wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2024 – 02:54 pm BST

PDB ID	:	5DGF
Title	:	Complex of yeast 80S ribosome with hypusine-containing/non-modified eIF5A and/or a peptidyl-tRNA analog
Authors	:	Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.; Dever, T.E.; Yusupov, M.
Deposited on	:	2015-08-27
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

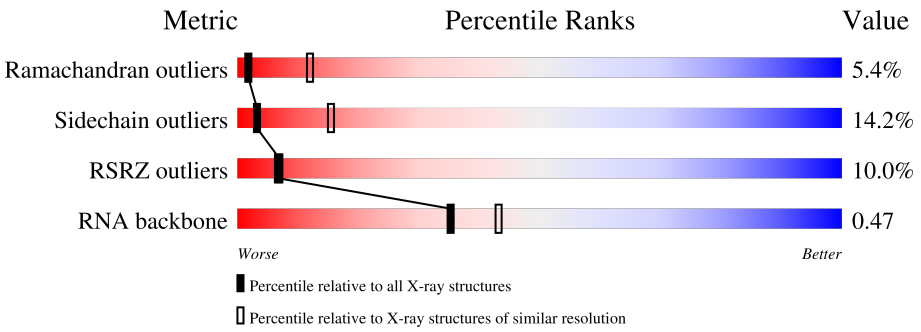
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	2	1800	5%, 72%, 26%, ••
1	6	1800	3%, 74%, 25%, •
2	S0	251	20%, 65%, 16%, •, 18%
2	s0	251	20%, 67%, 15%, 18%
3	S1	254	30%, 68%, 16%, •, 16%
3	s1	254	17%, 69%, 15%, 15%

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Mol	Chain	Length	Quality of chain
4	S2	253	12% 73% 12% 14%
4	s2	253	4% 66% 20% 14%
5	S3	239	10% 80% 13% 7%
5	s3	239	30% 81% 13% 7%
6	S4	260	25% 86% 13%
6	s4	260	23% 83% 14%
7	S5	224	17% 81% 10% 8%
7	s5	224	9% 74% 18% 8%
8	S6	236	17% 83% 13%
8	s6	236	9% 78% 14% 8%
9	S7	189	16% 77% 19%
9	s7	189	12% 85% 12%
10	S8	200	10% 82% 12% 6%
10	s8	200	14% 81% 13% 6%
11	S9	196	36% 77% 16% 6%
11	s9	196	22% 77% 17% 6%
12	C0	96	54% 91% 9%
12	c0	96	42% 82% 17%
13	C1	155	14% 87% 12%
13	c1	155	6% 80% 14% 6%
14	C2	142	10% 71% 15% 13%
14	c2	142	11% 76% 10% 13%
15	C3	150	11% 87% 12%
15	c3	150	3% 83% 16%
16	C4	136	26% 77% 14% 7%

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Mol	Chain	Length	Quality of chain
16	c4	136	32% 71% 21% 6%
17	C5	141	15% 74% 10% 12%
17	c5	141	11% 80% 13%
18	C6	142	32% 85% 13%
18	c6	142	18% 82% 18%
19	C7	136	24% 71% 15% 12%
19	c7	136	7% 74% 11% 14%
20	C8	145	17% 78% 21%
20	c8	145	16% 83% 15%
21	C9	143	26% 84% 15%
21	c9	143	36% 85% 15%
22	D0	120	17% 76% 13% 11%
22	d0	120	48% 78% 14% 8%
23	D1	87	18% 80% 20%
23	d1	87	10% 85% 15%
24	D2	129	9% 86% 12%
24	d2	129	8% 84% 15%
25	D3	144	12% 83% 17%
25	d3	144	5% 90% 10%
26	D4	134	25% 87% 13%
26	d4	134	7% 84% 15%
27	D5	107	22% 47% 18% 35%
27	d5	107	18% 55% 8% 36%
28	D6	97	45% 72% 27%
28	d6	97	27% 79% 19%

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Mol	Chain	Length	Quality of chain
29	D7	81	21% 86% 14%
29	d7	81	16% 85% 15%
30	D8	66	20% 80% 15% 5%
30	d8	66	15% 77% 17% 5%
31	D9	55	22% 78% 15%
31	d9	55	47% 75% 22%
32	E0	62	34% 87% 10%
32	e0	62	18% 66% 32%
33	E1	76	12% 63% 24% 7% 7%
33	e1	76	26% 67% 29%
34	SR	318	32% 85% 14%
34	sR	318	33% 91% 9%
35	SM	273	8% 48% 10% 42%
35	sM	273	8% 33% 62%
36	1	3396	% 71% 20% 7%
36	5	3396	% 72% 21% 7%
37	3	121	91% 9%
37	7	121	88% 11%
38	4	158	% 79% 20%
38	8	158	% 78% 21%
39	L2	253	4% 85% 15%
39	l2	253	4% 82% 17%
40	L3	386	5% 82% 18%
40	l3	386	2% 82% 16%
41	L4	361	84% 16%

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Mol	Chain	Length	Quality of chain
41	l4	361	%, 84%, 15%
42	L5	296	23%, 83%, 16%
42	l5	296	7%, 83%, 15%
43	L6	175	6%, 78%, 11%, 11%
43	l6	175	3%, 77%, 13%, 10%
44	L7	243	%, 78%, 12%, 9%
44	l7	243	80%, 11%, 8%
45	L8	255	16%, 79%, 12%, 9%
45	l8	255	16%, 76%, 15%, 9%
46	L9	191	5%, 74%, 26%
46	l9	191	%, 83%, 16%
47	M0	220	18%, 77%, 18%
47	m0	220	13%, 78%, 18%
48	M1	173	14%, 75%, 22%
48	m1	173	3%, 78%, 19%
49	M3	198	4%, 83%, 15%
49	m3	198	15%, 78%, 19%
50	M4	137	%, 85%, 13%
50	m4	137	%, 88%, 12%
51	M5	203	%, 86%, 13%
51	m5	203	5%, 88%, 12%
52	M6	198	2%, 83%, 15%
52	m6	198	%, 87%, 12%
53	M7	183	13%, 86%, 14%
53	m7	183	73%, 11%, 15%

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Mol	Chain	Length	Quality of chain
54	M8	185	2%, 86%, 14%
54	m8	185	83%, 16%
55	M9	188	10%, 88%, 12%
55	m9	188	6%, 88%, 12%
56	N0	172	2%, 84%, 16%
56	n0	172	%, 85%, 15%
57	N1	159	3%, 80%, 18%
57	n1	159	7%, 84%, 16%
58	N2	120	21%, 73%, 9%, 17%
58	n2	120	18%, 69%, 12%, 18%
59	N3	136	8%, 87%, 12%
59	n3	136	2%, 85%, 14%
60	N4	155	19%, 54%, 9%, 37%
60	n4	155	12%, 79%, 8%, 13%
61	N5	141	10%, 69%, 16%, 14%
61	n5	141	%, 70%, 13%, 15%
62	N6	126	15%, 84%, 14%
62	n6	126	3%, 84%, 15%
63	N7	135	36%, 84%, 13%
63	n7	135	32%, 84%, 14%
64	N8	148	%, 82%, 18%
64	n8	148	2%, 82%, 17%
65	N9	58	7%, 84%, 16%
65	n9	58	9%, 83%, 14%
66	O0	104	9%, 81%, 12%, 7%

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Mol	Chain	Length	Quality of chain
66	o0	104	2%, 83%, 13%
67	O1	112	12%, 83%, 13%
67	o1	112	4%, 77%, 19%
68	O2	129	2%, 84%, 15%
68	o2	129	5%, 80%, 17%
69	O3	106	%, 85%, 14%
69	o3	106	85%, 15%
70	O4	120	6%, 82%, 12%, 7%
70	o4	120	7%, 82%, 11%, 7%
71	O5	119	5%, 84%, 16%
71	o5	119	7%, 87%, 13%
72	O6	99	5%, 80%, 15%, 5%
72	o6	99	4%, 72%, 25%
73	O7	87	%, 86%, 13%
73	o7	87	2%, 91%, 8%
74	O8	77	10%, 82%, 18%
74	o8	77	32%, 81%, 19%
75	O9	50	2%, 82%, 16%
75	o9	50	2%, 94%, 6%
76	Q0	52	13%, 81%, 17%
76	q0	52	2%, 83%, 17%
77	Q1	25	24%, 88%, 12%
77	q1	25	8%, 72%, 28%
78	Q2	105	2%, 80%, 19%
78	q2	105	%, 77%, 22%

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Mol	Chain	Length	Quality of chain
79	Q3	91	2%, 84%, 14%
79	q3	91	3%, 88%, 12%
80	m2	165	91%, 9%
81	p0	311	10%, 41%, 5%, 54%
82	p1	47	100%
82	p2	47	98%
83	f	157	59%, 73%, 19%, 6%

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 404292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	2	1781	37970	16975	6720	12493	1782	0	1	0
1	6	1795	38260	17105	6763	12596	1796	0	1	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S0	206	1577	1014	278	283	2	0	0	0
2	s0	206	1583	1017	281	283	2	0	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	S1	214	1709	1084	310	311	4	0	0	0
3	s1	216	1722	1091	312	315	4	0	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	S2	217	1635	1047	289	297	2	0	0	0
4	s2	217	1635	1047	289	297	2	0	0	0

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	S3	223	1734	1101	313	314	6	0	0	0
5	s3	223	1734	1101	313	314	6	0	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	S4	260	2068	1316	389	360	3	0	0	0
6	s4	260	2068	1316	389	360	3	0	0	0

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	S5	206	1609	1007	300	299	3	0	0	0
7	s5	206	1609	1007	300	299	3	0	0	0

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	S6	226	1799	1129	346	321	3	0	0	0
8	s6	218	1755	1102	337	313	3	0	0	0

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	S7	184	1481	951	265	265	0	0	0
9	s7	186	1491	957	267	267	0	0	0

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	S8	188	1489	925	298	264	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	s8	188	1489	925	298	264	2	0	0	0

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	S9	185	1494	943	289	261	1	0	0	0
11	s9	185	1494	943	289	261	1	0	0	0

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	C0	96	773	500	126	145	2	0	0	0
12	c0	96	762	491	125	144	2	0	0	0

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	C1	155	1214	775	230	206	3	0	0	0
13	c1	146	1168	747	221	197	3	0	0	0

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	C2	124	892	562	156	172	2	0	0	0
14	c2	124	892	562	156	172	2	0	0	0

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	C3	150	1192	759	224	207	2	0	0	0
15	c3	150	1192	759	224	207	2	0	0	0

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	C4	127	891	545	182	163	1	0	0	0
16	c4	128	949	582	188	176	3	0	0	0

- Molecule 17 is a protein called 40S ribosomal protein S15 (uS19).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	C5	124	977	622	182	166	7	0	0	0
17	c5	135	1039	658	196	178	7	0	0	0

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	C6	141	1105	708	203	194	0	0	0
18	c6	142	1111	711	204	196	0	0	0

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	C7	120	926	577	177	170	2	0	0	0
19	c7	117	906	563	174	167	2	0	0	0

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	C8	145	1192	743	237	210	2	0	0	0
20	c8	145	1192	743	237	210	2	0	0	0

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	C9	143	1112	694	208	208	2	0	0	0
21	c9	143	1112	694	208	208	2	0	0	0

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	D0	107	855	539	156	159	1	0	0	0
22	d0	110	882	554	161	166	1	0	0	0

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	D1	87	684	420	125	137	2	0	0	0
23	d1	87	684	420	125	137	2	0	0	0

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	D2	129	1021	650	188	180	3	0	0	0
24	d2	129	1021	650	188	180	3	0	0	0

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	D3	144	1121	708	220	191	2	0	0	0
25	d3	144	1121	708	220	191	2	0	0	0

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
26	D4	134	1073	676	208	189	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
26	d4	134	1073	676	208	189	0	0	0

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
27	D5	70	563	360	104	99	0	0	0
27	d5	69	558	357	103	98	0	0	0

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	D6	97	769	475	160	129	5	0	0	0
28	d6	97	769	475	160	129	5	0	0	0

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	D7	81	610	382	110	113	5	0	0	0
29	d7	81	610	382	110	113	5	0	0	0

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	D8	63	497	306	99	91	1	0	0	0
30	d8	63	497	306	99	91	1	0	0	0

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	D9	53	442	274	92	72	4	0	0	0
31	d9	53	442	274	92	72	4	0	0	0

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	E0	60	475	299	98	77	1	0	0	0
32	e0	62	491	309	101	80	1	0	0	0

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	E1	71	566	362	106	94	4	0	0	0
33	e1	76	608	388	117	99	4	0	0	0

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	SR	318	2437	1541	418	470	8	0	0	0
34	sR	318	2442	1544	418	472	8	0	0	0

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	159	1105	653	221	231	0	0	0
35	sM	104	680	403	140	137	0	0	0

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	1	3149	67355	30086	12142	21978	3149	0	0	0
36	5	3169	67780	30276	12216	22120	3168	0	0	0

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
37	3	121	2579	1152	461	845	121	0	0	0
37	7	121	2579	1152	461	845	121	0	0	0

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
38	4	158	3353	1500	586	1109	158	0	0	0
38	8	158	3353	1500	586	1109	158	0	0	0

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	L2	252	1914	1191	388	334	1	0	0	0
39	l2	252	1912	1190	388	333	1	0	0	0

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L3	386	3075	1950	584	533	8	0	0	0
40	l3	386	3075	1950	584	533	8	0	0	0

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	L4	361	2748	1729	522	494	3	0	0	0
41	l4	361	2748	1729	522	494	3	0	0	0

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	L5	296	2375	1501	414	458	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	l5	294	2359	1489	412	456	2	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	L6	156	1239	800	222	216	1	0	0	0
			Total	C	N	O	S			
43	l6	157	1248	806	224	217	1	0	0	0

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	L7	222	1784	1151	324	308	1	0	0	0
			Total	C	N	O	S			
44	l7	223	1791	1155	325	310	1	0	0	0

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L8	233	1804	1151	323	327	3	0	0	0
			Total	C	N	O	S			
45	l8	231	1764	1131	316	314	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L8	119	ALA	GLY	conflict	UNP P17076
l8	119	ALA	GLY	conflict	UNP P17076

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	L9	191	1518	963	274	277	4	0	0	0
			Total	C	N	O	S			
46	l9	191	1518	963	274	277	4	0	0	0

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	M0	211	1705	1083	322	294	6	0	0	0
47	m0	213	1722	1094	325	297	6	0	0	0

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	M1	169	1353	847	253	249	4	0	0	0
48	m1	169	1353	847	253	249	4	0	0	0

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	M3	193	1543	962	315	266	0	0	0
49	m3	194	1548	965	316	267	0	0	0

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	M4	136	1053	675	199	177	2	0	0	0
50	m4	137	1059	678	200	179	2	0	0	0

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	M5	203	1720	1077	361	281	1	0	0	0
51	m5	203	1720	1077	361	281	1	0	0	0

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	M6	197	1555	1003	289	262	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	m6	197	1555	1003	289	262	1	0	0	0

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
53	M7	183	1420	882	281	257	0	0	0
53	m7	155	1227	764	238	225	0	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	M8	185	1441	908	290	241	2	0	0	0
54	m8	185	1441	908	290	241	2	0	0	0

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
55	M9	188	1521	935	326	260	0	0	0
55	m9	188	1521	935	326	260	0	0	0

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	N0	172	1445	930	267	244	4	0	0	0
56	n0	172	1445	930	267	244	4	0	0	0

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	N1	159	1276	805	246	221	4	0	0	0
57	n1	159	1276	805	246	221	4	0	0	0

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
58	N2	100	796	516	131	149	0	0	0
58	n2	98	778	505	127	146	0	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	N3	136	1003	628	189	179	7	0	0	0
59	n3	136	1003	628	189	179	7	0	0	0

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
60	N4	98	699	443	137	118	1	0	0	0
60	n4	135	1038	651	206	180	1	0	0	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
61	N5	121	964	620	169	173	2	0	0	0
61	n5	120	959	617	168	172	2	0	0	0

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
62	N6	126	993	625	192	176	0	0	0
62	n6	126	993	625	192	176	0	0	0

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
63	N7	135	1092	710	202	180	0	0	0
63	n7	135	1092	710	202	180	0	0	0

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
64	N8	148	1173	749	231	190	3	0	0	0
64	n8	148	1173	749	231	190	3	0	0	0

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
65	N9	58	462	289	100	73	0	0	0
65	n9	58	462	289	100	73	0	0	0

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
66	O0	97	743	479	124	139	1	0	0	0
66	o0	100	767	492	128	146	1	0	0	0

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
67	O1	109	876	556	167	152	1	0	0	0
67	o1	109	883	559	167	156	1	0	0	0

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
68	O2	127	1020	647	205	167	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
68	o2	127	1020	647	205	167	1	0	0	0

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
69	O3	106	850	540	165	144	1	0	0	0
			Total	C	N	O	S			
69	o3	106	850	540	165	144	1	0	0	0

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
70	O4	112	880	545	179	152	4	0	0	0
			Total	C	N	O	S			
70	o4	112	880	545	179	152	4	0	0	0

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
71	O5	119	969	615	186	167	1	0	0	0
			Total	C	N	O	S			
71	o5	119	965	612	185	167	1	0	0	0

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
72	O6	99	771	481	156	132	2	0	0	0
			Total	C	N	O	S			
72	o6	99	770	481	156	131	2	0	0	0

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
73	O7	87	681	414	148	114	5	0	0	0
			Total	C	N	O	S			
73	o7	87	681	414	148	114	5	0	0	0

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
74	O8	77	612	391	115	106	0	0	0
74	o8	77	608	388	114	106	0	0	0

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
75	O9	50	436	272	97	65	2	0	0	0
75	o9	50	436	272	97	65	2	0	0	0

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
76	Q0	52	417	259	86	67	5	0	0	0
76	q0	52	417	259	86	67	5	0	0	0

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
77	Q1	25	233	142	63	27	1	0	0	0
77	q1	25	233	142	63	27	1	0	0	0

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
78	Q2	105	847	534	170	138	5	0	0	0
78	q2	105	847	534	170	138	5	0	0	0

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
79	Q3	91	694	429	138	121	6	0	0	0
79	q3	91	694	429	138	121	6	0	0	0

- Molecule 80 is a protein called 60S ribosomal protein L12-A (uL11).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
80	m2	150	750	450	150	150	0	0	0

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	p0	143	1077	687	192	195	3	0	0	0

- Molecule 82 is a protein called 60S ribosomal protein P1 alpha/P2 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
82	p1	47	235	141	47	47	0	0	0
82	p2	46	230	138	46	46	0	0	0

- Molecule 83 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
83	f	148	1116	692	188	227	9	0	0	0

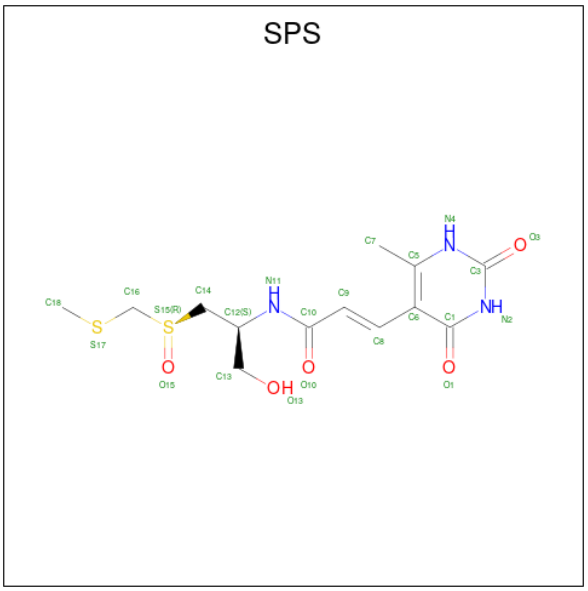
- Molecule 84 is an unknown type called CH-CH-8AN-PRO-PRO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
84	B	5	76	38	14	21	3	0	0
84	C	5	73	38	14	19	2	0	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
85	D6	1	1	1	0	0
85	D7	1	1	1	0	0
85	D9	1	1	1	0	0
85	E1	1	1	1	0	0
85	O7	1	1	1	0	0
85	Q0	1	1	1	0	0
85	Q2	1	1	1	0	0
85	Q3	1	1	1	0	0
85	d6	1	1	1	0	0
85	d7	1	1	1	0	0
85	d9	1	1	1	0	0
85	e1	1	1	1	0	0
85	o7	1	1	1	0	0
85	q0	1	1	1	0	0
85	q2	1	1	1	0	0
85	q3	1	1	1	0	0

- Molecule 86 is SPARSOMYCIN (three-letter code: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).

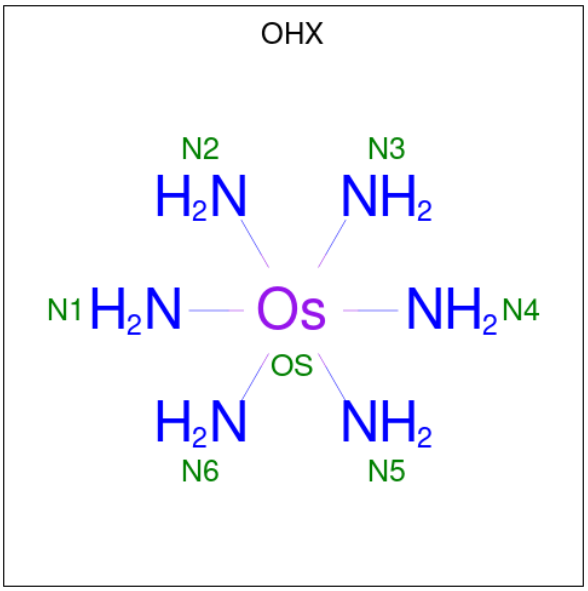


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
86	1	1	23	13	3	5	2	0	0
			Total	C	N	O	S		
86	B	1	23	13	3	5	2	0	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
87	1	3	3	3	0	0
			Total	Mg		
87	5	5	5	5	0	0
			Total	Mg		
87	f	2	2	2	0	0
			Total	Mg		
87	B	1	1	1	0	0
			Total	Mg		
87	C	1	1	1	0	0

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	1	1	Total N Os 7 6 1	0	0
88	1	1	Total N Os 7 6 1	0	0
88	5	1	Total N Os 7 6 1	0	0

- Molecule 89 is water.

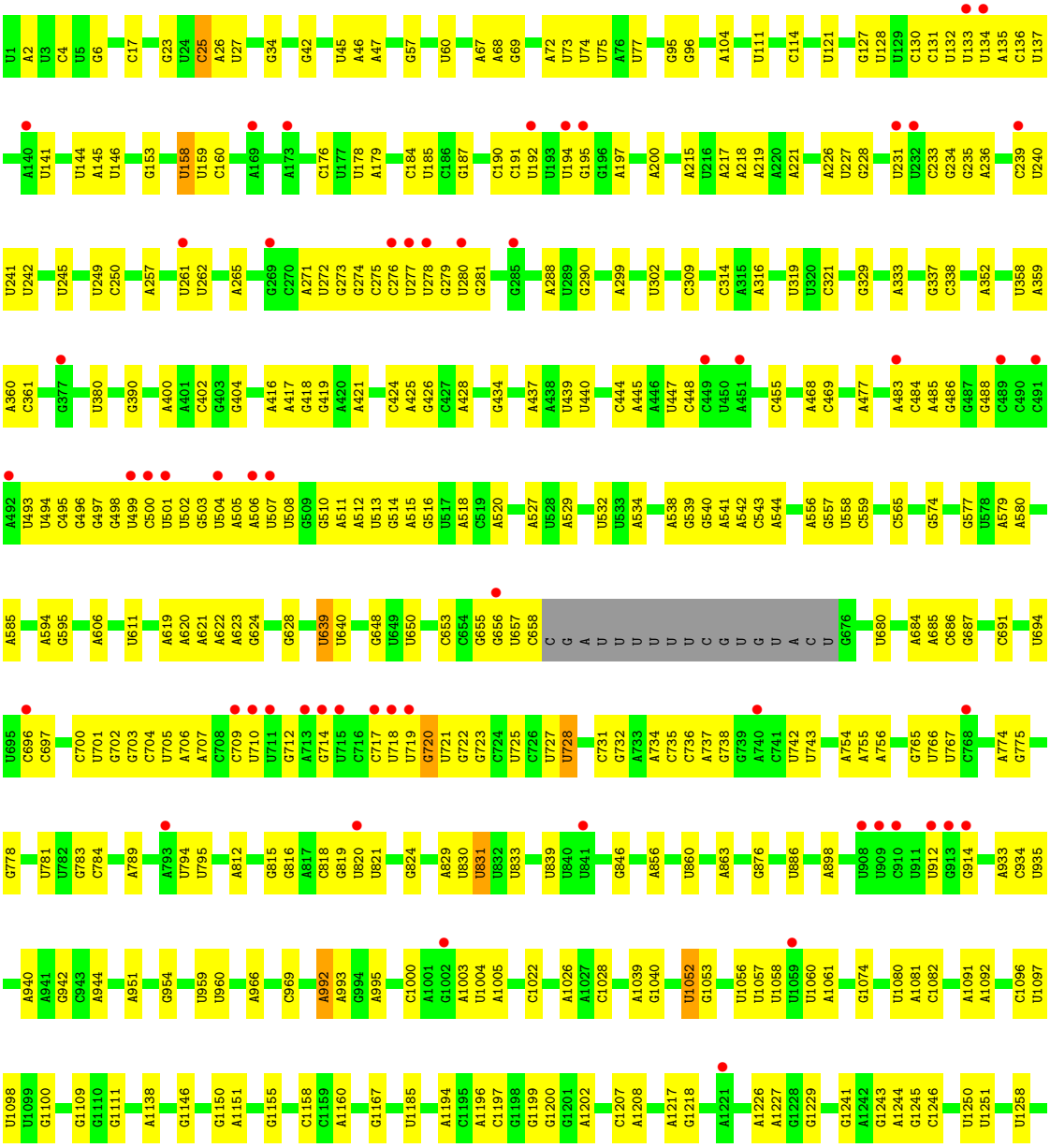
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	5	2	Total O 2 2	0	0
89	f	10	Total O 10 10	0	0

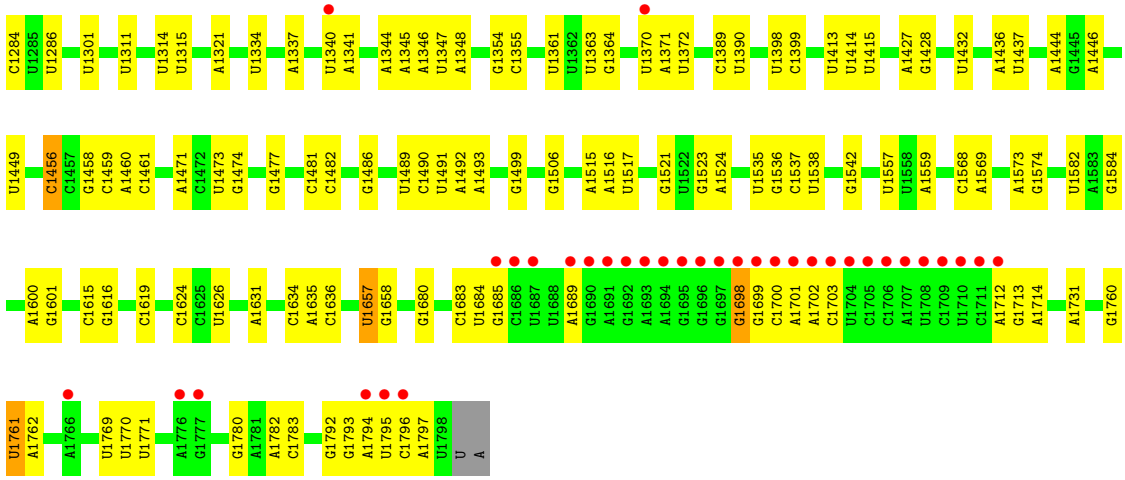
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 18S ribosomal RNA

