



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:42 PM UTC

PDB ID : 5VYC / pdb_00005vyc
Title : Crystal structure of the human 40S ribosomal subunit in complex with DENR-MCT-1.
Authors : Lomakin, I.B.; Stolboushkina, E.A.; Vaidya, A.T.; Garber, M.B.; Dmitriev, S.E.; Steitz, T.A.
Deposited on : 2017-05-24
Resolution : 6.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

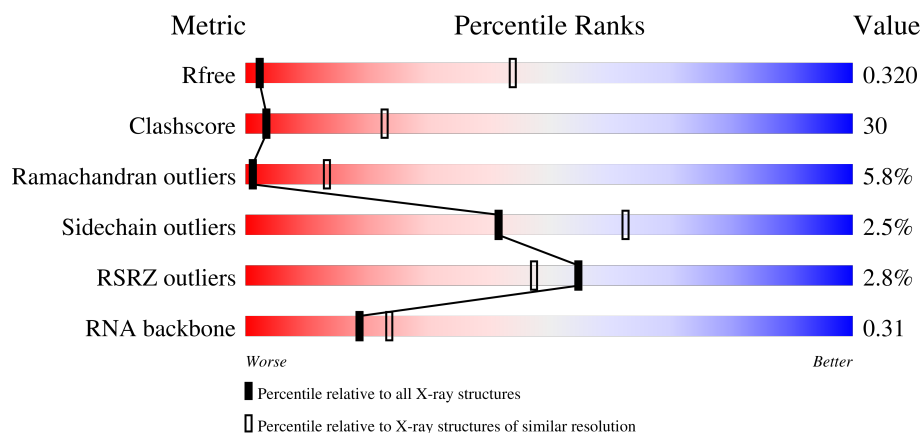
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)
RNA backbone	3983	1054 (8.70-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T1	145	4% 58% 37% ..
1	T2	145	% 57% 39% ..
1	T3	145	6% 54% 43% ..
1	T4	145	2% 54% 41% ..

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Mol	Chain	Length	Quality of chain
1	T5	145	
1	T6	145	
2	U1	119	
2	U2	119	
2	U3	119	
2	U4	119	
2	U5	119	
2	U6	119	
3	V1	83	
3	V2	83	
3	V3	83	
3	V4	83	
3	V5	83	
3	V6	83	
4	X1	143	
4	X2	143	
4	X3	143	
4	X4	143	
4	X5	143	
4	X6	143	
5	a1	115	
5	a2	115	
5	a3	115	
5	a4	115	
5	a5	115	

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Mol	Chain	Length	Quality of chain
5	a6	115	
6	c1	69	
6	c2	69	
6	c3	69	
6	c4	69	
6	c5	69	
6	c6	69	
7	d1	56	
7	d2	56	
7	d3	56	
7	d4	56	
7	d5	56	
7	d6	56	
8	f1	156	
8	f2	156	
8	f3	156	
8	f4	156	
8	f5	156	
8	f6	156	
9	g1	317	
9	g2	317	
9	g3	317	
9	g4	317	
9	g5	317	
9	g6	317	

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Mol	Chain	Length	Quality of chain
10	C1	293	
10	C2	293	
10	C3	293	
10	C4	293	
10	C5	293	
10	C6	293	
11	G1	249	
11	G2	249	
11	G3	249	
11	G4	249	
11	G5	249	
11	G6	249	
12	J1	194	
12	J2	194	
12	J3	194	
12	J4	194	
12	J5	194	
12	J6	194	
13	M1	132	
13	M2	132	
13	M3	132	
13	M4	132	
13	M5	132	
13	M6	132	
14	N1	151	

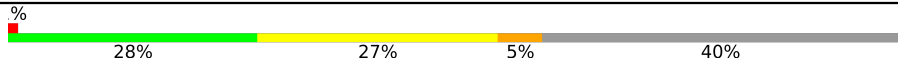
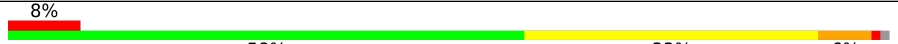
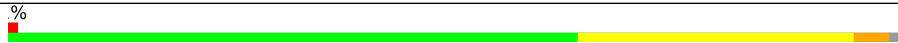
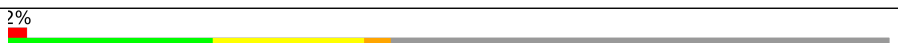
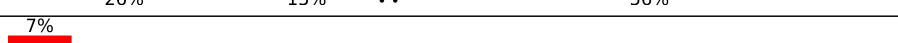
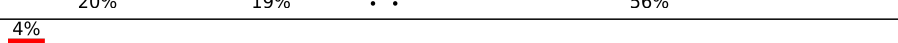
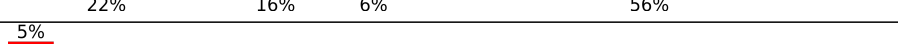
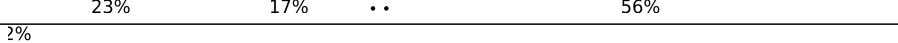
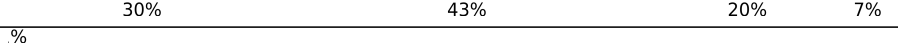
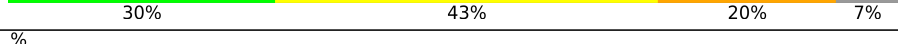
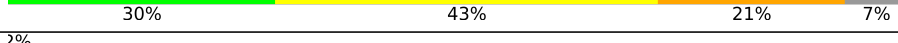
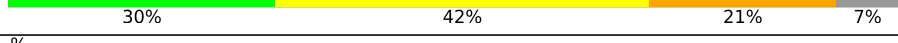
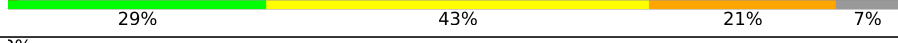
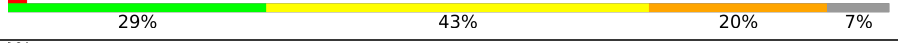
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Mol	Chain	Length	Quality of chain
14	N2	151	3% 49% 45% 5%
14	N3	151	% 46% 47% 7%
14	N4	151	46% 48% 5%
14	N5	151	% 44% 48% 7%
14	N6	151	48% 46% 6%
15	O1	151	5% 42% 44% 7% 7%
15	O2	151	3% 42% 44% 7% 7%
15	O3	151	14% 42% 44% 6% 7%
15	O4	151	12% 44% 42% 7% 7%
15	O5	151	2% 44% 42% 7% 7%
15	O6	151	% 43% 42% 7% 7%
16	W1	130	47% 50%
16	W2	130	2% 48% 48%
16	W3	130	2% 45% 51%
16	W4	130	6% 48% 49%
16	W5	130	% 48% 48%
16	W6	130	49% 48%
17	Y1	133	7% 52% 46%
17	Y2	133	8% 52% 46%
17	Y3	133	14% 50% 48%
17	Y4	133	3% 52% 46%
17	Y5	133	6% 52% 47%
17	Y6	133	2% 50% 47%
18	Z1	125	30% 25% 5% 40%
18	Z2	125	2% 30% 26% 5% 40%

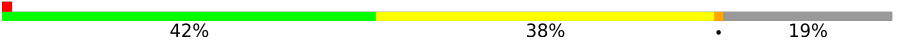
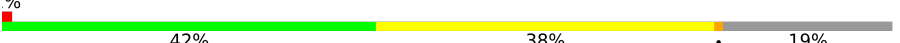
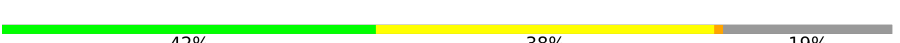
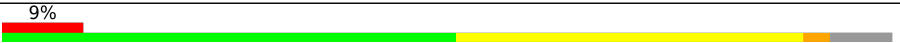
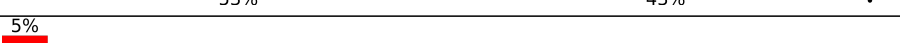
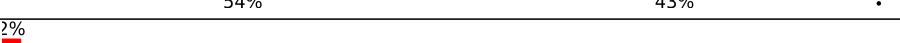
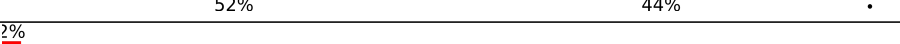
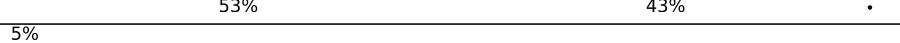
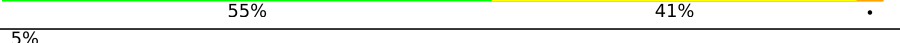
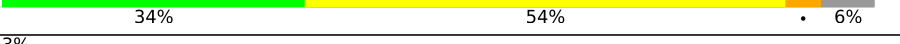
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Mol	Chain	Length	Quality of chain
18	Z3	125	
18	Z4	125	
18	Z5	125	
18	Z6	125	
19	b1	84	
19	b2	84	
19	b3	84	
19	b4	84	
19	b5	84	
19	b6	84	
20	e1	133	
20	e2	133	
20	e3	133	
20	e4	133	
20	e5	133	
20	e6	133	
21	i1	1869	
21	i2	1869	
21	i3	1869	
21	i4	1869	
21	i5	1869	
21	i6	1869	
22	A1	295	
22	A2	295	
22	A3	295	

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Mol	Chain	Length	Quality of chain
22	A4	295	
22	A5	295	
22	A6	295	
23	B1	264	
23	B2	264	
23	B3	264	
23	B4	264	
23	B5	264	
23	B6	264	
24	D1	243	
24	D2	243	
24	D3	243	
24	D4	243	
24	D5	243	
24	D6	243	
25	E1	263	
25	E2	263	
25	E3	263	
25	E4	263	
25	E5	263	
25	E6	263	
26	F1	204	
26	F2	204	
26	F3	204	
26	F4	204	

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Mol	Chain	Length	Quality of chain
26	F5	204	
26	F6	204	
27	H1	194	
27	H2	194	
27	H3	194	
27	H4	194	
27	H5	194	
27	H6	194	
28	I1	208	
28	I2	208	
28	I3	208	
28	I4	208	
28	I5	208	
28	I6	208	
29	K1	165	
29	K2	165	
29	K3	165	
29	K4	165	
29	K5	165	
29	K6	165	
30	L1	158	
30	L2	158	
30	L3	158	
30	L4	158	
30	L5	158	

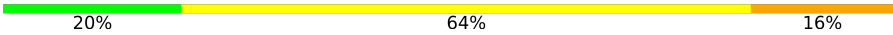
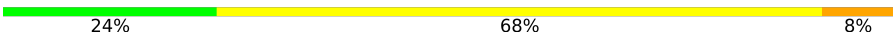
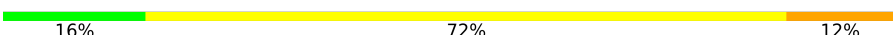
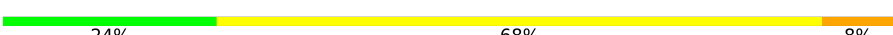
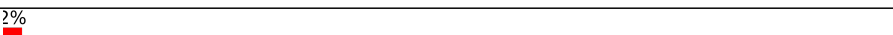
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Mol	Chain	Length	Quality of chain
30	L6	158	
31	P1	145	
31	P2	145	
31	P3	145	
31	P4	145	
31	P5	145	
31	P6	145	
32	Q1	146	
32	Q2	146	
32	Q3	146	
32	Q4	146	
32	Q5	146	
32	Q6	146	
33	R1	135	
33	R2	135	
33	R3	135	
33	R4	135	
33	R5	135	
33	R6	135	
34	S1	152	
34	S2	152	
34	S3	152	
34	S4	152	
34	S5	152	
34	S6	152	

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Mol	Chain	Length	Quality of chain
35	j1	25	
35	j2	25	
35	j3	25	
35	j4	25	
35	j5	25	
35	j6	25	
36	k1	181	
36	k2	181	
36	k3	181	
36	k4	181	
36	k5	181	
36	k6	181	
37	l1	198	
37	l2	198	
37	l3	198	
37	l4	198	
37	l5	198	
37	l6	198	

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
38	ZN	f1	500	-	-	X	-
38	ZN	f5	500	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 470574 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 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T1	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T2	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T3	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T4	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T5	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T6	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			

- Molecule 2 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U1	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U2	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U3	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U4	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U5	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U6	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			

- Molecule 3 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V1	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V2	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V3	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V4	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V5	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V6	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			

- Molecule 4 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X1	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X2	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X3	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X4	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X5	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X6	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			

- Molecule 5 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	a1	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a2	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a3	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a4	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a5	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a6	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			

- Molecule 6 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	c1	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c2	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c3	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c4	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c5	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c6	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			

- Molecule 7 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	d1	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d2	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d3	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d4	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d5	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d6	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			

- Molecule 8 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	f1	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			
8	f2	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			
8	f3	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			
8	f4	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			
8	f5	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	f6	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			

- Molecule 9 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	g1	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g2	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g3	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g4	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g5	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g6	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			

- Molecule 10 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	C1	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C2	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C3	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C4	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C5	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C6	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G1	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			
11	G2	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G3	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			
11	G4	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			
11	G5	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			
11	G6	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			

- Molecule 12 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J1	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J2	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J3	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J4	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J5	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J6	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			

- Molecule 13 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M1	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M2	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M3	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M4	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M5	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M6	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N1	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N2	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N3	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N4	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N5	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N6	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O1	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O2	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O3	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O4	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O5	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O6	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			

- Molecule 16 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	W1	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W2	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W3	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W4	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W5	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W6	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y1	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y2	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y3	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y4	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y5	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y6	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			

- Molecule 18 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z1	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z2	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z3	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z4	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z5	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z6	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			

- Molecule 19 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	b1	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			
19	b2	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			
19	b3	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			
19	b4	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			
19	b5	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	b6	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			

- Molecule 20 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	e1	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e2	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e3	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e4	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e5	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e6	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e1	-48	ALA	-	insertion	UNP E9PR30
e1	-47	HIS	-	insertion	UNP E9PR30
e1	-46	VAL	-	insertion	UNP E9PR30
e1	-45	ALA	-	insertion	UNP E9PR30
e1	-44	SER	-	insertion	UNP E9PR30
e1	-43	LEU	-	insertion	UNP E9PR30
e1	-42	GLU	-	insertion	UNP E9PR30
e1	-41	GLY	-	insertion	UNP E9PR30
e1	-40	ILE	-	insertion	UNP E9PR30
e1	-39	ALA	-	insertion	UNP E9PR30
e1	-38	PRO	-	insertion	UNP E9PR30
e1	-37	GLU	-	insertion	UNP E9PR30
e1	-36	ASP	-	insertion	UNP E9PR30
e1	-35	GLN	-	insertion	UNP E9PR30
e1	-34	VAL	-	insertion	UNP E9PR30
e1	-33	VAL	-	insertion	UNP E9PR30
e1	-32	LEU	-	insertion	UNP E9PR30
e1	-31	LEU	-	insertion	UNP E9PR30
e1	-30	ALA	-	insertion	UNP E9PR30
e1	-29	GLY	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e1	-28	ALA	-	insertion	UNP E9PR30
e1	-27	PRO	-	insertion	UNP E9PR30
e1	-26	LEU	-	insertion	UNP E9PR30
e1	-25	GLU	-	insertion	UNP E9PR30
e1	-24	ASP	-	insertion	UNP E9PR30
e1	-23	GLU	-	insertion	UNP E9PR30
e1	-22	ALA	-	insertion	UNP E9PR30
e1	-21	THR	-	insertion	UNP E9PR30
e1	-20	LEU	-	insertion	UNP E9PR30
e1	-19	GLY	-	insertion	UNP E9PR30
e1	-18	GLN	-	insertion	UNP E9PR30
e1	-17	CYS	-	insertion	UNP E9PR30
e1	-16	GLY	-	insertion	UNP E9PR30
e1	-15	VAL	-	insertion	UNP E9PR30
e1	-14	GLU	-	insertion	UNP E9PR30
e2	-48	ALA	-	insertion	UNP E9PR30
e2	-47	HIS	-	insertion	UNP E9PR30
e2	-46	VAL	-	insertion	UNP E9PR30
e2	-45	ALA	-	insertion	UNP E9PR30
e2	-44	SER	-	insertion	UNP E9PR30
e2	-43	LEU	-	insertion	UNP E9PR30
e2	-42	GLU	-	insertion	UNP E9PR30
e2	-41	GLY	-	insertion	UNP E9PR30
e2	-40	ILE	-	insertion	UNP E9PR30
e2	-39	ALA	-	insertion	UNP E9PR30
e2	-38	PRO	-	insertion	UNP E9PR30
e2	-37	GLU	-	insertion	UNP E9PR30
e2	-36	ASP	-	insertion	UNP E9PR30
e2	-35	GLN	-	insertion	UNP E9PR30
e2	-34	VAL	-	insertion	UNP E9PR30
e2	-33	VAL	-	insertion	UNP E9PR30
e2	-32	LEU	-	insertion	UNP E9PR30
e2	-31	LEU	-	insertion	UNP E9PR30
e2	-30	ALA	-	insertion	UNP E9PR30
e2	-29	GLY	-	insertion	UNP E9PR30
e2	-28	ALA	-	insertion	UNP E9PR30
e2	-27	PRO	-	insertion	UNP E9PR30
e2	-26	LEU	-	insertion	UNP E9PR30
e2	-25	GLU	-	insertion	UNP E9PR30
e2	-24	ASP	-	insertion	UNP E9PR30
e2	-23	GLU	-	insertion	UNP E9PR30
e2	-22	ALA	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e2	-21	THR	-	insertion	UNP E9PR30
e2	-20	LEU	-	insertion	UNP E9PR30
e2	-19	GLY	-	insertion	UNP E9PR30
e2	-18	GLN	-	insertion	UNP E9PR30
e2	-17	CYS	-	insertion	UNP E9PR30
e2	-16	GLY	-	insertion	UNP E9PR30
e2	-15	VAL	-	insertion	UNP E9PR30
e2	-14	GLU	-	insertion	UNP E9PR30
e3	-48	ALA	-	insertion	UNP E9PR30
e3	-47	HIS	-	insertion	UNP E9PR30
e3	-46	VAL	-	insertion	UNP E9PR30
e3	-45	ALA	-	insertion	UNP E9PR30
e3	-44	SER	-	insertion	UNP E9PR30
e3	-43	LEU	-	insertion	UNP E9PR30
e3	-42	GLU	-	insertion	UNP E9PR30
e3	-41	GLY	-	insertion	UNP E9PR30
e3	-40	ILE	-	insertion	UNP E9PR30
e3	-39	ALA	-	insertion	UNP E9PR30
e3	-38	PRO	-	insertion	UNP E9PR30
e3	-37	GLU	-	insertion	UNP E9PR30
e3	-36	ASP	-	insertion	UNP E9PR30
e3	-35	GLN	-	insertion	UNP E9PR30
e3	-34	VAL	-	insertion	UNP E9PR30
e3	-33	VAL	-	insertion	UNP E9PR30
e3	-32	LEU	-	insertion	UNP E9PR30
e3	-31	LEU	-	insertion	UNP E9PR30
e3	-30	ALA	-	insertion	UNP E9PR30
e3	-29	GLY	-	insertion	UNP E9PR30
e3	-28	ALA	-	insertion	UNP E9PR30
e3	-27	PRO	-	insertion	UNP E9PR30
e3	-26	LEU	-	insertion	UNP E9PR30
e3	-25	GLU	-	insertion	UNP E9PR30
e3	-24	ASP	-	insertion	UNP E9PR30
e3	-23	GLU	-	insertion	UNP E9PR30
e3	-22	ALA	-	insertion	UNP E9PR30
e3	-21	THR	-	insertion	UNP E9PR30
e3	-20	LEU	-	insertion	UNP E9PR30
e3	-19	GLY	-	insertion	UNP E9PR30
e3	-18	GLN	-	insertion	UNP E9PR30
e3	-17	CYS	-	insertion	UNP E9PR30
e3	-16	GLY	-	insertion	UNP E9PR30
e3	-15	VAL	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e3	-14	GLU	-	insertion	UNP E9PR30
e4	-48	ALA	-	insertion	UNP E9PR30
e4	-47	HIS	-	insertion	UNP E9PR30
e4	-46	VAL	-	insertion	UNP E9PR30
e4	-45	ALA	-	insertion	UNP E9PR30
e4	-44	SER	-	insertion	UNP E9PR30
e4	-43	LEU	-	insertion	UNP E9PR30
e4	-42	GLU	-	insertion	UNP E9PR30
e4	-41	GLY	-	insertion	UNP E9PR30
e4	-40	ILE	-	insertion	UNP E9PR30
e4	-39	ALA	-	insertion	UNP E9PR30
e4	-38	PRO	-	insertion	UNP E9PR30
e4	-37	GLU	-	insertion	UNP E9PR30
e4	-36	ASP	-	insertion	UNP E9PR30
e4	-35	GLN	-	insertion	UNP E9PR30
e4	-34	VAL	-	insertion	UNP E9PR30
e4	-33	VAL	-	insertion	UNP E9PR30
e4	-32	LEU	-	insertion	UNP E9PR30
e4	-31	LEU	-	insertion	UNP E9PR30
e4	-30	ALA	-	insertion	UNP E9PR30
e4	-29	GLY	-	insertion	UNP E9PR30
e4	-28	ALA	-	insertion	UNP E9PR30
e4	-27	PRO	-	insertion	UNP E9PR30
e4	-26	LEU	-	insertion	UNP E9PR30
e4	-25	GLU	-	insertion	UNP E9PR30
e4	-24	ASP	-	insertion	UNP E9PR30
e4	-23	GLU	-	insertion	UNP E9PR30
e4	-22	ALA	-	insertion	UNP E9PR30
e4	-21	THR	-	insertion	UNP E9PR30
e4	-20	LEU	-	insertion	UNP E9PR30
e4	-19	GLY	-	insertion	UNP E9PR30
e4	-18	GLN	-	insertion	UNP E9PR30
e4	-17	CYS	-	insertion	UNP E9PR30
e4	-16	GLY	-	insertion	UNP E9PR30
e4	-15	VAL	-	insertion	UNP E9PR30
e4	-14	GLU	-	insertion	UNP E9PR30
e5	-48	ALA	-	insertion	UNP E9PR30
e5	-47	HIS	-	insertion	UNP E9PR30
e5	-46	VAL	-	insertion	UNP E9PR30
e5	-45	ALA	-	insertion	UNP E9PR30
e5	-44	SER	-	insertion	UNP E9PR30
e5	-43	LEU	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e5	-42	GLU	-	insertion	UNP E9PR30
e5	-41	GLY	-	insertion	UNP E9PR30
e5	-40	ILE	-	insertion	UNP E9PR30
e5	-39	ALA	-	insertion	UNP E9PR30
e5	-38	PRO	-	insertion	UNP E9PR30
e5	-37	GLU	-	insertion	UNP E9PR30
e5	-36	ASP	-	insertion	UNP E9PR30
e5	-35	GLN	-	insertion	UNP E9PR30
e5	-34	VAL	-	insertion	UNP E9PR30
e5	-33	VAL	-	insertion	UNP E9PR30
e5	-32	LEU	-	insertion	UNP E9PR30
e5	-31	LEU	-	insertion	UNP E9PR30
e5	-30	ALA	-	insertion	UNP E9PR30
e5	-29	GLY	-	insertion	UNP E9PR30
e5	-28	ALA	-	insertion	UNP E9PR30
e5	-27	PRO	-	insertion	UNP E9PR30
e5	-26	LEU	-	insertion	UNP E9PR30
e5	-25	GLU	-	insertion	UNP E9PR30
e5	-24	ASP	-	insertion	UNP E9PR30
e5	-23	GLU	-	insertion	UNP E9PR30
e5	-22	ALA	-	insertion	UNP E9PR30
e5	-21	THR	-	insertion	UNP E9PR30
e5	-20	LEU	-	insertion	UNP E9PR30
e5	-19	GLY	-	insertion	UNP E9PR30
e5	-18	GLN	-	insertion	UNP E9PR30
e5	-17	CYS	-	insertion	UNP E9PR30
e5	-16	GLY	-	insertion	UNP E9PR30
e5	-15	VAL	-	insertion	UNP E9PR30
e5	-14	GLU	-	insertion	UNP E9PR30
e6	-48	ALA	-	insertion	UNP E9PR30
e6	-47	HIS	-	insertion	UNP E9PR30
e6	-46	VAL	-	insertion	UNP E9PR30
e6	-45	ALA	-	insertion	UNP E9PR30
e6	-44	SER	-	insertion	UNP E9PR30
e6	-43	LEU	-	insertion	UNP E9PR30
e6	-42	GLU	-	insertion	UNP E9PR30
e6	-41	GLY	-	insertion	UNP E9PR30
e6	-40	ILE	-	insertion	UNP E9PR30
e6	-39	ALA	-	insertion	UNP E9PR30
e6	-38	PRO	-	insertion	UNP E9PR30
e6	-37	GLU	-	insertion	UNP E9PR30
e6	-36	ASP	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e6	-35	GLN	-	insertion	UNP E9PR30
e6	-34	VAL	-	insertion	UNP E9PR30
e6	-33	VAL	-	insertion	UNP E9PR30
e6	-32	LEU	-	insertion	UNP E9PR30
e6	-31	LEU	-	insertion	UNP E9PR30
e6	-30	ALA	-	insertion	UNP E9PR30
e6	-29	GLY	-	insertion	UNP E9PR30
e6	-28	ALA	-	insertion	UNP E9PR30
e6	-27	PRO	-	insertion	UNP E9PR30
e6	-26	LEU	-	insertion	UNP E9PR30
e6	-25	GLU	-	insertion	UNP E9PR30
e6	-24	ASP	-	insertion	UNP E9PR30
e6	-23	GLU	-	insertion	UNP E9PR30
e6	-22	ALA	-	insertion	UNP E9PR30
e6	-21	THR	-	insertion	UNP E9PR30
e6	-20	LEU	-	insertion	UNP E9PR30
e6	-19	GLY	-	insertion	UNP E9PR30
e6	-18	GLN	-	insertion	UNP E9PR30
e6	-17	CYS	-	insertion	UNP E9PR30
e6	-16	GLY	-	insertion	UNP E9PR30
e6	-15	VAL	-	insertion	UNP E9PR30
e6	-14	GLU	-	insertion	UNP E9PR30

- Molecule 21 is a RNA chain called Human 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	i1	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i2	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i3	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i4	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i5	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i6	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i1	582	C	U	conflict	GB 36162

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Chain	Residue	Modelled	Actual	Comment	Reference
i1	583	C	A	conflict	GB 36162
i1	584	G	A	conflict	GB 36162
i1	798	A	G	conflict	GB 36162
i1	1095	U	C	conflict	GB 36162
i2	582	C	U	conflict	GB 36162
i2	583	C	A	conflict	GB 36162
i2	584	G	A	conflict	GB 36162
i2	798	A	G	conflict	GB 36162
i2	1095	U	C	conflict	GB 36162
i3	582	C	U	conflict	GB 36162
i3	583	C	A	conflict	GB 36162
i3	584	G	A	conflict	GB 36162
i3	798	A	G	conflict	GB 36162
i3	1095	U	C	conflict	GB 36162
i4	582	C	U	conflict	GB 36162
i4	583	C	A	conflict	GB 36162
i4	584	G	A	conflict	GB 36162
i4	798	A	G	conflict	GB 36162
i4	1095	U	C	conflict	GB 36162
i5	582	C	U	conflict	GB 36162
i5	583	C	A	conflict	GB 36162
i5	584	G	A	conflict	GB 36162
i5	798	A	G	conflict	GB 36162
i5	1095	U	C	conflict	GB 36162
i6	582	C	U	conflict	GB 36162
i6	583	C	A	conflict	GB 36162
i6	584	G	A	conflict	GB 36162
i6	798	A	G	conflict	GB 36162
i6	1095	U	C	conflict	GB 36162

- Molecule 22 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A1	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			
22	A2	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			
22	A3	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			
22	A4	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			
22	A5	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A6	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			

- Molecule 23 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	B1	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B2	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B3	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B4	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B5	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B6	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			

- Molecule 24 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D1	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D2	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D3	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D4	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D5	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D6	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			

- Molecule 25 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	E1	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			
25	E2	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	E3	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			
25	E4	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			
25	E5	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			
25	E6	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			

- Molecule 26 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	F1	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F2	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F3	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F4	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F5	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F6	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			

- Molecule 27 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	H1	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H2	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H3	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H4	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H5	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H6	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			

- Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	I1	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I2	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I3	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I4	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I5	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I6	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			

- Molecule 29 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	K1	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K2	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K3	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K4	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K5	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K6	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			

- Molecule 30 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	L1	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L2	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L3	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L4	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L5	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L6	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			

- Molecule 31 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	P1	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P2	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P3	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P4	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P5	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P6	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			

- Molecule 32 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Q1	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q2	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q3	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q4	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q5	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q6	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			

- Molecule 33 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R1	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			
33	R2	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			
33	R3	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			
33	R4	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			
33	R5	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R6	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			

- Molecule 34 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	S1	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S2	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S3	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S4	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S5	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S6	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			

- Molecule 35 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	j1	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j2	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j3	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j4	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j5	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j6	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			

- Molecule 36 is a protein called Malignant T-cell-amplified sequence 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	k1	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			
36	k2	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	k3	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			
36	k4	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			
36	k5	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			
36	k6	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			

- Molecule 37 is a protein called Density-regulated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	l1	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l2	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l3	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l4	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l5	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l6	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			

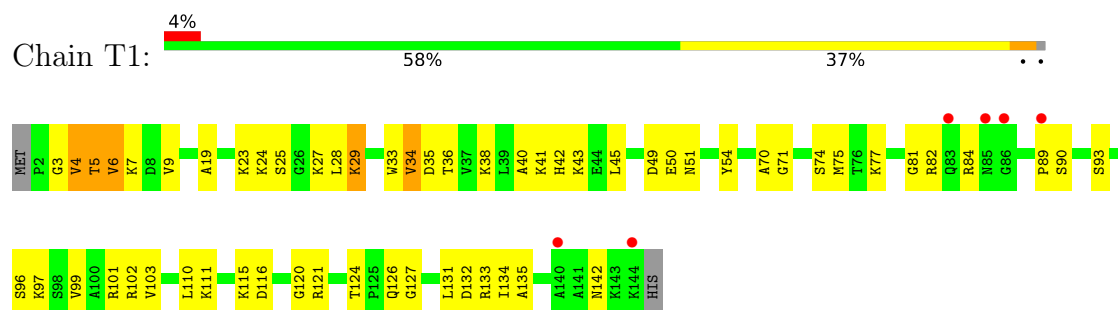
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	f1	1	Total	Zn	0	0
			1	1		
38	f2	1	Total	Zn	0	0
			1	1		
38	f3	1	Total	Zn	0	0
			1	1		
38	f4	1	Total	Zn	0	0
			1	1		
38	f5	1	Total	Zn	0	0
			1	1		
38	f6	1	Total	Zn	0	0
			1	1		

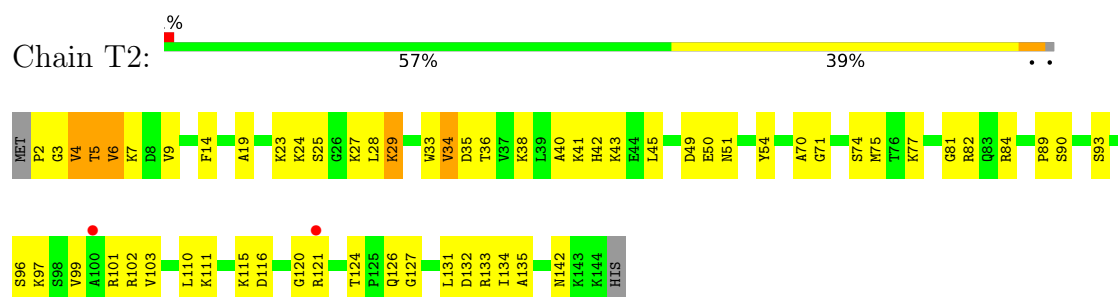
3 Residue-property plots [i](#)

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.

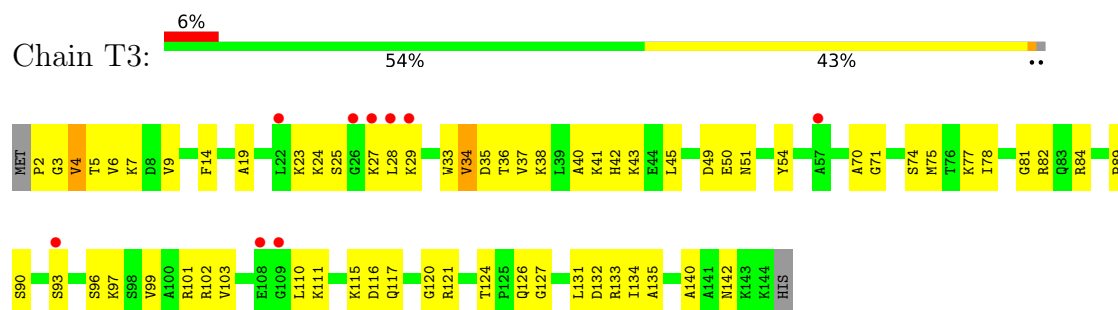
- Molecule 1: 40S ribosomal protein S19



- Molecule 1: 40S ribosomal protein S19

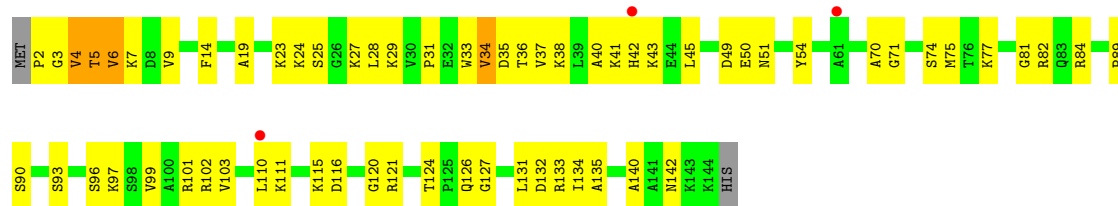


- Molecule 1: 40S ribosomal protein S19

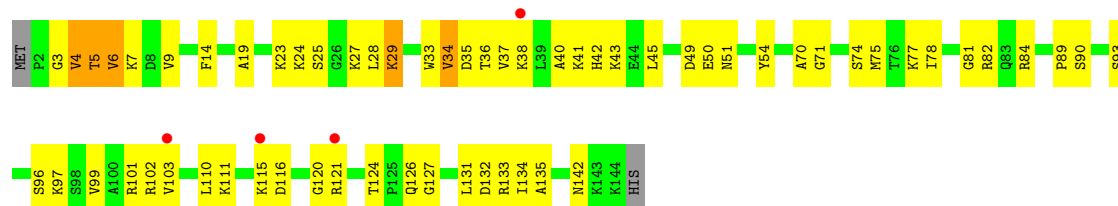


- Molecule 1: 40S ribosomal protein S19

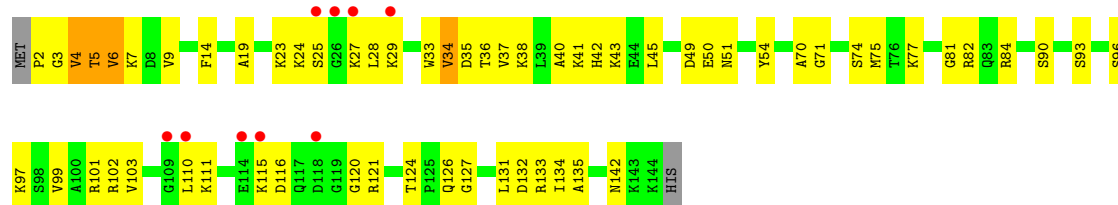




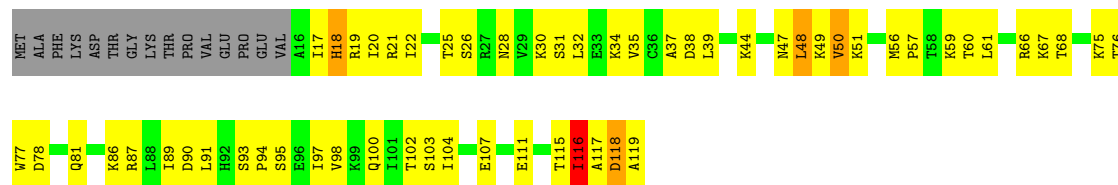
• Molecule 1: 40S ribosomal protein S19



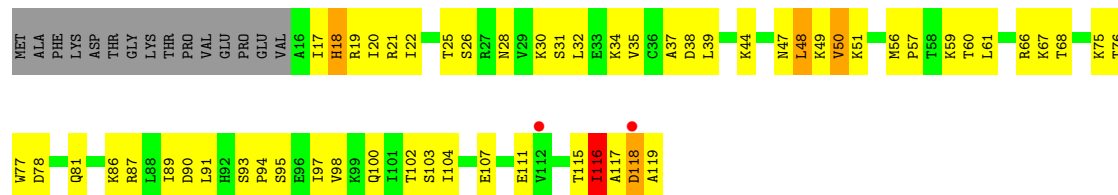
• Molecule 1: 40S ribosomal protein S19



• Molecule 2: 40S ribosomal protein S20



• Molecule 2: 40S ribosomal protein S20



- Molecule 2: 40S ribosomal protein S20

Chain U3: 



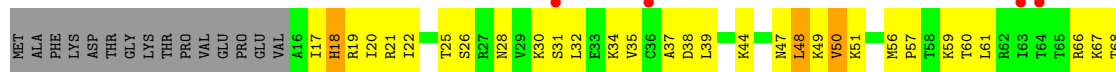
- Molecule 2: 40S ribosomal protein S20

Chain U4: 



- Molecule 2: 40S ribosomal protein S20

Chain U5: 



- Molecule 2: 40S ribosomal protein S20

Chain U6: 

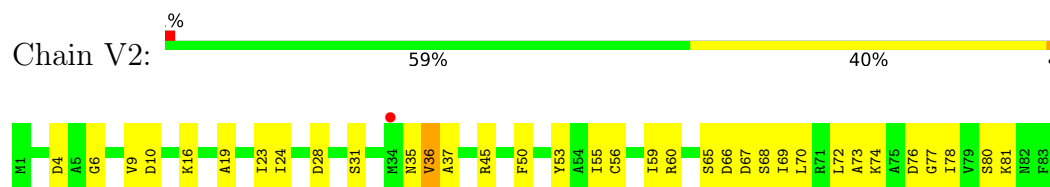


- Molecule 3: 40S ribosomal protein S21

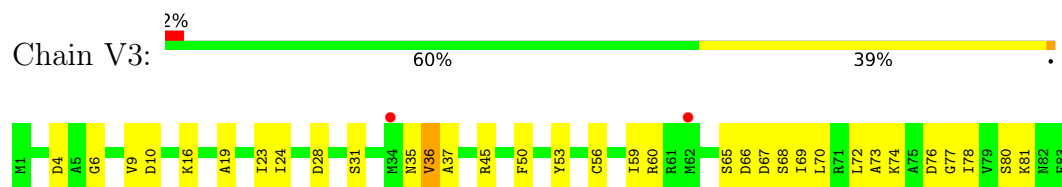
Chain V1: 



