wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 08:51 pm GMT

PDB ID	:	4U3N
Title	:	Crystal structure of CCA trinucleotide bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-22
Resolution	:	3.20 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 (1)) were used in the production of this report:

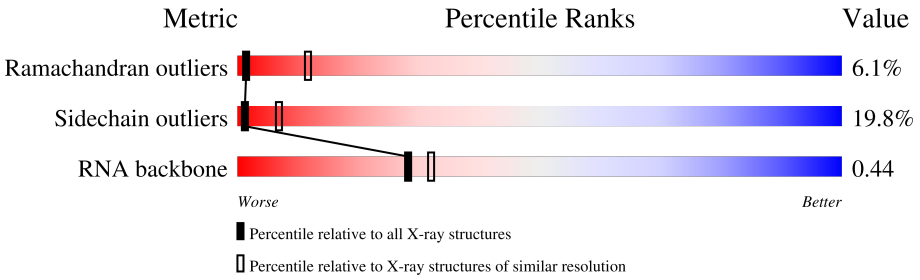
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	64% 29% • •
1	6	1800	64% 30% 5%
2	S0	251	64% 15% • 18%
2	s0	251	61% 20% • 18%
3	S1	254	57% 24% • 16%
3	s1	254	65% 19% • 15%
4	S2	253	63% 22% • 14%
4	s2	253	64% 20% • 14%

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Mol	Chain	Length	Quality of chain
5	S3	239	73% 17% 7%
5	s3	239	72% 20% 7%
6	S4	260	78% 21%
6	s4	260	79% 20%
7	S5	224	73% 18% 8%
7	s5	224	67% 23% 8%
8	S6	236	76% 19%
8	s6	236	73% 19% 8%
9	S7	189	72% 23%
9	s7	189	75% 21%
10	S8	200	74% 19% 6%
10	s8	200	74% 18% 6%
11	S9	196	73% 19% 6%
11	s9	196	76% 17% 6%
12	C0	105	71% 18% 9%
13	C1	155	78% 19%
13	c1	155	77% 15% 6%
14	C2	142	60% 24% 13%
14	c2	142	56% 29% 13%
15	C3	150	79% 18%
15	c3	150	78% 20%
16	C4	136	70% 19% 7%
16	c4	136	67% 26% 6%
17	C5	141	67% 18% 12%
17	c5	141	67% 26%

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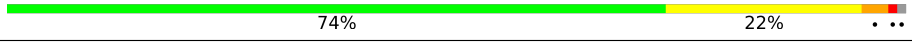
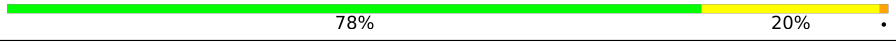
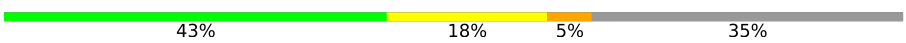
Mol	Chain	Length	Quality of chain
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	

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Mol	Chain	Length	Quality of chain
30	d8	66	67% 27% 5%
31	D9	55	82% 13%
31	d9	55	67% 29%
32	E0	60	85% 13%
33	E1	76	51% 37% 7%
34	SR	318	78% 21%
34	sR	318	89% 10%
35	SM	273	46% 11% 42%
35	sM	273	29% 8% 62%
36	1	3396	55% 32% 6% 7%
36	5	3396	54% 34% 6% 7%
37	3	121	79% 21%
37	7	121	62% 34%
38	4	158	61% 36%
38	8	158	65% 32%
39	L2	253	81% 17%
39	l2	253	80% 19%
40	L3	386	81% 18%
40	l3	386	82% 16%
41	L4	361	80% 18%
41	l4	361	80% 19%
42	L5	296	79% 19%
42	l5	296	80% 18%
43	L6	175	74% 15% 11%
43	l6	175	73% 16% 10%

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Mol	Chain	Length	Quality of chain
44	L7	243	79% 11% • 9%
44	l7	243	80% 11% • 8%
45	L8	255	74% 16% • 9%
45	l8	255	72% 18% • 9%
46	L9	191	81% 19% •
46	l9	191	77% 21% •
47	M0	220	74% 21% • •
47	m0	220	76% 19% • •
48	M1	173	73% 20% 5% •
48	m1	173	73% 22% • •
49	M3	198	77% 19% • •
49	m3	198	80% 16% • •
50	M4	137	80% 19% ••
50	m4	137	82% 16% •
51	M5	203	85% 14% •
51	m5	203	83% 16% •
52	M6	198	83% 15% •••
52	m6	198	84% 15% •••
53	M7	183	81% 18% •
53	m7	183	70% 15% 15%
54	M8	185	82% 17% •
54	m8	185	83% 17% •
55	M9	188	87% 13%
55	m9	188	81% 18% •
56	N0	172	80% 17% •

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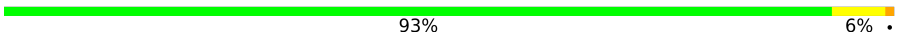
Mol	Chain	Length	Quality of chain
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	

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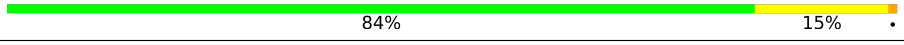
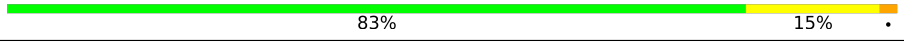
Mol	Chain	Length	Quality of chain
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	c0	105	
81	e0	62	
82	e1	76	

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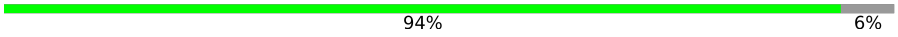
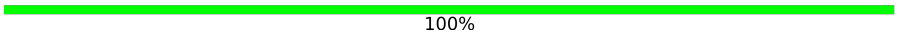
Mol	Chain	Length	Quality of chain
83	m2	160	
84	p0	311	
85	p1	47	
86	p2	46	

2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 411288 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
1	2	1750	Total	C	N	O	P	0	0	0
			37283	16668	6591	12274	1750			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47
c1	147	ALA	GLY	conflict	UNP P0CX47

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	104	ALA	GLY	conflict	UNP P48589
C2	110	ALA	GLY	conflict	UNP P48589
c2	104	ALA	GLY	conflict	UNP P48589
c2	110	ALA	GLY	conflict	UNP P48589

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total 1104	C 652	N 221	O 231	0	0	0
35	sM	104	Total 680	C 403	N 140	O 137	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total 67355	C 30086	N 12142	O 21978	P 3149	0	0	0
36	5	3150	Total 67376	C 30095	N 12145	O 21987	P 3149	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c0	89	ALA	GLY	conflict	UNP Q08745

- Molecule 81 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 83 is a protein called UNKNOWN PROTEIN m2.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
85	p1	47	Total 235	C 141	N 47	O 47	0	0	0

- Molecule 86 is a protein called UNKNOWN PROTEIN p2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
86	p2	46	Total 230	C 138	N 46	O 46	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	2	124	Total 124	Mg 124	0	0
87	S4	2	Total 2	Mg 2	0	0
87	S8	1	Total 1	Mg 1	0	0
87	D3	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	1	477	Total 477	Mg 477	0	0
87	3	14	Total 14	Mg 14	0	0
87	4	19	Total 19	Mg 19	0	0
87	L2	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	L3	3	Total Mg 3 3	0	0
87	L4	1	Total Mg 1 1	0	0
87	L5	1	Total Mg 1 1	0	0
87	L7	4	Total Mg 4 4	0	0
87	L8	1	Total Mg 1 1	0	0
87	M0	2	Total Mg 2 2	0	0
87	M1	1	Total Mg 1 1	0	0
87	M3	2	Total Mg 2 2	0	0
87	M5	2	Total Mg 2 2	0	0
87	M6	1	Total Mg 1 1	0	0
87	M7	4	Total Mg 4 4	0	0
87	M9	1	Total Mg 1 1	0	0
87	N0	1	Total Mg 1 1	0	0
87	N3	3	Total Mg 3 3	0	0
87	N5	1	Total Mg 1 1	0	0
87	N8	5	Total Mg 5 5	0	0
87	O2	1	Total Mg 1 1	0	0
87	O4	1	Total Mg 1 1	0	0
87	O5	1	Total Mg 1 1	0	0
87	O7	1	Total Mg 1 1	0	0
87	6	144	Total Mg 144 144	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	s1	1	Total Mg 1 1	0	0
87	s6	1	Total Mg 1 1	0	0
87	s8	3	Total Mg 3 3	0	0
87	c1	1	Total Mg 1 1	0	0
87	c7	2	Total Mg 2 2	0	0
87	c8	1	Total Mg 1 1	0	0
87	c9	1	Total Mg 1 1	0	0
87	d3	1	Total Mg 1 1	0	0
87	d4	1	Total Mg 1 1	0	0
87	d6	1	Total Mg 1 1	0	0
87	sM	1	Total Mg 1 1	0	0
87	5	502	Total Mg 502 502	0	0
87	7	15	Total Mg 15 15	0	0
87	8	16	Total Mg 16 16	0	0
87	l2	1	Total Mg 1 1	0	0
87	l3	3	Total Mg 3 3	0	0
87	l4	2	Total Mg 2 2	0	0
87	l5	2	Total Mg 2 2	0	0
87	l7	1	Total Mg 1 1	0	0
87	m1	2	Total Mg 2 2	0	0
87	m5	5	Total Mg 5 5	0	0

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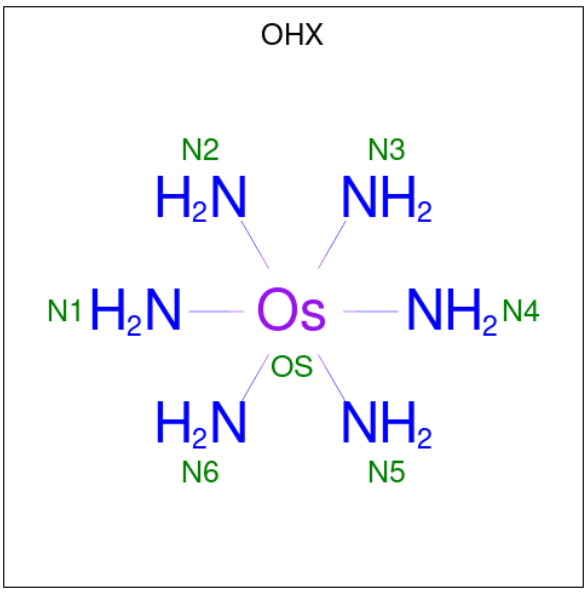
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	m6	2	Total Mg 2 2	0	0
87	m7	5	Total Mg 5 5	0	0
87	n0	3	Total Mg 3 3	0	0
87	n3	2	Total Mg 2 2	0	0
87	n6	2	Total Mg 2 2	0	0
87	n8	3	Total Mg 3 3	0	0
87	o1	1	Total Mg 1 1	0	0
87	o3	1	Total Mg 1 1	0	0
87	o4	1	Total Mg 1 1	0	0
87	q0	1	Total Mg 1 1	0	0
87	q1	1	Total Mg 1 1	0	0
87	q3	2	Total Mg 2 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0
88	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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88	L3	1	Total N Os 7 6 1	0	0
88	L3	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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88	M0	1	Total N Os 7 6 1	0	0
88	M5	1	Total N Os 7 6 1	0	0
88	M7	1	Total N Os 7 6 1	0	0
88	M7	1	Total N Os 7 6 1	0	0
88	M8	1	Total N Os 7 6 1	0	0
88	M9	1	Total N Os 7 6 1	0	0
88	N9	1	Total N Os 7 6 1	0	0
88	O3	1	Total N Os 7 6 1	0	0
88	O7	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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88	s1	1	Total N Os 7 6 1	0	0
88	s1	1	Total N Os 7 6 1	0	0
88	s8	1	Total N Os 7 6 1	0	0
88	c1	1	Total N Os 7 6 1	0	0
88	c3	1	Total N Os 7 6 1	0	0
88	c5	1	Total N Os 7 6 1	0	0
88	c8	1	Total N Os 7 6 1	0	0
88	d4	1	Total N Os 7 6 1	0	0
88	d9	1	Total N Os 7 6 1	0	0
88	sR	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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88	5	1	Total N Os 7 6 1	0	0
88	5	1	Total N Os 7 6 1	0	0
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88	5	1	Total N Os 7 6 1	0	0
88	5	1	Total N Os 7 6 1	0	0
88	5	1	Total N Os 7 6 1	0	0
88	5	1	Total N Os 7 6 1	0	0
88	5	1	Total N Os 7 6 1	0	0

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	7	1	Total N Os 7 6 1	0	0
88	7	1	Total N Os 7 6 1	0	0
88	7	1	Total N Os 7 6 1	0	0
88	7	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
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88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	8	1	Total N Os 7 6 1	0	0
88	l3	1	Total N Os 7 6 1	0	0
88	l3	1	Total N Os 7 6 1	0	0
88	l3	1	Total N Os 7 6 1	0	0

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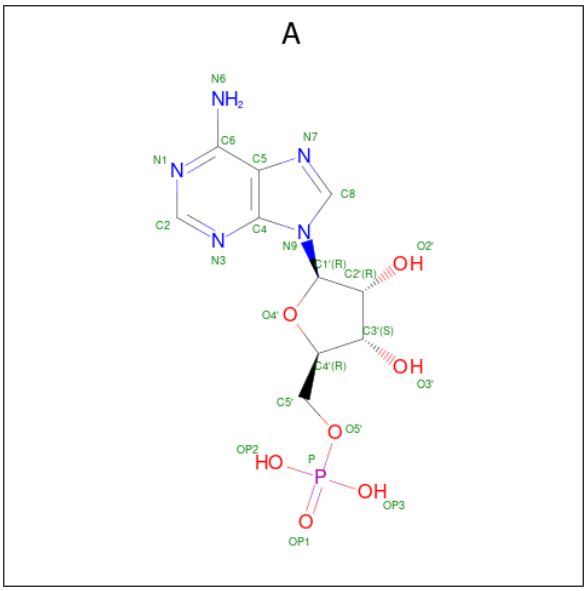
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	l4	1	Total N Os 7 6 1	0	0
88	l4	1	Total N Os 7 6 1	0	0
88	l5	1	Total N Os 7 6 1	0	0
88	l5	1	Total N Os 7 6 1	0	0
88	l5	1	Total N Os 7 6 1	0	0
88	l5	1	Total N Os 7 6 1	0	0
88	l9	1	Total N Os 7 6 1	0	0
88	m0	1	Total N Os 7 6 1	0	0
88	m0	1	Total N Os 7 6 1	0	0
88	m1	1	Total N Os 7 6 1	0	0
88	m4	1	Total N Os 7 6 1	0	0
88	m5	1	Total N Os 7 6 1	0	0
88	m6	1	Total N Os 7 6 1	0	0
88	n3	1	Total N Os 7 6 1	0	0
88	n3	1	Total N Os 7 6 1	0	0
88	n9	1	Total N Os 7 6 1	0	0
88	o3	1	Total N Os 7 6 1	0	0
88	o7	1	Total N Os 7 6 1	0	0
88	q2	1	Total N Os 7 6 1	0	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

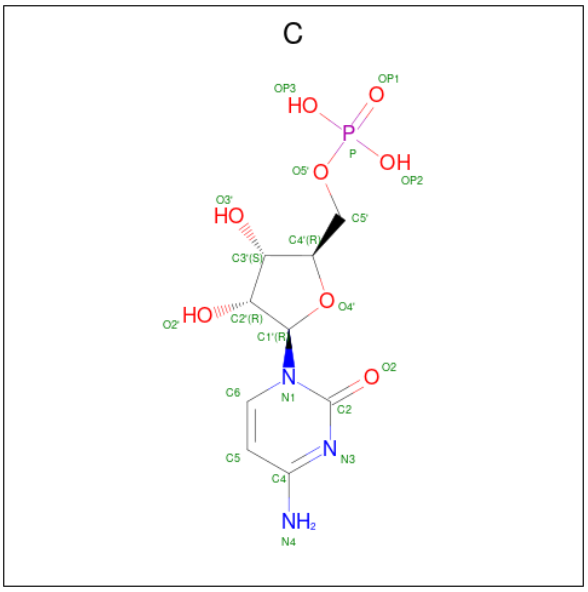
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	D6	1	Total Zn 1 1	0	0
89	D7	1	Total Zn 1 1	0	0
89	D9	1	Total Zn 1 1	0	0
89	E1	1	Total Zn 1 1	0	0
89	O7	1	Total Zn 1 1	0	0
89	Q0	1	Total Zn 1 1	0	0
89	Q2	1	Total Zn 1 1	0	0
89	Q3	1	Total Zn 1 1	0	0
89	d6	1	Total Zn 1 1	0	0
89	d7	1	Total Zn 1 1	0	0
89	d9	1	Total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

- Molecule 90 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
90	1	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
90	5	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 91 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

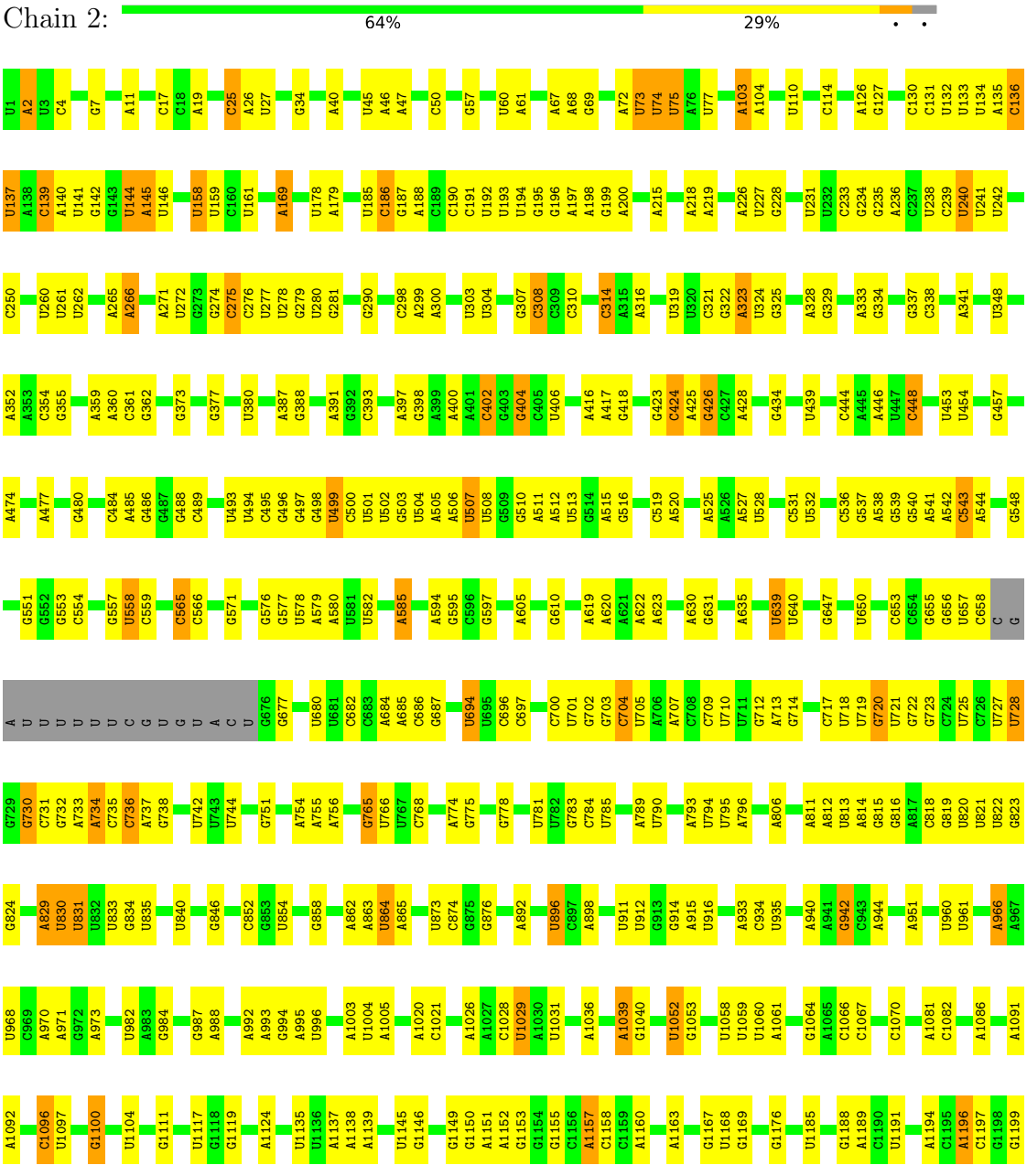
3 Residue-property plots (i)

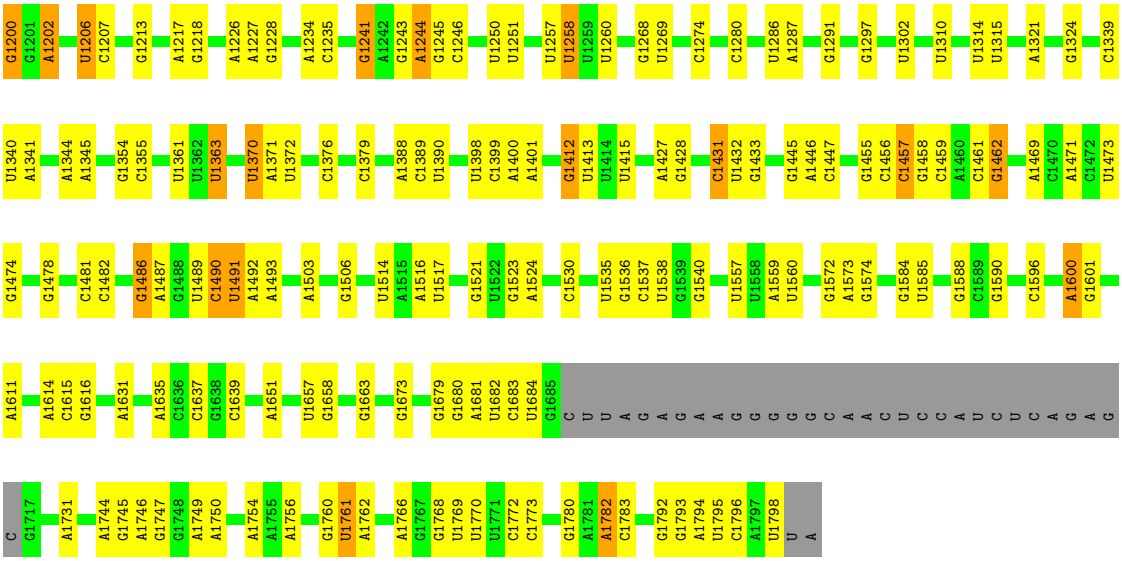
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

- Molecule 1: 18S ribosomal RNA

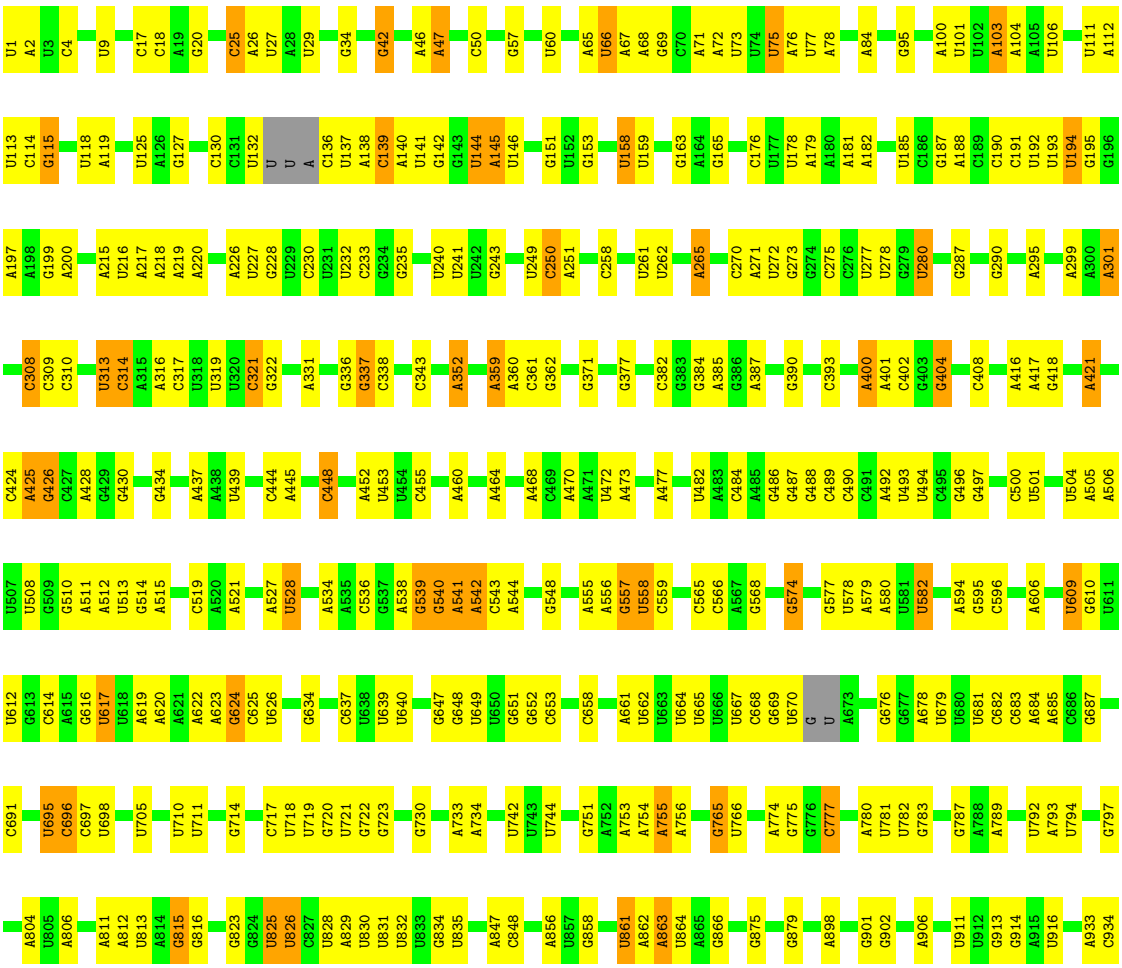
Chain 2:

