wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 07:33 am GMT

PDB ID	:	4PJO
Title	:	Minimal U1 snRNP
Authors	:	Kondo, Y.; Oubridge, C.; van Roon, A.M.; Nagai, K.
Deposited on	:	2014-05-12
Resolution	:	3.30 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 (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 (i)) were used in the production of this report:

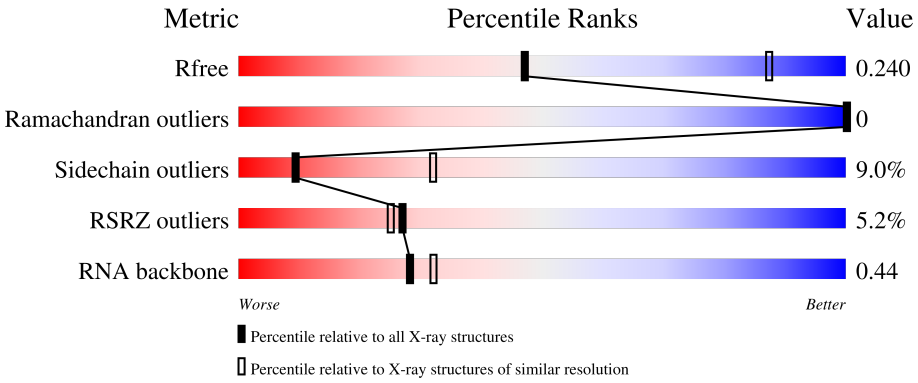
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	126	2% 59% 8% 33%
1	O	126	19% 58% 6% 35%
1	a	126	60% 5% 34%
1	o	126	9% 56% 6% 36%
2	B	95	3% 82% 5% 13%

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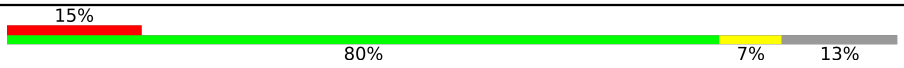
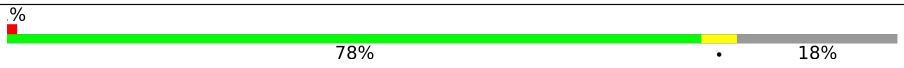
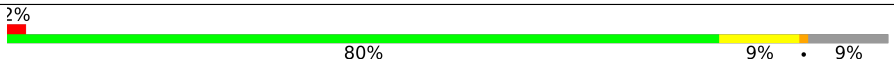
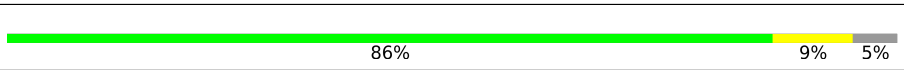
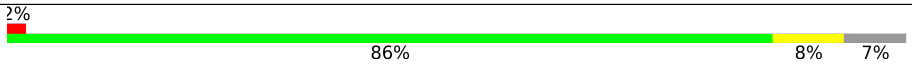
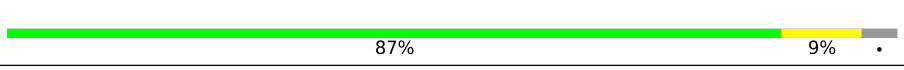
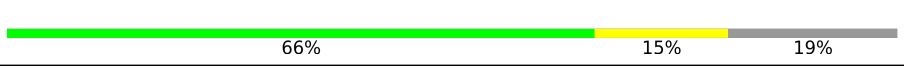
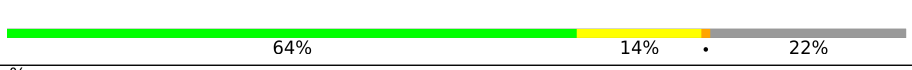
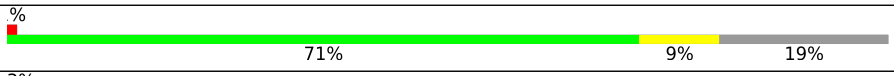
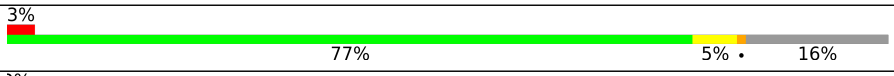
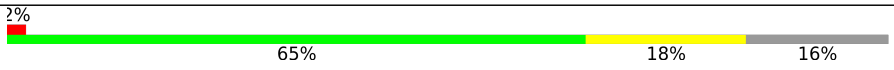
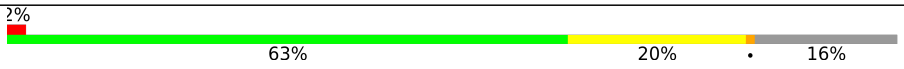
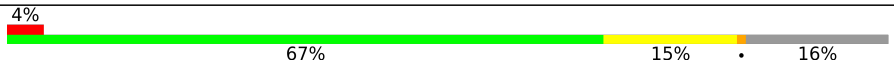
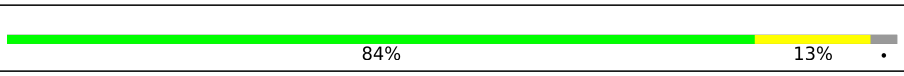
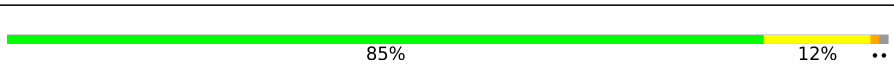
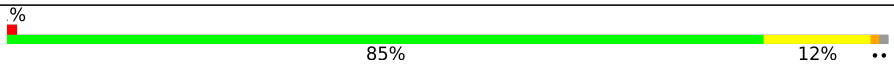
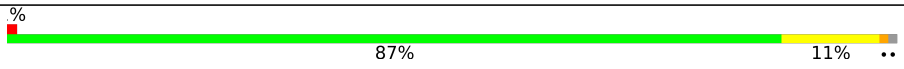
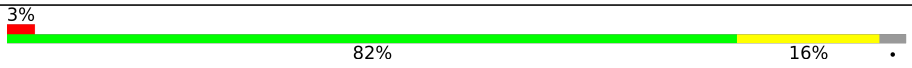
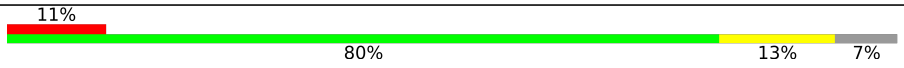
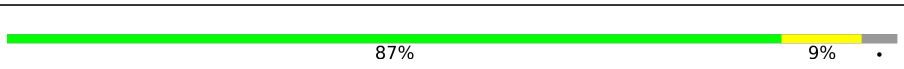
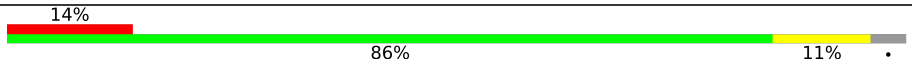
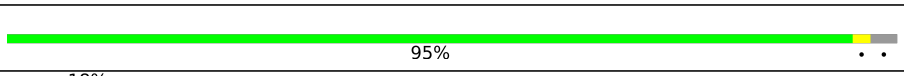
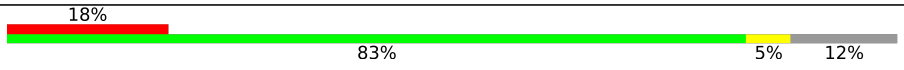
Mol	Chain	Length	Quality of chain
2	P	95	
2	b	95	
2	p	95	
3	C	91	
3	Q	91	
3	c	91	
3	q	91	
4	D	118	
4	R	118	
4	d	118	
4	r	118	
5	E	92	
5	S	92	
5	e	92	
5	s	92	
6	F	75	
6	T	75	
6	f	75	
6	t	75	
7	G	76	
7	U	76	
7	g	76	
7	u	76	
8	K	60	
8	N	60	