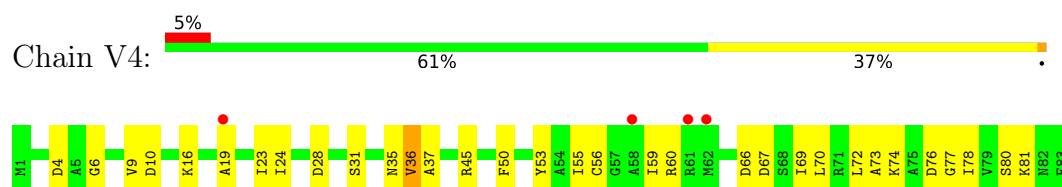
• Molecule 3: 40S ribosomal protein S21



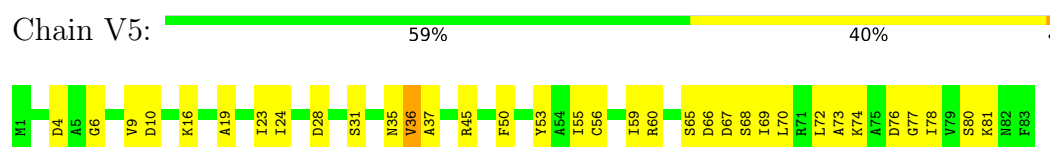
• Molecule 3: 40S ribosomal protein S21



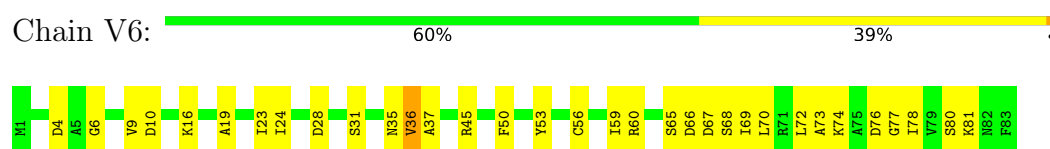
• Molecule 3: 40S ribosomal protein S21



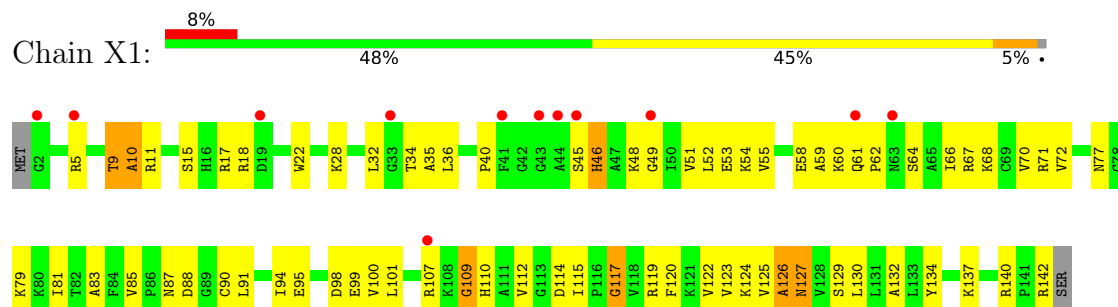
• Molecule 3: 40S ribosomal protein S21



• Molecule 3: 40S ribosomal protein S21

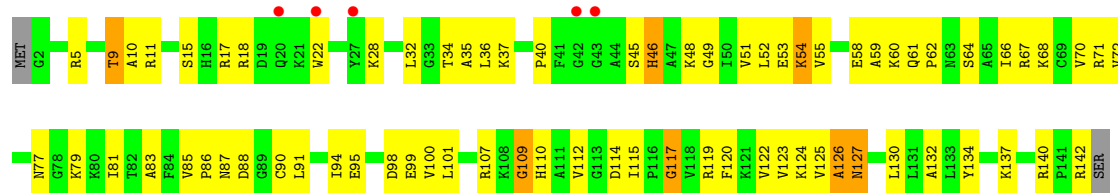


• Molecule 4: 40S ribosomal protein S23

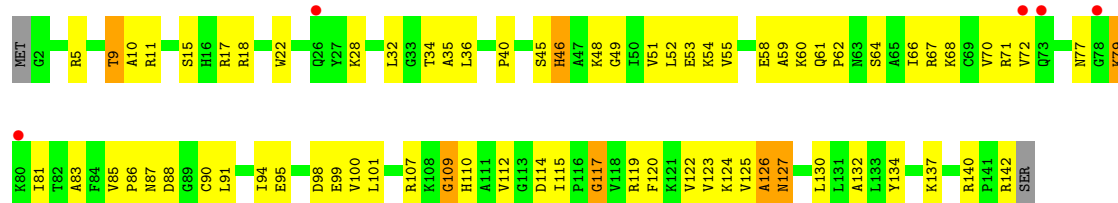


• Molecule 4: 40S ribosomal protein S23

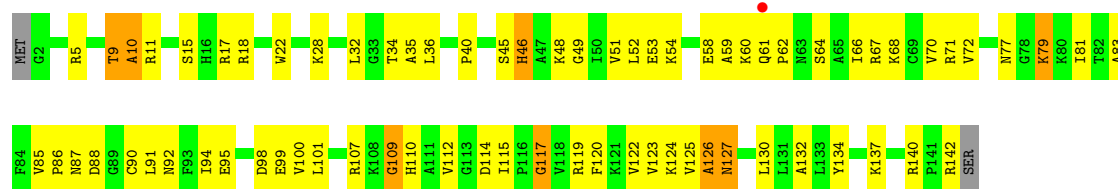




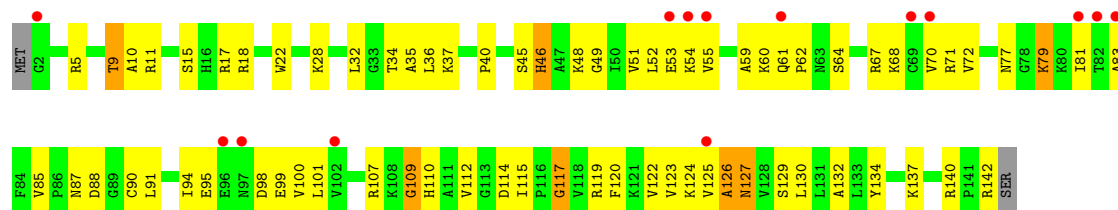
• Molecule 4: 40S ribosomal protein S23



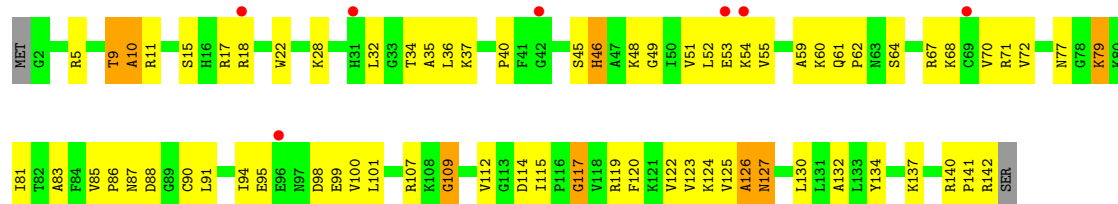
• Molecule 4: 40S ribosomal protein S23



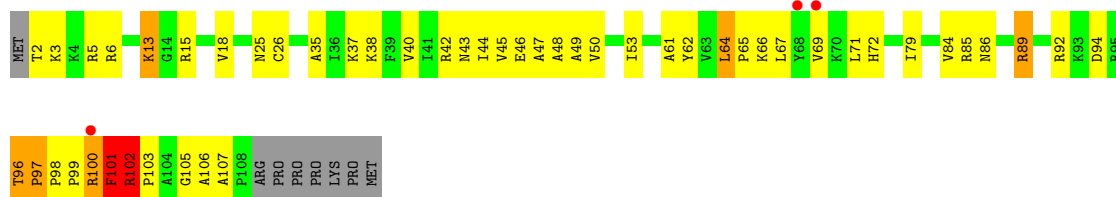
• Molecule 4: 40S ribosomal protein S23



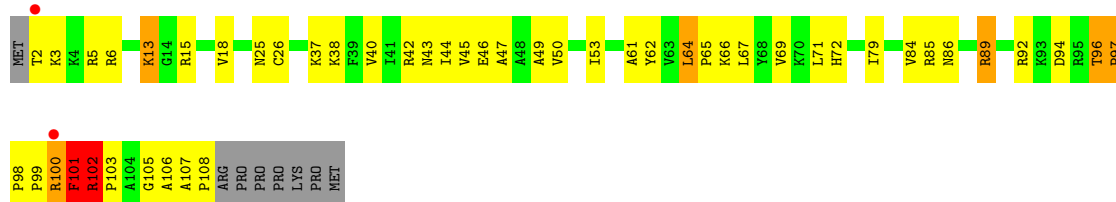
• Molecule 4: 40S ribosomal protein S23



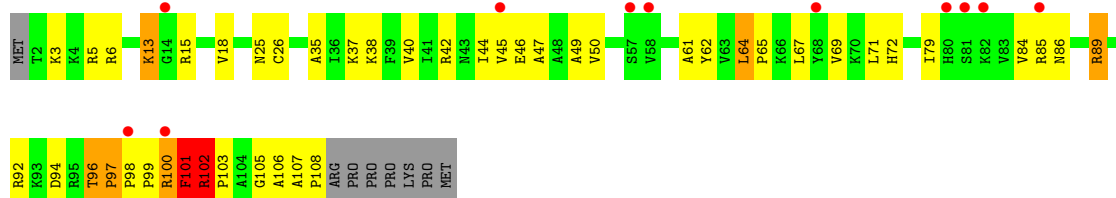
• Molecule 5: 40S ribosomal protein S26

Chain a1: 

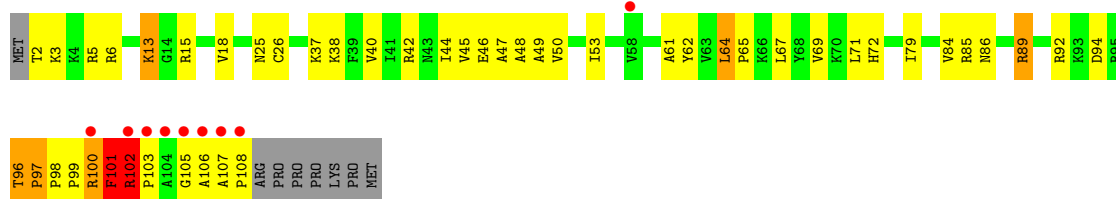
• Molecule 5: 40S ribosomal protein S26

Chain a2: 

• Molecule 5: 40S ribosomal protein S26

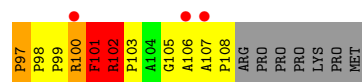
Chain a3: 

• Molecule 5: 40S ribosomal protein S26

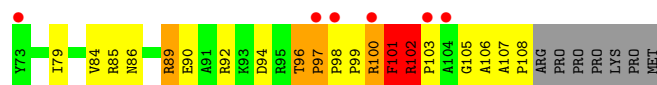
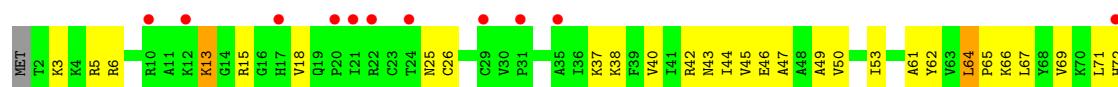
Chain a4: 

• Molecule 5: 40S ribosomal protein S26

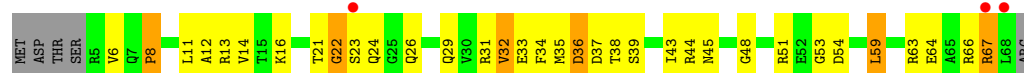
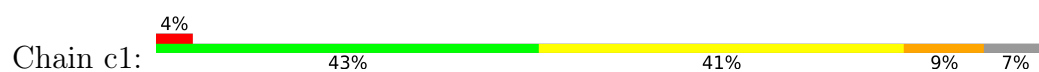
Chain a5: 



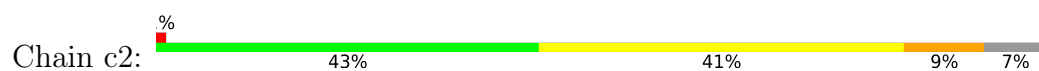
• Molecule 5: 40S ribosomal protein S26



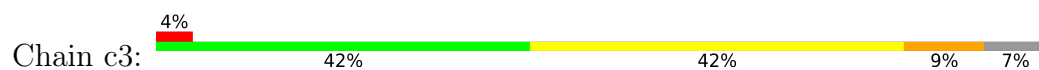
• Molecule 6: 40S ribosomal protein S28



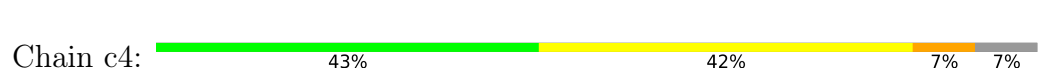
• Molecule 6: 40S ribosomal protein S28



• Molecule 6: 40S ribosomal protein S28



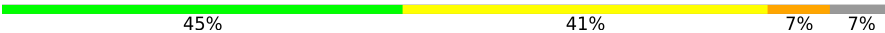
• Molecule 6: 40S ribosomal protein S28



• Molecule 6: 40S ribosomal protein S28



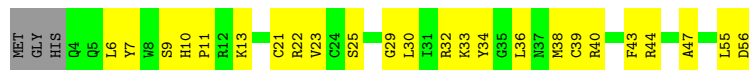
- Molecule 6: 40S ribosomal protein S28

Chain c6: 



- Molecule 7: 40S ribosomal protein S29

Chain d1: 

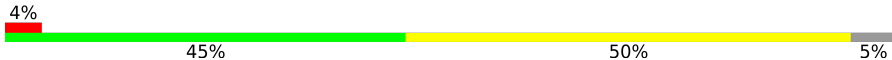


- Molecule 7: 40S ribosomal protein S29

Chain d2: 



- Molecule 7: 40S ribosomal protein S29

Chain d3: 



- Molecule 7: 40S ribosomal protein S29

Chain d4: 



- Molecule 7: 40S ribosomal protein S29

Chain d5: 

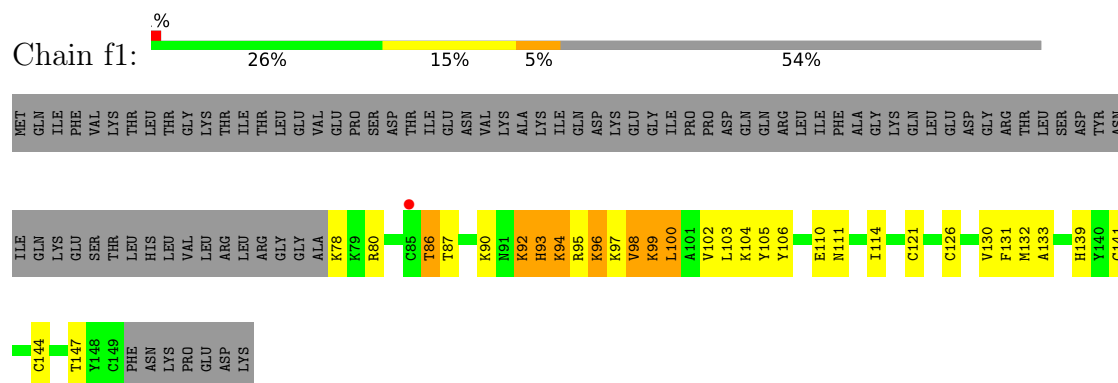


- Molecule 7: 40S ribosomal protein S29

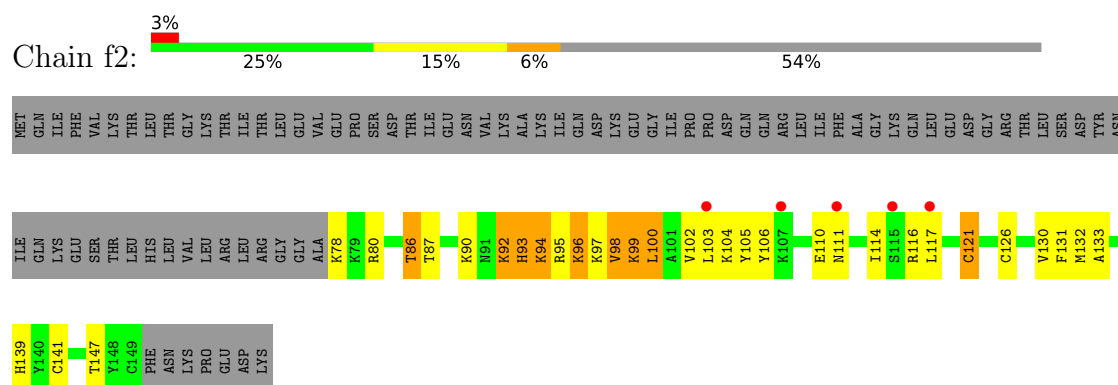
Chain d6: 



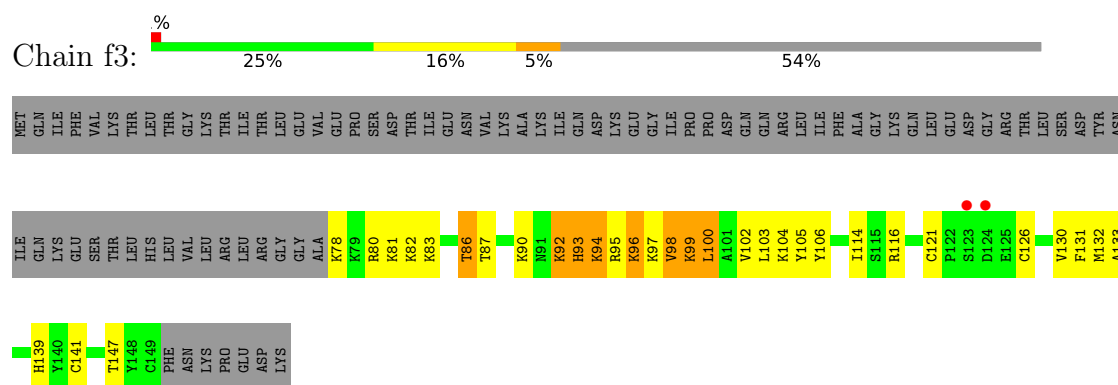
● Molecule 8: Ribosomal protein S27a



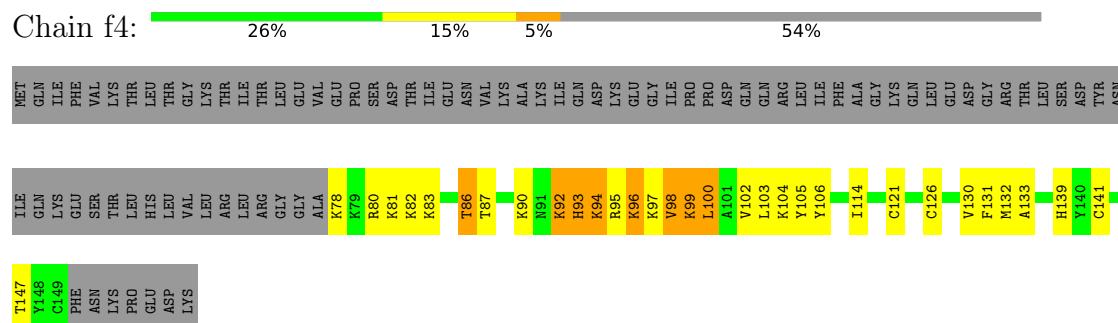
● Molecule 8: Ribosomal protein S27a



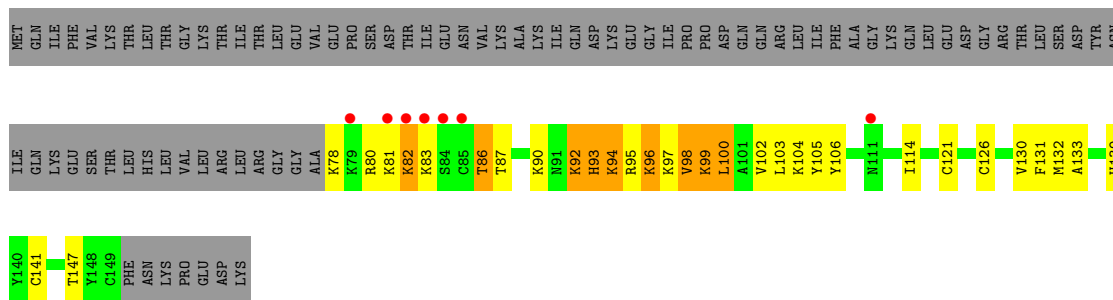
● Molecule 8: Ribosomal protein S27a



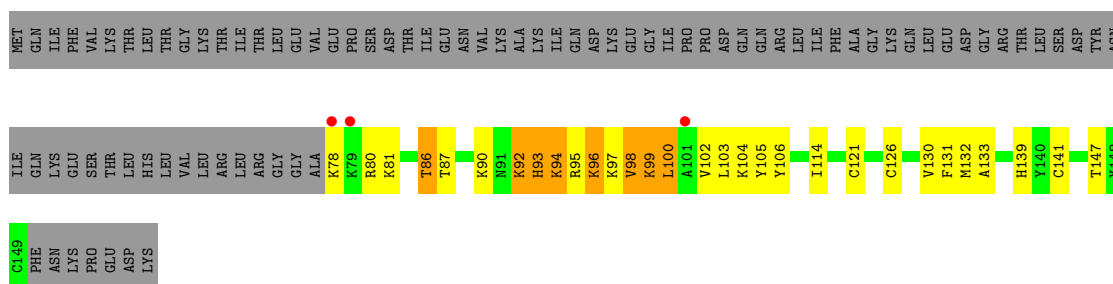
● Molecule 8: Ribosomal protein S27a



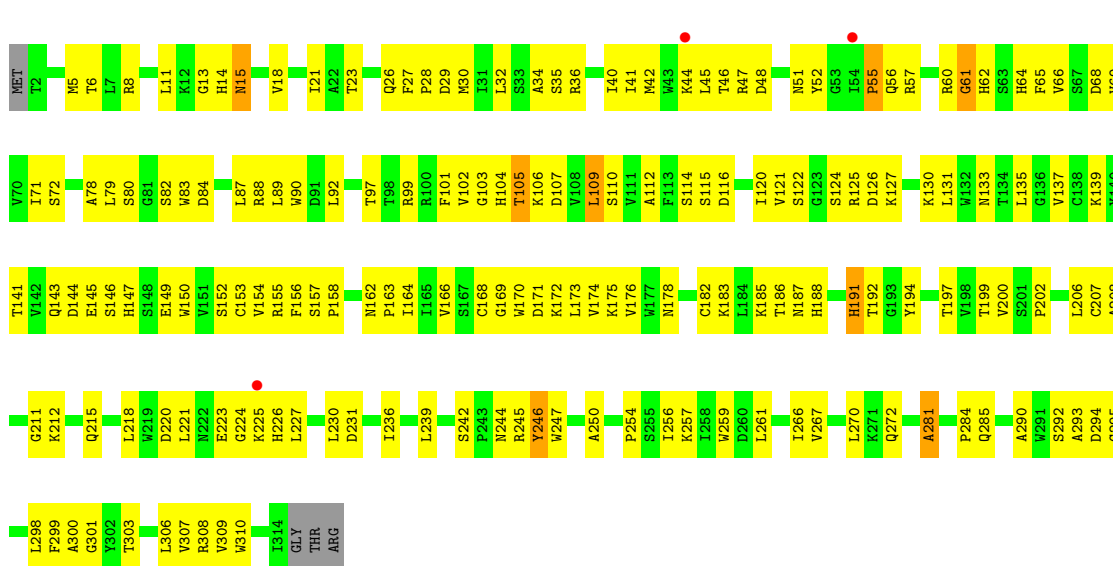
Chain f5:



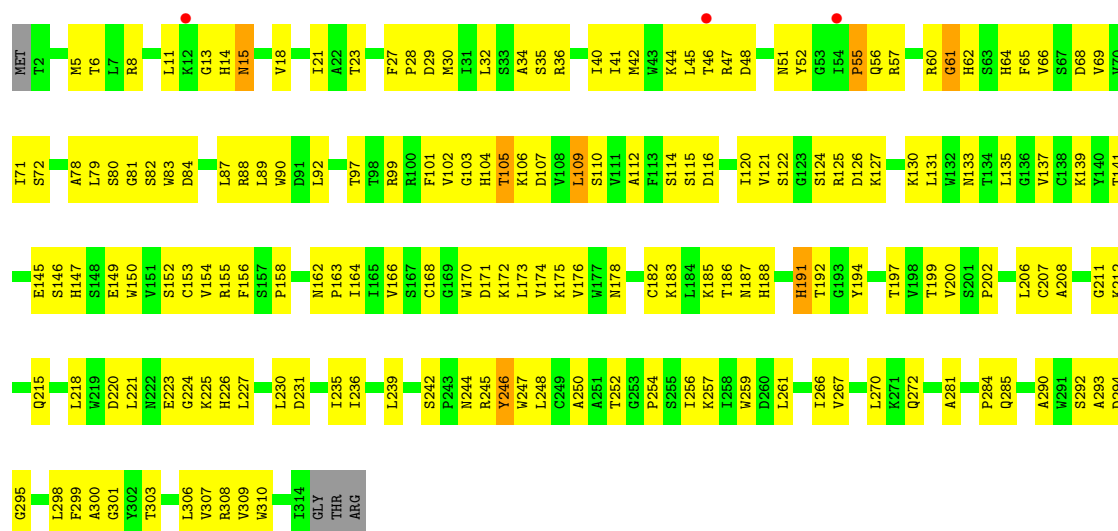
Chain f6:



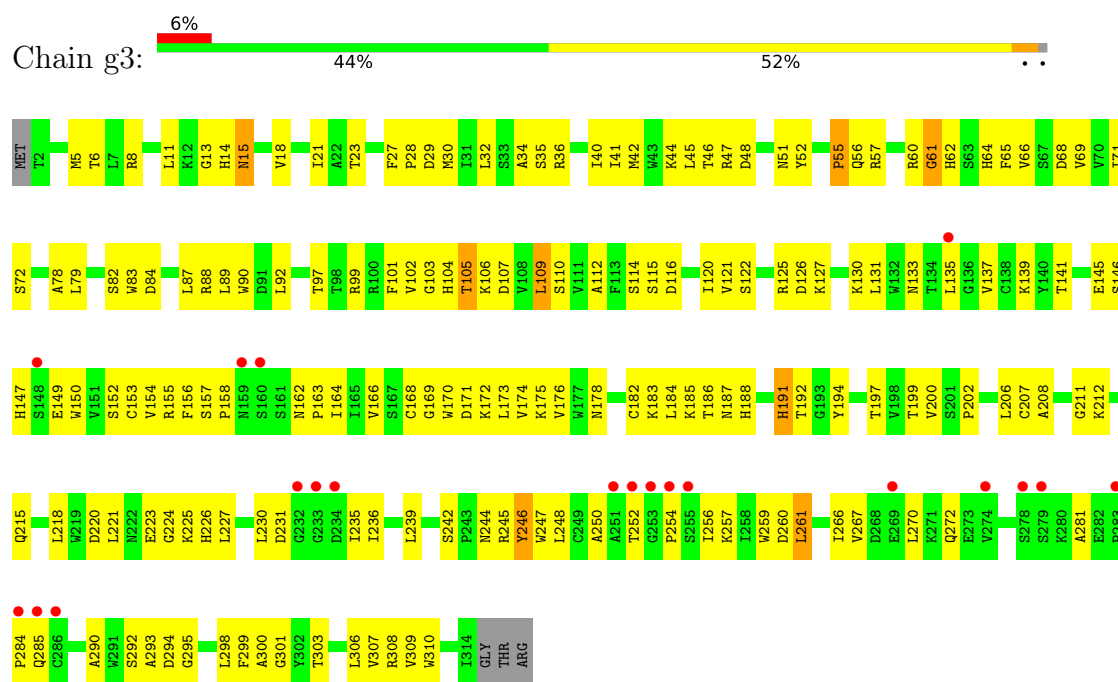
Chain g1: %



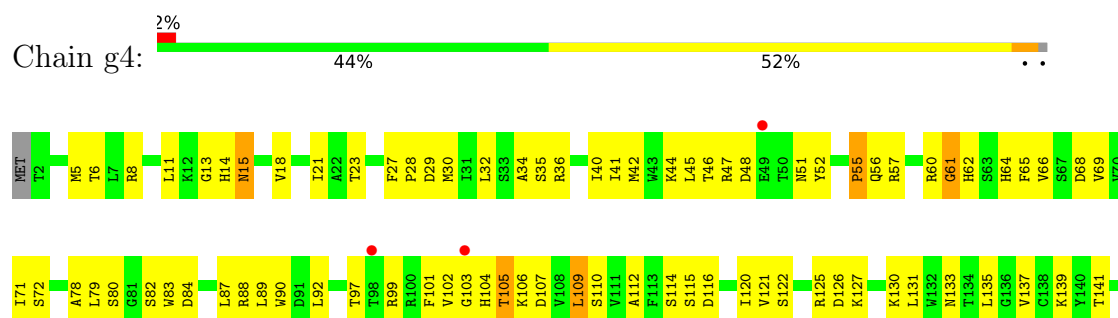
Chain g2: %



• Molecule 9: Receptor of activated protein C kinase 1

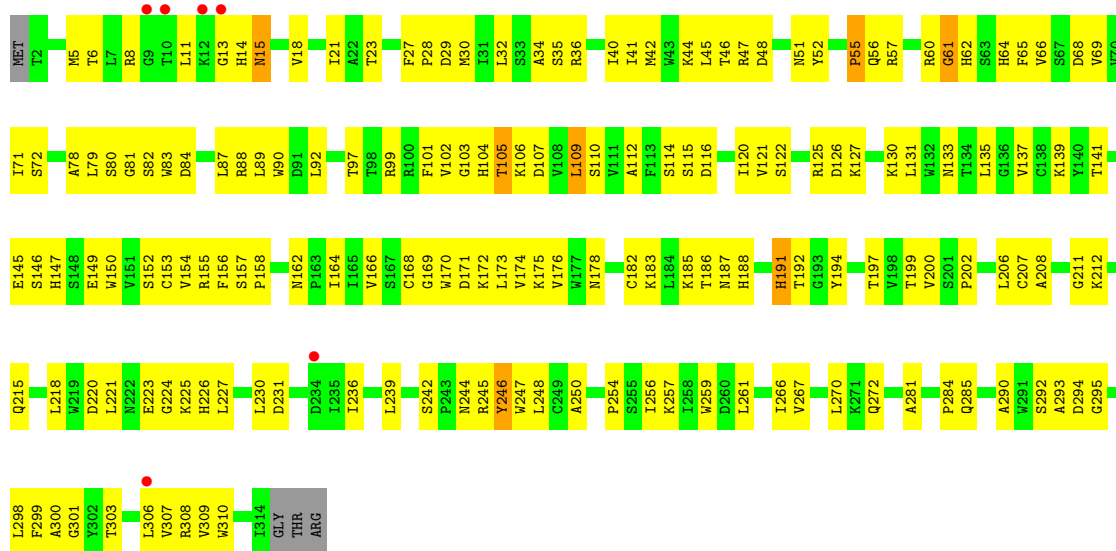


• Molecule 9: Receptor of activated protein C kinase 1

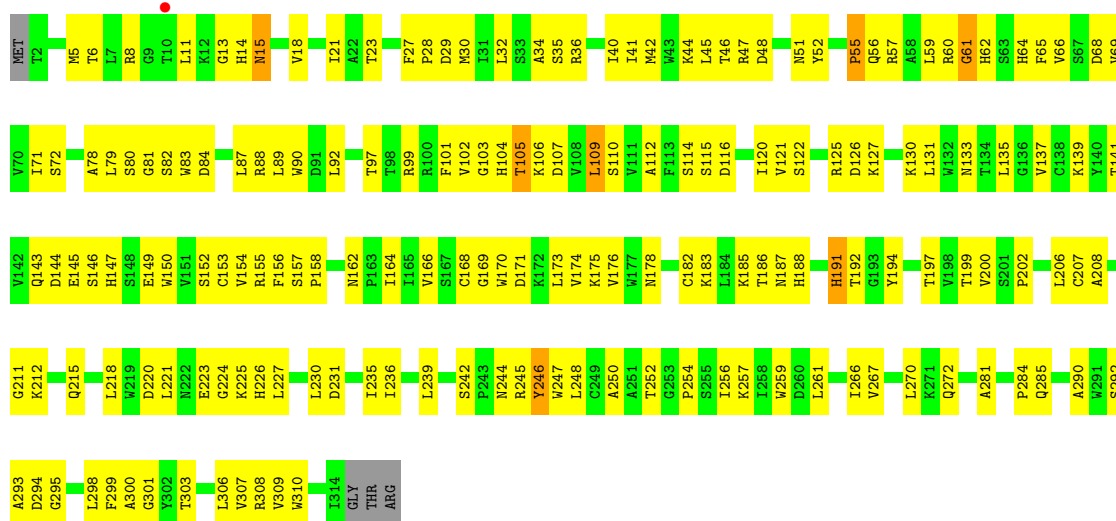




● Molecule 9: Receptor of activated protein C kinase 1



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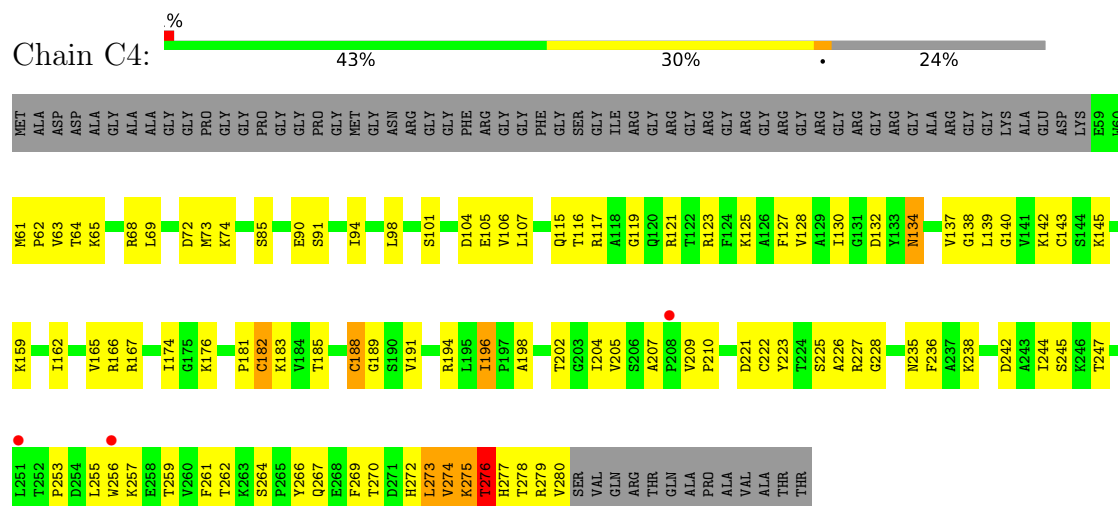
Chain C1:

[illegible]

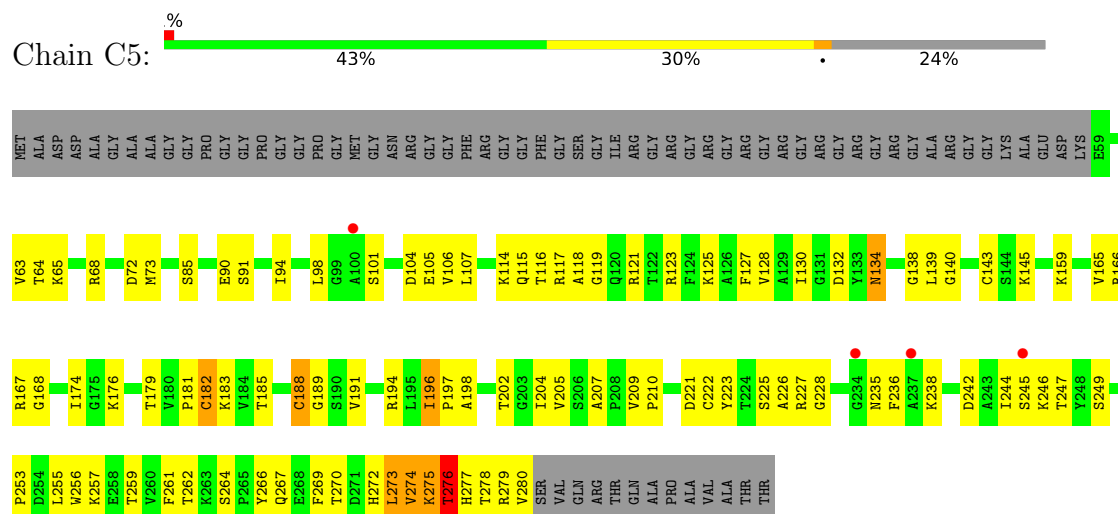
Chain C3:

Amino Acid	Category
K159	Green
K162	Green
V165	Green
R166	Green
R167	Green
G168	Green
I174	Green
G175	Green
K176	Green
T179	Green
V180	Green
P181	Green
C182	Green
K183	Green
C188	Green
G189	Green
S190	Green
V191	Green
R194	Green
L195	Green
L196	Green
P197	Green
A198	Green
T202	Green
G203	Green
I204	Green
V205	Green
S206	Green
A207	Green
P208	Green
G209	Green
R210	Green
L214	Green
I219	Green
D220	Green
D221	Green
C222	Green
Y223	Green
T224	Green
S225	Green
A226	Green
G228	Green
G234	Green
N235	Green
F236	Green
A237	Green
K238	Green
D242	Green
K159	Yellow
K162	Yellow
V165	Yellow
R166	Yellow
R167	Yellow
G168	Yellow
I174	Yellow
G175	Yellow
K176	Yellow
T179	Yellow
V180	Yellow
P181	Yellow
C182	Yellow
K183	Yellow
C188	Yellow
G189	Yellow
S190	Yellow
V191	Yellow
R194	Yellow
L195	Yellow
L196	Yellow
P197	Yellow
A198	Yellow
T202	Yellow
G203	Yellow
I204	Yellow
V205	Yellow
S206	Yellow
A207	Yellow
P208	Yellow
G209	Yellow
R210	Yellow
L214	Yellow
I219	Yellow
D220	Yellow
D221	Yellow
C222	Yellow
Y223	Yellow
T224	Yellow
S225	Yellow
A226	Yellow
G228	Yellow
G234	Yellow
N235	Yellow
F236	Yellow
A237	Yellow
K238	Yellow
D242	Yellow
K159	Grey
K162	Grey
V165	Grey
R166	Grey
R167	Grey
G168	Grey
I174	Grey
G175	Grey
K176	Grey
T179	Grey
V180	Grey
P181	Grey
C182	Grey
K183	Grey
C188	Grey
G189	Grey
S190	Grey
V191	Grey
R194	Grey
L195	Grey
L196	Grey
P197	Grey
A198	Grey
T202	Grey
G203	Grey
I204	Grey
V205	Grey
S206	Grey
A207	Grey
P208	Grey
G209	Grey
R210	Grey
L214	Grey
I219	Grey
D220	Grey
D221	Grey
C222	Grey
Y223	Grey
T224	Grey
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N235	Grey
F236	Grey
A237	Grey
K238	Grey
D242	Grey