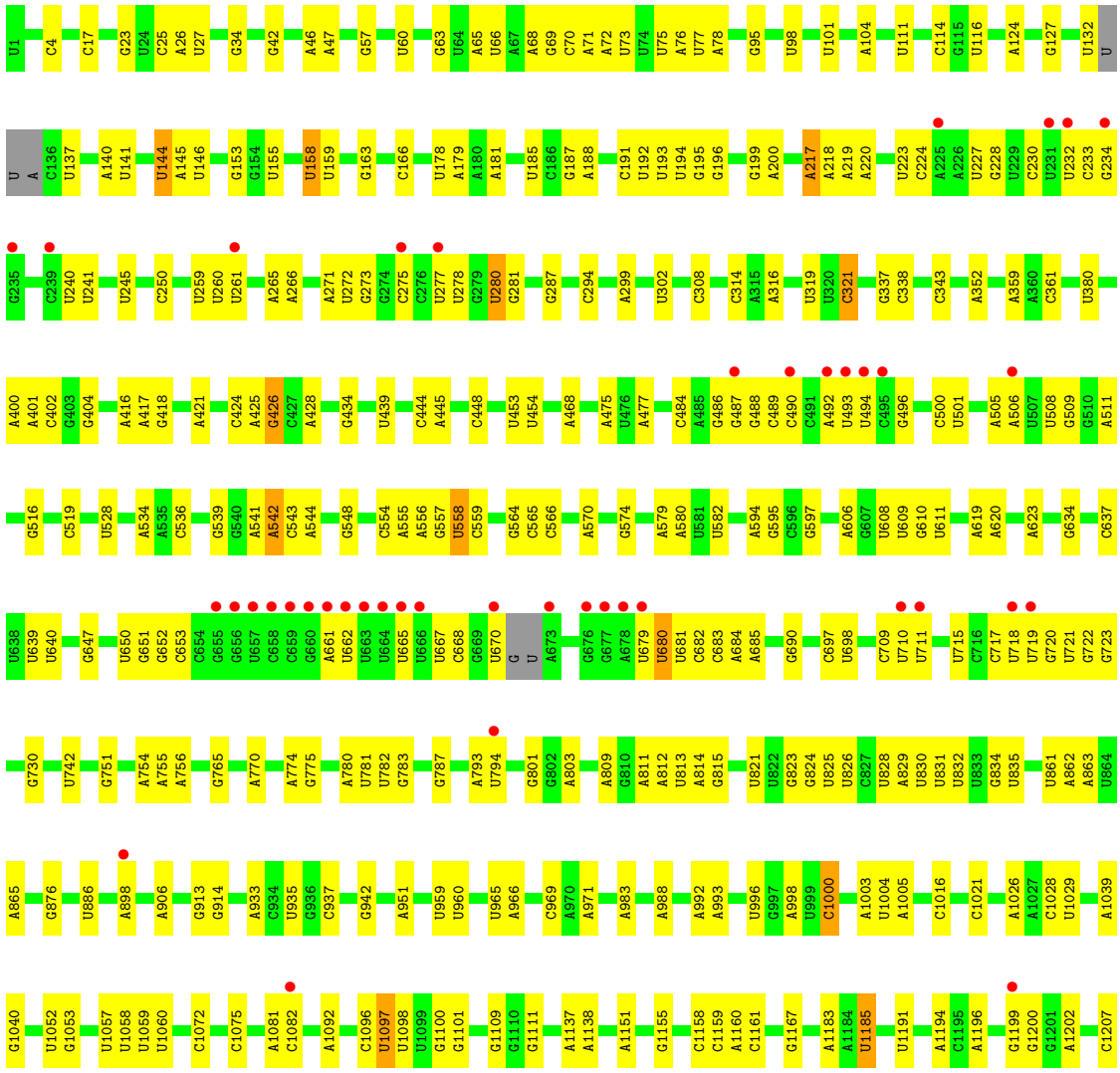
Chain 2:

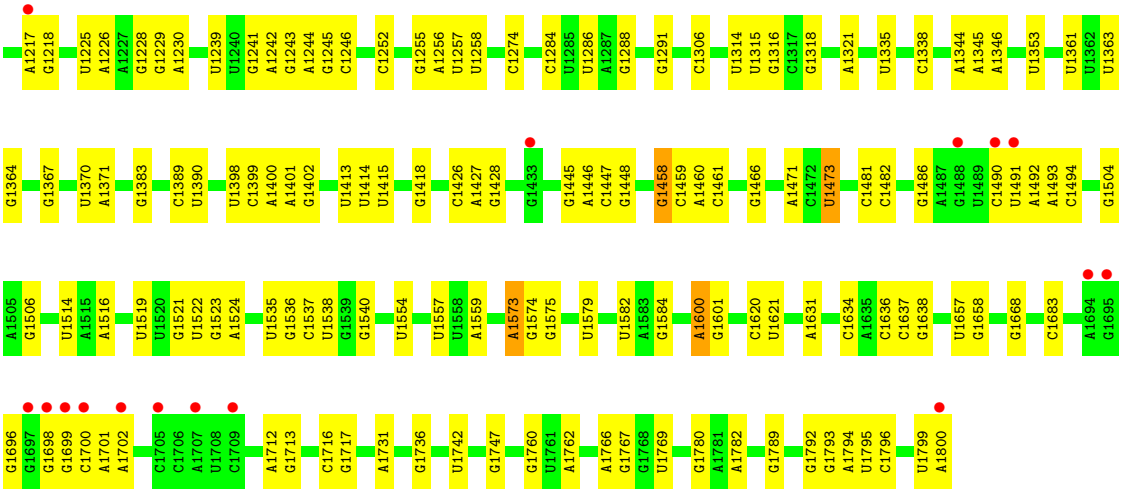




- Molecule 1: 18S ribosomal RNA

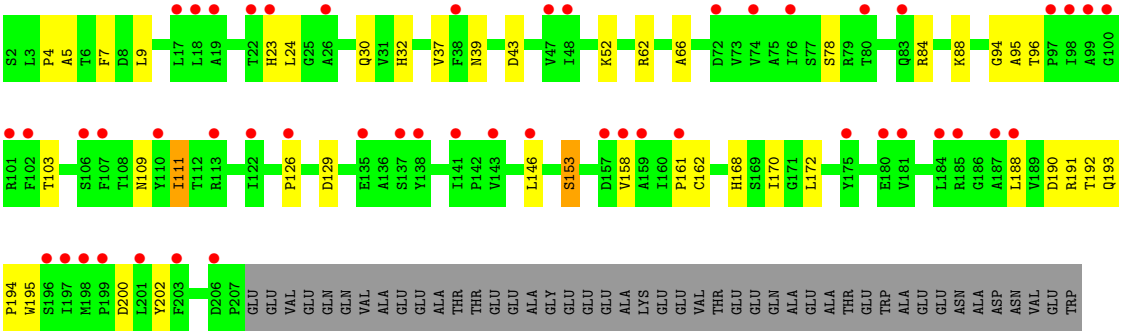
Chain 6:





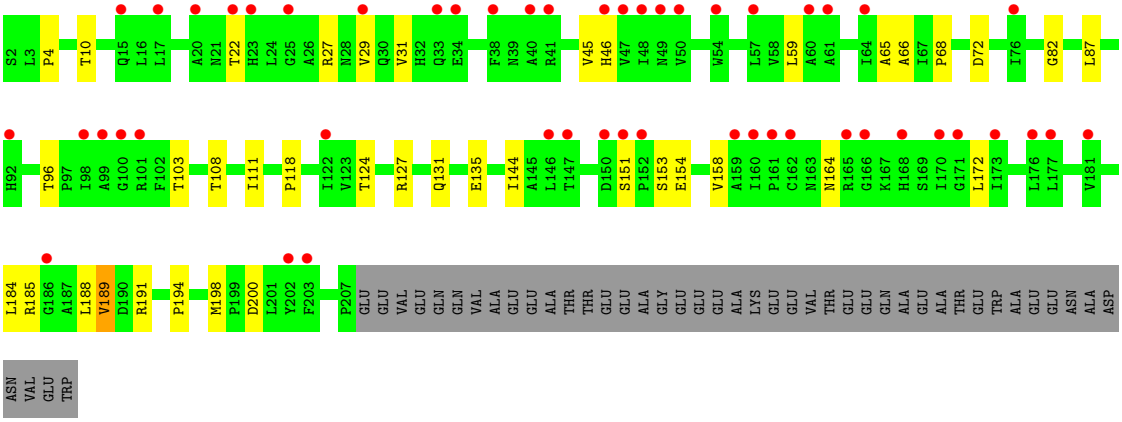
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



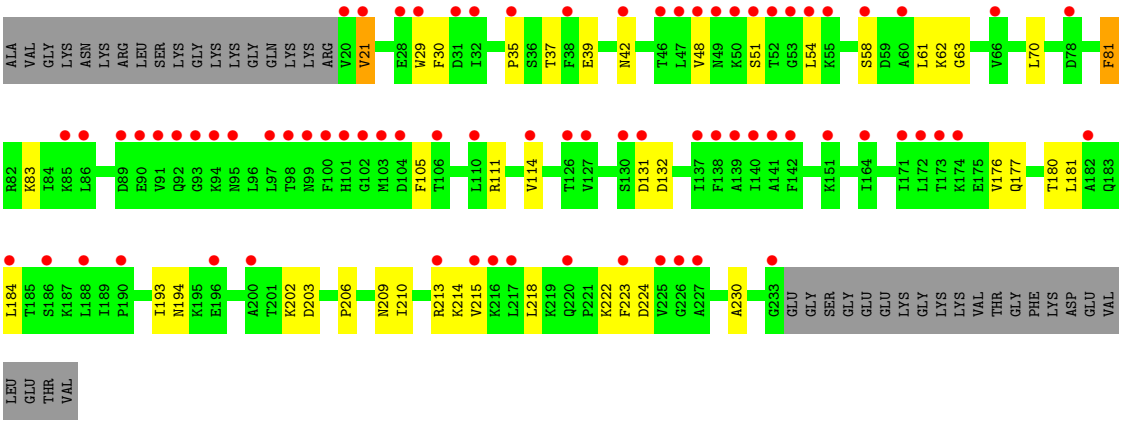
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



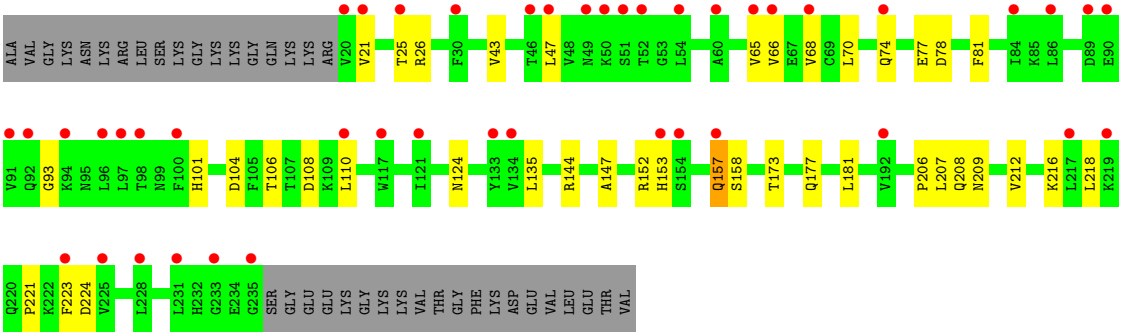
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



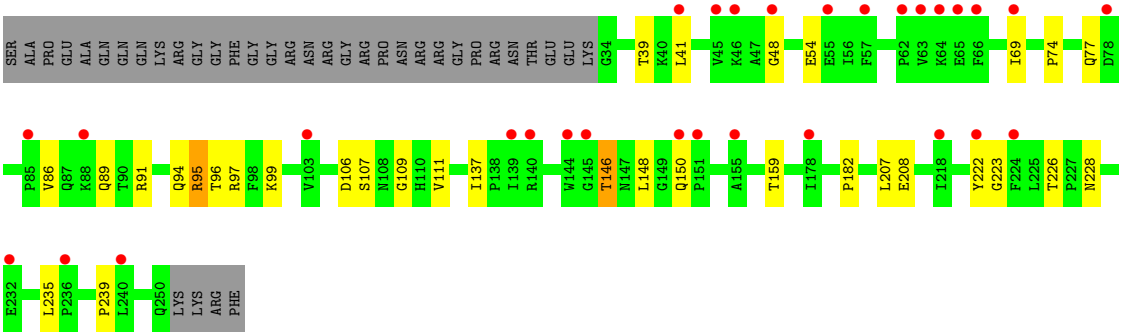
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



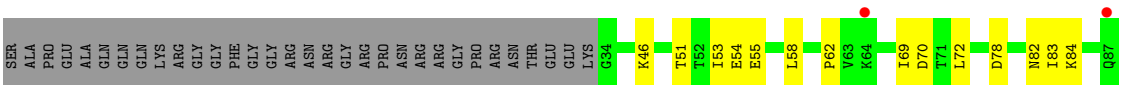
• Molecule 4: 40S ribosomal protein S2

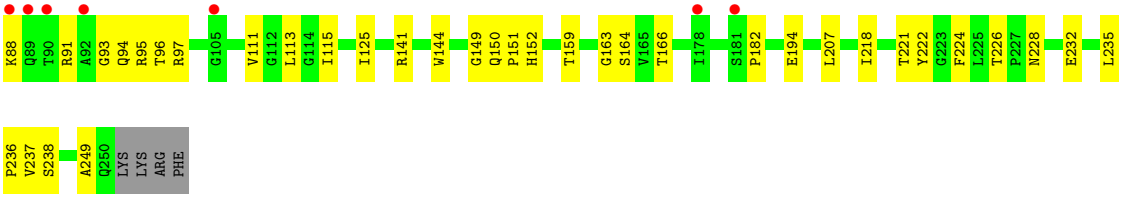
Chain S2:



• Molecule 4: 40S ribosomal protein S2

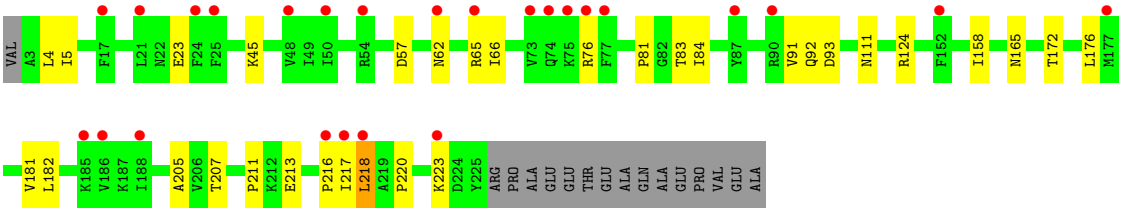
Chain s2:





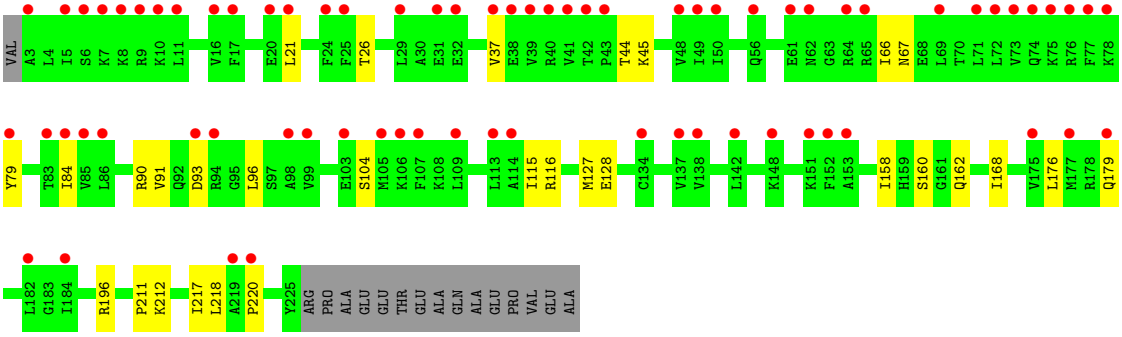
• Molecule 5: 40S ribosomal protein S3

Chain S3:



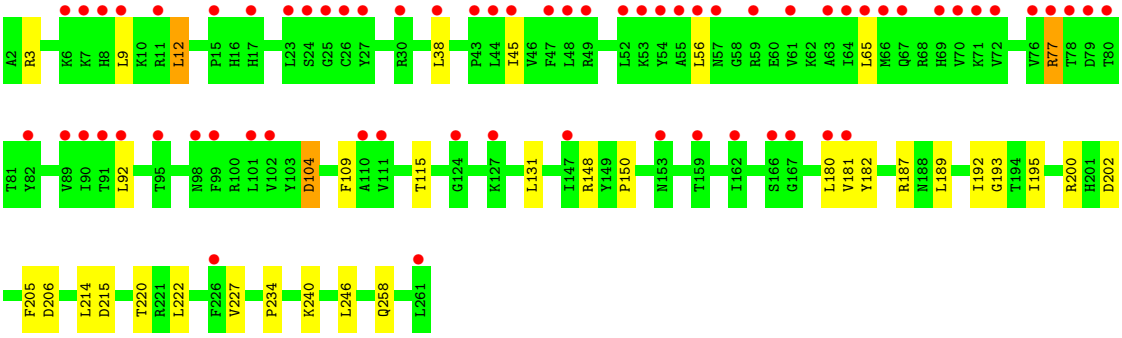
• Molecule 5: 40S ribosomal protein S3

Chain s3:



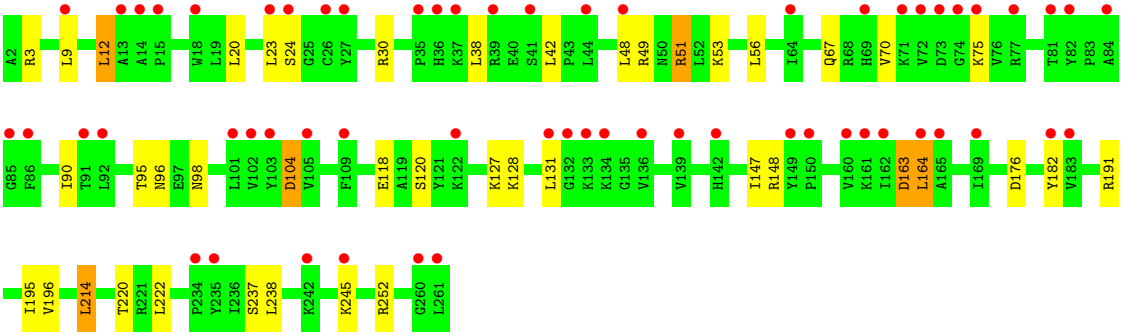
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



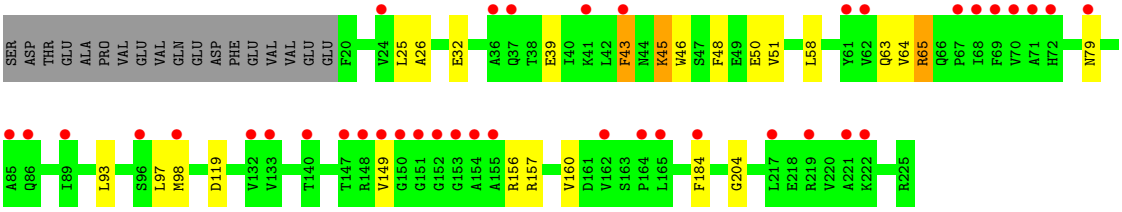
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



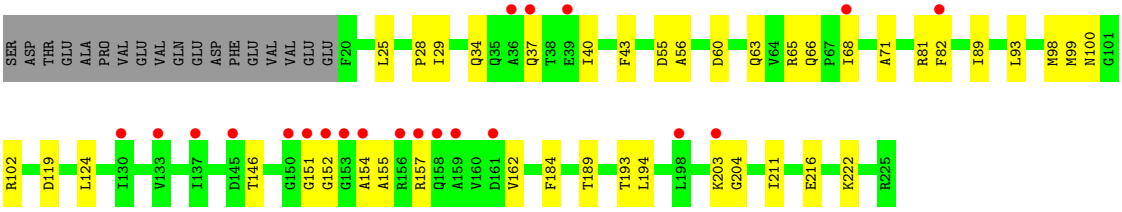
- Molecule 7: 40S ribosomal protein S5

Chain S5:



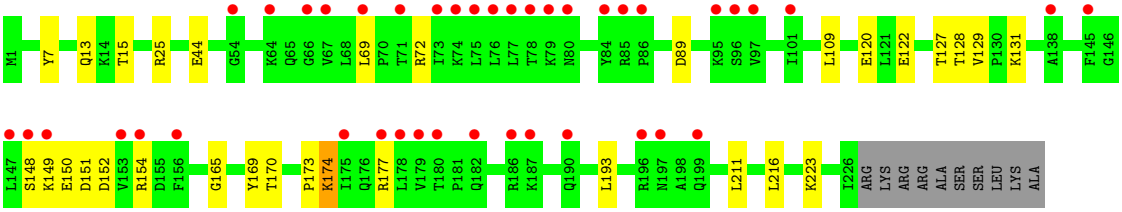
- Molecule 7: 40S ribosomal protein S5

Chain s5:



- Molecule 8: 40S ribosomal protein S6-A

Chain S6:



- Molecule 8: 40S ribosomal protein S6-A

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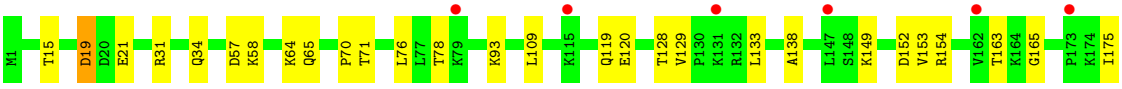
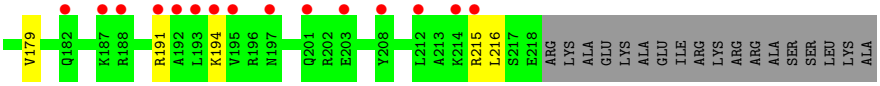
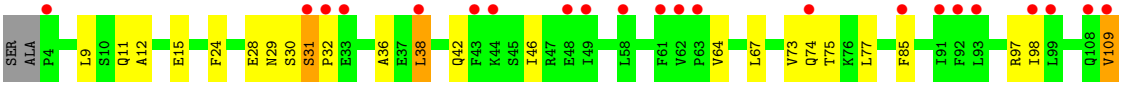
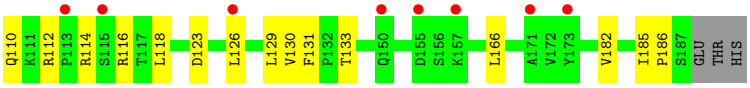




• Molecule 9: 40S ribosomal protein S7-A

Chain S7:





• Molecule 9: 40S ribosomal protein S7-A

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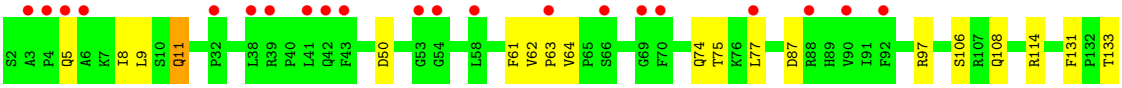
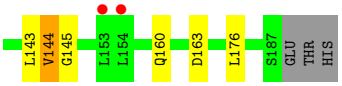
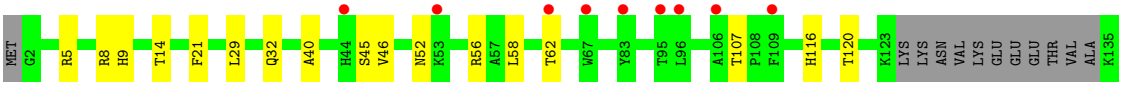
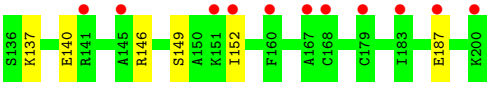




• Molecule 10: 40S ribosomal protein S8-A

Chain S8:





• Molecule 10: 40S ribosomal protein S8-A

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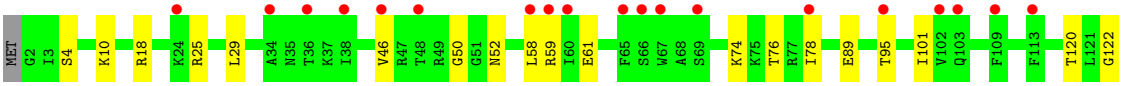
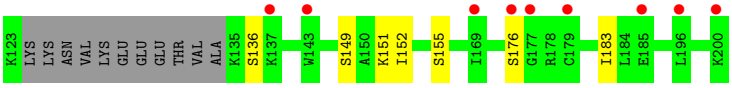
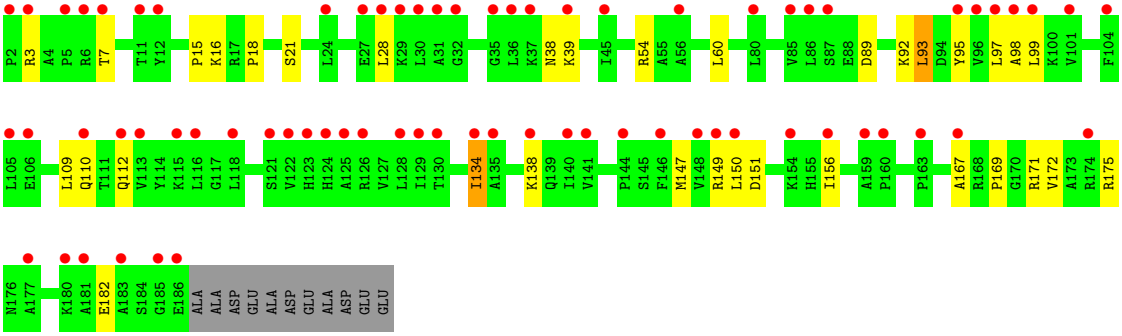




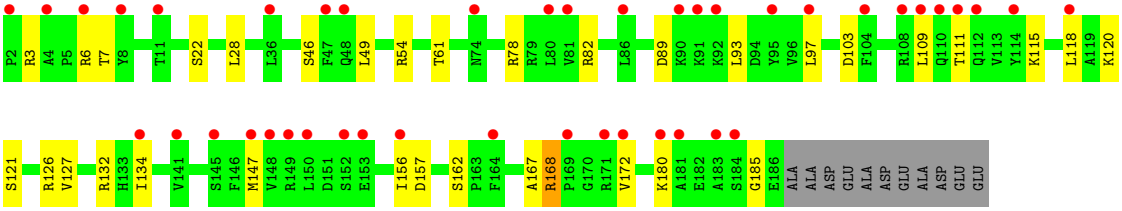
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



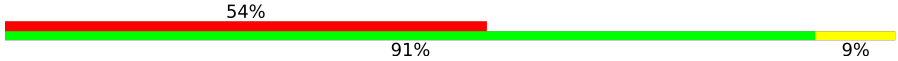
- Molecule 11: 40S ribosomal protein S9-A