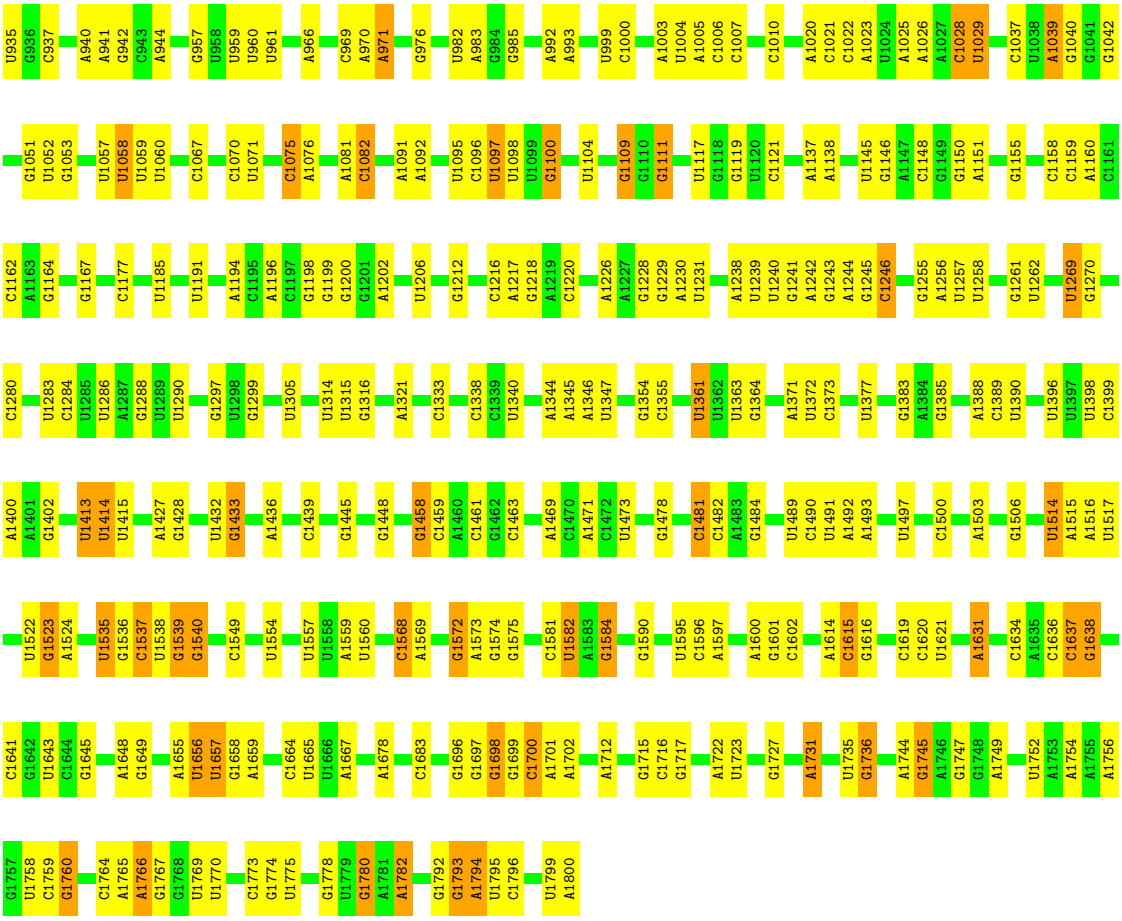




• Molecule 1: 18S ribosomal RNA

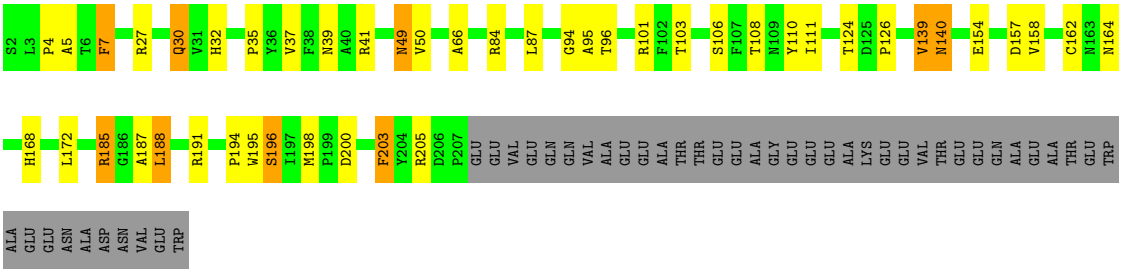
Chain 6:





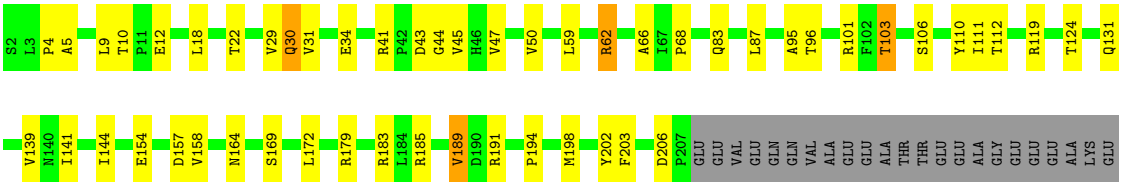
• Molecule 2: 40S ribosomal protein S0-A

Chain S0:



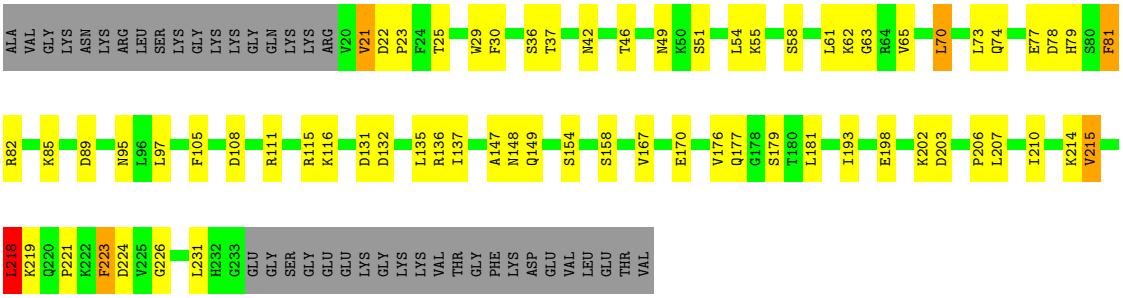
• Molecule 2: 40S ribosomal protein S0-A

Chain s0:



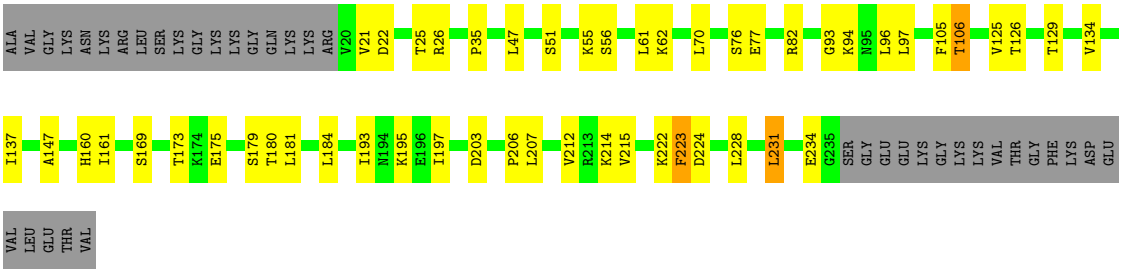
• Molecule 3: 40S ribosomal protein S1-A

Chain S1:



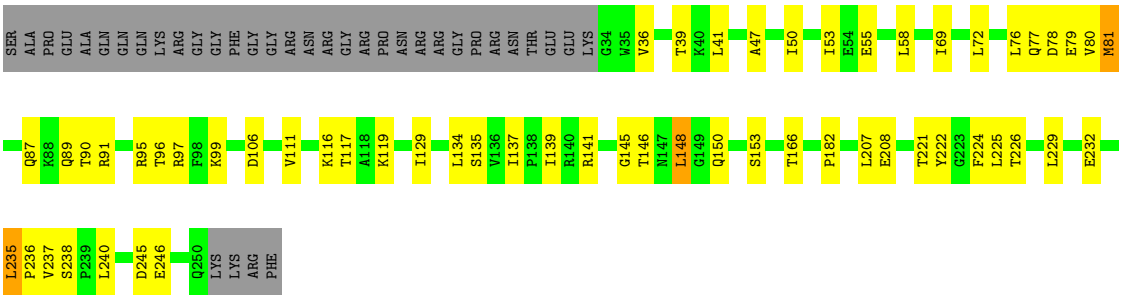
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



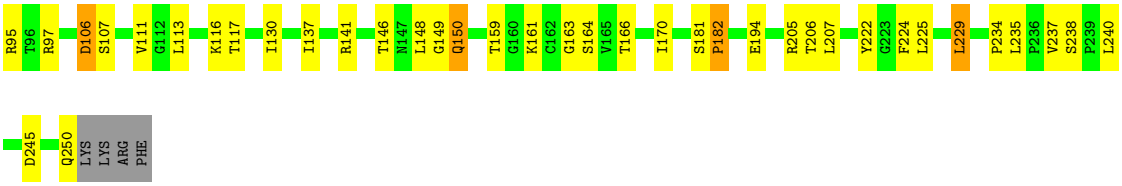
• Molecule 4: 40S ribosomal protein S2

Chain S2:



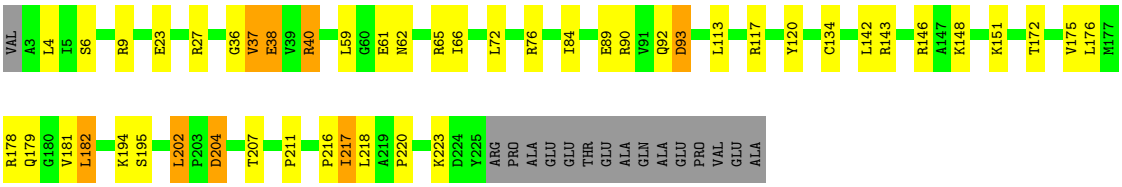
• Molecule 4: 40S ribosomal protein S2

Chain s2:



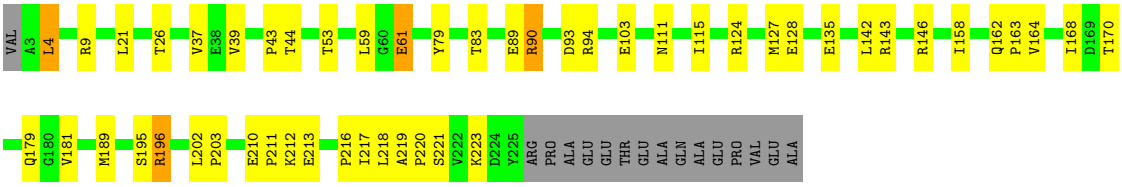
• Molecule 5: 40S ribosomal protein S3

Chain S3:



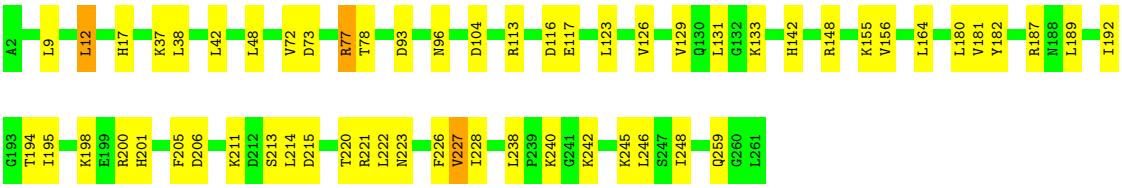
• Molecule 5: 40S ribosomal protein S3

Chain s3:



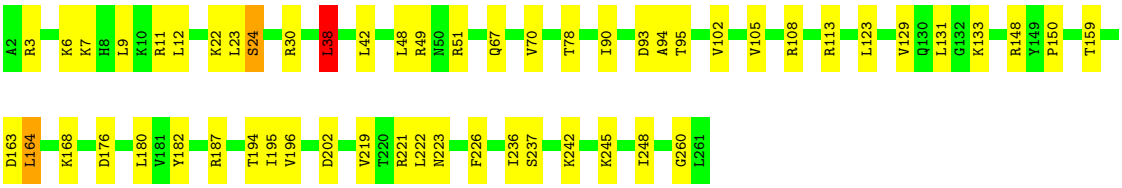
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



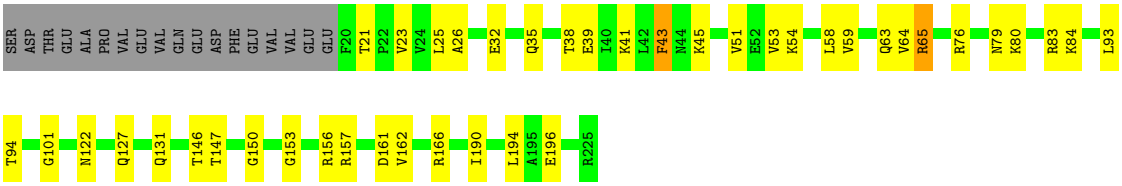
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



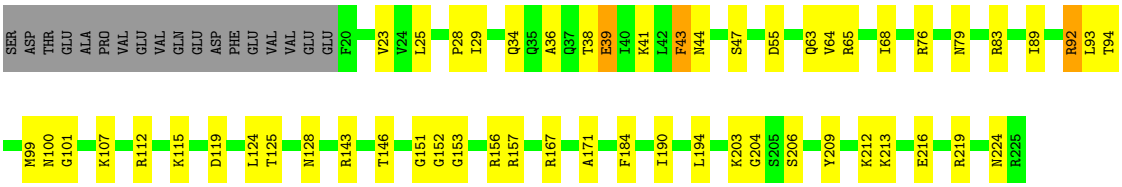
• Molecule 7: 40S ribosomal protein S5

Chain S5:



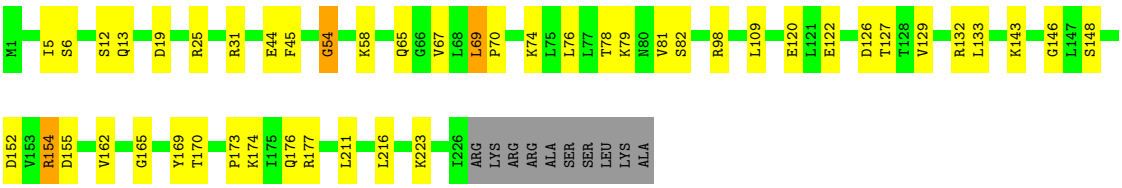
• Molecule 7: 40S ribosomal protein S5

Chain s5:



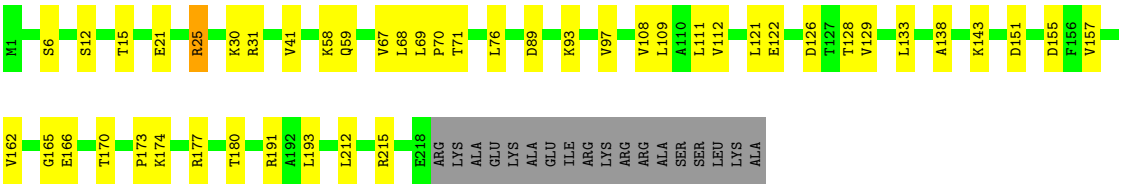
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



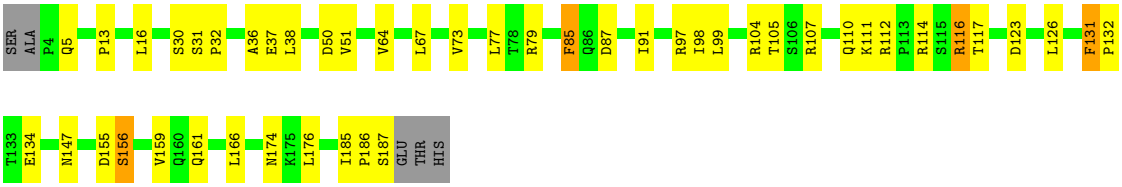
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



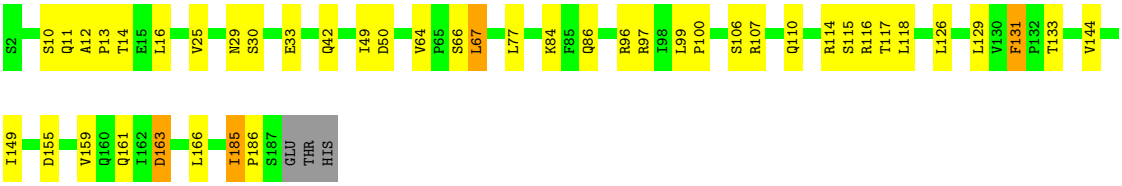
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



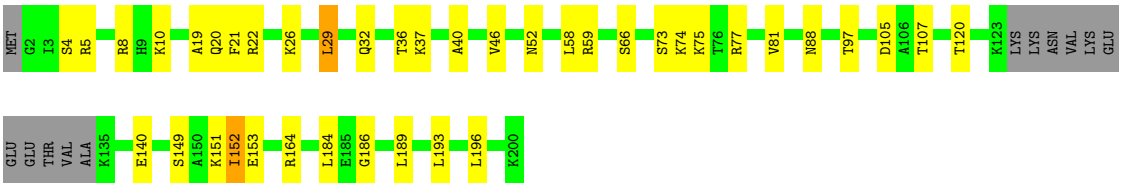
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



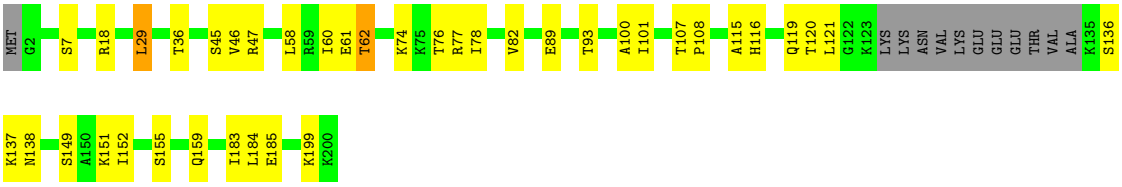
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



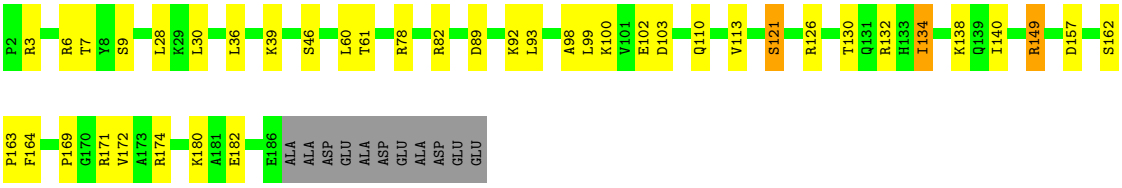
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



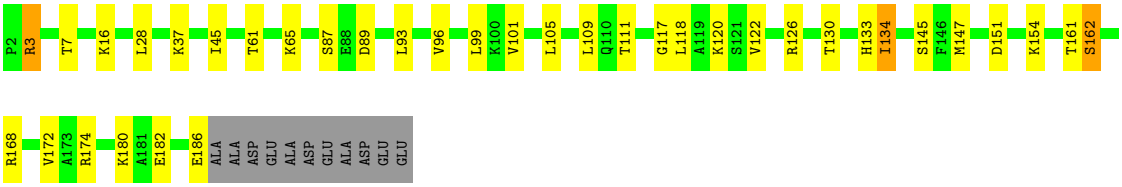
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



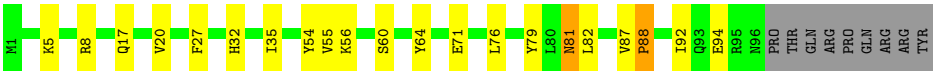
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



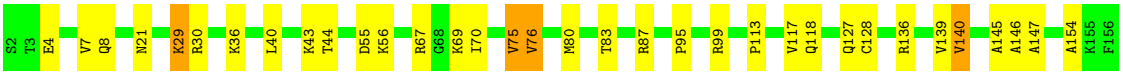
• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



• Molecule 13: 40S ribosomal protein S11-A

Chain C1:

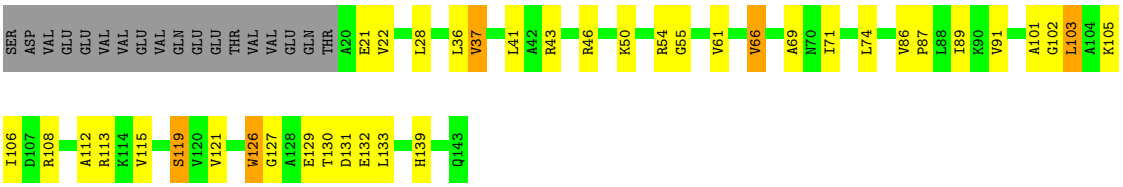


• Molecule 13: 40S ribosomal protein S11-A

Chain c1:

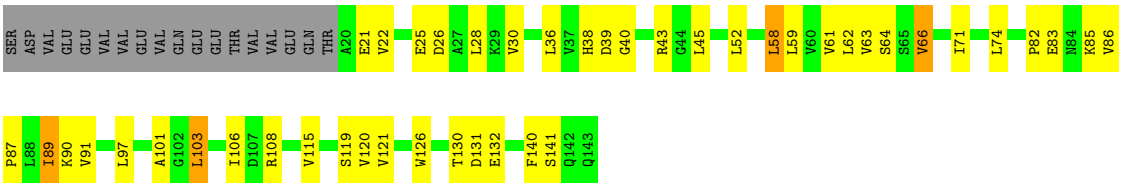
• Molecule 14: 40S ribosomal protein S12

Chain C2:



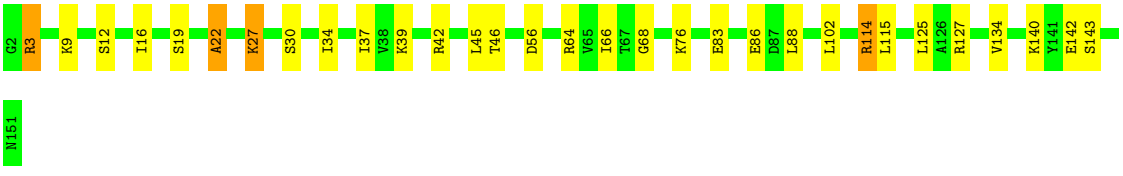
• Molecule 14: 40S ribosomal protein S12

Chain c2:



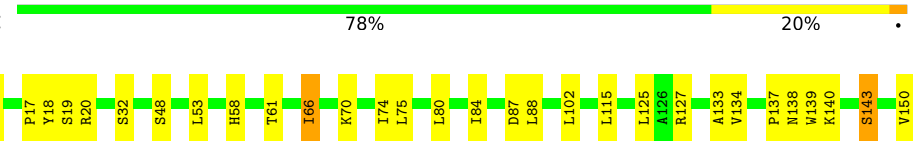
• Molecule 15: 40S ribosomal protein S13

Chain C3:



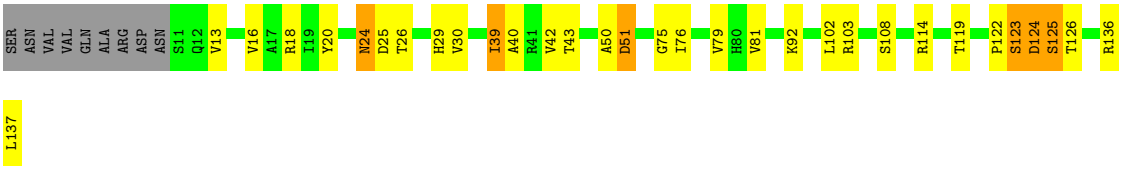
• Molecule 15: 40S ribosomal protein S13

Chain c3:



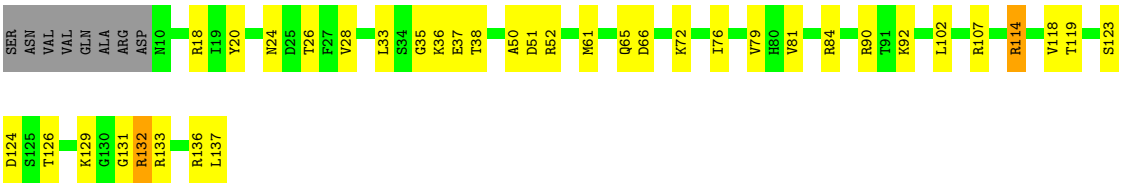
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



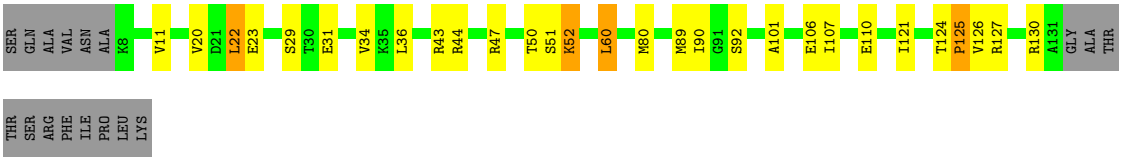
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



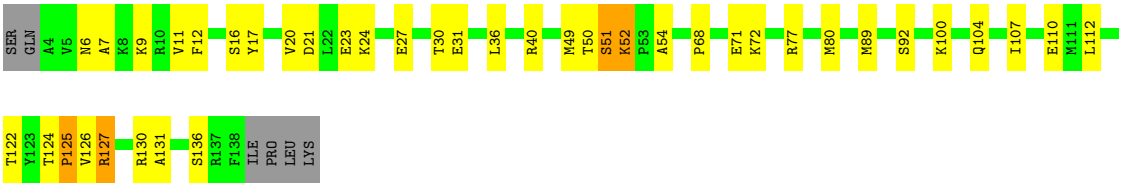
• Molecule 17: 40S ribosomal protein S15

Chain C5:



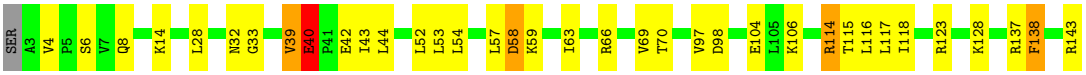
• Molecule 17: 40S ribosomal protein S15

Chain c5:



• Molecule 18: 40S ribosomal protein S16-A

Chain C6:

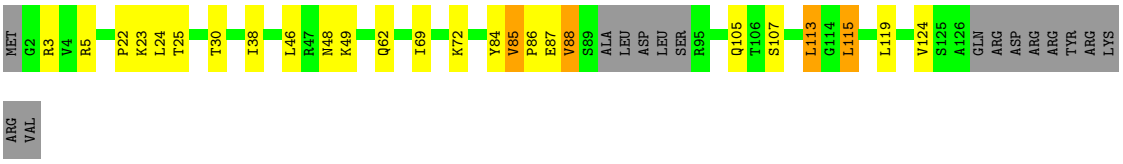


• Molecule 18: 40S ribosomal protein S16-A

Chain c6:

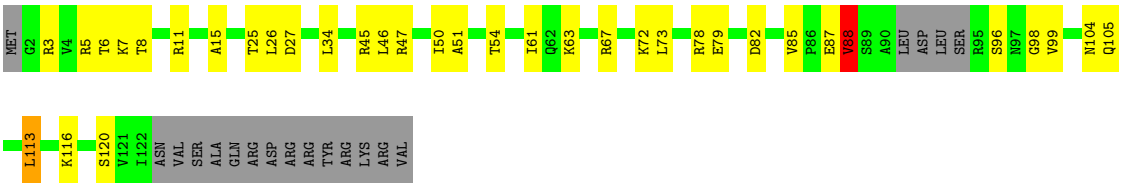
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