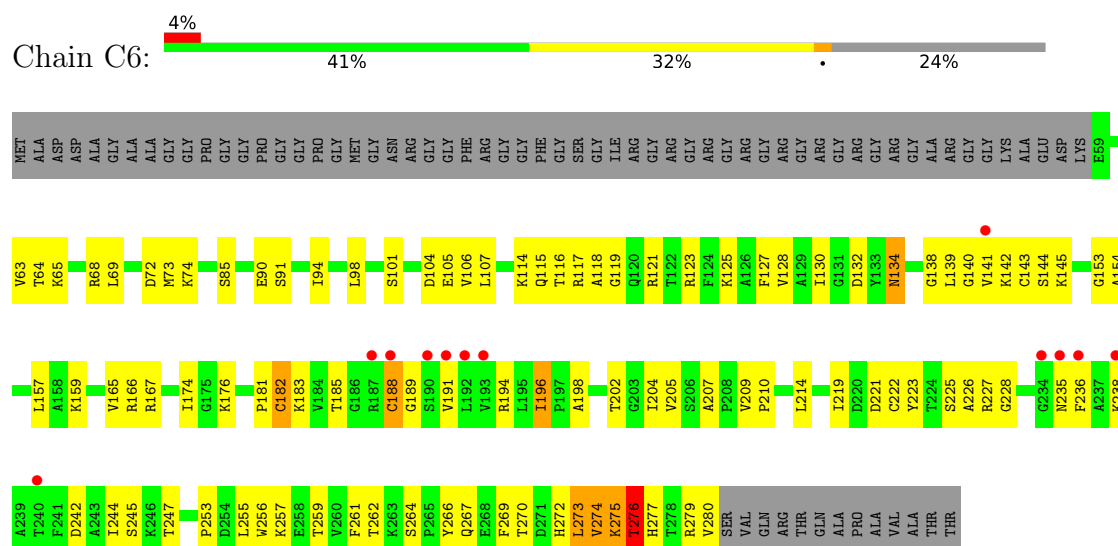
- Molecule 10: 40S ribosomal protein S2



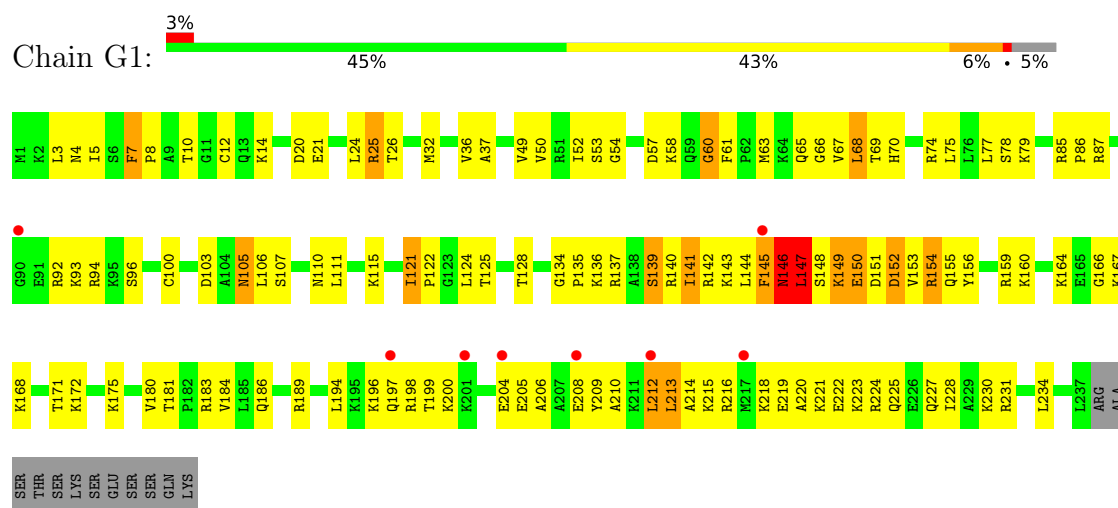
- Molecule 10: 40S ribosomal protein S2



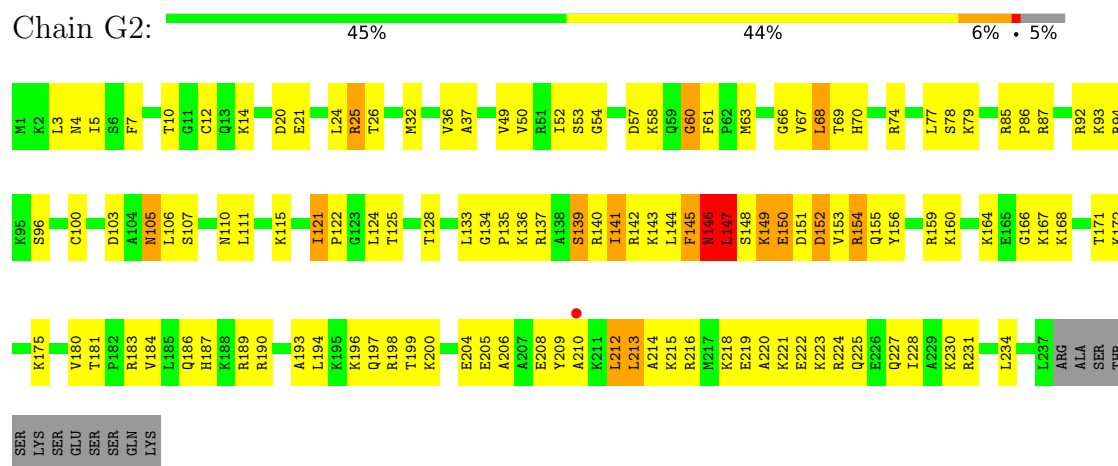
- Molecule 10: 40S ribosomal protein S2



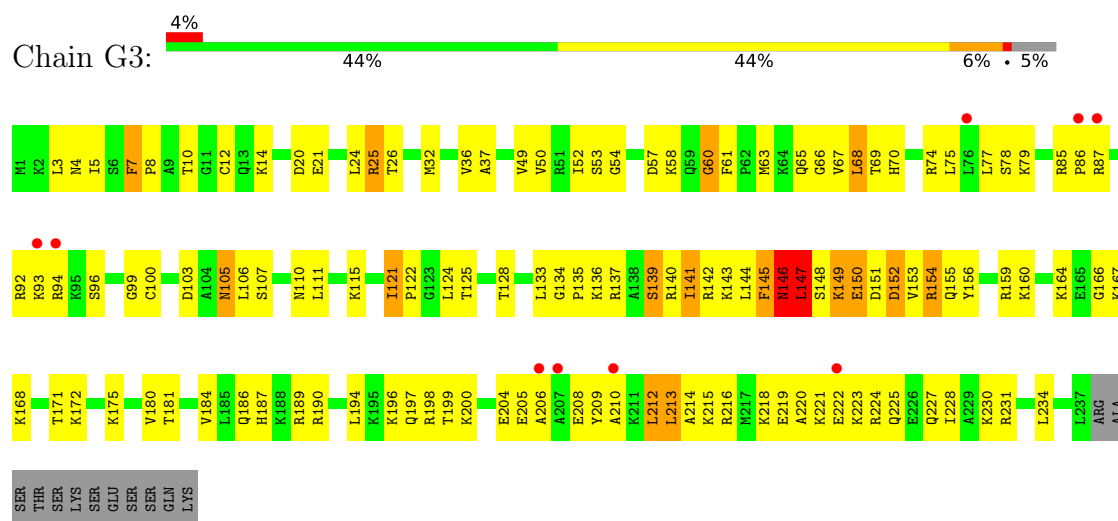
• Molecule 11: 40S ribosomal protein S6



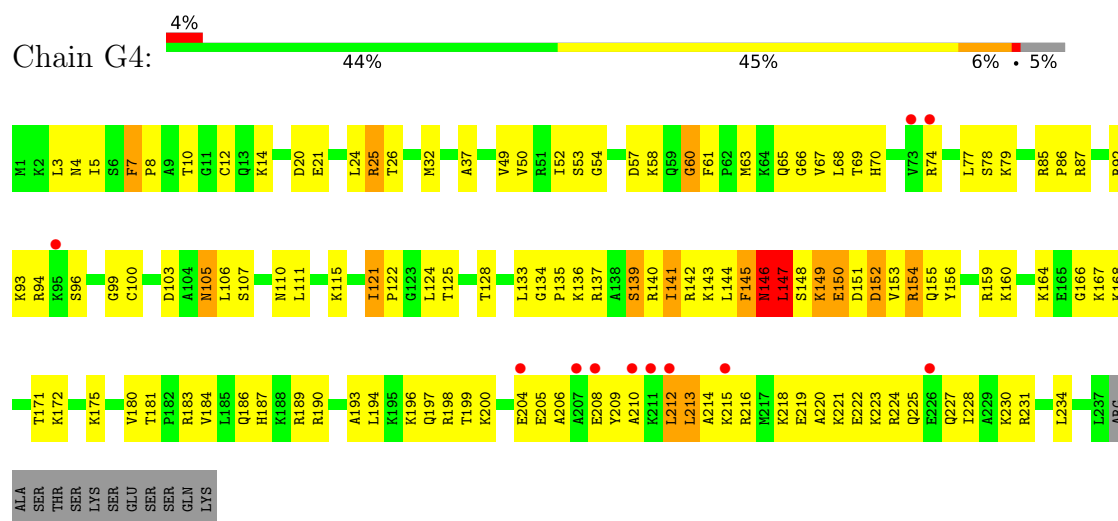
• Molecule 11: 40S ribosomal protein S6



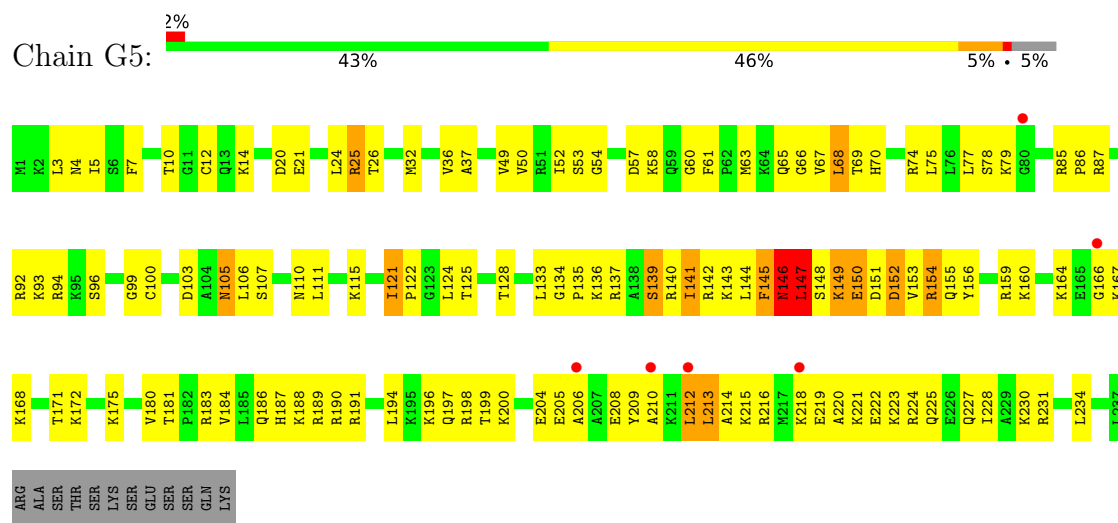
• Molecule 11: 40S ribosomal protein S6



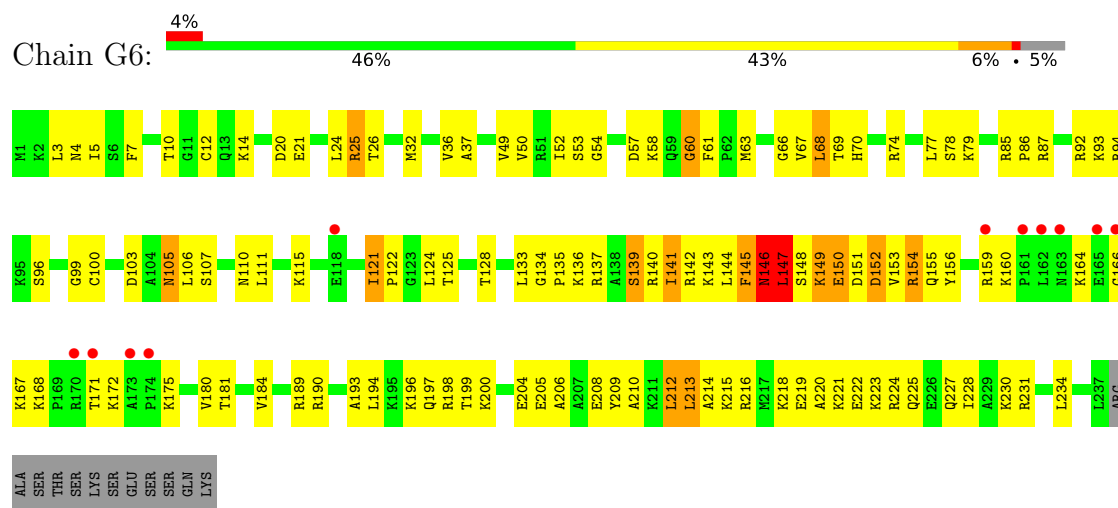
• Molecule 11: 40S ribosomal protein S6



• Molecule 11: 40S ribosomal protein S6

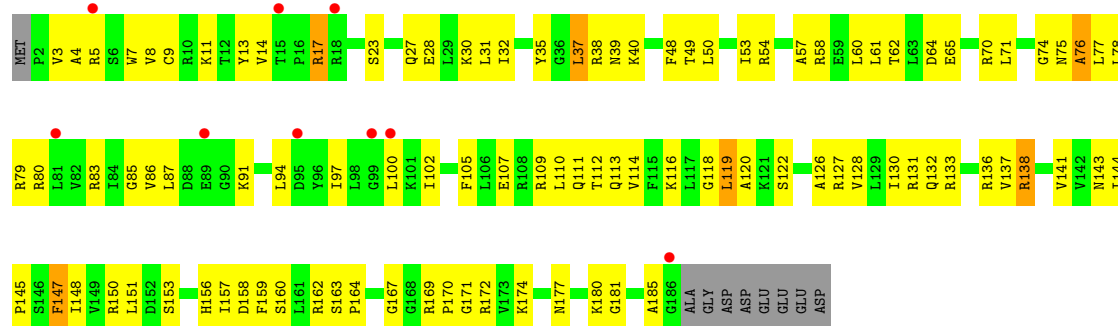


• Molecule 11: 40S ribosomal protein S6



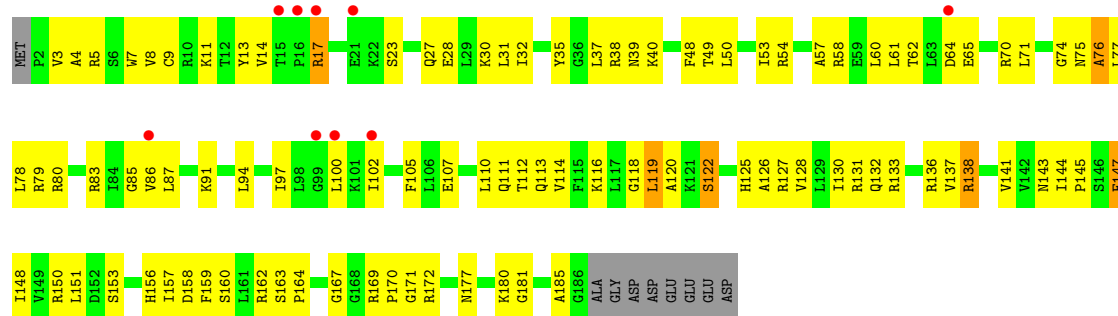
• Molecule 12: 40S ribosomal protein S9

Chain J1:  5% 43% 49% 5%



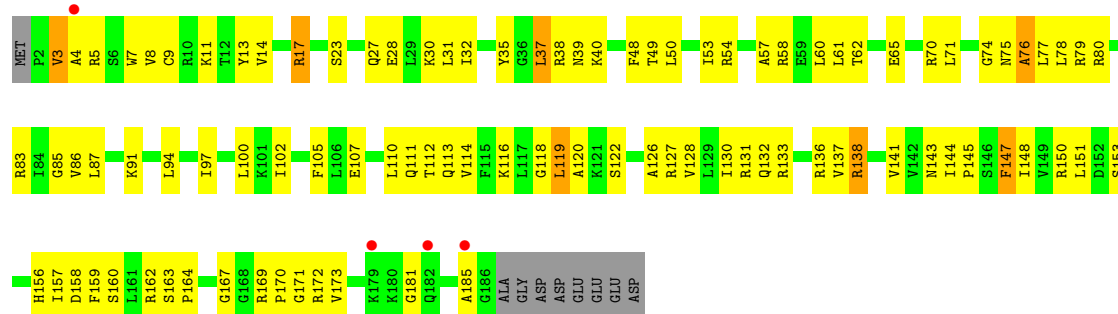
• Molecule 12: 40S ribosomal protein S9

Chain J2:  5% 44% 48% 5%



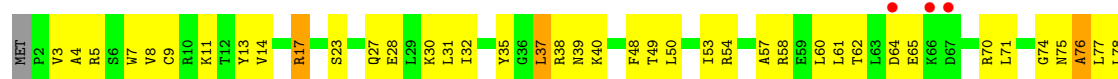
• Molecule 12: 40S ribosomal protein S9

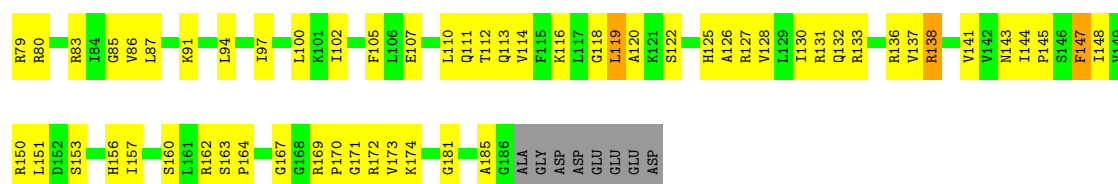
Chain J3:  2% 45% 46% 5%



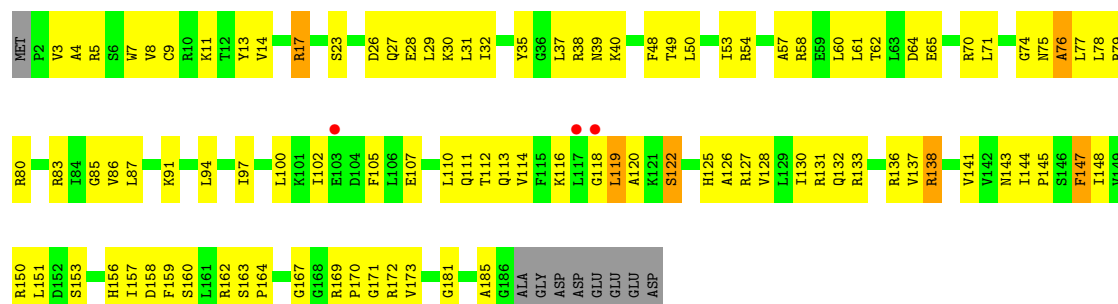
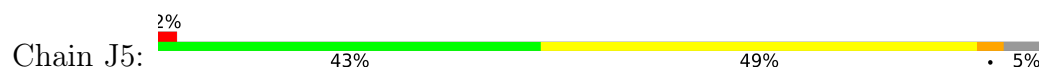
• Molecule 12: 40S ribosomal protein S9

Chain J4:  2% 45% 47% 5%

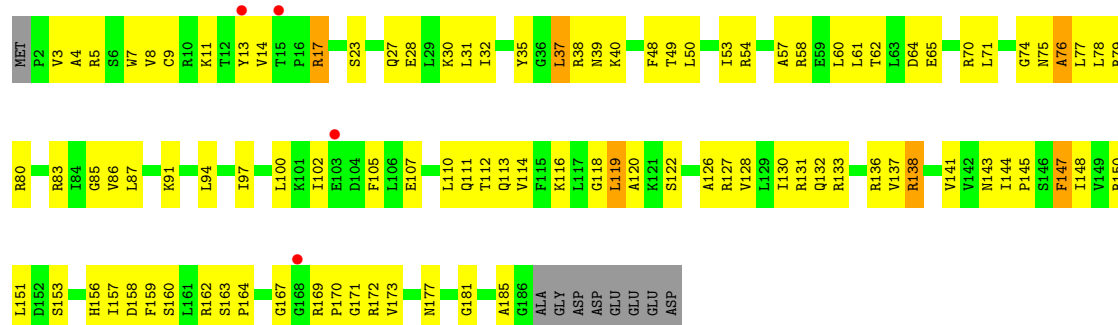
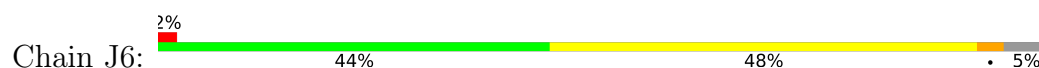




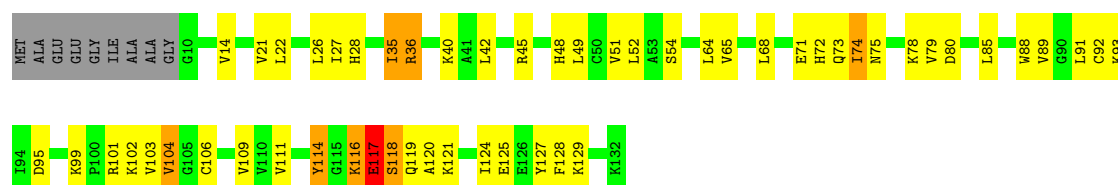
• Molecule 12: 40S ribosomal protein S9



• Molecule 12: 40S ribosomal protein S9

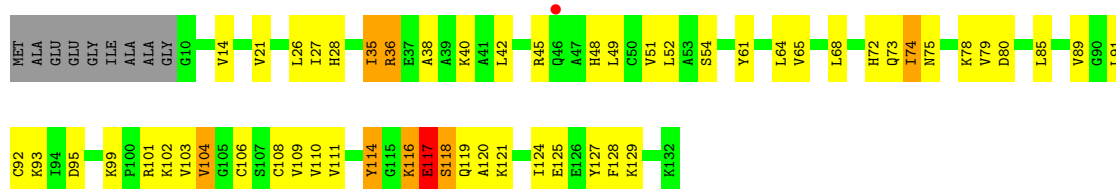


• Molecule 13: 40S ribosomal protein S12



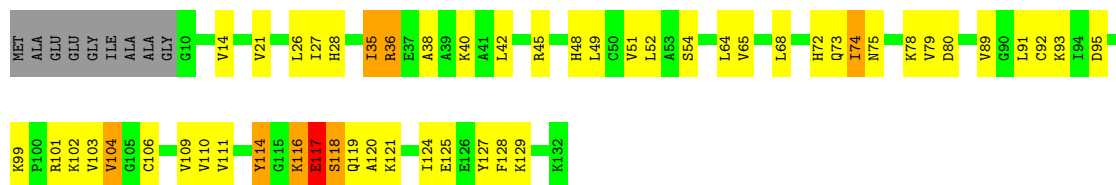
• Molecule 13: 40S ribosomal protein S12





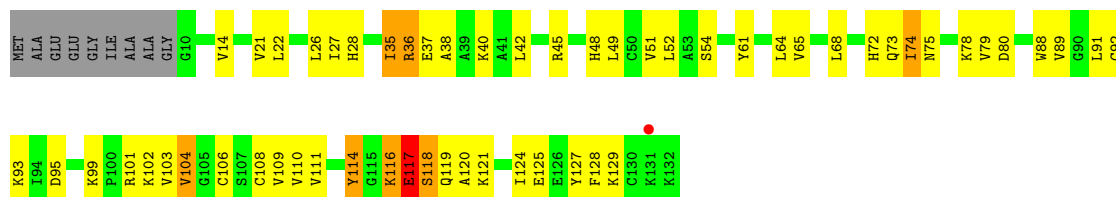
• Molecule 13: 40S ribosomal protein S12

Chain M3: 54% 33% 5% • 7%



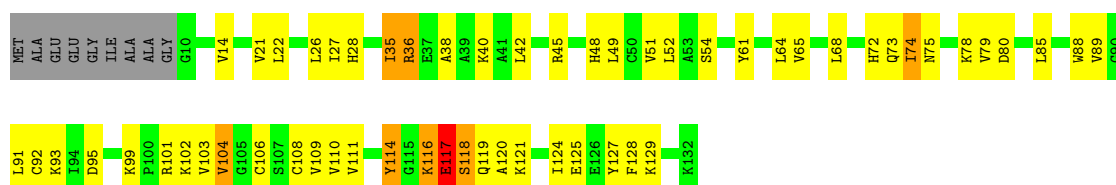
• Molecule 13: 40S ribosomal protein S12

Chain M4: 50% 37% 5% • 7%



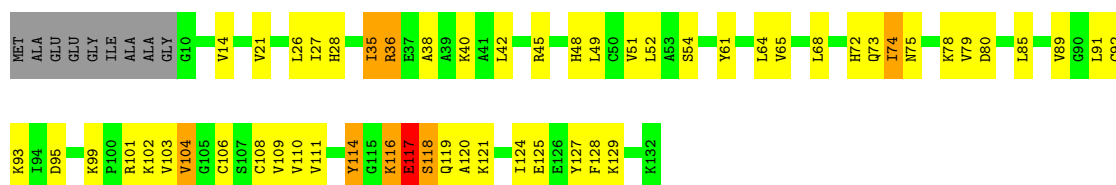
• Molecule 13: 40S ribosomal protein S12

Chain M5: 50% 37% 5% • 7%

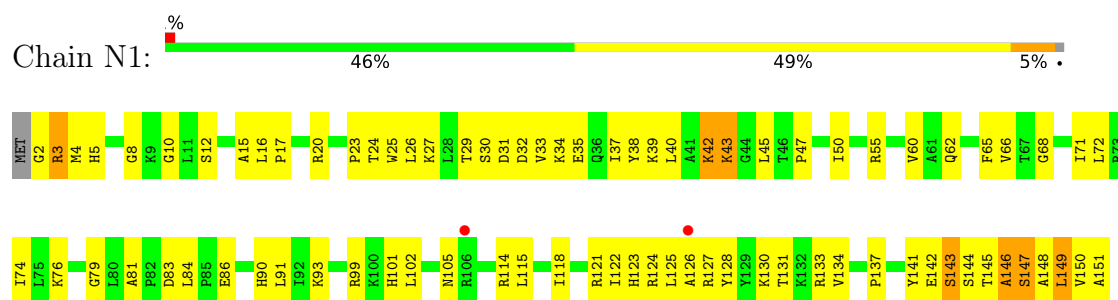


• Molecule 13: 40S ribosomal protein S12

Chain M6: 52% 36% 5% • 7%



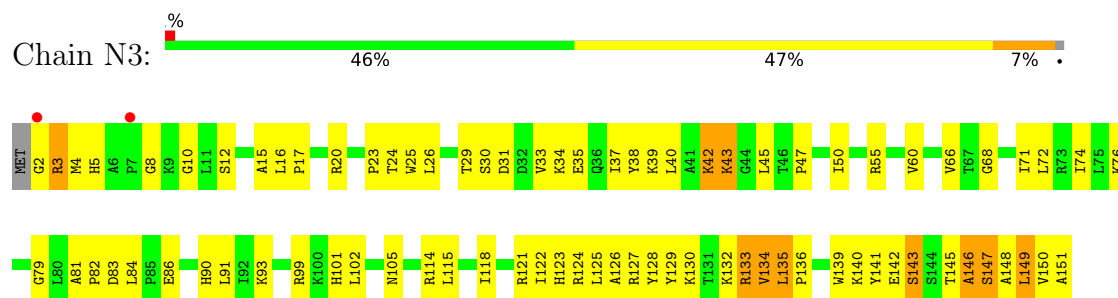
• Molecule 14: 40S ribosomal protein S13



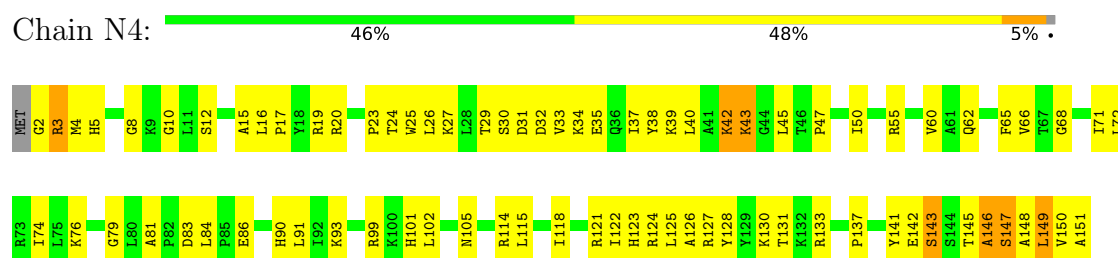
- Molecule 14: 40S ribosomal protein S13



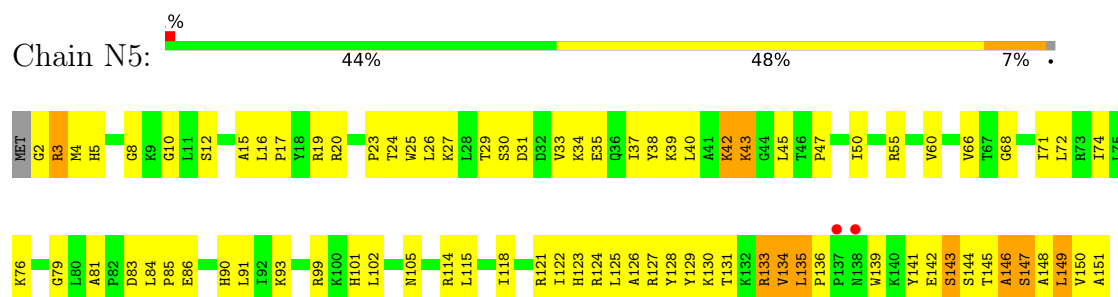
- Molecule 14: 40S ribosomal protein S13



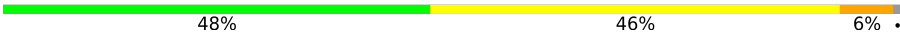
- Molecule 14: 40S ribosomal protein S13

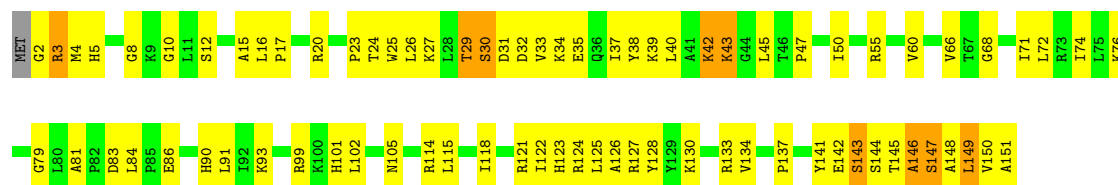


- Molecule 14: 40S ribosomal protein S13



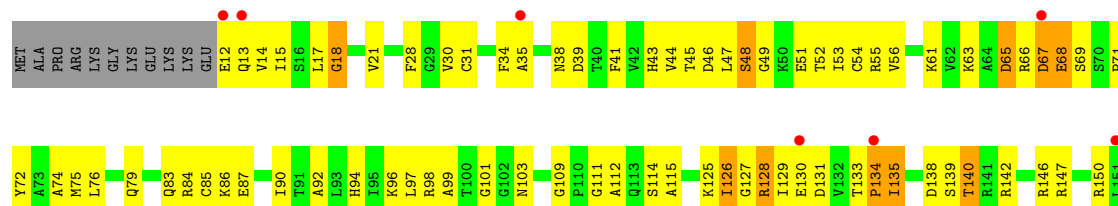
- Molecule 14: 40S ribosomal protein S13

Chain N6:  48% 46% 6%



- Molecule 15: 40S ribosomal protein S14

Chain O1:  5% 42% 44% 7% 7%



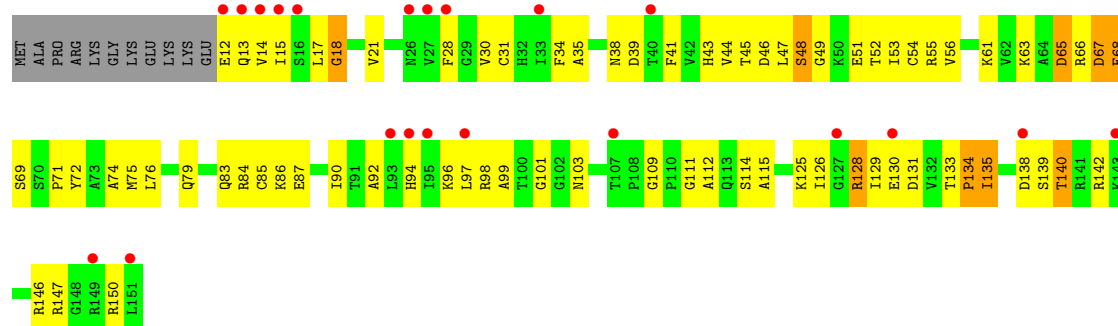
- Molecule 15: 40S ribosomal protein S14

Chain O2:  3% 42% 44% 7% 7%

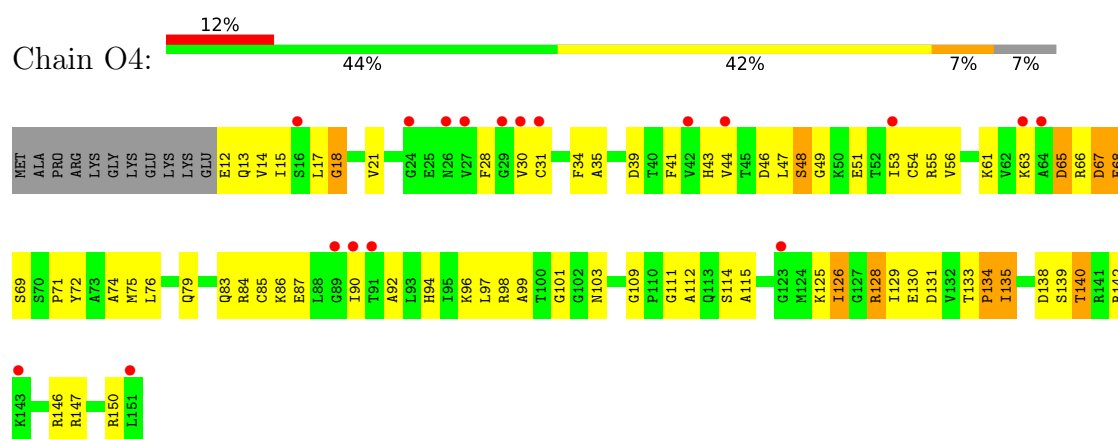


- Molecule 15: 40S ribosomal protein S14

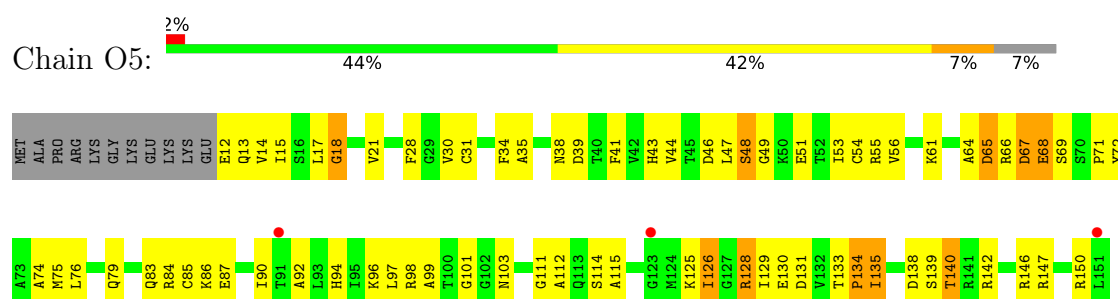
Chain O3:  14% 42% 44% 6% 7%



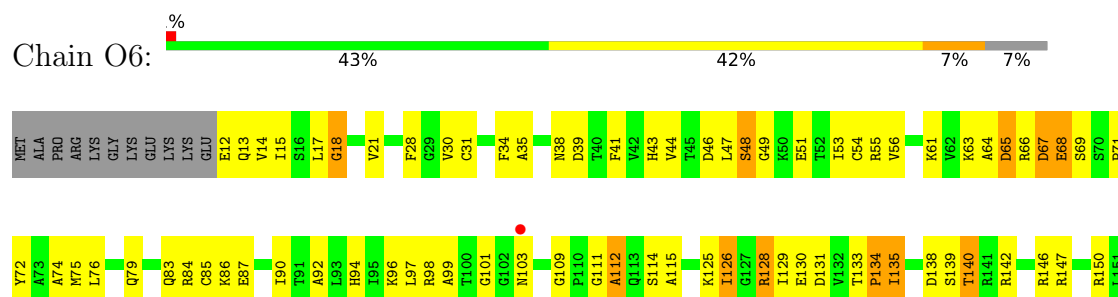
- Molecule 15: 40S ribosomal protein S14



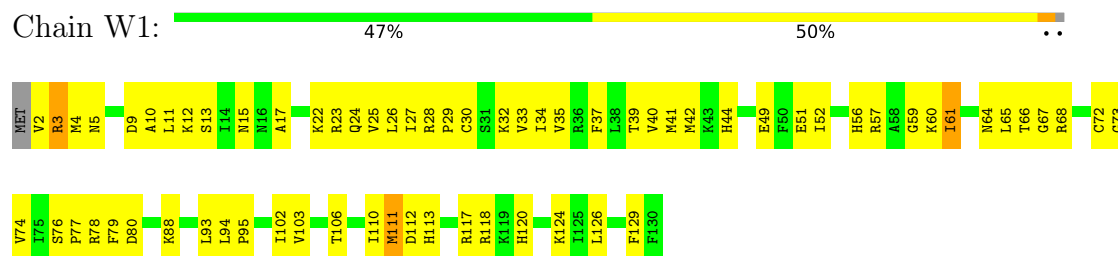
- Molecule 15: 40S ribosomal protein S14



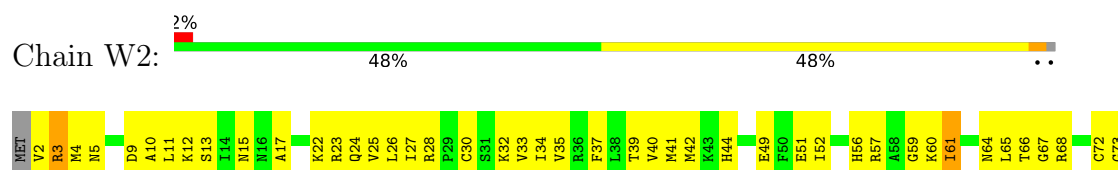
- Molecule 15: 40S ribosomal protein S14



- Molecule 16: 40S ribosomal protein S15a

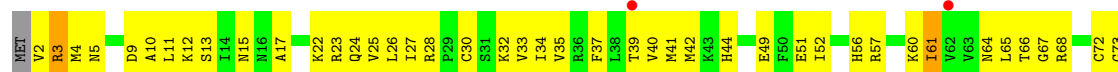


- Molecule 16: 40S ribosomal protein S15a

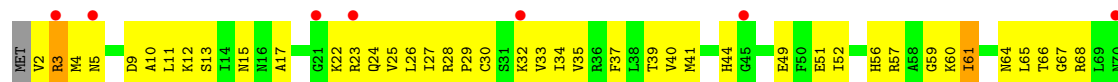




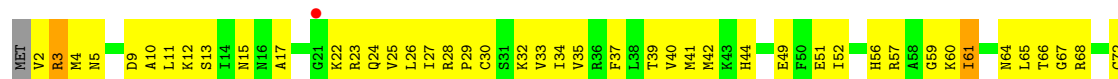
- Molecule 16: 40S ribosomal protein S15a



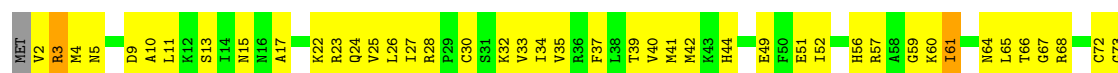
- Molecule 16: 40S ribosomal protein S15a



- Molecule 16: 40S ribosomal protein S15a

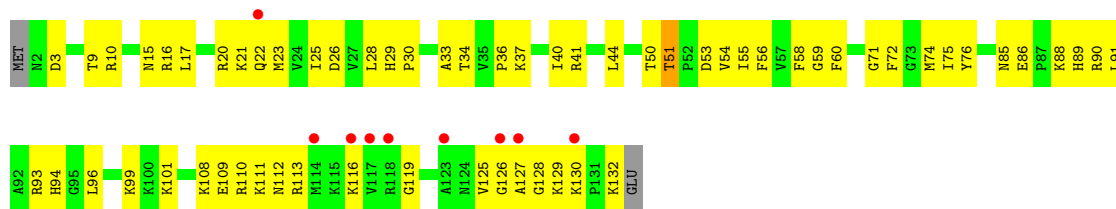


- Molecule 16: 40S ribosomal protein S15a

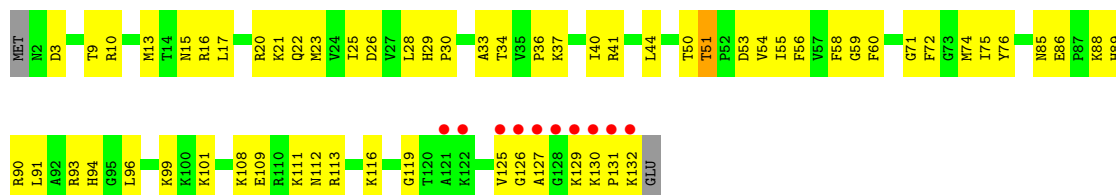


- Molecule 17: 40S ribosomal protein S24

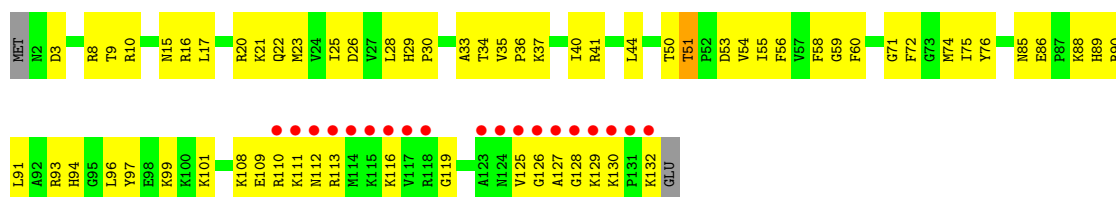




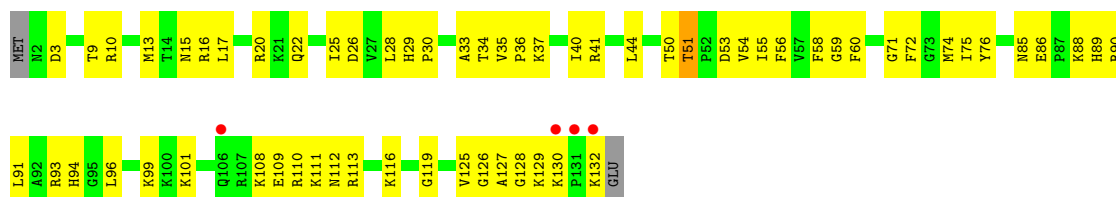
• Molecule 17: 40S ribosomal protein S24