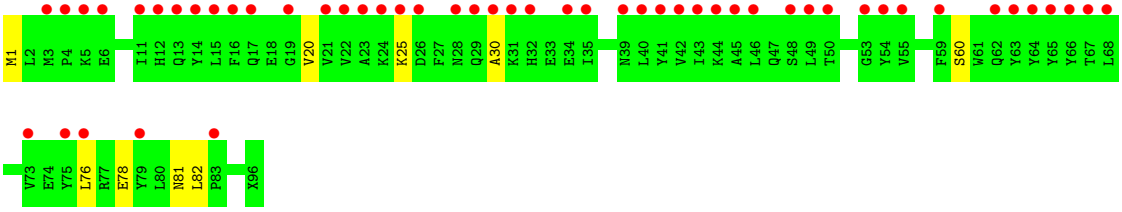
Chain s9:



- Molecule 12: 40S ribosomal protein S10-A

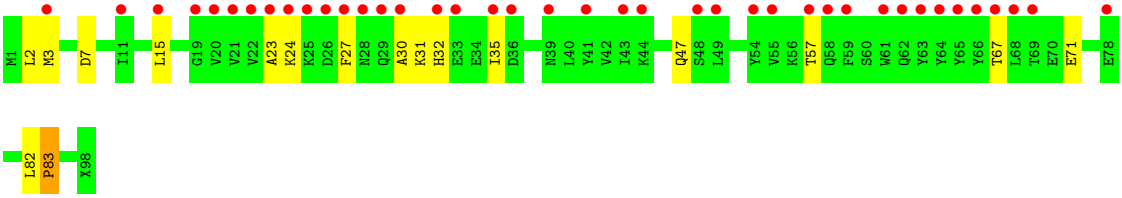
Chain C0:





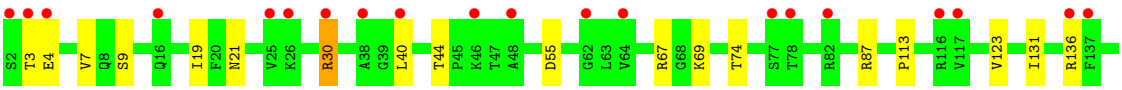
- Molecule 12: 40S ribosomal protein S10-A

Chain c0:



- Molecule 13: 40S ribosomal protein S11-A

Chain C1:

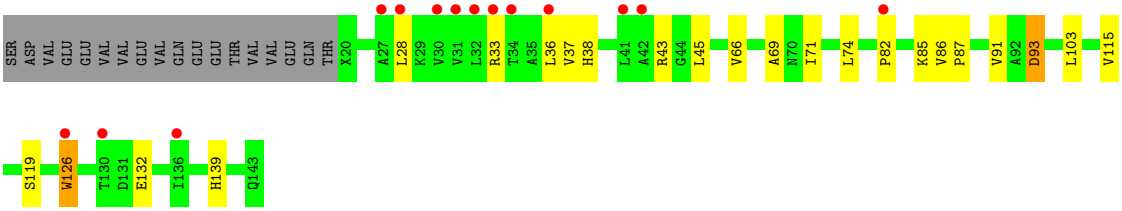


• Molecule 13: 40S ribosomal protein S11-A

Chain c1:

• Molecule 14: 40S ribosomal protein S12

Chain C2:



• Molecule 14: 40S ribosomal protein S12

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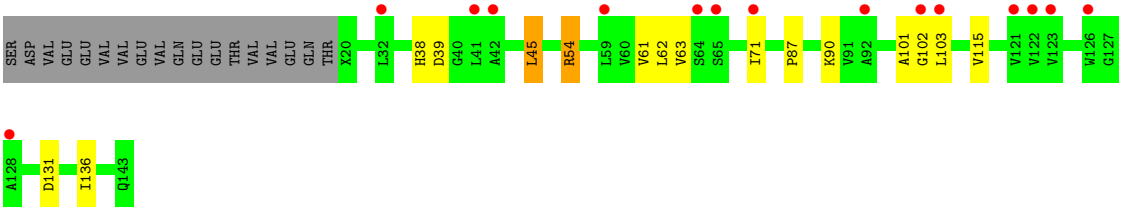
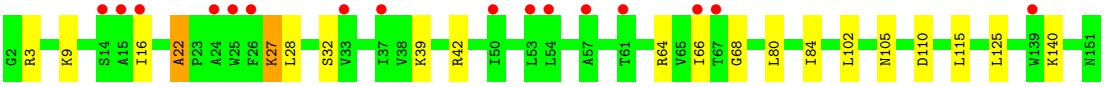


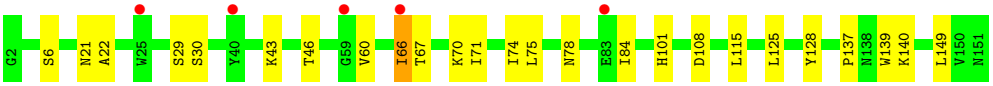
• Molecule 15: 40S ribosomal protein S13

Chain C3:



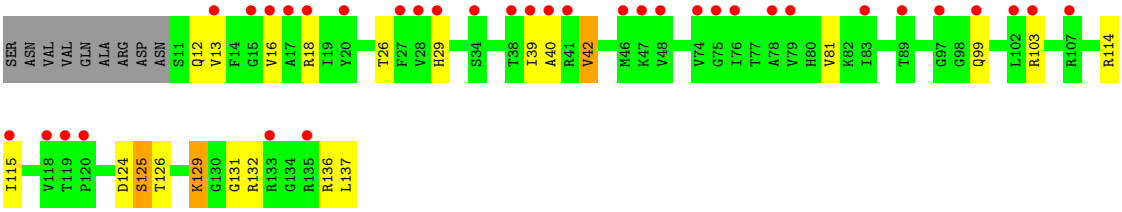
• Molecule 15: 40S ribosomal protein S13

Chain c3:



• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



- Molecule 16: 40S ribosomal protein S14-A

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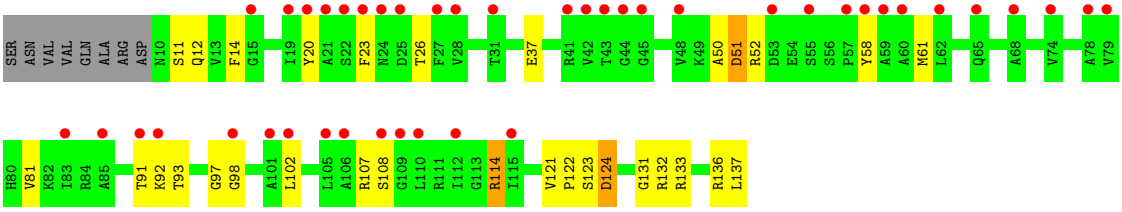
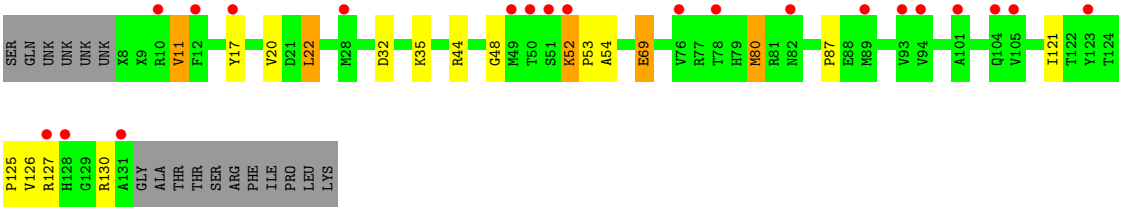


- Molecule 17: 40S ribosomal protein S15 (uS19)

Chain C5:

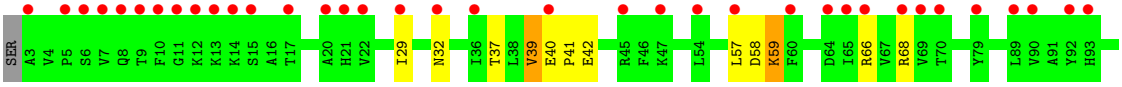


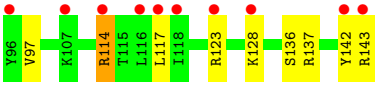
- Molecule 17: 40S ribosomal protein S15 (uS19)

Chain c5:

- Molecule 18: 40S ribosomal protein S16-A

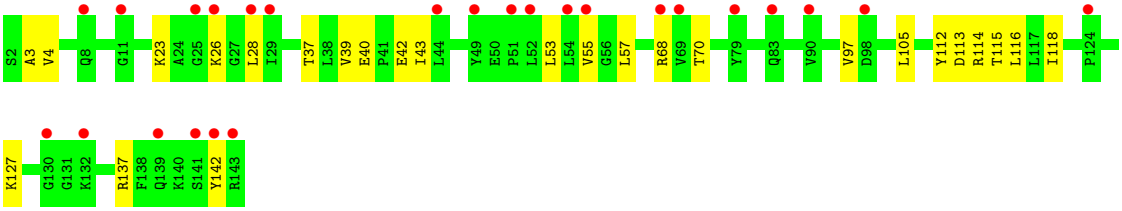
Chain C6:





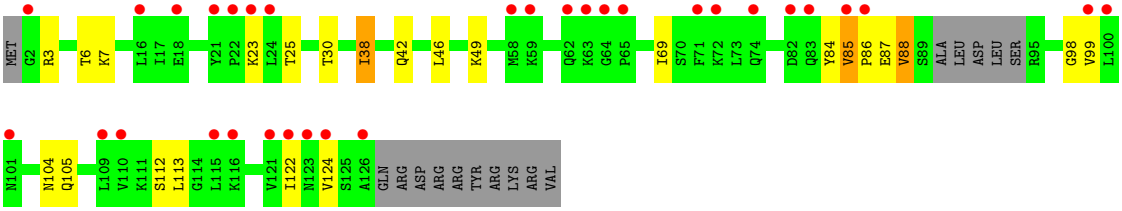
• Molecule 18: 40S ribosomal protein S16-A

Chain c6:



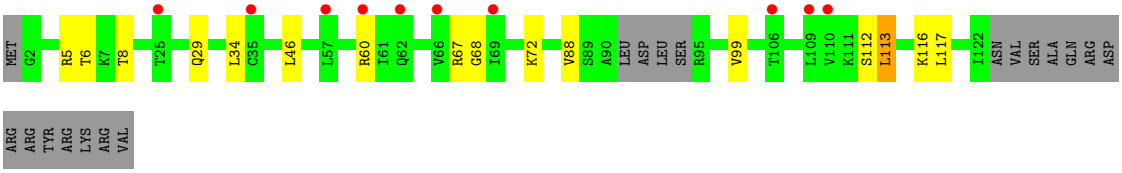
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



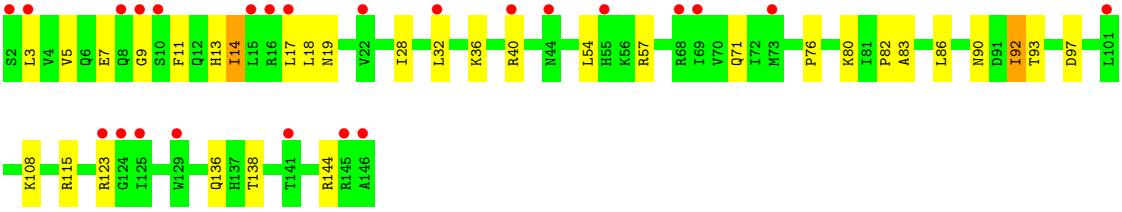
• Molecule 19: 40S ribosomal protein S17-A

Chain c7:



• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



• Molecule 20: 40S ribosomal protein S18-A

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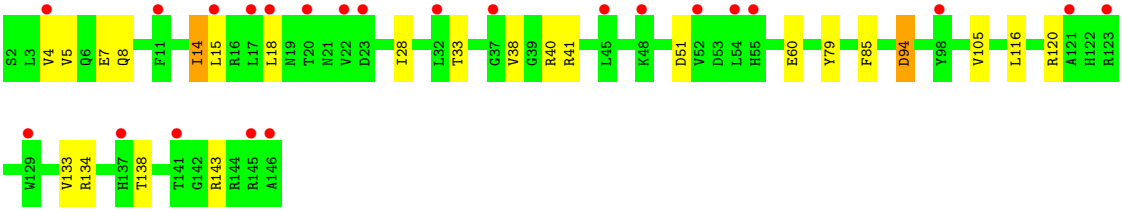
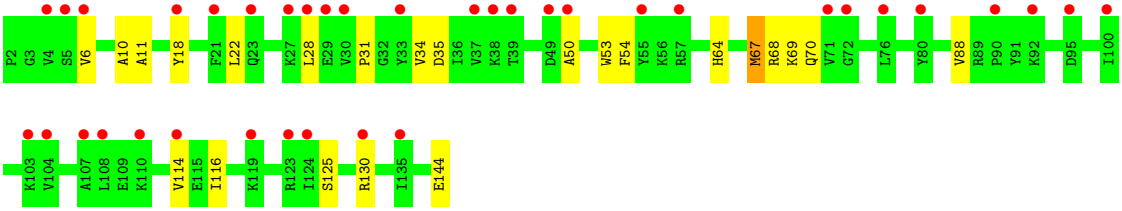


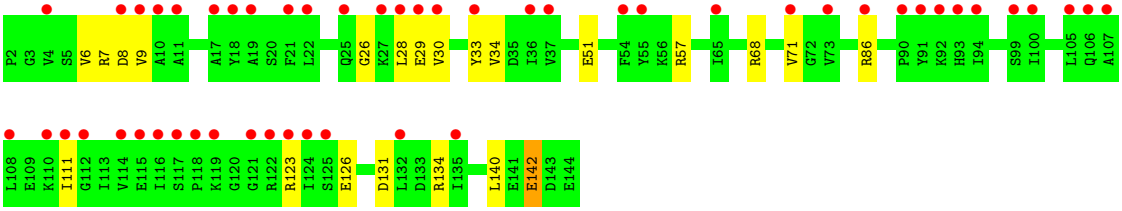
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



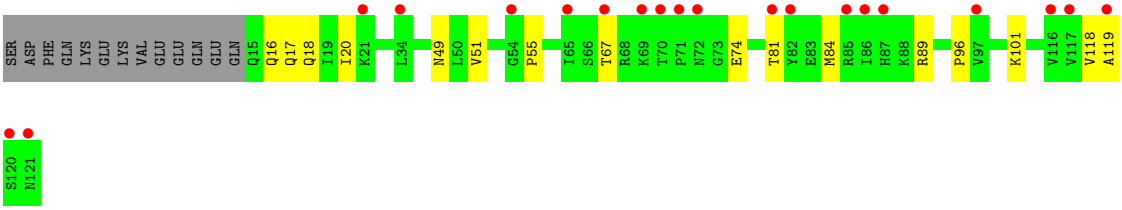
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



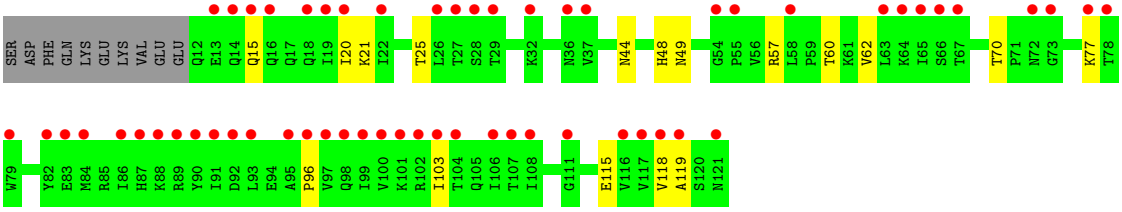
- Molecule 22: 40S ribosomal protein S20

Chain D0:



- Molecule 22: 40S ribosomal protein S20

Chain d0:

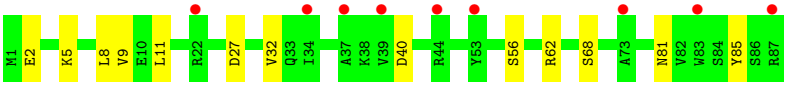


• Molecule 23: 40S ribosomal protein S21-A

Chain D1:

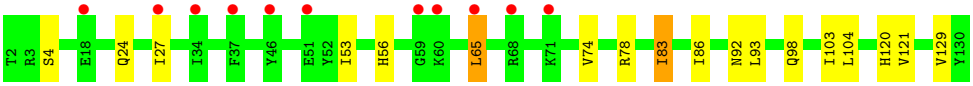
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

Chain D2:



• Molecule 24: 40S ribosomal protein S22-A

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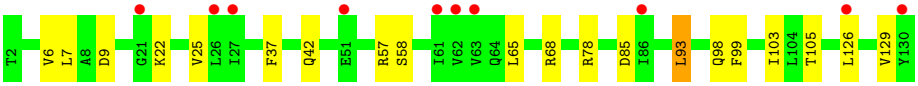
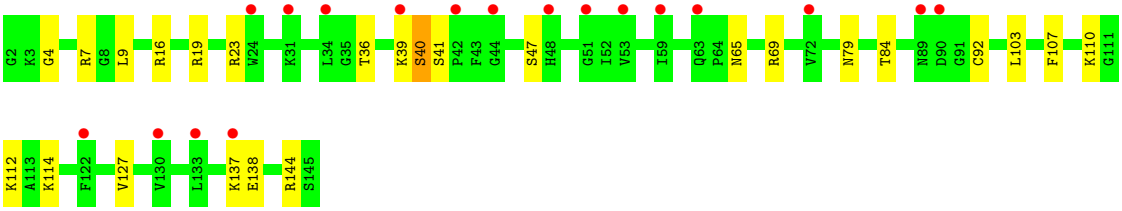


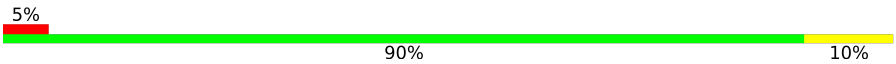
• Molecule 25: 40S ribosomal protein S23-A

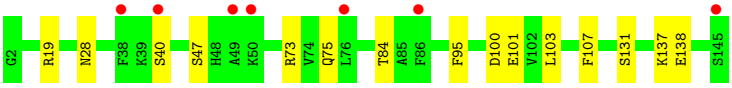
Chain D3:



• Molecule 25: 40S ribosomal protein S23-A

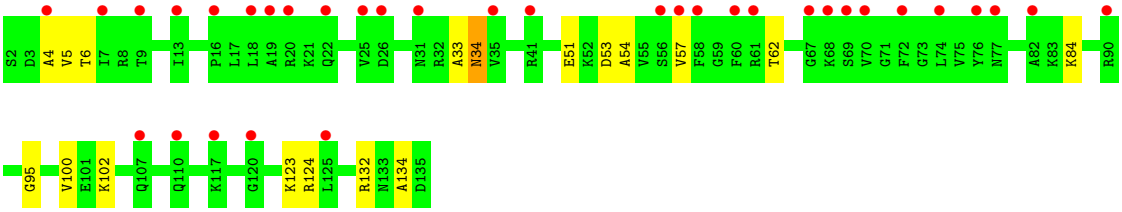
Chain d3:





• Molecule 26: 40S ribosomal protein S24-A

Chain D4:

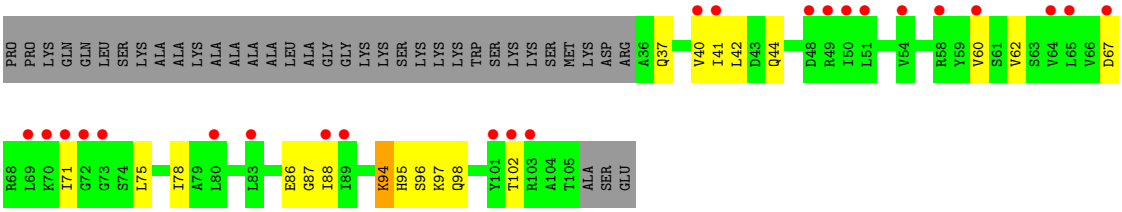


• Molecule 26: 40S ribosomal protein S24-A

Chain d4:

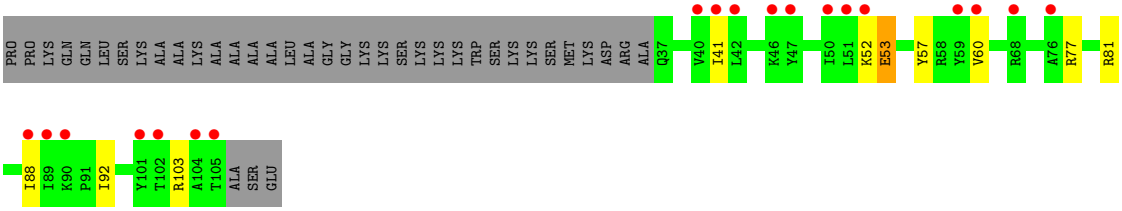
• Molecule 27: 40S ribosomal protein S25-A

Chain D5:



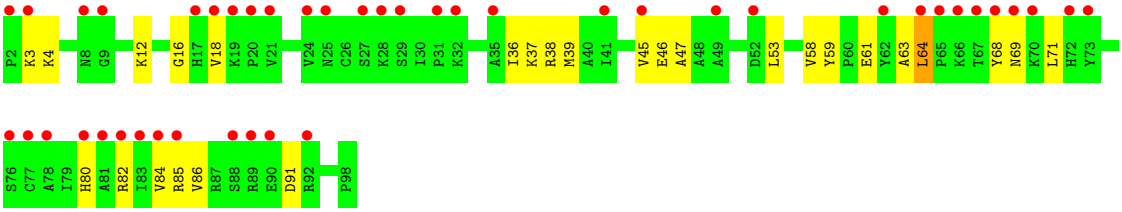
• Molecule 27: 40S ribosomal protein S25-A

Chain d5:



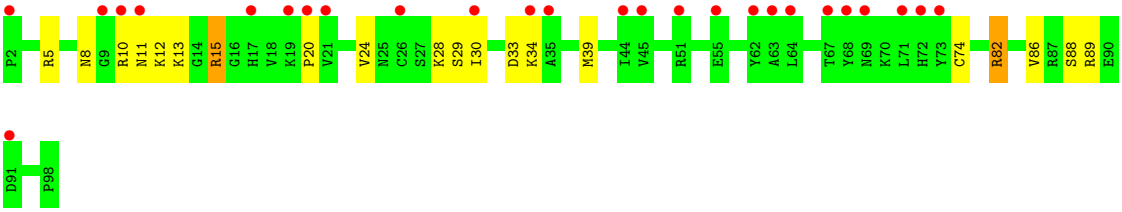
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



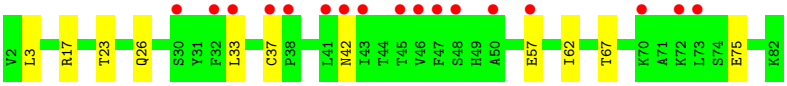
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



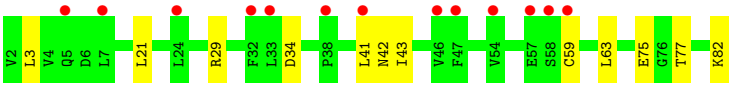
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



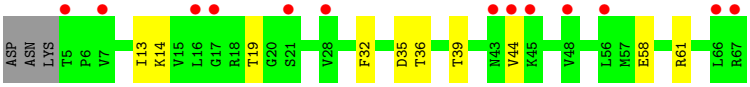
• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



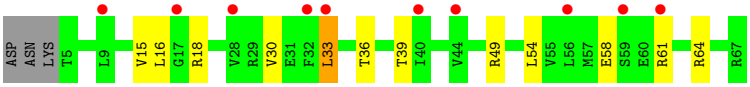
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



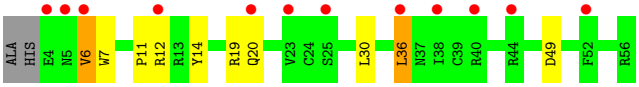
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



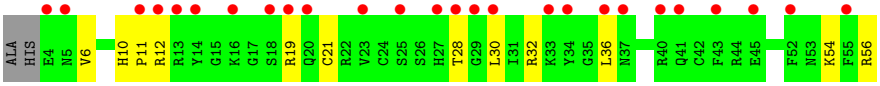
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



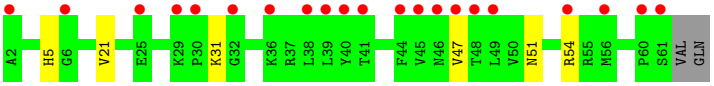
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



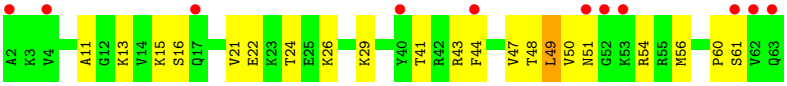
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



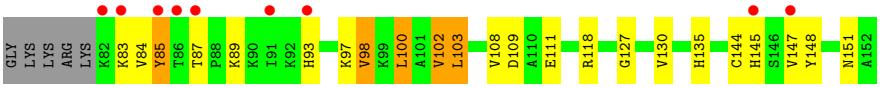
• Molecule 32: 40S ribosomal protein S30-A

Chain e0:



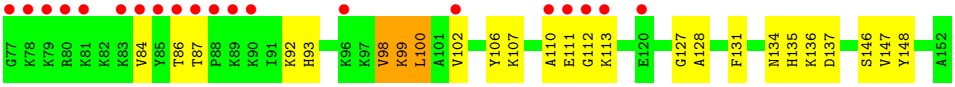
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



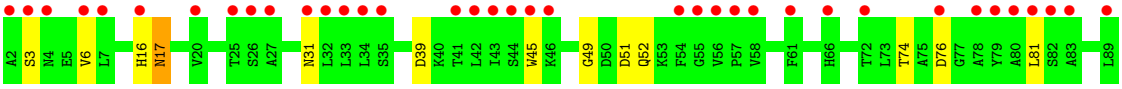
• Molecule 33: Ubiquitin-40S ribosomal protein S31

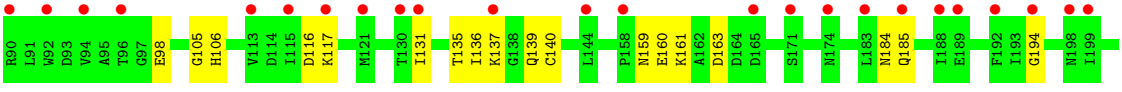
Chain e1:

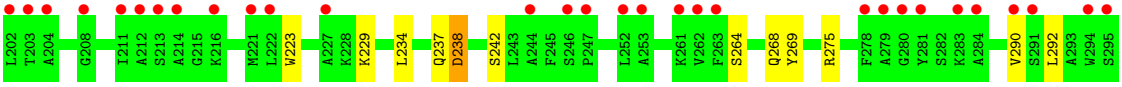


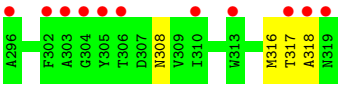
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