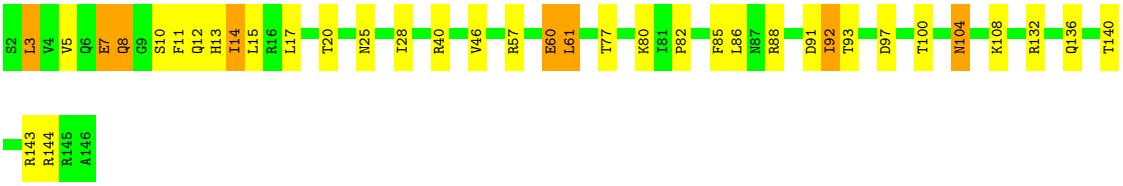
• Molecule 19: 40S ribosomal protein S17-A

Chain c7:



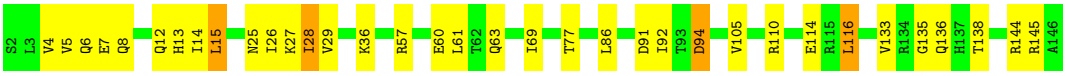
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



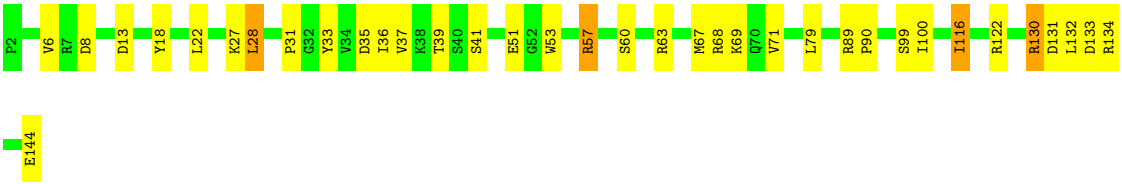
• Molecule 20: 40S ribosomal protein S18-A

Chain c8:



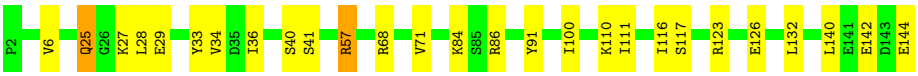
• Molecule 21: 40S ribosomal protein S19-A

Chain C9:



• Molecule 21: 40S ribosomal protein S19-A

Chain c9:

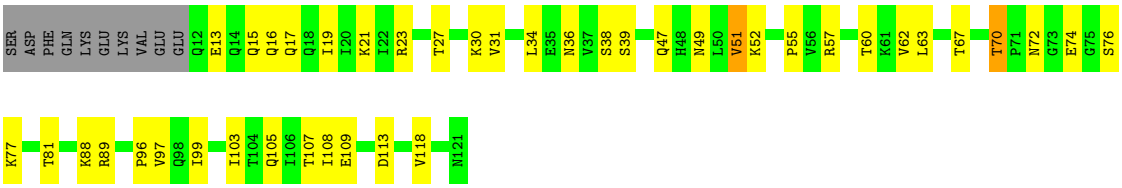


• Molecule 22: 40S ribosomal protein S20

Chain D0:

• Molecule 22: 40S ribosomal protein S20

Chain d0:

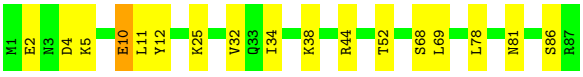


• Molecule 23: 40S ribosomal protein S21-A

Chain D1:

• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

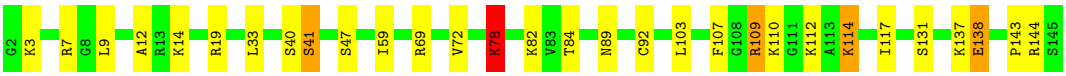
Chain D2:

• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

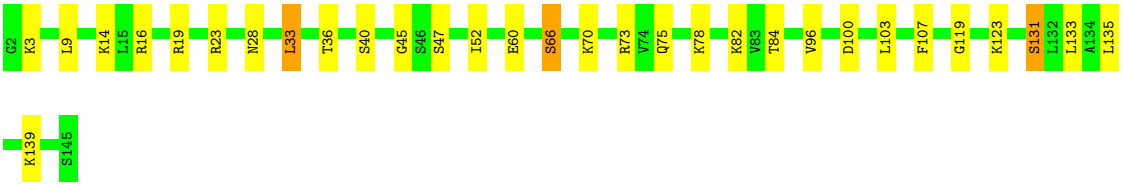
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



• Molecule 25: 40S ribosomal protein S23-A

Chain d3:

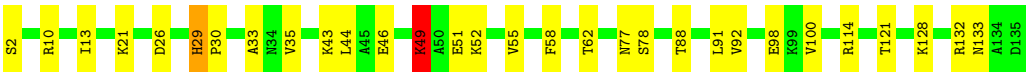


• Molecule 26: 40S ribosomal protein S24-A

Chain D4:

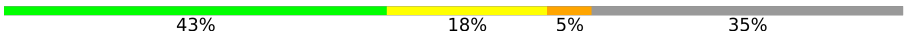
• Molecule 26: 40S ribosomal protein S24-A

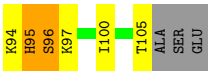
Chain d4:



• Molecule 27: 40S ribosomal protein S25-A

Chain D5:



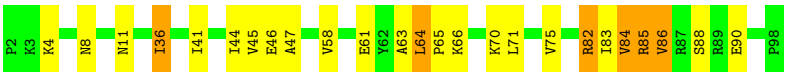


• Molecule 27: 40S ribosomal protein S25-A

Chain d5:

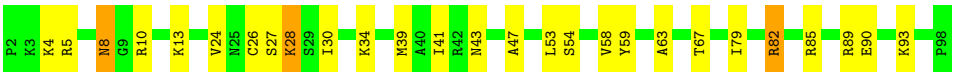
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



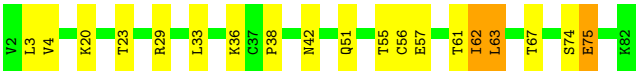
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



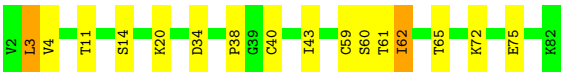
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



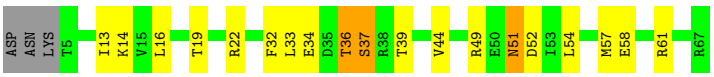
• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



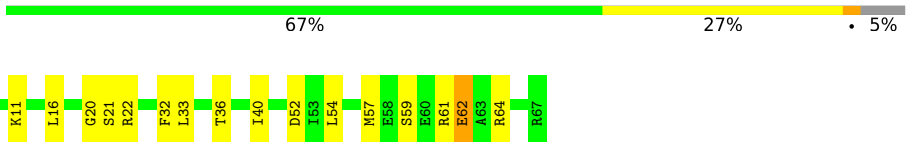
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



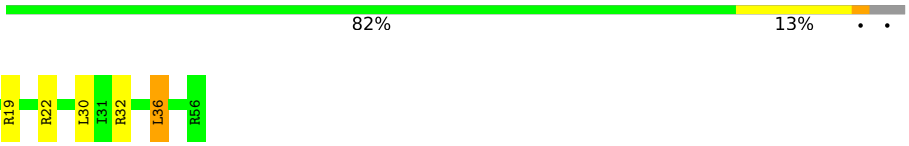
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



• Molecule 31: 40S ribosomal protein S29-A

Chain D9:

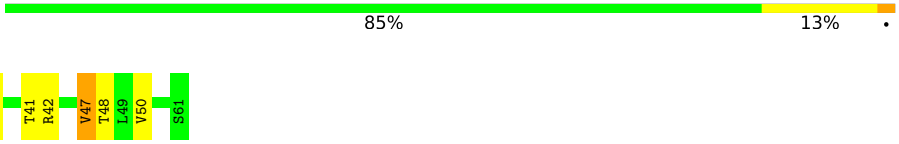


• Molecule 31: 40S ribosomal protein S29-A

Chain d9:

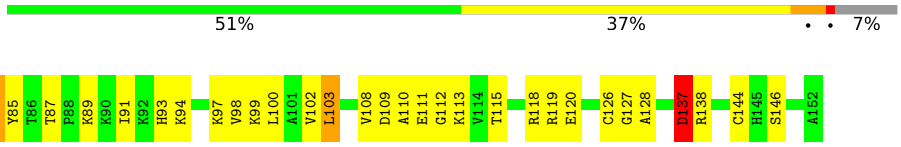
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



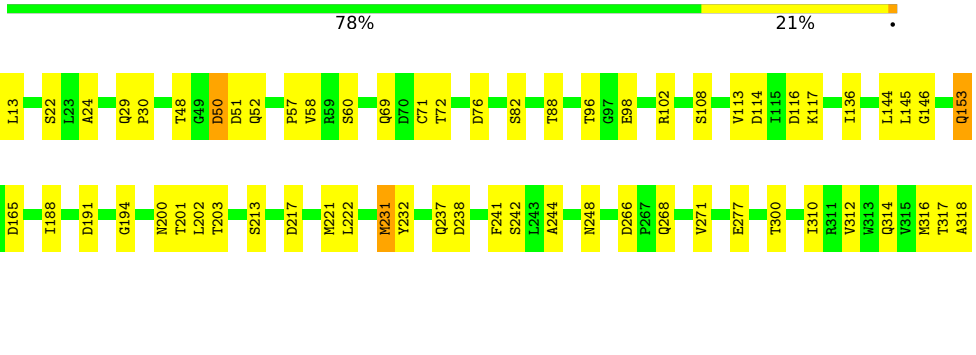
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



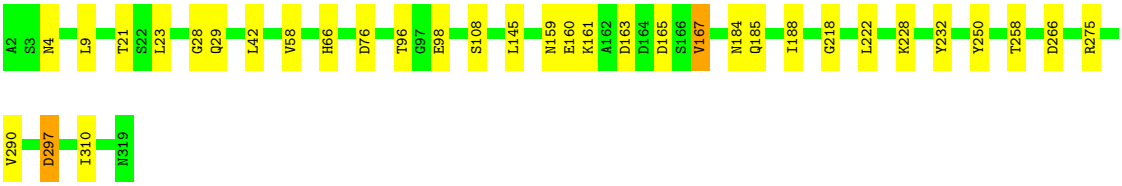
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



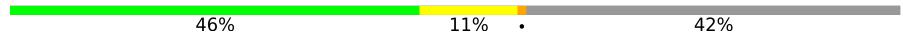
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

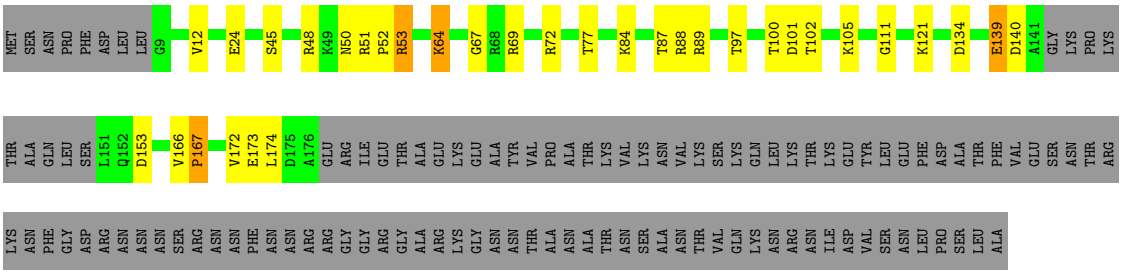
Chain sR:



• Molecule 35: Suppressor protein STM1

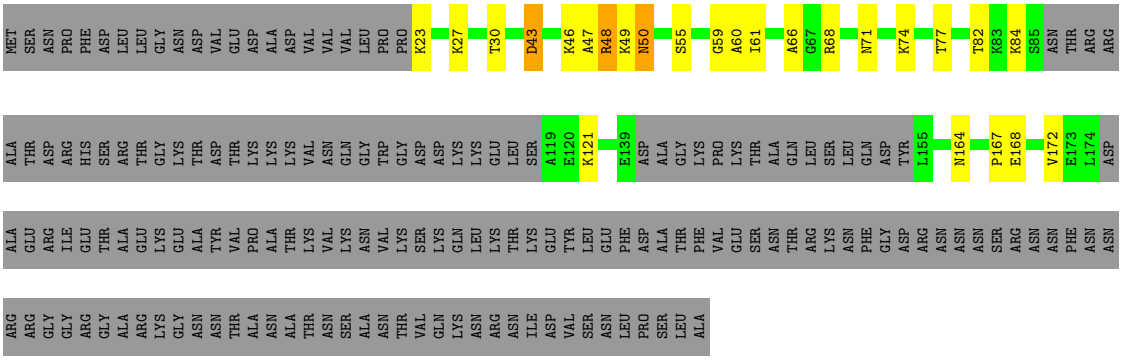
Chain SM:





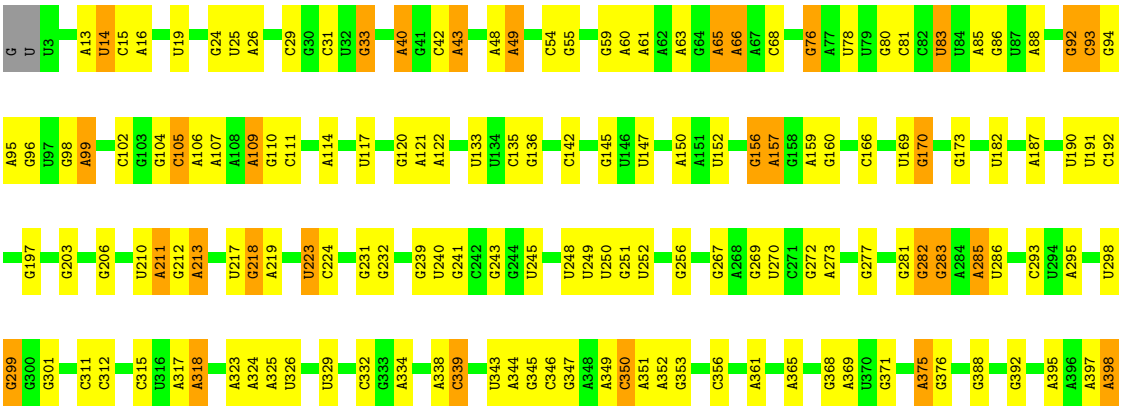
• Molecule 35: Suppressor protein STM1

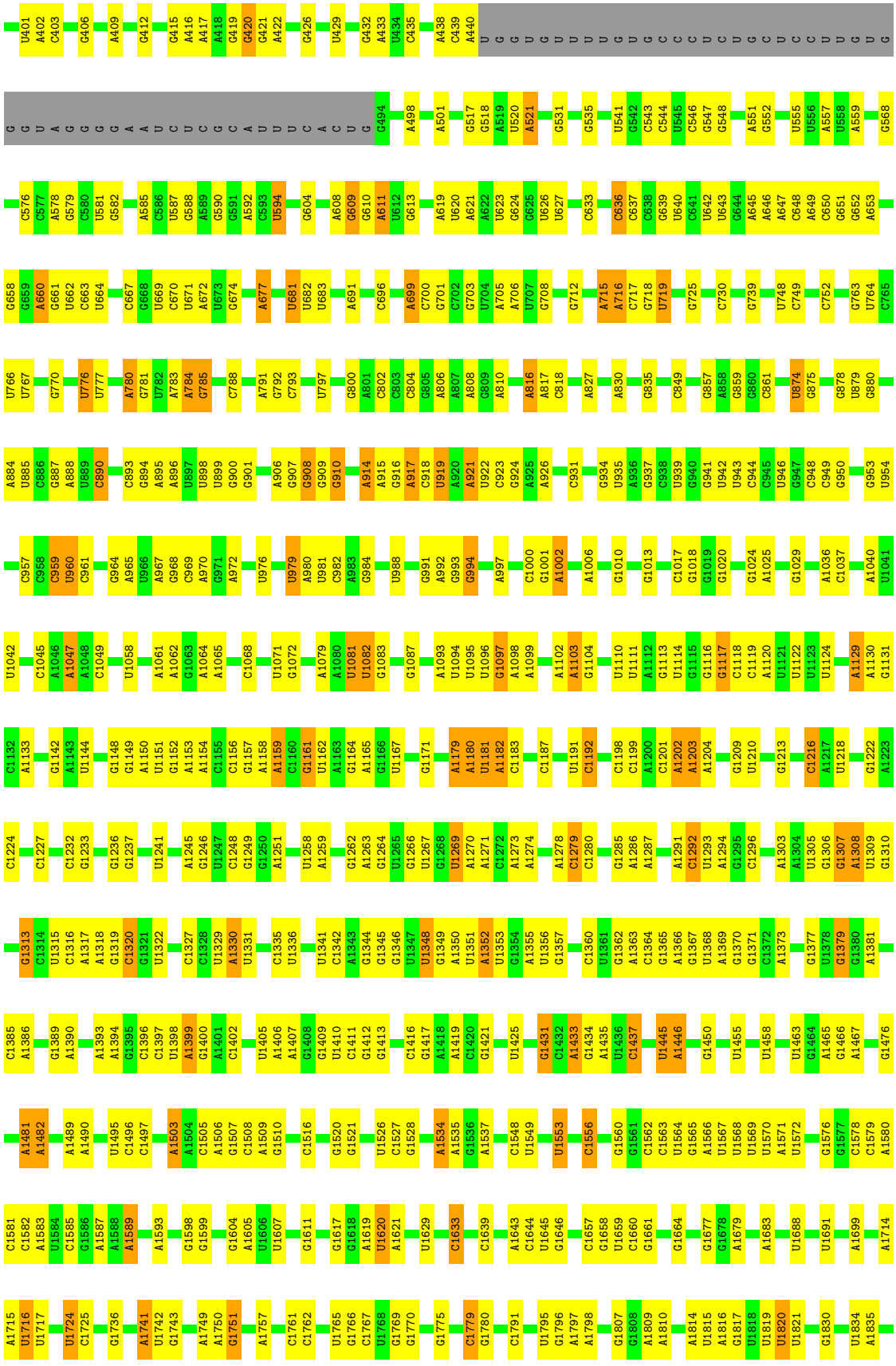
Chain sM:

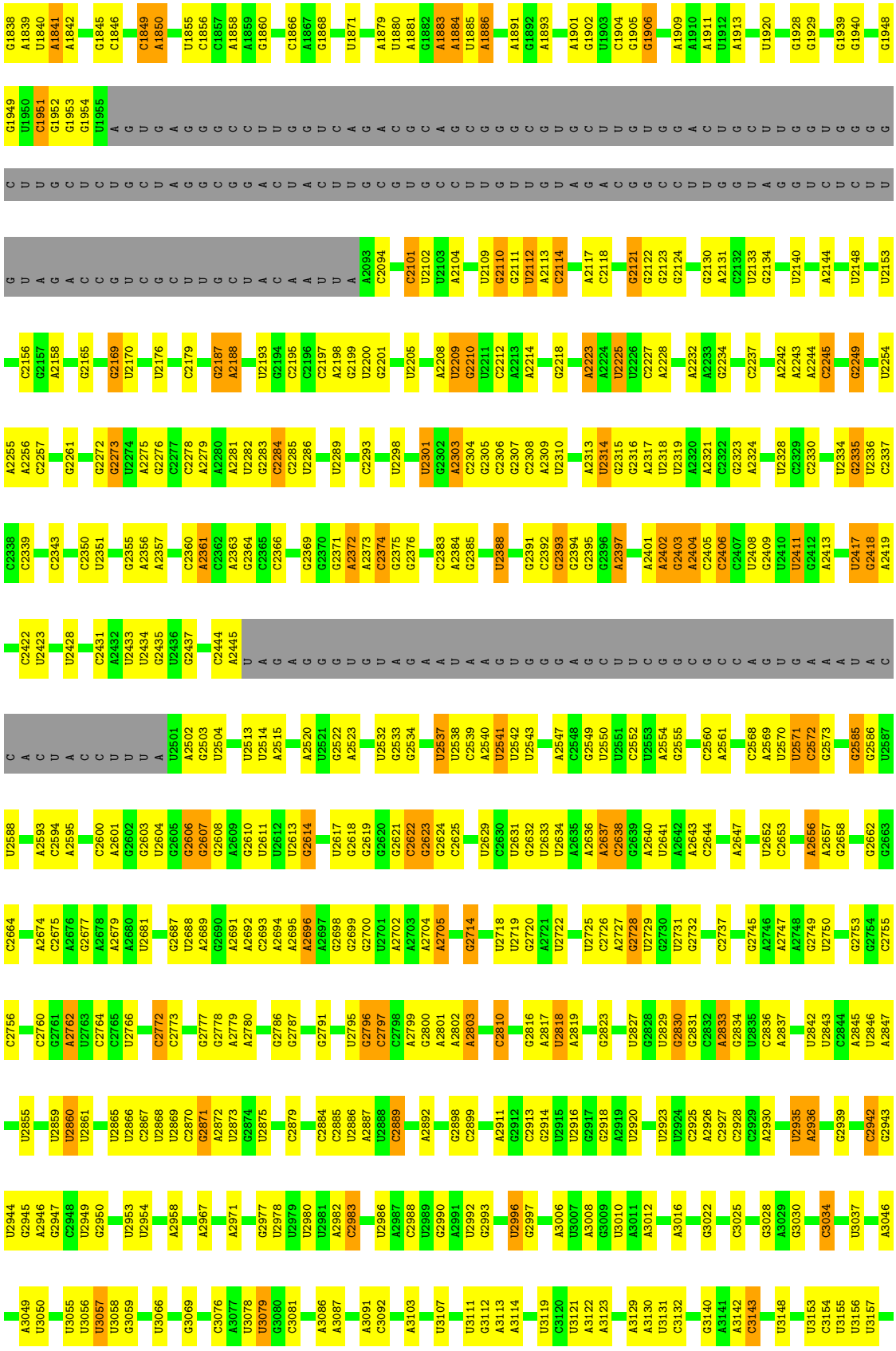


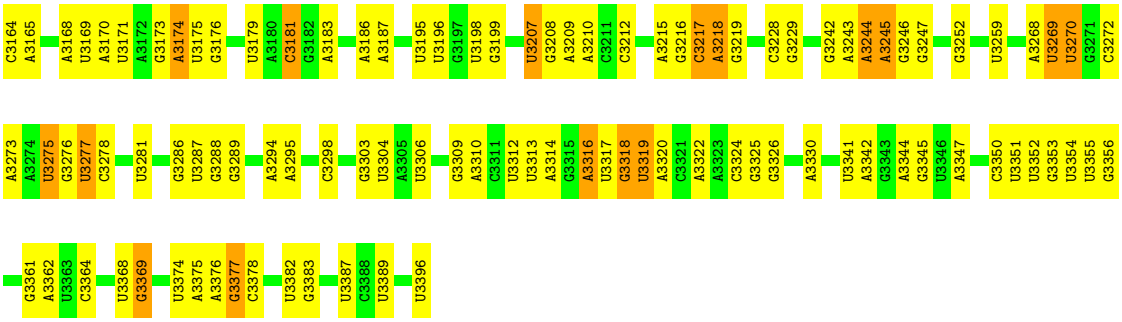
• Molecule 36: 25S ribosomal RNA

Chain 1:



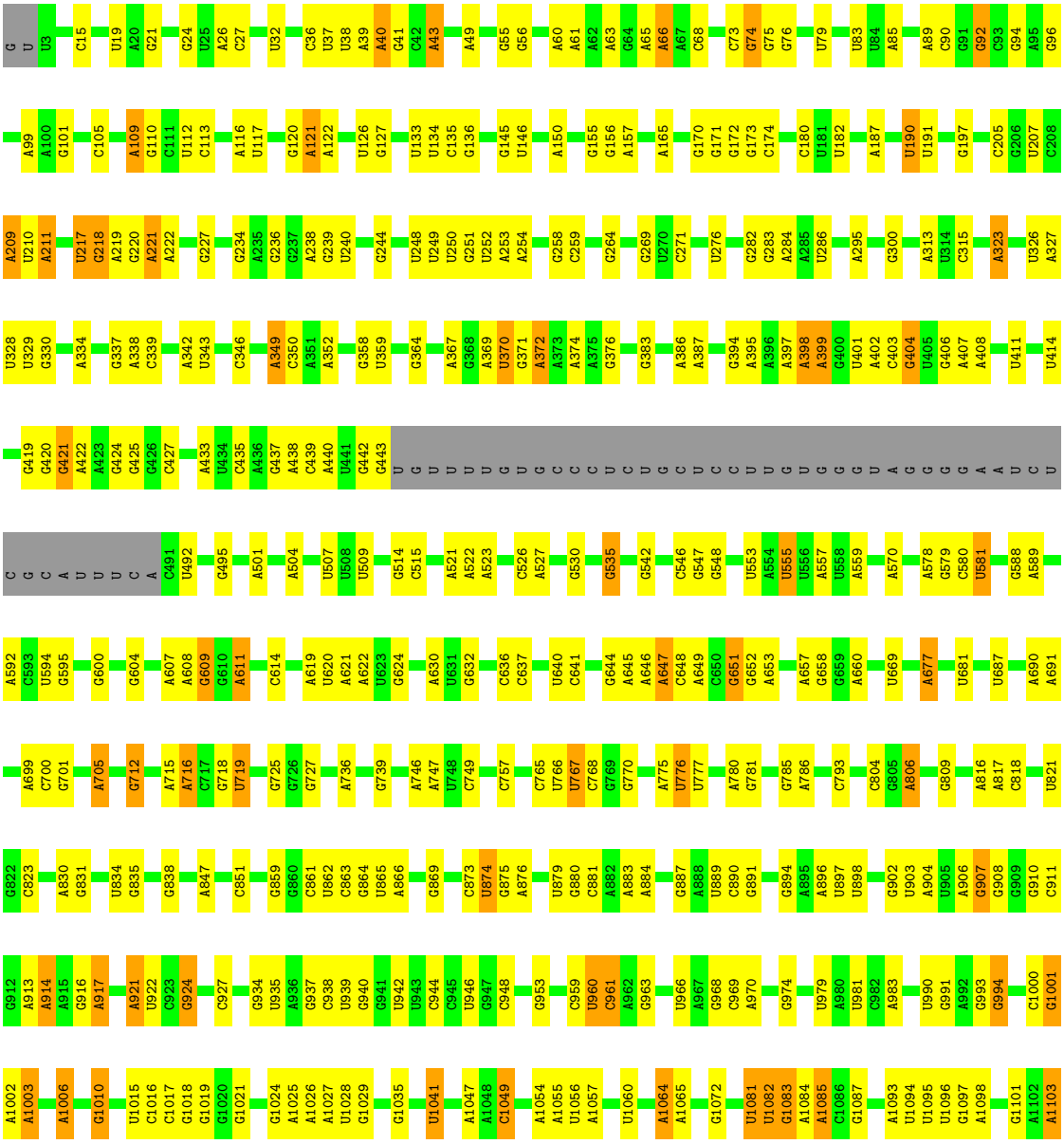


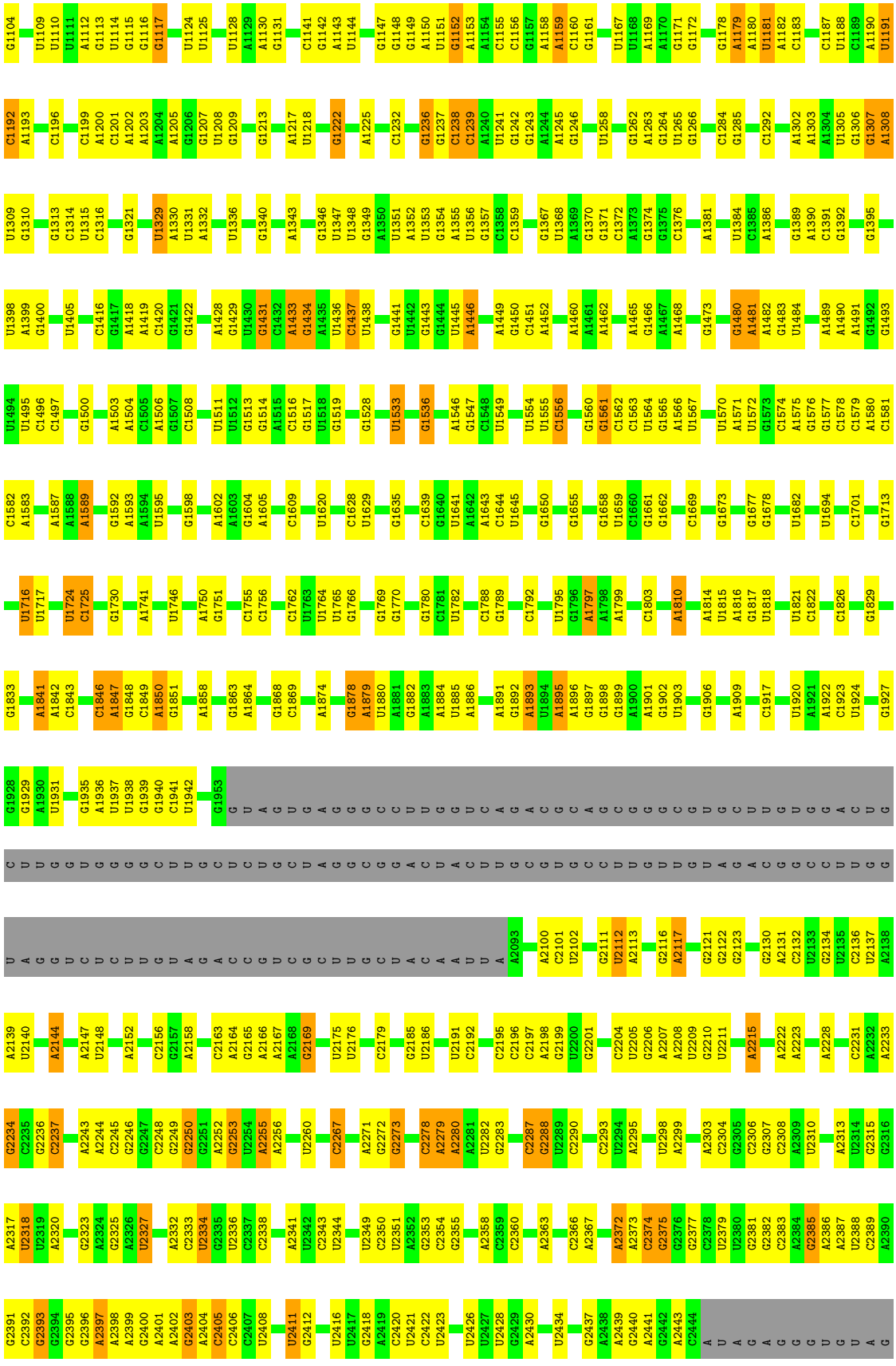


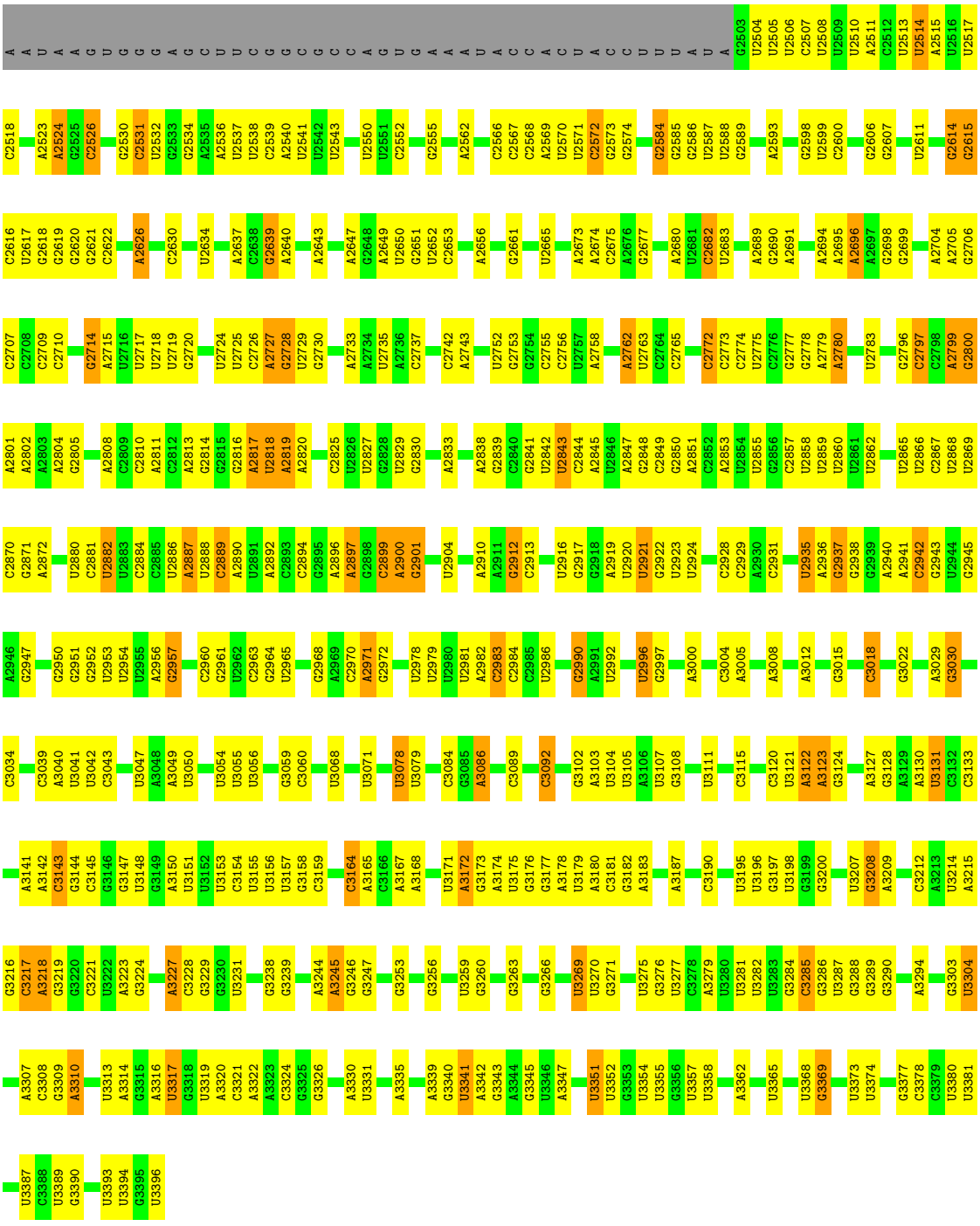


• Molecule 36: 25S ribosomal RNA

Chain 5:

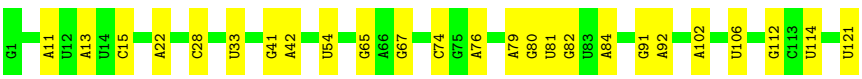






• Molecule 37: 5S ribosomal RNA

Chain 3:

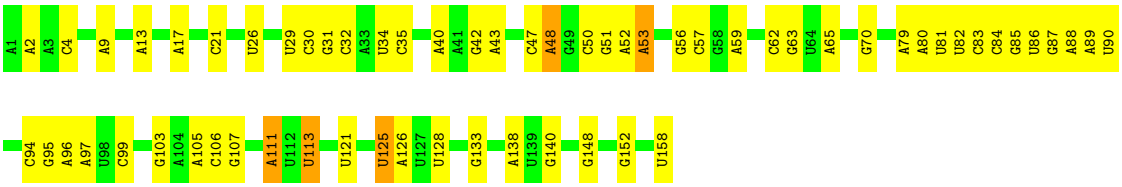


• Molecule 37: 5S ribosomal RNA

Chain 7:

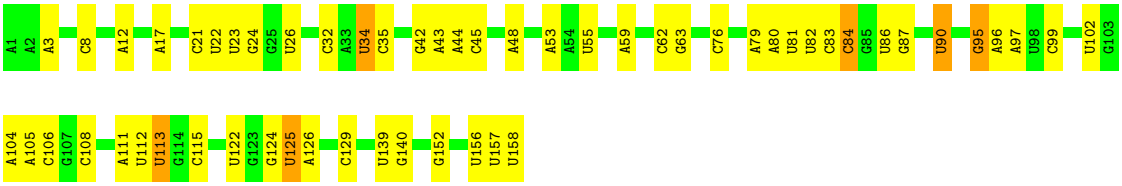
• Molecule 38: 5.8S ribosomal RNA

Chain 4:



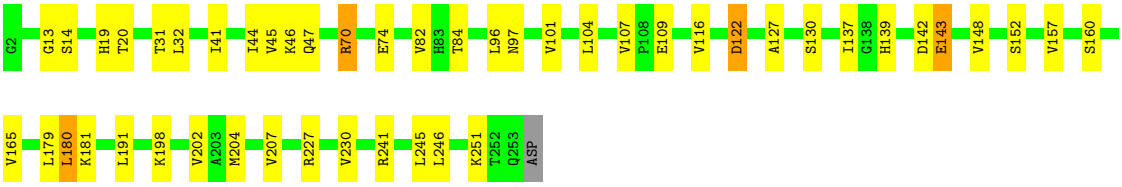
• Molecule 38: 5.8S ribosomal RNA

Chain 8:



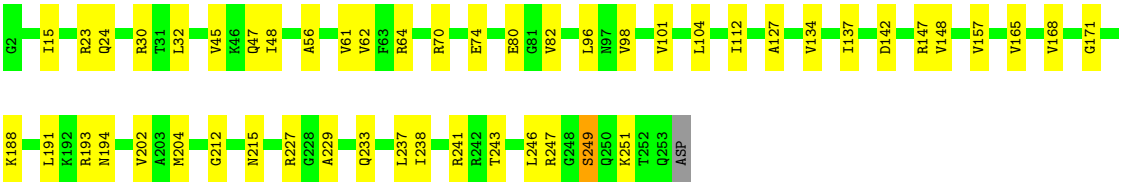
• Molecule 39: 60S ribosomal protein L2-A

Chain L2:



• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



• Molecule 40: 60S ribosomal protein L3

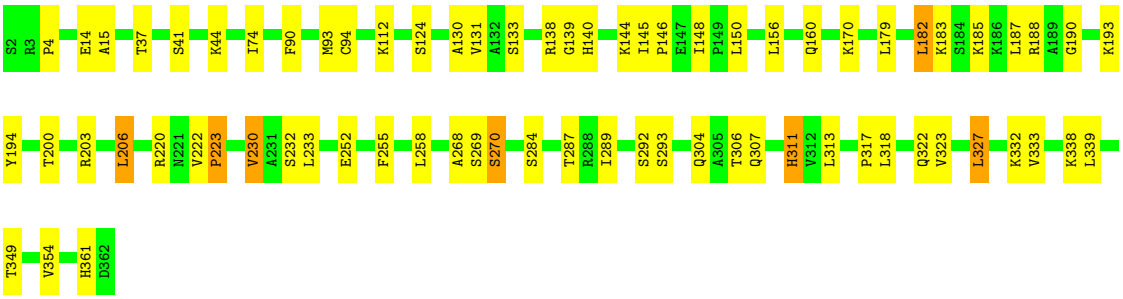
Chain L3:

• Molecule 40: 60S ribosomal protein L3

Chain l3:

• Molecule 41: 60S ribosomal protein L4-A

Chain L4:

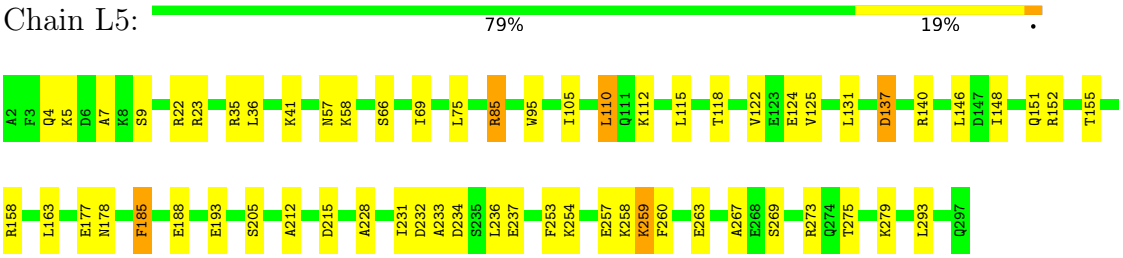


• Molecule 41: 60S ribosomal protein L4-A

Chain l4:

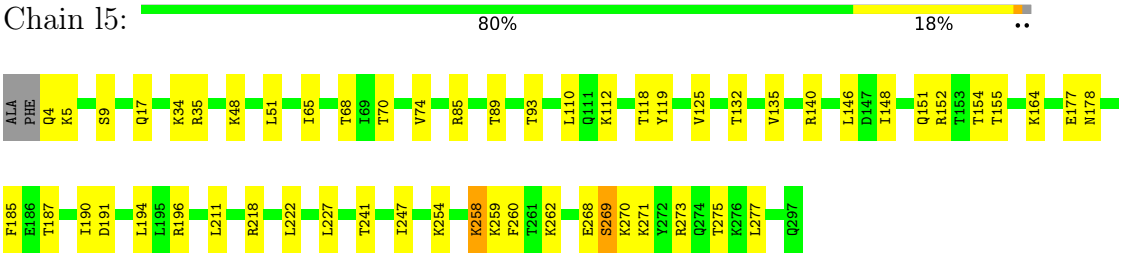
• Molecule 42: 60S ribosomal protein L5

Chain L5:



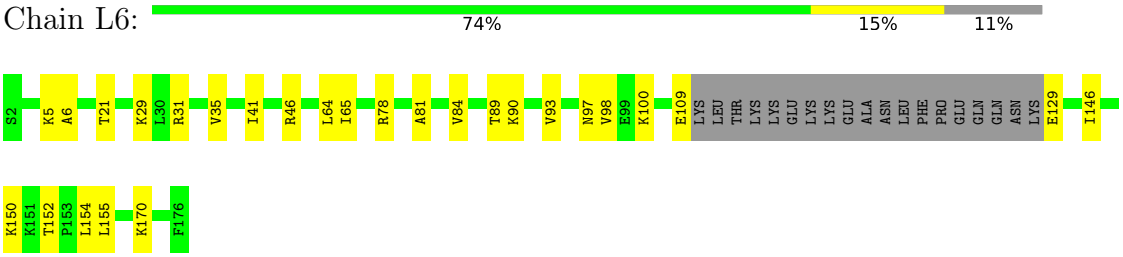
• Molecule 42: 60S ribosomal protein L5

Chain l5:



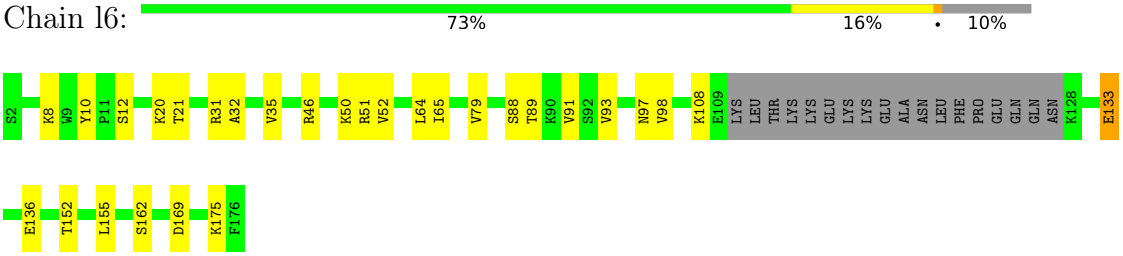
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



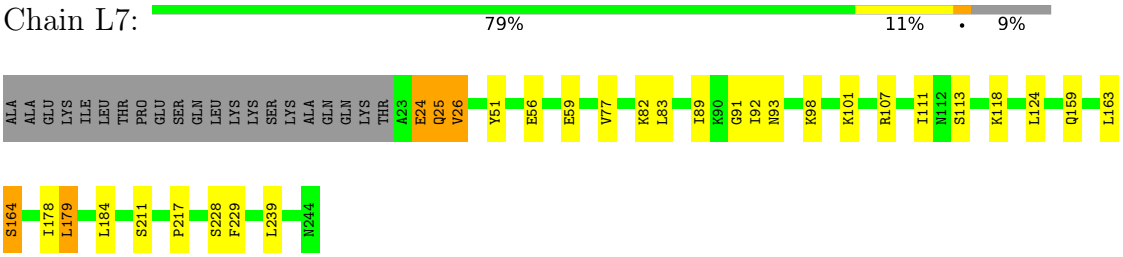
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



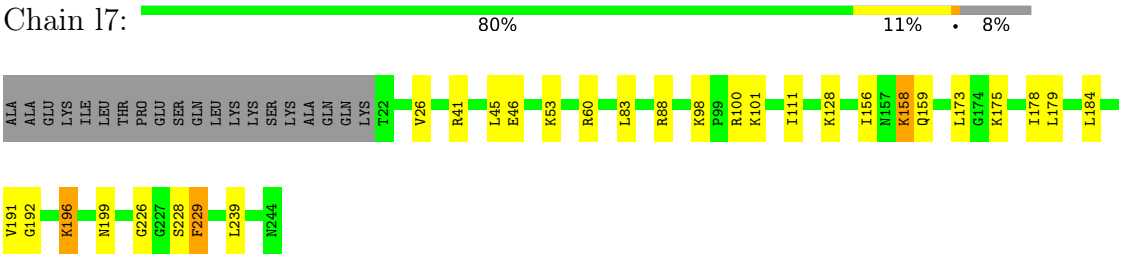
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



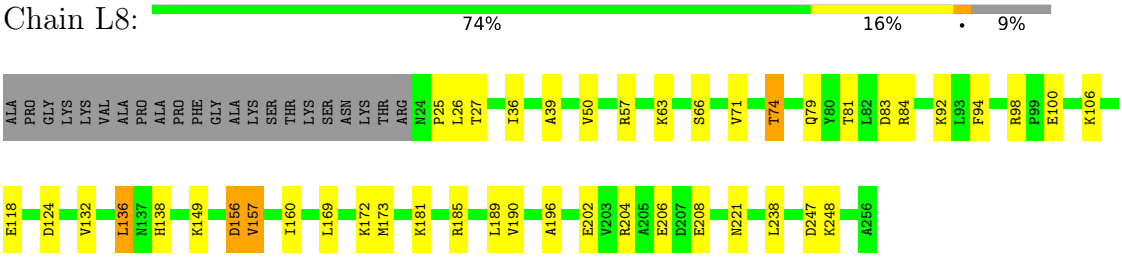
• Molecule 44: 60S ribosomal protein L7-A

Chain l7:



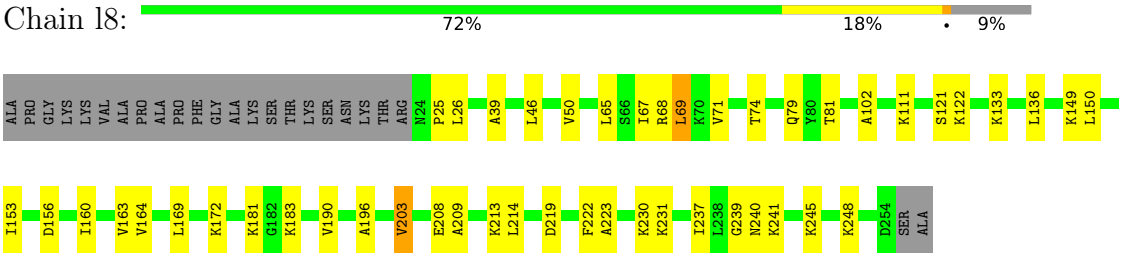
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



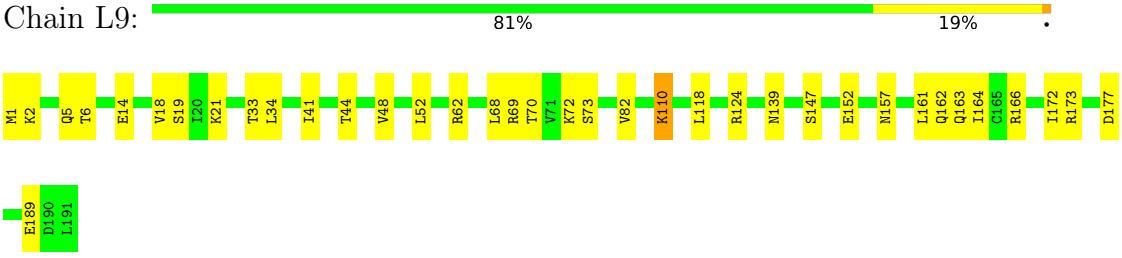
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



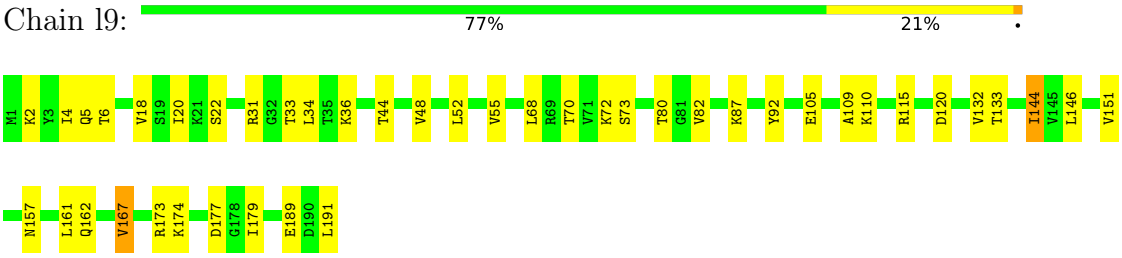
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



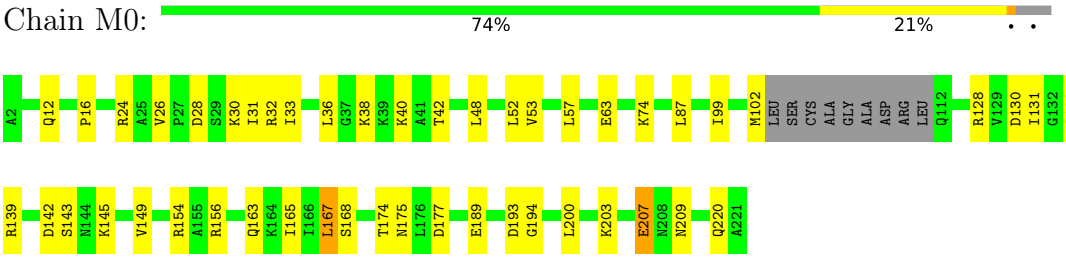
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



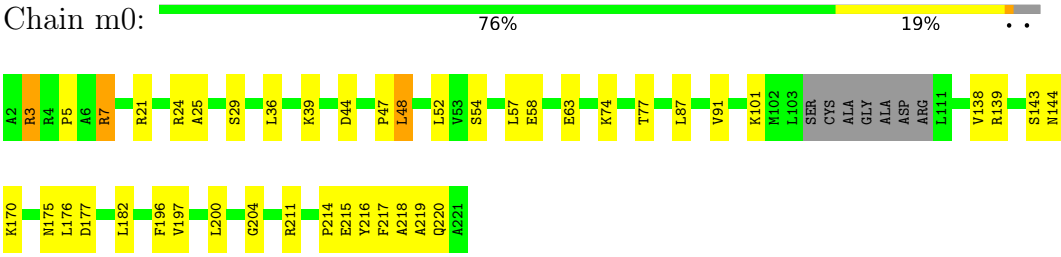
• Molecule 47: 60S ribosomal protein L10

Chain M0:



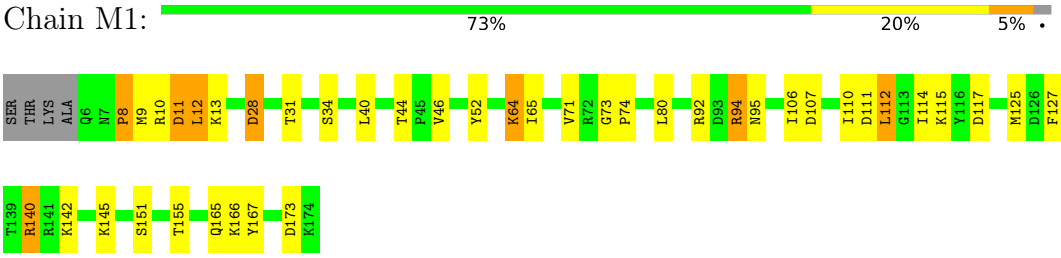
• Molecule 47: 60S ribosomal protein L10

Chain m0:



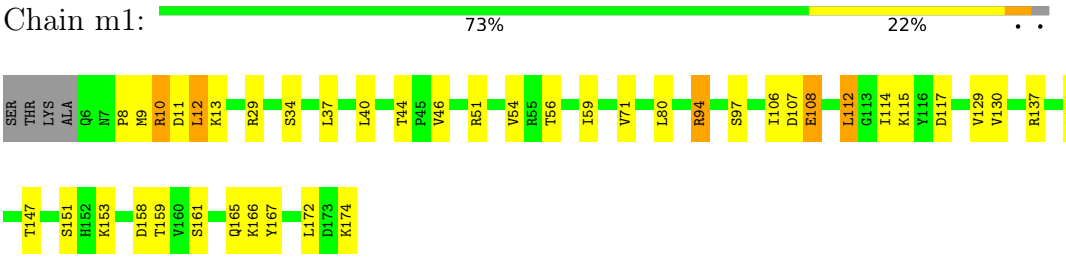
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