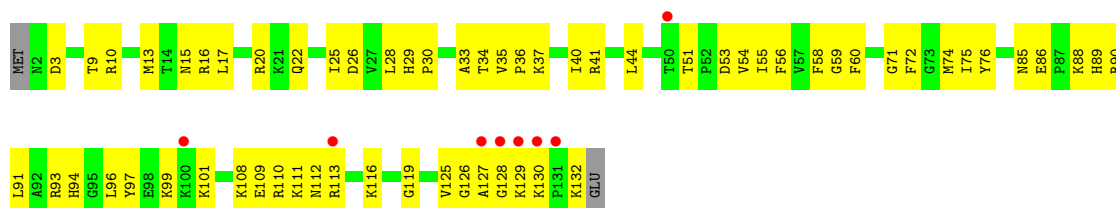
• Molecule 17: 40S ribosomal protein S24



• Molecule 17: 40S ribosomal protein S24



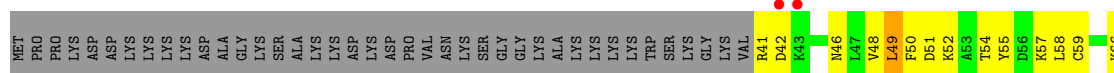
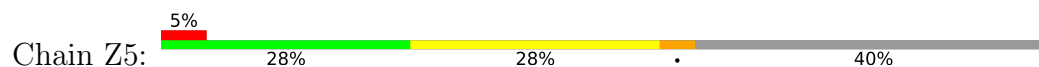
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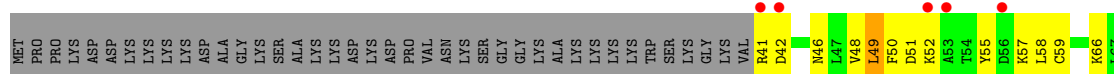
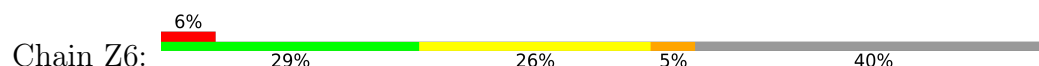
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|-----|
| MET | PRO | PRO | ASP | ASP | LYS | LYS | LYS | LYS | ASP | ALA | GLY | LYS | SER | ALA | LYS | LYS | ASP | ASP | PRO | VAL | ASN | LYS | SER | GLY | GLY | LYS | ALA | LYS | LYS | LYS | LYS | TRP | SER | LYS | GLY | LYS | VAL | R41 | D42 | N46 | V48 | L49 | F50 | D51 | K52 | V55 | D56 | K57 | L58 | C59 | K66 | L67 | I68 |
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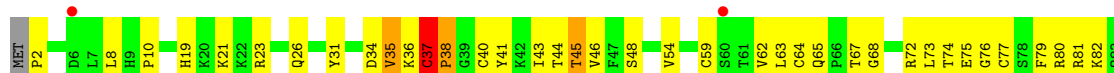
- Molecule 18: 40S ribosomal protein S25



- Molecule 18: 40S ribosomal protein S25



- Molecule 19: 40S ribosomal protein S27



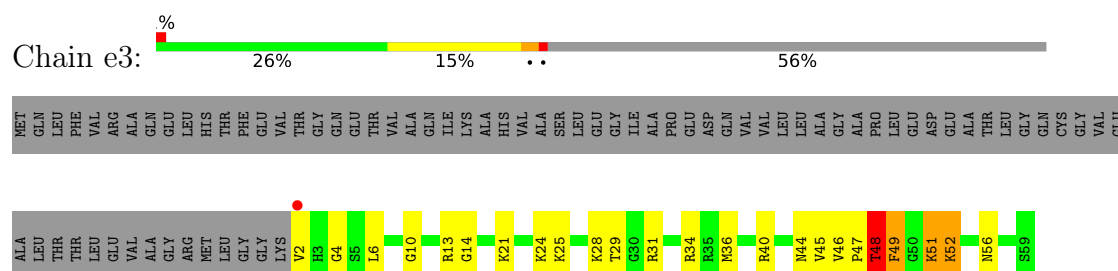
- Molecule 19: 40S ribosomal protein S27



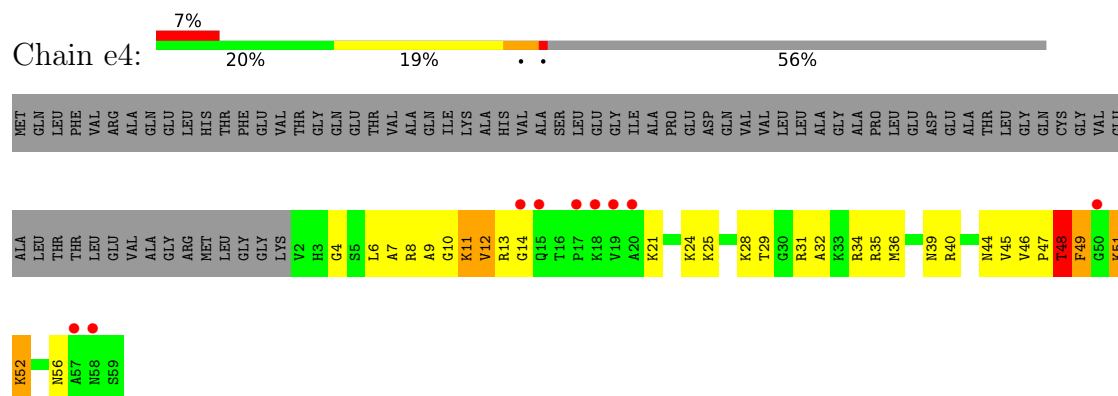
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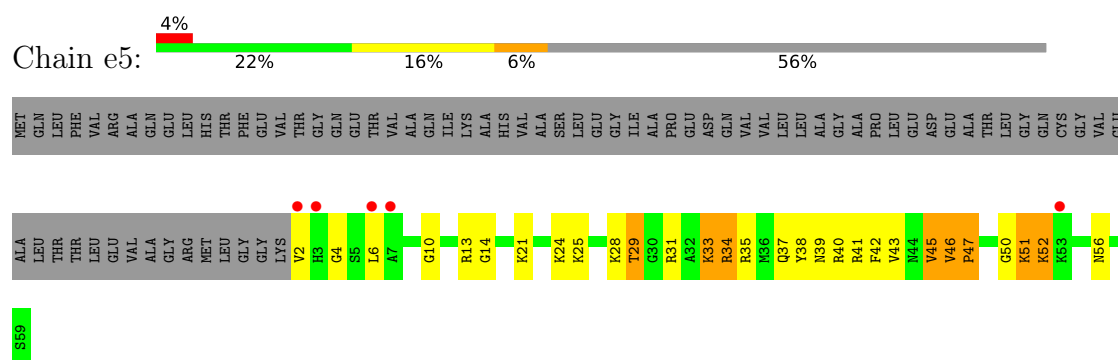
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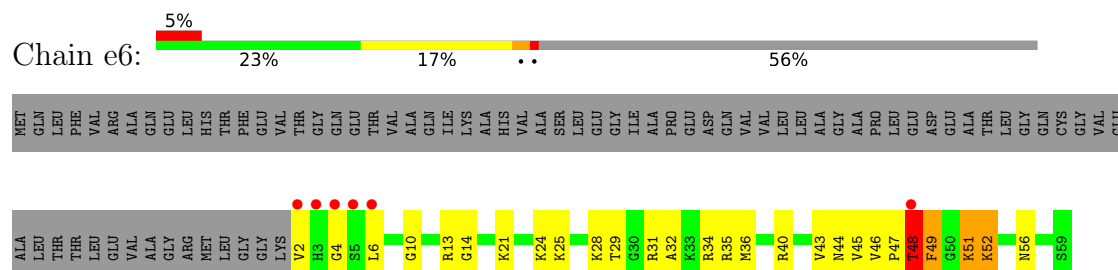
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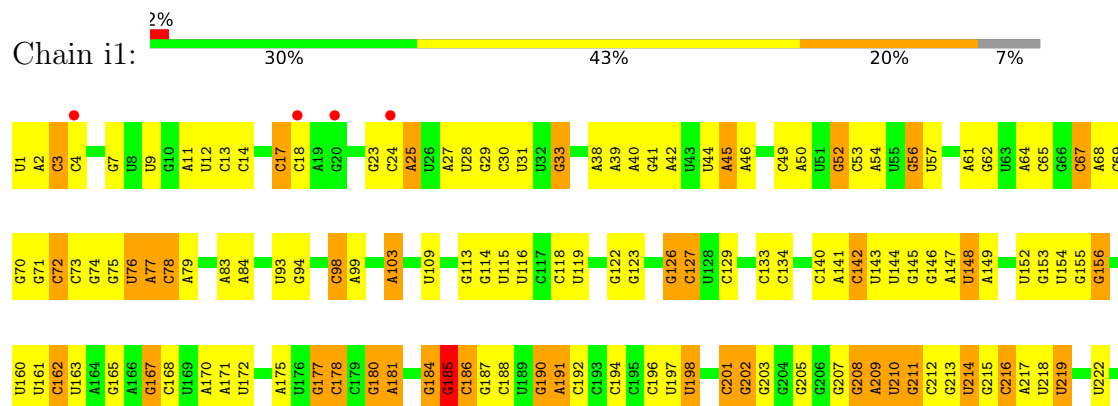
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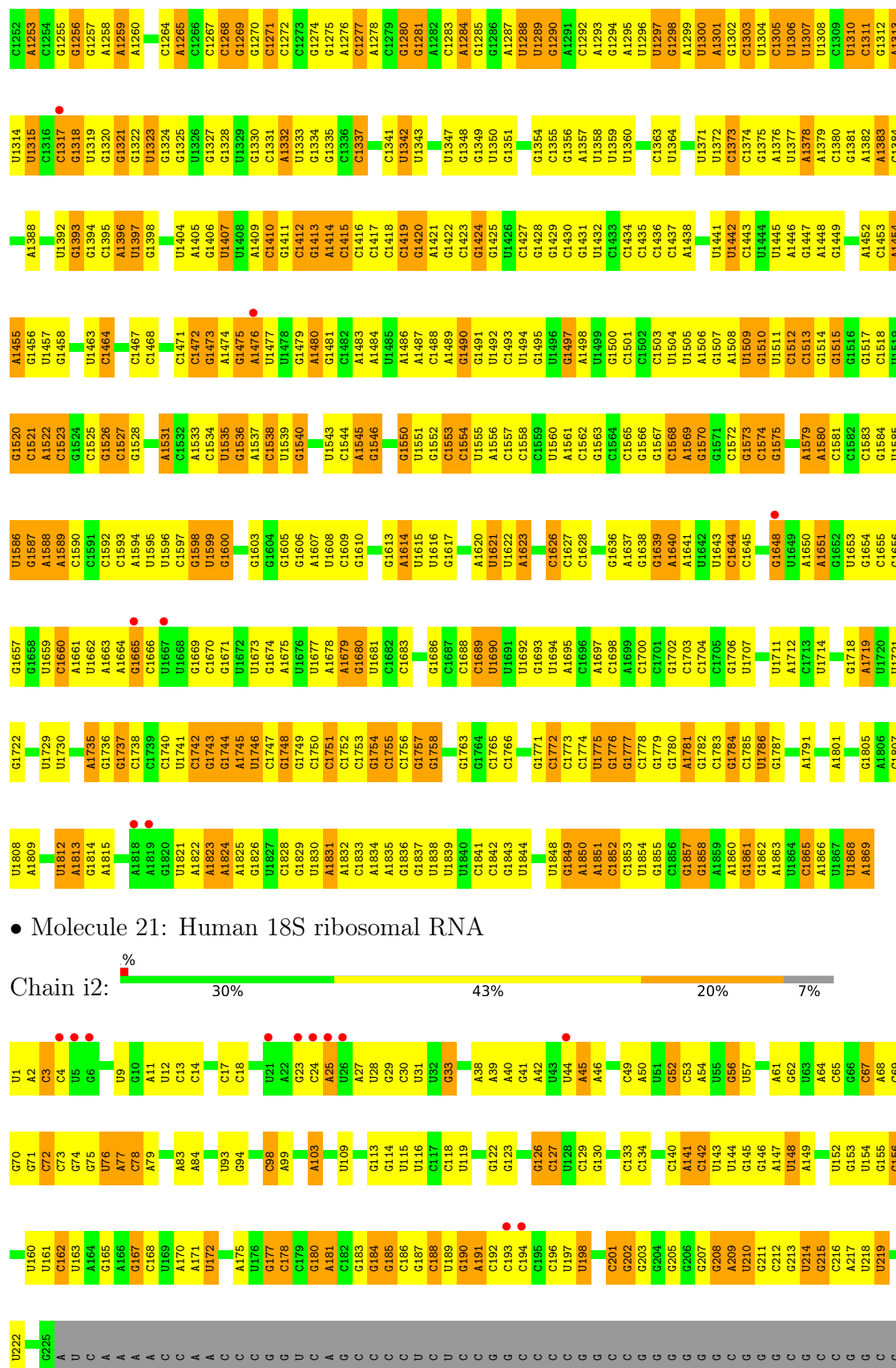
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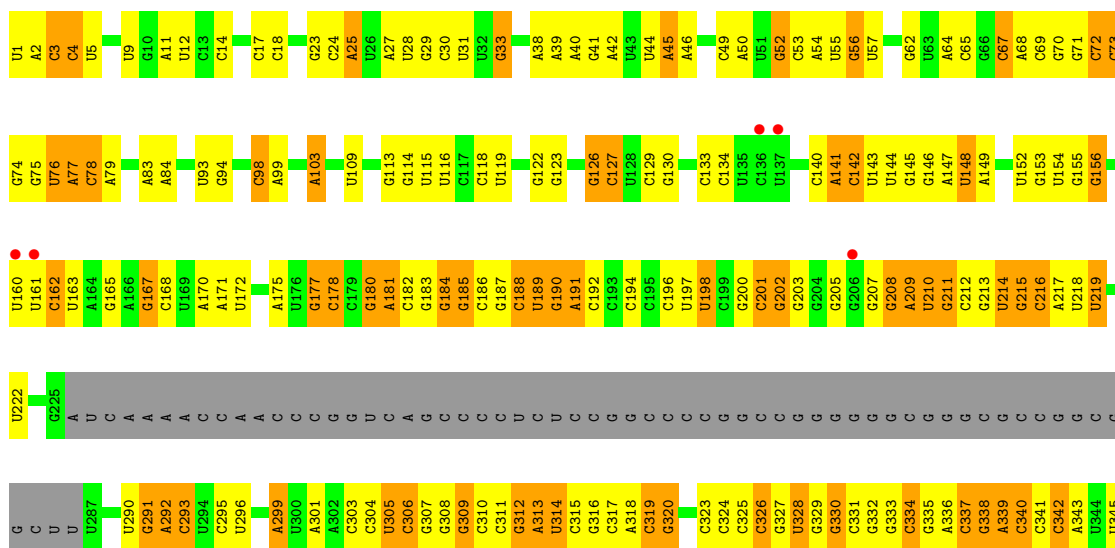
• Molecule 21: Human 18S ribosomal RNA



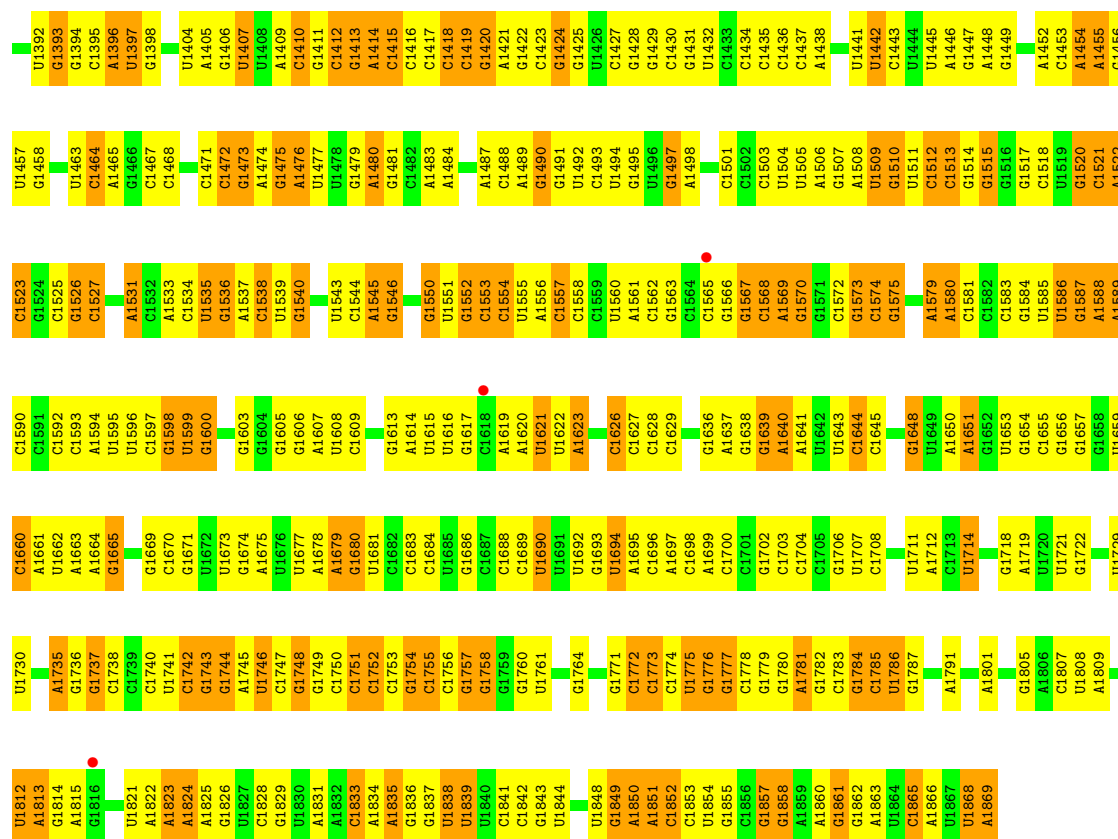
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G1187	C1117	G1037	A962	U896	U822	U	G	C632	U556	C494	U426	U352	U
A1188	C1118	A963	U897	U896	U823	G	G	C633	U557	C495	A426	C353	C
A1189	A1119	A964	U898	U899	C824	A	C	A634	G558	C496	C429	U354	A
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		A972	C905	C905	C836	U	G	U642	G565	C504	G435	U296	C
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A1200		G1054	A908	G908	C838	G	G	U647	U570	G507	G439	C303	C
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C1215	C1145	G1068	A990	A922	C852	G	C	C660	A587	A522	A455	C315	U
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G1235	G1166		U1017	A944	C877	U	U	G684	U609	U542	G477	C335	C
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G1243	C1175	C1103	A1023	C951	U883	C	C	U749	A811	C618	C483	C341	C
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G1245	U1177		U1025	C953	U887	C	C	G751	A813	G549	A485	C343	C
		C1109	A1027	U954	U888	C	C	G752	A814	C548	A486	A343	C
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C1249	A1182	U1112	U958	U958	U892	C	C	G696	A629	G552	C490	G346	C
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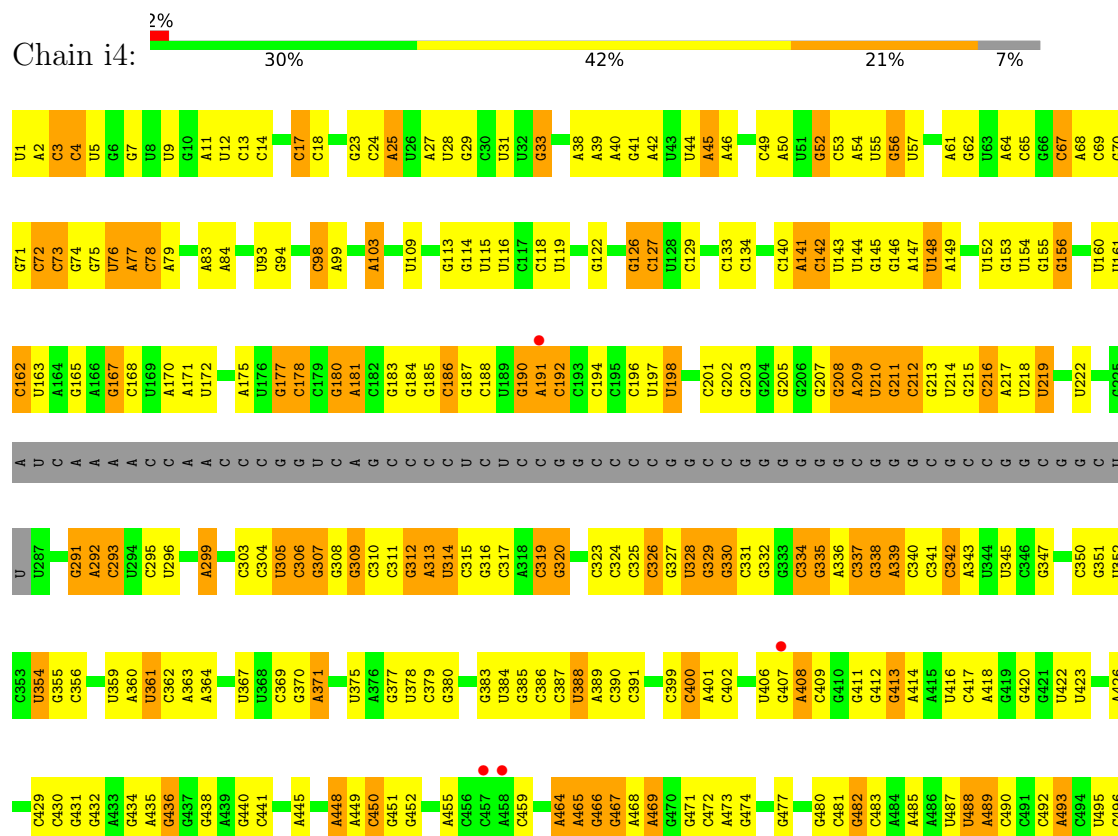
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C1309	U1247	U1111	G958	U893	U894	C	G696	G626	U551	C417	A344	
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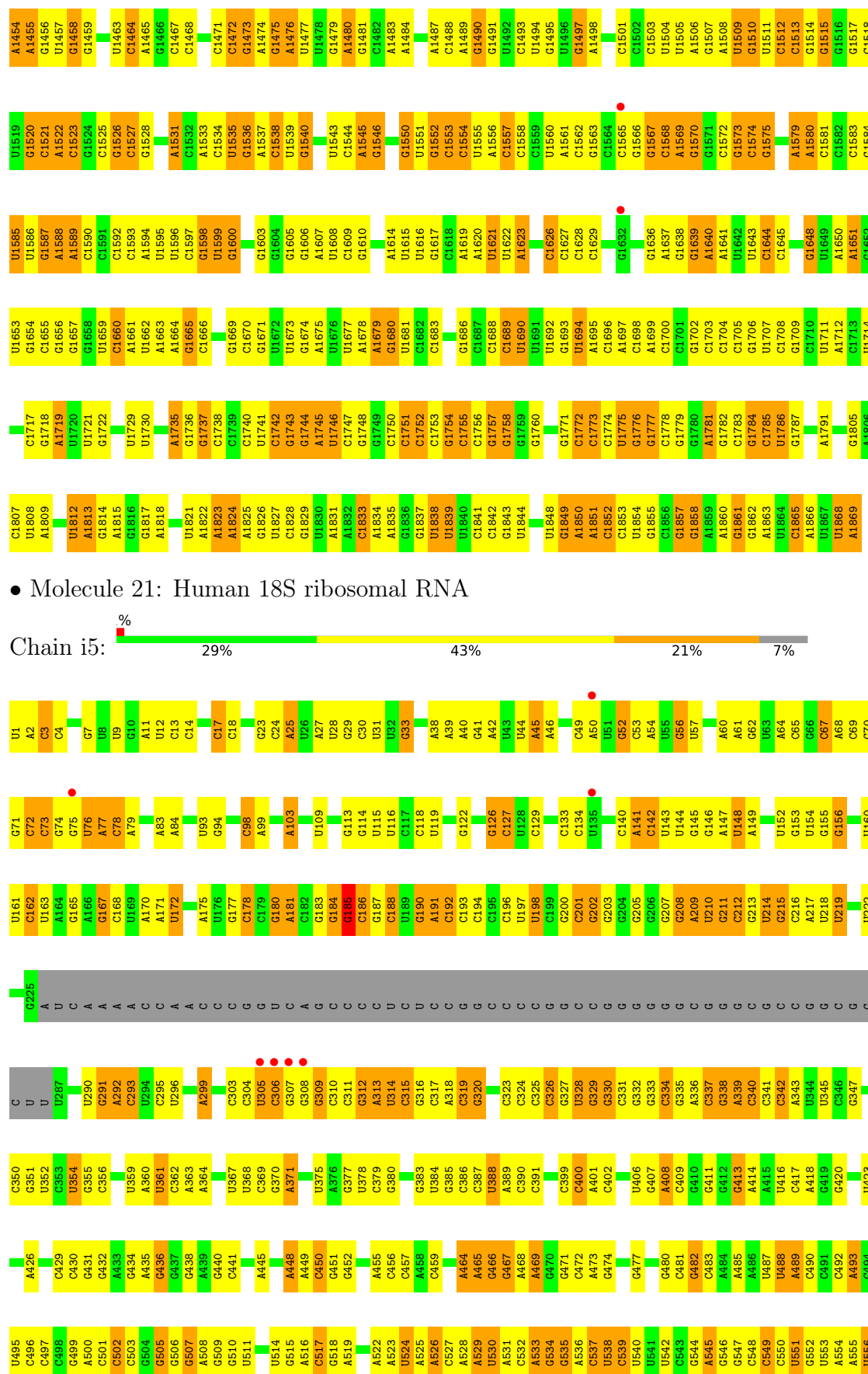




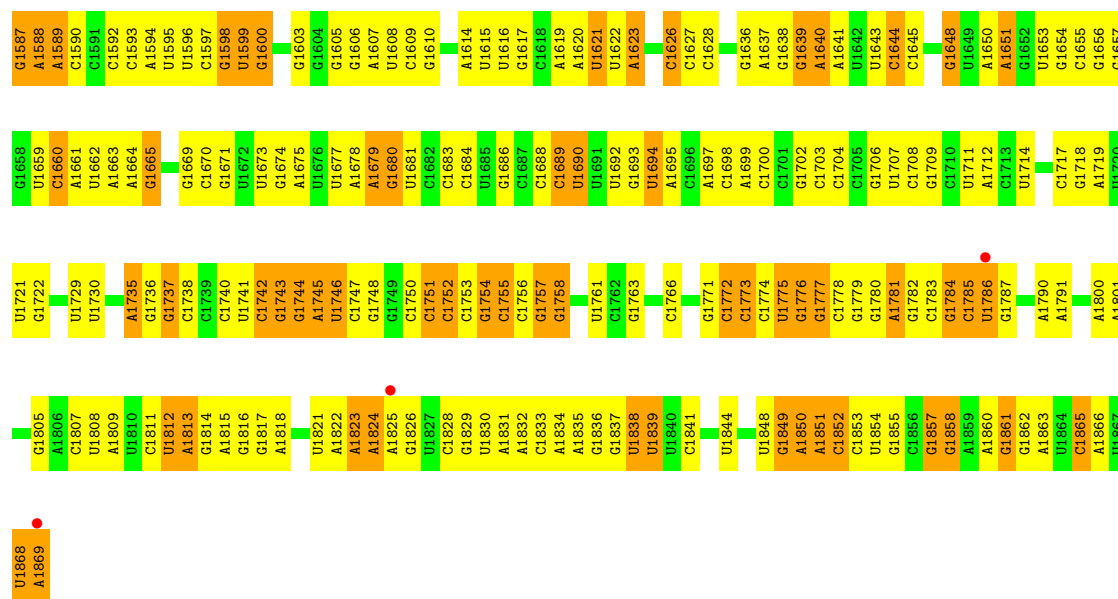
● Molecule 21: Human 18S ribosomal RNA



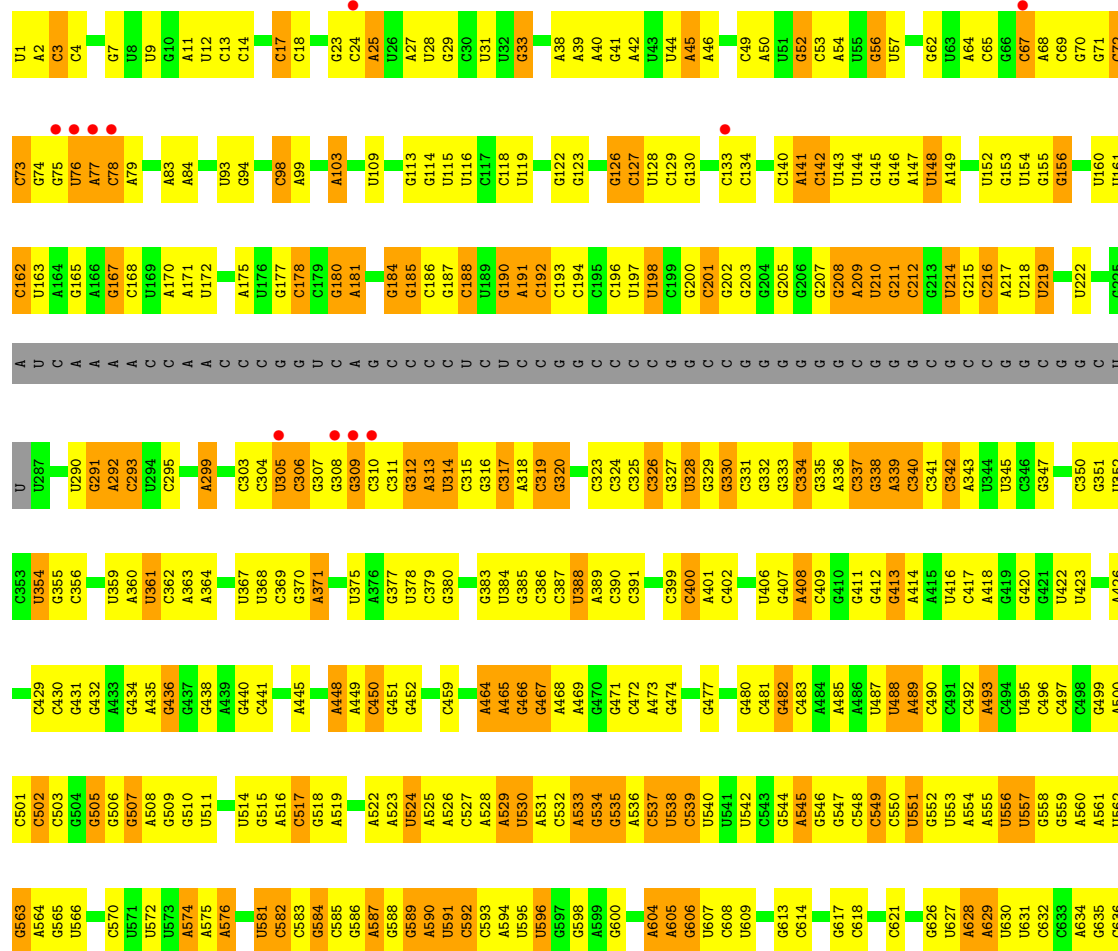
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A1035	A1036	G1037	G1041	A1042	G1043	G1044	C1047	A1052	G1053	G1054	U1055	U1056	C1057	A1058	G1059	A1060	A1061	A1062	G1065	G1068	U1069	A1070	G1071	G1072	A1073	C1077	C1078	C1079	A1080	U1081	A1082	A1083	C1084	G1085	U1087	U1088	C1094	U1095	G1096	G1097	C1098	G1099	G1102	C1103	G1104	C1109	G1110	U1111	C1180	A1181	A1182	A1183													
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C559	A560	A561	U562	A563	A564	G565	U566	C570	U571	U572	U573	A574	A575	A576	U581	C582	C583	G584	C585	G586	A587	G588	G589	A590	C591	C592	C593	A594	U595	U596	G597	G598	A599	G600	A604	A605	G606	U607	C608	U609	G610	G611	U612	G613	C614	C615	A616	C617	C618	C621	G626	U627	A628	A629											
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U1531	G1466	G1321	A1259	A1194	G1051	C974	G907	G836	U	C	U642	A564
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C1544	G1479	U1333	C1273	G1207	A1062	G866	A919	A847	C	C	U657	C582
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U1554	G1488	U1344	U1282	C1216	A1078	C1000	G928	A865	C	C	U667	C589
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U1556	G1490	U1348	A1284	C1218	A1078	U1002	C930	G868	U	C	A670	C593
C1557	G1491	G1349	G1285	G1219	C1079	U1003	C931	A869	G	C	A671	A594
U1558	U1492	U1350	U1286	A1220	A1080	U1004	G932	A870	C	C	A672	U596
C1559	C1493	G1354	A1287	G1223	U1081	U1005	G933	U871	C	C	G673	G597
U1560	U1494	C1355	U1288	A1224	A1082	A1008	G934	A872	C	C	U675	G598
A1561	G1495	G1356	C1289	G1225	U1083	U1013	A938	A874	U	C	A679	A599
C1562	U1496	G1357	A1290	U1226	A1084	U1016	U939	A875	C	C	U682	A604
G1563	G1497	U1358	C1292	G1226	U1085	U1017	C941	C877	U	C	G683	A605
C1564	A1498	U1359	A1293	C1231	G1086	U1018	G942	C878	U	C	G684	G606
U1565	C1501	U1360	G1294	U1232	U1087	U1019	C950	C881	C	C	A685	U607
G1566	G1502	G1361	A1295	G1233	U1088	C1018	C951	C884	C	C	U686	C608
C1567	U1503	C1363	U1296	C1234	G1096	C1019	G952	U887	C	C	U687	U609
U1568	U1504	U1364	U1297	G1235	U1097	A1020	C953	U888	C	C	G613	G614
G1570	A1505	U1364	G1298	G1236	C1098	U1021	U954	U889	C	C	G691	C614
C1571	U1506	U1371	A1299	C1237	G1099	U1022	A955	U890	C	C	G692	G617
U1572	G1507	U1372	U1300	U1238	U1100	A1023	G956	C891	C	C	A693	C618
G1573	U1508	C1373	G1294	U1239	U1111	A1024	C957	U892	C	C	G694	C621
C1574	U1509	G1374	A1301	U1239	U1112	G1033	A957	U893	C	C	G695	U627
U1575	G1510	C1375	G1302	A1240	U1113	A1036	G958	U894	C	C	G696	A628
G1576	U1511	A1376	C1303	A1241	U1114	A1036	G959	C895	C	C	G697	A629
C1577	C1512	U1377	U1304	U1242	U1115	G1037	U960	U896	C	C	G698	U630
U1578	G1513	U1378	C1305	U1243	G1109	G1037	G961	U897	C	C	G	U630
A1579	U1514	A1379	U1306	U1244	U1110	G1033	A962	U898	C	C	G	U630
U1580	G1515	U1380	U1307	G1245	U1111	A1034	A963	U899	C	C	G	U630
C1581	U1516	G1381	U1308	A1246	U1112	A1034	A964	U899	C	C	G	U630
G1582	G1517	A1382	C1309	G1247	U1113	A1036	A965	U899	C	C	G	U630
C1583	U1518	A1383	U1310	U1248	U1114	A1036	A966	U899	C	C	G	U630
U1584	A1519	C1384	C1311	G1249	U1115	G1037	A967	U899	C	C	G	U630
G1585	U1520	U1385	G1312	A1250	U1116	G1041	A968	U899	C	C	G	U630
U1586	C1521	A1455	A1313	A1251	C1117	A1042	A969	U899	C	C	G	U630
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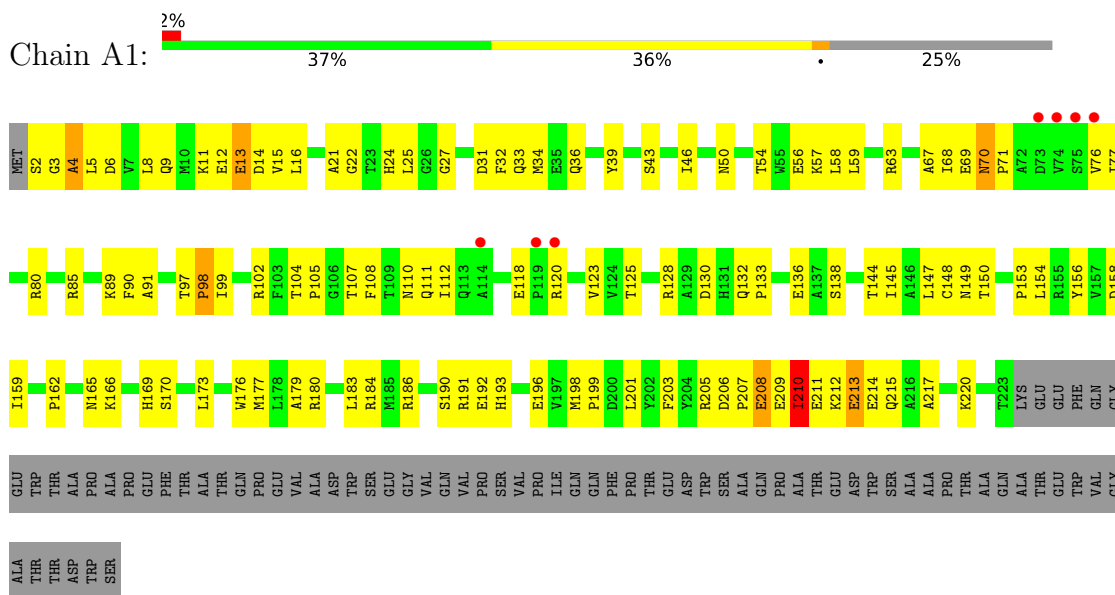