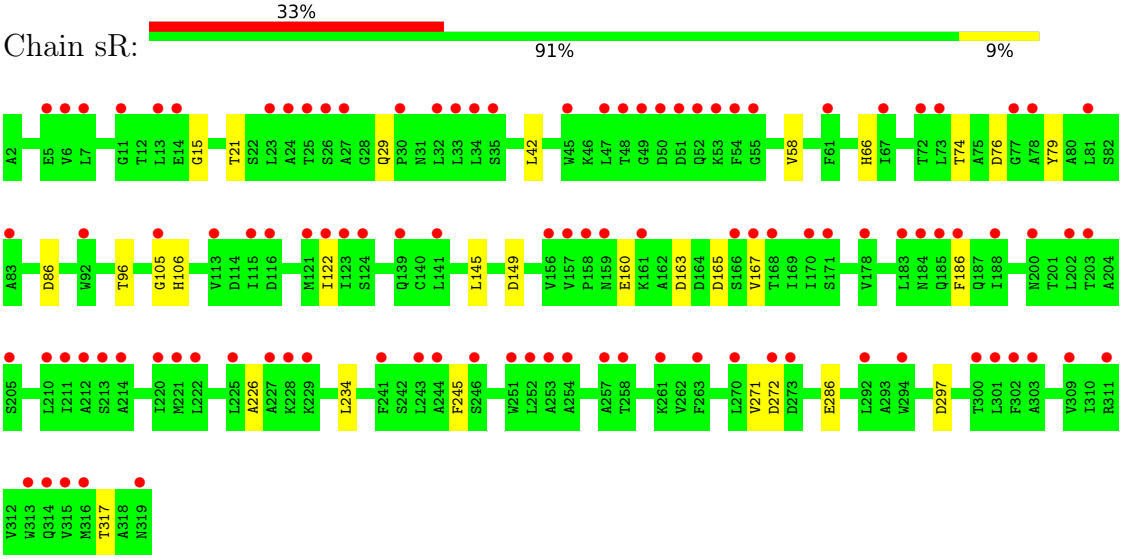






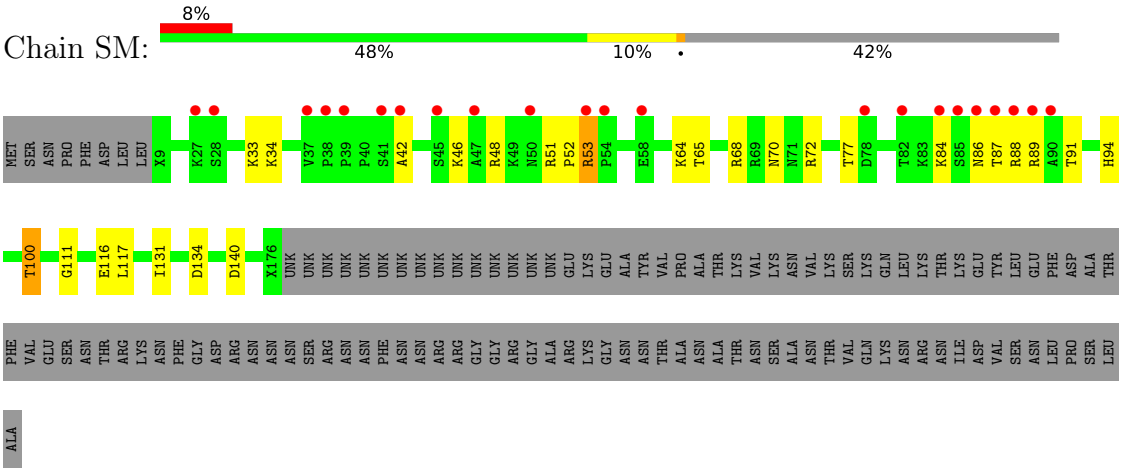
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



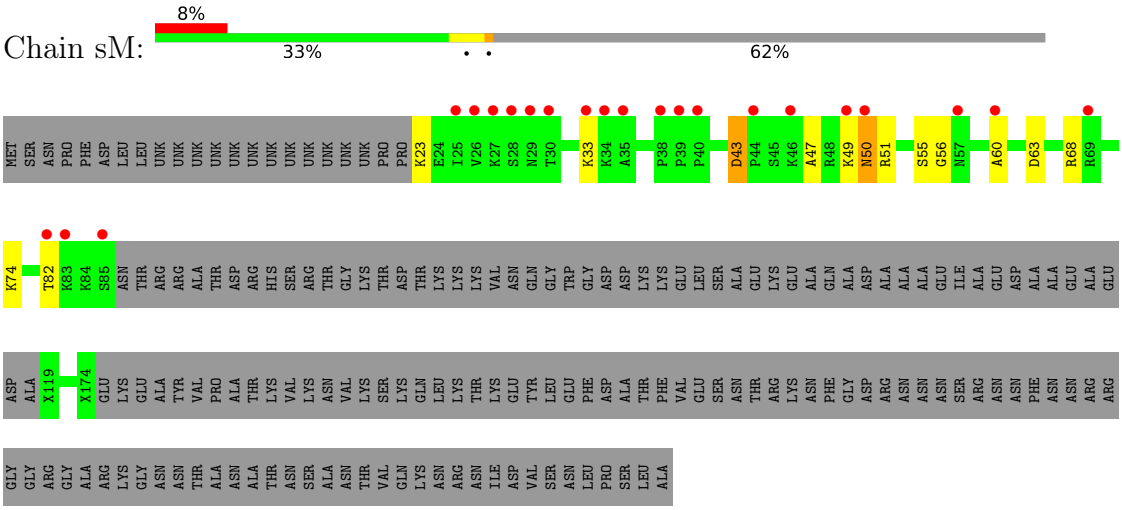
• Molecule 35: Suppressor protein STM1

Chain SM:

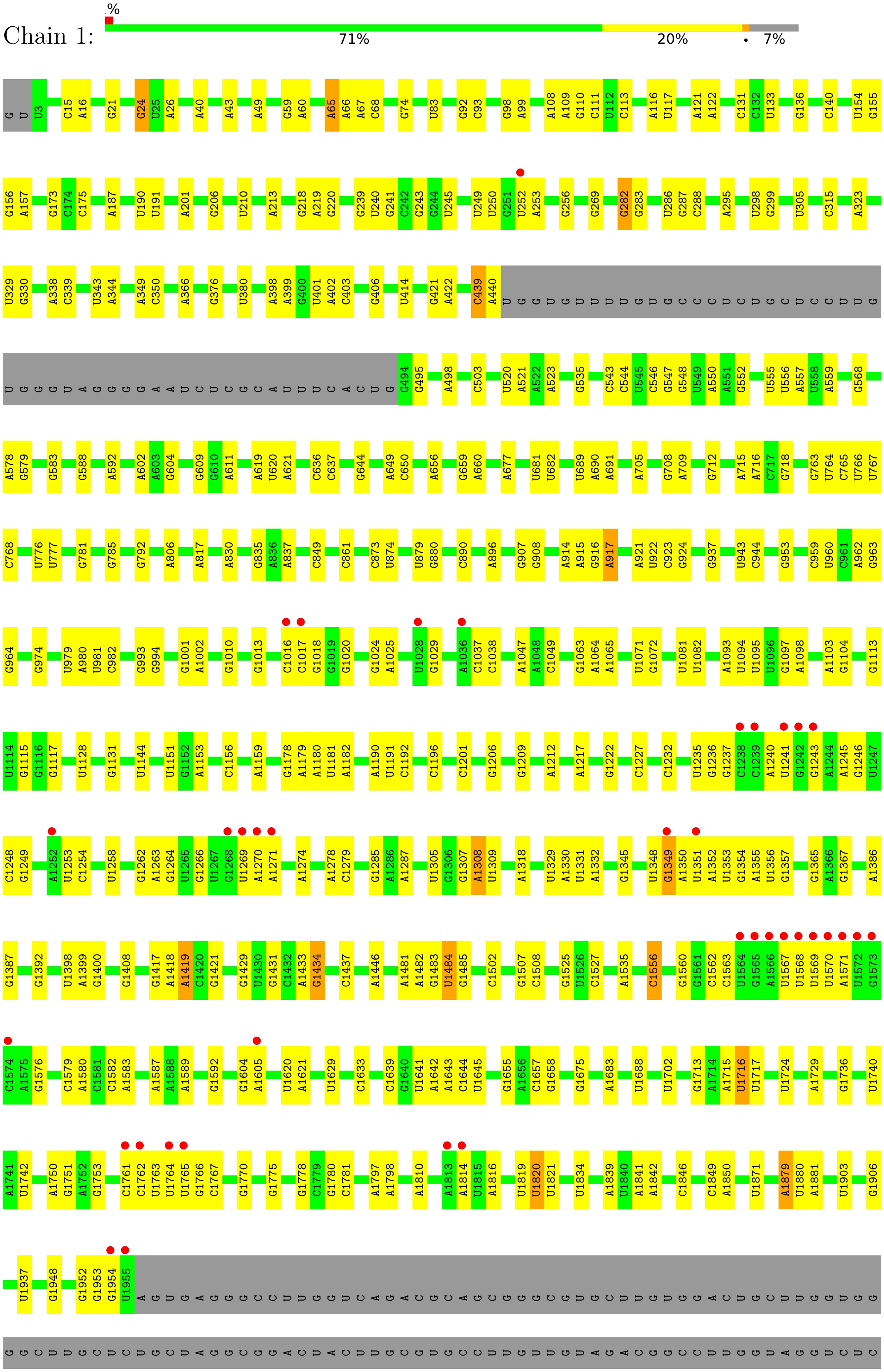


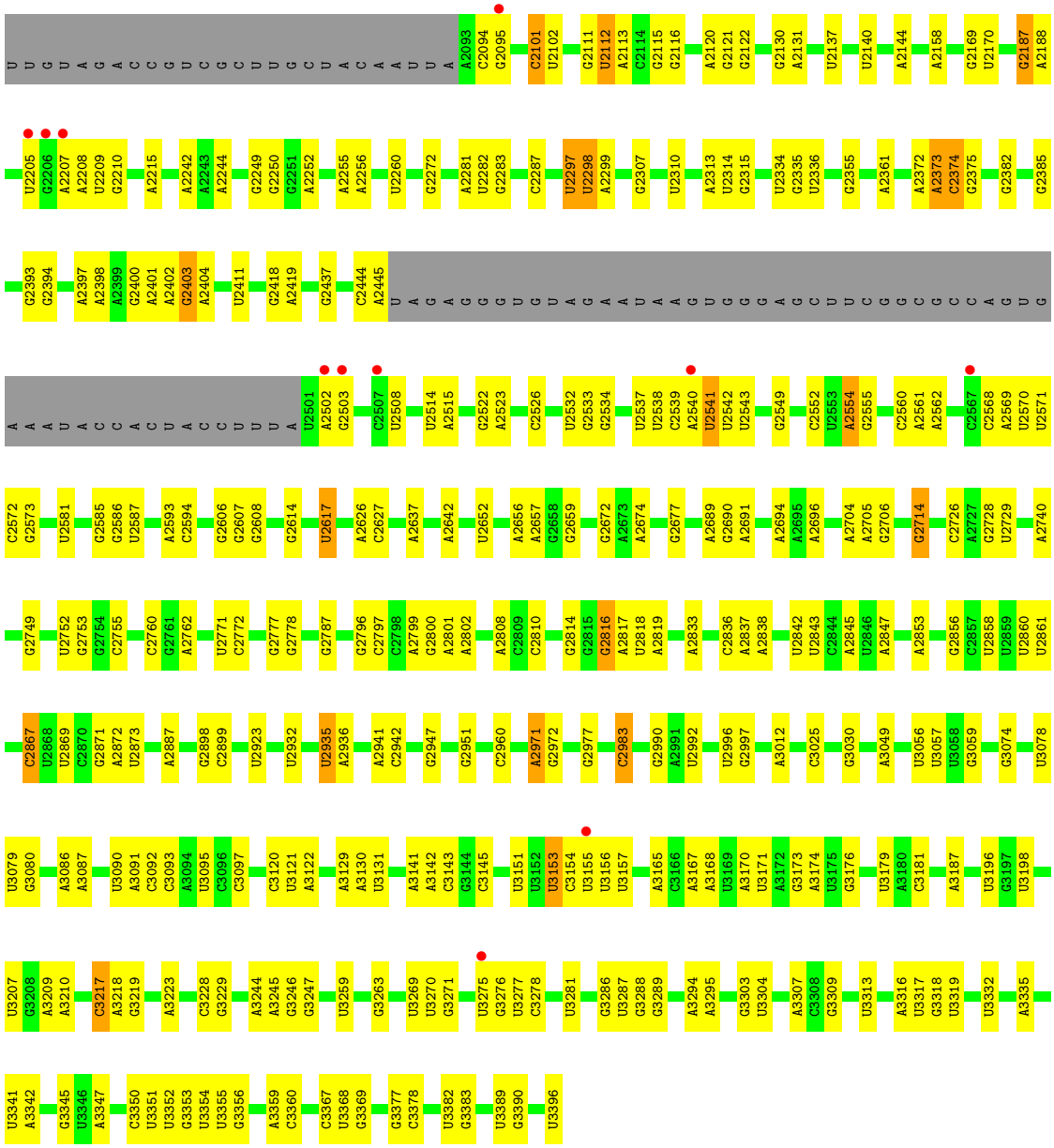
• Molecule 35: Suppressor protein STM1

Chain sM:



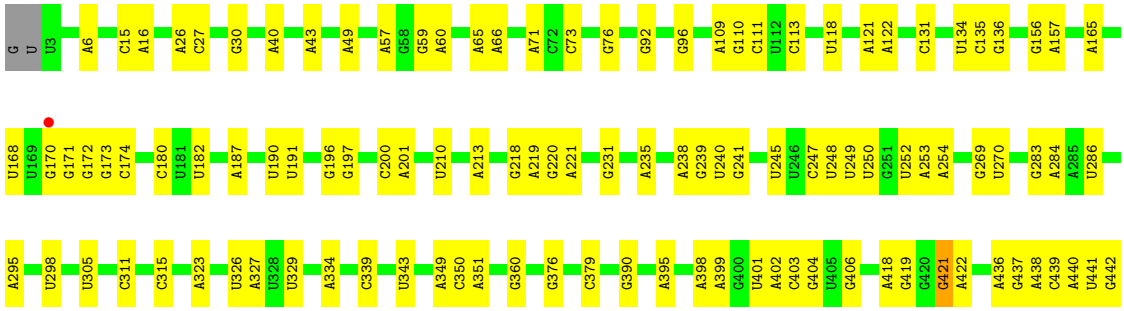
• Molecule 36: 25S ribosomal RNA

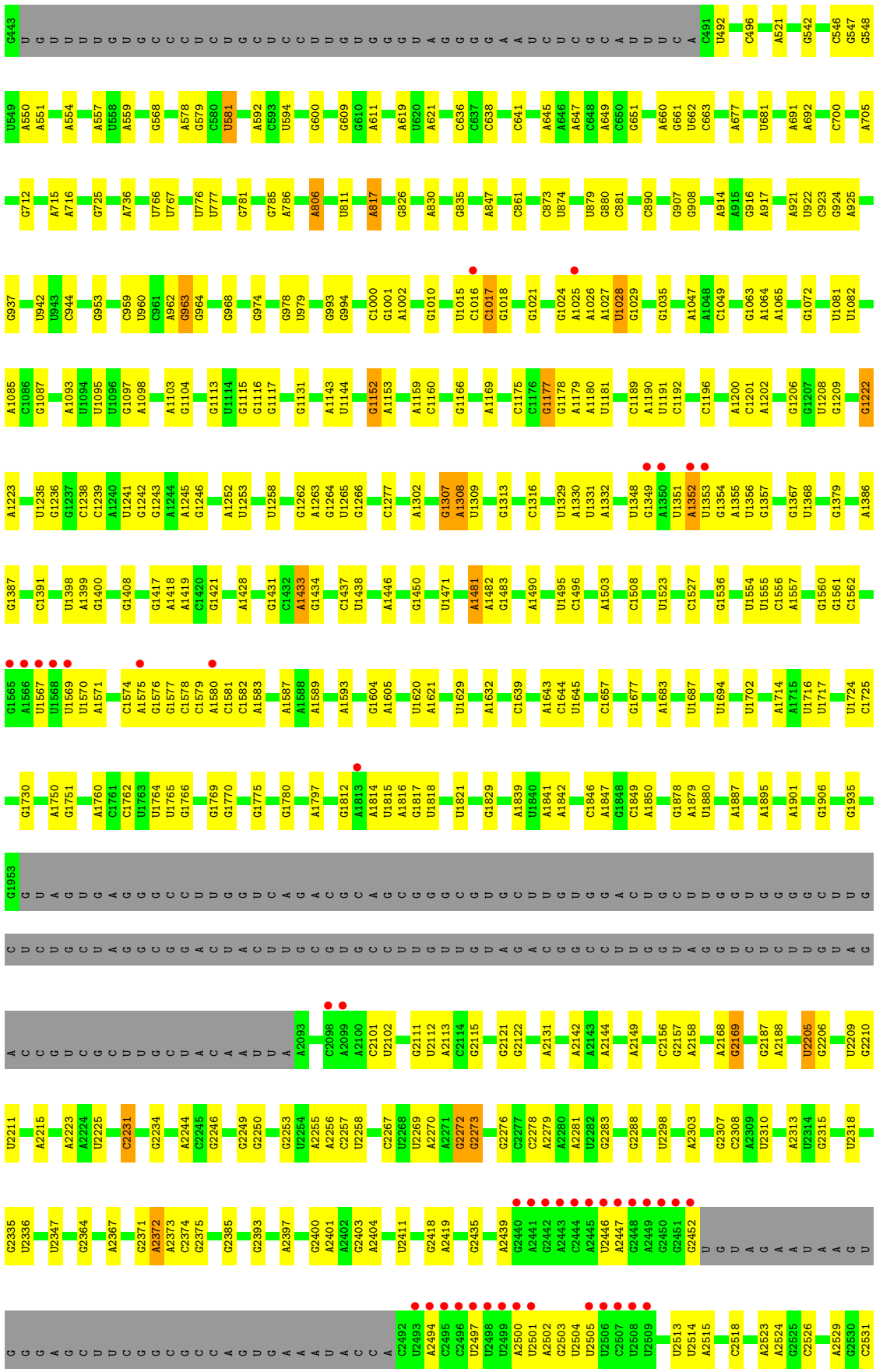




- Molecule 36: 25S ribosomal RNA

Chain 5:




G443 U U U U U G U G C C C U C U U G C U U C C U U G U G G G U A G G G G A A U U C U C G G A C491 U492 C496 A521 G542 C546 G547 G548
U549 A550 A551 A554 A557 U558 A559 G568 A578 G579 C580 U581 A592 C593 U594 G600 G609 G610 A611 A619 U620 A621 C636 C637 C638 C641 A645 A646 A647 C648 A649 C650 G651 A660 G661 U662 C663 A677 U681 A691 A692 C700 A705
G712 A715 A716 G725 A736 U766 U767 U776 U777 G781 G785 A786 A806 U811 A817 G826 A830 G835 A847 C861 C873 U874 U879 G880 C881 C890 G907 G908 A914 A915 G916 A917 A921 U922 C923 G924 A925
G937 U942 U943 G944 G953 C959 U960 C961 A962 G963 G964 G968 G974 G978 U979 G993 G994 C1000 G1001 A1002 G1010 U1015 C1016 C1017 G1018 G1021 G1024 A1025 A1026 A1027 U1028 G1029 G1035 A1047 A1048 C1049 G1063 A1064 A1065 G1072 U1081 U1082
A1085 C1086 G1087 A1093 U1094 U1095 U1096 G1097 A1098 A1103 G1104 G1113 U1114 G1115 G1116 G1117 G1131 A1143 U1144 G1152 A1153 A1159 C1160 G1166 A1169 C1175 C1176 G1177 G1178 A1179 A1180 U1181 C1189 A1190 U1191 C1192 C1196 A1200 C1201 A1202 G1206 G1207 U1208 G1209 G1222
A1223 U1235 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 A1252 U1253 U1258 G1262 A1263 G1264 U1265 G1266 C1277 A1302 G1307 A1308 U1309 G1313 C1316 U1329 A1330 U1331 A1332 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 G1367 U1368 G1379 A1386
G1387 C1391 U1398 A1399 G1400 G1408 G1417 A1418 A1419 C1420 G1421 A1428 G1431 C1432 A1433 G1434 C1437 U1438 A1446 G1450 U1471 A1481 A1482 G1483 A1490 U1495 C1496 A1503 C1508 U1523 C1527 G1536 U1554 U1555 C1556 A1557 G1560 G1561 C1562
G1565 A1566 U1567 U1568 U1569 U1570 A1571 C1574 A1575 G1576 G1577 C1578 C1579 A1580 C1581 C1582 A1583 A1587 A1588 A1589 A1593 G1604 A1605 U1620 A1621 U1629 A1632 C1639 A1643 C1644 U1645 C1657 G1677 A1683 U1687 U1694 U1702 A1714 A1715 U1716 U1717 U1724 C1725
G1730 A1750 G1751 A1760 C1761 C1762 U1763 U1764 U1765 G1766 G1769 G1770 G1775 G1780 A1797 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1821 G1829 A1839 U1840 A1841 A1842 C1846 A1847 G1848 C1849 A1850 G1878 A1879 U1880 A1887 A1895 A1901 G1906 G1935
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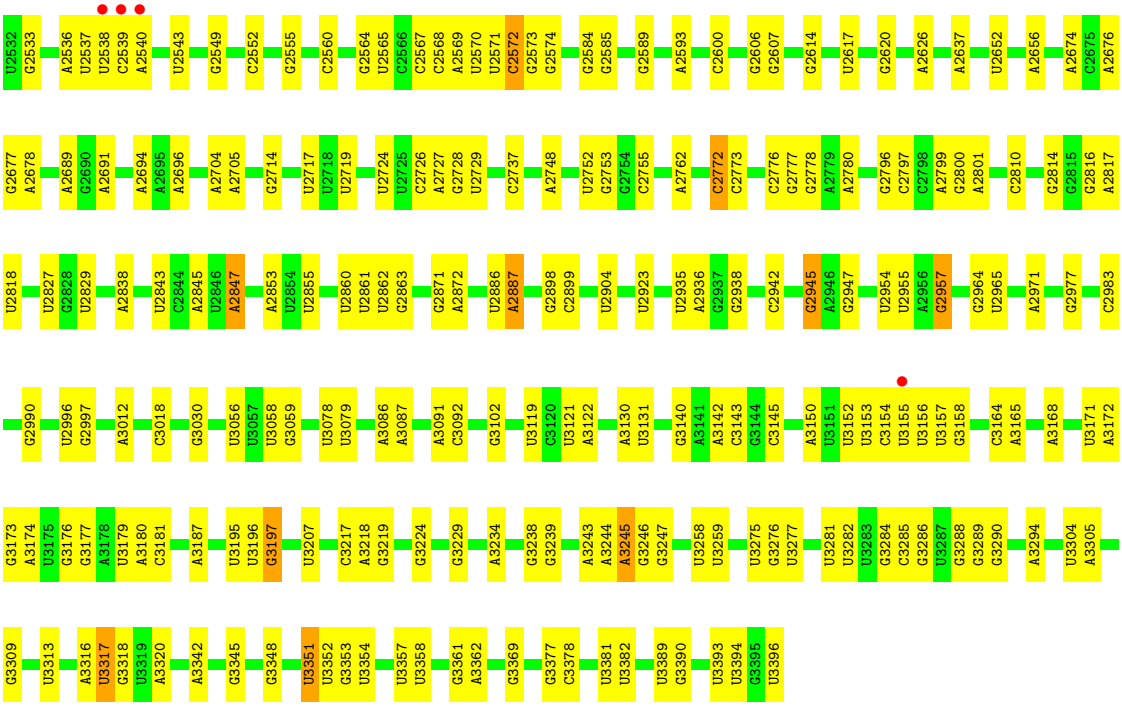
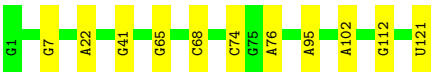


- Molecule 37: 5S ribosomal RNA

Chain 3:

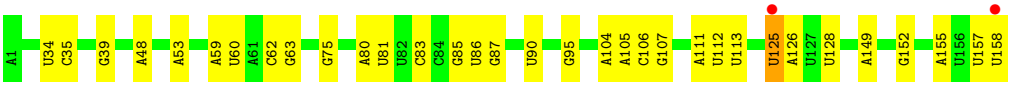


- Molecule 37: 5S ribosomal RNA

Chain 7:

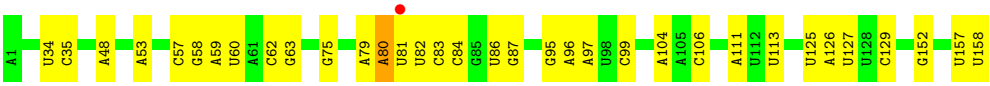
- Molecule 38: 5.8S ribosomal RNA

Chain 4:



- Molecule 38: 5.8S ribosomal RNA

Chain 8:



- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 4% 85% 15%

G2 G13 S14 T17 T20 K28 L32 I44 V45 G55 A59 R70 L71 R72 V82 H83 T84 V101 T111 I112 V113 S114 N115 V116 A125 S130 V134 N144 R149 V157 V165 D176 L179 L180 K192 T199

M204 V207 D208 S223 T224 R227 K234 A235 I238 L246 Q250 K251 T252 Q253 ASP

- Molecule 39: 60S ribosomal protein L2-A

Chain l2: 4% 82% 17%

G2 K10 H19 Q24 L29 L32 I44 V45 K46 Q47 A56 A59 K60 V61 V62 Y69 R72 E73 E74 E80 G81 V82 L96 V101 L104 E109 S114 N115 A125 S130 V134 I137 D142 E143 R147 V148 R149

D161 G164 V165 V168 I169 A170 R174 L179 L180 R193 N194 T199 V202 A203 M204 V207 G212 L237 I238 A239 A240 R241 R242 L246 R247 G248 S249 Q250 K251 T252 Q253 ASP

- Molecule 40: 60S ribosomal protein L3

Chain L3: 5% 82% 18%

S2 H3 R4 K5 Y6 E7 L17 P18 R19 K20 R21 I25 K30 S38 L47 G48 Y49 K50 A51 T55 I56 V57 F67 V72 V76 T77 V78 V79 D80 V84 V85 P96 R97 T103 T104 V114 K115 R116 K120 N121 K128 D140 G141 A142

A155 T164 R167 L171 A172 Q173 K174 H177 L183 S187 I188 R196 D206 E213 A217 T221 F226 T235 L238 R244 G245 L246 I252 P257 A258 R275 T276 S277 R284 N293 T296 S297 F298 T301 T304 I305

I317 D320 M323 I328 N331 R332 V336 T337 L338 Y343 T344 N345 T346 S347 L351 E352 E353 V354 D360 D386 L387

- Molecule 40: 60S ribosomal protein L3

Chain l3: 2% 82% 16%

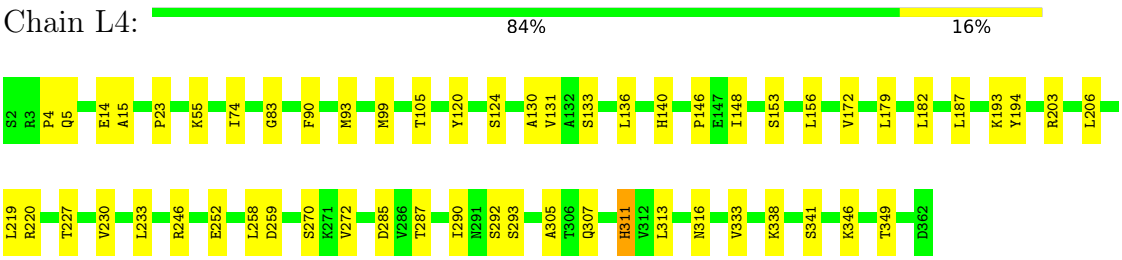
S2 H3 R4 K5 Y6 E7 L17 P18 R19 A23 S24 K30 R37 P40 L47 K50 I56 R70 V79 V85 V93 T103 T104 H109 L110 S111 D112 E113 V114 K115 R116 Y123 K124 S125 A129 Q139 D140 R146 E147 L148 A155

S156 T164 R167 P170 K175 L178 L183 S187 I188 V192 R196 V208 Q211 H231 R232 W233 G234 T235 G245 V249 V264 A265 R266 S274 R284 T296 S297 R300 T304 V324 I328 R332 I335 K340 S341