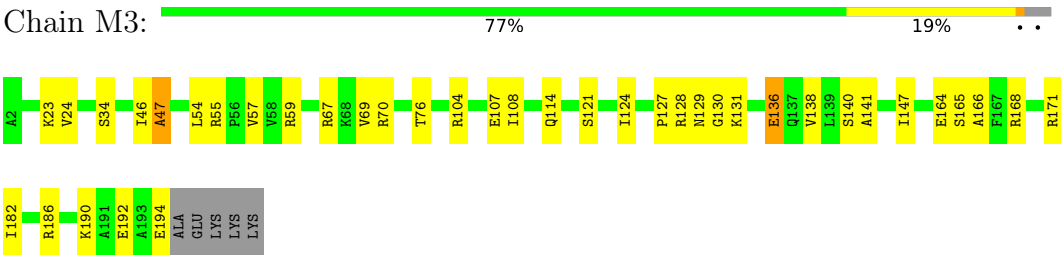
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



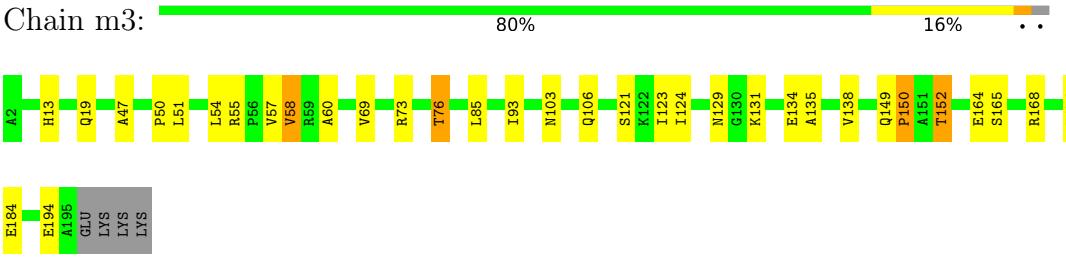
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



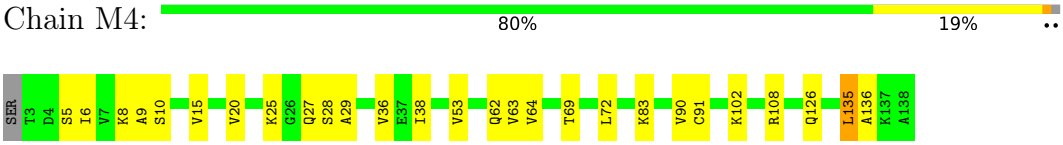
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



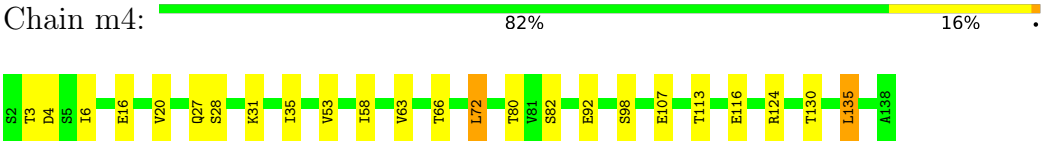
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



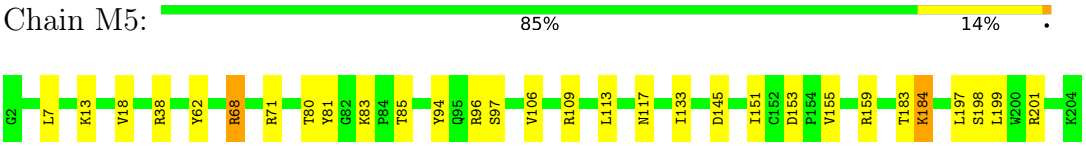
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



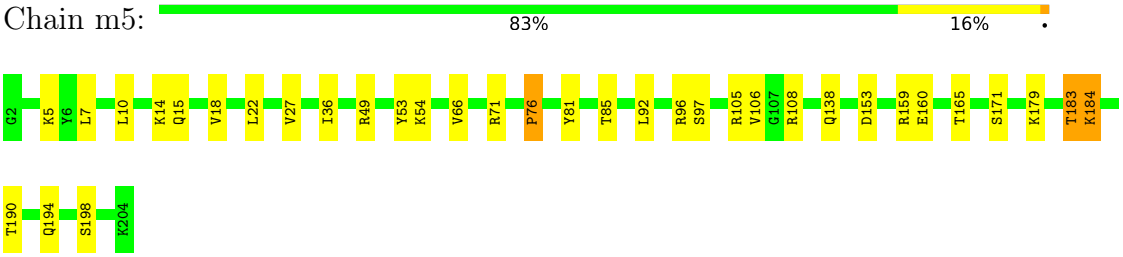
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



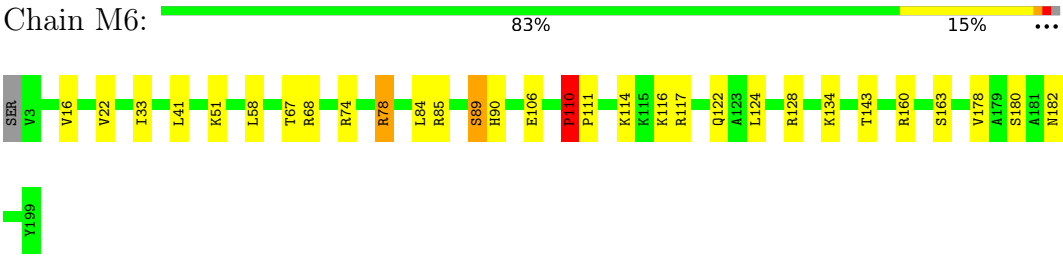
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



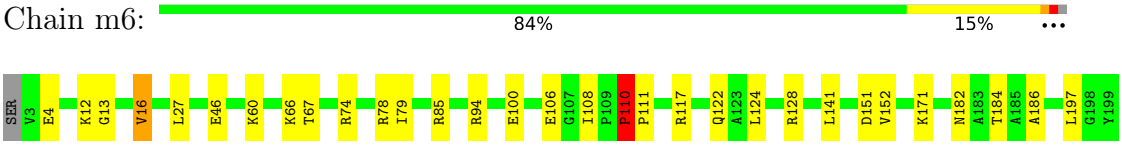
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



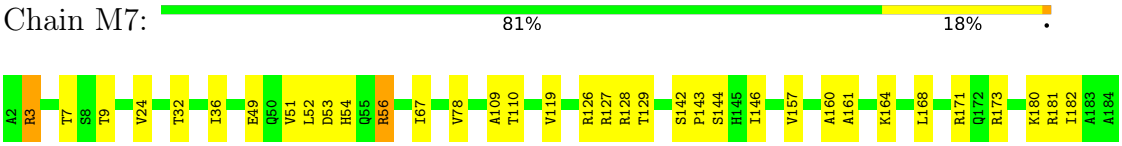
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



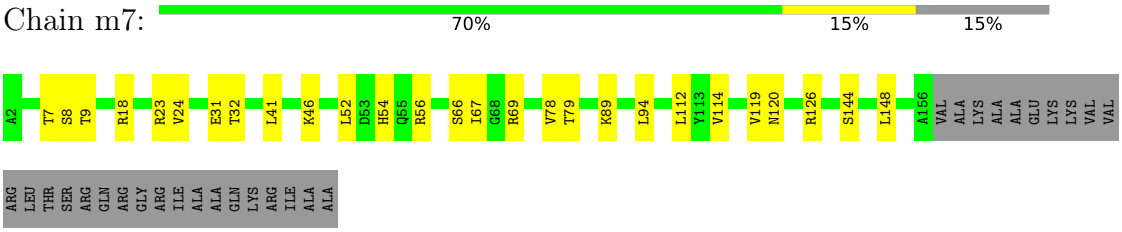
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



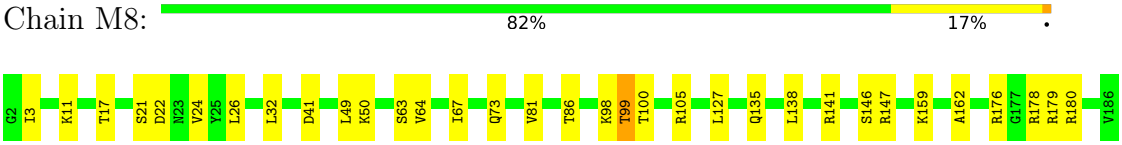
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



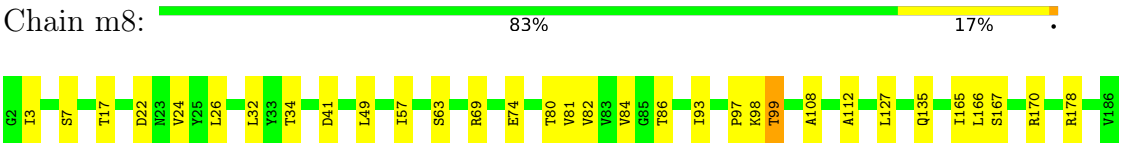
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



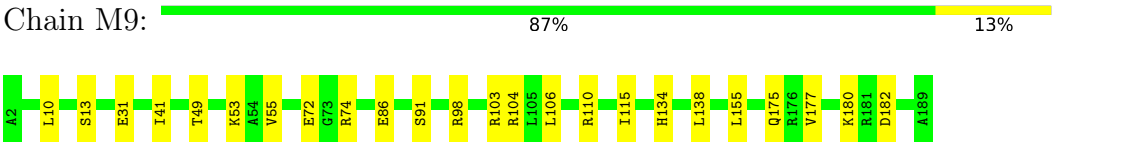
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



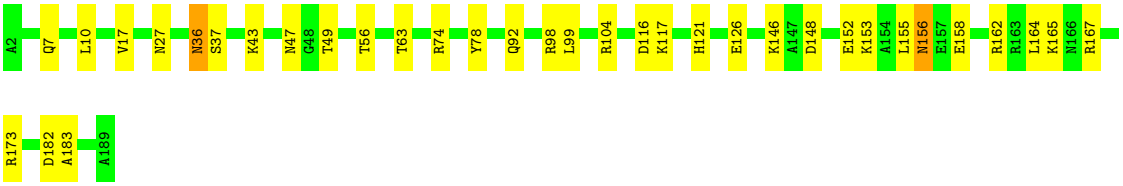
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



• Molecule 55: 60S ribosomal protein L19-A

Chain m9:

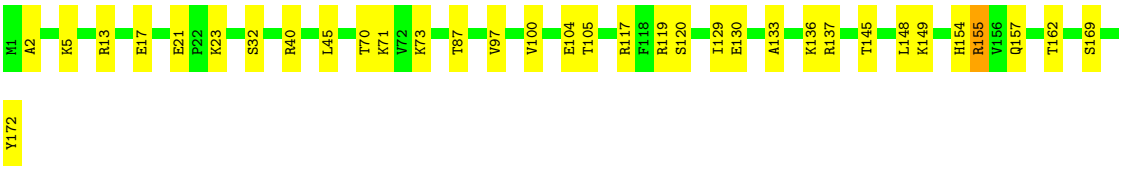


• Molecule 56: 60S ribosomal protein L20-A

Chain N0:

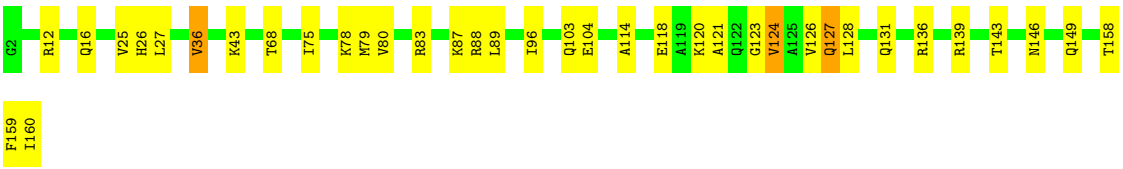
• Molecule 56: 60S ribosomal protein L20-A

Chain n0:



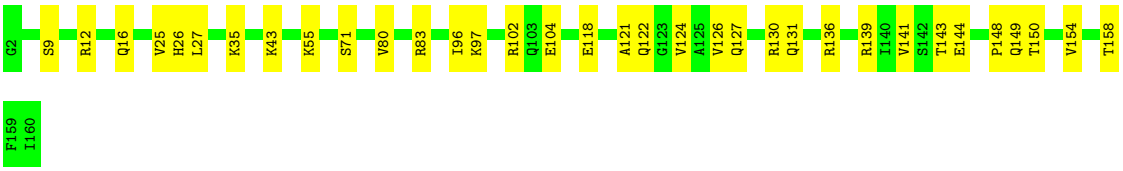
• Molecule 57: 60S ribosomal protein L21-A

Chain N1:



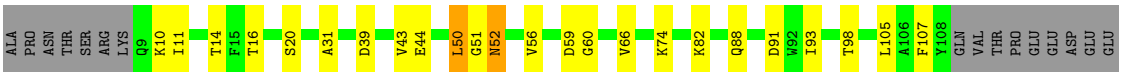
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



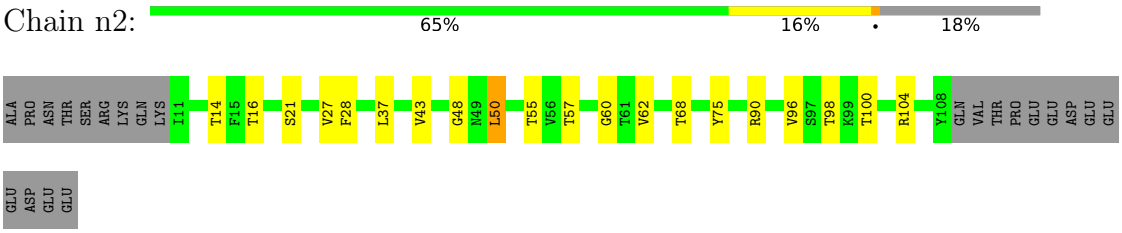
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



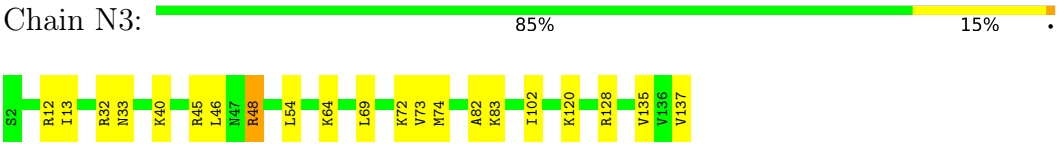
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



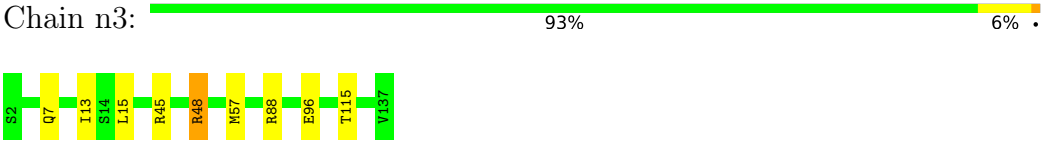
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



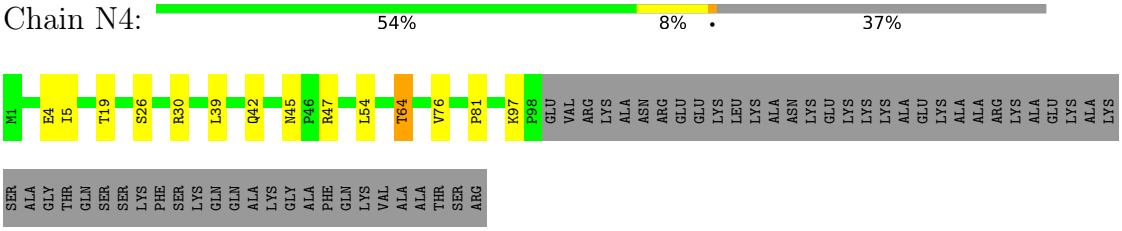
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



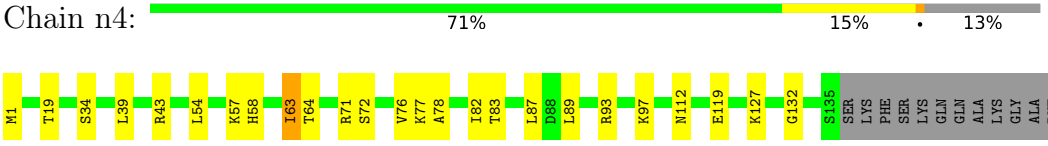
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



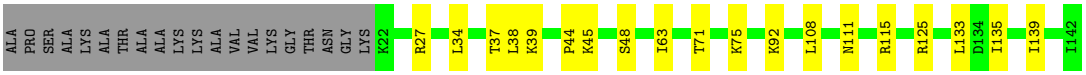
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



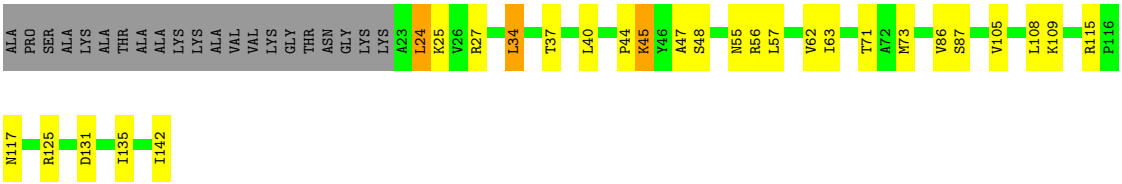
• Molecule 61: 60S ribosomal protein L25

Chain N5:



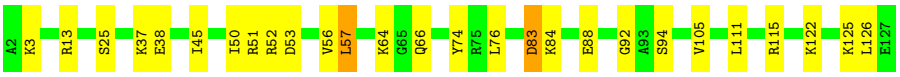
• Molecule 61: 60S ribosomal protein L25

Chain n5:



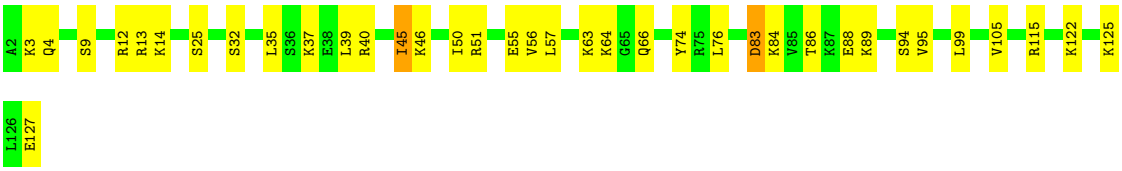
• Molecule 62: 60S ribosomal protein L26-A

Chain N6:



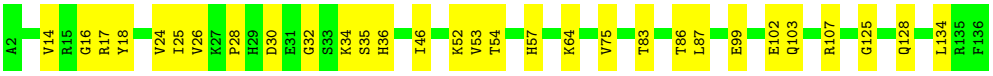
• Molecule 62: 60S ribosomal protein L26-A

Chain n6:



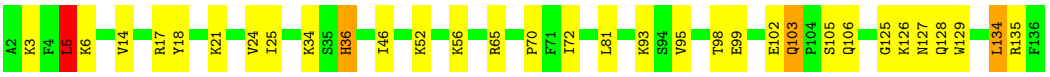
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



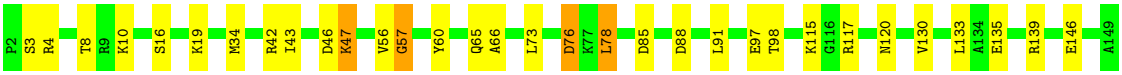
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



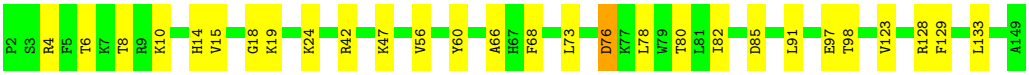
• Molecule 64: 60S ribosomal protein L28

Chain N8:



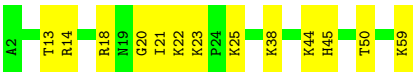
• Molecule 64: 60S ribosomal protein L28

Chain n8:



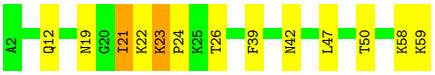
• Molecule 65: 60S ribosomal protein L29

Chain N9:



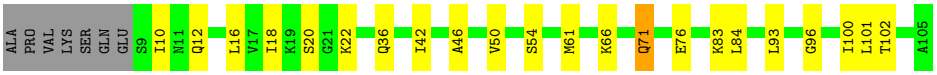
• Molecule 65: 60S ribosomal protein L29

Chain n9:



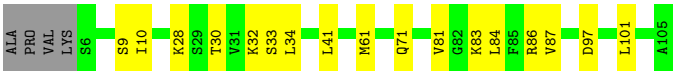
• Molecule 66: 60S ribosomal protein L30

Chain O0:



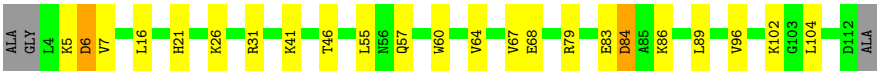
• Molecule 66: 60S ribosomal protein L30

Chain o0:



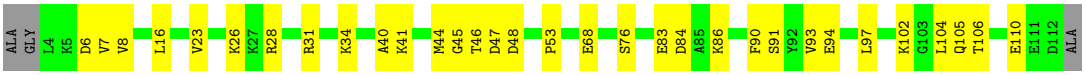
• Molecule 67: 60S ribosomal protein L31-A

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

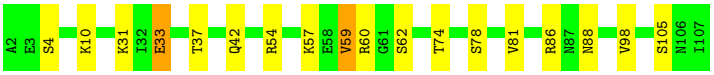
Chain o2:

• Molecule 69: 60S ribosomal protein L33-A

Chain O3:

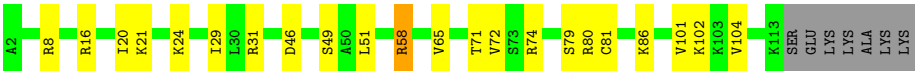
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



• Molecule 70: 60S ribosomal protein L34-A

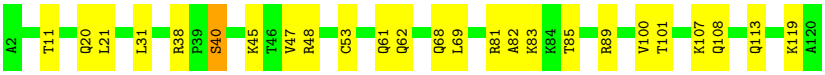
Chain o4:

• Molecule 71: 60S ribosomal protein L35-A

Chain O5:

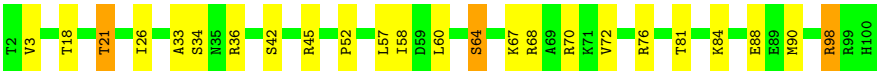
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



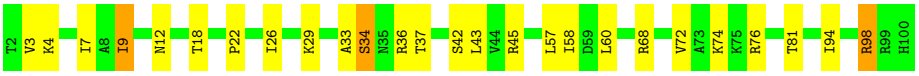
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



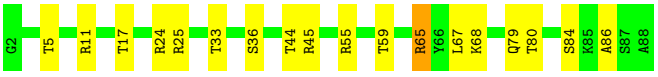
• Molecule 72: 60S ribosomal protein L36-A

Chain o6:



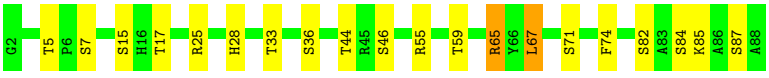
• Molecule 73: 60S ribosomal protein L37-A

Chain O7:



• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



• Molecule 74: 60S ribosomal protein L38

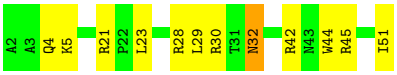
Chain O8:

• Molecule 74: 60S ribosomal protein L38

Chain o8:

• Molecule 75: 60S ribosomal protein L39

Chain O9:

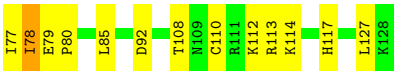


• Molecule 75: 60S ribosomal protein L39

Chain o9:

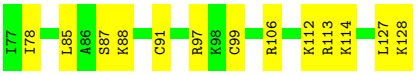
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



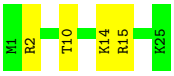
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



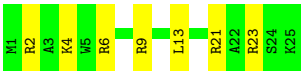
• Molecule 77: 60S ribosomal protein L41-A

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

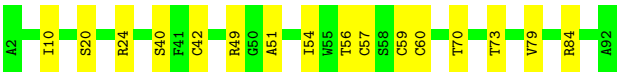
Chain q2:

• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:

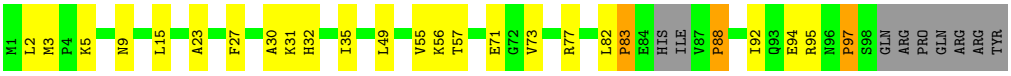
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



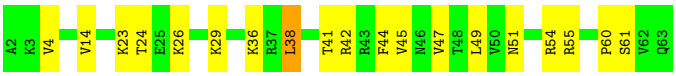
• Molecule 80: 40S ribosomal protein S10-A

Chain c0:



• Molecule 81: 40S ribosomal protein S30-A

Chain e0:

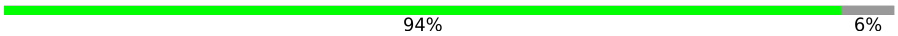


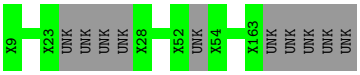
• Molecule 82: Ubiquitin-40S ribosomal protein S31

Chain e1:

• Molecule 83: UNKNOWN PROTEIN m2

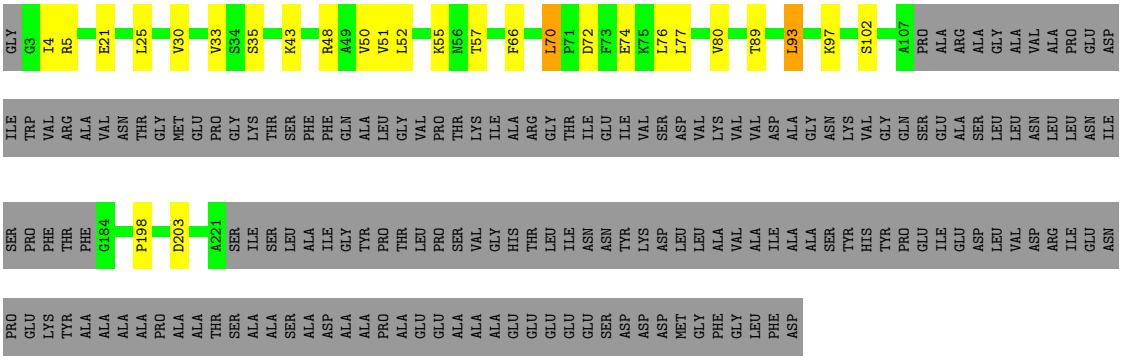
Chain m2:





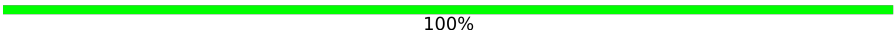
• Molecule 84: 60S acidic ribosomal protein P0

Chain p0:



• Molecule 85: UNKNOWN PROTEIN p1

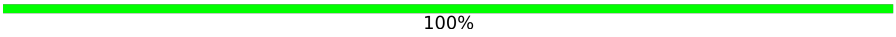
Chain p1:



There are no outlier residues recorded for this chain.