• Molecule 21: Human 18S ribosomal RNA

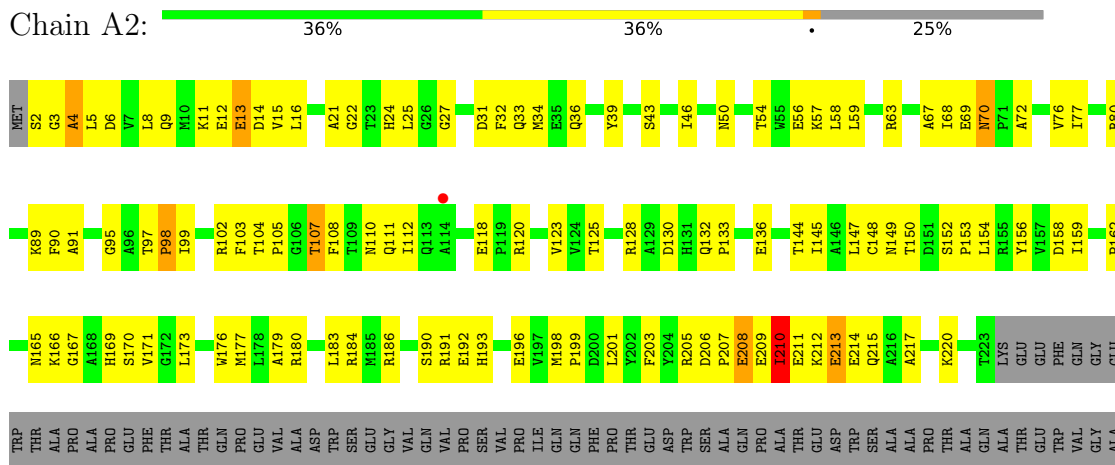


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U1519	A1454	G1385	G1385	C1316	C1254	A1188	G1041	U965	G902	C933	C	U	A641
G1520	A1455	C1317	C1317	C1317	C1255	A1189	A1042	U968	A903	C834	C	C	A642
C1521	G1456	G1318	G1318	U1319	G1256	A1190	G1043	U969	A904	C835	C	C	A643
A1522	U1457	U1319	U1319	G1320	G1257	C1191	G1044	G970	C905	G836	C	C	G644
G1523	G1458	G1320	G1320	G1321	A1258	U1192	C1047	G971	U906	A837	C	C	G645
G1524	G1459	G1322	G1322	A1260	U1259	U1193	G1048	A972	G907	G838	G	G	G646
C1525	U1463	U1323	U1323	G1324	C1261	A1194	A1052	C973	A908	C839	C	C	U647
G1526	A1464	A1396	A1396	G1324	G1262	C974	G1053	C974	G909	C840	C	C	A648
C1527	G1465	U1397	U1397	G1325	U1263	G975	A1054	G975	C911	G841	G	A	U649
G1528	G1466	G1398	G1398	U1326	C1264	G976	A1055	G976	C912	G842	G	G	A650
A1531	C1467	U1404	U1404	G1327	C1265	C977	U1056	C977	U914	C843	C	C	U651
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A1533	U1471	G1406	G1406	U1329	C1267	A1200	C1058	A980	U917	G845	G	A	A655
C1534	C1472	U1407	U1407	C1330	G1268	U1201	A1059	A981	U918	G846	C	C	G656
U1535	G1473	A1408	A1408	C1331	C1269	G1203	U1060	A982	U919	A847	C	C	U657
G1536	A1474	A1409	A1409	A1332	C1270	A1204	U1061	G983	U918	U848	C	C	U658
A1537	G1475	G1410	G1410	U1333	C1271	G1205	U1062	A983	A920	C851	G	A	G659
C1538	A1476	G1411	G1411	G1334	G1272	U1206	A1063	G986	G921	G852	C	C	C660
U1539	U1477	A1412	A1412	G1335	G1273	A1208	G1064	U987	A922	C853	C	C	U661
G1540	C1478	G1413	G1413	C1336	U1274	A1209	G1065	A988	G923	C854	C	C	G662
U1543	U1479	A1414	A1414	C1337	G1275	G1212	G1068	G990	G924	U863	C	C	U666
C1544	A1480	C1415	C1415	G1341	G1276	C1213	U1069	A992	G925	A864	C	C	U667
A1545	G1481	G1416	G1416	U1342	G1277	A1214	G1070	A996	A926	A865	C	C	A668
G1546	A1482	C1417	C1417	U1343	C1278	C1215	A1071	A997	G928	U866	C	C	A669
U1550	A1483	A1418	A1418	U1347	A1281	G1216	G1072	A998	G929	G867	C	C	G732
G1551	G1484	C1419	C1419	U1348	C1282	A1217	A1073	G999	C930	G868	C	C	G733
U1552	U1485	G1420	G1420	G1349	A1283	C1218	A1074	C1000	C931	A869	C	C	A670
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C1556	A1489	G1424	G1424	G1353	U1288	U1154	U1081	U1004	G937	G873	C	C	C674
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G1559	U1492	C1427	C1427	C1356	A1291	G1225	A1084	U1017	U939	C376	U	U	U682
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A1561	U1494	A1357	A1357	U1358	A1293	G1232	G1086	U1019	U940	G878	C	C	A684
C1562	U1495	U1358	U1358	U1359	G1294	U1233	A1087	C1010	C941	C879	C	C	G685
G1563	U1496	G1430	G1430	U1360	A1295	G1234	U1088	U1015	G942	G880	C	C	U686
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C1566	C1501	C1434	C1434	C1363	G1298	U1237	G1097	U1018	G947	U883	C	C	U689
G1567	C1502	C1435	C1435	U1364	A1299	G1171	C1098	U1019	C950	C884	C	C	G690
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G1570	A1505	U1438	U1438	C1373	C1303	U1242	G1103	A1022	C953	U888	C	C	A693
C1571	G1507	U1441	U1441	C1374	U1304	U1243	G1104	A1024	U954	U889	C	C	G694
U1572	A1508	U1442	U1442	G1375	C1305	G1244	C1109	A1027	U955	U890	C	C	C695
G1573	U1509	C1443	C1443	A1376	U1306	G1245	G1110	G956	A955	G891	C	C	G696
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A1579	C1512	G1447	G1447	A1379	C1309	U1248	A1113	G1033	G959	G894	C	C	C
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C1581	G1514	G1449	G1449	C1381	C1312	A1251	C1115	A1035	G961	U896	C	C	G
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- Molecule 22: 40S ribosomal protein SA



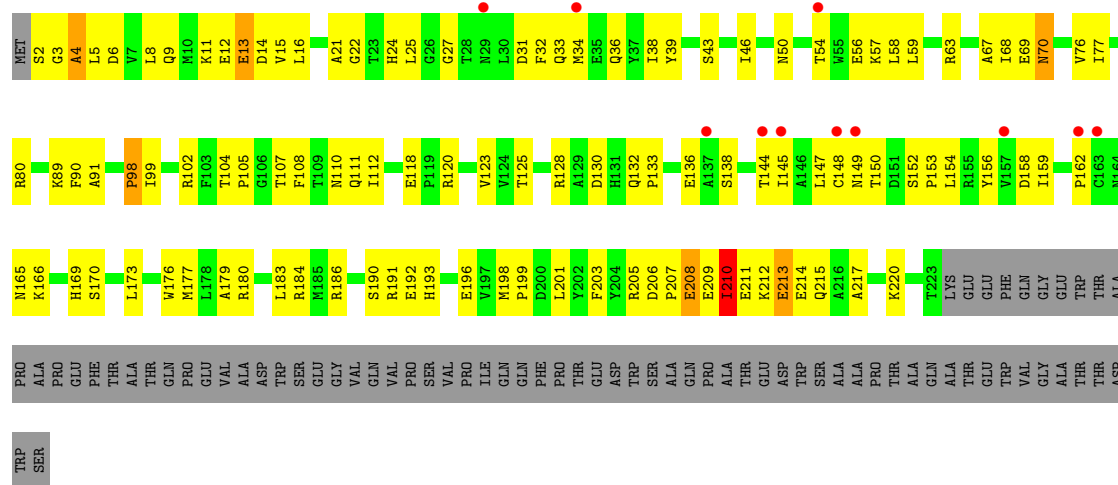
- Molecule 22: 40S ribosomal protein SA



PHE THR ALA THR GLN PRO PRO GLU VAL ALA ASP TRP SER GLU GLY VAL GLN VAL PRO PRO SER VAL PRO PRO ILE GLN GLN PHE PRO THR GLU ASP TRP SER ALA GLN PRO ALA THR ASP TRP VAL GLY VAL GLY THR THR THR ASP TRP SER

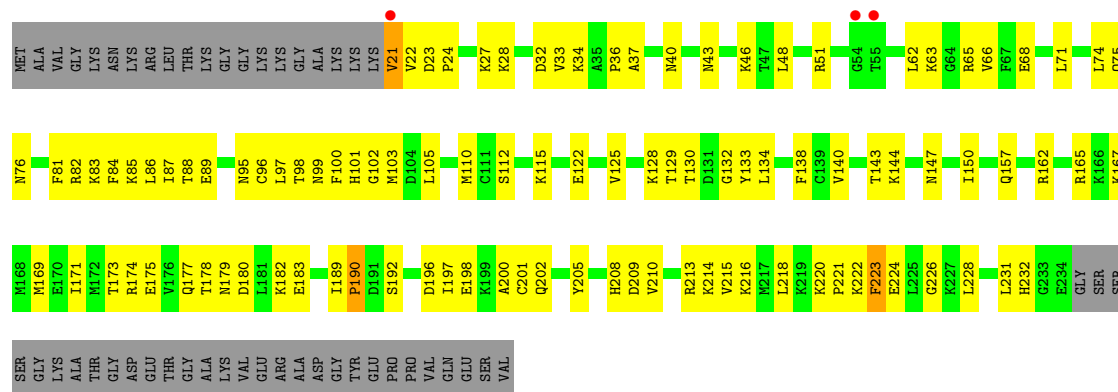
• Molecule 22: 40S ribosomal protein SA

Chain A6: 4% 38% 35% 25%



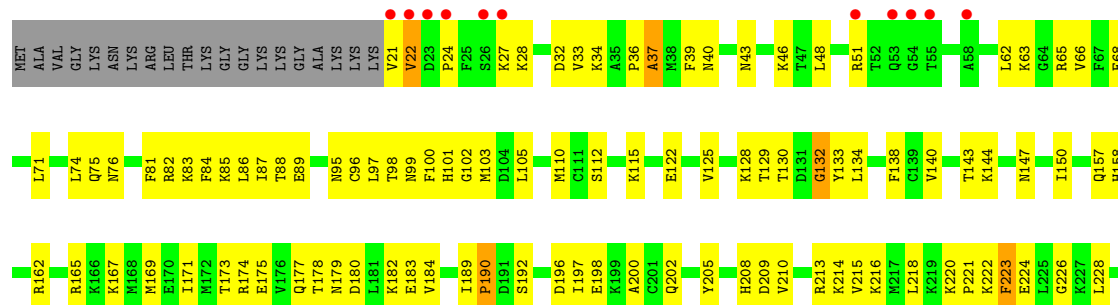
• Molecule 23: 40S ribosomal protein S3a

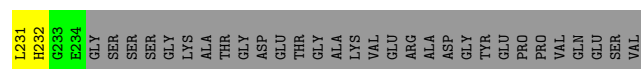
Chain B1: % 42% 38% 19%



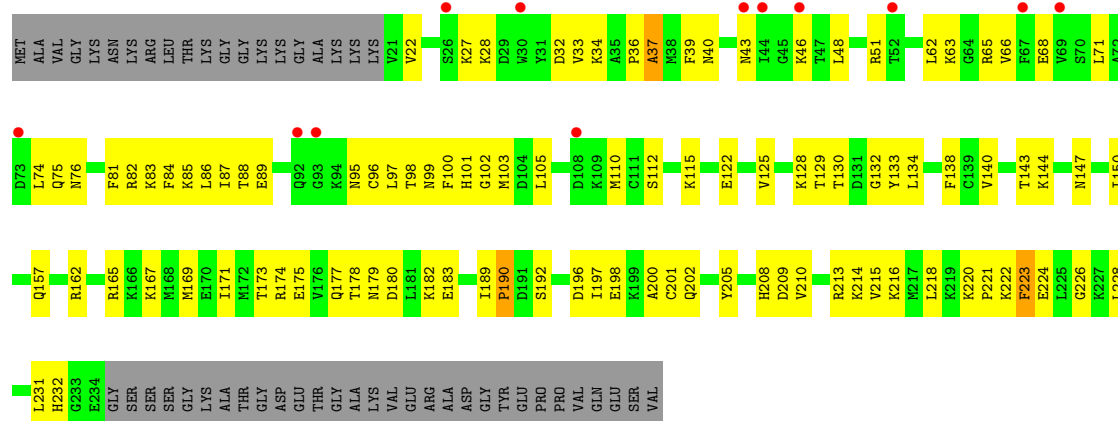
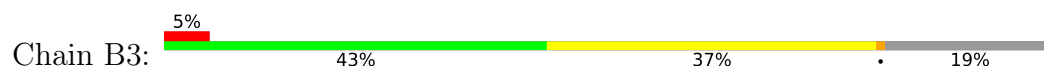
• Molecule 23: 40S ribosomal protein S3a

Chain B2: 4% 42% 38% 19%

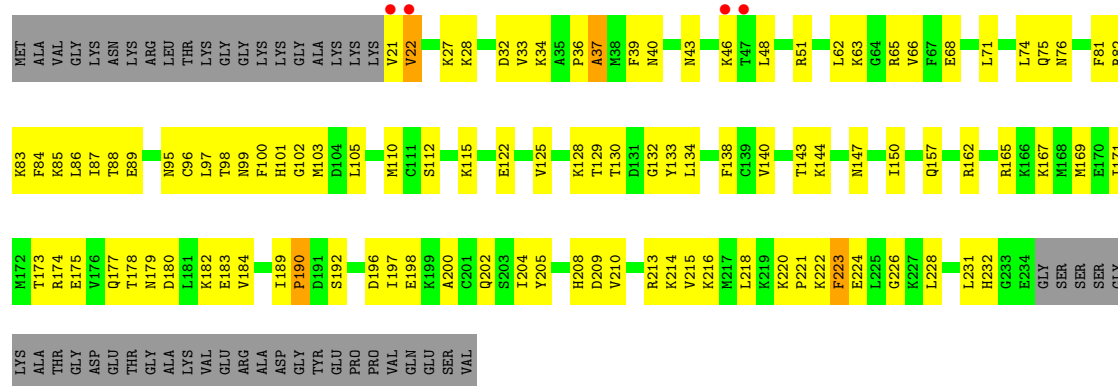




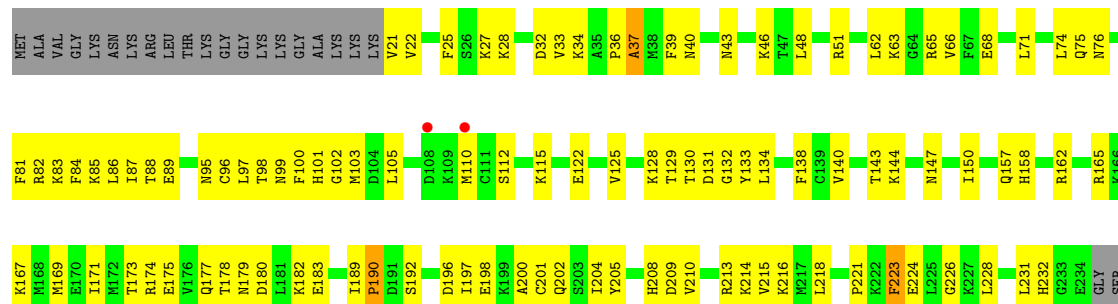
• Molecule 23: 40S ribosomal protein S3a



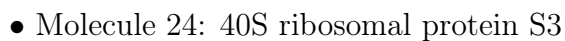
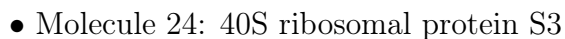
• Molecule 23: 40S ribosomal protein S3a

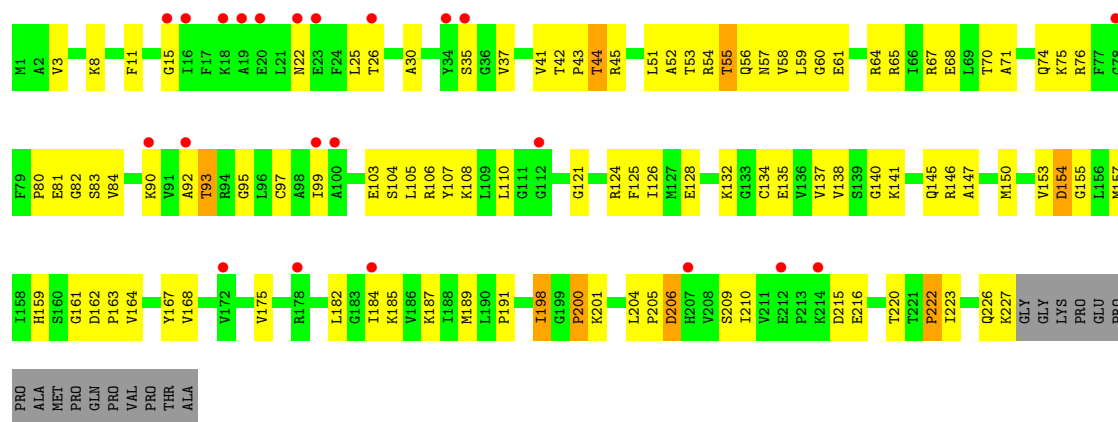


• Molecule 23: 40S ribosomal protein S3a

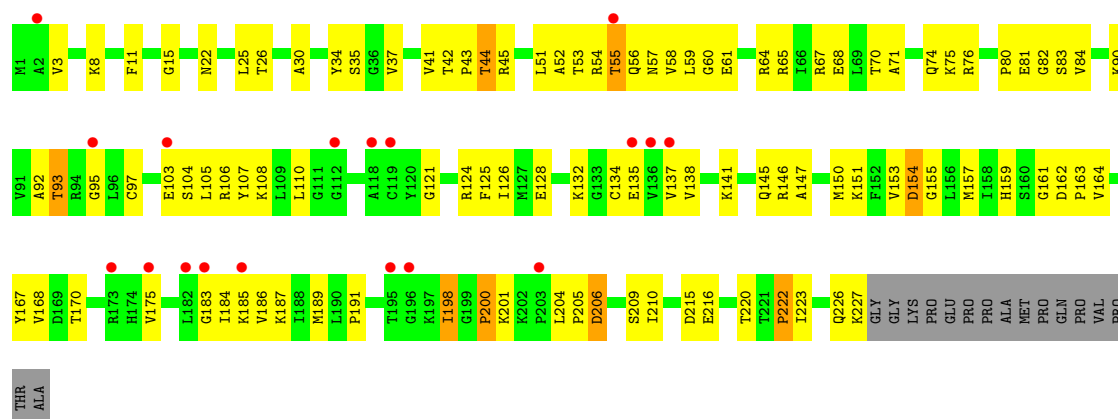


Chain B6: 42% 38% . 19%

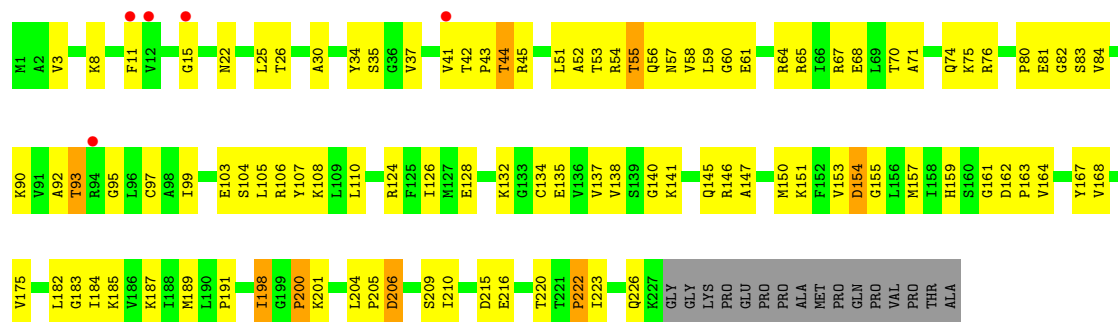




• Molecule 24: 40S ribosomal protein S3

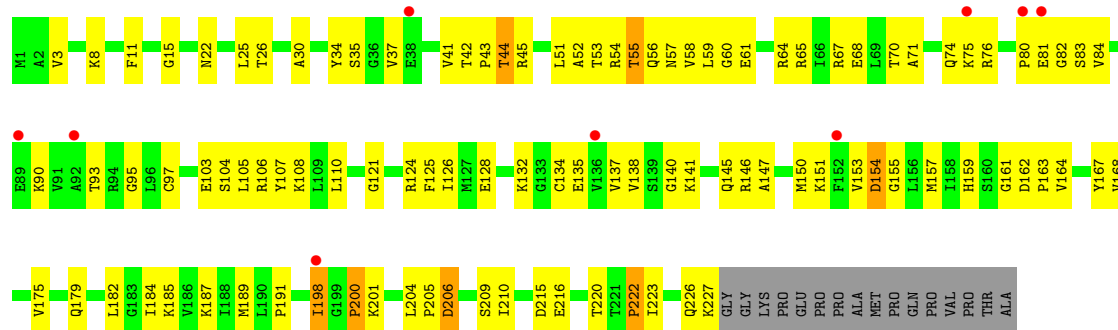


• Molecule 24: 40S ribosomal protein S3

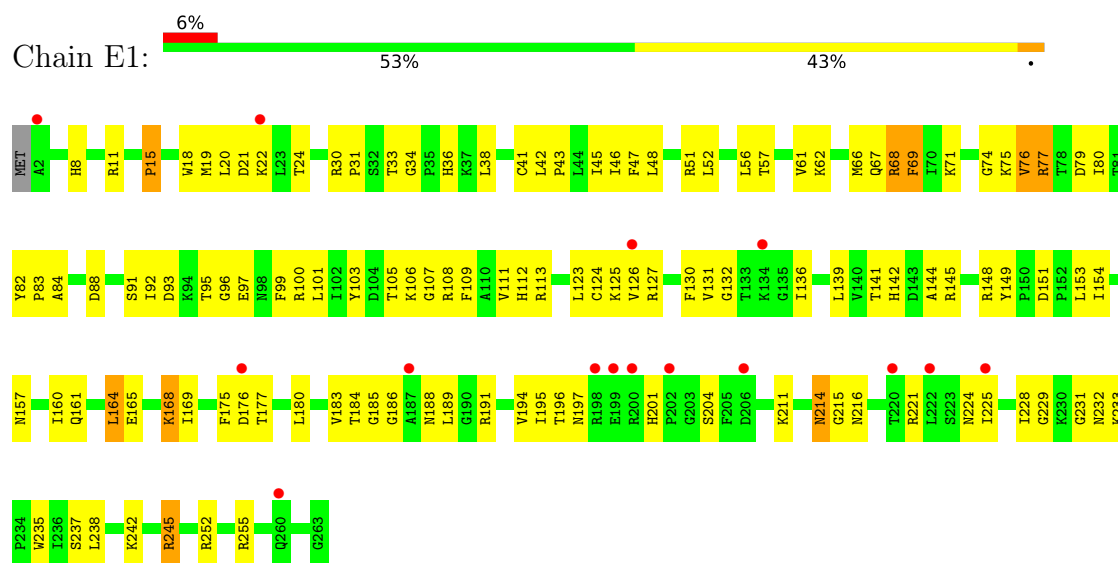


• Molecule 24: 40S ribosomal protein S3

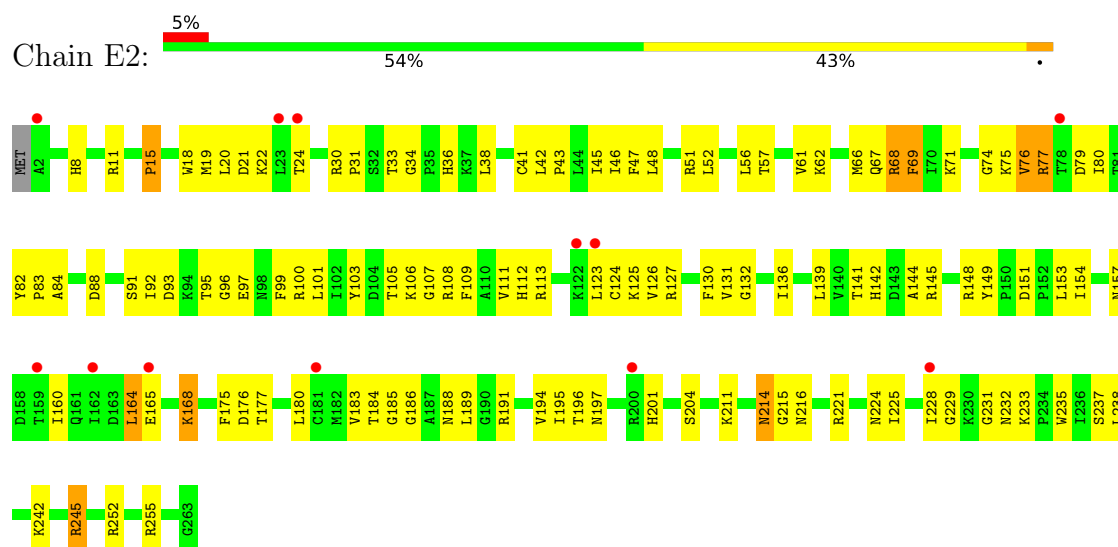




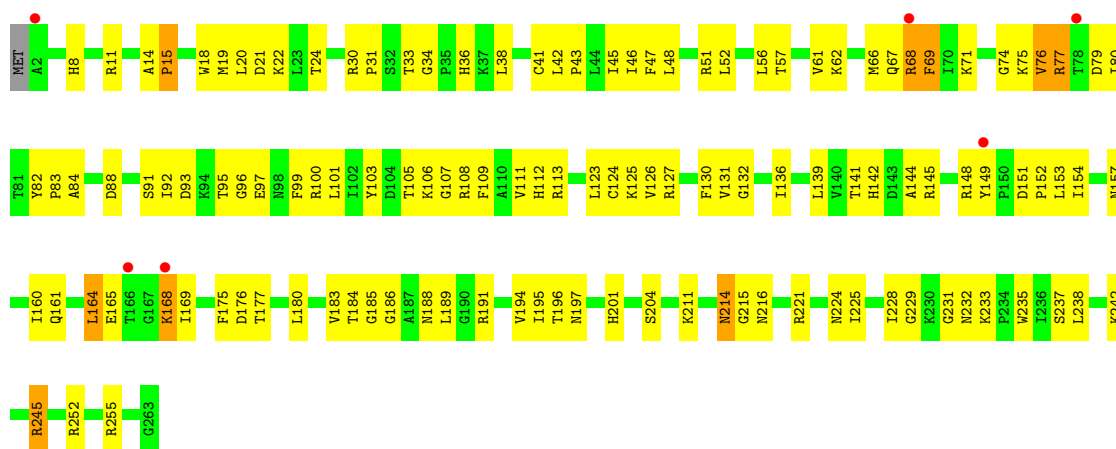
• Molecule 25: 40S ribosomal protein S4, X isoform



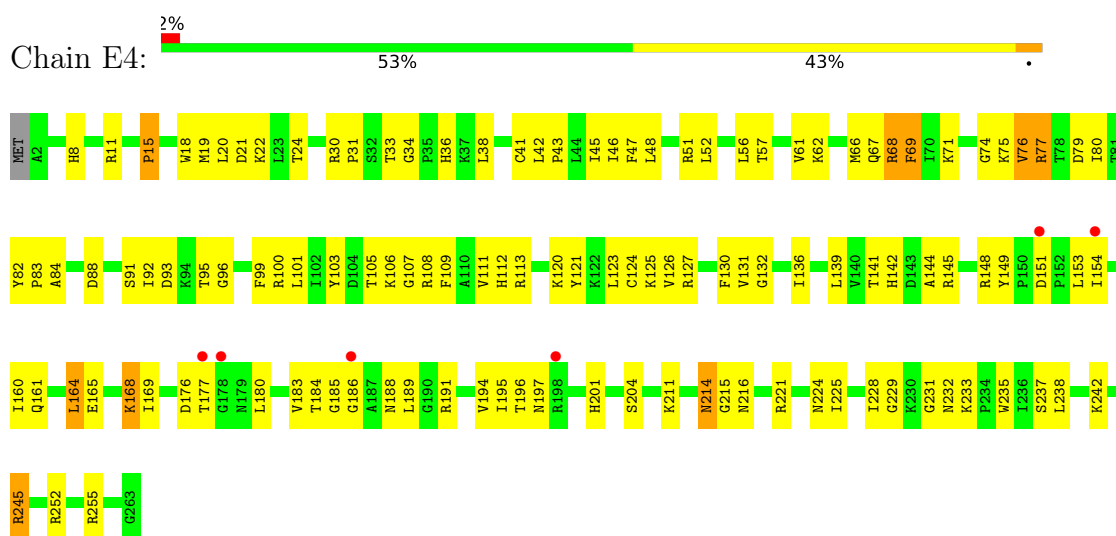
• Molecule 25: 40S ribosomal protein S4, X isoform



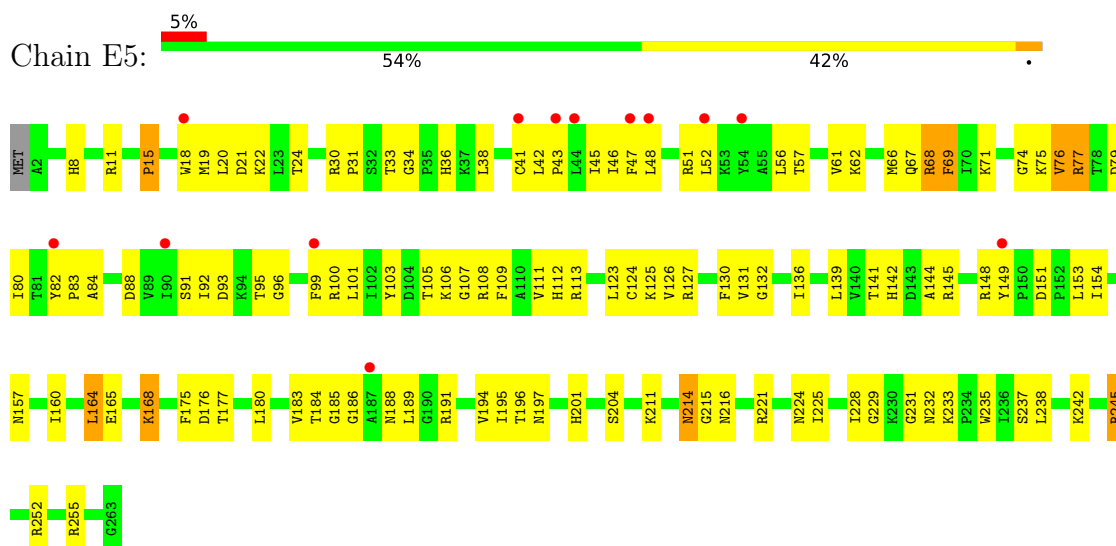
• Molecule 25: 40S ribosomal protein S4, X isoform



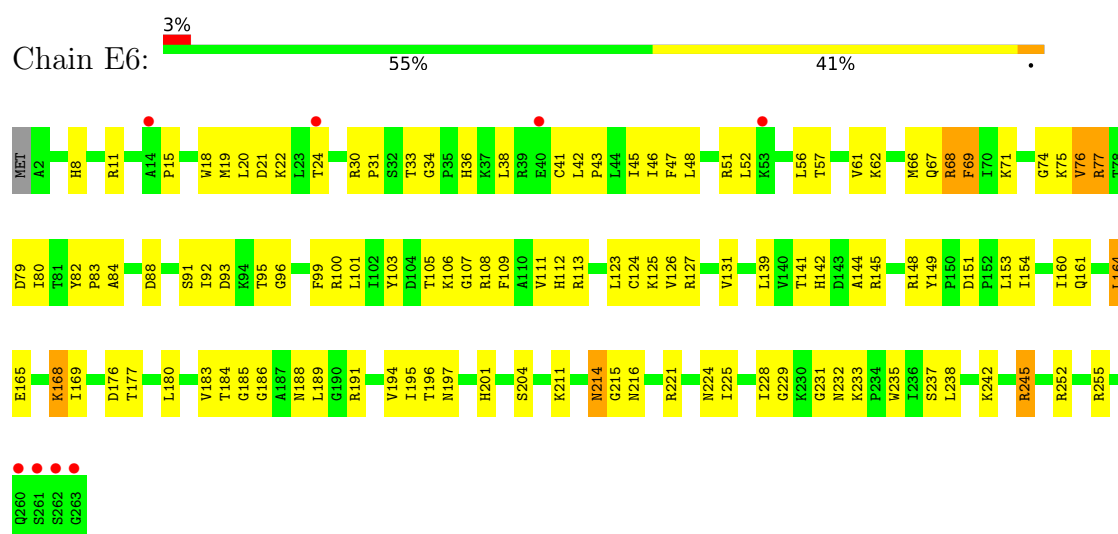
- Molecule 25: 40S ribosomal protein S4, X isoform



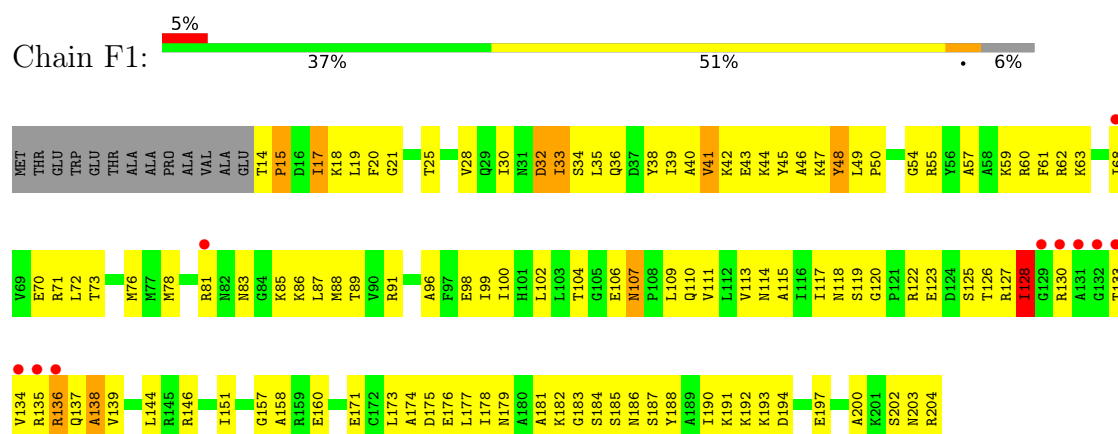
- Molecule 25: 40S ribosomal protein S4, X isoform



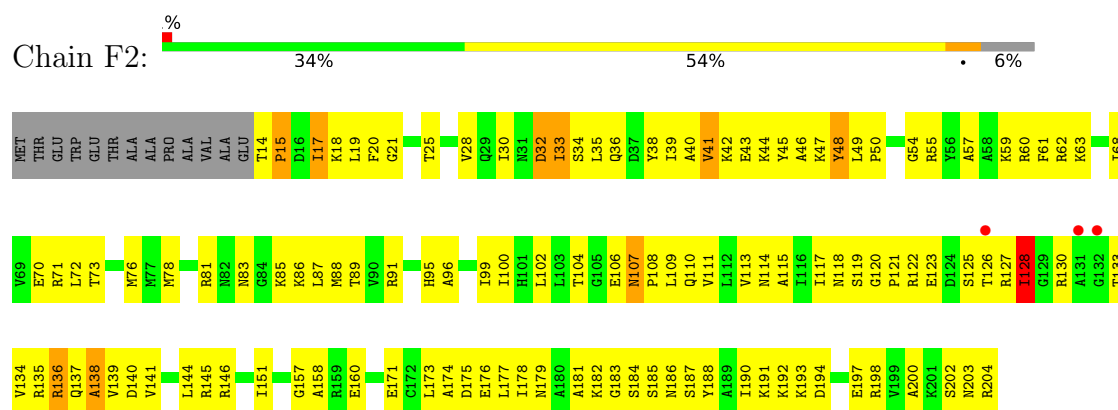
- Molecule 25: 40S ribosomal protein S4, X isoform



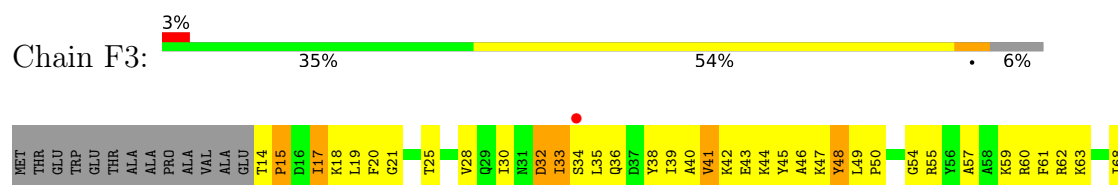
- Molecule 26: 40S ribosomal protein S5

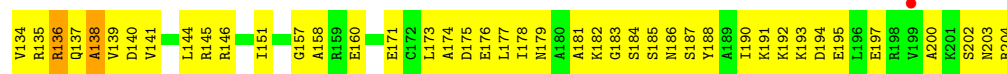


- Molecule 26: 40S ribosomal protein S5

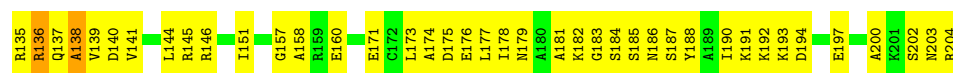
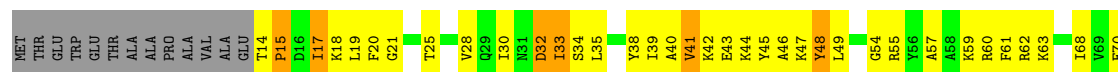


- Molecule 26: 40S ribosomal protein S5

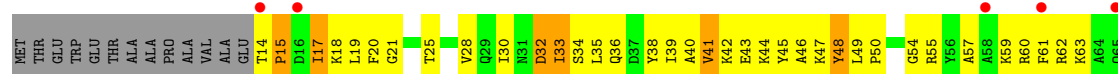




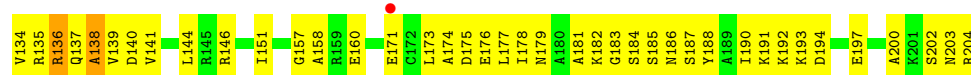
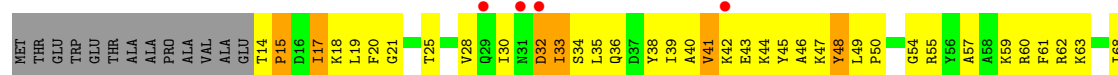
• Molecule 26: 40S ribosomal protein S5



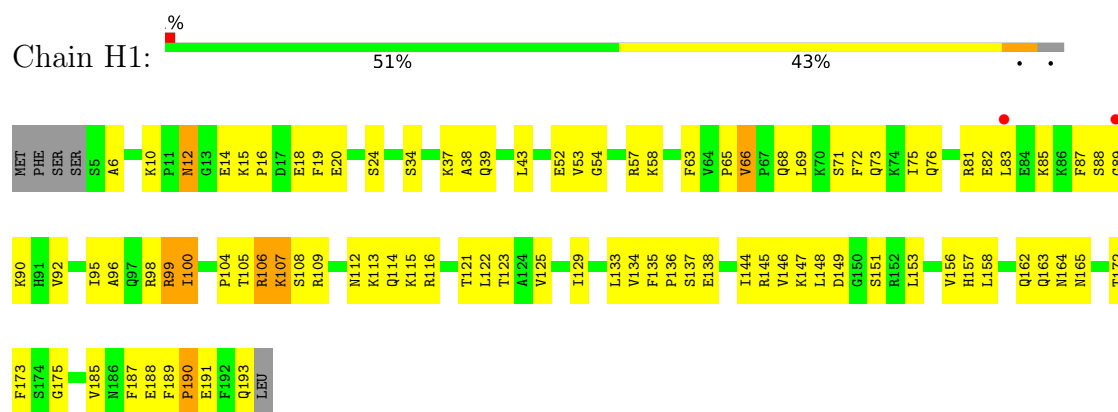
• Molecule 26: 40S ribosomal protein S5



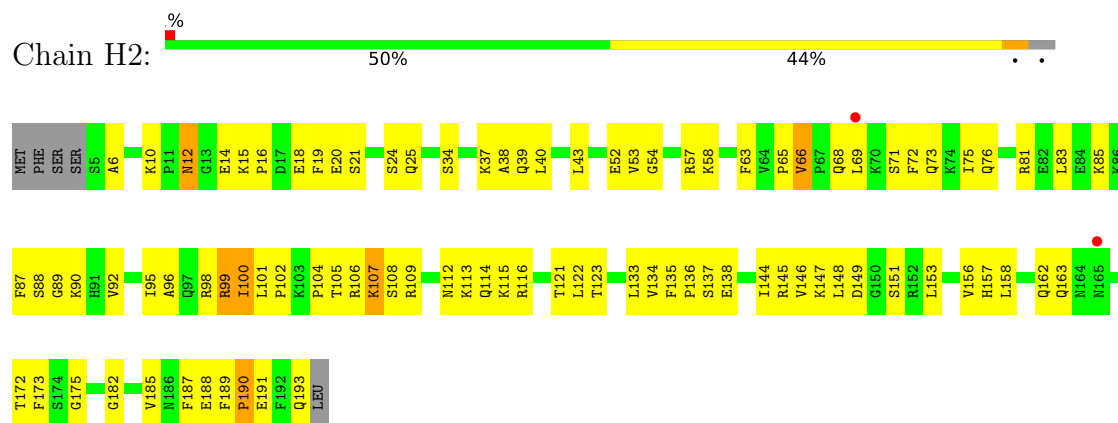
• Molecule 26: 40S ribosomal protein S5



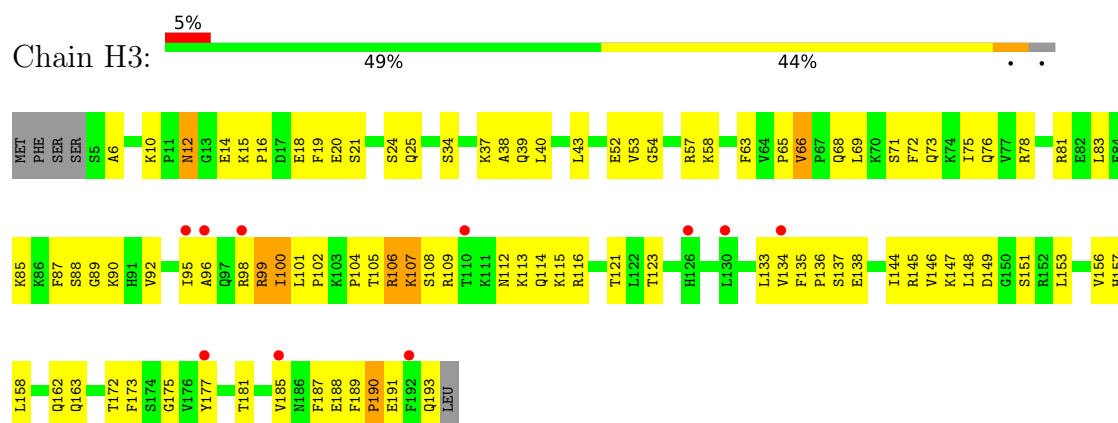
• Molecule 27: 40S ribosomal protein S7



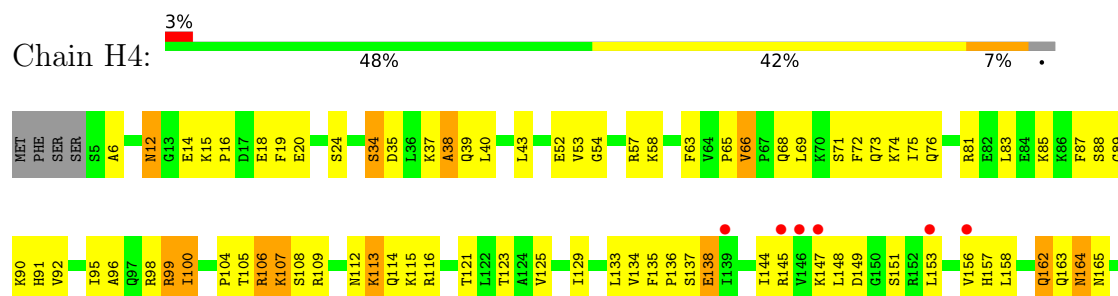
• Molecule 27: 40S ribosomal protein S7

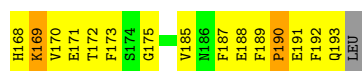


• Molecule 27: 40S ribosomal protein S7

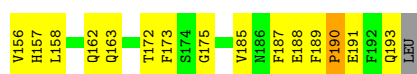
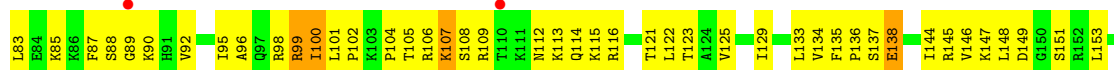
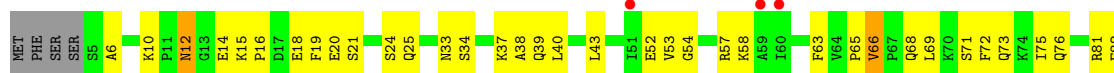