T346 S347 R348 S355 K385 D386 L387

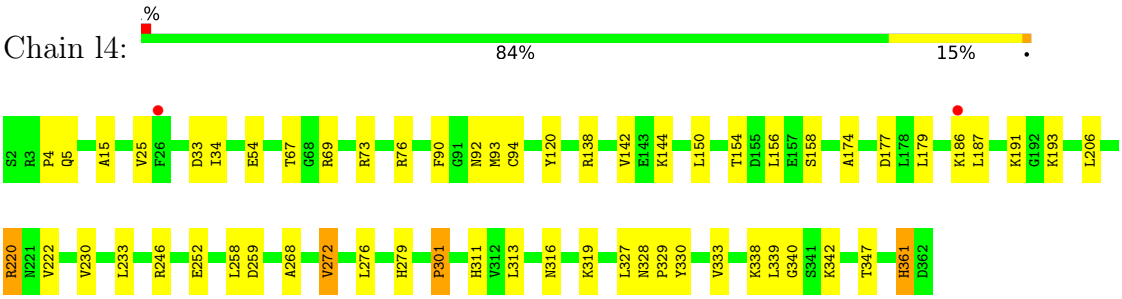
- Molecule 41: 60S ribosomal protein L4-A

Chain L4:



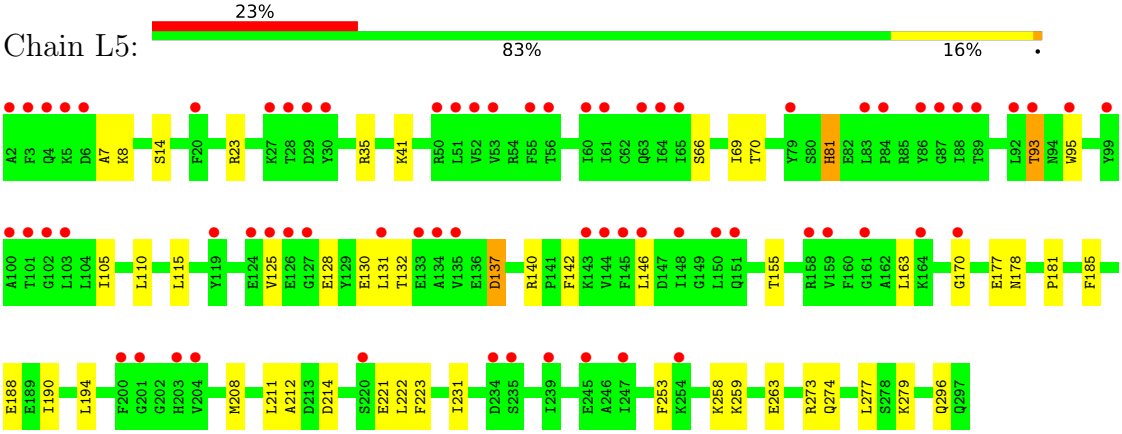
- Molecule 41: 60S ribosomal protein L4-A

Chain l4:



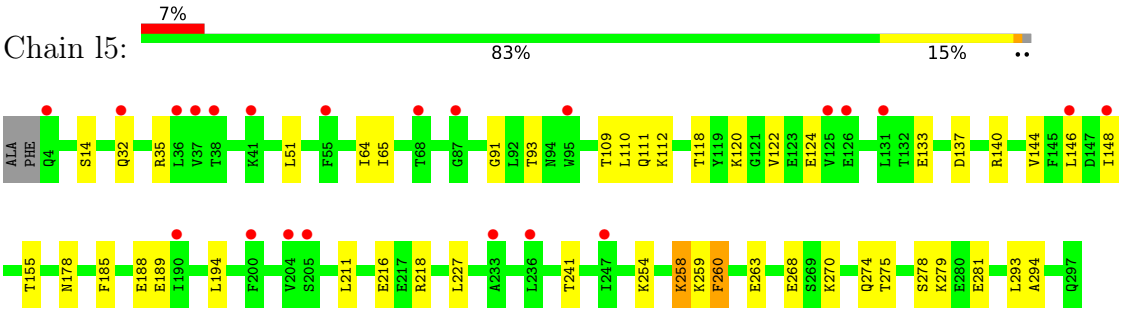
- Molecule 42: 60S ribosomal protein L5

Chain L5:



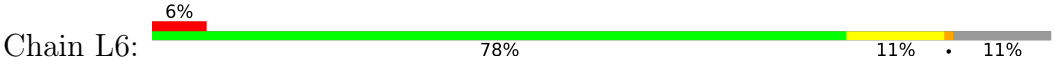
- Molecule 42: 60S ribosomal protein L5

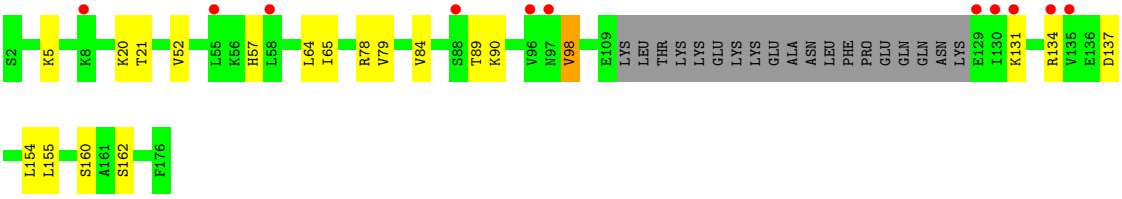
Chain l5:



- Molecule 43: 60S ribosomal protein L6-A

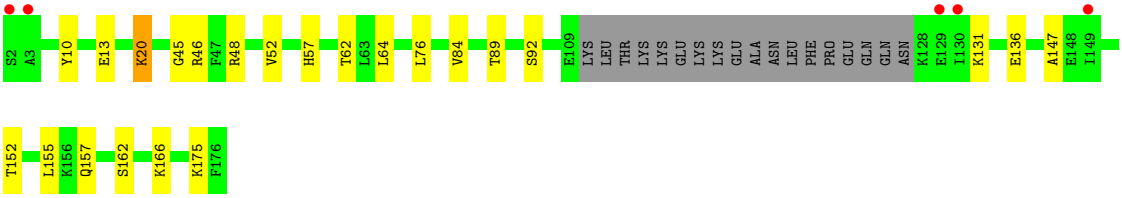
Chain L6:





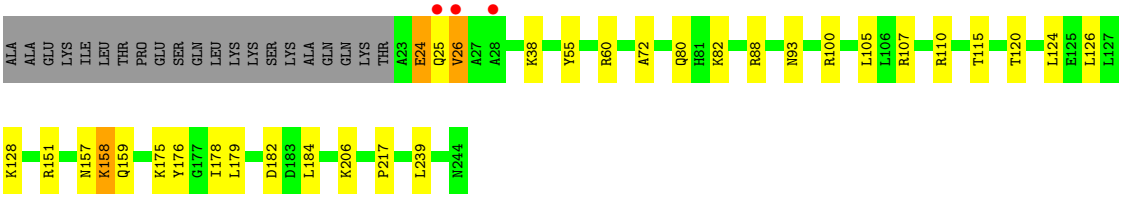
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



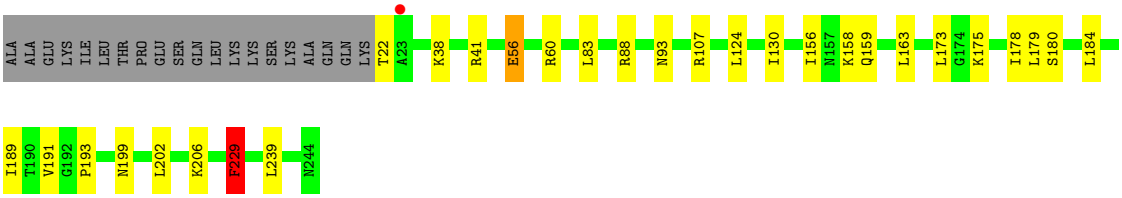
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



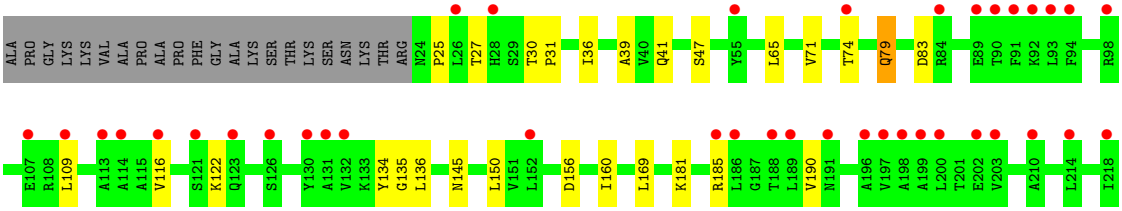
• Molecule 44: 60S ribosomal protein L7-A

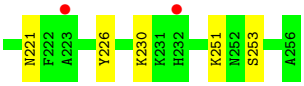
Chain l7:



• Molecule 45: 60S ribosomal protein L8-A

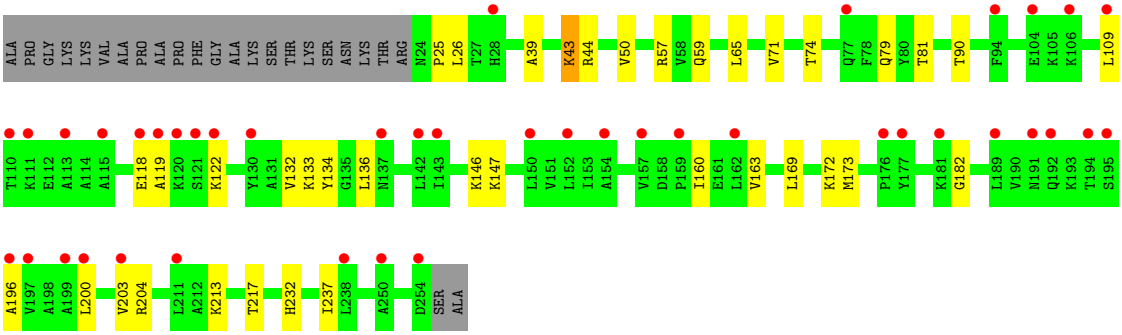
Chain L8:





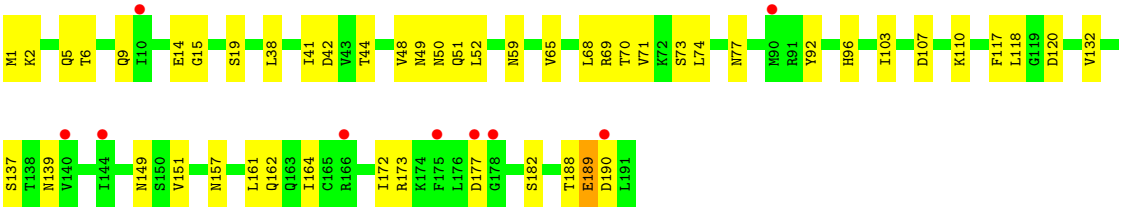
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



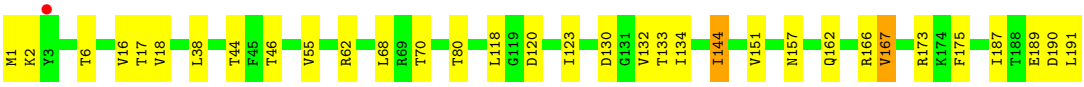
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



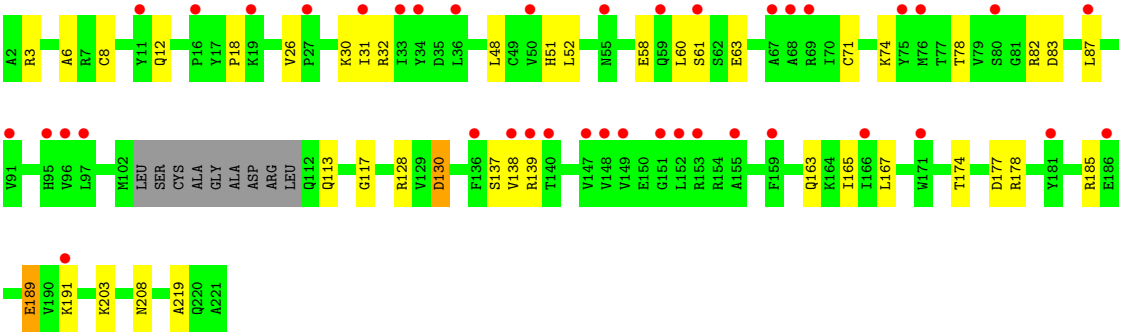
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



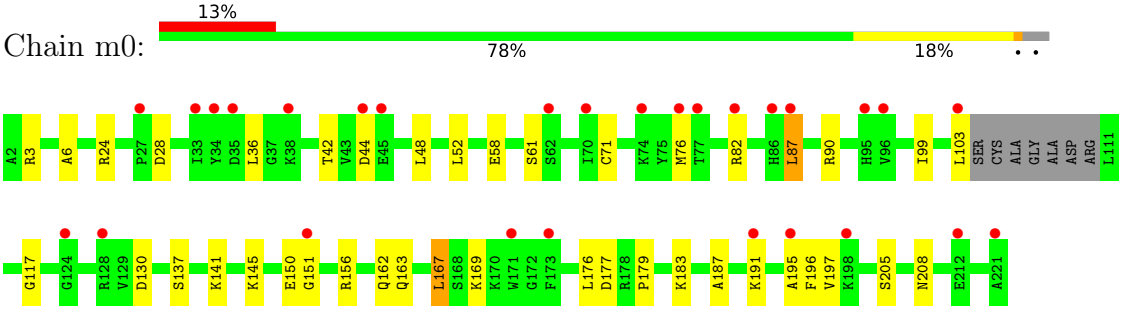
• Molecule 47: 60S ribosomal protein L10

Chain M0:



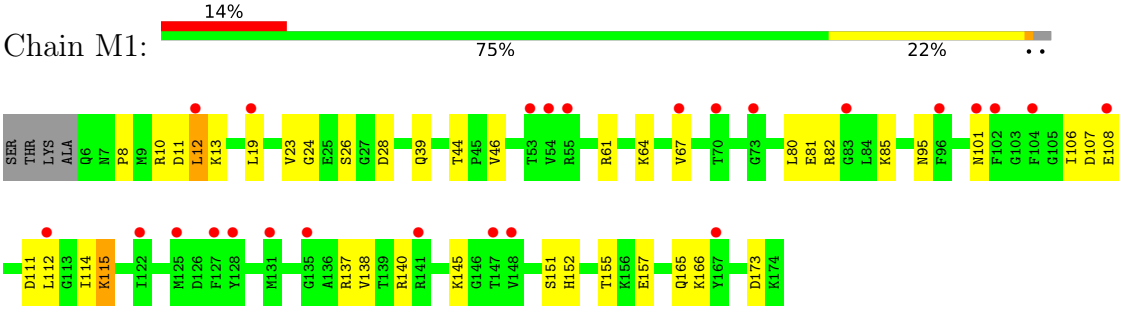
• Molecule 47: 60S ribosomal protein L10

Chain m0:



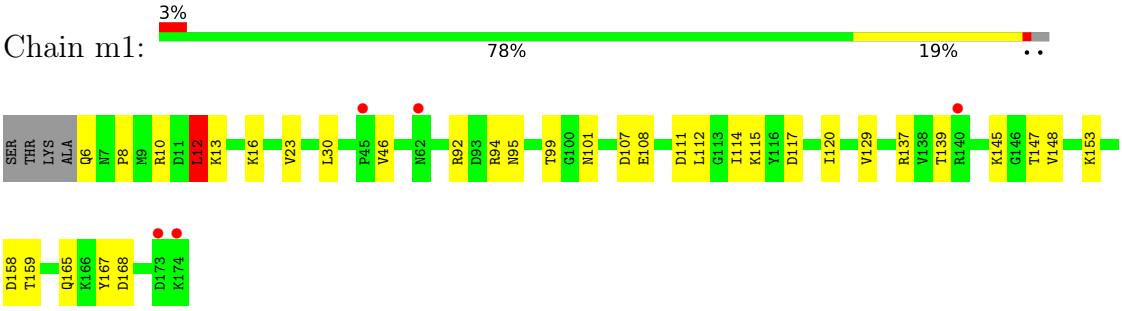
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



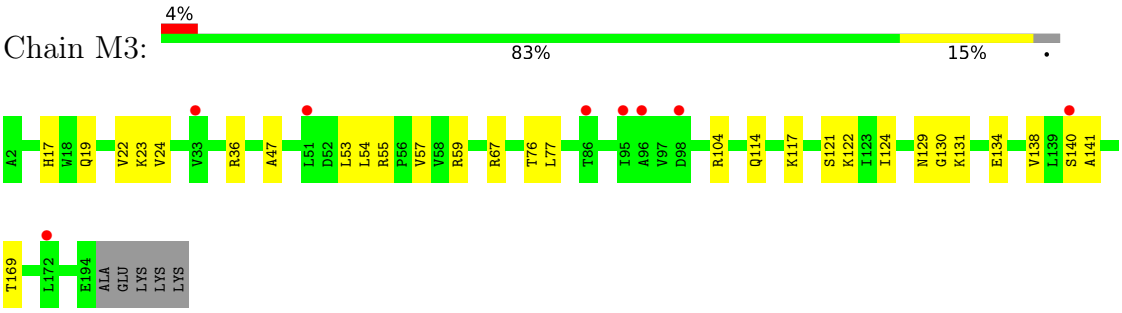
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



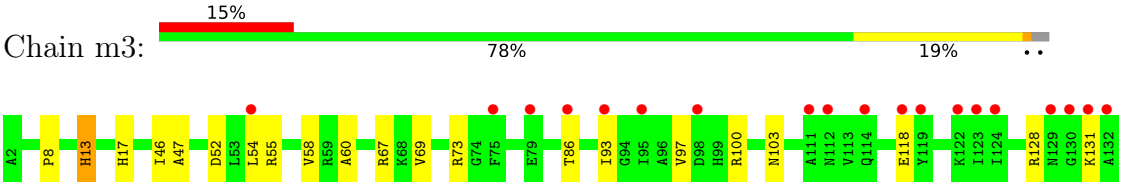
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



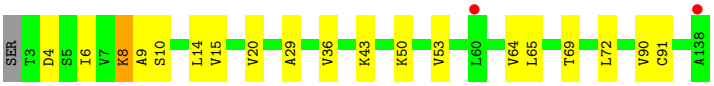
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



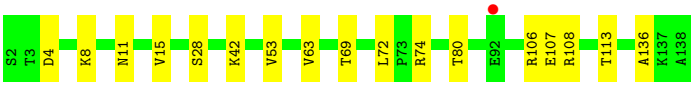
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



• Molecule 50: 60S ribosomal protein L14-A

Chain m4:

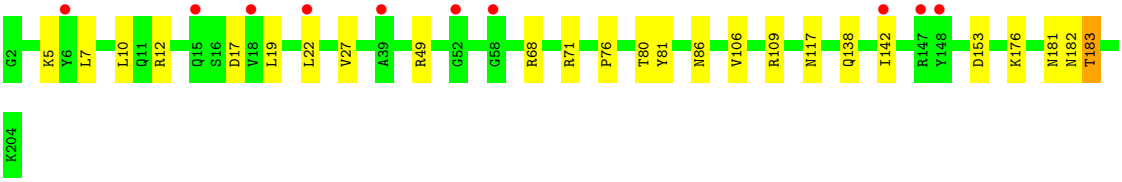


• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

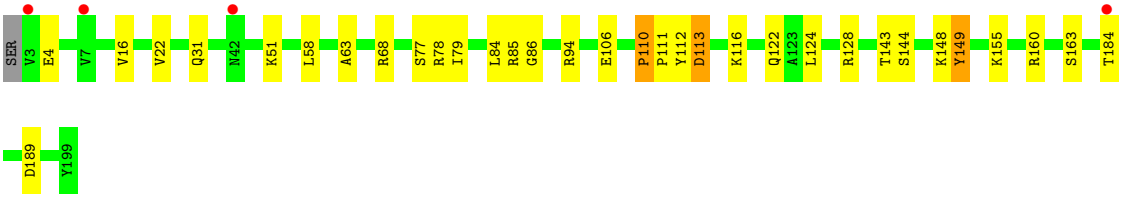
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



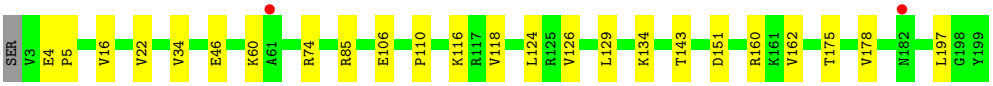
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



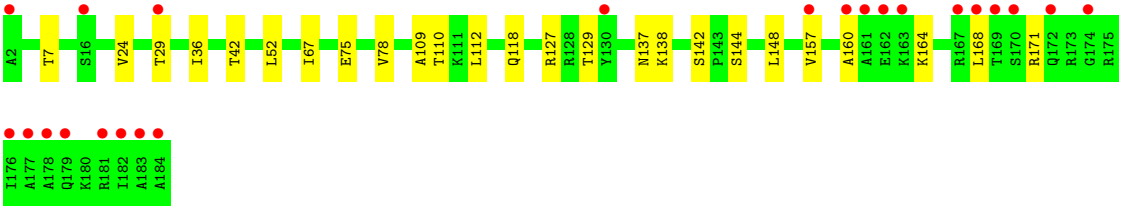
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



• Molecule 53: 60S ribosomal protein L17-A

Chain M7:

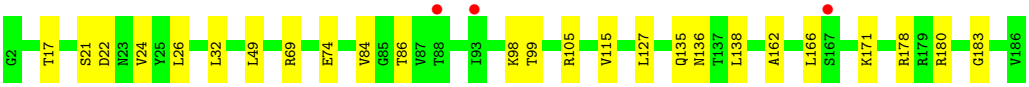


• Molecule 53: 60S ribosomal protein L17-A

Chain m7:

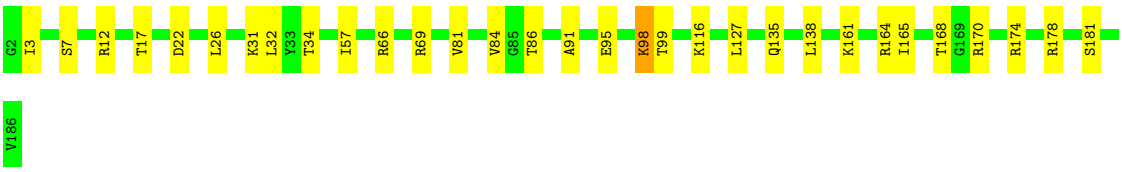
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



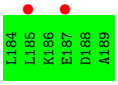
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



• Molecule 55: 60S ribosomal protein L19-A

Chain M9:

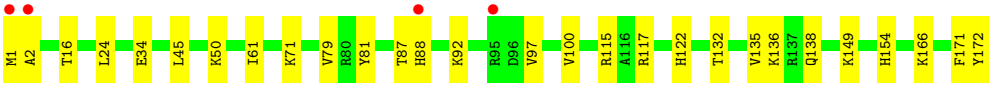


• Molecule 55: 60S ribosomal protein L19-A

Chain m9:

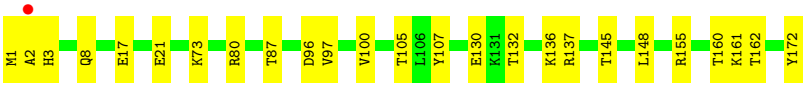
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

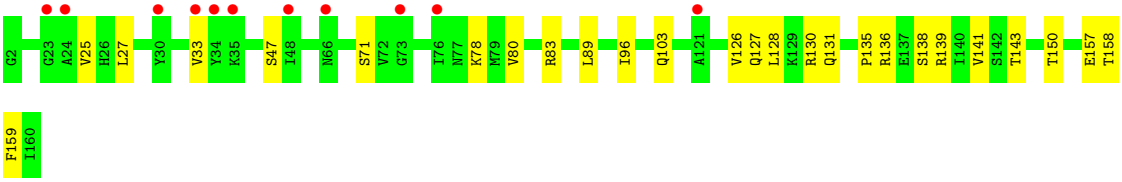


• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

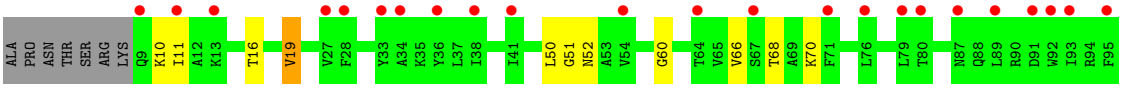
• Molecule 57: 60S ribosomal protein L21-A

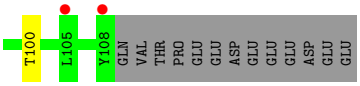
Chain n1:



• Molecule 58: 60S ribosomal protein L22-A

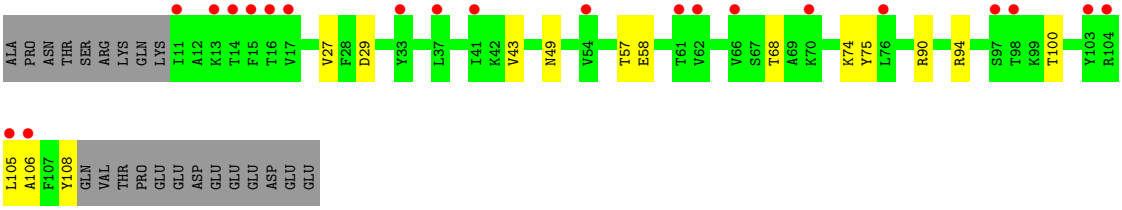
Chain N2:





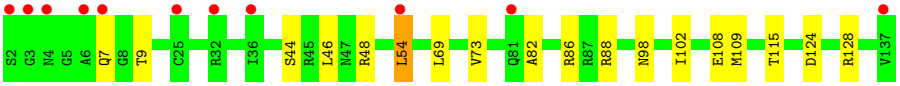
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



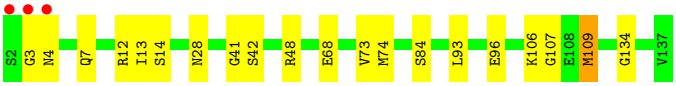
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



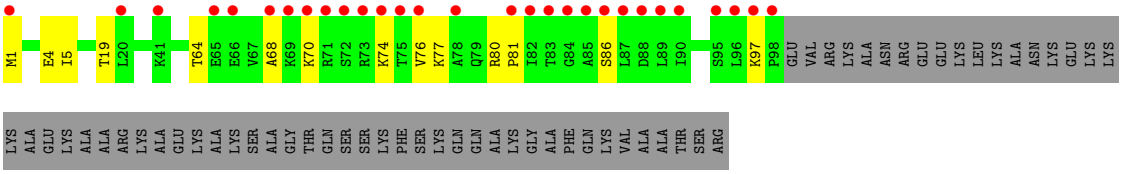
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



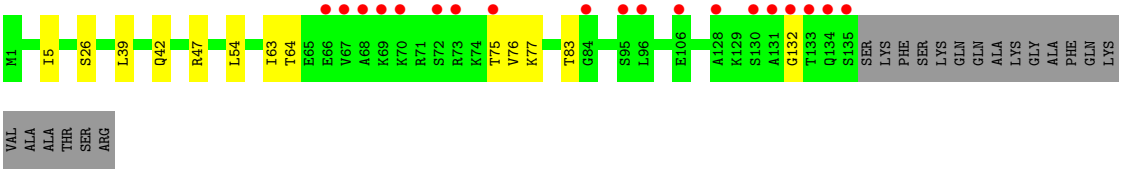
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