• Molecule 86: UNKNOWN PROTEIN p2

Chain p2:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.02Å 287.59Å 304.52Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	49.82 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (49.82-3.20)	Depositor
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.181 , 0.237	Depositor
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.157	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411288	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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

5.1 Standard geometry

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

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	0.68	1/41698 (0.0%)	1.28	292/64972 (0.4%)
1	6	0.81	13/42765 (0.0%)	1.38	456/66634 (0.7%)
2	S0	0.43	0/1617	0.67	0/2215
2	s0	0.49	0/1623	0.72	0/2222
3	S1	0.37	0/1735	0.69	2/2335 (0.1%)
3	s1	0.51	0/1748	0.70	1/2352 (0.0%)
4	S2	0.45	0/1665	0.65	0/2263
4	s2	0.54	0/1665	0.72	1/2263 (0.0%)
5	S3	0.45	0/1759	0.68	2/2368 (0.1%)
5	s3	0.45	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.71	0/2839
6	s4	0.52	0/2109	0.75	2/2839 (0.1%)
7	S5	0.38	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.71	1/2202 (0.0%)
8	S6	0.45	0/1823	0.63	1/2439 (0.0%)
8	s6	0.51	0/1779	0.68	0/2379
9	S7	0.42	0/1506	0.63	0/2028
9	s7	0.44	0/1516	0.70	1/2043 (0.0%)
10	S8	0.51	0/1514	0.76	1/2021 (0.0%)
10	s8	0.59	0/1514	0.77	1/2021 (0.0%)
11	S9	0.43	0/1519	0.65	0/2035
11	s9	0.53	0/1519	0.75	1/2035 (0.0%)
12	C0	0.43	0/790	0.66	1/1069 (0.1%)
13	C1	0.55	0/1240	0.69	0/1675
13	c1	0.60	0/1194	0.80	2/1610 (0.1%)
14	C2	0.35	0/900	0.65	1/1224 (0.1%)
14	c2	0.32	0/900	0.60	1/1224 (0.1%)
15	C3	0.47	0/1215	0.69	3/1638 (0.2%)
15	c3	0.54	0/1215	0.75	1/1638 (0.1%)
16	C4	0.37	0/901	0.64	0/1217
16	c4	0.52	0/960	0.73	0/1290
17	C5	0.44	0/998	0.66	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	c5	0.47	0/1060	0.66	0/1426
18	C6	0.43	0/1125	0.69	2/1510 (0.1%)
18	c6	0.48	0/1131	0.71	1/1518 (0.1%)
19	C7	0.40	0/935	0.66	0/1254
19	c7	0.48	0/914	0.72	0/1224
20	C8	0.43	0/1211	0.66	1/1628 (0.1%)
20	c8	0.50	0/1211	0.70	2/1628 (0.1%)
21	C9	0.44	0/1130	0.67	1/1517 (0.1%)
21	c9	0.49	0/1130	0.72	2/1517 (0.1%)
22	D0	0.45	0/865	0.66	0/1169
22	d0	0.49	0/892	0.70	0/1205
23	D1	0.39	0/693	0.59	0/935
23	d1	0.49	0/693	0.70	0/935
24	D2	0.46	0/1038	0.75	2/1395 (0.1%)
24	d2	0.64	0/1038	0.78	1/1395 (0.1%)
25	D3	0.58	0/1139	0.74	0/1518
25	d3	0.64	0/1139	0.82	2/1518 (0.1%)
26	D4	0.41	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.69	0/1449
27	D5	0.39	0/571	0.77	2/768 (0.3%)
27	d5	0.42	0/566	0.69	0/761
28	D6	0.40	0/782	0.60	0/1047
28	d6	0.53	0/782	0.69	0/1047
29	D7	0.42	0/620	0.68	0/838
29	d7	0.44	0/620	0.68	0/838
30	D8	0.34	0/499	0.62	0/670
30	d8	0.38	0/499	0.64	0/670
31	D9	0.50	0/452	0.74	1/600 (0.2%)
31	d9	0.56	0/452	0.71	0/600
32	E0	0.40	0/483	0.64	0/643
33	E1	0.41	0/577	0.78	0/770
34	SR	0.39	0/2494	0.63	0/3393
34	sR	0.39	0/2495	0.60	0/3395
35	SM	0.45	0/1113	0.68	2/1502 (0.1%)
35	sM	0.41	0/683	0.63	1/923 (0.1%)
36	1	1.01	59/75394 (0.1%)	1.57	1453/117545 (1.2%)
36	5	1.05	74/75414 (0.1%)	1.58	1442/117575 (1.2%)
37	3	0.87	0/2883	1.32	14/4491 (0.3%)
37	7	1.02	1/2883 (0.0%)	1.60	54/4491 (1.2%)
38	4	0.95	1/3746 (0.0%)	1.51	47/5832 (0.8%)
38	8	0.89	0/3746	1.43	43/5832 (0.7%)
39	L2	0.65	0/1948	0.81	2/2617 (0.1%)
39	l2	0.64	0/1946	0.83	0/2614

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
40	L3	0.62	0/3146	0.77	0/4228
40	l3	0.76	0/3146	0.84	3/4228 (0.1%)
41	L4	0.70	1/2800 (0.0%)	0.88	3/3790 (0.1%)
41	l4	0.68	1/2800 (0.0%)	0.85	3/3790 (0.1%)
42	L5	0.51	0/2425	0.67	0/3271
42	l5	0.65	0/2408	0.76	0/3248
43	L6	0.65	0/1260	0.79	0/1694
43	l6	0.66	0/1269	0.76	1/1705 (0.1%)
44	L7	0.68	0/1821	0.85	2/2451 (0.1%)
44	l7	0.74	0/1828	0.80	2/2461 (0.1%)
45	L8	0.51	0/1836	0.69	0/2481
45	l8	0.52	0/1795	0.67	0/2429
46	L9	0.60	0/1539	0.71	0/2073
46	l9	0.70	0/1539	0.80	0/2073
47	M0	0.64	0/1741	0.76	2/2335 (0.1%)
47	m0	0.67	0/1758	0.80	3/2358 (0.1%)
48	M1	0.49	0/1374	0.71	1/1842 (0.1%)
48	m1	0.59	0/1374	0.81	2/1842 (0.1%)
49	M3	0.68	0/1568	0.80	1/2106 (0.0%)
49	m3	0.61	0/1573	0.78	0/2113
50	M4	0.61	0/1068	0.74	0/1438
50	m4	0.68	0/1074	0.80	1/1446 (0.1%)
51	M5	0.65	0/1757	0.79	1/2354 (0.0%)
51	m5	0.64	0/1757	0.77	0/2354
52	M6	0.70	0/1585	0.86	3/2128 (0.1%)
52	m6	0.84	0/1585	0.92	3/2128 (0.1%)
53	M7	0.67	0/1443	0.80	1/1944 (0.1%)
53	m7	0.78	0/1250	0.81	0/1683
54	M8	0.67	0/1465	0.85	2/1965 (0.1%)
54	m8	0.66	0/1465	0.86	2/1965 (0.1%)
55	M9	0.51	0/1538	0.66	0/2050
55	m9	0.57	0/1538	0.65	0/2050
56	N0	0.64	0/1481	0.82	3/1990 (0.2%)
56	n0	0.73	0/1481	0.83	2/1990 (0.1%)
57	N1	0.68	0/1300	0.79	0/1743
57	n1	0.74	0/1300	0.79	0/1743
58	N2	0.44	0/812	0.63	0/1099
58	n2	0.46	0/794	0.62	0/1076
59	N3	0.62	0/1018	0.78	1/1369 (0.1%)
59	n3	0.69	0/1018	0.83	1/1369 (0.1%)
60	N4	0.50	0/712	0.64	0/958
60	n4	0.61	0/1052	0.70	0/1398
61	N5	0.53	0/979	0.74	1/1321 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
61	n5	0.58	0/974	0.74	1/1314 (0.1%)
62	N6	0.63	0/1004	0.82	1/1341 (0.1%)
62	n6	0.57	0/1004	0.78	1/1341 (0.1%)
63	N7	0.49	0/1118	0.66	0/1497
63	n7	0.47	0/1118	0.67	0/1497
64	N8	0.72	0/1204	0.86	1/1612 (0.1%)
64	n8	0.69	0/1204	0.82	0/1612
65	N9	0.60	0/473	0.78	0/629
65	n9	0.63	0/473	0.89	1/629 (0.2%)
66	O0	0.47	0/751	0.64	0/1008
66	o0	0.49	0/775	0.69	0/1040
67	O1	0.60	0/890	0.74	0/1196
67	o1	0.66	0/897	0.81	0/1205
68	O2	0.79	0/1041	0.87	0/1394
68	o2	0.74	0/1041	0.87	2/1394 (0.1%)
69	O3	0.79	0/868	0.85	0/1168
69	o3	0.79	0/868	0.83	0/1168
70	O4	0.59	0/890	0.79	2/1189 (0.2%)
70	o4	0.57	0/890	0.81	0/1189
71	O5	0.62	0/978	0.77	0/1301
71	o5	0.53	0/974	0.67	0/1297
72	O6	0.57	0/778	0.74	0/1034
72	o6	0.55	0/777	0.70	0/1033
73	O7	0.67	0/696	0.94	4/923 (0.4%)
73	o7	0.64	0/696	0.81	1/923 (0.1%)
74	O8	0.48	0/618	0.64	1/826 (0.1%)
74	o8	0.45	0/614	0.64	0/822
75	O9	0.64	0/443	0.83	0/588
75	o9	0.63	0/443	0.76	0/588
76	Q0	0.64	0/423	0.73	0/562
76	q0	0.81	1/423 (0.2%)	0.85	0/562
77	Q1	0.66	0/234	0.84	0/300
77	q1	0.65	0/234	0.98	2/300 (0.7%)
78	Q2	0.74	1/860 (0.1%)	0.83	0/1136
78	q2	0.69	0/860	0.79	1/1136 (0.1%)
79	Q3	0.67	0/701	0.77	0/934
79	q3	0.65	0/701	0.80	0/934
80	c0	0.40	0/777	0.66	3/1049 (0.3%)
81	e0	0.49	0/499	0.72	0/665
82	e1	0.38	0/619	0.74	1/822 (0.1%)
84	p0	0.44	0/1092	0.63	1/1474 (0.1%)
All	All	0.80	153/430074 (0.0%)	1.26	3913/631364 (0.6%)

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
3	s1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	s8	0	1
13	C1	0	1
15	c3	0	1
16	C4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	3
22	d0	0	1
25	D3	0	1
26	d4	0	2
27	D5	0	3
27	d5	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	2
42	l5	0	2
43	l6	0	1
44	l7	0	2
45	L8	0	2
48	M1	0	2
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	2
56	n0	0	1
57	N1	0	1
60	n4	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
82	e1	0	1
All	All	0	52

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.64	1.28	1.38
36	5	3008	A	N9-C4	-8.98	1.32	1.37
36	5	2358	A	N9-C4	-8.04	1.33	1.37
36	1	1114	U	C2-N3	-7.72	1.32	1.37
36	1	2714	G	N9-C4	-7.69	1.31	1.38

The worst 5 of 3913 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C4-N9	-21.84	112.90	126.00
36	5	1152	G	N3-C4-C5	21.63	139.41	128.60
36	5	1152	G	C2-N3-C4	-18.18	102.81	111.90
36	1	2714	G	N3-C4-C5	17.75	137.47	128.60
36	1	1308	A	O5'-P-OP2	-16.96	90.35	110.70

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	127	GLN	Peptide
16	C4	124	ASP	Peptide
18	C6	40	GLU	Peptide
19	C7	22	PRO	Peptide
9	S7	131	PHE	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%)	143 (70%)	34 (17%)	27 (13%)	0 1
2	s0	204/251 (81%)	152 (74%)	33 (16%)	19 (9%)	0 3
3	S1	212/254 (84%)	141 (66%)	38 (18%)	33 (16%)	0 1
3	s1	214/254 (84%)	171 (80%)	30 (14%)	13 (6%)	1 12
4	S2	215/253 (85%)	173 (80%)	27 (13%)	15 (7%)	1 8
4	s2	215/253 (85%)	184 (86%)	21 (10%)	10 (5%)	2 17
5	S3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	1 9
5	s3	221/239 (92%)	174 (79%)	31 (14%)	16 (7%)	1 7
6	S4	258/260 (99%)	206 (80%)	34 (13%)	18 (7%)	1 8
6	s4	258/260 (99%)	210 (81%)	28 (11%)	20 (8%)	1 6
7	S5	204/224 (91%)	154 (76%)	34 (17%)	16 (8%)	1 6
7	s5	204/224 (91%)	154 (76%)	35 (17%)	15 (7%)	1 7
8	S6	224/236 (95%)	197 (88%)	15 (7%)	12 (5%)	2 14
8	s6	216/236 (92%)	184 (85%)	22 (10%)	10 (5%)	2 18
9	S7	182/189 (96%)	136 (75%)	25 (14%)	21 (12%)	0 2
9	s7	184/189 (97%)	141 (77%)	28 (15%)	15 (8%)	1 5
10	S8	184/200 (92%)	148 (80%)	23 (12%)	13 (7%)	1 8
10	s8	184/200 (92%)	155 (84%)	16 (9%)	13 (7%)	1 8
11	S9	183/196 (93%)	147 (80%)	26 (14%)	10 (6%)	2 14
11	s9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	3 22
12	C0	94/105 (90%)	68 (72%)	17 (18%)	9 (10%)	0 3
13	C1	153/155 (99%)	114 (74%)	24 (16%)	15 (10%)	0 3
13	c1	144/155 (93%)	122 (85%)	16 (11%)	6 (4%)	3 20
14	C2	122/142 (86%)	67 (55%)	34 (28%)	21 (17%)	0 0
14	c2	122/142 (86%)	67 (55%)	32 (26%)	23 (19%)	0 0
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	3 21
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	1 9
16	C4	125/136 (92%)	90 (72%)	19 (15%)	16 (13%)	0 1
16	c4	126/136 (93%)	96 (76%)	19 (15%)	11 (9%)	1 4
17	C5	122/141 (86%)	88 (72%)	22 (18%)	12 (10%)	0 3
17	c5	133/141 (94%)	94 (71%)	20 (15%)	19 (14%)	0 1
18	C6	139/142 (98%)	117 (84%)	11 (8%)	11 (8%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	1 14
19	C7	116/136 (85%)	87 (75%)	21 (18%)	8 (7%)	1 8
19	c7	113/136 (83%)	84 (74%)	19 (17%)	10 (9%)	1 4
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1 5
20	c8	143/145 (99%)	115 (80%)	18 (13%)	10 (7%)	1 8
21	C9	141/143 (99%)	120 (85%)	14 (10%)	7 (5%)	2 16
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	2 20
22	D0	105/120 (88%)	82 (78%)	19 (18%)	4 (4%)	3 22
22	d0	108/120 (90%)	87 (81%)	10 (9%)	11 (10%)	0 3
23	D1	85/87 (98%)	64 (75%)	12 (14%)	9 (11%)	0 2
23	d1	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	3 24
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	6 34
24	d2	127/129 (98%)	112 (88%)	14 (11%)	1 (1%)	19 58
25	D3	142/144 (99%)	109 (77%)	19 (13%)	14 (10%)	0 3
25	d3	142/144 (99%)	119 (84%)	18 (13%)	5 (4%)	3 24
26	D4	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	1 12
26	d4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	1 7
27	D5	68/107 (64%)	44 (65%)	11 (16%)	13 (19%)	0 0
27	d5	67/107 (63%)	49 (73%)	11 (16%)	7 (10%)	0 3
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0 1
28	d6	95/97 (98%)	67 (70%)	18 (19%)	10 (10%)	0 3
29	D7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1 4
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1 4
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	0 3
30	d8	61/66 (92%)	43 (70%)	13 (21%)	5 (8%)	1 5
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3 22
31	d9	51/55 (93%)	36 (71%)	9 (18%)	6 (12%)	0 2
32	E0	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	9 42
33	E1	69/76 (91%)	38 (55%)	12 (17%)	19 (28%)	0 0
34	SR	316/318 (99%)	244 (77%)	45 (14%)	27 (8%)	1 4
34	sR	316/318 (99%)	261 (83%)	42 (13%)	13 (4%)	3 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	SM	155/273 (57%)	111 (72%)	27 (17%)	17 (11%)	0 2
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0 1
39	L2	250/253 (99%)	224 (90%)	17 (7%)	9 (4%)	3 23
39	l2	250/253 (99%)	214 (86%)	23 (9%)	13 (5%)	2 15
40	L3	384/386 (100%)	322 (84%)	45 (12%)	17 (4%)	2 19
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	3 24
41	L4	359/361 (99%)	297 (83%)	34 (10%)	28 (8%)	1 6
41	l4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	1 12
42	L5	294/296 (99%)	237 (81%)	35 (12%)	22 (8%)	1 7
42	l5	292/296 (99%)	253 (87%)	32 (11%)	7 (2%)	6 34
43	L6	152/175 (87%)	134 (88%)	12 (8%)	6 (4%)	3 22
43	l6	153/175 (87%)	130 (85%)	17 (11%)	6 (4%)	3 22
44	L7	220/243 (90%)	184 (84%)	26 (12%)	10 (4%)	2 18
44	l7	221/243 (91%)	189 (86%)	27 (12%)	5 (2%)	6 34
45	L8	231/255 (91%)	189 (82%)	31 (13%)	11 (5%)	2 17
45	l8	229/255 (90%)	188 (82%)	23 (10%)	18 (8%)	1 6
46	L9	189/191 (99%)	166 (88%)	21 (11%)	2 (1%)	14 51
46	l9	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	4 26
47	M0	207/220 (94%)	171 (83%)	28 (14%)	8 (4%)	3 22
47	m0	209/220 (95%)	172 (82%)	23 (11%)	14 (7%)	1 9
48	M1	167/173 (96%)	122 (73%)	29 (17%)	16 (10%)	0 3
48	m1	167/173 (96%)	141 (84%)	15 (9%)	11 (7%)	1 9
49	M3	191/198 (96%)	154 (81%)	26 (14%)	11 (6%)	1 13
49	m3	192/198 (97%)	150 (78%)	28 (15%)	14 (7%)	1 7
50	M4	134/137 (98%)	113 (84%)	12 (9%)	9 (7%)	1 9
50	m4	135/137 (98%)	118 (87%)	16 (12%)	1 (1%)	22 61
51	M5	201/203 (99%)	183 (91%)	14 (7%)	4 (2%)	7 38
51	m5	201/203 (99%)	181 (90%)	16 (8%)	4 (2%)	7 38
52	M6	195/198 (98%)	176 (90%)	12 (6%)	7 (4%)	3 23
52	m6	195/198 (98%)	179 (92%)	10 (5%)	6 (3%)	4 26
53	M7	181/183 (99%)	144 (80%)	27 (15%)	10 (6%)	2 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	m7	153/183 (84%)	132 (86%)	18 (12%)	3 (2%)	7 38
54	M8	183/185 (99%)	154 (84%)	24 (13%)	5 (3%)	5 30
54	m8	183/185 (99%)	151 (82%)	26 (14%)	6 (3%)	4 25
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29 67
55	m9	186/188 (99%)	167 (90%)	14 (8%)	5 (3%)	5 30
56	N0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	8 41
56	n0	170/172 (99%)	160 (94%)	7 (4%)	3 (2%)	8 41
57	N1	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	2 18
57	n1	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	4 26
58	N2	98/120 (82%)	72 (74%)	15 (15%)	11 (11%)	0 2
58	n2	96/120 (80%)	78 (81%)	15 (16%)	3 (3%)	4 26
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	10 44
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100 100
60	N4	96/155 (62%)	78 (81%)	13 (14%)	5 (5%)	2 15
60	n4	133/155 (86%)	109 (82%)	15 (11%)	9 (7%)	1 9
61	N5	119/141 (84%)	106 (89%)	11 (9%)	2 (2%)	9 42
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1 7
62	N6	124/126 (98%)	104 (84%)	14 (11%)	6 (5%)	2 17
62	n6	124/126 (98%)	112 (90%)	8 (6%)	4 (3%)	4 26
63	N7	133/135 (98%)	111 (84%)	11 (8%)	11 (8%)	1 5
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	1 5
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	2 17
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	3 24
65	N9	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	2 14
65	n9	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1 4
66	O0	95/104 (91%)	76 (80%)	15 (16%)	4 (4%)	3 20
66	o0	98/104 (94%)	85 (87%)	13 (13%)	0	100 100
67	O1	107/112 (96%)	91 (85%)	8 (8%)	8 (8%)	1 7
67	o1	107/112 (96%)	85 (79%)	13 (12%)	9 (8%)	1 5
68	O2	125/129 (97%)	108 (86%)	17 (14%)	0	100 100
68	o2	125/129 (97%)	109 (87%)	9 (7%)	7 (6%)	2 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
69	O3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	4 28
69	o3	104/106 (98%)	96 (92%)	4 (4%)	4 (4%)	3 22
70	O4	110/119 (92%)	94 (86%)	14 (13%)	2 (2%)	8 41
70	o4	110/119 (92%)	100 (91%)	9 (8%)	1 (1%)	17 56
71	O5	117/119 (98%)	99 (85%)	10 (8%)	8 (7%)	1 9
71	o5	117/119 (98%)	95 (81%)	17 (14%)	5 (4%)	2 20
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1 11
72	o6	97/99 (98%)	76 (78%)	15 (16%)	6 (6%)	1 11
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	3 24
73	o7	85/87 (98%)	70 (82%)	11 (13%)	4 (5%)	2 17
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	3 21
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	3 21
75	O9	48/50 (96%)	40 (83%)	6 (12%)	2 (4%)	3 20
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100 100
76	Q0	50/52 (96%)	39 (78%)	9 (18%)	2 (4%)	3 21
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	7 38
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100 100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2 20
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	1 13
78	q2	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	8 39
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	3 24
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	14 51
80	c0	92/105 (88%)	59 (64%)	16 (17%)	17 (18%)	0 0
81	e0	60/62 (97%)	43 (72%)	10 (17%)	7 (12%)	0 2
82	e1	74/76 (97%)	34 (46%)	21 (28%)	19 (26%)	0 0
84	p0	139/311 (45%)	116 (84%)	16 (12%)	7 (5%)	2 16
All	All	22333/24141 (92%)	18253 (82%)	2722 (12%)	1358 (6%)	1 12

5 of 1358 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN

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Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	66	ALA
2	S0	111	ILE

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%)	136 (83%)	28 (17%)	2 10
2	s0	165/209 (79%)	127 (77%)	38 (23%)	1 3
3	S1	191/223 (86%)	151 (79%)	40 (21%)	1 6
3	s1	192/223 (86%)	153 (80%)	39 (20%)	1 6
4	S2	176/204 (86%)	130 (74%)	46 (26%)	0 2
4	s2	176/204 (86%)	129 (73%)	47 (27%)	0 2
5	S3	182/194 (94%)	143 (79%)	39 (21%)	1 5
5	s3	182/194 (94%)	143 (79%)	39 (21%)	1 5
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1 7
6	s4	221/221 (100%)	184 (83%)	37 (17%)	2 10
7	S5	173/190 (91%)	145 (84%)	28 (16%)	2 11
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1 3
8	S6	188/201 (94%)	151 (80%)	37 (20%)	1 7
8	s6	187/201 (93%)	150 (80%)	37 (20%)	1 7
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2 9
9	s7	165/169 (98%)	134 (81%)	31 (19%)	1 8
10	S8	150/161 (93%)	122 (81%)	28 (19%)	1 8
10	s8	150/161 (93%)	124 (83%)	26 (17%)	2 10
11	S9	158/165 (96%)	124 (78%)	34 (22%)	1 5
11	s9	158/165 (96%)	126 (80%)	32 (20%)	1 6
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2 10
13	c1	129/136 (95%)	109 (84%)	20 (16%)	2 12
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0 2
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0 1
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1 5
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1 8
16	C4	81/104 (78%)	60 (74%)	21 (26%)	0 2
16	c4	97/104 (93%)	69 (71%)	28 (29%)	0 1
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1 6
17	c5	103/117 (88%)	78 (76%)	25 (24%)	0 2
18	C6	117/118 (99%)	89 (76%)	28 (24%)	0 3
18	c6	118/118 (100%)	95 (80%)	23 (20%)	1 7
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1 6
19	c7	92/124 (74%)	66 (72%)	26 (28%)	0 1
20	C8	128/128 (100%)	96 (75%)	32 (25%)	0 2
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1 6
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0 1
21	c9	115/115 (100%)	93 (81%)	22 (19%)	1 8
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2 10
22	d0	103/113 (91%)	71 (69%)	32 (31%)	0 0
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1 6
23	d1	74/74 (100%)	59 (80%)	15 (20%)	1 6
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1 6
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2 12
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2 9
25	d3	119/119 (100%)	92 (77%)	27 (23%)	1 4
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2 9
26	d4	112/112 (100%)	91 (81%)	21 (19%)	1 8
27	D5	61/88 (69%)	50 (82%)	11 (18%)	1 9
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1 7
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	d6	83/83 (100%)	63 (76%)	20 (24%)	0 3
29	D7	70/70 (100%)	55 (79%)	15 (21%)	1 5
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2 12
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0 1
30	d8	56/59 (95%)	41 (73%)	15 (27%)	0 2
31	D9	47/48 (98%)	41 (87%)	6 (13%)	4 20
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1 5
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2 9
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0 1
34	SR	260/261 (100%)	214 (82%)	46 (18%)	2 9
34	sR	260/261 (100%)	237 (91%)	23 (9%)	10 36
35	SM	97/228 (42%)	79 (81%)	18 (19%)	1 8
35	sM	54/228 (24%)	40 (74%)	14 (26%)	0 2
39	L2	193/195 (99%)	153 (79%)	40 (21%)	1 6
39	l2	192/195 (98%)	156 (81%)	36 (19%)	1 8
40	L3	320/322 (99%)	260 (81%)	60 (19%)	1 8
40	l3	319/322 (99%)	259 (81%)	60 (19%)	1 8
41	L4	288/288 (100%)	241 (84%)	47 (16%)	2 11
41	l4	288/288 (100%)	236 (82%)	52 (18%)	1 8
42	L5	244/244 (100%)	199 (82%)	45 (18%)	1 8
42	l5	243/244 (100%)	194 (80%)	49 (20%)	1 6
43	L6	134/152 (88%)	113 (84%)	21 (16%)	2 12
43	l6	135/152 (89%)	113 (84%)	22 (16%)	2 11
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4 19
44	l7	187/204 (92%)	163 (87%)	24 (13%)	4 20
45	L8	187/207 (90%)	151 (81%)	36 (19%)	1 8
45	l8	177/207 (86%)	145 (82%)	32 (18%)	1 8
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1 6
46	l9	171/171 (100%)	132 (77%)	39 (23%)	1 4
47	M0	177/186 (95%)	136 (77%)	41 (23%)	1 3
47	m0	179/186 (96%)	148 (83%)	31 (17%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1 5
48	m1	147/150 (98%)	112 (76%)	35 (24%)	0 3
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1 7
49	m3	154/158 (98%)	129 (84%)	25 (16%)	2 11
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2 9
50	m4	108/108 (100%)	84 (78%)	24 (22%)	1 4
51	M5	175/175 (100%)	148 (85%)	27 (15%)	2 13
51	m5	175/175 (100%)	142 (81%)	33 (19%)	1 8
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2 11
52	m6	160/161 (99%)	136 (85%)	24 (15%)	3 14
53	M7	140/145 (97%)	114 (81%)	26 (19%)	1 8
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1 8
54	M8	150/150 (100%)	123 (82%)	27 (18%)	1 9
54	m8	150/150 (100%)	125 (83%)	25 (17%)	2 10
55	M9	153/153 (100%)	130 (85%)	23 (15%)	3 14
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1 6
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1 6
56	n0	156/156 (100%)	127 (81%)	29 (19%)	1 8
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1 3
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1 5
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2 10
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1 5
59	N3	104/104 (100%)	85 (82%)	19 (18%)	1 8
59	n3	104/104 (100%)	95 (91%)	9 (9%)	10 37
60	N4	57/129 (44%)	47 (82%)	10 (18%)	2 9
60	n4	100/129 (78%)	84 (84%)	16 (16%)	2 11
61	N5	104/117 (89%)	88 (85%)	16 (15%)	2 13
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1 6
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1 6
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0 0
63	N7	115/115 (100%)	96 (84%)	19 (16%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
63	n7	115/115 (100%)	89 (77%)	26 (23%)	1 4
64	N8	118/118 (100%)	90 (76%)	28 (24%)	1 3
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1 8
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1 7
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2 10
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1 3
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1 6
67	O1	92/96 (96%)	75 (82%)	17 (18%)	1 8
67	o1	94/96 (98%)	71 (76%)	23 (24%)	0 2
68	O2	109/110 (99%)	82 (75%)	27 (25%)	0 2
68	o2	109/110 (99%)	89 (82%)	20 (18%)	1 8
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2 10
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2 9
70	O4	95/101 (94%)	76 (80%)	19 (20%)	1 6
70	o4	95/101 (94%)	78 (82%)	17 (18%)	2 9
71	O5	104/104 (100%)	79 (76%)	25 (24%)	0 3
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1 6
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0 2
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0 1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	1 8
73	o7	70/70 (100%)	53 (76%)	17 (24%)	0 2
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0 2
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2 9
75	O9	45/45 (100%)	34 (76%)	11 (24%)	0 2
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2 9
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0 2
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1 3
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2 10
77	q1	23/23 (100%)	18 (78%)	5 (22%)	1 5
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	0 2
78	q2	90/90 (100%)	65 (72%)	25 (28%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2 10
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1 6
80	c0	73/98 (74%)	65 (89%)	8 (11%)	6 26
81	e0	53/53 (100%)	40 (76%)	13 (24%)	0 2
82	e1	66/66 (100%)	45 (68%)	21 (32%)	0 0
84	p0	105/253 (42%)	84 (80%)	21 (20%)	1 6
All	All	18727/20239 (92%)	15017 (80%)	3710 (20%)	1 7