• Molecule 27: 40S ribosomal protein S7

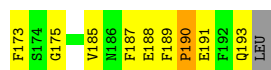
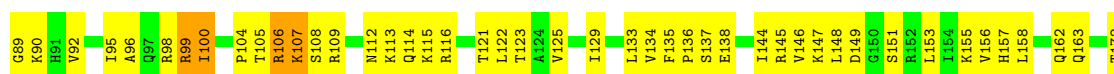
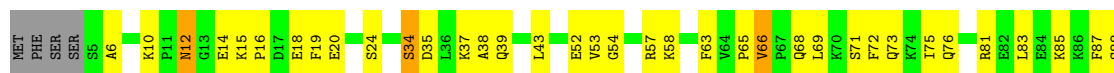




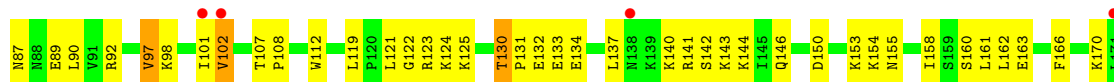
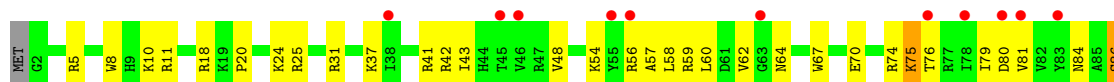
- Molecule 27: 40S ribosomal protein S7



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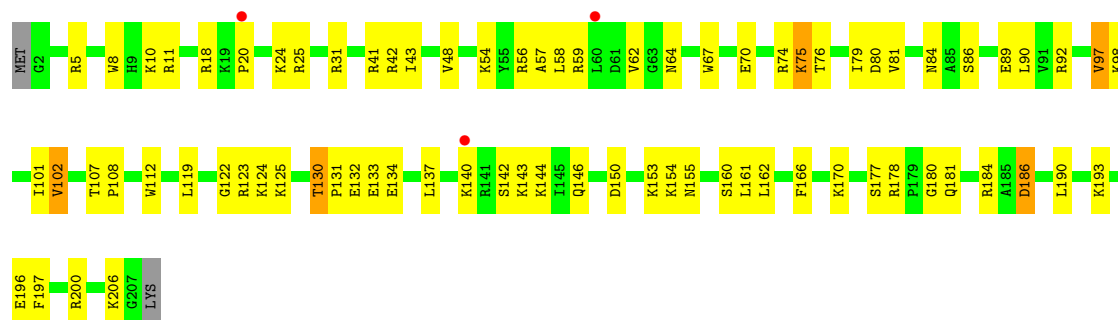


- Molecule 28: 40S ribosomal protein S8

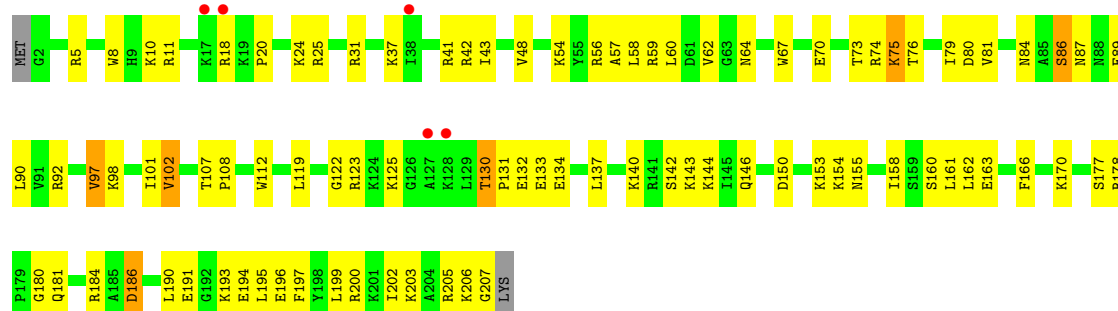


- Molecule 28: 40S ribosomal protein S8

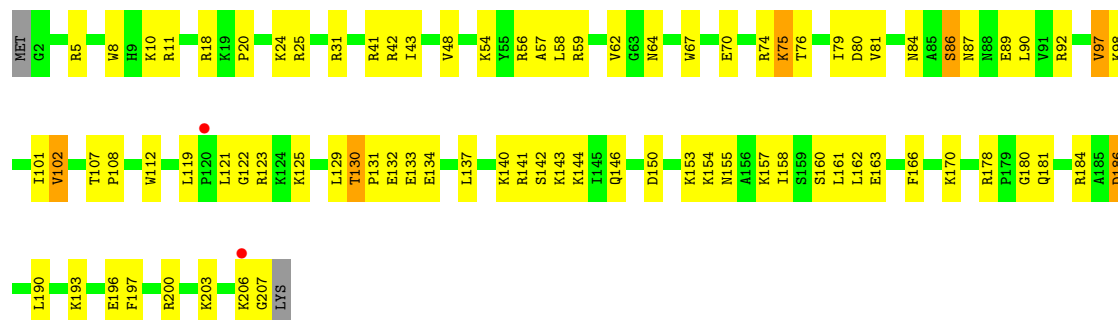




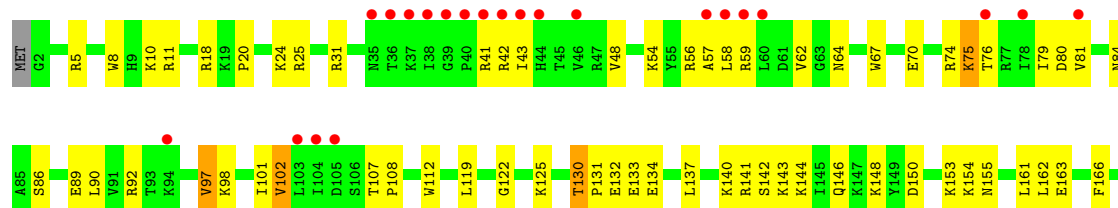
- Molecule 28: 40S ribosomal protein S8



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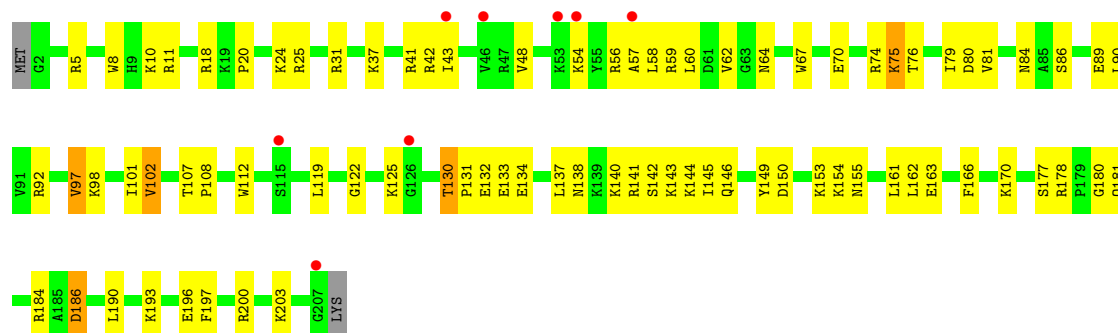


- Molecule 28: 40S ribosomal protein S8

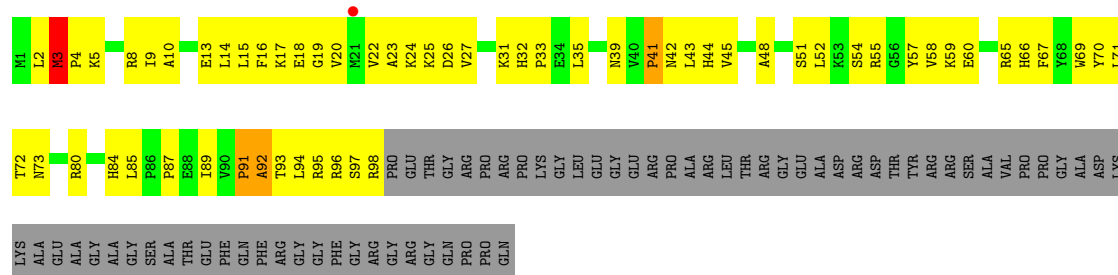
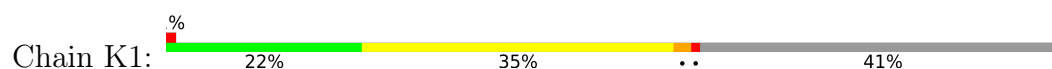




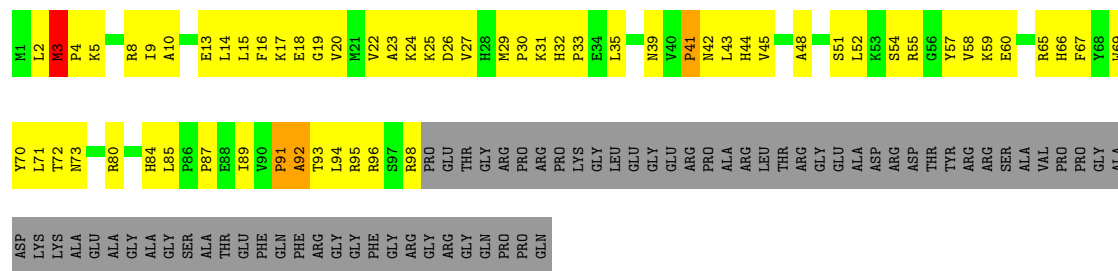
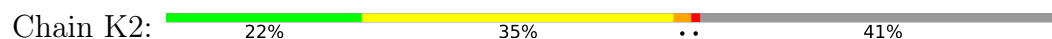
- Molecule 28: 40S ribosomal protein S8



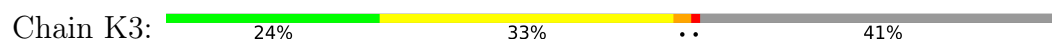
- Molecule 29: 40S ribosomal protein S10

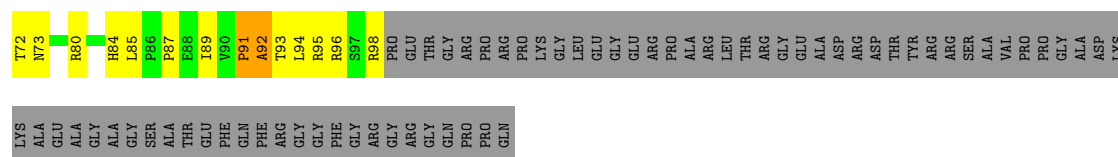


- Molecule 29: 40S ribosomal protein S10

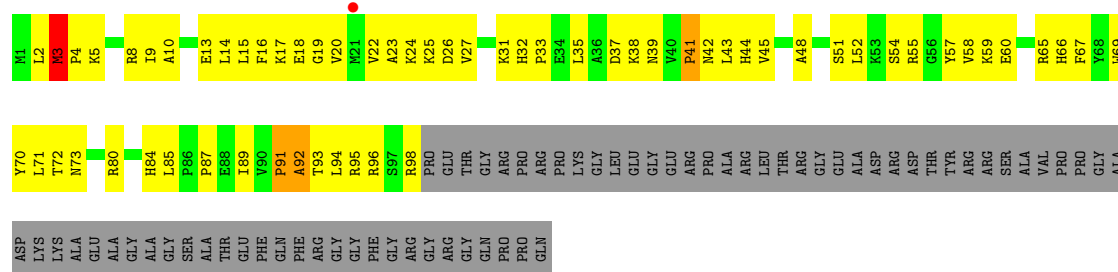
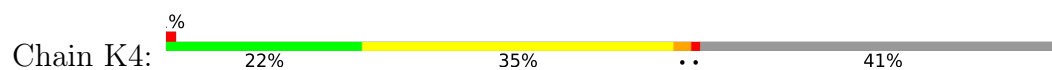


- Molecule 29: 40S ribosomal protein S10

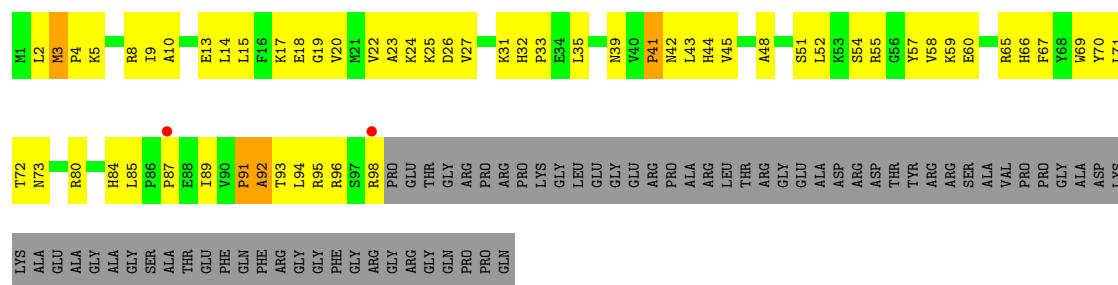
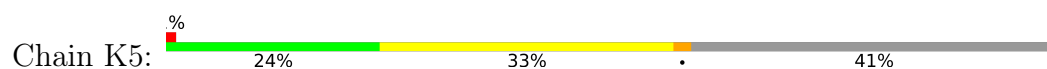




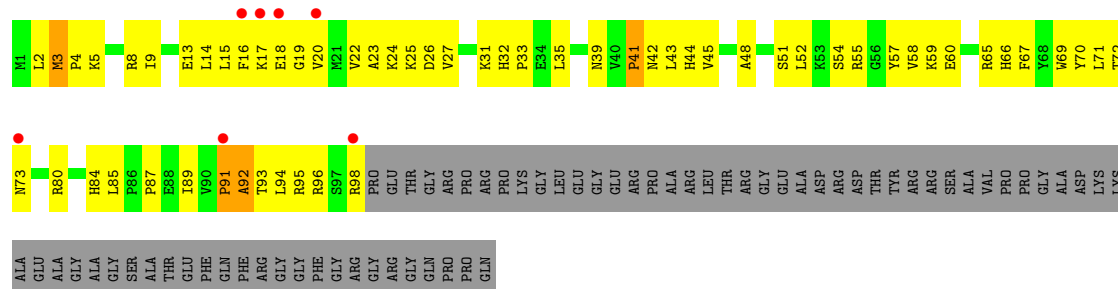
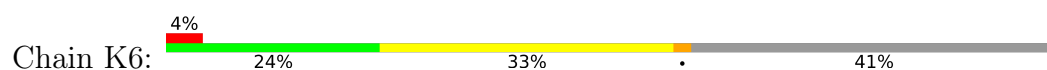
• Molecule 29: 40S ribosomal protein S10



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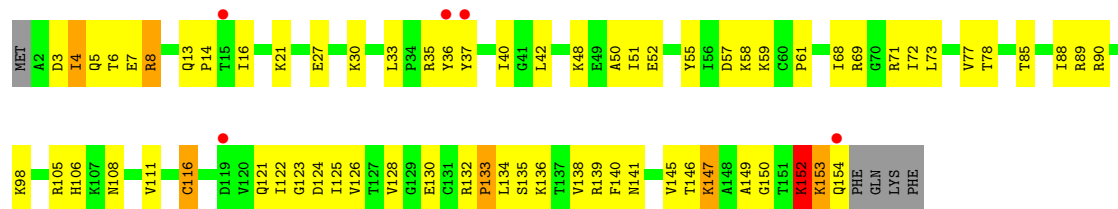


• Molecule 29: 40S ribosomal protein S10



• Molecule 30: 40S ribosomal protein S11





• Molecule 30: 40S ribosomal protein S11



• Molecule 30: 40S ribosomal protein S11



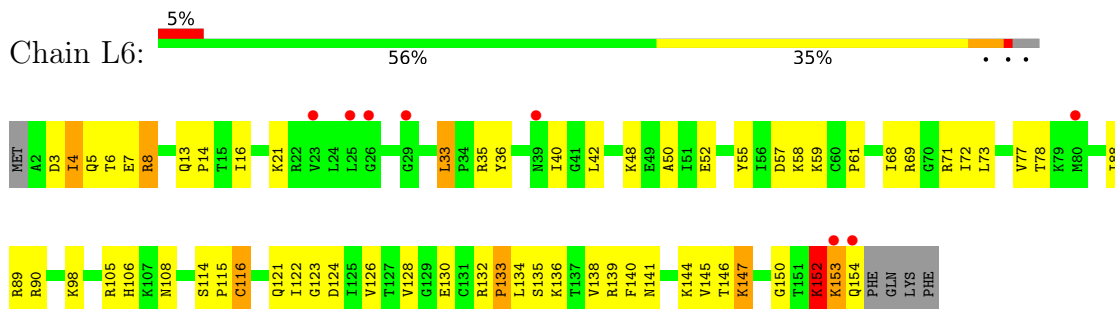
• Molecule 30: 40S ribosomal protein S11



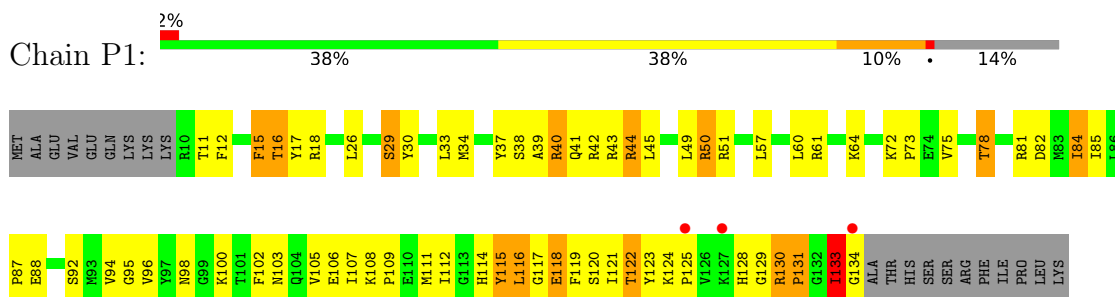
• Molecule 30: 40S ribosomal protein S11



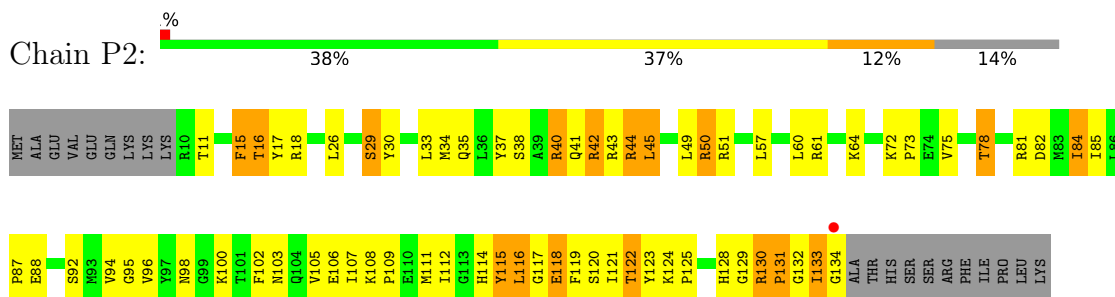
- Molecule 30: 40S ribosomal protein S11



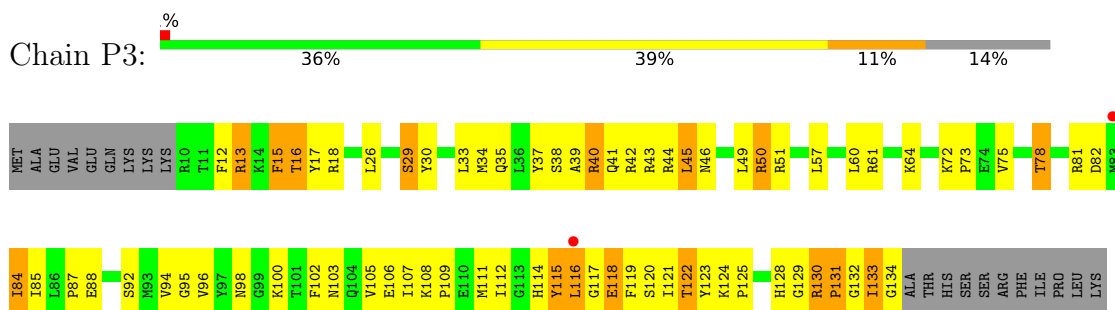
- Molecule 31: 40S ribosomal protein S15



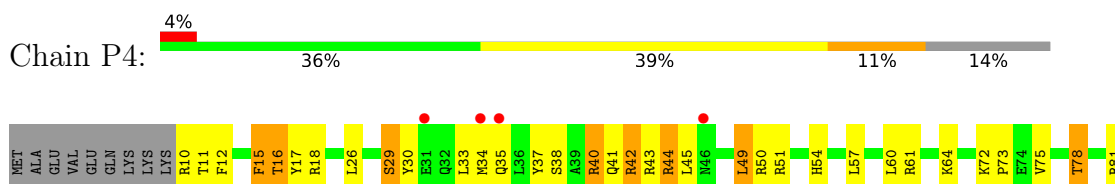
- Molecule 31: 40S ribosomal protein S15



- Molecule 31: 40S ribosomal protein S15



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- Molecule 31: 40S ribosomal protein S15



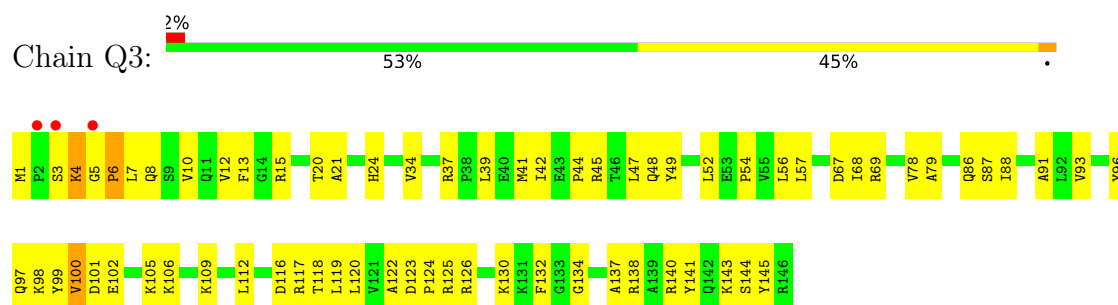
- Molecule 32: 40S ribosomal protein S16



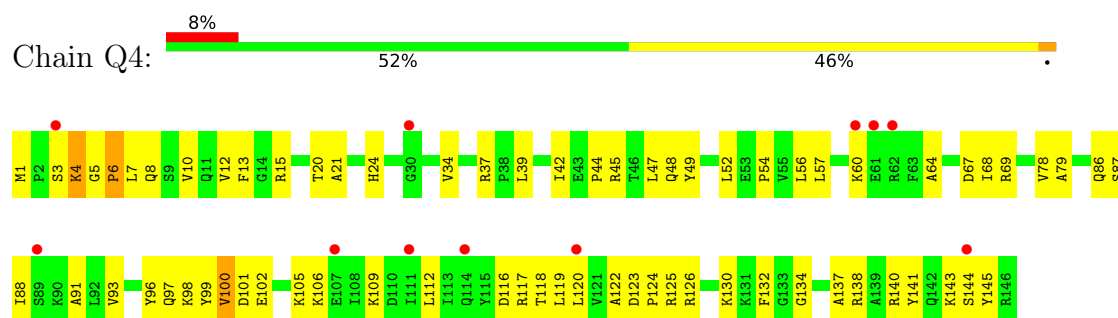
- Molecule 32: 40S ribosomal protein S16



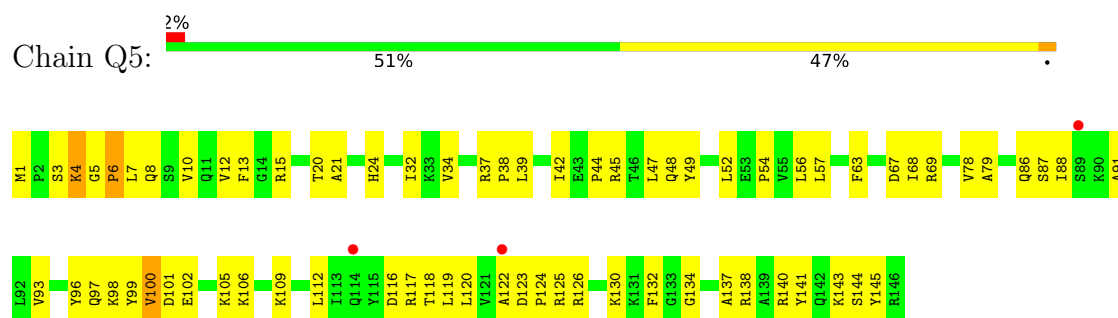
- Molecule 32: 40S ribosomal protein S16



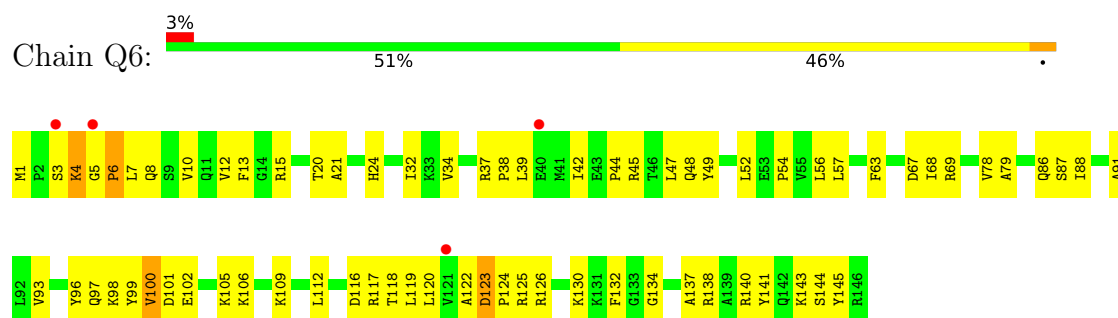
- Molecule 32: 40S ribosomal protein S16



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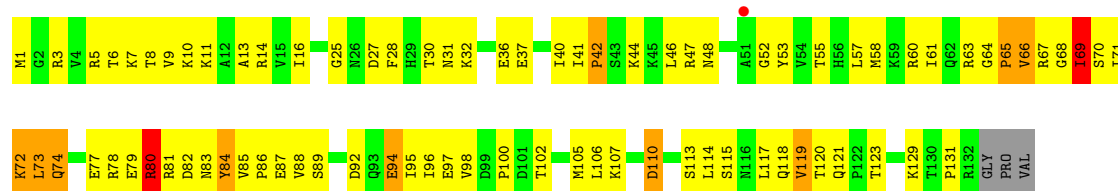


- Molecule 32: 40S ribosomal protein S16



- Molecule 33: 40S ribosomal protein S17





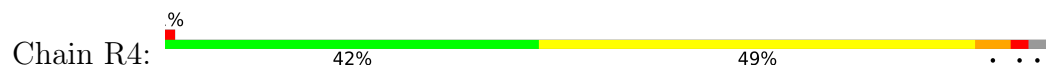
- Molecule 33: 40S ribosomal protein S17



- Molecule 33: 40S ribosomal protein S17



- Molecule 33: 40S ribosomal protein S17

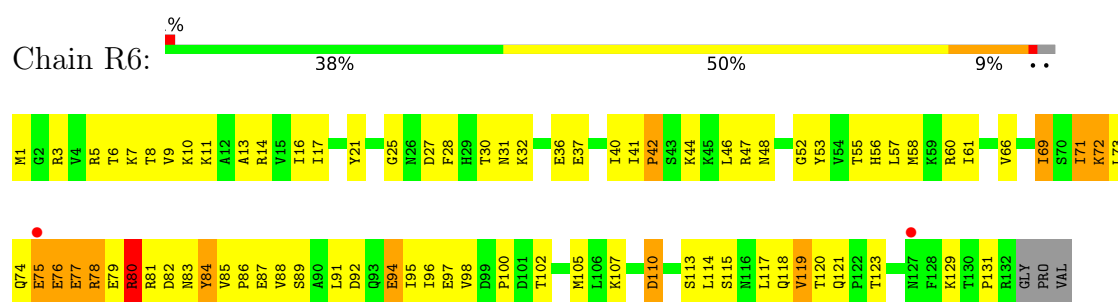


- Molecule 33: 40S ribosomal protein S17

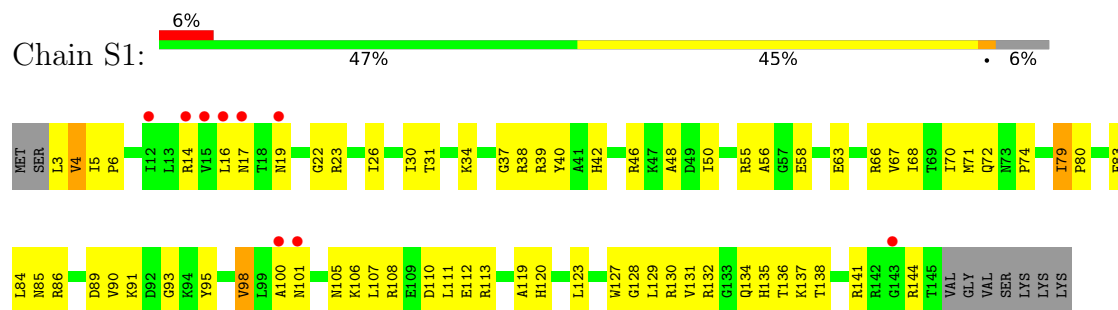


- Molecule 33: 40S ribosomal protein S17

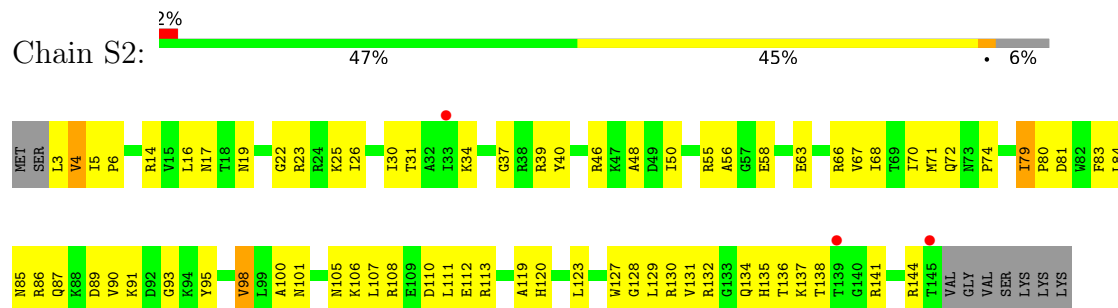




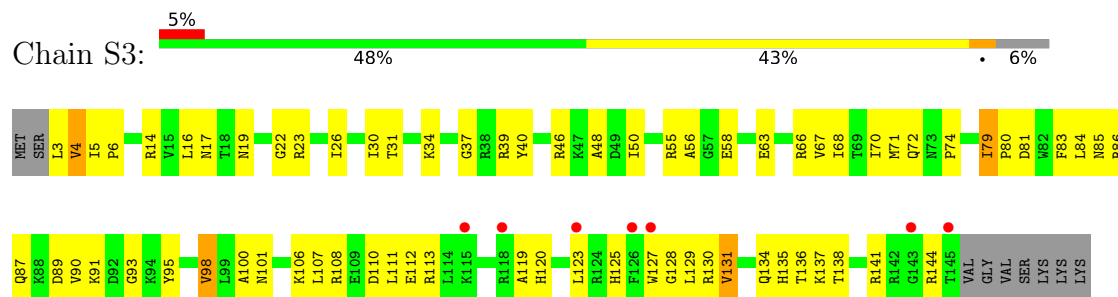
• Molecule 34: 40S ribosomal protein S18



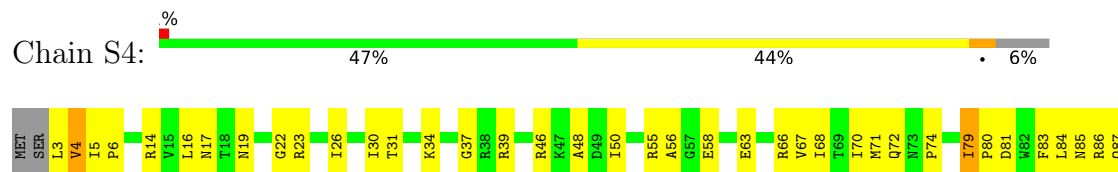
• Molecule 34: 40S ribosomal protein S18



• Molecule 34: 40S ribosomal protein S18



• Molecule 34: 40S ribosomal protein S18





- Molecule 34: 40S ribosomal protein S18



- Molecule 34: 40S ribosomal protein S18



- Molecule 35: 60S ribosomal protein L41



- Molecule 35: 60S ribosomal protein L41

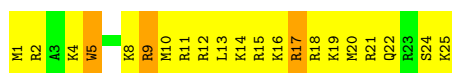


- Molecule 35: 60S ribosomal protein L41

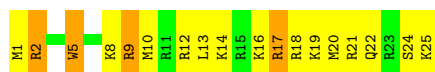


- Molecule 35: 60S ribosomal protein L41





- Molecule 35: 60S ribosomal protein L41



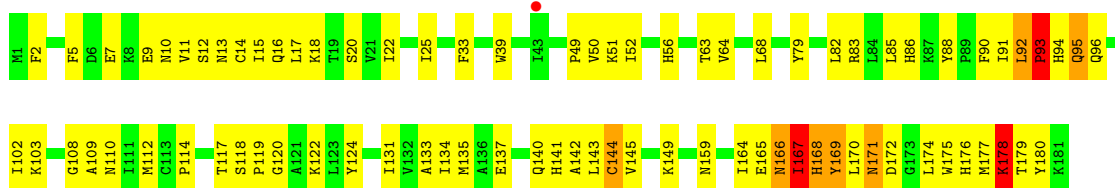
- Molecule 35: 60S ribosomal protein L41



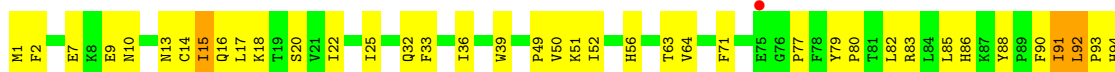
- Molecule 36: Malignant T-cell-amplified sequence 1



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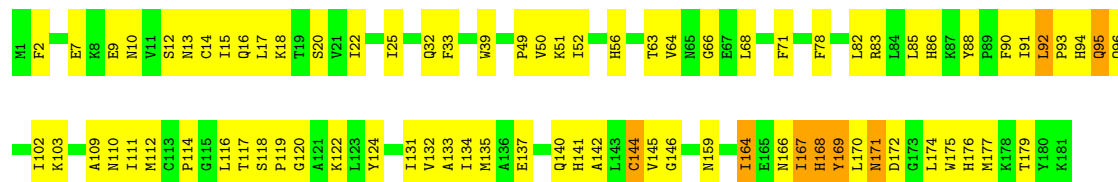
- Molecule 36: Malignant T-cell-amplified sequence 1





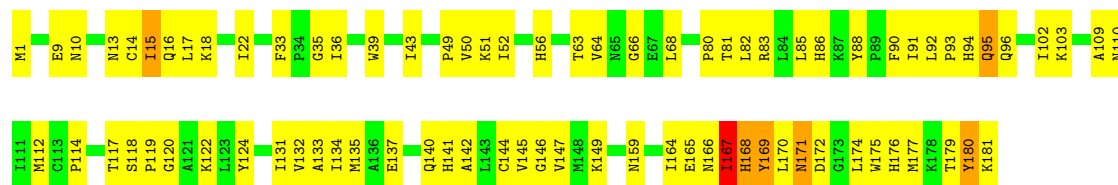
- Molecule 36: Malignant T-cell-amplified sequence 1

Chain k4: 56% 40%



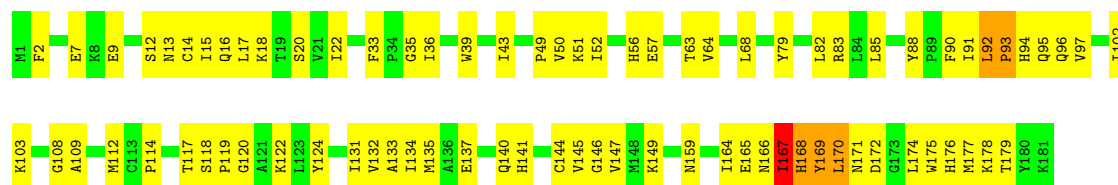
- Molecule 36: Malignant T-cell-amplified sequence 1

Chain k5: 55% 41%



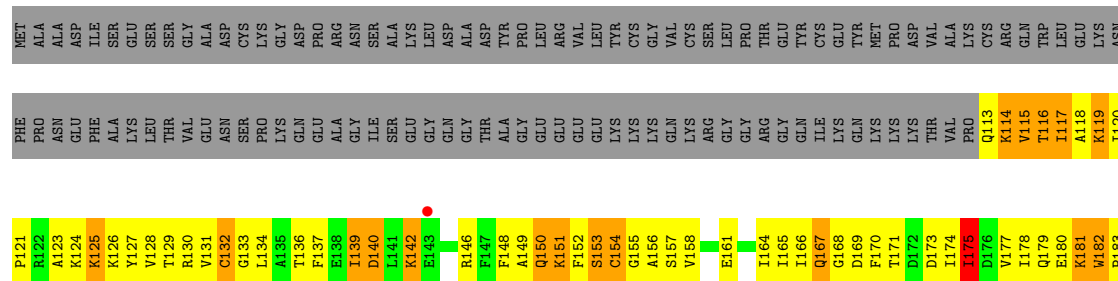
- Molecule 36: Malignant T-cell-amplified sequence 1

Chain k6: 56% 41%



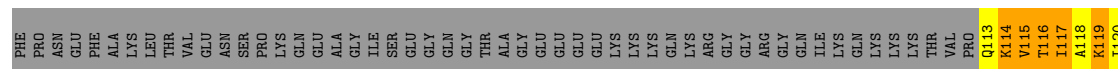
- Molecule 37: Density-regulated protein

Chain l1: 8% 21% 10% 60%

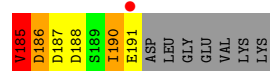
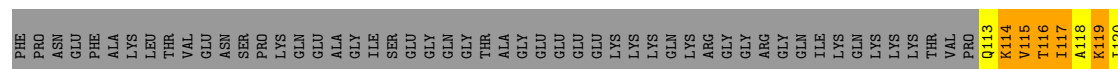




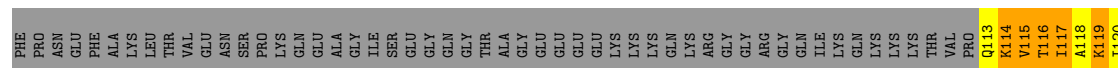
• Molecule 37: Density-regulated protein