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Mol	Chain	Length	Quality of chain
8	k	60	87% 8% 5%
8	n	60	18% 83% 12%
9	L	61	3% 74% 13% 13%
9	M	61	23% 64% 23% 13%
9	l	61	5% 77% 10% 13%
9	m	61	23% 70% 10% 18%
10	1	60	55% 15% 10% 20%
10	2	60	52% 23% 5% 20%
10	3	60	55% 15% 8% 22%
10	4	60	53% 20% 8% 18%
11	X	10	50% 50%
11	Y	10	60% 40%
11	x	10	80% 20%
11	y	10	10% 80% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	MG	l	202	-	-	-	X
16	EOH	4	201	-	-	-	X
18	SO4	y	103	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 26921 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	84	Total	C	N	O	S	0	0	0
			657	412	116	123	6			
1	a	83	Total	C	N	O	S	0	0	0
			652	409	115	122	6			
1	O	82	Total	C	N	O	S	0	0	0
			643	403	113	121	6			
1	o	81	Total	C	N	O	S	0	0	0
			637	400	112	119	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			673	425	123	118	7			
2	b	78	Total	C	N	O	S	0	0	0
			635	402	114	112	7			
2	P	83	Total	C	N	O	S	0	0	0
			673	425	123	118	7			
2	p	86	Total	C	N	O	S	0	0	0
			692	435	126	124	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	86	Total	C	N	O	S	0	0	0
			668	423	117	125	3			
3	c	87	Total	C	N	O	S	0	0	0
			675	428	118	126	3			
3	Q	85	Total	C	N	O	S	0	0	0
			664	421	116	124	3			
3	q	87	Total	C	N	O	S	0	0	0
			674	426	118	127	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	linker	UNP P62314
C	-4	SER	-	linker	UNP P62314
C	-3	GLY	-	linker	UNP P62314
C	-2	SER	-	linker	UNP P62314
C	-1	GLY	-	linker	UNP P62314
C	0	SER	-	linker	UNP P62314
C	1	VAL	-	linker	UNP P62314
c	-5	GLY	-	linker	UNP P62314
c	-4	SER	-	linker	UNP P62314
c	-3	GLY	-	linker	UNP P62314
c	-2	SER	-	linker	UNP P62314
c	-1	GLY	-	linker	UNP P62314
c	0	SER	-	linker	UNP P62314
c	1	VAL	-	linker	UNP P62314
Q	-5	GLY	-	linker	UNP P62314
Q	-4	SER	-	linker	UNP P62314
Q	-3	GLY	-	linker	UNP P62314
Q	-2	SER	-	linker	UNP P62314
Q	-1	GLY	-	linker	UNP P62314
Q	0	SER	-	linker	UNP P62314
Q	1	VAL	-	linker	UNP P62314
q	-5	GLY	-	linker	UNP P62314
q	-4	SER	-	linker	UNP P62314
q	-3	GLY	-	linker	UNP P62314
q	-2	SER	-	linker	UNP P62314
q	-1	GLY	-	linker	UNP P62314
q	0	SER	-	linker	UNP P62314
q	1	VAL	-	linker	UNP P62314

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	98	Total	C	N	O	S	0	0	0
			796	498	144	148	6			
4	d	92	Total	C	N	O	S	0	0	0
			753	472	138	138	5			
4	R	96	Total	C	N	O	S	0	1	0
			790	497	141	146	6			
4	r	95	Total	C	N	O	S	0	0	0
			777	486	141	144	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
5	e	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
5	S	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
5	s	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	73	Total	C	N	O	S	0	0	0
			568	367	94	102	5			
6	f	74	Total	C	N	O	S	0	0	0
			577	373	95	104	5			
6	T	74	Total	C	N	O	S	0	0	0
			577	373	95	104	5			
6	t	74	Total	C	N	O	S	0	0	0
			577	373	95	104	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	1	0
			584	369	106	103	6			
7	g	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	U	71	Total	C	N	O	S	0	0	0
			558	353	100	99	6			
7	u	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	58	Total	C	N	O	S	0	0	0
			477	313	82	81	1			
8	k	57	Total	C	N	O	S	0	0	0
			470	309	81	79	1			
8	N	53	Total	C	N	O	S	0	0	0
			431	283	73	74	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	58	Total	C	N	O	S	0	0	0
			477	313	82	81	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	GLY	-	expression tag	UNP P08621
k	1	GLY	-	expression tag	UNP P08621
N	1	GLY	-	expression tag	UNP P08621
n	1	GLY	-	expression tag	UNP P08621

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	53	Total	C	N	O	S	0	0	0
			448	280	77	87	4			
9	l	53	Total	C	N	O	S	0	0	0
			448	280	77	87	4			
9	M	53	Total	C	N	O	S	0	0	0
			448	280	77	87	4			
9	m	50	Total	C	N	O	S	0	0	0
			425	266	73	82	4			

- Molecule 10 is a RNA chain called U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1	48	Total	C	N	O	P	0	0	0
			1036	458	183	345	50			
10	2	48	Total	C	N	O	P	0	0	0
			1036	458	183	345	50			
10	3	47	Total	C	N	O	P	0	0	0
			1013	448	178	338	49			
10	4	49	Total	C	N	O	P	0	0	0
			1059	468	188	352	51			

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	X	10	Total	C	N	O	P	0	0	0
			212	96	40	67	9			

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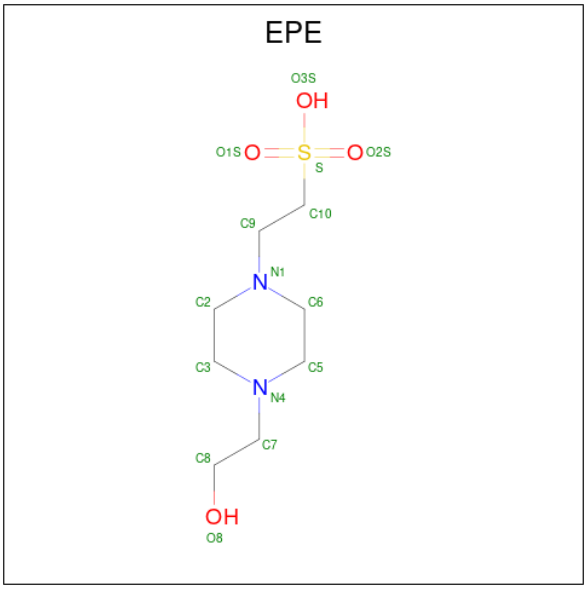
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	x	10	Total C N O P 212 96 40 67 9	0	0	0
11	Y	10	Total C N O P 212 96 40 67 9	0	0	0
11	y	10	Total C N O P 212 96 40 67 9	0	0	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total Zn 1 1	0	0
12	l	1	Total Zn 1 1	0	0
12	M	1	Total Zn 1 1	0	0
12	m	1	Total Zn 1 1	0	0

- Molecule 13 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	1	1	Total C N O S 15 8 2 4 1	0	0
13	2	1	Total C N O S 15 8 2 4 1	0	0

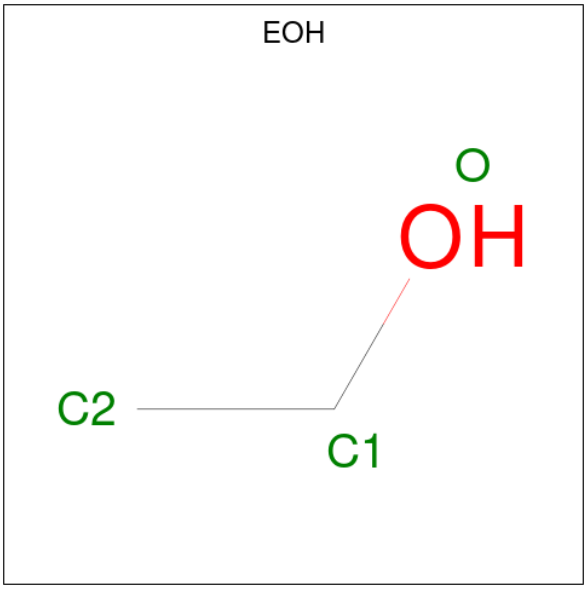
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	1	8	Total Mg 8 8	0	0
14	l	1	Total Mg 1 1	0	0
14	2	4	Total Mg 4 4	0	0
14	3	4	Total Mg 4 4	0	0
14	4	1	Total Mg 1 1	0	0
14	y	2	Total Mg 2 2	0	0

- Molecule 15 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	1	1	Total K 1 1	0	0
15	b	2	Total K 2 2	0	0
15	Q	1	Total K 1 1	0	0
15	3	2	Total K 2 2	0	0

- Molecule 16 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).