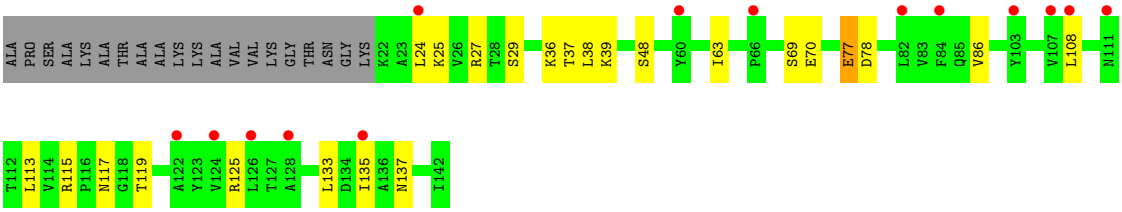
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



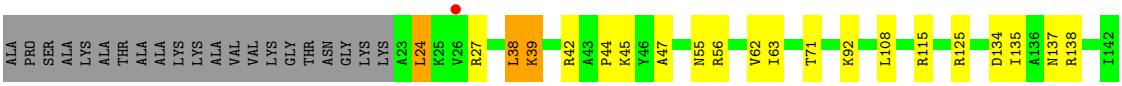
• Molecule 61: 60S ribosomal protein L25

Chain N5:



- Molecule 61: 60S ribosomal protein L25

Chain n5:

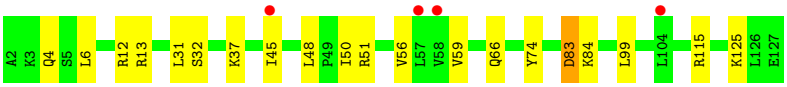


- Molecule 62: 60S ribosomal protein L26-A

Chain N6:

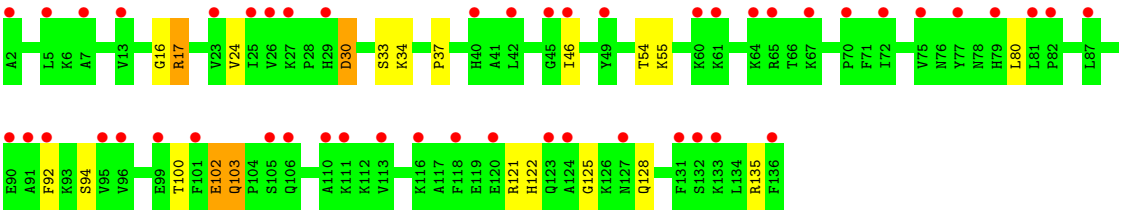
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



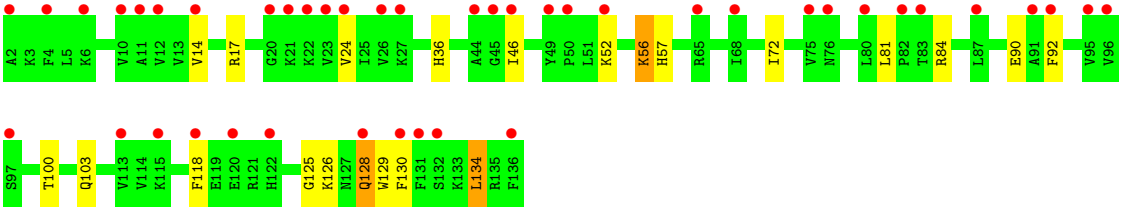
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



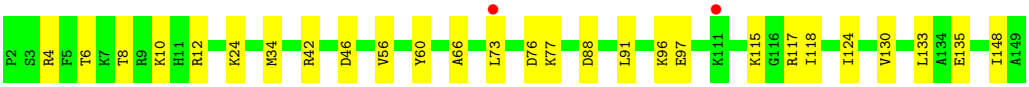
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



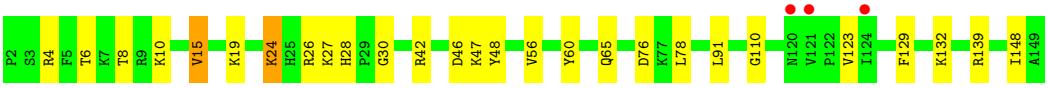
- Molecule 64: 60S ribosomal protein L28

Chain N8:



- Molecule 64: 60S ribosomal protein L28

Chain n8:

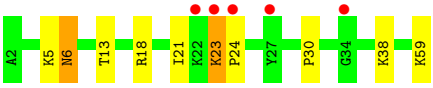


- Molecule 65: 60S ribosomal protein L29

Chain N9:

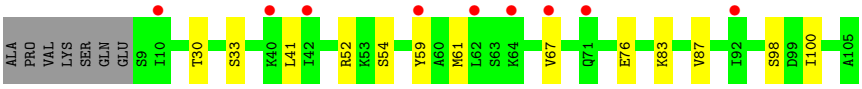
- Molecule 65: 60S ribosomal protein L29

Chain n9:



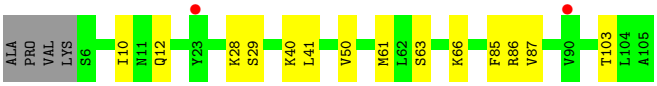
- Molecule 66: 60S ribosomal protein L30

Chain O0:



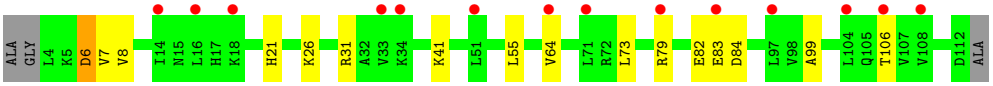
- Molecule 66: 60S ribosomal protein L30

Chain o0:



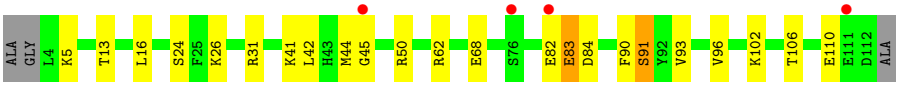
• Molecule 67: 60S ribosomal protein L31-A

Chain O1:



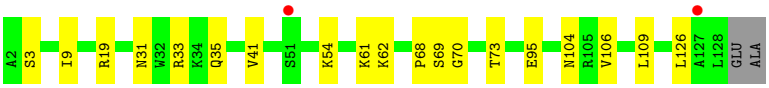
• Molecule 67: 60S ribosomal protein L31-A

Chain o1:



• Molecule 68: 60S ribosomal protein L32

Chain O2:

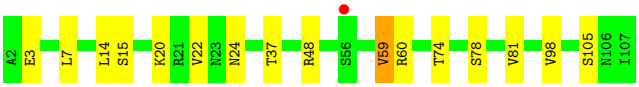


• Molecule 68: 60S ribosomal protein L32

Chain o2:

• Molecule 69: 60S ribosomal protein L33-A

Chain O3:

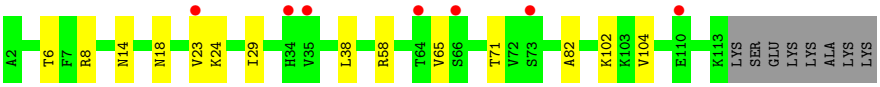


• Molecule 69: 60S ribosomal protein L33-A

Chain o3:

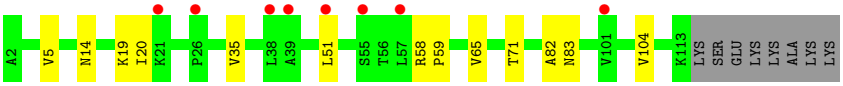
• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



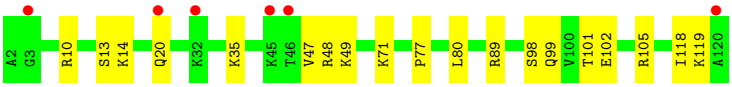
• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



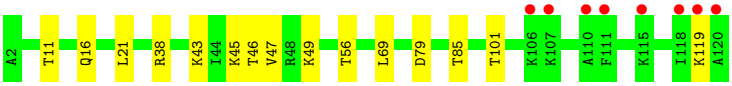
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



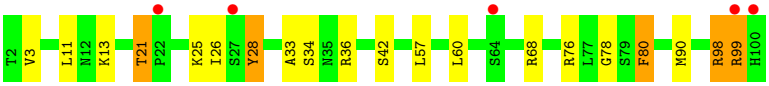
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



• Molecule 72: 60S ribosomal protein L36-A

Chain O6:

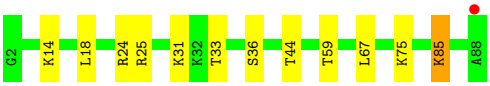


• Molecule 72: 60S ribosomal protein L36-A

Chain o6:

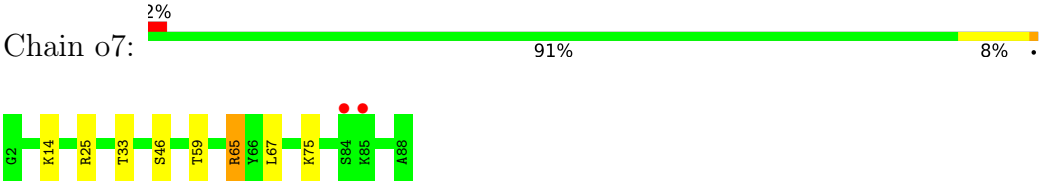
• Molecule 73: 60S ribosomal protein L37-A

Chain O7:



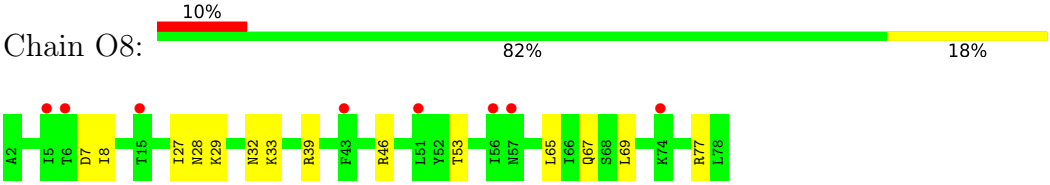
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



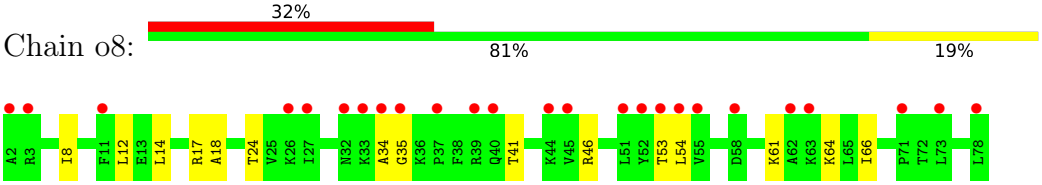
• Molecule 74: 60S ribosomal protein L38

Chain O8:



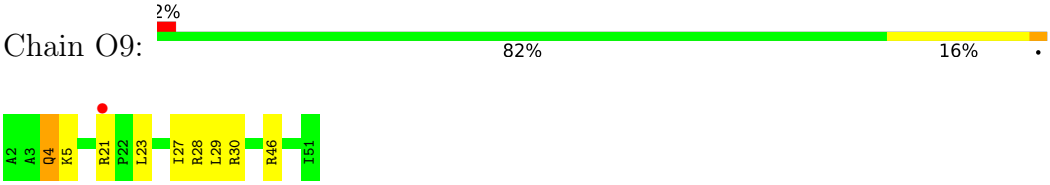
• Molecule 74: 60S ribosomal protein L38

Chain o8:



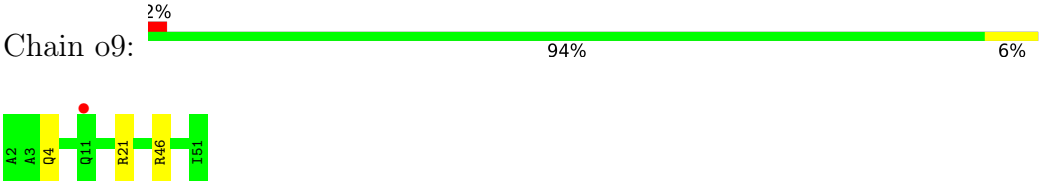
• Molecule 75: 60S ribosomal protein L39

Chain O9:



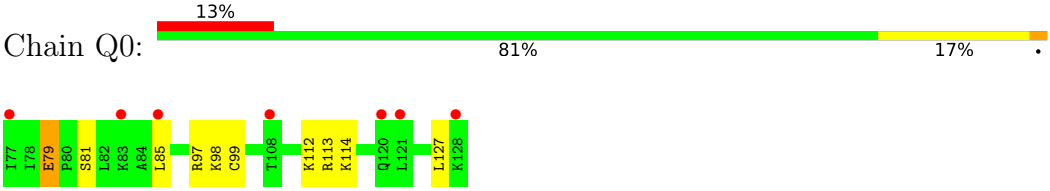
• Molecule 75: 60S ribosomal protein L39

Chain o9:



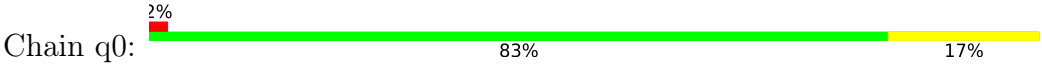
• Molecule 76: Ubiquitin-60S ribosomal protein L40

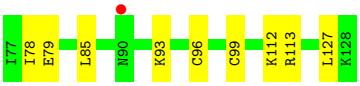
Chain Q0:



• Molecule 76: Ubiquitin-60S ribosomal protein L40

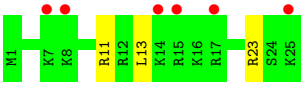
Chain q0:





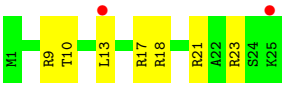
• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



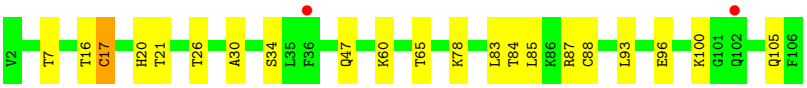
• Molecule 77: 60S ribosomal protein L41-A

Chain q1:



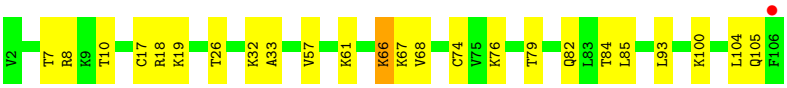
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



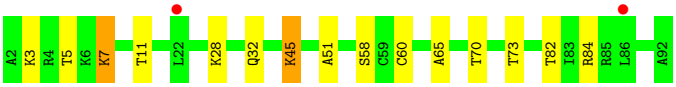
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



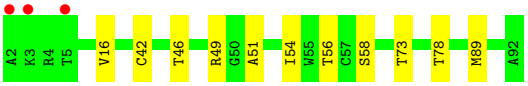
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



• Molecule 79: 60S ribosomal protein L43-A

Chain q3:

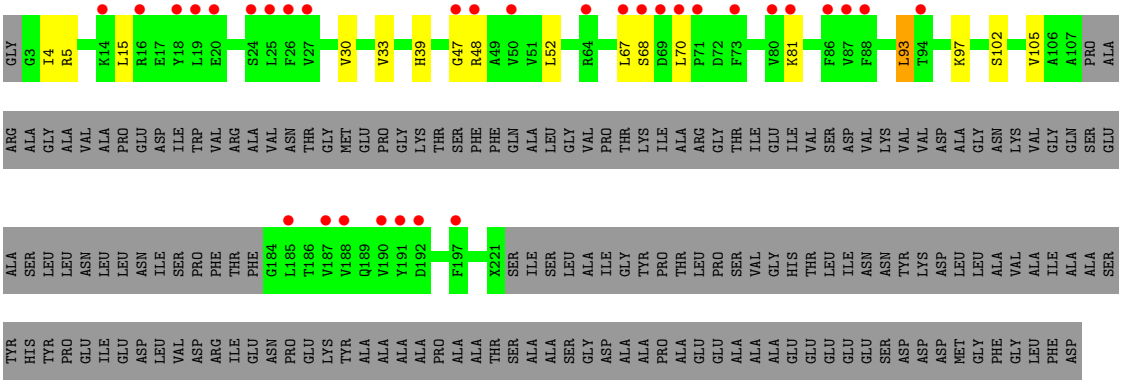


• Molecule 80: 60S ribosomal protein L12-A (uL11)

Chain m2:

• Molecule 81: 60S acidic ribosomal protein P0

Chain p0:



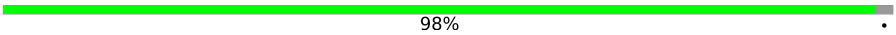
• Molecule 82: 60S ribosomal protein P1 alpha/P2 beta

Chain p1:

There are no outlier residues recorded for this chain.

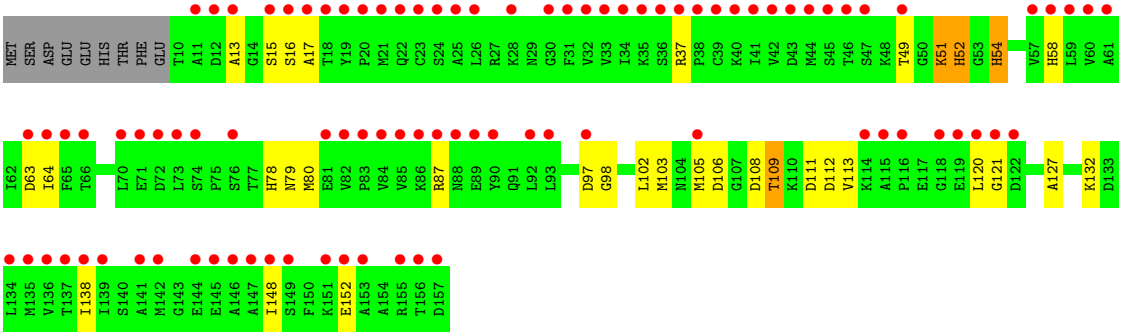
• Molecule 82: 60S ribosomal protein P1 alpha/P2 beta

Chain p2:



• Molecule 83: Eukaryotic translation initiation factor 5A-1

Chain f:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	435.58Å 287.33Å 303.82Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	99.53 – 3.30 99.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.53-3.30) 99.9 (99.53-3.30)	Depositor EDS
R_{merge}	0.59	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.310 0.255 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 74.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	404292	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CH, 8AN, SPS, MG, OHX, 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	2	0.36	0/42467	0.89	42/66169 (0.1%)
1	6	0.43	0/42790	0.93	50/66673 (0.1%)
2	S0	0.28	0/1617	0.50	0/2215
2	s0	0.29	0/1623	0.51	0/2222
3	S1	0.26	0/1735	0.50	0/2335
3	s1	0.32	0/1748	0.53	0/2352
4	S2	0.30	0/1665	0.52	0/2263
4	s2	0.33	0/1665	0.55	1/2263 (0.0%)
5	S3	0.29	0/1759	0.47	0/2368
5	s3	0.27	0/1759	0.47	0/2368
6	S4	0.29	0/2109	0.53	0/2839
6	s4	0.34	0/2109	0.55	0/2839
7	S5	0.27	0/1629	0.50	0/2202
7	s5	0.28	0/1629	0.48	0/2202
8	S6	0.29	0/1823	0.47	0/2439
8	s6	0.33	0/1779	0.53	0/2379
9	S7	0.28	0/1506	0.53	1/2028 (0.0%)
9	s7	0.29	0/1516	0.52	0/2043
10	S8	0.30	0/1514	0.51	0/2021
10	s8	0.34	0/1514	0.52	0/2021
11	S9	0.29	0/1519	0.48	0/2035
11	s9	0.31	0/1519	0.50	0/2035
12	C0	0.28	0/725	0.44	0/978
12	c0	0.27	0/713	0.51	1/961 (0.1%)
13	C1	0.31	0/1185	0.50	0/1598
13	c1	0.36	0/1185	0.55	0/1598
14	C2	0.26	0/819	0.49	0/1109
14	c2	0.22	0/819	0.47	0/1109
15	C3	0.31	0/1215	0.52	1/1638 (0.1%)
15	c3	0.33	0/1215	0.51	0/1638
16	C4	0.26	0/901	0.51	0/1217
16	c4	0.30	0/960	0.54	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.31	0/988	0.54	0/1327
17	c5	0.29	0/1030	0.52	0/1384
18	C6	0.29	0/1125	0.54	2/1510 (0.1%)
18	c6	0.29	0/1131	0.51	0/1518
19	C7	0.30	0/935	0.52	0/1254
19	c7	0.27	0/914	0.50	0/1224
20	C8	0.30	0/1211	0.51	0/1628
20	c8	0.28	0/1211	0.49	0/1628
21	C9	0.29	0/1130	0.48	0/1517
21	c9	0.29	0/1130	0.47	0/1517
22	D0	0.30	0/865	0.52	0/1169
22	d0	0.29	0/892	0.49	0/1205
23	D1	0.29	0/693	0.49	0/935
23	d1	0.31	0/693	0.50	0/935
24	D2	0.30	0/1038	0.55	1/1395 (0.1%)
24	d2	0.35	0/1038	0.56	1/1395 (0.1%)
25	D3	0.35	0/1139	0.55	0/1518
25	d3	0.38	0/1139	0.57	0/1518
26	D4	0.29	0/1087	0.47	0/1449
26	d4	0.31	0/1087	0.51	0/1449
27	D5	0.26	0/571	0.55	0/768
27	d5	0.26	0/566	0.47	0/761
28	D6	0.29	0/782	0.53	0/1047
28	d6	0.34	0/782	0.53	0/1047
29	D7	0.29	0/620	0.51	0/838
29	d7	0.28	0/620	0.49	0/838
30	D8	0.27	0/499	0.47	0/670
30	d8	0.28	0/499	0.49	0/670
31	D9	0.32	0/452	0.55	1/600 (0.2%)
31	d9	0.33	0/452	0.50	0/600
32	E0	0.28	0/483	0.48	0/643
32	e0	0.32	0/499	0.54	0/665
33	E1	0.29	0/577	0.56	0/770
33	e1	0.29	0/619	0.58	0/822
34	SR	0.26	0/2490	0.49	0/3389
34	sR	0.25	0/2495	0.44	0/3395
35	SM	0.31	0/925	0.54	1/1240 (0.1%)
35	sM	0.31	0/480	0.53	0/642
36	1	0.56	0/75394	1.03	115/117545 (0.1%)
36	5	0.59	2/75865 (0.0%)	1.05	143/118275 (0.1%)
37	3	0.46	0/2883	0.91	0/4491
37	7	0.55	0/2883	1.00	2/4491 (0.0%)
38	4	0.53	0/3746	1.00	5/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	8	0.52	0/3746	0.97	2/5832 (0.0%)
39	L2	0.37	0/1948	0.57	0/2617
39	l2	0.40	0/1946	0.62	0/2614
40	L3	0.39	0/3146	0.56	0/4228
40	l3	0.45	0/3146	0.58	0/4228
41	L4	0.41	0/2800	0.61	0/3790
41	l4	0.41	1/2800 (0.0%)	0.63	2/3790 (0.1%)
42	L5	0.35	0/2425	0.53	0/3271
42	l5	0.42	0/2408	0.55	0/3248
43	L6	0.39	0/1260	0.55	0/1694
43	l6	0.41	0/1269	0.57	0/1705
44	L7	0.42	0/1821	0.59	0/2451
44	l7	0.43	0/1828	0.62	2/2461 (0.1%)
45	L8	0.31	0/1836	0.53	0/2481
45	l8	0.32	0/1796	0.51	0/2431
46	L9	0.36	0/1539	0.56	0/2073
46	l9	0.40	0/1539	0.57	0/2073
47	M0	0.40	1/1741 (0.1%)	0.55	0/2335
47	m0	0.43	0/1758	0.61	2/2358 (0.1%)
48	M1	0.31	0/1374	0.50	0/1842
48	m1	0.38	0/1374	0.59	1/1842 (0.1%)
49	M3	0.40	0/1568	0.59	0/2106
49	m3	0.37	0/1573	0.57	0/2113
50	M4	0.40	0/1068	0.54	0/1438
50	m4	0.41	0/1074	0.57	0/1446
51	M5	0.38	0/1757	0.56	0/2354
51	m5	0.36	0/1757	0.55	0/2354
52	M6	0.44	0/1585	0.59	0/2128
52	m6	0.50	0/1585	0.61	0/2128
53	M7	0.41	0/1443	0.58	0/1944
53	m7	0.44	0/1250	0.59	0/1683
54	M8	0.39	0/1465	0.60	0/1965
54	m8	0.39	0/1465	0.60	0/1965
55	M9	0.31	0/1538	0.49	0/2050
55	m9	0.34	0/1538	0.51	0/2050
56	N0	0.39	0/1481	0.56	0/1990
56	n0	0.44	0/1481	0.59	0/1990
57	N1	0.40	0/1300	0.56	1/1743 (0.1%)
57	n1	0.43	0/1300	0.55	0/1743
58	N2	0.30	0/812	0.48	0/1099
58	n2	0.32	0/794	0.52	0/1076
59	N3	0.39	0/1018	0.57	0/1369
59	n3	0.45	0/1018	0.61	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	N4	0.31	0/712	0.50	0/958
60	n4	0.35	0/1052	0.51	0/1398
61	N5	0.33	0/979	0.55	0/1321
61	n5	0.36	0/974	0.57	0/1314
62	N6	0.35	0/1004	0.62	2/1341 (0.1%)
62	n6	0.35	0/1004	0.57	0/1341
63	N7	0.30	0/1118	0.50	0/1497
63	n7	0.31	0/1118	0.51	0/1497
64	N8	0.41	0/1204	0.62	0/1612
64	n8	0.40	0/1204	0.61	0/1612
65	N9	0.38	0/473	0.60	0/629
65	n9	0.43	0/473	0.67	0/629
66	O0	0.30	0/751	0.47	0/1008
66	o0	0.31	0/775	0.52	0/1040
67	O1	0.34	0/890	0.52	0/1196
67	o1	0.41	0/897	0.60	0/1205
68	O2	0.43	0/1041	0.63	0/1394
68	o2	0.44	0/1041	0.62	0/1394
69	O3	0.48	0/868	0.56	0/1168
69	o3	0.48	0/868	0.58	0/1168
70	O4	0.34	0/890	0.54	0/1189
70	o4	0.34	0/890	0.58	0/1189
71	O5	0.37	0/978	0.57	0/1301
71	o5	0.34	0/974	0.53	0/1297
72	O6	0.37	0/778	0.60	0/1034
72	o6	0.34	0/777	0.54	0/1033
73	O7	0.42	0/696	0.61	0/923
73	o7	0.40	0/696	0.59	0/923
74	O8	0.30	0/618	0.47	0/826
74	o8	0.31	0/614	0.54	0/822
75	O9	0.39	0/443	0.58	0/588
75	o9	0.39	0/443	0.53	0/588
76	Q0	0.43	0/423	0.60	0/562
76	q0	0.45	0/423	0.55	0/562
77	Q1	0.36	0/234	0.59	0/300
77	q1	0.43	0/234	0.62	0/300
78	Q2	0.53	1/860 (0.1%)	0.63	0/1136
78	q2	0.52	1/860 (0.1%)	0.63	1/1136 (0.1%)
79	Q3	0.37	0/701	0.59	0/934
79	q3	0.43	0/701	0.56	0/934
81	p0	0.27	0/977	0.48	0/1313
83	f	0.34	0/1131	0.58	0/1522
84	B	0.31	0/15	0.54	0/20

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
84	C	0.41	0/15	0.80	0/20
All	All	0.46	6/431576 (0.0%)	0.85	380/633602 (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
18	c6	0	1
19	C7	0	1
27	D5	0	1
39	l2	0	1
44	L7	0	1
52	M6	0	1
64	n8	0	1
65	N9	0	1
65	n9	0	1
83	f	0	1
All	All	0	10