5 of 3710 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	s0	96	THR
70	o4	61	GLN
16	c4	81	VAL
68	o2	61	LYS
54	m8	57	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
80	c0	29	GLN
29	d7	19	HIS
80	c0	32	HIS
20	c8	90	ASN
34	sR	184	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	488 (27%)	56 (3%)
1	6	1792/1800 (99%)	474 (26%)	57 (3%)
36	1	3145/3396 (92%)	688 (21%)	83 (2%)
36	5	3145/3396 (92%)	687 (21%)	76 (2%)
37	3	120/121 (99%)	14 (11%)	0
37	7	120/121 (99%)	24 (20%)	1 (0%)
38	4	157/158 (99%)	38 (24%)	2 (1%)
38	8	157/158 (99%)	37 (23%)	2 (1%)
All	All	10383/10950 (94%)	2450 (23%)	277 (2%)

5 of 2450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 277 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	1716	U
36	5	2112	U
36	5	3078	U
36	1	1820	U
36	1	1751	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2563 ligands modelled in this entry, 1424 are monoatomic - leaving 1139 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	3897	-	0,6,6	-	-	-		
88	OHX	5	4017	-	0,6,6	-	-	-		
88	OHX	5	4215	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4168	-	0,6,6	-	-	-		
88	OHX	5	4082	-	0,6,6	-	-	-		
88	OHX	5	3980	-	0,6,6	-	-	-		
88	OHX	5	3989	-	0,6,6	-	-	-		
88	OHX	2	2044	-	0,6,6	-	-	-		
88	OHX	5	4074	-	0,6,6	-	-	-		
88	OHX	5	4076	-	0,6,6	-	-	-		
88	OHX	5	3924	-	0,6,6	-	-	-		
88	OHX	5	4165	-	0,6,6	-	-	-		
88	OHX	5	3948	-	0,6,6	-	-	-		
88	OHX	5	3995	-	0,6,6	-	-	-		
88	OHX	m1	203	-	0,6,6	-	-	-		
88	OHX	5	4084	-	0,6,6	-	-	-		
88	OHX	6	2192	-	0,6,6	-	-	-		
88	OHX	2	2112	-	0,6,6	-	-	-		
88	OHX	2	2122	-	0,6,6	-	-	-		
88	OHX	1	3952	-	0,6,6	-	-	-		
88	OHX	1	4162	-	0,6,6	-	-	-		
88	OHX	1	4003	-	0,6,6	-	-	-		
88	OHX	2	2169	-	0,6,6	-	-	-		
88	OHX	N9	101	-	0,6,6	-	-	-		
88	OHX	5	4070	-	0,6,6	-	-	-		
88	OHX	1	4048	-	0,6,6	-	-	-		
88	OHX	5	4073	-	0,6,6	-	-	-		
88	OHX	3	223	-	0,6,6	-	-	-		
88	OHX	L3	405	-	0,6,6	-	-	-		
88	OHX	1	4062	-	0,6,6	-	-	-		
88	OHX	1	3958	-	0,6,6	-	-	-		
88	OHX	1	4054	-	0,6,6	-	-	-		
88	OHX	5	4182	-	0,6,6	-	-	-		
91	C	q2	502	-	18,21,22	0.37	0	26,30,33	0.63	0
88	OHX	1	4142	-	0,6,6	-	-	-		
88	OHX	1	3982	-	0,6,6	-	-	-		
88	OHX	5	4208	-	0,6,6	-	-	-		
88	OHX	5	4237	-	0,6,6	-	-	-		
88	OHX	8	219	-	0,6,6	-	-	-		
88	OHX	1	4134	-	0,6,6	-	-	-		
88	OHX	2	2173	-	0,6,6	-	-	-		
88	OHX	4	225	-	0,6,6	-	-	-		
88	OHX	6	2199	-	0,6,6	-	-	-		
88	OHX	SR	401	-	0,6,6	-	-	-		
88	OHX	5	3984	-	0,6,6	-	-	-		
88	OHX	5	4079	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4218	-	0,6,6	-	-	-		
88	OHX	2	2127	-	0,6,6	-	-	-		
88	OHX	2	2137	-	0,6,6	-	-	-		
88	OHX	5	4201	-	0,6,6	-	-	-		
88	OHX	4	222	-	0,6,6	-	-	-		
88	OHX	2	2149	-	0,6,6	-	-	-		
88	OHX	2	2111	-	0,6,6	-	-	-		
88	OHX	5	4127	-	0,6,6	-	-	-		
88	OHX	1	4035	-	0,6,6	-	-	-		
88	OHX	5	4106	-	0,6,6	-	-	-		
88	OHX	5	3946	-	0,6,6	-	-	-		
88	OHX	1	3927	-	0,6,6	-	-	-		
88	OHX	8	223	-	0,6,6	-	-	-		
88	OHX	o7	502	-	0,6,6	-	-	-		
88	OHX	5	3957	-	0,6,6	-	-	-		
88	OHX	2	2148	-	0,6,6	-	-	-		
88	OHX	5	4022	-	0,6,6	-	-	-		
88	OHX	5	4001	-	0,6,6	-	-	-		
88	OHX	5	3910	-	0,6,6	-	-	-		
88	OHX	2	2142	-	0,6,6	-	-	-		
88	OHX	1	4127	-	0,6,6	-	-	-		
88	OHX	1	4187	-	0,6,6	-	-	-		
88	OHX	6	2169	-	0,6,6	-	-	-		
88	OHX	1	4102	-	0,6,6	-	-	-		
88	OHX	5	4089	-	0,6,6	-	-	-		
88	OHX	8	230	-	0,6,6	-	-	-		
88	OHX	2	2095	-	0,6,6	-	-	-		
88	OHX	5	4232	-	0,6,6	-	-	-		
88	OHX	6	2054	-	0,6,6	-	-	-		
88	OHX	6	2141	-	0,6,6	-	-	-		
88	OHX	1	4166	-	0,6,6	-	-	-		
88	OHX	6	2135	-	0,6,6	-	-	-		
88	OHX	1	4176	-	0,6,6	-	-	-		
88	OHX	1	3898	-	0,6,6	-	-	-		
88	OHX	5	4019	-	0,6,6	-	-	-		
88	OHX	5	4147	-	0,6,6	-	-	-		
88	OHX	2	2153	-	0,6,6	-	-	-		
88	OHX	M7	205	-	0,6,6	-	-	-		
88	OHX	5	4023	-	0,6,6	-	-	-		
88	OHX	1	4178	-	0,6,6	-	-	-		
88	OHX	1	4024	-	0,6,6	-	-	-		
88	OHX	1	4186	-	0,6,6	-	-	-		
88	OHX	7	220	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	L3	406	-	0,6,6	-	-	-		
88	OHX	5	4009	-	0,6,6	-	-	-		
88	OHX	1	4219	-	0,6,6	-	-	-		
88	OHX	2	2125	-	0,6,6	-	-	-		
88	OHX	1	4068	-	0,6,6	-	-	-		
88	OHX	1	4073	-	0,6,6	-	-	-		
88	OHX	5	3983	-	0,6,6	-	-	-		
88	OHX	2	2093	-	0,6,6	-	-	-		
88	OHX	5	4154	-	0,6,6	-	-	-		
88	OHX	1	4199	-	0,6,6	-	-	-		
88	OHX	6	2106	-	0,6,6	-	-	-		
88	OHX	7	226	-	0,6,6	-	-	-		
88	OHX	5	4095	-	0,6,6	-	-	-		
88	OHX	6	2084	-	0,6,6	-	-	-		
88	OHX	6	2179	-	0,6,6	-	-	-		
88	OHX	5	3962	-	0,6,6	-	-	-		
88	OHX	1	4159	-	0,6,6	-	-	-		
88	OHX	2	2029	-	0,6,6	-	-	-		
88	OHX	1	3938	-	0,6,6	-	-	-		
88	OHX	1	4222	-	0,6,6	-	-	-		
88	OHX	2	2176	-	0,6,6	-	-	-		
88	OHX	5	3952	-	0,6,6	-	-	-		
88	OHX	6	2160	-	0,6,6	-	-	-		
88	OHX	2	2079	-	0,6,6	-	-	-		
88	OHX	2	2158	-	0,6,6	-	-	-		
88	OHX	5	4146	-	0,6,6	-	-	-		
88	OHX	6	2062	-	0,6,6	-	-	-		
88	OHX	6	2059	-	0,6,6	-	-	-		
88	OHX	5	3958	-	0,6,6	-	-	-		
88	OHX	5	4129	-	0,6,6	-	-	-		
88	OHX	2	2102	-	0,6,6	-	-	-		
88	OHX	1	3884	-	0,6,6	-	-	-		
88	OHX	5	4034	-	0,6,6	-	-	-		
88	OHX	1	4198	-	0,6,6	-	-	-		
88	OHX	5	3968	-	0,6,6	-	-	-		
88	OHX	6	2060	-	0,6,6	-	-	-		
88	OHX	l5	304	-	0,6,6	-	-	-		
88	OHX	O7	104	-	0,6,6	-	-	-		
88	OHX	5	4238	-	0,6,6	-	-	-		
88	OHX	1	4175	-	0,6,6	-	-	-		
88	OHX	1	4098	-	0,6,6	-	-	-		
88	OHX	6	2070	-	0,6,6	-	-	-		
88	OHX	5	3922	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	2	2161	-	0,6,6	-	-	-		
88	OHX	1	4116	-	0,6,6	-	-	-		
88	OHX	5	3923	-	0,6,6	-	-	-		
88	OHX	2	2045	-	0,6,6	-	-	-		
88	OHX	3	217	-	0,6,6	-	-	-		
88	OHX	1	4104	-	0,6,6	-	-	-		
88	OHX	2	2026	-	0,6,6	-	-	-		
88	OHX	1	4220	-	0,6,6	-	-	-		
88	OHX	6	2154	-	0,6,6	-	-	-		
90	A	5	3401	-	18,24,25	0.68	0	18,35,38	0.99	1 (5%)
88	OHX	2	2052	-	0,6,6	-	-	-		
88	OHX	7	218	-	0,6,6	-	-	-		
88	OHX	2	2134	-	0,6,6	-	-	-		
88	OHX	1	3988	-	0,6,6	-	-	-		
88	OHX	5	4096	-	0,6,6	-	-	-		
88	OHX	2	2027	-	0,6,6	-	-	-		
88	OHX	1	3943	-	0,6,6	-	-	-		
88	OHX	2	2155	-	0,6,6	-	-	-		
88	OHX	5	4189	-	0,6,6	-	-	-		
88	OHX	2	2141	-	0,6,6	-	-	-		
88	OHX	6	2187	-	0,6,6	-	-	-		
88	OHX	5	4054	-	0,6,6	-	-	-		
88	OHX	1	4029	-	0,6,6	-	-	-		
88	OHX	6	2050	-	0,6,6	-	-	-		
88	OHX	1	4128	-	0,6,6	-	-	-		
88	OHX	6	2202	-	0,6,6	-	-	-		
88	OHX	1	4157	-	0,6,6	-	-	-		
88	OHX	2	2060	-	0,6,6	-	-	-		
88	OHX	1	3873	-	0,6,6	-	-	-		
88	OHX	5	4149	-	0,6,6	-	-	-		
88	OHX	5	4166	-	0,6,6	-	-	-		
88	OHX	5	4162	-	0,6,6	-	-	-		
88	OHX	1	4124	-	0,6,6	-	-	-		
88	OHX	5	4003	-	0,6,6	-	-	-		
88	OHX	5	4179	-	0,6,6	-	-	-		
88	OHX	1	4096	-	0,6,6	-	-	-		
88	OHX	5	4239	-	0,6,6	-	-	-		
88	OHX	6	2053	-	0,6,6	-	-	-		
88	OHX	6	2173	-	0,6,6	-	-	-		
88	OHX	5	4145	-	0,6,6	-	-	-		
88	OHX	5	4062	-	0,6,6	-	-	-		
88	OHX	6	2104	-	0,6,6	-	-	-		
88	OHX	5	4242	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4025	-	0,6,6	-	-	-		
88	OHX	5	4068	-	0,6,6	-	-	-		
88	OHX	2	2051	-	0,6,6	-	-	-		
88	OHX	5	3901	-	0,6,6	-	-	-		
88	OHX	5	3966	-	0,6,6	-	-	-		
88	OHX	l3	404	-	0,6,6	-	-	-		
88	OHX	6	2047	-	0,6,6	-	-	-		
88	OHX	2	2154	-	0,6,6	-	-	-		
88	OHX	5	3982	-	0,6,6	-	-	-		
88	OHX	2	2157	-	0,6,6	-	-	-		
88	OHX	1	4121	-	0,6,6	-	-	-		
88	OHX	5	3976	-	0,6,6	-	-	-		
88	OHX	5	4027	-	0,6,6	-	-	-		
88	OHX	5	4078	-	0,6,6	-	-	-		
88	OHX	5	4245	-	0,6,6	-	-	-		
88	OHX	1	3968	-	0,6,6	-	-	-		
91	C	Q2	502	-	18,21,22	0.40	0	26,30,33	0.75	0
88	OHX	5	4227	-	0,6,6	-	-	-		
88	OHX	5	4063	-	0,6,6	-	-	-		
88	OHX	5	3955	-	0,6,6	-	-	-		
88	OHX	d4	202	-	0,6,6	-	-	-		
88	OHX	5	4139	-	0,6,6	-	-	-		
88	OHX	5	4029	-	0,6,6	-	-	-		
88	OHX	2	2046	-	0,6,6	-	-	-		
88	OHX	1	3974	-	0,6,6	-	-	-		
88	OHX	5	3999	-	0,6,6	-	-	-		
88	OHX	5	4060	-	0,6,6	-	-	-		
88	OHX	5	4125	-	0,6,6	-	-	-		
88	OHX	1	3977	-	0,6,6	-	-	-		
88	OHX	6	2097	-	0,6,6	-	-	-		
88	OHX	2	2171	-	0,6,6	-	-	-		
88	OHX	6	2180	-	0,6,6	-	-	-		
88	OHX	1	3964	-	0,6,6	-	-	-		
88	OHX	1	4110	-	0,6,6	-	-	-		
88	OHX	5	3964	-	0,6,6	-	-	-		
88	OHX	2	2037	-	0,6,6	-	-	-		
88	OHX	2	2028	-	0,6,6	-	-	-		
88	OHX	1	3885	-	0,6,6	-	-	-		
88	OHX	5	4102	-	0,6,6	-	-	-		
88	OHX	8	224	-	0,6,6	-	-	-		
88	OHX	1	3981	-	0,6,6	-	-	-		
88	OHX	5	3990	-	0,6,6	-	-	-		
88	OHX	5	4206	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	C8	201	-	0,6,6	-	-	-		
88	OHX	5	4105	-	0,6,6	-	-	-		
88	OHX	5	4180	-	0,6,6	-	-	-		
88	OHX	1	4181	-	0,6,6	-	-	-		
88	OHX	6	2130	-	0,6,6	-	-	-		
88	OHX	5	3942	-	0,6,6	-	-	-		
88	OHX	6	2177	-	0,6,6	-	-	-		
88	OHX	6	2123	-	0,6,6	-	-	-		
88	OHX	5	4205	-	0,6,6	-	-	-		
88	OHX	6	2115	-	0,6,6	-	-	-		
88	OHX	5	4225	-	0,6,6	-	-	-		
88	OHX	c1	202	-	0,6,6	-	-	-		
88	OHX	1	4223	-	0,6,6	-	-	-		
88	OHX	6	2152	-	0,6,6	-	-	-		
88	OHX	1	3903	-	0,6,6	-	-	-		
88	OHX	2	2166	-	0,6,6	-	-	-		
88	OHX	5	3935	-	0,6,6	-	-	-		
88	OHX	1	4021	-	0,6,6	-	-	-		
88	OHX	6	2120	-	0,6,6	-	-	-		
88	OHX	2	2144	-	0,6,6	-	-	-		
88	OHX	1	3931	-	0,6,6	-	-	-		
88	OHX	1	4145	-	0,6,6	-	-	-		
88	OHX	l4	404	-	0,6,6	-	-	-		
88	OHX	2	2065	-	0,6,6	-	-	-		
88	OHX	1	4131	-	0,6,6	-	-	-		
88	OHX	1	4101	-	0,6,6	-	-	-		
88	OHX	2	2180	-	0,6,6	-	-	-		
88	OHX	1	4183	-	0,6,6	-	-	-		
88	OHX	6	2190	-	0,6,6	-	-	-		
88	OHX	2	2050	-	0,6,6	-	-	-		
88	OHX	l4	403	-	0,6,6	-	-	-		
88	OHX	8	217	-	0,6,6	-	-	-		
88	OHX	2	2090	-	0,6,6	-	-	-		
88	OHX	5	4041	-	0,6,6	-	-	-		
88	OHX	5	4142	-	0,6,6	-	-	-		
88	OHX	5	4196	-	0,6,6	-	-	-		
88	OHX	1	3951	-	0,6,6	-	-	-		
88	OHX	6	2185	-	0,6,6	-	-	-		
88	OHX	1	3908	-	0,6,6	-	-	-		
88	OHX	5	4100	-	0,6,6	-	-	-		
88	OHX	2	2105	-	0,6,6	-	-	-		
88	OHX	1	3915	-	0,6,6	-	-	-		
88	OHX	1	4055	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
88	OHX	3	218	-	0,6,6	-	-	-		
88	OHX	6	2196	-	0,6,6	-	-	-		
88	OHX	5	4000	-	0,6,6	-	-	-		
88	OHX	1	4185	-	0,6,6	-	-	-		
88	OHX	5	4049	-	0,6,6	-	-	-		
88	OHX	5	4080	-	0,6,6	-	-	-		
88	OHX	6	2175	-	0,6,6	-	-	-		
88	OHX	5	4246	-	0,6,6	-	-	-		
88	OHX	5	4153	-	0,6,6	-	-	-		
88	OHX	5	4175	-	0,6,6	-	-	-		
88	OHX	5	4004	-	0,6,6	-	-	-		
88	OHX	5	4249	-	0,6,6	-	-	-		
88	OHX	6	2195	-	0,6,6	-	-	-		
88	OHX	6	2153	-	0,6,6	-	-	-		
88	OHX	1	4032	-	0,6,6	-	-	-		
88	OHX	6	2058	-	0,6,6	-	-	-		
88	OHX	5	4006	-	0,6,6	-	-	-		
88	OHX	1	3879	-	0,6,6	-	-	-		
88	OHX	1	3950	-	0,6,6	-	-	-		
88	OHX	6	2068	-	0,6,6	-	-	-		
88	OHX	6	2144	-	0,6,6	-	-	-		
88	OHX	5	3950	-	0,6,6	-	-	-		
88	OHX	1	4064	-	0,6,6	-	-	-		
88	OHX	5	3963	-	0,6,6	-	-	-		
88	OHX	2	2064	-	0,6,6	-	-	-		
88	OHX	1	3906	-	0,6,6	-	-	-		
88	OHX	1	3949	-	0,6,6	-	-	-		
88	OHX	1	3924	-	0,6,6	-	-	-		
88	OHX	1	3886	-	0,6,6	-	-	-		
88	OHX	1	3970	-	0,6,6	-	-	-		
88	OHX	2	2123	-	0,6,6	-	-	-		
88	OHX	1	3940	-	0,6,6	-	-	-		
88	OHX	1	4052	-	0,6,6	-	-	-		
88	OHX	4	230	-	0,6,6	-	-	-		
88	OHX	6	2150	-	0,6,6	-	-	-		
88	OHX	1	4105	-	0,6,6	-	-	-		
88	OHX	5	3970	-	0,6,6	-	-	-		
88	OHX	2	2108	-	0,6,6	-	-	-		
88	OHX	3	215	-	0,6,6	-	-	-		
88	OHX	l9	600	-	0,6,6	-	-	-		
88	OHX	5	3943	-	0,6,6	-	-	-		
88	OHX	6	2117	-	0,6,6	-	-	-		
88	OHX	8	225	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
88	OHX	5	4016	-	0,6,6	-	-	-		
88	OHX	5	4090	-	0,6,6	-	-	-		
88	OHX	1	4043	-	0,6,6	-	-	-		
88	OHX	1	4172	-	0,6,6	-	-	-		
88	OHX	1	3944	-	0,6,6	-	-	-		
88	OHX	2	2097	-	0,6,6	-	-	-		
88	OHX	2	2177	-	0,6,6	-	-	-		
88	OHX	2	2071	-	0,6,6	-	-	-		
88	OHX	1	3907	-	0,6,6	-	-	-		
88	OHX	1	4117	-	0,6,6	-	-	-		
88	OHX	6	2110	-	0,6,6	-	-	-		
88	OHX	5	3951	-	0,6,6	-	-	-		
88	OHX	5	4059	-	0,6,6	-	-	-		
88	OHX	5	4224	-	0,6,6	-	-	-		
88	OHX	2	2055	-	0,6,6	-	-	-		
88	OHX	1	4152	-	0,6,6	-	-	-		
88	OHX	1	3926	-	0,6,6	-	-	-		
88	OHX	2	2175	-	0,6,6	-	-	-		
88	OHX	1	4067	-	0,6,6	-	-	-		
88	OHX	2	2023	-	0,6,6	-	-	-		
88	OHX	1	3928	-	0,6,6	-	-	-		
88	OHX	1	3894	-	0,6,6	-	-	-		
88	OHX	1	3962	-	0,6,6	-	-	-		
88	OHX	1	4031	-	0,6,6	-	-	-		
88	OHX	1	4057	-	0,6,6	-	-	-		
88	OHX	6	2109	-	0,6,6	-	-	-		
88	OHX	6	2189	-	0,6,6	-	-	-		
88	OHX	5	4158	-	0,6,6	-	-	-		
88	OHX	5	4231	-	0,6,6	-	-	-		
88	OHX	1	4195	-	0,6,6	-	-	-		
88	OHX	5	4067	-	0,6,6	-	-	-		
88	OHX	1	4026	-	0,6,6	-	-	-		
88	OHX	6	2102	-	0,6,6	-	-	-		
88	OHX	1	4038	-	0,6,6	-	-	-		
88	OHX	5	4190	-	0,6,6	-	-	-		
88	OHX	2	2115	-	0,6,6	-	-	-		
88	OHX	D9	102	-	0,6,6	-	-	-		
88	OHX	5	3971	-	0,6,6	-	-	-		
88	OHX	5	3991	-	0,6,6	-	-	-		
88	OHX	1	3921	-	0,6,6	-	-	-		
88	OHX	2	2109	-	0,6,6	-	-	-		
88	OHX	1	4009	-	0,6,6	-	-	-		
88	OHX	1	4165	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	6	2114	-	0,6,6	-	-	-		
88	OHX	1	3995	-	0,6,6	-	-	-		
88	OHX	1	3960	-	0,6,6	-	-	-		
88	OHX	5	3953	-	0,6,6	-	-	-		
88	OHX	5	4240	-	0,6,6	-	-	-		
88	OHX	1	3946	-	0,6,6	-	-	-		
88	OHX	2	2038	-	0,6,6	-	-	-		
88	OHX	1	4085	-	0,6,6	-	-	-		
88	OHX	5	3913	-	0,6,6	-	-	-		
88	OHX	5	3920	-	0,6,6	-	-	-		
88	OHX	1	3985	-	0,6,6	-	-	-		
88	OHX	2	2135	-	0,6,6	-	-	-		
88	OHX	6	2118	-	0,6,6	-	-	-		
88	OHX	5	3956	-	0,6,6	-	-	-		
88	OHX	5	3981	-	0,6,6	-	-	-		
88	OHX	5	4092	-	0,6,6	-	-	-		
88	OHX	n3	204	-	0,6,6	-	-	-		
88	OHX	1	3998	-	0,6,6	-	-	-		
88	OHX	6	2083	-	0,6,6	-	-	-		
88	OHX	6	2165	-	0,6,6	-	-	-		
88	OHX	5	4021	-	0,6,6	-	-	-		
88	OHX	1	4042	-	0,6,6	-	-	-		
88	OHX	5	4111	-	0,6,6	-	-	-		
88	OHX	5	4185	-	0,6,6	-	-	-		
88	OHX	1	4194	-	0,6,6	-	-	-		
88	OHX	5	3938	-	0,6,6	-	-	-		
88	OHX	2	2106	-	0,6,6	-	-	-		
88	OHX	1	3973	-	0,6,6	-	-	-		
88	OHX	1	4034	-	0,6,6	-	-	-		
88	OHX	5	4183	-	0,6,6	-	-	-		
88	OHX	5	4221	-	0,6,6	-	-	-		
88	OHX	5	4110	-	0,6,6	-	-	-		
88	OHX	2	2165	-	0,6,6	-	-	-		
88	OHX	5	4187	-	0,6,6	-	-	-		
88	OHX	5	4200	-	0,6,6	-	-	-		
88	OHX	2	2151	-	0,6,6	-	-	-		
88	OHX	2	2179	-	0,6,6	-	-	-		
88	OHX	6	2174	-	0,6,6	-	-	-		
88	OHX	1	4167	-	0,6,6	-	-	-		