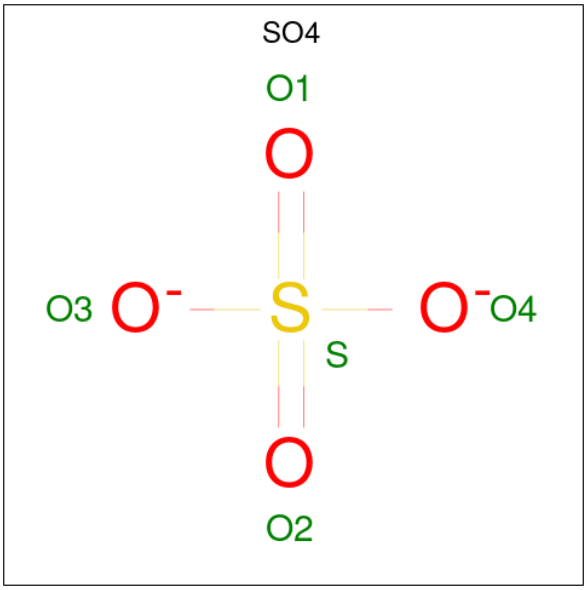


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	4	1	Total C O 3 2 1	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	4	1	Total Cl 1 1	0	0

- Molecule 18 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	y	1	Total O S 5 4 1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	5	Total O 5 5	0	0
19	G	2	Total O 2 2	0	0
19	K	1	Total O 1 1	0	0
19	1	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

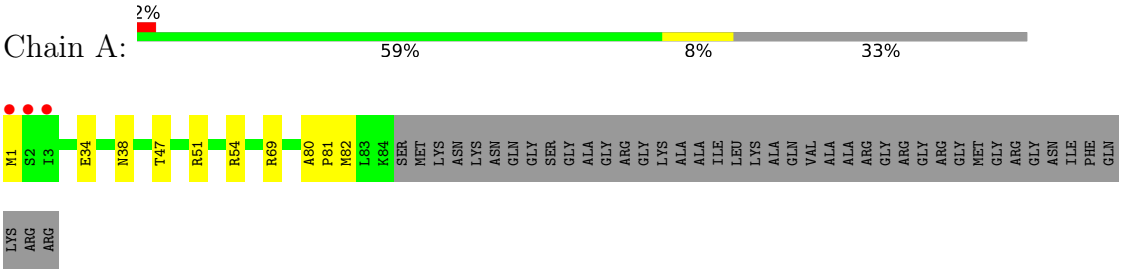
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	a	1	Total O 1 1	0	0
19	b	1	Total O 1 1	0	0
19	c	2	Total O 2 2	0	0
19	d	6	Total O 6 6	0	0
19	g	1	Total O 1 1	0	0
19	2	4	Total O 4 4	0	0
19	P	2	Total O 2 2	0	0
19	R	1	Total O 1 1	0	0
19	S	1	Total O 1 1	0	0
19	T	1	Total O 1 1	0	0
19	N	1	Total O 1 1	0	0
19	3	2	Total O 2 2	0	0
19	Y	1	Total O 1 1	0	0
19	p	1	Total O 1 1	0	0
19	q	2	Total O 2 2	0	0
19	r	1	Total O 1 1	0	0
19	t	1	Total O 1 1	0	0
19	m	1	Total O 1 1	0	0
19	4	4	Total O 4 4	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.

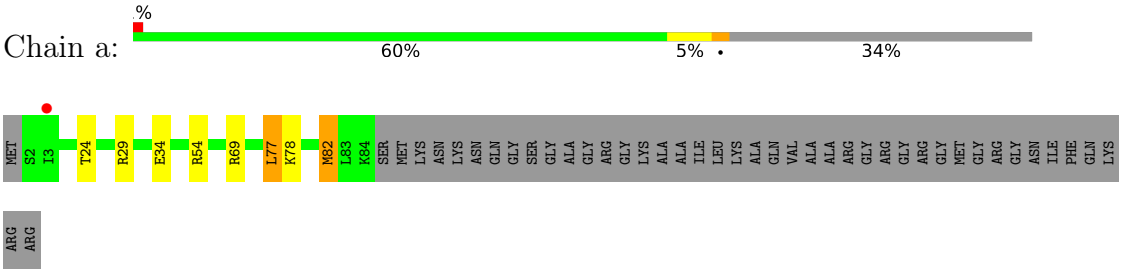
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain A:



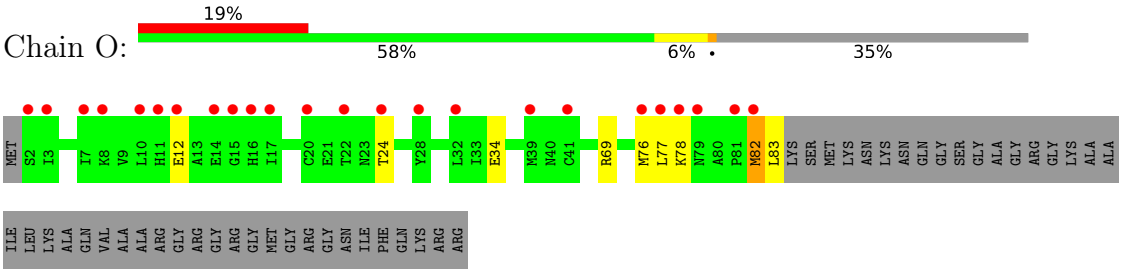
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain a:



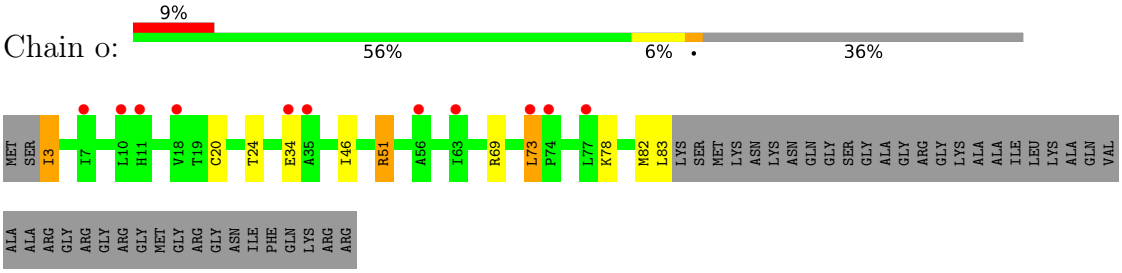
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain O:



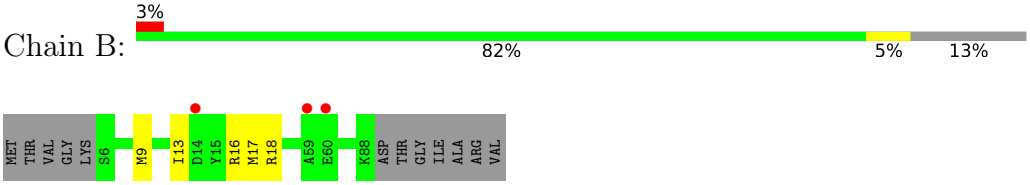
• Molecule 1: Small nuclear ribonucleoprotein Sm D3

Chain o:



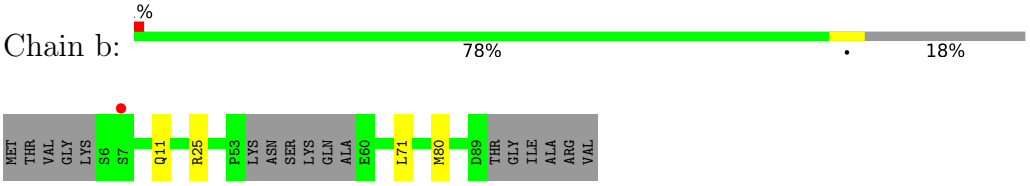
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain B:



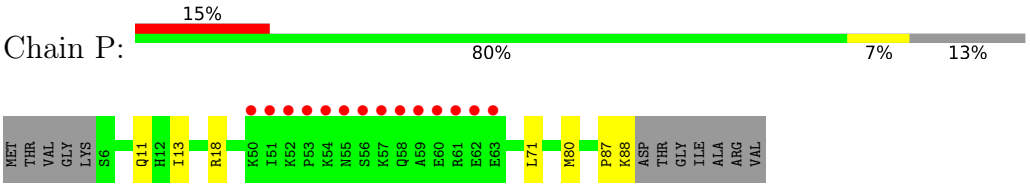
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain b:



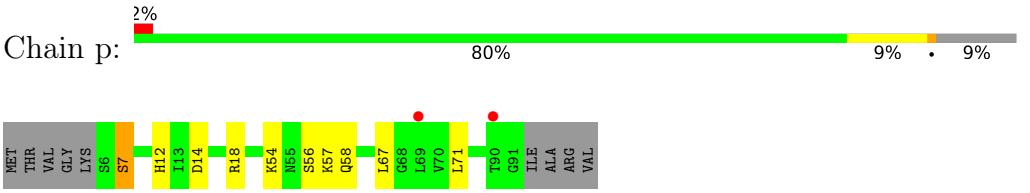
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain P:



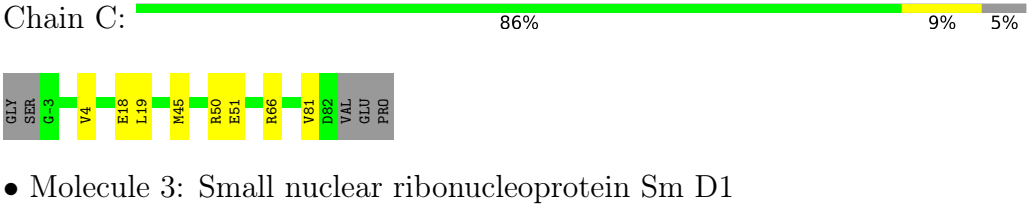
• Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain p:



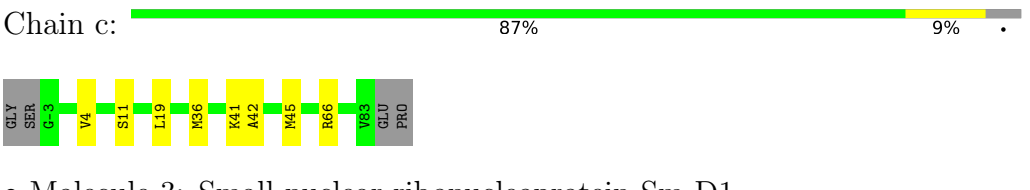
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain C:



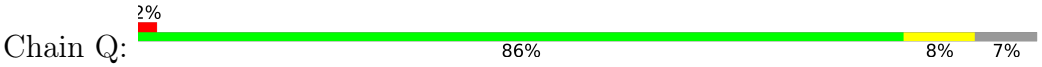
• Molecule 3: Small nuclear ribonucleoprotein Sm D1

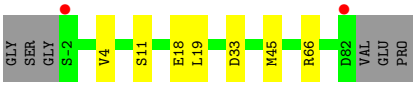
Chain c:



• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain Q:



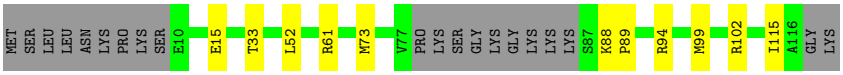


• Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain q:

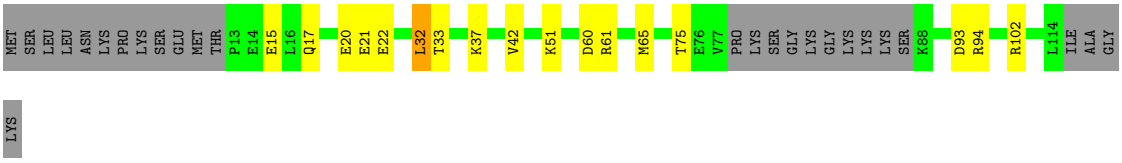
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain D:



• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain d:

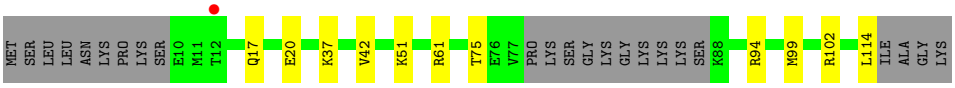


• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain R:

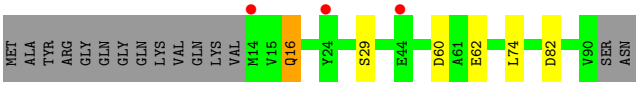
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain r:

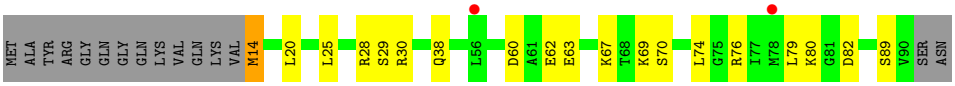


• Molecule 5: Small nuclear ribonucleoprotein E

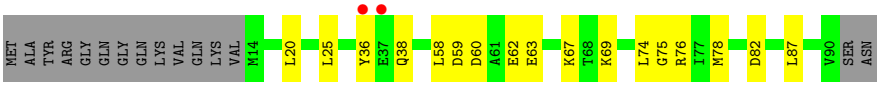
Chain E:



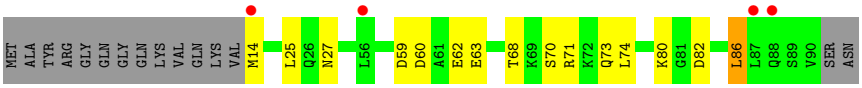
• Molecule 5: Small nuclear ribonucleoprotein E



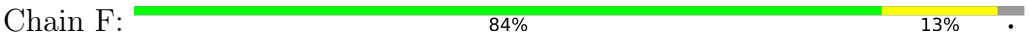
• Molecule 5: Small nuclear ribonucleoprotein E

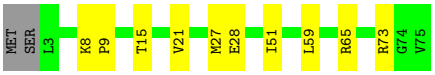


• Molecule 5: Small nuclear ribonucleoprotein E

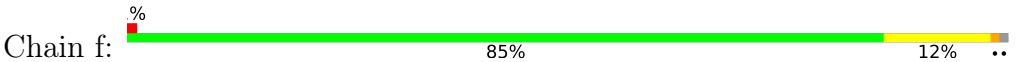


• Molecule 6: Small nuclear ribonucleoprotein F

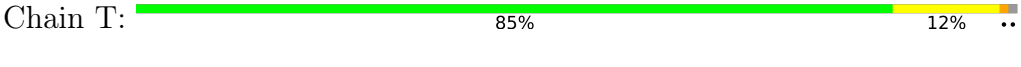


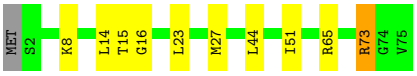


• Molecule 6: Small nuclear ribonucleoprotein F



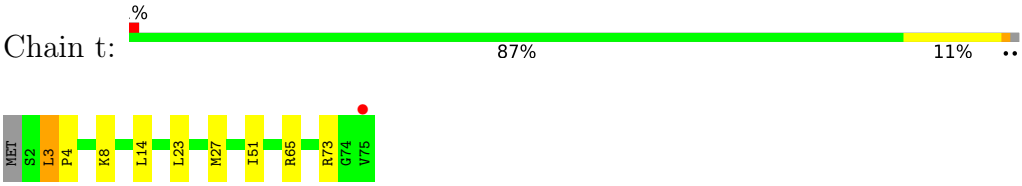
• Molecule 6: Small nuclear ribonucleoprotein F