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	8.77	1.97	1.82
78	Q2	17	CYS	CB-SG	7.99	1.95	1.82
36	5	1152	G	N9-C4	-5.86	1.33	1.38
36	5	942	U	C4-O4	5.25	1.27	1.23
47	M0	8	CYS	CB-SG	-5.03	1.73	1.81

The worst 5 of 380 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C4-N9	-11.60	119.04	126.00
36	5	1152	G	N3-C4-C5	11.31	134.25	128.60
36	5	2726	C	C6-N1-C2	-9.68	116.43	120.30
36	5	1152	G	C2-N3-C4	-9.61	107.10	111.90
36	1	406	G	O4'-C1'-N9	9.54	115.83	108.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
44	L7	157	ASN	Peptide
52	M6	110	PRO	Peptide
65	N9	20	GLY	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S0	204/251 (81%)	151 (74%)	30 (15%)	23 (11%)	0 2
2	s0	204/251 (81%)	164 (80%)	25 (12%)	15 (7%)	1 7
3	S1	212/254 (84%)	152 (72%)	38 (18%)	22 (10%)	0 3
3	s1	214/254 (84%)	168 (78%)	33 (15%)	13 (6%)	1 10
4	S2	215/253 (85%)	168 (78%)	33 (15%)	14 (6%)	1 9
4	s2	215/253 (85%)	168 (78%)	33 (15%)	14 (6%)	1 9
5	S3	221/239 (92%)	187 (85%)	26 (12%)	8 (4%)	3 20
5	s3	221/239 (92%)	176 (80%)	35 (16%)	10 (4%)	2 15
6	S4	258/260 (99%)	202 (78%)	46 (18%)	10 (4%)	3 18
6	s4	258/260 (99%)	189 (73%)	53 (20%)	16 (6%)	1 10
7	S5	204/224 (91%)	155 (76%)	37 (18%)	12 (6%)	1 10
7	s5	204/224 (91%)	160 (78%)	29 (14%)	15 (7%)	1 7
8	S6	224/236 (95%)	193 (86%)	22 (10%)	9 (4%)	3 18
8	s6	216/236 (92%)	182 (84%)	22 (10%)	12 (6%)	2 11
9	S7	182/189 (96%)	134 (74%)	27 (15%)	21 (12%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	s7	184/189 (97%)	152 (83%)	20 (11%)	12 (6%)	1	9
10	S8	184/200 (92%)	151 (82%)	24 (13%)	9 (5%)	2	14
10	s8	184/200 (92%)	157 (85%)	20 (11%)	7 (4%)	3	19
11	S9	183/196 (93%)	149 (81%)	23 (13%)	11 (6%)	1	10
11	s9	183/196 (93%)	147 (80%)	27 (15%)	9 (5%)	2	14
12	C0	82/96 (85%)	71 (87%)	8 (10%)	3 (4%)	3	20
12	c0	82/96 (85%)	56 (68%)	16 (20%)	10 (12%)	0	1
13	C1	143/155 (92%)	116 (81%)	18 (13%)	9 (6%)	1	9
13	c1	143/155 (92%)	115 (80%)	21 (15%)	7 (5%)	2	14
14	C2	107/142 (75%)	70 (65%)	27 (25%)	10 (9%)	0	4
14	c2	107/142 (75%)	75 (70%)	22 (21%)	10 (9%)	0	4
15	C3	148/150 (99%)	124 (84%)	20 (14%)	4 (3%)	5	26
15	c3	148/150 (99%)	116 (78%)	23 (16%)	9 (6%)	1	10
16	C4	125/136 (92%)	81 (65%)	33 (26%)	11 (9%)	1	5
16	c4	126/136 (93%)	96 (76%)	15 (12%)	15 (12%)	0	2
17	C5	121/141 (86%)	95 (78%)	12 (10%)	14 (12%)	0	2
17	c5	128/141 (91%)	98 (77%)	19 (15%)	11 (9%)	1	5
18	C6	139/142 (98%)	116 (84%)	14 (10%)	9 (6%)	1	9
18	c6	140/142 (99%)	118 (84%)	13 (9%)	9 (6%)	1	9
19	C7	116/136 (85%)	82 (71%)	23 (20%)	11 (10%)	0	4
19	c7	113/136 (83%)	93 (82%)	13 (12%)	7 (6%)	1	10
20	C8	143/145 (99%)	116 (81%)	17 (12%)	10 (7%)	1	7
20	c8	143/145 (99%)	120 (84%)	16 (11%)	7 (5%)	2	14
21	C9	141/143 (99%)	115 (82%)	18 (13%)	8 (6%)	1	11
21	c9	141/143 (99%)	120 (85%)	15 (11%)	6 (4%)	2	16
22	D0	105/120 (88%)	89 (85%)	9 (9%)	7 (7%)	1	8
22	d0	108/120 (90%)	89 (82%)	14 (13%)	5 (5%)	2	15
23	D1	85/87 (98%)	66 (78%)	11 (13%)	8 (9%)	0	4
23	d1	85/87 (98%)	63 (74%)	17 (20%)	5 (6%)	1	10
24	D2	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	6	28
24	d2	127/129 (98%)	107 (84%)	17 (13%)	3 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D3	142/144 (99%)	109 (77%)	21 (15%)	12 (8%)	1	5
25	d3	142/144 (99%)	117 (82%)	20 (14%)	5 (4%)	3	21
26	D4	132/134 (98%)	109 (83%)	13 (10%)	10 (8%)	1	6
26	d4	132/134 (98%)	110 (83%)	15 (11%)	7 (5%)	2	12
27	D5	68/107 (64%)	48 (71%)	13 (19%)	7 (10%)	0	3
27	d5	67/107 (63%)	51 (76%)	15 (22%)	1 (2%)	10	38
28	D6	95/97 (98%)	56 (59%)	21 (22%)	18 (19%)	0	1
28	d6	95/97 (98%)	66 (70%)	20 (21%)	9 (10%)	0	4
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	3	19
29	d7	79/81 (98%)	61 (77%)	14 (18%)	4 (5%)	2	13
30	D8	61/66 (92%)	50 (82%)	9 (15%)	2 (3%)	4	22
30	d8	61/66 (92%)	47 (77%)	11 (18%)	3 (5%)	2	14
31	D9	51/55 (93%)	39 (76%)	9 (18%)	3 (6%)	1	10
31	d9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	18
32	E0	58/62 (94%)	46 (79%)	10 (17%)	2 (3%)	3	22
32	e0	60/62 (97%)	40 (67%)	12 (20%)	8 (13%)	0	1
33	E1	69/76 (91%)	35 (51%)	17 (25%)	17 (25%)	0	0
33	e1	74/76 (97%)	36 (49%)	21 (28%)	17 (23%)	0	0
34	SR	316/318 (99%)	263 (83%)	36 (11%)	17 (5%)	2	12
34	sR	316/318 (99%)	252 (80%)	53 (17%)	11 (4%)	3	21
35	SM	120/273 (44%)	91 (76%)	18 (15%)	11 (9%)	1	4
35	sM	61/273 (22%)	42 (69%)	11 (18%)	8 (13%)	0	1
39	L2	250/253 (99%)	213 (85%)	27 (11%)	10 (4%)	3	18
39	l2	250/253 (99%)	205 (82%)	30 (12%)	15 (6%)	1	10
40	L3	384/386 (100%)	316 (82%)	49 (13%)	19 (5%)	2	14
40	l3	384/386 (100%)	330 (86%)	39 (10%)	15 (4%)	3	18
41	L4	359/361 (99%)	291 (81%)	46 (13%)	22 (6%)	1	10
41	l4	359/361 (99%)	296 (82%)	43 (12%)	20 (6%)	2	11
42	L5	294/296 (99%)	232 (79%)	44 (15%)	18 (6%)	1	10
42	l5	292/296 (99%)	248 (85%)	38 (13%)	6 (2%)	7	31
43	L6	152/175 (87%)	122 (80%)	27 (18%)	3 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	5	27
44	L7	220/243 (90%)	185 (84%)	24 (11%)	11 (5%)	2	14
44	l7	221/243 (91%)	192 (87%)	21 (10%)	8 (4%)	3	20
45	L8	231/255 (91%)	190 (82%)	30 (13%)	11 (5%)	2	14
45	l8	229/255 (90%)	174 (76%)	40 (18%)	15 (7%)	1	8
46	L9	189/191 (99%)	145 (77%)	29 (15%)	15 (8%)	1	6
46	l9	189/191 (99%)	158 (84%)	24 (13%)	7 (4%)	3	20
47	M0	207/220 (94%)	161 (78%)	37 (18%)	9 (4%)	2	16
47	m0	209/220 (95%)	169 (81%)	29 (14%)	11 (5%)	2	12
48	M1	167/173 (96%)	128 (77%)	27 (16%)	12 (7%)	1	7
48	m1	167/173 (96%)	145 (87%)	9 (5%)	13 (8%)	1	6
49	M3	191/198 (96%)	153 (80%)	30 (16%)	8 (4%)	3	17
49	m3	192/198 (97%)	152 (79%)	27 (14%)	13 (7%)	1	8
50	M4	134/137 (98%)	116 (87%)	12 (9%)	6 (4%)	2	15
50	m4	135/137 (98%)	117 (87%)	15 (11%)	3 (2%)	6	30
51	M5	201/203 (99%)	175 (87%)	20 (10%)	6 (3%)	4	24
51	m5	201/203 (99%)	178 (89%)	18 (9%)	5 (2%)	5	27
52	M6	195/198 (98%)	174 (89%)	12 (6%)	9 (5%)	2	15
52	m6	195/198 (98%)	172 (88%)	20 (10%)	3 (2%)	10	38
53	M7	181/183 (99%)	151 (83%)	25 (14%)	5 (3%)	5	25
53	m7	153/183 (84%)	137 (90%)	14 (9%)	2 (1%)	12	40
54	M8	183/185 (99%)	156 (85%)	20 (11%)	7 (4%)	3	19
54	m8	183/185 (99%)	154 (84%)	21 (12%)	8 (4%)	2	16
55	M9	186/188 (99%)	164 (88%)	17 (9%)	5 (3%)	5	26
55	m9	186/188 (99%)	164 (88%)	20 (11%)	2 (1%)	14	45
56	N0	170/172 (99%)	151 (89%)	15 (9%)	4 (2%)	6	28
56	n0	170/172 (99%)	159 (94%)	9 (5%)	2 (1%)	13	42
57	N1	157/159 (99%)	131 (83%)	20 (13%)	6 (4%)	3	19
57	n1	157/159 (99%)	138 (88%)	16 (10%)	3 (2%)	8	34
58	N2	98/120 (82%)	73 (74%)	20 (20%)	5 (5%)	2	13
58	n2	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	N3	134/136 (98%)	117 (87%)	12 (9%)	5 (4%)	3	20
59	n3	134/136 (98%)	122 (91%)	4 (3%)	8 (6%)	1	10
60	N4	96/155 (62%)	66 (69%)	21 (22%)	9 (9%)	0	4
60	n4	133/155 (86%)	102 (77%)	23 (17%)	8 (6%)	1	10
61	N5	119/141 (84%)	103 (87%)	12 (10%)	4 (3%)	3	22
61	n5	118/141 (84%)	91 (77%)	17 (14%)	10 (8%)	1	5
62	N6	124/126 (98%)	104 (84%)	19 (15%)	1 (1%)	19	51
62	n6	124/126 (98%)	102 (82%)	17 (14%)	5 (4%)	3	18
63	N7	133/135 (98%)	112 (84%)	12 (9%)	9 (7%)	1	8
63	n7	133/135 (98%)	100 (75%)	26 (20%)	7 (5%)	2	12
64	N8	146/148 (99%)	113 (77%)	26 (18%)	7 (5%)	2	14
64	n8	146/148 (99%)	110 (75%)	25 (17%)	11 (8%)	1	7
65	N9	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	3	20
65	n9	56/58 (97%)	41 (73%)	9 (16%)	6 (11%)	0	3
66	O0	95/104 (91%)	83 (87%)	11 (12%)	1 (1%)	14	45
66	o0	98/104 (94%)	86 (88%)	10 (10%)	2 (2%)	7	32
67	O1	107/112 (96%)	96 (90%)	6 (6%)	5 (5%)	2	14
67	o1	107/112 (96%)	85 (79%)	15 (14%)	7 (6%)	1	9
68	O2	125/129 (97%)	110 (88%)	11 (9%)	4 (3%)	4	22
68	o2	125/129 (97%)	105 (84%)	16 (13%)	4 (3%)	4	22
69	O3	104/106 (98%)	96 (92%)	6 (6%)	2 (2%)	8	34
69	o3	104/106 (98%)	93 (89%)	9 (9%)	2 (2%)	8	34
70	O4	110/120 (92%)	96 (87%)	11 (10%)	3 (3%)	5	26
70	o4	110/120 (92%)	88 (80%)	18 (16%)	4 (4%)	3	20
71	O5	117/119 (98%)	95 (81%)	12 (10%)	10 (8%)	1	5
71	o5	117/119 (98%)	94 (80%)	21 (18%)	2 (2%)	9	35
72	O6	97/99 (98%)	76 (78%)	12 (12%)	9 (9%)	0	4
72	o6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	0	3
73	O7	85/87 (98%)	69 (81%)	14 (16%)	2 (2%)	6	28
73	o7	85/87 (98%)	70 (82%)	14 (16%)	1 (1%)	13	42
74	O8	75/77 (97%)	66 (88%)	7 (9%)	2 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
74	o8	75/77 (97%)	61 (81%)	9 (12%)	5 (7%)	1 8
75	O9	48/50 (96%)	35 (73%)	10 (21%)	3 (6%)	1 9
75	o9	48/50 (96%)	39 (81%)	9 (19%)	0	100 100
76	Q0	50/52 (96%)	43 (86%)	6 (12%)	1 (2%)	7 32
76	q0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	7 32
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100 100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2 16
78	Q2	103/105 (98%)	85 (82%)	13 (13%)	5 (5%)	2 14
78	q2	103/105 (98%)	88 (85%)	9 (9%)	6 (6%)	1 11
79	Q3	89/91 (98%)	70 (79%)	13 (15%)	6 (7%)	1 8
79	q3	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	14 45
81	p0	117/311 (38%)	97 (83%)	14 (12%)	6 (5%)	2 13
83	f	146/157 (93%)	91 (62%)	35 (24%)	20 (14%)	0 1
All	All	22316/24284 (92%)	18108 (81%)	2992 (13%)	1216 (5%)	2 12

5 of 1216 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	95	ALA
2	S0	158	VAL
2	S0	190	ASP
2	S0	192	THR
3	S1	35	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S0	164/209 (78%)	143 (87%)	21 (13%)	4 18
2	s0	165/209 (79%)	140 (85%)	25 (15%)	3 13
3	S1	191/223 (86%)	169 (88%)	22 (12%)	5 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	s1	192/223 (86%)	164 (85%)	28 (15%)	3	14
4	S2	176/204 (86%)	155 (88%)	21 (12%)	5	21
4	s2	176/204 (86%)	141 (80%)	35 (20%)	1	5
5	S3	182/194 (94%)	157 (86%)	25 (14%)	3	16
5	s3	182/194 (94%)	162 (89%)	20 (11%)	6	24
6	S4	221/221 (100%)	192 (87%)	29 (13%)	4	17
6	s4	221/221 (100%)	188 (85%)	33 (15%)	3	13
7	S5	173/190 (91%)	157 (91%)	16 (9%)	9	31
7	s5	173/190 (91%)	147 (85%)	26 (15%)	3	13
8	S6	188/201 (94%)	165 (88%)	23 (12%)	5	20
8	s6	187/201 (93%)	165 (88%)	22 (12%)	5	21
9	S7	165/169 (98%)	145 (88%)	20 (12%)	5	20
9	s7	165/169 (98%)	150 (91%)	15 (9%)	9	31
10	S8	150/161 (93%)	136 (91%)	14 (9%)	9	30
10	s8	150/161 (93%)	131 (87%)	19 (13%)	4	19
11	S9	158/165 (96%)	133 (84%)	25 (16%)	2	11
11	s9	158/165 (96%)	132 (84%)	26 (16%)	2	10
12	C0	77/77 (100%)	71 (92%)	6 (8%)	12	38
12	c0	73/77 (95%)	66 (90%)	7 (10%)	8	29
13	C1	129/129 (100%)	117 (91%)	12 (9%)	9	30
13	c1	129/129 (100%)	113 (88%)	16 (12%)	4	19
14	C2	88/106 (83%)	73 (83%)	15 (17%)	2	9
14	c2	88/106 (83%)	80 (91%)	8 (9%)	9	31
15	C3	127/127 (100%)	110 (87%)	17 (13%)	4	16
15	c3	127/127 (100%)	110 (87%)	17 (13%)	4	16
16	C4	81/104 (78%)	67 (83%)	14 (17%)	2	8
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	5
17	C5	101/113 (89%)	91 (90%)	10 (10%)	8	28
17	c5	103/113 (91%)	89 (86%)	14 (14%)	3	16
18	C6	117/118 (99%)	103 (88%)	14 (12%)	5	20
18	c6	118/118 (100%)	102 (86%)	16 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	C7	94/124 (76%)	79 (84%)	15 (16%)	2	11
19	c7	92/124 (74%)	82 (89%)	10 (11%)	6	24
20	C8	128/128 (100%)	104 (81%)	24 (19%)	1	6
20	c8	128/128 (100%)	109 (85%)	19 (15%)	3	13
21	C9	115/115 (100%)	99 (86%)	16 (14%)	3	16
21	c9	115/115 (100%)	98 (85%)	17 (15%)	3	13
22	D0	100/113 (88%)	91 (91%)	9 (9%)	9	32
22	d0	103/113 (91%)	91 (88%)	12 (12%)	5	21
23	D1	74/74 (100%)	65 (88%)	9 (12%)	5	20
23	d1	74/74 (100%)	66 (89%)	8 (11%)	6	24
24	D2	110/110 (100%)	94 (86%)	16 (14%)	3	14
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2	12
25	D3	119/119 (100%)	105 (88%)	14 (12%)	5	21
25	d3	119/119 (100%)	109 (92%)	10 (8%)	11	35
26	D4	112/112 (100%)	103 (92%)	9 (8%)	12	37
26	d4	112/112 (100%)	97 (87%)	15 (13%)	4	16
27	D5	61/88 (69%)	48 (79%)	13 (21%)	1	4
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	10
28	D6	83/83 (100%)	73 (88%)	10 (12%)	5	20
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2	12
29	D7	70/70 (100%)	62 (89%)	8 (11%)	5	22
29	d7	70/70 (100%)	62 (89%)	8 (11%)	5	22
30	D8	56/59 (95%)	48 (86%)	8 (14%)	3	15
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2	8
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	9
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	4
32	E0	51/53 (96%)	47 (92%)	4 (8%)	12	38
32	e0	53/53 (100%)	39 (74%)	14 (26%)	0	1
33	E1	62/66 (94%)	51 (82%)	11 (18%)	2	8
33	e1	66/66 (100%)	55 (83%)	11 (17%)	2	10
34	SR	259/261 (99%)	227 (88%)	32 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	sR	260/261 (100%)	243 (94%)	17 (6%)	17	46
35	SM	97/183 (53%)	79 (81%)	18 (19%)	1	7
35	sM	54/183 (30%)	46 (85%)	8 (15%)	3	13
39	L2	193/195 (99%)	166 (86%)	27 (14%)	3	16
39	l2	192/195 (98%)	161 (84%)	31 (16%)	2	10
40	L3	319/322 (99%)	267 (84%)	52 (16%)	2	10
40	l3	319/322 (99%)	261 (82%)	58 (18%)	1	7
41	L4	288/288 (100%)	252 (88%)	36 (12%)	4	19
41	l4	288/288 (100%)	248 (86%)	40 (14%)	3	16
42	L5	244/244 (100%)	208 (85%)	36 (15%)	3	13
42	l5	243/244 (100%)	200 (82%)	43 (18%)	2	8
43	L6	134/152 (88%)	116 (87%)	18 (13%)	4	16
43	l6	135/152 (89%)	115 (85%)	20 (15%)	3	13
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	18
44	l7	187/204 (92%)	164 (88%)	23 (12%)	4	20
45	L8	187/207 (90%)	165 (88%)	22 (12%)	5	21
45	l8	177/207 (86%)	153 (86%)	24 (14%)	3	16
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	4
46	l9	171/171 (100%)	143 (84%)	28 (16%)	2	10
47	M0	177/186 (95%)	144 (81%)	33 (19%)	1	7
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	9
48	M1	147/150 (98%)	117 (80%)	30 (20%)	1	4
48	m1	147/150 (98%)	125 (85%)	22 (15%)	3	13
49	M3	154/158 (98%)	133 (86%)	21 (14%)	3	16
49	m3	154/158 (98%)	127 (82%)	27 (18%)	2	8
50	M4	107/108 (99%)	93 (87%)	14 (13%)	4	17
50	m4	108/108 (100%)	94 (87%)	14 (13%)	4	17
51	M5	175/175 (100%)	151 (86%)	24 (14%)	3	16
51	m5	175/175 (100%)	154 (88%)	21 (12%)	5	20
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2	10
52	m6	160/161 (99%)	139 (87%)	21 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	M7	140/145 (97%)	120 (86%)	20 (14%)	3	15
53	m7	125/145 (86%)	106 (85%)	19 (15%)	3	13
54	M8	150/150 (100%)	132 (88%)	18 (12%)	5	20
54	m8	150/150 (100%)	126 (84%)	24 (16%)	2	11
55	M9	153/153 (100%)	136 (89%)	17 (11%)	6	23
55	m9	153/153 (100%)	133 (87%)	20 (13%)	4	17
56	N0	156/156 (100%)	132 (85%)	24 (15%)	2	12
56	n0	156/156 (100%)	133 (85%)	23 (15%)	3	14
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	4
57	n1	136/136 (100%)	113 (83%)	23 (17%)	2	9
58	N2	87/106 (82%)	79 (91%)	8 (9%)	9	31
58	n2	85/106 (80%)	73 (86%)	12 (14%)	3	16
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	16
59	n3	104/104 (100%)	91 (88%)	13 (12%)	4	19
60	N4	57/129 (44%)	52 (91%)	5 (9%)	10	33
60	n4	100/129 (78%)	95 (95%)	5 (5%)	24	55
61	N5	104/117 (89%)	83 (80%)	21 (20%)	1	5
61	n5	104/117 (89%)	90 (86%)	14 (14%)	4	16
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	8
62	n6	109/109 (100%)	93 (85%)	16 (15%)	3	14
63	N7	115/115 (100%)	99 (86%)	16 (14%)	3	16
63	n7	115/115 (100%)	97 (84%)	18 (16%)	2	12
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2	9
64	n8	118/118 (100%)	101 (86%)	17 (14%)	3	15
65	N9	46/46 (100%)	40 (87%)	6 (13%)	4	17
65	n9	46/46 (100%)	41 (89%)	5 (11%)	6	24
66	O0	81/87 (93%)	69 (85%)	12 (15%)	3	13
66	o0	84/87 (97%)	72 (86%)	12 (14%)	3	15
67	O1	92/96 (96%)	80 (87%)	12 (13%)	4	17
67	o1	94/96 (98%)	76 (81%)	18 (19%)	1	6
68	O2	109/110 (99%)	94 (86%)	15 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
68	o2	109/110 (99%)	87 (80%)	22 (20%)	1 5
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2 10
69	o3	90/90 (100%)	76 (84%)	14 (16%)	2 12
70	O4	95/102 (93%)	84 (88%)	11 (12%)	5 22
70	o4	95/102 (93%)	86 (90%)	9 (10%)	8 29
71	O5	104/104 (100%)	95 (91%)	9 (9%)	10 34
71	o5	103/104 (99%)	90 (87%)	13 (13%)	4 19
72	O6	81/81 (100%)	65 (80%)	16 (20%)	1 5
72	o6	80/81 (99%)	59 (74%)	21 (26%)	0 2
73	O7	70/70 (100%)	59 (84%)	11 (16%)	2 12
73	o7	70/70 (100%)	62 (89%)	8 (11%)	5 22
74	O8	68/68 (100%)	56 (82%)	12 (18%)	2 8
74	o8	67/68 (98%)	57 (85%)	10 (15%)	3 13
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2 12
75	o9	45/45 (100%)	42 (93%)	3 (7%)	16 45
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1 4
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2 9
77	Q1	23/23 (100%)	20 (87%)	3 (13%)	4 17
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0 2
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2 8
78	q2	90/90 (100%)	72 (80%)	18 (20%)	1 5
79	Q3	71/71 (100%)	60 (84%)	11 (16%)	2 12
79	q3	71/71 (100%)	61 (86%)	10 (14%)	3 16
81	p0	105/232 (45%)	93 (89%)	12 (11%)	5 22
83	f	124/133 (93%)	107 (86%)	17 (14%)	3 16
All	All	18849/20177 (93%)	16179 (86%)	2670 (14%)	3 15

5 of 2670 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	sM	43	ASP
54	m8	86	THR
40	l3	110	LEU

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Mol	Chain	Res	Type
35	sM	23	LYS
45	l8	74	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
26	d4	34	ASN
53	m7	137	ASN
32	e0	17	GLN
45	l8	59	GLN
65	n9	12	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	455 (25%)	40 (2%)
1	6	1791/1800 (99%)	447 (24%)	29 (1%)
36	1	3145/3396 (92%)	672 (21%)	53 (1%)
36	5	3163/3396 (93%)	649 (20%)	52 (1%)
37	3	120/121 (99%)	11 (9%)	0
37	7	120/121 (99%)	13 (10%)	0
38	4	157/158 (99%)	32 (20%)	3 (1%)
38	8	157/158 (99%)	34 (21%)	0
All	All	10429/10950 (95%)	2313 (22%)	177 (1%)

5 of 2313 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	6	G
1	2	17	C
1	2	23	G

5 of 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	6	1097	U
36	5	1331	U
1	6	1481	C

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Mol	Chain	Res	Type
36	5	916	G
36	5	1816	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 28 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
88	OHX	1	3406	-	0,6,6	-	-	-		
88	OHX	5	3406	-	0,6,6	-	-	-		
86	SPS	1	3401	-	20,23,23	3.43	10 (50%)	18,30,30	2.96	6 (33%)
88	OHX	1	3405	-	0,6,6	-	-	-		
86	SPS	B	3401	87	20,23,23	3.42	11 (55%)	18,30,30	3.02	7 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPS	B	3401	87	-	3/15/18/18	0/1/1/1
86	SPS	1	3401	-	-	3/15/18/18	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	3401	SPS	C9-C10	-8.24	1.31	1.48
86	B	3401	SPS	C9-C10	-7.97	1.31	1.48
86	B	3401	SPS	C9-C8	7.78	1.53	1.33
86	1	3401	SPS	C9-C8	7.48	1.52	1.33
86	B	3401	SPS	O13-C13	-5.45	1.19	1.42

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	B	3401	SPS	C3-N2-C1	8.31	122.15	115.14
86	1	3401	SPS	C3-N2-C1	7.60	121.56	115.14
86	1	3401	SPS	C6-C1-N2	-7.07	119.47	124.40
86	B	3401	SPS	C6-C1-N2	-6.31	120.00	124.40
86	B	3401	SPS	C18-S17-C16	3.98	111.12	100.10

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

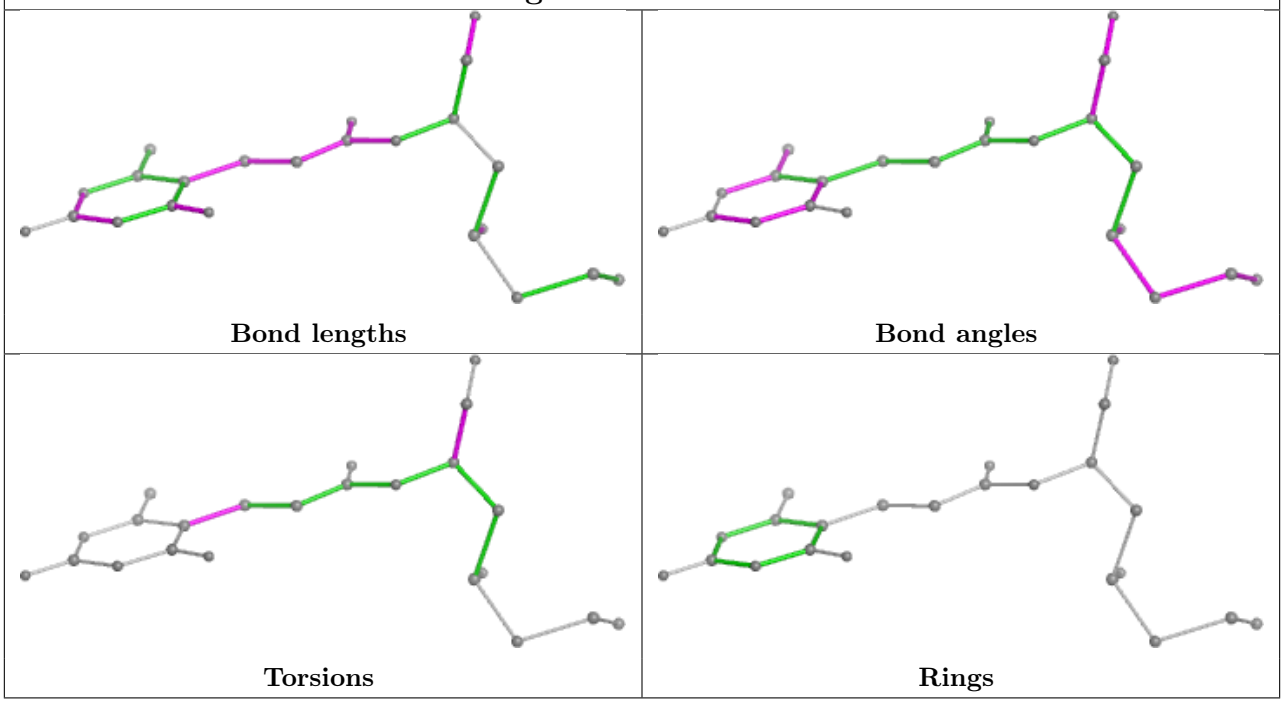
Mol	Chain	Res	Type	Atoms
86	B	3401	SPS	N11-C12-C13-O13
86	1	3401	SPS	C14-C12-C13-O13
86	B	3401	SPS	C14-C12-C13-O13
86	1	3401	SPS	N11-C12-C13-O13
86	1	3401	SPS	C5-C6-C8-C9

There are no ring outliers.