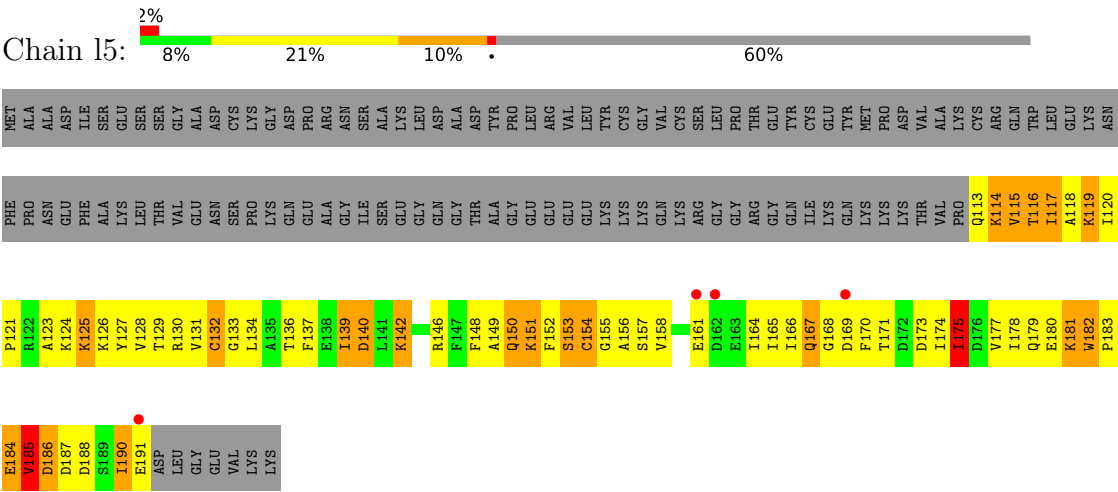
• Molecule 37: Density-regulated protein



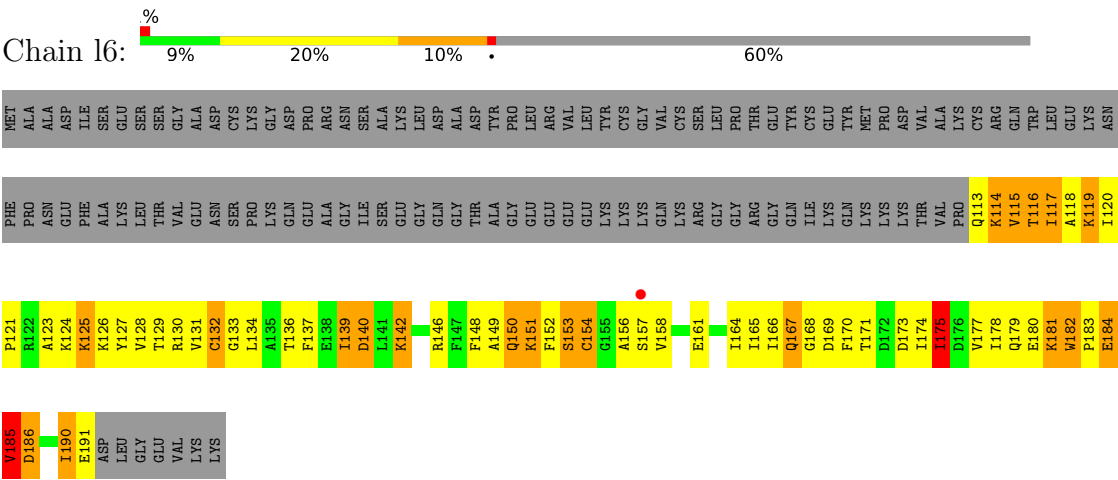
• Molecule 37: Density-regulated protein



● Molecule 37: Density-regulated protein



● Molecule 37: Density-regulated protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	334.67Å 597.13Å 336.50Å 90.00° 120.29° 90.00°	Depositor
Resolution (Å)	116.93 – 6.00 116.93 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (116.93-6.00) 98.8 (116.93-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 5.12Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.323 , 0.321 0.323 , 0.320	Depositor DCC
R_{free} test set	19868 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	278.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 5.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.094 for -h-l,k,h 0.094 for l,k,-h-l 0.099 for l,-k,h 0.097 for h,-k,-h-l 0.118 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	470574	wwPDB-VP
Average B, all atoms (Å ²)	204.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	T1	0.36	0/1131	0.82	1/1515 (0.1%)
1	T2	0.36	0/1131	0.82	1/1515 (0.1%)
1	T3	0.36	0/1131	0.82	1/1515 (0.1%)
1	T4	0.36	0/1131	0.82	1/1515 (0.1%)
1	T5	0.36	0/1131	0.82	1/1515 (0.1%)
1	T6	0.35	0/1131	0.82	1/1515 (0.1%)
2	U1	0.40	0/831	0.88	0/1115
2	U2	0.39	0/831	0.88	0/1115
2	U3	0.39	0/831	0.88	0/1115
2	U4	0.39	0/831	0.88	0/1115
2	U5	0.39	0/831	0.88	0/1115
2	U6	0.39	0/831	0.89	0/1115
3	V1	0.36	0/643	0.72	1/860 (0.1%)
3	V2	0.35	0/643	0.72	1/860 (0.1%)
3	V3	0.35	0/643	0.73	1/860 (0.1%)
3	V4	0.36	0/643	0.73	1/860 (0.1%)
3	V5	0.35	0/643	0.72	1/860 (0.1%)
3	V6	0.36	0/643	0.72	1/860 (0.1%)
4	X1	0.40	0/1116	0.79	0/1490
4	X2	0.40	0/1116	0.79	0/1490
4	X3	0.40	0/1116	0.79	0/1490
4	X4	0.40	0/1116	0.80	0/1490
4	X5	0.40	0/1116	0.79	0/1490
4	X6	0.40	0/1116	0.79	0/1490
5	a1	0.60	2/863 (0.2%)	0.97	5/1159 (0.4%)
5	a2	0.60	1/863 (0.1%)	0.97	5/1159 (0.4%)
5	a3	0.60	2/863 (0.2%)	0.97	5/1159 (0.4%)
5	a4	0.60	0/863	0.98	5/1159 (0.4%)
5	a5	0.61	2/863 (0.2%)	0.98	5/1159 (0.4%)
5	a6	0.60	1/863 (0.1%)	0.97	5/1159 (0.4%)
6	c1	0.36	0/508	0.88	3/680 (0.4%)
6	c2	0.37	0/508	0.88	3/680 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	c3	0.37	0/508	0.88	3/680 (0.4%)
6	c4	0.36	0/508	0.88	3/680 (0.4%)
6	c5	0.35	0/508	0.87	3/680 (0.4%)
6	c6	0.37	0/508	0.88	3/680 (0.4%)
7	d1	0.31	0/455	0.76	0/603
7	d2	0.31	0/455	0.77	0/603
7	d3	0.31	0/455	0.76	0/603
7	d4	0.30	0/455	0.76	0/603
7	d5	0.31	0/455	0.76	0/603
7	d6	0.31	0/455	0.76	0/603
8	f1	0.38	0/595	0.80	2/785 (0.3%)
8	f2	0.38	0/595	0.80	2/785 (0.3%)
8	f3	0.38	0/595	0.80	2/785 (0.3%)
8	f4	0.38	0/595	0.80	2/785 (0.3%)
8	f5	0.38	0/595	0.80	2/785 (0.3%)
8	f6	0.39	0/595	0.80	2/785 (0.3%)
9	g1	0.33	0/2493	0.81	2/3394 (0.1%)
9	g2	0.33	0/2493	0.81	2/3394 (0.1%)
9	g3	0.33	0/2493	0.81	2/3394 (0.1%)
9	g4	0.33	0/2493	0.81	2/3394 (0.1%)
9	g5	0.33	0/2493	0.81	2/3394 (0.1%)
9	g6	0.33	0/2493	0.82	2/3394 (0.1%)
10	C1	0.38	0/1762	0.84	7/2381 (0.3%)
10	C2	0.38	0/1762	0.84	7/2381 (0.3%)
10	C3	0.37	0/1762	0.84	7/2381 (0.3%)
10	C4	0.37	0/1762	0.84	7/2381 (0.3%)
10	C5	0.38	0/1762	0.84	7/2381 (0.3%)
10	C6	0.37	0/1762	0.84	7/2381 (0.3%)
11	G1	0.34	0/1946	0.89	9/2590 (0.3%)
11	G2	0.34	0/1946	0.89	9/2590 (0.3%)
11	G3	0.35	0/1946	0.89	9/2590 (0.3%)
11	G4	0.34	0/1946	0.90	9/2590 (0.3%)
11	G5	0.34	0/1946	0.89	8/2590 (0.3%)
11	G6	0.34	0/1946	0.89	9/2590 (0.3%)
12	J1	0.36	0/1550	0.77	0/2069
12	J2	0.36	0/1550	0.77	0/2069
12	J3	0.36	0/1550	0.77	0/2069
12	J4	0.36	0/1550	0.78	0/2069
12	J5	0.36	0/1550	0.77	0/2069
12	J6	0.36	0/1550	0.77	0/2069
13	M1	0.50	0/963	0.79	0/1291
13	M2	0.51	0/963	0.79	0/1291
13	M3	0.50	0/963	0.79	0/1291

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	M4	0.50	0/963	0.79	0/1291
13	M5	0.51	0/963	0.79	0/1291
13	M6	0.50	0/963	0.79	0/1291
14	N1	0.40	0/1232	0.80	1/1656 (0.1%)
14	N2	0.40	0/1232	0.80	1/1656 (0.1%)
14	N3	0.39	0/1232	0.77	0/1656
14	N4	0.40	0/1232	0.80	0/1656
14	N5	0.39	0/1232	0.77	0/1656
14	N6	0.39	0/1232	0.79	1/1656 (0.1%)
15	O1	0.42	0/1062	0.95	7/1425 (0.5%)
15	O2	0.42	0/1062	0.96	7/1425 (0.5%)
15	O3	0.42	0/1062	0.95	7/1425 (0.5%)
15	O4	0.42	0/1062	0.95	7/1425 (0.5%)
15	O5	0.42	0/1062	0.95	5/1425 (0.4%)
15	O6	0.42	0/1062	0.95	7/1425 (0.5%)
16	W1	0.40	0/1051	0.86	1/1406 (0.1%)
16	W2	0.40	0/1051	0.86	1/1406 (0.1%)
16	W3	0.39	0/1051	0.85	1/1406 (0.1%)
16	W4	0.40	0/1051	0.86	1/1406 (0.1%)
16	W5	0.40	0/1051	0.86	1/1406 (0.1%)
16	W6	0.40	0/1051	0.86	1/1406 (0.1%)
17	Y1	0.36	0/1083	0.76	0/1438
17	Y2	0.36	0/1083	0.76	0/1438
17	Y3	0.36	0/1083	0.76	0/1438
17	Y4	0.36	0/1083	0.76	0/1438
17	Y5	0.36	0/1083	0.76	0/1438
17	Y6	0.36	0/1083	0.76	0/1438
18	Z1	0.36	0/604	0.86	1/810 (0.1%)
18	Z2	0.37	0/604	0.86	1/810 (0.1%)
18	Z3	0.36	0/604	0.85	1/810 (0.1%)
18	Z4	0.35	0/604	0.85	1/810 (0.1%)
18	Z5	0.36	0/604	0.86	1/810 (0.1%)
18	Z6	0.37	0/604	0.86	1/810 (0.1%)
19	b1	0.35	0/665	0.92	1/891 (0.1%)
19	b2	0.36	0/665	0.88	2/891 (0.2%)
19	b3	0.36	0/665	0.88	0/891
19	b4	0.34	0/665	0.93	3/891 (0.3%)
19	b5	0.35	0/665	0.89	2/891 (0.2%)
19	b6	0.36	0/665	0.89	2/891 (0.2%)
20	e1	0.33	0/465	0.79	1/612 (0.2%)
20	e2	0.38	0/465	0.70	0/612
20	e3	0.39	0/465	0.73	0/612
20	e4	0.37	0/465	0.71	0/612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	e5	0.31	0/465	0.63	0/612
20	e6	0.40	0/465	0.72	0/612
21	i1	0.20	0/41243	0.32	6/64257 (0.0%)
21	i2	0.20	0/41242	0.30	1/64253 (0.0%)
21	i3	0.20	0/41242	0.30	1/64253 (0.0%)
21	i4	0.22	1/41243 (0.0%)	0.31	4/64257 (0.0%)
21	i5	0.27	1/41243 (0.0%)	0.31	6/64257 (0.0%)
21	i6	0.25	1/41243 (0.0%)	0.31	4/64257 (0.0%)
22	A1	0.35	0/1784	0.80	3/2424 (0.1%)
22	A2	0.35	0/1784	0.80	3/2424 (0.1%)
22	A3	0.36	0/1784	0.80	3/2424 (0.1%)
22	A4	0.36	0/1784	0.80	3/2424 (0.1%)
22	A5	0.36	0/1784	0.80	3/2424 (0.1%)
22	A6	0.36	0/1784	0.80	3/2424 (0.1%)
23	B1	0.36	0/1765	0.78	0/2362
23	B2	0.37	0/1765	0.79	0/2362
23	B3	0.37	0/1765	0.79	0/2362
23	B4	0.37	0/1765	0.79	0/2362
23	B5	0.37	0/1765	0.79	0/2362
23	B6	0.37	0/1765	0.78	0/2362
24	D1	0.38	0/1793	0.79	0/2414
24	D2	0.38	0/1793	0.79	0/2414
24	D3	0.38	0/1793	0.79	0/2414
24	D4	0.38	0/1793	0.79	0/2414
24	D5	0.38	0/1793	0.79	0/2414
24	D6	0.38	0/1793	0.79	0/2414
25	E1	0.35	0/2118	0.83	1/2849 (0.0%)
25	E2	0.35	0/2118	0.84	1/2849 (0.0%)
25	E3	0.35	0/2118	0.84	1/2849 (0.0%)
25	E4	0.35	0/2118	0.84	1/2849 (0.0%)
25	E5	0.35	0/2118	0.84	1/2849 (0.0%)
25	E6	0.35	0/2118	0.84	1/2849 (0.0%)
26	F1	0.40	0/1531	0.83	2/2059 (0.1%)
26	F2	0.40	0/1531	0.83	2/2059 (0.1%)
26	F3	0.40	0/1531	0.83	2/2059 (0.1%)
26	F4	0.40	0/1531	0.83	2/2059 (0.1%)
26	F5	0.40	0/1531	0.83	2/2059 (0.1%)
26	F6	0.39	0/1531	0.82	2/2059 (0.1%)
27	H1	0.35	0/1544	0.81	1/2068 (0.0%)
27	H2	0.36	0/1544	0.80	0/2068
27	H3	0.36	0/1544	0.81	1/2068 (0.0%)
27	H4	0.35	0/1544	0.81	1/2068 (0.0%)
27	H5	0.36	0/1544	0.81	0/2068

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	H6	0.36	0/1544	0.80	1/2068 (0.0%)
28	I1	0.35	0/1715	0.76	0/2287
28	I2	0.35	0/1715	0.76	0/2287
28	I3	0.34	0/1715	0.76	0/2287
28	I4	0.36	0/1715	0.77	0/2287
28	I5	0.36	0/1715	0.76	0/2287
28	I6	0.35	0/1715	0.76	0/2287
29	K1	0.36	0/851	0.91	2/1147 (0.2%)
29	K2	0.38	0/851	0.90	2/1147 (0.2%)
29	K3	0.37	0/851	0.91	2/1147 (0.2%)
29	K4	0.37	0/851	0.91	2/1147 (0.2%)
29	K5	0.37	0/851	0.91	0/1147
29	K6	0.37	0/851	0.91	0/1147
30	L1	0.36	0/1268	0.76	0/1696
30	L2	0.37	0/1268	0.77	0/1696
30	L3	0.36	0/1268	0.77	0/1696
30	L4	0.38	0/1268	0.77	0/1696
30	L5	0.37	0/1268	0.77	0/1696
30	L6	0.37	0/1268	0.77	0/1696
31	P1	0.38	0/1053	0.69	0/1406
31	P2	0.38	0/1053	0.69	0/1406
31	P3	0.38	0/1053	0.71	1/1406 (0.1%)
31	P4	0.38	0/1053	0.69	0/1406
31	P5	0.37	0/1053	0.69	0/1406
31	P6	0.38	0/1053	0.69	0/1406
32	Q1	0.39	0/1177	0.81	2/1575 (0.1%)
32	Q2	0.39	0/1177	0.82	2/1575 (0.1%)
32	Q3	0.40	0/1177	0.82	2/1575 (0.1%)
32	Q4	0.40	0/1177	0.82	2/1575 (0.1%)
32	Q5	0.39	0/1177	0.82	2/1575 (0.1%)
32	Q6	0.39	0/1177	0.82	2/1575 (0.1%)
33	R1	0.39	0/1086	0.90	3/1457 (0.2%)
33	R2	0.39	0/1086	0.89	3/1457 (0.2%)
33	R3	0.39	0/1086	0.89	3/1457 (0.2%)
33	R4	0.39	0/1086	0.89	3/1457 (0.2%)
33	R5	0.39	0/1086	0.89	3/1457 (0.2%)
33	R6	0.39	0/1086	0.89	3/1457 (0.2%)
34	S1	0.48	0/1202	0.86	2/1610 (0.1%)
34	S2	0.48	0/1202	0.86	2/1610 (0.1%)
34	S3	0.48	0/1202	0.86	2/1610 (0.1%)
34	S4	0.48	0/1202	0.86	2/1610 (0.1%)
34	S5	0.48	0/1202	0.86	2/1610 (0.1%)
34	S6	0.48	0/1202	0.86	2/1610 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	j1	0.25	0/240	0.57	0/305
35	j2	0.25	0/240	0.58	0/305
35	j3	0.25	0/240	0.58	0/305
35	j4	0.25	0/240	0.58	0/305
35	j5	0.25	0/240	0.57	0/305
35	j6	0.26	0/240	0.57	0/305
36	k1	0.72	0/1455	0.79	2/1968 (0.1%)
36	k2	0.91	2/1455 (0.1%)	1.39	7/1968 (0.4%)
36	k3	0.74	0/1455	1.53	3/1968 (0.2%)
36	k4	0.73	0/1455	0.76	0/1968
36	k5	0.77	1/1455 (0.1%)	1.12	4/1968 (0.2%)
36	k6	0.73	0/1455	0.75	0/1968
37	l1	0.42	0/638	1.01	4/859 (0.5%)
37	l2	0.41	0/638	1.00	4/859 (0.5%)
37	l3	0.41	0/638	1.01	4/859 (0.5%)
37	l4	0.42	0/638	1.00	4/859 (0.5%)
37	l5	0.42	0/638	1.01	4/859 (0.5%)
37	l6	0.42	0/638	1.01	4/859 (0.5%)
All	All	0.33	14/500884 (0.0%)	0.61	398/725470 (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
33	R1	0	1
33	R2	0	1
33	R3	0	1
33	R4	0	1
33	R5	0	1
36	k2	0	1
36	k3	0	2
36	k5	0	1
All	All	0	9

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	i5	1689	C	O3'-P	35.83	2.14	1.61
21	i6	1689	C	O3'-P	30.72	2.07	1.61
21	i4	1689	C	O3'-P	20.05	1.91	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k2	92	LEU	C-N	17.95	1.55	1.33
36	k2	93	PRO	C-N	9.78	1.48	1.33

The worst 5 of 398 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	k3	180	TYR	O-C-N	-45.37	62.25	122.59
36	k5	167	ILE	O-C-N	-33.89	80.21	122.57
36	k2	92	LEU	CA-C-N	-27.58	91.06	120.85
36	k2	92	LEU	C-N-CA	-27.58	91.06	120.85
36	k3	180	TYR	CA-C-N	26.71	169.78	121.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	R1	69	ILE	Peptide
33	R2	69	ILE	Peptide
33	R3	69	ILE	Peptide
33	R4	69	ILE	Peptide
33	R5	69	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T1	1112	0	1146	49	0
1	T2	1112	0	1146	52	0
1	T3	1112	0	1146	53	3
1	T4	1112	0	1146	53	3
1	T5	1112	0	1146	52	0
1	T6	1112	0	1146	52	0
2	U1	821	0	883	84	0
2	U2	821	0	883	87	0
2	U3	821	0	883	87	0
2	U4	821	0	883	86	0
2	U5	821	0	883	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U6	821	0	883	87	0
3	V1	636	0	637	25	0
3	V2	636	0	637	27	0
3	V3	636	0	637	25	0
3	V4	636	0	637	25	0
3	V5	636	0	637	27	0
3	V6	636	0	637	27	0
4	X1	1098	0	1167	60	0
4	X2	1098	0	1167	84	0
4	X3	1098	0	1167	65	0
4	X4	1098	0	1167	63	0
4	X5	1098	0	1167	61	0
4	X6	1098	0	1167	59	0
5	a1	847	0	899	60	0
5	a2	847	0	899	59	0
5	a3	847	0	899	58	0
5	a4	847	0	899	60	0
5	a5	847	0	899	59	0
5	a6	847	0	899	57	0
6	c1	506	0	536	24	0
6	c2	506	0	536	24	0
6	c3	506	0	536	25	0
6	c4	506	0	536	26	0
6	c5	506	0	536	25	0
6	c6	506	0	536	23	0
7	d1	445	0	442	30	0
7	d2	445	0	442	31	0
7	d3	445	0	442	31	0
7	d4	445	0	442	31	0
7	d5	445	0	442	31	0
7	d6	445	0	442	32	0
8	f1	585	0	617	190	0
8	f2	585	0	617	184	0
8	f3	585	0	618	181	3
8	f4	585	0	616	168	0
8	f5	585	0	617	180	0
8	f6	585	0	618	174	0
9	g1	2436	0	2393	124	3
9	g2	2436	0	2393	129	1
9	g3	2436	0	2393	131	1
9	g4	2436	0	2393	130	2
9	g5	2436	0	2393	124	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	g6	2436	0	2393	131	3
10	C1	1725	0	1806	176	0
10	C2	1725	0	1810	180	0
10	C3	1725	0	1811	172	0
10	C4	1725	0	1809	163	0
10	C5	1725	0	1809	160	0
10	C6	1725	0	1808	200	0
11	G1	1923	0	2089	180	0
11	G2	1923	0	2089	197	0
11	G3	1923	0	2089	168	0
11	G4	1923	0	2089	183	0
11	G5	1923	0	2086	203	0
11	G6	1923	0	2089	157	0
12	J1	1525	0	1640	88	0
12	J2	1525	0	1640	96	0
12	J3	1525	0	1640	84	0
12	J4	1525	0	1640	95	0
12	J5	1525	0	1640	100	0
12	J6	1525	0	1640	99	0
13	M1	953	0	990	103	0
13	M2	953	0	990	100	0
13	M3	953	0	990	100	1
13	M4	953	0	990	101	0
13	M5	953	0	990	103	0
13	M6	953	0	990	100	0
14	N1	1208	0	1294	112	8
14	N2	1208	0	1294	113	1
14	N3	1208	0	1294	121	0
14	N4	1208	0	1294	102	4
14	N5	1208	0	1294	117	0
14	N6	1208	0	1294	112	5
15	O1	1049	0	1073	87	0
15	O2	1049	0	1071	94	0
15	O3	1049	0	1072	71	0
15	O4	1049	0	1073	77	0
15	O5	1049	0	1071	77	0
15	O6	1049	0	1071	102	0
16	W1	1034	0	1080	65	0
16	W2	1034	0	1080	58	0
16	W3	1034	0	1080	70	0
16	W4	1034	0	1080	74	0
16	W5	1034	0	1080	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	W6	1034	0	1080	58	0
17	Y1	1065	0	1142	62	0
17	Y2	1065	0	1142	75	0
17	Y3	1065	0	1142	56	0
17	Y4	1065	0	1142	53	0
17	Y5	1065	0	1142	54	0
17	Y6	1065	0	1142	55	0
18	Z1	598	0	655	113	0
18	Z2	598	0	655	118	0
18	Z3	598	0	655	132	0
18	Z4	598	0	655	121	0
18	Z5	598	0	655	120	0
18	Z6	598	0	654	121	0
19	b1	651	0	672	48	16
19	b2	651	0	672	18	2
19	b3	651	0	672	20	9
19	b4	651	0	672	35	11
19	b5	651	0	672	19	6
19	b6	651	0	672	23	0
20	e1	459	0	503	77	0
20	e2	459	0	502	109	0
20	e3	459	0	503	50	0
20	e4	459	0	503	81	0
20	e5	459	0	503	82	0
20	e6	459	0	502	55	0
21	i1	36900	0	18592	1544	2
21	i2	36900	0	18590	1492	15
21	i3	36900	0	18593	1436	8
21	i4	36900	0	18594	1447	14
21	i5	36900	0	18589	1519	7
21	i6	36900	0	18589	1482	7
22	A1	1747	0	1749	153	0
22	A2	1747	0	1751	159	0
22	A3	1747	0	1749	158	0
22	A4	1747	0	1748	140	0
22	A5	1747	0	1748	149	0
22	A6	1747	0	1748	160	0
23	B1	1738	0	1809	83	0
23	B2	1738	0	1809	110	0
23	B3	1738	0	1809	77	0
23	B4	1738	0	1809	106	0
23	B5	1738	0	1809	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B6	1738	0	1809	91	0
24	D1	1765	0	1865	100	6
24	D2	1765	0	1865	106	12
24	D3	1765	0	1865	105	0
24	D4	1765	0	1865	104	0
24	D5	1765	0	1865	106	0
24	D6	1765	0	1865	113	0
25	E1	2076	0	2177	96	0
25	E2	2076	0	2177	96	0
25	E3	2076	0	2177	99	0
25	E4	2076	0	2177	93	0
25	E5	2076	0	2177	93	0
25	E6	2076	0	2177	93	0
26	F1	1509	0	1563	134	0
26	F2	1509	0	1561	148	0
26	F3	1509	0	1562	153	0
26	F4	1509	0	1561	150	0
26	F5	1509	0	1562	134	0
26	F6	1509	0	1563	142	0
27	H1	1521	0	1616	75	19
27	H2	1521	0	1616	89	0
27	H3	1521	0	1616	84	2
27	H4	1521	0	1616	85	28
27	H5	1521	0	1616	74	5
27	H6	1521	0	1616	72	0
28	I1	1686	0	1769	154	0
28	I2	1686	0	1769	81	0
28	I3	1686	0	1772	119	0
28	I4	1686	0	1767	127	0
28	I5	1686	0	1772	94	0
28	I6	1686	0	1772	83	0
29	K1	827	0	854	83	1
29	K2	827	0	854	84	2
29	K3	827	0	854	82	0
29	K4	827	0	854	85	0
29	K5	827	0	854	82	0
29	K6	827	0	854	83	0
30	L1	1247	0	1323	124	0
30	L2	1247	0	1323	99	0
30	L3	1247	0	1323	74	0
30	L4	1247	0	1322	120	0
30	L5	1247	0	1323	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	L6	1247	0	1323	87	0
31	P1	1033	0	1079	193	0
31	P2	1033	0	1079	179	0
31	P3	1033	0	1079	208	0
31	P4	1033	0	1079	187	0
31	P5	1033	0	1079	214	0
31	P6	1033	0	1078	202	0
32	Q1	1158	0	1232	54	0
32	Q2	1158	0	1232	55	0
32	Q3	1158	0	1232	55	0
32	Q4	1158	0	1232	55	0
32	Q5	1158	0	1232	58	0
32	Q6	1158	0	1232	58	0
33	R1	1072	0	1130	112	0
33	R2	1072	0	1130	121	2
33	R3	1072	0	1128	140	0
33	R4	1072	0	1128	111	0
33	R5	1072	0	1130	121	0
33	R6	1072	0	1130	118	5
34	S1	1184	0	1240	140	0
34	S2	1184	0	1241	145	0
34	S3	1184	0	1241	123	0
34	S4	1184	0	1242	119	0
34	S5	1184	0	1242	141	0
34	S6	1184	0	1242	122	0
35	j1	239	0	287	86	0
35	j2	239	0	288	55	0
35	j3	239	0	286	56	0
35	j4	239	0	288	92	0
35	j5	239	0	289	79	0
35	j6	239	0	287	40	0
36	k1	1421	0	1436	327	0
36	k2	1421	0	1433	288	0
36	k3	1421	0	1436	256	0
36	k4	1421	0	1437	256	0
36	k5	1421	0	1436	247	0
36	k6	1421	0	1436	223	0
37	l1	629	0	626	199	0
37	l2	629	0	626	189	0
37	l3	629	0	626	205	0
37	l4	629	0	626	209	0
37	l5	629	0	626	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	l6	629	0	626	208	0
38	f1	1	0	0	2	0
38	f2	1	0	0	1	0
38	f3	1	0	0	0	0
38	f4	1	0	0	0	0
38	f5	1	0	0	3	0
38	f6	1	0	0	1	0
All	All	470574	0	372069	24796	109

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

The worst 5 of 24796 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M5:36:ARG:CZ	21:i5:1310:U:C5	1.74	1.68
36:k4:33:PHE:CE1	36:k4:92:LEU:HD11	1.28	1.67
13:M1:36:ARG:CZ	21:i1:1310:U:C5	1.74	1.66
13:M3:36:ARG:CZ	21:i3:1310:U:C5	1.74	1.66
13:M6:36:ARG:CZ	21:i6:1310:U:C5	1.74	1.66

The worst 5 of 109 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b1:81:ARG:CB	27:H4:35:ASP:O[2_545]	0.92	1.28
21:i2:1109:C:OP1	19:b3:41:TYR:CD2[2_555]	1.03	1.17
19:b5:41:TYR:OH	21:i6:1109:C:O4'[2_555]	1.05	1.15
27:H1:165:ASN:OD1	27:H4:164:ASN:N[2_545]	1.07	1.13
19:b5:41:TYR:OH	21:i6:1109:C:C4'[2_555]	1.09	1.11

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	T1	141/145 (97%)	119 (84%)	15 (11%)	7 (5%)	1	15
1	T2	141/145 (97%)	119 (84%)	15 (11%)	7 (5%)	1	15
1	T3	141/145 (97%)	119 (84%)	16 (11%)	6 (4%)	2	17
1	T4	141/145 (97%)	119 (84%)	16 (11%)	6 (4%)	2	17
1	T5	141/145 (97%)	119 (84%)	15 (11%)	7 (5%)	1	15
1	T6	141/145 (97%)	119 (84%)	16 (11%)	6 (4%)	2	17
2	U1	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	13
2	U2	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	13
2	U3	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	13
2	U4	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	13
2	U5	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	13
2	U6	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	13
3	V1	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	12
3	V2	81/83 (98%)	66 (82%)	10 (12%)	5 (6%)	1	12
3	V3	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	12
3	V4	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	12
3	V5	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	12
3	V6	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	12
4	X1	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	8
4	X2	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	8
4	X3	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	8
4	X4	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	8
4	X5	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	8
4	X6	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	8
5	a1	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	4
5	a2	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	4
5	a3	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	4
5	a4	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	4
5	a5	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	4
5	a6	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	4
6	c1	62/69 (90%)	47 (76%)	9 (14%)	6 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c2	62/69 (90%)	47 (76%)	10 (16%)	5 (8%)	1	9
6	c3	62/69 (90%)	47 (76%)	10 (16%)	5 (8%)	1	9
6	c4	62/69 (90%)	47 (76%)	10 (16%)	5 (8%)	1	9
6	c5	62/69 (90%)	47 (76%)	9 (14%)	6 (10%)	0	7
6	c6	62/69 (90%)	47 (76%)	10 (16%)	5 (8%)	1	9
7	d1	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d2	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d3	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d4	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d5	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d6	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
8	f1	70/156 (45%)	56 (80%)	10 (14%)	4 (6%)	1	14
8	f2	70/156 (45%)	56 (80%)	10 (14%)	4 (6%)	1	14
8	f3	70/156 (45%)	56 (80%)	10 (14%)	4 (6%)	1	14
8	f4	70/156 (45%)	57 (81%)	9 (13%)	4 (6%)	1	14
8	f5	70/156 (45%)	56 (80%)	10 (14%)	4 (6%)	1	14
8	f6	70/156 (45%)	55 (79%)	11 (16%)	4 (6%)	1	14
9	g1	311/317 (98%)	237 (76%)	58 (19%)	16 (5%)	1	15
9	g2	311/317 (98%)	236 (76%)	59 (19%)	16 (5%)	1	15
9	g3	311/317 (98%)	236 (76%)	59 (19%)	16 (5%)	1	15
9	g4	311/317 (98%)	237 (76%)	58 (19%)	16 (5%)	1	15
9	g5	311/317 (98%)	237 (76%)	58 (19%)	16 (5%)	1	15
9	g6	311/317 (98%)	236 (76%)	59 (19%)	16 (5%)	1	15
10	C1	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	1	15
10	C2	220/293 (75%)	181 (82%)	28 (13%)	11 (5%)	1	15
10	C3	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	1	15
10	C4	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	1	15
10	C5	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	1	15
10	C6	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	1	15
11	G1	235/249 (94%)	194 (83%)	25 (11%)	16 (7%)	1	11
11	G2	235/249 (94%)	195 (83%)	24 (10%)	16 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	G3	235/249 (94%)	194 (83%)	25 (11%)	16 (7%)	1	11
11	G4	235/249 (94%)	194 (83%)	26 (11%)	15 (6%)	1	12
11	G5	235/249 (94%)	194 (83%)	25 (11%)	16 (7%)	1	11
11	G6	235/249 (94%)	194 (83%)	25 (11%)	16 (7%)	1	11
12	J1	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	1	14
12	J2	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	1	14
12	J3	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	1	14
12	J4	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	1	14
12	J5	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	1	14
12	J6	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	1	14
13	M1	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	7	36
13	M2	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	7	36
13	M3	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	7	36
13	M4	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	7	36
13	M5	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	7	36
13	M6	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	7	36
14	N1	148/151 (98%)	125 (84%)	14 (10%)	9 (6%)	1	12
14	N2	148/151 (98%)	125 (84%)	14 (10%)	9 (6%)	1	12
14	N3	148/151 (98%)	124 (84%)	15 (10%)	9 (6%)	1	12
14	N4	148/151 (98%)	125 (84%)	14 (10%)	9 (6%)	1	12
14	N5	148/151 (98%)	124 (84%)	15 (10%)	9 (6%)	1	12
14	N6	148/151 (98%)	125 (84%)	13 (9%)	10 (7%)	1	11
15	O1	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	8
15	O2	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	8
15	O3	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	8
15	O4	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	8
15	O5	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	8
15	O6	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	8
16	W1	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	2	18
16	W2	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	2	18
16	W3	127/130 (98%)	108 (85%)	13 (10%)	6 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	W4	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	2	18
16	W5	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	2	18
16	W6	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	2	18
17	Y1	129/133 (97%)	108 (84%)	16 (12%)	5 (4%)	2	18
17	Y2	129/133 (97%)	109 (84%)	15 (12%)	5 (4%)	2	18
17	Y3	129/133 (97%)	109 (84%)	15 (12%)	5 (4%)	2	18
17	Y4	129/133 (97%)	109 (84%)	15 (12%)	5 (4%)	2	18
17	Y5	129/133 (97%)	109 (84%)	15 (12%)	5 (4%)	2	18
17	Y6	129/133 (97%)	108 (84%)	16 (12%)	5 (4%)	2	18
18	Z1	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	1	14
18	Z2	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	1	14
18	Z3	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	1	14
18	Z4	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	1	14
18	Z5	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	1	14
18	Z6	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	1	14
19	b1	81/84 (96%)	64 (79%)	12 (15%)	5 (6%)	1	12
19	b2	81/84 (96%)	67 (83%)	12 (15%)	2 (2%)	4	26
19	b3	81/84 (96%)	67 (83%)	11 (14%)	3 (4%)	2	19
19	b4	81/84 (96%)	65 (80%)	11 (14%)	5 (6%)	1	12
19	b5	81/84 (96%)	67 (83%)	10 (12%)	4 (5%)	1	15
19	b6	81/84 (96%)	67 (83%)	12 (15%)	2 (2%)	4	26
20	e1	56/133 (42%)	41 (73%)	11 (20%)	4 (7%)	1	10
20	e2	56/133 (42%)	37 (66%)	12 (21%)	7 (12%)	0	4
20	e3	56/133 (42%)	38 (68%)	12 (21%)	6 (11%)	0	6
20	e4	56/133 (42%)	35 (62%)	15 (27%)	6 (11%)	0	6
20	e5	56/133 (42%)	38 (68%)	11 (20%)	7 (12%)	0	4
20	e6	56/133 (42%)	38 (68%)	12 (21%)	6 (11%)	0	6
22	A1	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	2	20
22	A2	220/295 (75%)	180 (82%)	32 (14%)	8 (4%)	2	20
22	A3	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	2	20
22	A4	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	A5	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	2	20
22	A6	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	2	20
23	B1	212/264 (80%)	174 (82%)	31 (15%)	7 (3%)	3	21
23	B2	212/264 (80%)	174 (82%)	29 (14%)	9 (4%)	2	17
23	B3	212/264 (80%)	174 (82%)	30 (14%)	8 (4%)	2	19
23	B4	212/264 (80%)	174 (82%)	30 (14%)	8 (4%)	2	19
23	B5	212/264 (80%)	174 (82%)	30 (14%)	8 (4%)	2	19
23	B6	212/264 (80%)	174 (82%)	31 (15%)	7 (3%)	3	21
24	D1	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	9
24	D2	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	9
24	D3	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	9
24	D4	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	9
24	D5	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	9
24	D6	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	9
25	E1	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	13
25	E2	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	13
25	E3	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	13
25	E4	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	13
25	E5	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	13
25	E6	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	13
26	F1	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	9
26	F2	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	9
26	F3	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	9
26	F4	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	9
26	F5	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	9
26	F6	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	9
27	H1	187/194 (96%)	145 (78%)	28 (15%)	14 (8%)	1	10
27	H2	187/194 (96%)	145 (78%)	28 (15%)	14 (8%)	1	10
27	H3	187/194 (96%)	145 (78%)	28 (15%)	14 (8%)	1	10
27	H4	187/194 (96%)	146 (78%)	27 (14%)	14 (8%)	1	10
27	H5	187/194 (96%)	146 (78%)	27 (14%)	14 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	H6	187/194 (96%)	146 (78%)	27 (14%)	14 (8%)	1	10
28	I1	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	13
28	I2	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	13
28	I3	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	13
28	I4	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	13
28	I5	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	13
28	I6	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	13
29	K1	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	1	14
29	K2	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	1	14
29	K3	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	1	14
29	K4	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	1	14
29	K5	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	1	14
29	K6	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	1	14
30	L1	151/158 (96%)	129 (85%)	11 (7%)	11 (7%)	1	10
30	L2	151/158 (96%)	125 (83%)	15 (10%)	11 (7%)	1	10
30	L3	151/158 (96%)	128 (85%)	14 (9%)	9 (6%)	1	13
30	L4	151/158 (96%)	127 (84%)	13 (9%)	11 (7%)	1	10
30	L5	151/158 (96%)	128 (85%)	14 (9%)	9 (6%)	1	13
30	L6	151/158 (96%)	126 (83%)	15 (10%)	10 (7%)	1	12
31	P1	123/145 (85%)	111 (90%)	6 (5%)	6 (5%)	1	15
31	P2	123/145 (85%)	111 (90%)	6 (5%)	6 (5%)	1	15
31	P3	123/145 (85%)	108 (88%)	11 (9%)	4 (3%)	3	21
31	P4	123/145 (85%)	111 (90%)	6 (5%)	6 (5%)	1	15
31	P5	123/145 (85%)	112 (91%)	6 (5%)	5 (4%)	2	17
31	P6	123/145 (85%)	111 (90%)	6 (5%)	6 (5%)	1	15
32	Q1	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	11
32	Q2	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	11
32	Q3	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	11
32	Q4	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	11
32	Q5	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	11
32	Q6	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	R1	130/135 (96%)	94 (72%)	25 (19%)	11 (8%)	0	9
33	R2	130/135 (96%)	95 (73%)	22 (17%)	13 (10%)	0	7
33	R3	130/135 (96%)	95 (73%)	24 (18%)	11 (8%)	0	9
33	R4	130/135 (96%)	97 (75%)	23 (18%)	10 (8%)	1	9
33	R5	130/135 (96%)	93 (72%)	26 (20%)	11 (8%)	0	9
33	R6	130/135 (96%)	93 (72%)	27 (21%)	10 (8%)	1	9
34	S1	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S2	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S3	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S4	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S5	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S6	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
35	j1	23/25 (92%)	23 (100%)	0	0	100	100
35	j2	23/25 (92%)	23 (100%)	0	0	100	100
35	j3	23/25 (92%)	23 (100%)	0	0	100	100
35	j4	23/25 (92%)	23 (100%)	0	0	100	100
35	j5	23/25 (92%)	23 (100%)	0	0	100	100
35	j6	23/25 (92%)	23 (100%)	0	0	100	100
36	k1	179/181 (99%)	162 (90%)	13 (7%)	4 (2%)	5	29
36	k2	179/181 (99%)	161 (90%)	16 (9%)	2 (1%)	11	46
36	k3	179/181 (99%)	164 (92%)	14 (8%)	1 (1%)	21	59
36	k4	179/181 (99%)	160 (89%)	17 (10%)	2 (1%)	11	46
36	k5	179/181 (99%)	164 (92%)	13 (7%)	2 (1%)	11	46
36	k6	179/181 (99%)	164 (92%)	13 (7%)	2 (1%)	11	46
37	l1	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	4
37	l2	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	4
37	l3	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	4
37	l4	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	4
37	l5	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	4
37	l6	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	4
All	All	30804/35724 (86%)	25074 (81%)	3953 (13%)	1777 (6%)	1	13