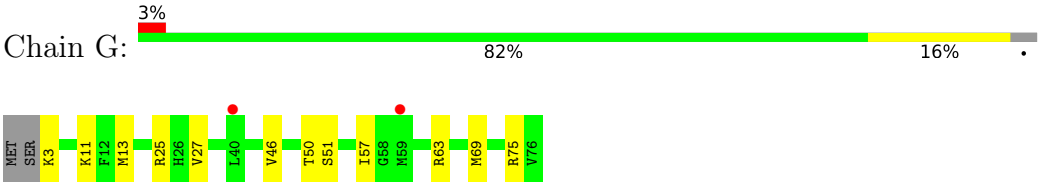
• Molecule 6: Small nuclear ribonucleoprotein F

Chain t:



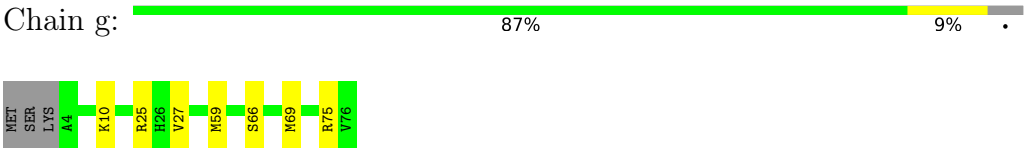
• Molecule 7: Small nuclear ribonucleoprotein G

Chain G:



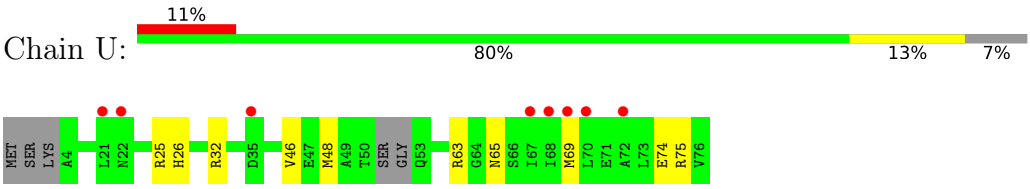
• Molecule 7: Small nuclear ribonucleoprotein G

Chain g:



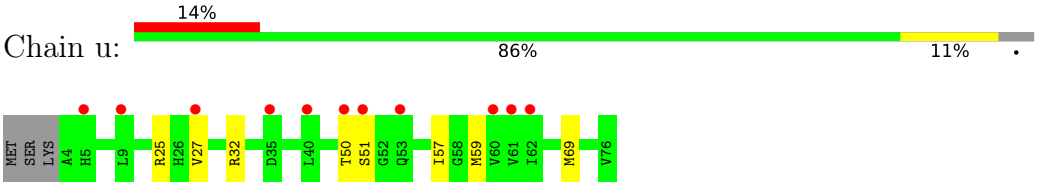
• Molecule 7: Small nuclear ribonucleoprotein G

Chain U:



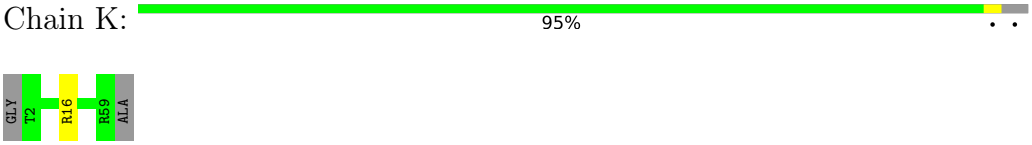
• Molecule 7: Small nuclear ribonucleoprotein G

Chain u:



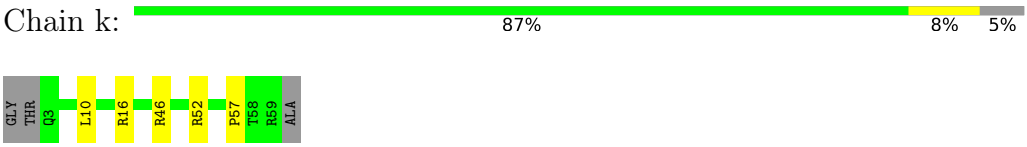
• Molecule 8: U1 small nuclear ribonucleoprotein 70 kDa

Chain K:



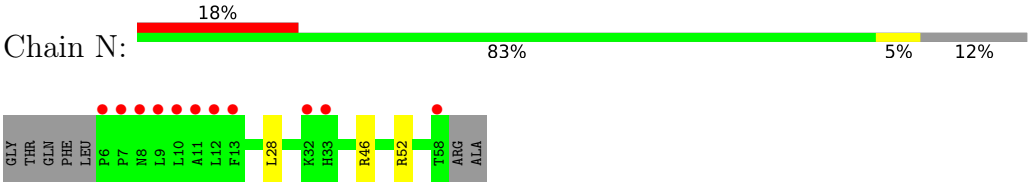
• Molecule 8: U1 small nuclear ribonucleoprotein 70 kDa

Chain k:



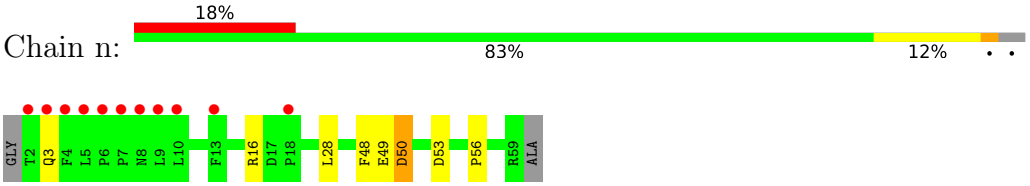
• Molecule 8: U1 small nuclear ribonucleoprotein 70 kDa

Chain N:



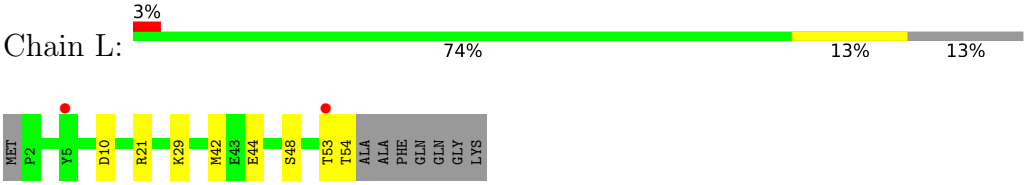
• Molecule 8: U1 small nuclear ribonucleoprotein 70 kDa

Chain n:



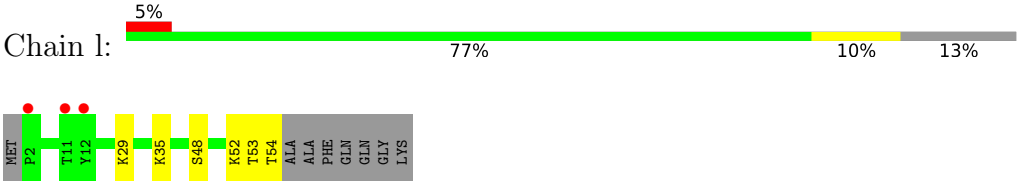
• Molecule 9: U1 small nuclear ribonucleoprotein C

Chain L:



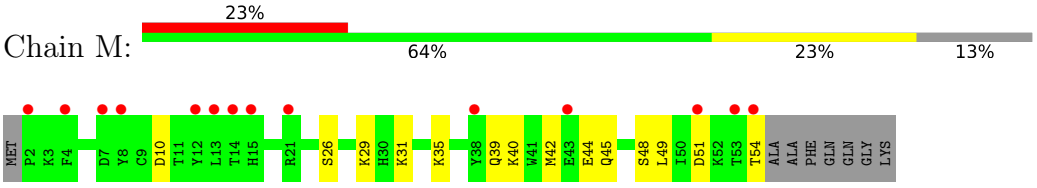
• Molecule 9: U1 small nuclear ribonucleoprotein C