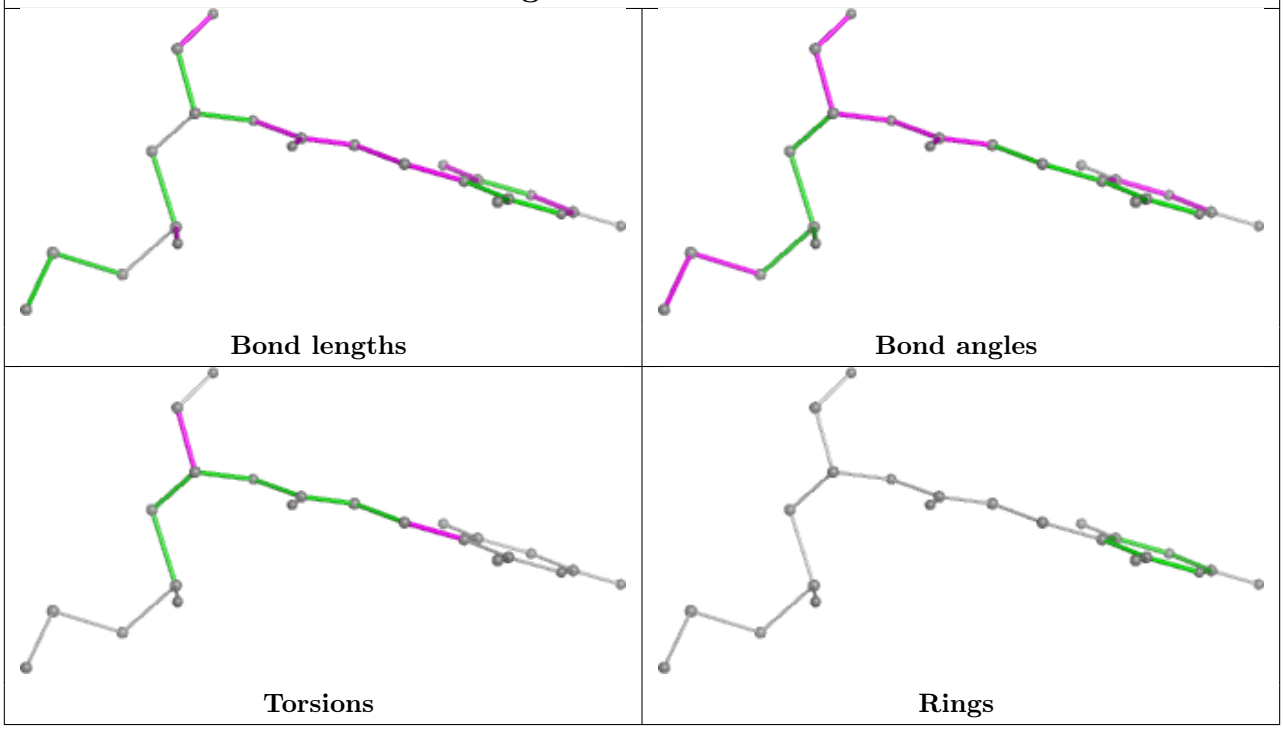
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SPS 1 3401



Ligand SPS B 3401



5.7 Other polymers (i)

10 such residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
84	CH	C	75	84,87	16,21,22	0.96	2 (12%)	20,30,33	1.91	2 (10%)
84	CH	B	75	84,87	16,21,22	0.73	0	20,30,33	1.91	2 (10%)
84	8AN	B	76	84,87	19,24,25	1.06	1 (5%)	13,35,38	1.55	3 (23%)
84	CH	C	74	84	16,18,22	0.92	1 (6%)	20,26,33	1.75	2 (10%)
84	8AN	C	76	84,87	19,24,25	1.11	1 (5%)	13,35,38	1.52	2 (15%)
84	CH	B	74	84	16,21,22	1.02	1 (6%)	20,30,33	1.81	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	CH	C	75	84,87	-	1/5/25/26	0/2/2/2
84	CH	B	75	84,87	-	0/5/25/26	0/2/2/2
84	8AN	B	76	84,87	-	3/3/25/26	0/3/3/3
84	CH	C	74	84	-	2/4/22/26	0/2/2/2
84	8AN	C	76	84,87	-	3/3/25/26	0/3/3/3
84	CH	B	74	84	-	0/5/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	B	74	CH	C4-N3	-2.99	1.33	1.37
84	C	74	CH	C4-N3	-2.79	1.33	1.37
84	B	76	8AN	C5-C4	2.61	1.47	1.40
84	C	75	CH	C5-C4	2.46	1.43	1.39
84	C	76	8AN	C5-C4	2.34	1.47	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	B	74	CH	C5-C4-N3	7.27	122.18	118.04
84	C	75	CH	C5-C4-N3	7.25	122.17	118.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	B	75	CH	C5-C4-N3	6.07	121.50	118.04
84	C	74	CH	C5-C4-N3	5.87	121.38	118.04
84	B	75	CH	C5-C4-N4	-5.28	118.74	123.88

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	C	74	CH	C3'-C4'-C5'-O5'
84	C	74	CH	O4'-C4'-C5'-O5'
84	C	76	8AN	C3'-C4'-C5'-O5'
84	B	76	8AN	C3'-C4'-C5'-O5'
84	C	76	8AN	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
80	m2	2
35	sM	1
35	SM	1
12	c0	1
36	5	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	38.68
1	SM	141:ALA	C	151:UNK	N	26.53
1	c0	84:UNK	C	87:UNK	N	8.84
1	2	1716:C	O3'	1717:G	P	5.83
1	5	2437:G	O3'	2438:A	P	4.00

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	2	1781/1800 (98%)	0.48	91 (5%)	28	26	60, 98, 170, 210	0
1	6	1795/1800 (99%)	0.27	58 (3%)	47	46	44, 86, 157, 204	0
2	S0	206/251 (82%)	1.22	50 (24%)	0	0	100, 112, 123, 128	0
2	s0	206/251 (82%)	1.16	50 (24%)	0	0	80, 97, 111, 117	0
3	S1	214/254 (84%)	1.60	76 (35%)	0	0	110, 145, 169, 175	0
3	s1	216/254 (85%)	1.03	44 (20%)	1	1	80, 96, 114, 123	0
4	S2	217/253 (85%)	0.73	30 (13%)	2	2	83, 96, 109, 113	0
4	s2	217/253 (85%)	0.45	9 (4%)	37	35	68, 79, 93, 108	0
5	S3	223/239 (93%)	0.67	25 (11%)	5	5	91, 100, 123, 128	0
5	s3	223/239 (93%)	1.46	72 (32%)	0	0	86, 112, 131, 137	0
6	S4	260/260 (100%)	1.31	66 (25%)	0	0	77, 99, 107, 124	0
6	s4	260/260 (100%)	1.20	60 (23%)	0	1	60, 82, 92, 119	0
7	S5	206/224 (91%)	1.21	39 (18%)	1	1	104, 124, 131, 134	0
7	s5	206/224 (91%)	0.62	21 (10%)	6	6	87, 108, 123, 130	0
8	S6	226/236 (95%)	0.85	41 (18%)	1	1	77, 105, 126, 132	0
8	s6	218/236 (92%)	0.49	21 (9%)	8	8	60, 89, 106, 114	0
9	S7	184/189 (97%)	0.90	30 (16%)	1	2	102, 121, 136, 142	0
9	s7	186/189 (98%)	0.67	23 (12%)	4	3	77, 104, 130, 134	0
10	S8	188/200 (94%)	0.78	20 (10%)	6	6	70, 86, 119, 129	0
10	s8	188/200 (94%)	1.01	28 (14%)	2	2	56, 73, 113, 130	0
11	S9	185/196 (94%)	1.69	71 (38%)	0	0	89, 106, 130, 141	0
11	s9	185/196 (94%)	1.21	43 (23%)	0	1	71, 88, 115, 126	0
12	C0	83/96 (86%)	2.34	52 (62%)	0	0	94, 112, 122, 126	0
12	c0	83/96 (86%)	2.04	40 (48%)	0	0	103, 131, 145, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	C1	144/155 (92%)	1.04	21 (14%)	2	2	73, 83, 101, 113	0
13	c1	144/155 (92%)	0.84	9 (6%)	20	20	59, 70, 91, 113	0
14	C2	108/142 (76%)	0.53	14 (12%)	3	3	137, 145, 150, 152	0
14	c2	108/142 (76%)	0.82	15 (13%)	2	2	167, 183, 196, 199	0
15	C3	150/150 (100%)	0.59	16 (10%)	6	5	82, 95, 111, 115	0
15	c3	150/150 (100%)	0.14	5 (3%)	46	44	66, 79, 95, 100	0
16	C4	127/136 (93%)	1.42	35 (27%)	0	0	84, 142, 156, 161	0
16	c4	128/136 (94%)	1.53	43 (33%)	0	0	67, 101, 113, 116	0
17	C5	122/141 (86%)	0.94	21 (17%)	1	1	88, 99, 111, 117	0
17	c5	129/141 (91%)	0.67	16 (12%)	4	3	86, 103, 113, 119	0
18	C6	141/142 (99%)	1.70	46 (32%)	0	0	91, 112, 117, 120	0
18	c6	142/142 (100%)	0.81	25 (17%)	1	1	83, 102, 115, 126	0
19	C7	120/136 (88%)	1.44	32 (26%)	0	0	97, 109, 125, 129	0
19	c7	117/136 (86%)	0.37	10 (8%)	10	10	88, 101, 115, 119	0
20	C8	145/145 (100%)	0.95	24 (16%)	1	2	85, 110, 131, 138	0
20	c8	145/145 (100%)	0.81	23 (15%)	1	2	86, 101, 116, 126	0
21	C9	143/143 (100%)	1.40	37 (25%)	0	0	96, 112, 122, 126	0
21	c9	143/143 (100%)	1.63	51 (35%)	0	0	85, 97, 112, 118	0
22	D0	107/120 (89%)	0.98	20 (18%)	1	1	86, 112, 123, 125	0
22	d0	110/120 (91%)	2.37	58 (52%)	0	0	84, 114, 138, 147	0
23	D1	87/87 (100%)	0.91	16 (18%)	1	1	96, 104, 119, 127	0
23	d1	87/87 (100%)	0.70	9 (10%)	6	6	76, 88, 104, 112	0
24	D2	129/129 (100%)	0.64	11 (8%)	10	10	83, 95, 101, 109	0
24	d2	129/129 (100%)	0.47	10 (7%)	13	12	64, 74, 81, 87	0
25	D3	144/144 (100%)	0.81	18 (12%)	3	3	69, 77, 86, 96	0
25	d3	144/144 (100%)	0.60	7 (4%)	29	27	56, 61, 71, 79	0
26	D4	134/134 (100%)	1.30	34 (25%)	0	0	86, 107, 118, 129	0
26	d4	134/134 (100%)	0.36	10 (7%)	14	13	68, 90, 105, 110	0
27	D5	70/107 (65%)	1.51	24 (34%)	0	0	119, 130, 139, 140	0
27	d5	69/107 (64%)	1.51	19 (27%)	0	0	99, 113, 123, 125	0
28	D6	97/97 (100%)	2.00	44 (45%)	0	0	88, 106, 154, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	1.37	26 (26%)	0	0	70, 87, 116, 123	0
29	D7	81/81 (100%)	1.23	17 (20%)	1	1	98, 110, 135, 141	0
29	d7	81/81 (100%)	0.94	13 (16%)	1	2	80, 93, 121, 128	0
30	D8	63/66 (95%)	1.20	13 (20%)	1	1	111, 127, 139, 143	0
30	d8	63/66 (95%)	1.06	10 (15%)	1	2	104, 116, 127, 129	0
31	D9	53/55 (96%)	1.26	12 (22%)	0	1	84, 91, 107, 112	0
31	d9	53/55 (96%)	2.26	26 (49%)	0	0	82, 92, 128, 139	0
32	E0	60/62 (96%)	1.83	21 (35%)	0	0	78, 107, 129, 134	0
32	e0	62/62 (100%)	0.84	11 (17%)	1	1	63, 88, 109, 122	0
33	E1	71/76 (93%)	0.66	9 (12%)	3	3	107, 133, 145, 148	0
33	e1	76/76 (100%)	1.08	20 (26%)	0	0	112, 158, 170, 175	0
34	SR	318/318 (100%)	1.49	102 (32%)	0	0	109, 120, 132, 146	0
34	sR	318/318 (100%)	1.56	105 (33%)	0	0	110, 126, 140, 150	0
35	SM	121/273 (44%)	0.86	22 (18%)	1	1	59, 94, 111, 116	0
35	sM	63/273 (23%)	1.59	22 (34%)	0	0	55, 105, 111, 112	0
36	1	3149/3396 (92%)	0.19	48 (1%)	73	72	35, 59, 123, 212	0
36	5	3169/3396 (93%)	0.21	48 (1%)	73	72	35, 54, 124, 188	0
37	3	121/121 (100%)	0.00	0	100	100	43, 76, 90, 96	0
37	7	121/121 (100%)	-0.09	0	100	100	39, 59, 70, 75	0
38	4	158/158 (100%)	0.12	2 (1%)	77	77	43, 61, 91, 130	0
38	8	158/158 (100%)	0.11	1 (0%)	89	90	43, 63, 96, 120	0
39	L2	252/253 (99%)	0.36	9 (3%)	42	40	42, 61, 77, 82	0
39	l2	252/253 (99%)	0.41	11 (4%)	34	33	43, 59, 74, 83	0
40	L3	386/386 (100%)	0.45	20 (5%)	27	25	42, 63, 77, 85	0
40	l3	386/386 (100%)	0.33	8 (2%)	63	62	34, 49, 62, 77	0
41	L4	361/361 (100%)	-0.03	0	100	100	40, 54, 70, 71	0
41	l4	361/361 (100%)	0.14	2 (0%)	89	90	40, 57, 73, 88	0
42	L5	296/296 (100%)	1.15	68 (22%)	0	1	58, 81, 97, 111	0
42	l5	294/296 (99%)	0.61	22 (7%)	14	13	49, 60, 84, 93	0
43	L6	156/175 (89%)	0.59	11 (7%)	16	16	49, 57, 72, 79	0
43	l6	157/175 (89%)	0.19	5 (3%)	47	46	49, 57, 75, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	L7	222/243 (91%)	0.19	3 (1%)	75	75	40, 49, 73, 106	0
44	l7	223/243 (91%)	-0.05	1 (0%)	92	93	39, 49, 80, 107	0
45	L8	233/255 (91%)	0.94	41 (17%)	1	1	67, 81, 104, 112	0
45	l8	231/255 (90%)	1.04	42 (18%)	1	1	73, 84, 106, 114	0
46	L9	191/191 (100%)	0.21	9 (4%)	31	29	60, 70, 82, 93	0
46	l9	191/191 (100%)	0.08	1 (0%)	91	91	44, 55, 71, 81	0
47	M0	211/220 (95%)	1.08	40 (18%)	1	1	45, 63, 92, 106	0
47	m0	213/220 (96%)	0.96	28 (13%)	3	3	40, 55, 80, 90	0
48	M1	169/173 (97%)	1.03	25 (14%)	2	2	68, 84, 94, 98	0
48	m1	169/173 (97%)	0.38	5 (2%)	50	49	52, 67, 77, 82	0
49	M3	193/198 (97%)	0.40	8 (4%)	37	35	39, 64, 92, 113	0
49	m3	194/198 (97%)	0.77	29 (14%)	2	2	41, 69, 100, 111	0
50	M4	136/137 (99%)	-0.04	2 (1%)	73	72	54, 61, 73, 83	0
50	m4	137/137 (100%)	-0.04	1 (0%)	87	88	48, 54, 69, 82	0
51	M5	203/203 (100%)	0.27	3 (1%)	73	72	41, 56, 66, 69	0
51	m5	203/203 (100%)	0.47	10 (4%)	29	27	44, 60, 71, 76	0
52	M6	197/198 (99%)	0.27	4 (2%)	65	64	42, 49, 65, 68	0
52	m6	197/198 (99%)	0.08	2 (1%)	82	82	34, 42, 64, 66	0
53	M7	183/183 (100%)	0.87	23 (12%)	3	3	47, 55, 98, 116	0
53	m7	155/183 (84%)	0.17	0	100	100	39, 46, 59, 77	0
54	M8	185/185 (100%)	0.22	3 (1%)	72	70	43, 55, 69, 88	0
54	m8	185/185 (100%)	0.11	0	100	100	42, 57, 66, 70	0
55	M9	188/188 (100%)	0.55	19 (10%)	7	6	65, 77, 135, 140	0
55	m9	188/188 (100%)	0.49	12 (6%)	19	19	51, 65, 121, 134	0
56	N0	172/172 (100%)	0.18	4 (2%)	60	59	49, 57, 69, 74	0
56	n0	172/172 (100%)	0.02	1 (0%)	89	90	43, 49, 59, 66	0
57	N1	159/159 (100%)	0.44	4 (2%)	57	54	42, 56, 93, 101	0
57	n1	159/159 (100%)	0.57	11 (6%)	16	16	40, 49, 83, 87	0
58	N2	100/120 (83%)	1.06	25 (25%)	0	0	93, 104, 120, 122	0
58	n2	98/120 (81%)	1.04	21 (21%)	0	1	75, 88, 94, 97	0
59	N3	136/136 (100%)	0.67	11 (8%)	12	11	51, 60, 70, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
59	n3	136/136 (100%)	0.41	3 (2%)	62	60	36, 45, 55, 58	0
60	N4	98/155 (63%)	1.83	29 (29%)	0	0	62, 72, 134, 147	0
60	n4	135/155 (87%)	0.74	19 (14%)	2	2	46, 91, 115, 116	0
61	N5	121/141 (85%)	0.80	14 (11%)	4	4	58, 69, 84, 95	0
61	n5	120/141 (85%)	0.27	1 (0%)	86	86	56, 68, 85, 93	0
62	N6	126/126 (100%)	0.84	19 (15%)	2	2	50, 62, 74, 79	0
62	n6	126/126 (100%)	0.42	4 (3%)	47	46	51, 64, 77, 83	0
63	N7	135/135 (100%)	1.78	49 (36%)	0	0	82, 94, 103, 109	0
63	n7	135/135 (100%)	1.44	43 (31%)	0	0	76, 91, 102, 105	0
64	N8	148/148 (100%)	0.36	2 (1%)	75	75	35, 56, 74, 82	0
64	n8	148/148 (100%)	0.16	3 (2%)	65	64	34, 59, 74, 77	0
65	N9	58/58 (100%)	0.54	4 (6%)	16	16	38, 61, 95, 106	0
65	n9	58/58 (100%)	0.36	5 (8%)	10	10	38, 58, 78, 85	0
66	O0	97/104 (93%)	0.64	9 (9%)	8	9	81, 89, 101, 102	0
66	o0	100/104 (96%)	0.44	2 (2%)	65	64	75, 82, 102, 108	0
67	O1	109/112 (97%)	0.97	14 (12%)	3	3	61, 72, 91, 103	0
67	o1	109/112 (97%)	0.45	4 (3%)	41	38	47, 58, 81, 90	0
68	O2	127/129 (98%)	0.16	2 (1%)	72	70	36, 49, 62, 68	0
68	o2	127/129 (98%)	0.54	7 (5%)	25	23	35, 52, 63, 71	0
69	O3	106/106 (100%)	0.31	1 (0%)	84	84	42, 47, 71, 78	0
69	o3	106/106 (100%)	0.14	0	100	100	40, 46, 69, 75	0
70	O4	112/120 (93%)	0.60	7 (6%)	20	20	57, 75, 101, 107	0
70	o4	112/120 (93%)	0.66	8 (7%)	16	16	50, 68, 99, 103	0
71	O5	119/119 (100%)	0.32	6 (5%)	28	27	55, 70, 78, 82	0
71	o5	119/119 (100%)	0.59	8 (6%)	17	17	59, 71, 87, 96	0
72	O6	99/99 (100%)	0.63	5 (5%)	28	26	60, 68, 91, 102	0
72	o6	99/99 (100%)	0.39	4 (4%)	38	36	64, 72, 88, 103	0
73	O7	87/87 (100%)	0.13	1 (1%)	80	81	43, 50, 65, 71	0
73	o7	87/87 (100%)	0.21	2 (2%)	60	59	41, 50, 73, 84	0
74	O8	77/77 (100%)	0.86	8 (10%)	6	6	83, 93, 108, 113	0
74	o8	77/77 (100%)	1.51	25 (32%)	0	0	77, 86, 94, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	O9	50/50 (100%)	0.49	1 (2%) 65 64	52, 57, 59, 60	0
75	o9	50/50 (100%)	0.27	1 (2%) 65 64	50, 55, 63, 63	0
76	Q0	52/52 (100%)	0.86	7 (13%) 3 3	53, 59, 74, 79	0
76	q0	52/52 (100%)	0.37	1 (1%) 66 65	41, 45, 55, 58	0
77	Q1	25/25 (100%)	1.26	6 (24%) 0 0	62, 66, 73, 74	0
77	q1	25/25 (100%)	0.99	2 (8%) 12 11	50, 56, 58, 58	0
78	Q2	105/105 (100%)	0.12	2 (1%) 66 65	41, 56, 76, 91	0
78	q2	105/105 (100%)	0.26	1 (0%) 82 82	44, 56, 70, 93	0
79	Q3	91/91 (100%)	0.21	2 (2%) 62 60	54, 65, 80, 85	0
79	q3	91/91 (100%)	0.38	3 (3%) 46 44	46, 59, 72, 84	0
80	m2	0/165	-	-	-	-
81	p0	120/311 (38%)	1.27	32 (26%) 0 0	101, 124, 144, 152	0
82	p1	0/47	-	-	-	-
82	p2	0/47	-	-	-	-
83	f	148/157 (94%)	2.86	92 (62%) 0 0	55, 96, 150, 153	75 (50%)
All	All	33080/35493 (93%)	0.60	3313 (10%) 7 7	34, 74, 132, 212	75 (0%)

The worst 5 of 3313 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	75	THR	13.9
1	2	1699	G	13.8
53	M7	161	ALA	12.0
1	2	1696	G	12.0
1	2	1697	G	11.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
85	ZN	e1	501	1/1	0.79	0.08	164,164,164,164	0
85	ZN	D7	101	1/1	0.81	0.21	141,141,141,141	0
85	ZN	d7	101	1/1	0.82	0.16	131,131,131,131	0
87	MG	5	3402	1/1	0.84	0.36	45,45,45,45	0
87	MG	1	3403	1/1	0.89	0.38	45,45,45,45	0
85	ZN	Q2	501	1/1	0.91	0.05	76,76,76,76	0
87	MG	1	3402	1/1	0.93	0.65	21,21,21,21	0
87	MG	f	1002	1/1	0.93	0.08	66,66,66,66	0
87	MG	1	3404	1/1	0.94	0.65	29,29,29,29	0
85	ZN	D6	500	1/1	0.94	0.07	105,105,105,105	0
86	SPS	1	3401	23/23	0.94	0.24	40,43,57,59	0
87	MG	C	101	1/1	0.94	0.31	49,49,49,49	0
87	MG	5	3405	1/1	0.95	0.74	42,42,42,42	0
87	MG	5	3401	1/1	0.95	0.38	41,41,41,41	0
87	MG	5	3404	1/1	0.95	0.48	36,36,36,36	0
87	MG	B	3402	1/1	0.96	0.32	40,40,40,40	0
86	SPS	B	3401	23/23	0.96	0.31	37,40,54,56	0
87	MG	f	1001	1/1	0.97	0.33	52,52,52,52	0
85	ZN	E1	501	1/1	0.97	0.05	136,136,136,136	0
85	ZN	d6	500	1/1	0.97	0.06	87,87,87,87	0
85	ZN	q2	501	1/1	0.97	0.05	77,77,77,77	0
85	ZN	D9	101	1/1	0.98	0.08	88,88,88,88	0
87	MG	5	3403	1/1	0.98	0.55	23,23,23,23	0
85	ZN	Q3	501	1/1	0.98	0.11	77,77,77,77	0
85	ZN	Q0	500	1/1	0.98	0.10	57,57,57,57	0
88	OHX	1	3405	7/7	0.98	0.09	91,91,91,91	0
88	OHX	5	3406	7/7	0.98	0.09	95,95,95,95	0
85	ZN	O7	100	1/1	0.99	0.14	52,52,52,52	0
85	ZN	o7	501	1/1	0.99	0.21	51,51,51,51	0
85	ZN	q0	500	1/1	0.99	0.13	42,42,42,42	0
88	OHX	1	3406	7/7	0.99	0.14	73,73,73,73	0
85	ZN	d9	101	1/1	0.99	0.09	94,94,94,94	0
85	ZN	q3	501	1/1	1.00	0.17	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.