5 of 1777 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T1	4	VAL
2	U1	50	VAL
2	U1	103	SER
2	U1	107	GLU
2	U1	116	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T1	113/115 (98%)	113 (100%)	0	100	100
1	T2	113/115 (98%)	113 (100%)	0	100	100
1	T3	113/115 (98%)	113 (100%)	0	100	100
1	T4	113/115 (98%)	113 (100%)	0	100	100
1	T5	113/115 (98%)	113 (100%)	0	100	100
1	T6	113/115 (98%)	113 (100%)	0	100	100
2	U1	94/107 (88%)	91 (97%)	3 (3%)	34	56
2	U2	94/107 (88%)	91 (97%)	3 (3%)	34	56
2	U3	94/107 (88%)	91 (97%)	3 (3%)	34	56
2	U4	94/107 (88%)	91 (97%)	3 (3%)	34	56
2	U5	94/107 (88%)	91 (97%)	3 (3%)	34	56
2	U6	94/107 (88%)	91 (97%)	3 (3%)	34	56
3	V1	67/67 (100%)	67 (100%)	0	100	100
3	V2	67/67 (100%)	67 (100%)	0	100	100
3	V3	67/67 (100%)	67 (100%)	0	100	100
3	V4	67/67 (100%)	67 (100%)	0	100	100
3	V5	67/67 (100%)	67 (100%)	0	100	100
3	V6	67/67 (100%)	67 (100%)	0	100	100
4	X1	113/115 (98%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X2	113/115 (98%)	113 (100%)	0	100	100
4	X3	113/115 (98%)	113 (100%)	0	100	100
4	X4	113/115 (98%)	113 (100%)	0	100	100
4	X5	113/115 (98%)	113 (100%)	0	100	100
4	X6	113/115 (98%)	113 (100%)	0	100	100
5	a1	90/98 (92%)	87 (97%)	3 (3%)	33	55
5	a2	90/98 (92%)	87 (97%)	3 (3%)	33	55
5	a3	90/98 (92%)	87 (97%)	3 (3%)	33	55
5	a4	90/98 (92%)	87 (97%)	3 (3%)	33	55
5	a5	90/98 (92%)	87 (97%)	3 (3%)	33	55
5	a6	90/98 (92%)	87 (97%)	3 (3%)	33	55
6	c1	57/62 (92%)	57 (100%)	0	100	100
6	c2	57/62 (92%)	57 (100%)	0	100	100
6	c3	57/62 (92%)	57 (100%)	0	100	100
6	c4	57/62 (92%)	57 (100%)	0	100	100
6	c5	57/62 (92%)	57 (100%)	0	100	100
6	c6	57/62 (92%)	57 (100%)	0	100	100
7	d1	47/49 (96%)	47 (100%)	0	100	100
7	d2	47/49 (96%)	47 (100%)	0	100	100
7	d3	47/49 (96%)	47 (100%)	0	100	100
7	d4	47/49 (96%)	47 (100%)	0	100	100
7	d5	47/49 (96%)	47 (100%)	0	100	100
7	d6	47/49 (96%)	47 (100%)	0	100	100
8	f1	65/140 (46%)	61 (94%)	4 (6%)	16	38
8	f2	65/140 (46%)	61 (94%)	4 (6%)	16	38
8	f3	65/140 (46%)	59 (91%)	6 (9%)	8	27
8	f4	65/140 (46%)	59 (91%)	6 (9%)	8	27
8	f5	65/140 (46%)	59 (91%)	6 (9%)	8	27
8	f6	65/140 (46%)	60 (92%)	5 (8%)	12	32
9	g1	272/275 (99%)	272 (100%)	0	100	100
9	g2	272/275 (99%)	272 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	g3	272/275 (99%)	272 (100%)	0	100	100
9	g4	272/275 (99%)	272 (100%)	0	100	100
9	g5	272/275 (99%)	272 (100%)	0	100	100
9	g6	272/275 (99%)	272 (100%)	0	100	100
10	C1	188/225 (84%)	186 (99%)	2 (1%)	65	76
10	C2	188/225 (84%)	186 (99%)	2 (1%)	65	76
10	C3	188/225 (84%)	186 (99%)	2 (1%)	65	76
10	C4	188/225 (84%)	186 (99%)	2 (1%)	65	76
10	C5	188/225 (84%)	186 (99%)	2 (1%)	65	76
10	C6	188/225 (84%)	186 (99%)	2 (1%)	65	76
11	G1	207/218 (95%)	201 (97%)	6 (3%)	37	58
11	G2	207/218 (95%)	201 (97%)	6 (3%)	37	58
11	G3	207/218 (95%)	201 (97%)	6 (3%)	37	58
11	G4	207/218 (95%)	201 (97%)	6 (3%)	37	58
11	G5	207/218 (95%)	201 (97%)	6 (3%)	37	58
11	G6	207/218 (95%)	201 (97%)	6 (3%)	37	58
12	J1	161/168 (96%)	161 (100%)	0	100	100
12	J2	161/168 (96%)	161 (100%)	0	100	100
12	J3	161/168 (96%)	161 (100%)	0	100	100
12	J4	161/168 (96%)	161 (100%)	0	100	100
12	J5	161/168 (96%)	161 (100%)	0	100	100
12	J6	161/168 (96%)	161 (100%)	0	100	100
13	M1	104/108 (96%)	92 (88%)	12 (12%)	5	18
13	M2	104/108 (96%)	92 (88%)	12 (12%)	5	18
13	M3	104/108 (96%)	92 (88%)	12 (12%)	5	18
13	M4	104/108 (96%)	92 (88%)	12 (12%)	5	18
13	M5	104/108 (96%)	92 (88%)	12 (12%)	5	18
13	M6	104/108 (96%)	92 (88%)	12 (12%)	5	18
14	N1	130/131 (99%)	127 (98%)	3 (2%)	44	64
14	N2	130/131 (99%)	127 (98%)	3 (2%)	44	64
14	N3	130/131 (99%)	124 (95%)	6 (5%)	24	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N4	130/131 (99%)	127 (98%)	3 (2%)	44	64
14	N5	130/131 (99%)	124 (95%)	6 (5%)	24	45
14	N6	130/131 (99%)	126 (97%)	4 (3%)	35	56
15	O1	110/119 (92%)	110 (100%)	0	100	100
15	O2	110/119 (92%)	110 (100%)	0	100	100
15	O3	110/119 (92%)	110 (100%)	0	100	100
15	O4	110/119 (92%)	110 (100%)	0	100	100
15	O5	110/119 (92%)	110 (100%)	0	100	100
15	O6	110/119 (92%)	110 (100%)	0	100	100
16	W1	112/113 (99%)	112 (100%)	0	100	100
16	W2	112/113 (99%)	112 (100%)	0	100	100
16	W3	112/113 (99%)	112 (100%)	0	100	100
16	W4	112/113 (99%)	112 (100%)	0	100	100
16	W5	112/113 (99%)	112 (100%)	0	100	100
16	W6	112/113 (99%)	112 (100%)	0	100	100
17	Y1	113/115 (98%)	113 (100%)	0	100	100
17	Y2	113/115 (98%)	113 (100%)	0	100	100
17	Y3	113/115 (98%)	113 (100%)	0	100	100
17	Y4	113/115 (98%)	113 (100%)	0	100	100
17	Y5	113/115 (98%)	113 (100%)	0	100	100
17	Y6	113/115 (98%)	113 (100%)	0	100	100
18	Z1	66/103 (64%)	64 (97%)	2 (3%)	36	57
18	Z2	66/103 (64%)	64 (97%)	2 (3%)	36	57
18	Z3	66/103 (64%)	64 (97%)	2 (3%)	36	57
18	Z4	66/103 (64%)	64 (97%)	2 (3%)	36	57
18	Z5	66/103 (64%)	64 (97%)	2 (3%)	36	57
18	Z6	66/103 (64%)	64 (97%)	2 (3%)	36	57
19	b1	75/76 (99%)	74 (99%)	1 (1%)	61	74
19	b2	75/76 (99%)	75 (100%)	0	100	100
19	b3	75/76 (99%)	75 (100%)	0	100	100
19	b4	75/76 (99%)	74 (99%)	1 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	b5	75/76 (99%)	75 (100%)	0	100	100
19	b6	75/76 (99%)	75 (100%)	0	100	100
20	e1	47/104 (45%)	44 (94%)	3 (6%)	16	37
20	e2	47/104 (45%)	44 (94%)	3 (6%)	16	37
20	e3	47/104 (45%)	45 (96%)	2 (4%)	26	47
20	e4	47/104 (45%)	43 (92%)	4 (8%)	10	29
20	e5	47/104 (45%)	43 (92%)	4 (8%)	10	29
20	e6	47/104 (45%)	45 (96%)	2 (4%)	26	47
22	A1	184/243 (76%)	182 (99%)	2 (1%)	65	76
22	A2	184/243 (76%)	181 (98%)	3 (2%)	55	70
22	A3	184/243 (76%)	182 (99%)	2 (1%)	65	76
22	A4	184/243 (76%)	182 (99%)	2 (1%)	65	76
22	A5	184/243 (76%)	182 (99%)	2 (1%)	65	76
22	A6	184/243 (76%)	182 (99%)	2 (1%)	65	76
23	B1	195/231 (84%)	194 (100%)	1 (0%)	81	83
23	B2	195/231 (84%)	195 (100%)	0	100	100
23	B3	195/231 (84%)	195 (100%)	0	100	100
23	B4	195/231 (84%)	195 (100%)	0	100	100
23	B5	195/231 (84%)	195 (100%)	0	100	100
23	B6	195/231 (84%)	195 (100%)	0	100	100
24	D1	190/202 (94%)	190 (100%)	0	100	100
24	D2	190/202 (94%)	190 (100%)	0	100	100
24	D3	190/202 (94%)	190 (100%)	0	100	100
24	D4	190/202 (94%)	190 (100%)	0	100	100
24	D5	190/202 (94%)	190 (100%)	0	100	100
24	D6	190/202 (94%)	190 (100%)	0	100	100
25	E1	224/225 (100%)	224 (100%)	0	100	100
25	E2	224/225 (100%)	224 (100%)	0	100	100
25	E3	224/225 (100%)	224 (100%)	0	100	100
25	E4	224/225 (100%)	224 (100%)	0	100	100
25	E5	224/225 (100%)	224 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	E6	224/225 (100%)	224 (100%)	0	100	100
26	F1	161/170 (95%)	157 (98%)	4 (2%)	42	62
26	F2	161/170 (95%)	157 (98%)	4 (2%)	42	62
26	F3	161/170 (95%)	157 (98%)	4 (2%)	42	62
26	F4	161/170 (95%)	157 (98%)	4 (2%)	42	62
26	F5	161/170 (95%)	157 (98%)	4 (2%)	42	62
26	F6	161/170 (95%)	157 (98%)	4 (2%)	42	62
27	H1	169/174 (97%)	169 (100%)	0	100	100
27	H2	169/174 (97%)	169 (100%)	0	100	100
27	H3	169/174 (97%)	169 (100%)	0	100	100
27	H4	169/174 (97%)	166 (98%)	3 (2%)	51	68
27	H5	169/174 (97%)	169 (100%)	0	100	100
27	H6	169/174 (97%)	169 (100%)	0	100	100
28	I1	178/180 (99%)	178 (100%)	0	100	100
28	I2	178/180 (99%)	178 (100%)	0	100	100
28	I3	178/180 (99%)	177 (99%)	1 (1%)	78	82
28	I4	178/180 (99%)	178 (100%)	0	100	100
28	I5	178/180 (99%)	178 (100%)	0	100	100
28	I6	178/180 (99%)	178 (100%)	0	100	100
29	K1	89/136 (65%)	89 (100%)	0	100	100
29	K2	89/136 (65%)	89 (100%)	0	100	100
29	K3	89/136 (65%)	89 (100%)	0	100	100
29	K4	89/136 (65%)	89 (100%)	0	100	100
29	K5	89/136 (65%)	89 (100%)	0	100	100
29	K6	89/136 (65%)	89 (100%)	0	100	100
30	L1	137/142 (96%)	134 (98%)	3 (2%)	45	64
30	L2	137/142 (96%)	134 (98%)	3 (2%)	45	64
30	L3	137/142 (96%)	134 (98%)	3 (2%)	45	64
30	L4	137/142 (96%)	134 (98%)	3 (2%)	45	64
30	L5	137/142 (96%)	134 (98%)	3 (2%)	45	64
30	L6	137/142 (96%)	134 (98%)	3 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	P1	112/130 (86%)	97 (87%)	15 (13%)	4	14
31	P2	112/130 (86%)	96 (86%)	16 (14%)	3	13
31	P3	112/130 (86%)	98 (88%)	14 (12%)	4	16
31	P4	112/130 (86%)	96 (86%)	16 (14%)	3	13
31	P5	112/130 (86%)	96 (86%)	16 (14%)	3	13
31	P6	112/130 (86%)	99 (88%)	13 (12%)	5	18
32	Q1	121/121 (100%)	119 (98%)	2 (2%)	53	69
32	Q2	121/121 (100%)	119 (98%)	2 (2%)	53	69
32	Q3	121/121 (100%)	119 (98%)	2 (2%)	53	69
32	Q4	121/121 (100%)	119 (98%)	2 (2%)	53	69
32	Q5	121/121 (100%)	119 (98%)	2 (2%)	53	69
32	Q6	121/121 (100%)	119 (98%)	2 (2%)	53	69
33	R1	120/122 (98%)	113 (94%)	7 (6%)	18	40
33	R2	120/122 (98%)	113 (94%)	7 (6%)	18	40
33	R3	120/122 (98%)	114 (95%)	6 (5%)	22	43
33	R4	120/122 (98%)	113 (94%)	7 (6%)	18	40
33	R5	120/122 (98%)	114 (95%)	6 (5%)	22	43
33	R6	120/122 (98%)	112 (93%)	8 (7%)	15	36
34	S1	124/132 (94%)	116 (94%)	8 (6%)	15	37
34	S2	124/132 (94%)	116 (94%)	8 (6%)	15	37
34	S3	124/132 (94%)	116 (94%)	8 (6%)	15	37
34	S4	124/132 (94%)	116 (94%)	8 (6%)	15	37
34	S5	124/132 (94%)	116 (94%)	8 (6%)	15	37
34	S6	124/132 (94%)	116 (94%)	8 (6%)	15	37
35	j1	24/24 (100%)	18 (75%)	6 (25%)	0	4
35	j2	24/24 (100%)	18 (75%)	6 (25%)	0	4
35	j3	24/24 (100%)	18 (75%)	6 (25%)	0	4
35	j4	24/24 (100%)	19 (79%)	5 (21%)	1	6
35	j5	24/24 (100%)	18 (75%)	6 (25%)	0	4
35	j6	24/24 (100%)	18 (75%)	6 (25%)	0	4
36	k1	152/159 (96%)	145 (95%)	7 (5%)	24	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k2	152/159 (96%)	144 (95%)	8 (5%)	20	41
36	k3	152/159 (96%)	145 (95%)	7 (5%)	24	45
36	k4	152/159 (96%)	145 (95%)	7 (5%)	24	45
36	k5	152/159 (96%)	148 (97%)	4 (3%)	40	61
36	k6	152/159 (96%)	145 (95%)	7 (5%)	24	45
37	l1	69/168 (41%)	54 (78%)	15 (22%)	1	6
37	l2	69/168 (41%)	54 (78%)	15 (22%)	1	6
37	l3	69/168 (41%)	54 (78%)	15 (22%)	1	6
37	l4	69/168 (41%)	54 (78%)	15 (22%)	1	6
37	l5	69/168 (41%)	54 (78%)	15 (22%)	1	6
37	l6	69/168 (41%)	54 (78%)	15 (22%)	1	6
All	All	26880/30402 (88%)	26220 (98%)	660 (2%)	42	62

5 of 660 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	G6	151	ASP
37	l1	140	ASP
14	N6	27	LYS
11	G6	149	LYS
34	S6	98	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 435 such sidechains are listed below:

Mol	Chain	Res	Type
14	N4	36	GLN
9	g5	178	ASN
31	P6	79	HIS
17	Y4	85	ASN
28	I4	99	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	i1	1714/1869 (91%)	684 (39%)	0
21	i2	1714/1869 (91%)	687 (40%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	i3	1714/1869 (91%)	683 (39%)	0
21	i4	1714/1869 (91%)	683 (39%)	0
21	i5	1714/1869 (91%)	682 (39%)	0
21	i6	1714/1869 (91%)	682 (39%)	0
All	All	10284/11214 (91%)	4101 (39%)	0

5 of 4101 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	i1	2	A
21	i1	3	C
21	i1	4	C
21	i1	9	U
21	i1	17	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	i2	1
21	i3	1
21	i5	1
21	i6	1
21	i4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i2	1689:C	O3'	1690:U	P	2.39
1	i3	1689:C	O3'	1690:U	P	2.27
1	i5	1689:C	O3'	1690:U	P	2.14
1	i6	1689:C	O3'	1690:U	P	2.07
1	i4	1689:C	O3'	1690:U	P	1.91

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	T1	143/145 (98%)	-0.32	6 (4%)	40	39	166, 196, 227, 240	0
1	T2	143/145 (98%)	-0.25	2 (1%)	73	62	164, 191, 211, 219	0
1	T3	143/145 (98%)	-0.20	9 (6%)	26	30	235, 251, 270, 279	0
1	T4	143/145 (98%)	-0.39	3 (2%)	63	54	302, 349, 376, 382	0
1	T5	143/145 (98%)	-0.27	4 (2%)	55	47	182, 217, 239, 247	0
1	T6	143/145 (98%)	-0.30	9 (6%)	26	30	177, 203, 220, 229	0
2	U1	104/119 (87%)	-0.61	0	100	100	155, 178, 205, 213	0
2	U2	104/119 (87%)	-0.26	2 (1%)	66	56	153, 168, 189, 197	0
2	U3	104/119 (87%)	-0.12	4 (3%)	44	42	222, 235, 250, 257	0
2	U4	104/119 (87%)	0.27	5 (4%)	35	36	241, 266, 296, 311	0
2	U5	104/119 (87%)	0.27	7 (6%)	24	28	173, 200, 224, 233	0
2	U6	104/119 (87%)	-0.19	2 (1%)	66	56	168, 180, 196, 203	0
3	V1	83/83 (100%)	-0.01	5 (6%)	27	32	134, 163, 202, 215	0
3	V2	83/83 (100%)	-0.53	1 (1%)	76	65	128, 151, 181, 191	0
3	V3	83/83 (100%)	-0.57	2 (2%)	59	51	169, 194, 239, 250	0
3	V4	83/83 (100%)	-0.33	4 (4%)	35	36	161, 194, 236, 248	0
3	V5	83/83 (100%)	-0.79	0	100	100	162, 193, 232, 245	0
3	V6	83/83 (100%)	-0.51	0	100	100	153, 179, 211, 222	0
4	X1	141/143 (98%)	0.19	12 (8%)	16	23	112, 126, 143, 151	0
4	X2	141/143 (98%)	-0.19	5 (3%)	47	43	116, 130, 146, 153	0
4	X3	141/143 (98%)	-0.21	5 (3%)	47	43	131, 151, 176, 187	0
4	X4	141/143 (98%)	-0.36	1 (0%)	84	73	129, 166, 204, 218	0
4	X5	141/143 (98%)	0.42	14 (9%)	13	20	137, 151, 168, 180	0
4	X6	141/143 (98%)	-0.03	7 (4%)	34	35	138, 152, 169, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	a1	107/115 (93%)	-0.21	3 (2%) 55 47	111, 122, 148, 157	0
5	a2	107/115 (93%)	-0.30	2 (1%) 66 56	113, 123, 149, 155	0
5	a3	107/115 (93%)	0.31	11 (10%) 12 19	144, 161, 211, 220	0
5	a4	107/115 (93%)	0.09	9 (8%) 17 24	136, 154, 197, 204	0
5	a5	107/115 (93%)	0.04	7 (6%) 25 29	135, 144, 180, 188	0
5	a6	107/115 (93%)	0.45	17 (15%) 5 12	133, 141, 171, 176	0
6	c1	64/69 (92%)	-0.23	3 (4%) 36 36	182, 206, 232, 243	0
6	c2	64/69 (92%)	-0.41	1 (1%) 70 59	191, 213, 235, 252	0
6	c3	64/69 (92%)	-0.27	3 (4%) 36 36	209, 217, 229, 241	0
6	c4	64/69 (92%)	-0.88	0 100 100	237, 252, 280, 296	0
6	c5	64/69 (92%)	0.12	6 (9%) 14 21	187, 203, 217, 222	0
6	c6	64/69 (92%)	-0.83	0 100 100	196, 216, 234, 238	0
7	d1	53/56 (94%)	-0.58	0 100 100	156, 160, 181, 189	0
7	d2	53/56 (94%)	-0.57	0 100 100	154, 156, 172, 179	0
7	d3	53/56 (94%)	0.12	2 (3%) 44 42	217, 249, 308, 321	0
7	d4	53/56 (94%)	0.02	5 (9%) 14 21	244, 285, 361, 375	0
7	d5	53/56 (94%)	0.21	7 (13%) 7 15	175, 179, 191, 197	0
7	d6	53/56 (94%)	0.02	4 (7%) 20 26	169, 171, 191, 199	0
8	f1	72/156 (46%)	-0.58	1 (1%) 73 62	179, 218, 268, 285	0
8	f2	72/156 (46%)	-0.30	5 (6%) 23 28	174, 207, 248, 257	0
8	f3	72/156 (46%)	-0.71	2 (2%) 55 47	282, 365, 385, 393	0
8	f4	72/156 (46%)	-0.93	0 100 100	317, 397, 425, 435	0
8	f5	72/156 (46%)	-0.38	7 (9%) 13 20	182, 223, 255, 263	0
8	f6	72/156 (46%)	-0.52	3 (4%) 40 39	185, 229, 268, 282	0
9	g1	313/317 (98%)	-0.72	3 (0%) 79 68	191, 230, 269, 290	0
9	g2	313/317 (98%)	-0.88	3 (0%) 79 68	175, 207, 237, 248	0
9	g3	313/317 (98%)	-0.22	20 (6%) 25 30	208, 228, 248, 255	0
9	g4	313/317 (98%)	-0.63	5 (1%) 70 59	223, 250, 276, 286	0
9	g5	313/317 (98%)	-0.45	6 (1%) 66 56	204, 232, 260, 267	0
9	g6	313/317 (98%)	-0.82	1 (0%) 90 82	191, 224, 256, 271	0
10	C1	222/293 (75%)	-0.31	6 (2%) 56 48	117, 147, 182, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
10	C2	222/293 (75%)	-0.25	8 (3%) 46 43	118, 140, 168, 176	0
10	C3	222/293 (75%)	-0.75	2 (0%) 81 70	145, 179, 221, 235	0
10	C4	222/293 (75%)	-0.55	3 (1%) 73 62	144, 186, 226, 241	0
10	C5	222/293 (75%)	-0.38	4 (1%) 67 57	144, 176, 211, 221	0
10	C6	222/293 (75%)	-0.19	12 (5%) 31 33	141, 166, 194, 203	0
11	G1	237/249 (95%)	-0.35	8 (3%) 48 43	160, 218, 269, 295	0
11	G2	237/249 (95%)	-0.59	1 (0%) 88 79	168, 228, 256, 271	0
11	G3	237/249 (95%)	-0.50	9 (3%) 44 42	166, 225, 250, 256	0
11	G4	237/249 (95%)	-0.26	11 (4%) 37 37	174, 239, 267, 288	0
11	G5	237/249 (95%)	-0.56	6 (2%) 58 49	209, 290, 320, 341	0
11	G6	237/249 (95%)	-0.42	11 (4%) 37 37	212, 290, 318, 339	0
12	J1	185/194 (95%)	-0.09	9 (4%) 35 35	129, 171, 222, 262	0
12	J2	185/194 (95%)	-0.10	9 (4%) 35 35	128, 162, 204, 236	0
12	J3	185/194 (95%)	-0.56	4 (2%) 62 53	157, 197, 258, 306	0
12	J4	185/194 (95%)	-0.48	3 (1%) 70 59	164, 213, 300, 317	0
12	J5	185/194 (95%)	-0.45	3 (1%) 70 59	158, 209, 259, 296	0
12	J6	185/194 (95%)	-0.52	4 (2%) 62 53	154, 195, 238, 271	0
13	M1	123/132 (93%)	-0.57	0 100 100	215, 248, 278, 291	0
13	M2	123/132 (93%)	-0.65	1 (0%) 82 72	201, 226, 255, 268	0
13	M3	123/132 (93%)	-1.06	0 100 100	339, 364, 377, 381	0
13	M4	123/132 (93%)	-1.01	1 (0%) 82 72	369, 398, 417, 422	0
13	M5	123/132 (93%)	-0.80	0 100 100	217, 237, 257, 269	0
13	M6	123/132 (93%)	-0.94	0 100 100	212, 236, 257, 268	0
14	N1	150/151 (99%)	-0.40	2 (1%) 75 63	130, 172, 211, 221	0
14	N2	150/151 (99%)	-0.50	5 (3%) 49 44	124, 158, 185, 191	0
14	N3	150/151 (99%)	-0.42	2 (1%) 75 63	144, 166, 206, 219	0
14	N4	150/151 (99%)	-0.55	0 100 100	138, 166, 208, 222	0
14	N5	150/151 (99%)	-0.70	2 (1%) 75 63	148, 182, 217, 230	0
14	N6	150/151 (99%)	-0.61	0 100 100	144, 178, 207, 216	0
15	O1	140/151 (92%)	0.04	7 (5%) 34 35	121, 151, 185, 197	0
15	O2	140/151 (92%)	0.22	5 (3%) 46 43	124, 154, 181, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
15	O3	140/151 (92%)	0.70	21 (15%) 5 13	150, 202, 247, 260	0
15	O4	140/151 (92%)	0.47	18 (12%) 7 15	147, 199, 237, 259	0
15	O5	140/151 (92%)	-0.37	3 (2%) 63 54	139, 177, 213, 227	0
15	O6	140/151 (92%)	-0.83	1 (0%) 84 73	138, 169, 197, 211	0
16	W1	129/130 (99%)	-0.53	0 100 100	132, 149, 167, 175	0
16	W2	129/130 (99%)	-0.37	2 (1%) 70 59	127, 141, 155, 162	0
16	W3	129/130 (99%)	-0.18	2 (1%) 70 59	146, 165, 180, 186	0
16	W4	129/130 (99%)	0.35	8 (6%) 26 31	140, 162, 178, 187	0
16	W5	129/130 (99%)	-0.72	1 (0%) 82 72	156, 178, 195, 207	0
16	W6	129/130 (99%)	-0.47	0 100 100	152, 169, 184, 194	0
17	Y1	131/133 (98%)	-0.32	9 (6%) 23 28	159, 196, 223, 237	0
17	Y2	131/133 (98%)	-0.37	10 (7%) 20 26	164, 191, 214, 225	0
17	Y3	131/133 (98%)	-0.01	19 (14%) 6 14	180, 220, 252, 267	0
17	Y4	131/133 (98%)	-0.60	4 (3%) 51 45	191, 239, 278, 300	0
17	Y5	131/133 (98%)	-0.08	8 (6%) 27 31	210, 252, 285, 302	0
17	Y6	131/133 (98%)	-0.28	2 (1%) 72 60	208, 239, 266, 280	0
18	Z1	75/125 (60%)	-0.53	0 100 100	196, 226, 255, 258	0
18	Z2	75/125 (60%)	-0.38	2 (2%) 56 48	191, 228, 254, 264	0
18	Z3	75/125 (60%)	-0.76	1 (1%) 75 63	241, 264, 288, 300	0
18	Z4	75/125 (60%)	-0.98	0 100 100	325, 359, 372, 379	0
18	Z5	75/125 (60%)	0.18	6 (8%) 18 24	205, 223, 244, 248	0
18	Z6	75/125 (60%)	0.35	7 (9%) 14 21	195, 217, 236, 244	0
19	b1	83/84 (98%)	-0.45	2 (2%) 59 51	146, 177, 216, 229	0
19	b2	83/84 (98%)	-0.69	1 (1%) 76 65	136, 156, 185, 194	0
19	b3	83/84 (98%)	-0.30	0 100 100	166, 192, 221, 235	0
19	b4	83/84 (98%)	-0.13	7 (8%) 17 24	157, 182, 219, 236	0
19	b5	83/84 (98%)	-0.21	1 (1%) 76 65	169, 191, 221, 235	0
19	b6	83/84 (98%)	-0.56	1 (1%) 76 65	160, 179, 207, 219	0
20	e1	58/133 (43%)	-0.20	3 (5%) 33 34	134, 160, 176, 179	0
20	e2	58/133 (43%)	-0.09	5 (8%) 16 22	143, 155, 166, 168	0
20	e3	58/133 (43%)	-0.03	1 (1%) 69 58	163, 198, 215, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
20	e4	58/133 (43%)	0.53	9 (15%) 5 13	199, 226, 246, 253	0
20	e5	58/133 (43%)	-0.48	5 (8%) 16 22	154, 186, 202, 204	0
20	e6	58/133 (43%)	-0.39	6 (10%) 12 19	158, 181, 191, 194	0
21	i1	1742/1869 (93%)	-0.49	36 (2%) 63 54	110, 170, 323, 428	0
21	i2	1742/1869 (93%)	-0.55	28 (1%) 70 59	113, 169, 301, 421	0
21	i3	1742/1869 (93%)	-0.66	13 (0%) 84 73	130, 200, 353, 478	0
21	i4	1742/1869 (93%)	-0.52	36 (2%) 63 54	128, 212, 362, 457	0
21	i5	1742/1869 (93%)	-0.65	20 (1%) 78 66	133, 191, 362, 430	0
21	i6	1742/1869 (93%)	-0.59	33 (1%) 66 56	132, 188, 335, 417	0
22	A1	222/295 (75%)	-0.21	7 (3%) 50 45	134, 159, 193, 212	0
22	A2	222/295 (75%)	-0.42	1 (0%) 87 77	128, 149, 178, 190	0
22	A3	222/295 (75%)	-0.38	6 (2%) 56 48	172, 206, 247, 272	0
22	A4	222/295 (75%)	-0.95	0 100 100	161, 197, 237, 252	0
22	A5	222/295 (75%)	-0.53	3 (1%) 73 62	162, 191, 229, 245	0
22	A6	222/295 (75%)	-0.12	11 (4%) 34 35	154, 177, 211, 222	0
23	B1	214/264 (81%)	-0.57	3 (1%) 73 62	127, 168, 205, 214	0
23	B2	214/264 (81%)	-0.46	11 (5%) 33 35	124, 157, 193, 204	0
23	B3	214/264 (81%)	-0.20	12 (5%) 30 33	166, 208, 248, 254	0
23	B4	214/264 (81%)	-0.11	4 (1%) 66 56	151, 197, 248, 262	0
23	B5	214/264 (81%)	-0.88	2 (0%) 81 70	150, 186, 220, 228	0
23	B6	214/264 (81%)	-0.90	1 (0%) 87 77	144, 172, 204, 210	0
24	D1	227/243 (93%)	-0.39	3 (1%) 75 63	159, 173, 203, 250	0
24	D2	227/243 (93%)	-0.31	6 (2%) 57 49	156, 173, 205, 233	0
24	D3	227/243 (93%)	0.39	22 (9%) 13 20	211, 244, 269, 286	0
24	D4	227/243 (93%)	0.37	18 (7%) 18 25	217, 260, 298, 310	0
24	D5	227/243 (93%)	-0.08	5 (2%) 62 53	180, 191, 221, 254	0
24	D6	227/243 (93%)	-0.18	9 (3%) 42 40	171, 184, 221, 250	0
25	E1	262/263 (99%)	-0.03	15 (5%) 29 33	149, 195, 227, 236	0
25	E2	262/263 (99%)	-0.01	12 (4%) 37 37	151, 188, 219, 227	0
25	E3	262/263 (99%)	-0.48	6 (2%) 61 52	154, 197, 221, 238	0
25	E4	262/263 (99%)	-0.34	6 (2%) 61 52	158, 209, 239, 261	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	E5	262/263 (99%)	-0.15	13 (4%) 34 35	190, 242, 280, 296	0
25	E6	262/263 (99%)	-0.14	8 (3%) 51 45	189, 232, 270, 280	0
26	F1	191/204 (93%)	-0.10	10 (5%) 33 34	175, 204, 228, 236	0
26	F2	191/204 (93%)	-0.49	3 (1%) 70 59	172, 203, 224, 232	0
26	F3	191/204 (93%)	-0.45	6 (3%) 51 45	209, 229, 245, 255	0
26	F4	191/204 (93%)	-0.42	4 (2%) 63 54	242, 289, 324, 338	0
26	F5	191/204 (93%)	0.13	15 (7%) 18 25	185, 201, 218, 223	0
26	F6	191/204 (93%)	-0.29	5 (2%) 57 49	180, 203, 216, 221	0
27	H1	189/194 (97%)	-0.31	2 (1%) 78 66	173, 225, 287, 300	0
27	H2	189/194 (97%)	-0.55	2 (1%) 78 66	156, 196, 245, 258	0
27	H3	189/194 (97%)	0.04	10 (5%) 32 34	172, 222, 267, 278	0
27	H4	189/194 (97%)	-0.23	6 (3%) 50 45	176, 228, 290, 303	0
27	H5	189/194 (97%)	-0.39	5 (2%) 57 49	196, 242, 297, 312	0
27	H6	189/194 (97%)	-0.51	0 100 100	183, 227, 279, 291	0
28	I1	206/208 (99%)	0.11	15 (7%) 21 26	135, 223, 315, 326	0
28	I2	206/208 (99%)	-0.25	3 (1%) 72 60	139, 220, 301, 318	0
28	I3	206/208 (99%)	-0.15	5 (2%) 59 51	136, 188, 250, 272	0
28	I4	206/208 (99%)	-0.25	2 (0%) 79 68	139, 204, 286, 313	0
28	I5	206/208 (99%)	0.45	25 (12%) 8 16	163, 250, 344, 364	0
28	I6	206/208 (99%)	-0.00	8 (3%) 43 41	166, 255, 345, 361	0
29	K1	98/165 (59%)	-0.34	1 (1%) 79 68	164, 190, 213, 221	0
29	K2	98/165 (59%)	-0.66	0 100 100	159, 181, 202, 210	0
29	K3	98/165 (59%)	-0.50	0 100 100	255, 297, 324, 332	0
29	K4	98/165 (59%)	-0.63	1 (1%) 79 68	283, 331, 365, 374	0
29	K5	98/165 (59%)	-0.62	2 (2%) 65 55	182, 201, 219, 224	0
29	K6	98/165 (59%)	-0.23	7 (7%) 22 27	174, 192, 204, 210	0
30	L1	153/158 (96%)	-0.09	5 (3%) 49 44	124, 177, 257, 284	0
30	L2	153/158 (96%)	-0.11	5 (3%) 49 44	124, 169, 239, 265	0
30	L3	153/158 (96%)	0.07	12 (7%) 19 25	138, 161, 209, 227	0
30	L4	153/158 (96%)	0.11	9 (5%) 28 32	136, 167, 234, 258	0
30	L5	153/158 (96%)	0.18	13 (8%) 16 23	152, 202, 272, 302	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
30	L6	153/158 (96%)	-0.17	8 (5%)	33	34	150, 200, 273, 303	0
31	P1	125/145 (86%)	-0.90	3 (2%)	59	51	174, 193, 217, 230	0
31	P2	125/145 (86%)	-1.04	1 (0%)	82	72	174, 193, 222, 231	0
31	P3	125/145 (86%)	-0.54	2 (1%)	70	59	265, 327, 365, 374	0
31	P4	125/145 (86%)	-0.58	6 (4%)	35	36	306, 383, 399, 409	0
31	P5	125/145 (86%)	-0.77	1 (0%)	82	72	182, 204, 223, 228	0
31	P6	125/145 (86%)	-0.76	2 (1%)	70	59	187, 212, 240, 251	0
32	Q1	146/146 (100%)	-0.04	8 (5%)	30	33	156, 200, 232, 265	0
32	Q2	146/146 (100%)	-0.24	3 (2%)	63	54	156, 182, 200, 218	0
32	Q3	146/146 (100%)	-0.53	3 (2%)	63	54	212, 223, 233, 243	0
32	Q4	146/146 (100%)	-0.13	11 (7%)	20	26	249, 279, 311, 317	0
32	Q5	146/146 (100%)	-0.22	3 (2%)	63	54	174, 209, 233, 258	0
32	Q6	146/146 (100%)	-0.35	4 (2%)	56	48	170, 194, 210, 229	0
33	R1	132/135 (97%)	-0.52	1 (0%)	82	72	127, 177, 194, 200	0
33	R2	132/135 (97%)	-0.68	2 (1%)	72	60	124, 171, 196, 202	0
33	R3	132/135 (97%)	-0.56	2 (1%)	72	60	171, 211, 240, 249	0
33	R4	132/135 (97%)	-0.59	1 (0%)	82	72	154, 216, 227, 235	0
33	R5	132/135 (97%)	-0.06	5 (3%)	44	42	153, 202, 220, 228	0
33	R6	132/135 (97%)	-0.35	2 (1%)	72	60	146, 196, 217, 224	0
34	S1	143/152 (94%)	-0.28	9 (6%)	26	30	171, 201, 229, 247	0
34	S2	143/152 (94%)	-0.69	3 (2%)	63	54	172, 210, 240, 258	0
34	S3	143/152 (94%)	-0.57	7 (4%)	35	35	268, 296, 323, 339	0
34	S4	143/152 (94%)	-0.56	2 (1%)	73	62	321, 375, 385, 388	0
34	S5	143/152 (94%)	-0.53	1 (0%)	84	73	181, 213, 234, 246	0
34	S6	143/152 (94%)	-0.36	3 (2%)	63	54	183, 215, 233, 243	0
35	j1	25/25 (100%)	-0.25	0	100	100	113, 121, 137, 140	0
35	j2	25/25 (100%)	-0.28	0	100	100	119, 127, 143, 146	0
35	j3	25/25 (100%)	-0.74	0	100	100	137, 141, 145, 149	0
35	j4	25/25 (100%)	-0.67	0	100	100	139, 147, 157, 163	0
35	j5	25/25 (100%)	-0.59	0	100	100	133, 138, 152, 153	0
35	j6	25/25 (100%)	-0.33	0	100	100	134, 141, 155, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
36	k1	181/181 (100%)	-0.83	0 100 100	146, 198, 267, 284	0
36	k2	181/181 (100%)	-0.83	1 (0%) 85 75	147, 195, 253, 268	0
36	k3	181/181 (100%)	-0.97	1 (0%) 85 75	158, 205, 256, 270	0
36	k4	181/181 (100%)	-0.97	0 100 100	168, 233, 302, 315	0
36	k5	181/181 (100%)	-0.67	0 100 100	157, 199, 256, 270	0
36	k6	181/181 (100%)	-0.88	0 100 100	155, 193, 242, 252	0
37	l1	79/198 (39%)	-0.26	1 (1%) 75 63	174, 212, 268, 279	0
37	l2	79/198 (39%)	-0.17	3 (3%) 44 42	185, 206, 233, 240	0
37	l3	79/198 (39%)	-0.33	2 (2%) 58 49	237, 298, 351, 357	0
37	l4	79/198 (39%)	-0.32	1 (1%) 75 63	237, 274, 309, 327	0
37	l5	79/198 (39%)	-0.20	4 (5%) 33 35	199, 234, 288, 302	0
37	l6	79/198 (39%)	-0.14	1 (1%) 75 63	185, 220, 273, 287	0
All	All	41688/46938 (88%)	-0.41	1186 (2%) 55 47	110, 198, 315, 478	0

The worst 5 of 1186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	A3	223	THR	13.9
8	f5	82	LYS	12.9
21	i1	752	G	11.9
22	A3	222	VAL	11.4
21	i1	794	A	11.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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
38	ZN	f1	500	1/1	1.00	0.02	80,80,80,80	0
38	ZN	f2	500	1/1	1.00	0.06	80,80,80,80	0
38	ZN	f3	500	1/1	1.00	0.04	80,80,80,80	0
38	ZN	f4	500	1/1	1.00	0.01	80,80,80,80	0
38	ZN	f5	500	1/1	1.00	0.01	80,80,80,80	0
38	ZN	f6	500	1/1	1.00	0.03	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.