Chain l:



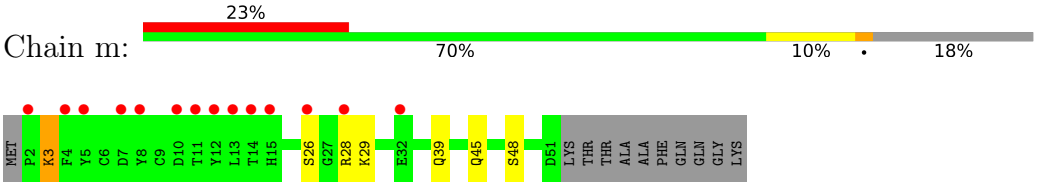
• Molecule 9: U1 small nuclear ribonucleoprotein C

Chain M:



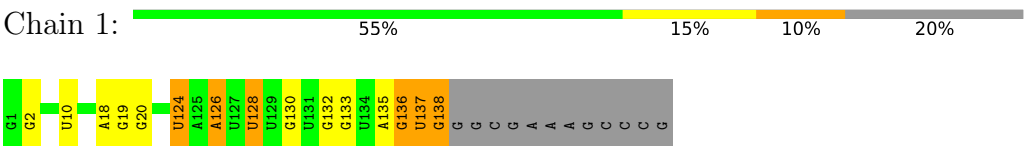
• Molecule 9: U1 small nuclear ribonucleoprotein C

Chain m:



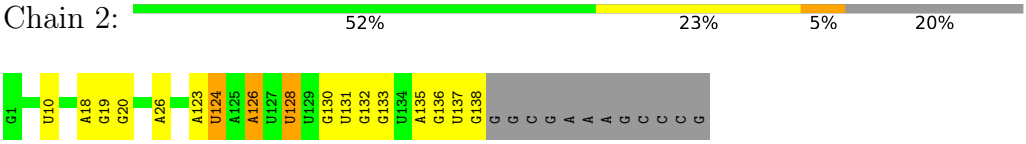
• Molecule 10: U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4.

Chain 1:



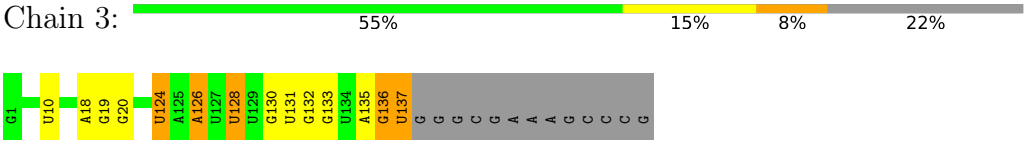
• Molecule 10: U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4.

Chain 2:



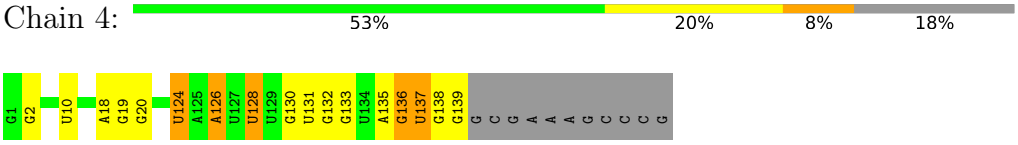
• Molecule 10: U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4.

Chain 3:



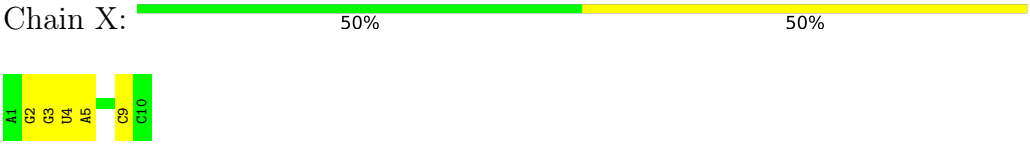
• Molecule 10: U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4.

Chain 4:



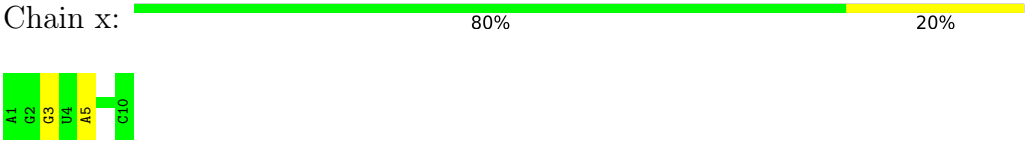
• Molecule 11: RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3')

Chain X:



• Molecule 11: RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3')

Chain x:

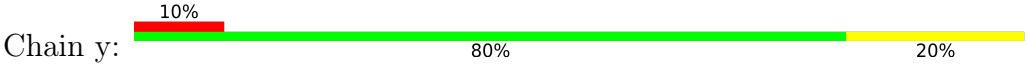


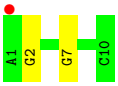
• Molecule 11: RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3')

Chain Y:

• Molecule 11: RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3')

Chain y:




A1
G2
G7
C10

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	120.36Å 172.63Å 256.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.30 69.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (70.00-3.30) 97.4 (69.67-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.255 0.196 , 0.240	Depositor DCC
R_{free} test set	3972 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	86.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 72.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	26921	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: EOH, CL, MG, EPE, GTP, K, ZN, SO4

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	0.74	1/665 (0.2%)	1.04	4/896 (0.4%)
1	O	0.52	0/651	1.15	5/878 (0.6%)
1	a	0.71	0/660	1.18	8/889 (0.9%)
1	o	0.53	0/645	1.19	6/870 (0.7%)
2	B	0.77	0/683	1.08	2/910 (0.2%)
2	P	0.65	0/683	1.08	1/910 (0.1%)
2	b	0.75	0/644	1.10	1/858 (0.1%)
2	p	0.63	0/702	1.16	3/936 (0.3%)
3	C	0.87	0/676	1.19	6/914 (0.7%)
3	Q	0.74	0/672	1.19	6/909 (0.7%)
3	c	0.84	0/683	1.28	4/924 (0.4%)
3	q	0.67	0/682	1.22	7/922 (0.8%)
4	D	0.75	1/805 (0.1%)	1.15	6/1081 (0.6%)
4	R	0.80	0/803	1.32	8/1079 (0.7%)
4	d	0.76	0/762	1.18	5/1022 (0.5%)
4	r	0.69	0/786	1.14	2/1055 (0.2%)
5	E	0.67	0/646	0.98	2/867 (0.2%)
5	S	0.64	0/646	1.30	6/867 (0.7%)
5	e	0.71	0/646	1.13	4/867 (0.5%)
5	s	0.62	0/646	1.27	5/867 (0.6%)
6	F	0.81	1/580 (0.2%)	1.17	3/783 (0.4%)
6	T	0.69	0/589	1.16	3/795 (0.4%)
6	f	0.77	0/589	1.24	4/795 (0.5%)
6	t	0.66	1/589 (0.2%)	1.18	4/795 (0.5%)
7	G	0.76	0/595	1.28	5/794 (0.6%)
7	U	0.57	0/564	1.06	1/752 (0.1%)
7	g	0.77	1/575 (0.2%)	1.27	4/768 (0.5%)
7	u	0.59	0/575	1.17	4/768 (0.5%)
8	K	0.76	0/499	1.10	1/688 (0.1%)
8	N	0.61	0/452	1.11	1/624 (0.2%)
8	k	0.77	0/492	1.10	2/678 (0.3%)
8	n	0.63	0/499	1.09	4/688 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	L	0.60	0/460	1.00	2/618 (0.3%)
9	M	0.61	0/460	1.12	6/618 (1.0%)
9	l	0.58	0/460	0.96	0/618
9	m	0.56	0/437	1.16	4/587 (0.7%)
10	1	0.62	0/1122	1.21	12/1747 (0.7%)
10	2	0.58	0/1122	1.16	7/1747 (0.4%)
10	3	0.49	0/1096	1.09	6/1706 (0.4%)
10	4	0.49	0/1148	1.10	7/1788 (0.4%)
11	X	0.44	0/237	1.33	5/368 (1.4%)
11	Y	0.43	0/237	1.26	4/368 (1.1%)
11	x	0.44	0/237	1.11	2/368 (0.5%)
11	y	0.40	0/237	0.94	0/368
All	All	0.67	5/27637 (0.0%)	1.16	182/38350 (0.5%)

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
1	A	0	1
2	P	0	1
3	C	0	1
3	c	0	1
4	R	0	1
4	r	0	1
6	T	0	1
8	k	0	1
8	n	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	89	PRO	N-CD	5.34	1.55	1.47
1	A	81	PRO	N-CD	5.18	1.55	1.47
6	F	9	PRO	N-CD	5.13	1.55	1.47
7	g	66	SER	CB-OG	-5.13	1.35	1.42
6	t	4	PRO	N-CD	5.04	1.54	1.47

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	87	LEU	CB-CG-CD2	13.57	134.07	111.00
9	m	28	ARG	NE-CZ-NH1	12.22	126.41	120.30
6	f	73	ARG	NE-CZ-NH1	-10.81	114.89	120.30
4	d	32	LEU	CB-CG-CD2	10.65	129.10	111.00
10	2	136	G	C4'-C3'-O3'	-10.48	87.40	109.40

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
3	C	81	VAL	Peptide
2	P	87	PRO	Peptide
3	c	42	ALA	Peptide
8	k	57	PRO	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 (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	82/126 (65%)	80 (98%)	2 (2%)	0	100	100
1	O	80/126 (64%)	74 (92%)	6 (8%)	0	100	100
1	a	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
1	o	79/126 (63%)	75 (95%)	4 (5%)	0	100	100
2	B	81/95 (85%)	80 (99%)	1 (1%)	0	100	100
2	P	81/95 (85%)	80 (99%)	1 (1%)	0	100	100
2	b	74/95 (78%)	73 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	p	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
3	C	84/91 (92%)	79 (94%)	5 (6%)	0	100	100
3	Q	83/91 (91%)	81 (98%)	2 (2%)	0	100	100
3	c	85/91 (93%)	81 (95%)	4 (5%)	0	100	100
3	q	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
4	D	94/118 (80%)	90 (96%)	4 (4%)	0	100	100
4	R	93/118 (79%)	87 (94%)	6 (6%)	0	100	100
4	d	88/118 (75%)	86 (98%)	2 (2%)	0	100	100
4	r	91/118 (77%)	85 (93%)	6 (7%)	0	100	100
5	E	75/92 (82%)	71 (95%)	4 (5%)	0	100	100
5	S	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
5	e	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
5	s	75/92 (82%)	70 (93%)	5 (7%)	0	100	100
6	F	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
6	T	72/75 (96%)	68 (94%)	4 (6%)	0	100	100
6	f	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
6	t	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
7	G	73/76 (96%)	69 (94%)	4 (6%)	0	100	100
7	U	67/76 (88%)	64 (96%)	3 (4%)	0	100	100
7	g	71/76 (93%)	68 (96%)	3 (4%)	0	100	100
7	u	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
8	K	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
8	N	51/60 (85%)	47 (92%)	4 (8%)	0	100	100
8	k	55/60 (92%)	53 (96%)	2 (4%)	0	100	100
8	n	56/60 (93%)	47 (84%)	9 (16%)	0	100	100
9	L	51/61 (84%)	48 (94%)	3 (6%)	0	100	100
9	M	51/61 (84%)	47 (92%)	4 (8%)	0	100	100
9	l	51/61 (84%)	48 (94%)	3 (6%)	0	100	100
9	m	48/61 (79%)	47 (98%)	1 (2%)	0	100	100
All	All	2633/3176 (83%)	2509 (95%)	124 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	73/101 (72%)	69 (94%)	4 (6%)	21 52
1	O	72/101 (71%)	67 (93%)	5 (7%)	15 44
1	a	73/101 (72%)	68 (93%)	5 (7%)	16 44
1	o	71/101 (70%)	61 (86%)	10 (14%)	3 16
2	B	76/85 (89%)	73 (96%)	3 (4%)	32 62
2	P	76/85 (89%)	71 (93%)	5 (7%)	16 46
2	b	72/85 (85%)	69 (96%)	3 (4%)	30 60
2	p	78/85 (92%)	70 (90%)	8 (10%)	7 26
3	C	79/83 (95%)	78 (99%)	1 (1%)	69 82
3	Q	79/83 (95%)	77 (98%)	2 (2%)	47 72
3	c	80/83 (96%)	77 (96%)	3 (4%)	33 62
3	q	80/83 (96%)	76 (95%)	4 (5%)	24 55
4	D	93/110 (84%)	88 (95%)	5 (5%)	22 53
4	R	92/110 (84%)	82 (89%)	10 (11%)	6 24
4	d	88/110 (80%)	75 (85%)	13 (15%)	3 13
4	r	91/110 (83%)	83 (91%)	8 (9%)	10 33
5	E	72/84 (86%)	68 (94%)	4 (6%)	21 52
5	S	72/84 (86%)	61 (85%)	11 (15%)	2 12
5	e	72/84 (86%)	57 (79%)	15 (21%)	1 4
5	s	72/84 (86%)	61 (85%)	11 (15%)	2 12
6	F	61/64 (95%)	55 (90%)	6 (10%)	8 29
6	T	63/64 (98%)	56 (89%)	7 (11%)	6 23
6	f	63/64 (98%)	54 (86%)	9 (14%)	3 15
6	t	63/64 (98%)	56 (89%)	7 (11%)	6 23
7	G	65/66 (98%)	57 (88%)	8 (12%)	4 20
7	U	62/66 (94%)	53 (86%)	9 (14%)	3 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	g	63/66 (96%)	59 (94%)	4 (6%)	18 47
7	u	63/66 (96%)	57 (90%)	6 (10%)	8 29
8	K	53/53 (100%)	53 (100%)	0	100 100
8	N	48/53 (91%)	46 (96%)	2 (4%)	30 60
8	k	52/53 (98%)	50 (96%)	2 (4%)	33 62
8	n	53/53 (100%)	49 (92%)	4 (8%)	13 39
9	L	51/56 (91%)	45 (88%)	6 (12%)	5 21
9	M	51/56 (91%)	42 (82%)	9 (18%)	2 8
9	l	51/56 (91%)	45 (88%)	6 (12%)	5 21
9	m	48/56 (86%)	42 (88%)	6 (12%)	4 19
All	All	2471/2808 (88%)	2250 (91%)	221 (9%)	9 32

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	51	LYS
7	U	69	MET
9	m	45	GLN
6	t	8	LYS
5	S	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	73	GLN
6	F	43	GLN
2	P	11	GLN
7	U	26	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	1	46/60 (76%)	14 (30%)	4 (8%)
10	2	46/60 (76%)	14 (30%)	3 (6%)
10	3	45/60 (75%)	14 (31%)	3 (6%)
10	4	47/60 (78%)	16 (34%)	4 (8%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	X	9/10 (90%)	1 (11%)	0
11	Y	9/10 (90%)	2 (22%)	0
11	x	9/10 (90%)	0	0
11	y	9/10 (90%)	2 (22%)	0
All	All	220/280 (78%)	63 (28%)	14 (6%)

5 of 63 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	1	10	U
10	1	18	A
10	1	19	G
10	1	20	G
10	1	124	U

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	3	126	A
10	3	128	U
10	4	138	G
10	4	128	U
10	4	136	G

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)

Of 35 ligands modelled in this entry, 31 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	EPE	1	201	-	15,15,15	1.93	1 (6%)	18,20,20	2.28	6 (33%)
16	EOH	4	201	-	2,2,2	0.56	0	1,1,1	0.19	0
18	SO4	y	103	-	4,4,4	0.38	0	6,6,6	0.60	0
13	EPE	2	201	-	15,15,15	1.97	1 (6%)	18,20,20	2.24	10 (55%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	EPE	1	201	-	-	1/9/19/19	0/1/1/1
13	EPE	2	201	-	-	4/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	201	EPE	C10-S	-6.98	1.67	1.77
13	2	201	EPE	C10-S	-6.93	1.67	1.77

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	201	EPE	O1S-S-C10	5.47	113.51	106.92
13	2	201	EPE	C6-C5-N4	4.83	120.56	110.64
13	1	201	EPE	C6-N1-C2	3.69	117.14	108.83
13	1	201	EPE	O2S-S-O1S	-3.52	101.77	113.95
13	2	201	EPE	O1S-S-C10	3.44	111.06	106.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	2	201	EPE	C9-C10-S-O2S
13	2	201	EPE	C9-C10-S-O3S
13	1	201	EPE	C8-C7-N4-C5
13	2	201	EPE	C9-C10-S-O1S
13	2	201	EPE	C10-C9-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	84/126 (66%)	0.18	3 (3%) 42 40	50, 68, 102, 155	0
1	O	82/126 (65%)	1.28	24 (29%) 0 0	96, 125, 152, 182	0
1	a	83/126 (65%)	-0.22	1 (1%) 79 78	46, 70, 103, 123	0
1	o	81/126 (64%)	0.83	11 (13%) 3 2	87, 137, 161, 176	0
2	B	83/95 (87%)	0.63	3 (3%) 42 40	41, 65, 189, 219	0
2	P	83/95 (87%)	0.98	14 (16%) 1 1	68, 111, 178, 219	0
2	b	78/95 (82%)	0.05	1 (1%) 77 77	45, 70, 135, 185	0
2	p	86/95 (90%)	0.08	2 (2%) 60 59	75, 122, 185, 221	0
3	C	86/91 (94%)	-0.11	0 100 100	39, 56, 120, 139	0
3	Q	85/91 (93%)	0.06	2 (2%) 59 56	55, 77, 125, 140	0
3	c	87/91 (95%)	0.04	0 100 100	42, 60, 124, 139	0
3	q	87/91 (95%)	-0.22	0 100 100	57, 82, 131, 150	0
4	D	98/118 (83%)	0.01	0 100 100	38, 62, 151, 181	0
4	R	96/118 (81%)	0.13	0 100 100	49, 73, 157, 176	0
4	d	92/118 (77%)	-0.05	0 100 100	41, 63, 154, 176	0
4	r	95/118 (80%)	-0.06	1 (1%) 80 81	63, 85, 172, 233	0
5	E	77/92 (83%)	0.52	3 (3%) 39 37	49, 75, 113, 134	0
5	S	77/92 (83%)	-0.30	2 (2%) 56 53	75, 117, 159, 177	0
5	e	77/92 (83%)	0.63	2 (2%) 56 53	52, 81, 126, 150	0
5	s	77/92 (83%)	0.23	4 (5%) 27 25	86, 115, 155, 171	0
6	F	73/75 (97%)	-0.04	0 100 100	45, 64, 95, 133	0
6	T	74/75 (98%)	-0.09	0 100 100	59, 88, 136, 175	0
6	f	74/75 (98%)	0.35	1 (1%) 75 75	52, 76, 101, 129	0
6	t	74/75 (98%)	0.28	1 (1%) 75 75	73, 100, 144, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	G	74/76 (97%)	0.62	2 (2%) 54 52	51, 80, 120, 137	0
7	U	71/76 (93%)	0.33	8 (11%) 5 5	95, 130, 165, 178	0
7	g	73/76 (96%)	-0.01	0 100 100	55, 83, 123, 168	0
7	u	73/76 (96%)	0.72	11 (15%) 2 2	98, 133, 171, 188	0
8	K	58/60 (96%)	-0.13	0 100 100	52, 83, 139, 159	0
8	N	53/60 (88%)	1.03	11 (20%) 1 1	57, 121, 162, 171	0
8	k	57/60 (95%)	-0.18	0 100 100	52, 90, 130, 155	0
8	n	58/60 (96%)	0.95	11 (18%) 1 1	80, 140, 185, 196	0
9	L	53/61 (86%)	0.25	2 (3%) 40 37	72, 106, 180, 197	0
9	M	53/61 (86%)	1.46	14 (26%) 0 0	102, 140, 194, 199	0
9	l	53/61 (86%)	0.27	3 (5%) 23 23	70, 112, 177, 202	0
9	m	50/61 (81%)	1.30	14 (28%) 0 0	116, 157, 210, 217	0
10	1	47/60 (78%)	-0.39	0 100 100	46, 93, 150, 176	0
10	2	47/60 (78%)	-0.23	0 100 100	47, 99, 158, 175	0
10	3	46/60 (76%)	-0.22	0 100 100	72, 127, 151, 178	0
10	4	48/60 (80%)	-0.05	0 100 100	77, 129, 173, 196	0
11	X	10/10 (100%)	-0.75	0 100 100	88, 119, 157, 164	0
11	Y	10/10 (100%)	-0.09	0 100 100	114, 143, 162, 164	0
11	x	10/10 (100%)	-0.06	0 100 100	89, 118, 165, 176	0
11	y	10/10 (100%)	0.56	1 (10%) 7 7	130, 152, 171, 177	0
All	All	2943/3456 (85%)	0.26	152 (5%) 27 25	38, 95, 165, 233	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	56	SER	18.1
8	n	2	THR	9.5
2	P	55	ASN	8.7
8	n	3	GLN	7.3
2	P	57	LYS	6.9

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	MG	2	203	1/1	0.35	0.18	87,87,87,87	0
18	SO4	y	103	5/5	0.39	0.60	192,193,205,208	0
16	EOH	4	201	3/3	0.42	1.11	112,112,115,119	0
14	MG	l	202	1/1	0.45	0.92	106,106,106,106	0
15	K	3	205	1/1	0.45	0.23	122,122,122,122	0
14	MG	3	202	1/1	0.47	0.13	91,91,91,91	0
14	MG	2	204	1/1	0.60	0.27	94,94,94,94	0
14	MG	1	209	1/1	0.65	0.27	95,95,95,95	0
14	MG	1	205	1/1	0.70	0.29	71,71,71,71	0
14	MG	1	208	1/1	0.72	0.27	75,75,75,75	0
13	EPE	1	201	15/15	0.77	0.35	131,146,150,162	0
14	MG	4	202	1/1	0.79	0.31	86,86,86,86	0
14	MG	1	202	1/1	0.80	0.27	100,100,100,100	0
14	MG	1	207	1/1	0.80	0.18	82,82,82,82	0
13	EPE	2	201	15/15	0.81	0.44	92,116,141,146	0
14	MG	3	204	1/1	0.81	0.25	97,97,97,97	0
14	MG	1	206	1/1	0.86	0.27	86,86,86,86	0
14	MG	1	203	1/1	0.87	0.20	52,52,52,52	0
14	MG	2	205	1/1	0.87	0.26	61,61,61,61	0
15	K	3	206	1/1	0.88	0.41	125,125,125,125	0
15	K	b	101	1/1	0.88	0.33	105,105,105,105	0
14	MG	y	102	1/1	0.88	0.21	100,100,100,100	0
14	MG	y	101	1/1	0.89	0.31	100,100,100,100	0
14	MG	3	201	1/1	0.89	0.15	75,75,75,75	0
14	MG	3	203	1/1	0.89	0.12	80,80,80,80	0
15	K	b	102	1/1	0.89	0.24	124,124,124,124	0
14	MG	2	202	1/1	0.92	0.36	69,69,69,69	0
15	K	Q	101	1/1	0.93	0.14	97,97,97,97	0
15	K	1	210	1/1	0.95	0.09	91,91,91,91	0
17	CL	4	203	1/1	0.95	0.11	111,111,111,111	0
14	MG	1	204	1/1	0.95	0.16	64,64,64,64	0
12	ZN	M	201	1/1	0.97	0.10	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	ZN	m	201	1/1	0.98	0.09	136,136,136,136	0
12	ZN	l	201	1/1	0.99	0.11	98,98,98,98	0
12	ZN	L	201	1/1	0.99	0.13	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.