88	OHX	1	3978	-	0,6,6	-	-	-		
88	OHX	5	4210	-	0,6,6	-	-	-		
88	OHX	5	4188	-	0,6,6	-	-	-		
88	OHX	1	4144	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	4123	-	0,6,6	-	-	-		
88	OHX	1	3997	-	0,6,6	-	-	-		
88	OHX	5	4244	-	0,6,6	-	-	-		
88	OHX	3	222	-	0,6,6	-	-	-		
88	OHX	5	4035	-	0,6,6	-	-	-		
88	OHX	1	3992	-	0,6,6	-	-	-		
88	OHX	6	2063	-	0,6,6	-	-	-		
88	OHX	1	4069	-	0,6,6	-	-	-		
88	OHX	2	2114	-	0,6,6	-	-	-		
88	OHX	1	4149	-	0,6,6	-	-	-		
88	OHX	6	2065	-	0,6,6	-	-	-		
88	OHX	5	3937	-	0,6,6	-	-	-		
88	OHX	5	3903	-	0,6,6	-	-	-		
88	OHX	l3	406	-	0,6,6	-	-	-		
88	OHX	1	4106	-	0,6,6	-	-	-		
88	OHX	5	4173	-	0,6,6	-	-	-		
88	OHX	1	4083	-	0,6,6	-	-	-		
88	OHX	5	4203	-	0,6,6	-	-	-		
88	OHX	5	4083	-	0,6,6	-	-	-		
88	OHX	1	4224	-	0,6,6	-	-	-		
88	OHX	5	4197	-	0,6,6	-	-	-		
88	OHX	2	2138	-	0,6,6	-	-	-		
88	OHX	5	4252	-	0,6,6	-	-	-		
88	OHX	5	3931	-	0,6,6	-	-	-		
88	OHX	5	4039	-	0,6,6	-	-	-		
88	OHX	1	4050	-	0,6,6	-	-	-		
88	OHX	1	3878	-	0,6,6	-	-	-		
88	OHX	1	4109	-	0,6,6	-	-	-		
88	OHX	O7	103	-	0,6,6	-	-	-		
88	OHX	6	2057	-	0,6,6	-	-	-		
88	OHX	6	2079	-	0,6,6	-	-	-		
88	OHX	1	4204	-	0,6,6	-	-	-		
88	OHX	6	2162	-	0,6,6	-	-	-		
88	OHX	5	4152	-	0,6,6	-	-	-		
88	OHX	3	216	-	0,6,6	-	-	-		
88	OHX	6	2131	-	0,6,6	-	-	-		
88	OHX	1	3991	-	0,6,6	-	-	-		
88	OHX	6	2101	-	0,6,6	-	-	-		
88	OHX	5	3985	-	0,6,6	-	-	-		
88	OHX	5	3994	-	0,6,6	-	-	-		
88	OHX	1	4019	-	0,6,6	-	-	-		
88	OHX	1	4129	-	0,6,6	-	-	-		
88	OHX	2	2174	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
88	OHX	1	3913	-	0,6,6	-	-	-		
88	OHX	2	2053	-	0,6,6	-	-	-		
88	OHX	1	3892	-	0,6,6	-	-	-		
88	OHX	6	2181	-	0,6,6	-	-	-		
88	OHX	4	227	-	0,6,6	-	-	-		
88	OHX	1	3983	-	0,6,6	-	-	-		
88	OHX	1	4061	-	0,6,6	-	-	-		
88	OHX	1	4033	-	0,6,6	-	-	-		
88	OHX	6	2143	-	0,6,6	-	-	-		
88	OHX	2	2039	-	0,6,6	-	-	-		
88	OHX	1	4022	-	0,6,6	-	-	-		
88	OHX	1	3901	-	0,6,6	-	-	-		
88	OHX	1	3936	-	0,6,6	-	-	-		
88	OHX	4	228	-	0,6,6	-	-	-		
88	OHX	4	229	-	0,6,6	-	-	-		
88	OHX	2	2132	-	0,6,6	-	-	-		
88	OHX	1	4015	-	0,6,6	-	-	-		
88	OHX	5	4056	-	0,6,6	-	-	-		
88	OHX	6	2052	-	0,6,6	-	-	-		
88	OHX	6	2061	-	0,6,6	-	-	-		
88	OHX	5	4140	-	0,6,6	-	-	-		
88	OHX	c5	201	-	0,6,6	-	-	-		
88	OHX	5	4052	-	0,6,6	-	-	-		
88	OHX	5	4002	-	0,6,6	-	-	-		
88	OHX	1	3876	-	0,6,6	-	-	-		
88	OHX	1	4156	-	0,6,6	-	-	-		
88	OHX	5	3961	-	0,6,6	-	-	-		
88	OHX	5	4103	-	0,6,6	-	-	-		
88	OHX	m6	203	-	0,6,6	-	-	-		
88	OHX	1	4213	-	0,6,6	-	-	-		
88	OHX	2	2047	-	0,6,6	-	-	-		
88	OHX	8	218	-	0,6,6	-	-	-		
88	OHX	5	3978	-	0,6,6	-	-	-		
88	OHX	1	4217	-	0,6,6	-	-	-		
88	OHX	5	4202	-	0,6,6	-	-	-		
88	OHX	1	4184	-	0,6,6	-	-	-		
88	OHX	2	2035	-	0,6,6	-	-	-		
88	OHX	1	4191	-	0,6,6	-	-	-		
88	OHX	1	3895	-	0,6,6	-	-	-		
88	OHX	6	2119	-	0,6,6	-	-	-		
88	OHX	8	229	-	0,6,6	-	-	-		
88	OHX	5	4058	-	0,6,6	-	-	-		
88	OHX	5	4114	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	2	2034	-	0,6,6	-	-	-		
88	OHX	S8	302	-	0,6,6	-	-	-		
88	OHX	1	4114	-	0,6,6	-	-	-		
88	OHX	5	4038	-	0,6,6	-	-	-		
88	OHX	5	4042	-	0,6,6	-	-	-		
88	OHX	2	2041	-	0,6,6	-	-	-		
88	OHX	1	4107	-	0,6,6	-	-	-		
88	OHX	1	4158	-	0,6,6	-	-	-		
88	OHX	5	3921	-	0,6,6	-	-	-		
88	OHX	7	217	-	0,6,6	-	-	-		
88	OHX	2	2098	-	0,6,6	-	-	-		
88	OHX	2	2146	-	0,6,6	-	-	-		
88	OHX	m0	302	-	0,6,6	-	-	-		
88	OHX	2	2100	-	0,6,6	-	-	-		
88	OHX	1	3965	-	0,6,6	-	-	-		
88	OHX	1	4177	-	0,6,6	-	-	-		
88	OHX	5	4107	-	0,6,6	-	-	-		
88	OHX	5	4174	-	0,6,6	-	-	-		
88	OHX	1	3976	-	0,6,6	-	-	-		
88	OHX	5	4209	-	0,6,6	-	-	-		
88	OHX	5	4251	-	0,6,6	-	-	-		
88	OHX	5	3912	-	0,6,6	-	-	-		
88	OHX	7	219	-	0,6,6	-	-	-		
88	OHX	6	2157	-	0,6,6	-	-	-		
88	OHX	6	2168	-	0,6,6	-	-	-		
88	OHX	1	3909	-	0,6,6	-	-	-		
88	OHX	1	4214	-	0,6,6	-	-	-		
88	OHX	5	3998	-	0,6,6	-	-	-		
88	OHX	1	3955	-	0,6,6	-	-	-		
88	OHX	2	2076	-	0,6,6	-	-	-		
88	OHX	1	3880	-	0,6,6	-	-	-		
88	OHX	1	4036	-	0,6,6	-	-	-		
88	OHX	6	2136	-	0,6,6	-	-	-		
88	OHX	l5	305	-	0,6,6	-	-	-		
88	OHX	6	2139	-	0,6,6	-	-	-		
88	OHX	2	2120	-	0,6,6	-	-	-		
88	OHX	1	4041	-	0,6,6	-	-	-		
88	OHX	5	4061	-	0,6,6	-	-	-		
88	OHX	5	4235	-	0,6,6	-	-	-		
88	OHX	1	4208	-	0,6,6	-	-	-		
88	OHX	M9	202	-	0,6,6	-	-	-		
88	OHX	1	4099	-	0,6,6	-	-	-		
88	OHX	1	4002	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4008	-	0,6,6	-	-	-		
88	OHX	1	4037	-	0,6,6	-	-	-		
88	OHX	1	4028	-	0,6,6	-	-	-		
88	OHX	5	3927	-	0,6,6	-	-	-		
88	OHX	1	4189	-	0,6,6	-	-	-		
88	OHX	2	2139	-	0,6,6	-	-	-		
88	OHX	sR	401	-	0,6,6	-	-	-		
88	OHX	1	4010	-	0,6,6	-	-	-		
88	OHX	1	3925	-	0,6,6	-	-	-		
88	OHX	5	4144	-	0,6,6	-	-	-		
88	OHX	1	3888	-	0,6,6	-	-	-		
88	OHX	6	2194	-	0,6,6	-	-	-		
88	OHX	1	4164	-	0,6,6	-	-	-		
88	OHX	1	3941	-	0,6,6	-	-	-		
88	OHX	1	3999	-	0,6,6	-	-	-		
88	OHX	1	3933	-	0,6,6	-	-	-		
88	OHX	L3	404	-	0,6,6	-	-	-		
88	OHX	M0	303	-	0,6,6	-	-	-		
88	OHX	6	2077	-	0,6,6	-	-	-		
88	OHX	6	2074	-	0,6,6	-	-	-		
88	OHX	2	2145	-	0,6,6	-	-	-		
88	OHX	5	3944	-	0,6,6	-	-	-		
88	OHX	1	4084	-	0,6,6	-	-	-		
88	OHX	1	3937	-	0,6,6	-	-	-		
88	OHX	5	4204	-	0,6,6	-	-	-		
88	OHX	1	4180	-	0,6,6	-	-	-		
88	OHX	5	4199	-	0,6,6	-	-	-		
88	OHX	5	3969	-	0,6,6	-	-	-		
88	OHX	6	2159	-	0,6,6	-	-	-		
88	OHX	1	3942	-	0,6,6	-	-	-		
88	OHX	1	4132	-	0,6,6	-	-	-		
88	OHX	5	4159	-	0,6,6	-	-	-		
88	OHX	1	4012	-	0,6,6	-	-	-		
88	OHX	2	2162	-	0,6,6	-	-	-		
88	OHX	6	2089	-	0,6,6	-	-	-		
88	OHX	5	4230	-	0,6,6	-	-	-		
88	OHX	7	222	-	0,6,6	-	-	-		
88	OHX	1	4136	-	0,6,6	-	-	-		
88	OHX	8	222	-	0,6,6	-	-	-		
88	OHX	1	4013	-	0,6,6	-	-	-		
88	OHX	2	2081	-	0,6,6	-	-	-		
88	OHX	2	2054	-	0,6,6	-	-	-		
88	OHX	8	221	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	6	2127	-	0,6,6	-	-	-		
88	OHX	5	4012	-	0,6,6	-	-	-		
88	OHX	5	4033	-	0,6,6	-	-	-		
88	OHX	5	4101	-	0,6,6	-	-	-		
88	OHX	1	4046	-	0,6,6	-	-	-		
88	OHX	6	2049	-	0,6,6	-	-	-		
88	OHX	2	2066	-	0,6,6	-	-	-		
88	OHX	1	3971	-	0,6,6	-	-	-		
88	OHX	2	2118	-	0,6,6	-	-	-		
88	OHX	1	3917	-	0,6,6	-	-	-		
88	OHX	6	2133	-	0,6,6	-	-	-		
88	OHX	5	4192	-	0,6,6	-	-	-		
88	OHX	3	224	-	0,6,6	-	-	-		
88	OHX	1	4143	-	0,6,6	-	-	-		
88	OHX	2	2033	-	0,6,6	-	-	-		
88	OHX	L4	402	-	0,6,6	-	-	-		
88	OHX	5	3947	-	0,6,6	-	-	-		
88	OHX	5	4024	-	0,6,6	-	-	-		
88	OHX	5	4191	-	0,6,6	-	-	-		
88	OHX	5	4194	-	0,6,6	-	-	-		
88	OHX	5	4253	-	0,6,6	-	-	-		
88	OHX	2	2049	-	0,6,6	-	-	-		
88	OHX	7	215	-	0,6,6	-	-	-		
88	OHX	2	2133	-	0,6,6	-	-	-		
88	OHX	5	4156	-	0,6,6	-	-	-		
88	OHX	4	226	-	0,6,6	-	-	-		
88	OHX	2	2160	-	0,6,6	-	-	-		
88	OHX	2	2061	-	0,6,6	-	-	-		
88	OHX	6	2140	-	0,6,6	-	-	-		
88	OHX	6	2095	-	0,6,6	-	-	-		
88	OHX	q2	504	-	0,6,6	-	-	-		
88	OHX	8	227	-	0,6,6	-	-	-		
88	OHX	1	4192	-	0,6,6	-	-	-		
88	OHX	c8	202	-	0,6,6	-	-	-		
88	OHX	2	2099	-	0,6,6	-	-	-		
88	OHX	1	4090	-	0,6,6	-	-	-		
88	OHX	5	4037	-	0,6,6	-	-	-		
88	OHX	6	2138	-	0,6,6	-	-	-		
88	OHX	2	2124	-	0,6,6	-	-	-		
88	OHX	l5	303	-	0,6,6	-	-	-		
88	OHX	5	3933	-	0,6,6	-	-	-		
88	OHX	5	3949	-	0,6,6	-	-	-		
88	OHX	8	228	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	6	2155	-	0,6,6	-	-	-		
88	OHX	5	4116	-	0,6,6	-	-	-		
88	OHX	5	3965	-	0,6,6	-	-	-		
88	OHX	5	3979	-	0,6,6	-	-	-		
88	OHX	5	3941	-	0,6,6	-	-	-		
88	OHX	1	4205	-	0,6,6	-	-	-		
88	OHX	5	4157	-	0,6,6	-	-	-		
88	OHX	1	4170	-	0,6,6	-	-	-		
88	OHX	2	2163	-	0,6,6	-	-	-		
88	OHX	1	4216	-	0,6,6	-	-	-		
88	OHX	2	2063	-	0,6,6	-	-	-		
88	OHX	6	2096	-	0,6,6	-	-	-		
88	OHX	2	2121	-	0,6,6	-	-	-		
88	OHX	5	4172	-	0,6,6	-	-	-		
88	OHX	5	3916	-	0,6,6	-	-	-		
88	OHX	5	4026	-	0,6,6	-	-	-		
88	OHX	6	2188	-	0,6,6	-	-	-		
88	OHX	5	3939	-	0,6,6	-	-	-		
88	OHX	6	2076	-	0,6,6	-	-	-		
88	OHX	1	3905	-	0,6,6	-	-	-		
88	OHX	1	4203	-	0,6,6	-	-	-		
88	OHX	1	4018	-	0,6,6	-	-	-		
88	OHX	5	4148	-	0,6,6	-	-	-		
88	OHX	5	4241	-	0,6,6	-	-	-		
88	OHX	1	4133	-	0,6,6	-	-	-		
88	OHX	2	2172	-	0,6,6	-	-	-		
88	OHX	1	4100	-	0,6,6	-	-	-		
88	OHX	5	3934	-	0,6,6	-	-	-		
88	OHX	5	4133	-	0,6,6	-	-	-		
88	OHX	2	2042	-	0,6,6	-	-	-		
88	OHX	2	2096	-	0,6,6	-	-	-		
88	OHX	1	4095	-	0,6,6	-	-	-		
88	OHX	5	4176	-	0,6,6	-	-	-		
88	OHX	2	2074	-	0,6,6	-	-	-		
88	OHX	5	4031	-	0,6,6	-	-	-		
88	OHX	5	4020	-	0,6,6	-	-	-		
88	OHX	5	4046	-	0,6,6	-	-	-		
88	OHX	5	4122	-	0,6,6	-	-	-		
88	OHX	6	2056	-	0,6,6	-	-	-		
88	OHX	5	3945	-	0,6,6	-	-	-		
88	OHX	5	3909	-	0,6,6	-	-	-		
88	OHX	5	4243	-	0,6,6	-	-	-		
88	OHX	s1	303	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
88	OHX	2	2129	-	0,6,6	-	-	-		
88	OHX	5	3925	-	0,6,6	-	-	-		
88	OHX	2	2067	-	0,6,6	-	-	-		
88	OHX	6	2201	-	0,6,6	-	-	-		
88	OHX	1	4040	-	0,6,6	-	-	-		
88	OHX	1	3993	-	0,6,6	-	-	-		
88	OHX	2	2056	-	0,6,6	-	-	-		
88	OHX	1	4074	-	0,6,6	-	-	-		
88	OHX	1	4078	-	0,6,6	-	-	-		
88	OHX	2	2159	-	0,6,6	-	-	-		
88	OHX	5	4099	-	0,6,6	-	-	-		
88	OHX	2	2057	-	0,6,6	-	-	-		
88	OHX	6	2087	-	0,6,6	-	-	-		
88	OHX	1	4155	-	0,6,6	-	-	-		
88	OHX	5	3930	-	0,6,6	-	-	-		
88	OHX	5	4121	-	0,6,6	-	-	-		
88	OHX	5	4131	-	0,6,6	-	-	-		
88	OHX	5	4047	-	0,6,6	-	-	-		
88	OHX	1	3923	-	0,6,6	-	-	-		
88	OHX	1	4200	-	0,6,6	-	-	-		
88	OHX	2	2128	-	0,6,6	-	-	-		
88	OHX	2	2025	-	0,6,6	-	-	-		
88	OHX	5	4141	-	0,6,6	-	-	-		
88	OHX	1	4014	-	0,6,6	-	-	-		
88	OHX	6	2113	-	0,6,6	-	-	-		
88	OHX	5	3960	-	0,6,6	-	-	-		
88	OHX	1	3900	-	0,6,6	-	-	-		
88	OHX	5	4130	-	0,6,6	-	-	-		
88	OHX	6	2100	-	0,6,6	-	-	-		
88	OHX	2	2117	-	0,6,6	-	-	-		
88	OHX	1	3948	-	0,6,6	-	-	-		
88	OHX	1	3967	-	0,6,6	-	-	-		
88	OHX	5	4223	-	0,6,6	-	-	-		
88	OHX	6	2091	-	0,6,6	-	-	-		
88	OHX	5	4013	-	0,6,6	-	-	-		
88	OHX	6	2080	-	0,6,6	-	-	-		
88	OHX	1	4079	-	0,6,6	-	-	-		
88	OHX	6	2081	-	0,6,6	-	-	-		
88	OHX	5	4088	-	0,6,6	-	-	-		
88	OHX	2	2085	-	0,6,6	-	-	-		
88	OHX	5	4195	-	0,6,6	-	-	-		
88	OHX	5	3993	-	0,6,6	-	-	-		
88	OHX	1	3996	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	2	2073	-	0,6,6	-	-	-		
88	OHX	1	4123	-	0,6,6	-	-	-		
88	OHX	1	4160	-	0,6,6	-	-	-		
88	OHX	1	4163	-	0,6,6	-	-	-		
88	OHX	1	4225	-	0,6,6	-	-	-		
88	OHX	6	2055	-	0,6,6	-	-	-		
88	OHX	6	2164	-	0,6,6	-	-	-		
88	OHX	5	4050	-	0,6,6	-	-	-		
88	OHX	3	221	-	0,6,6	-	-	-		
88	OHX	6	2044	-	0,6,6	-	-	-		
88	OHX	5	3915	-	0,6,6	-	-	-		
88	OHX	6	2066	-	0,6,6	-	-	-		
88	OHX	1	4092	-	0,6,6	-	-	-		
88	OHX	1	4179	-	0,6,6	-	-	-		
88	OHX	6	2147	-	0,6,6	-	-	-		
88	OHX	5	3905	-	0,6,6	-	-	-		
88	OHX	1	4137	-	0,6,6	-	-	-		
88	OHX	5	3908	-	0,6,6	-	-	-		
88	OHX	1	4112	-	0,6,6	-	-	-		
88	OHX	2	2147	-	0,6,6	-	-	-		
88	OHX	2	2152	-	0,6,6	-	-	-		
88	OHX	6	2092	-	0,6,6	-	-	-		
91	C	Q2	503	-	18,21,22	0.72	0	26,30,33	1.15	4 (15%)
88	OHX	5	3917	-	0,6,6	-	-	-		
88	OHX	4	231	-	0,6,6	-	-	-		
88	OHX	6	2161	-	0,6,6	-	-	-		
88	OHX	1	3957	-	0,6,6	-	-	-		
88	OHX	1	3918	-	0,6,6	-	-	-		
88	OHX	5	3932	-	0,6,6	-	-	-		
88	OHX	5	4143	-	0,6,6	-	-	-		
88	OHX	C3	201	-	0,6,6	-	-	-		
88	OHX	1	4060	-	0,6,6	-	-	-		
88	OHX	1	4097	-	0,6,6	-	-	-		
88	OHX	6	2111	-	0,6,6	-	-	-		
88	OHX	1	4138	-	0,6,6	-	-	-		
88	OHX	2	2087	-	0,6,6	-	-	-		
88	OHX	5	4236	-	0,6,6	-	-	-		
88	OHX	1	3911	-	0,6,6	-	-	-		
88	OHX	1	4049	-	0,6,6	-	-	-		
88	OHX	1	4120	-	0,6,6	-	-	-		
88	OHX	5	4177	-	0,6,6	-	-	-		
88	OHX	2	2084	-	0,6,6	-	-	-		
88	OHX	5	3936	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	6	2193	-	0,6,6	-	-	-		
88	OHX	6	2075	-	0,6,6	-	-	-		
88	OHX	1	4089	-	0,6,6	-	-	-		
88	OHX	5	3992	-	0,6,6	-	-	-		
88	OHX	1	3975	-	0,6,6	-	-	-		
88	OHX	5	4126	-	0,6,6	-	-	-		
88	OHX	5	4254	-	0,6,6	-	-	-		
88	OHX	6	2178	-	0,6,6	-	-	-		
88	OHX	5	4211	-	0,6,6	-	-	-		
88	OHX	5	4226	-	0,6,6	-	-	-		
88	OHX	1	3882	-	0,6,6	-	-	-		
88	OHX	1	4161	-	0,6,6	-	-	-		
88	OHX	6	2107	-	0,6,6	-	-	-		
88	OHX	M8	201	-	0,6,6	-	-	-		
88	OHX	5	4216	-	0,6,6	-	-	-		
88	OHX	2	2036	-	0,6,6	-	-	-		
88	OHX	1	3881	-	0,6,6	-	-	-		
88	OHX	1	4088	-	0,6,6	-	-	-		
88	OHX	1	4150	-	0,6,6	-	-	-		
88	OHX	M7	206	-	0,6,6	-	-	-		
88	OHX	5	4181	-	0,6,6	-	-	-		
88	OHX	1	4016	-	0,6,6	-	-	-		
88	OHX	5	3928	-	0,6,6	-	-	-		
88	OHX	1	3887	-	0,6,6	-	-	-		
88	OHX	1	3935	-	0,6,6	-	-	-		
88	OHX	1	4071	-	0,6,6	-	-	-		
88	OHX	5	4220	-	0,6,6	-	-	-		
88	OHX	8	226	-	0,6,6	-	-	-		
88	OHX	2	2150	-	0,6,6	-	-	-		
91	C	q2	503	-	18,21,22	0.61	0	26,30,33	0.76	1 (3%)
88	OHX	2	2077	-	0,6,6	-	-	-		
88	OHX	2	2088	-	0,6,6	-	-	-		
88	OHX	5	4118	-	0,6,6	-	-	-		
88	OHX	1	3910	-	0,6,6	-	-	-		
88	OHX	1	4146	-	0,6,6	-	-	-		
88	OHX	d9	102	-	0,6,6	-	-	-		
88	OHX	6	2132	-	0,6,6	-	-	-		
88	OHX	5	4044	-	0,6,6	-	-	-		
88	OHX	5	4212	-	0,6,6	-	-	-		
88	OHX	5	4163	-	0,6,6	-	-	-		
88	OHX	1	3939	-	0,6,6	-	-	-		
88	OHX	6	2078	-	0,6,6	-	-	-		
88	OHX	1	4209	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
88	OHX	1	4065	-	0,6,6	-	-	-		
88	OHX	6	2176	-	0,6,6	-	-	-		
88	OHX	6	2094	-	0,6,6	-	-	-		
88	OHX	2	2075	-	0,6,6	-	-	-		
88	OHX	2	2110	-	0,6,6	-	-	-		
88	OHX	5	4057	-	0,6,6	-	-	-		
88	OHX	1	4058	-	0,6,6	-	-	-		
88	OHX	5	4085	-	0,6,6	-	-	-		
88	OHX	C5	201	-	0,6,6	-	-	-		
88	OHX	6	2182	-	0,6,6	-	-	-		
88	OHX	1	4140	-	0,6,6	-	-	-		
88	OHX	5	4198	-	0,6,6	-	-	-		
88	OHX	2	2089	-	0,6,6	-	-	-		
88	OHX	5	3926	-	0,6,6	-	-	-		
88	OHX	1	3932	-	0,6,6	-	-	-		
88	OHX	1	4080	-	0,6,6	-	-	-		
88	OHX	5	4112	-	0,6,6	-	-	-		
88	OHX	5	4155	-	0,6,6	-	-	-		
88	OHX	1	3986	-	0,6,6	-	-	-		
88	OHX	1	4006	-	0,6,6	-	-	-		
88	OHX	1	4139	-	0,6,6	-	-	-		
88	OHX	1	4023	-	0,6,6	-	-	-		
88	OHX	1	3912	-	0,6,6	-	-	-		
88	OHX	1	4171	-	0,6,6	-	-	-		
88	OHX	2	2069	-	0,6,6	-	-	-		
88	OHX	5	4028	-	0,6,6	-	-	-		
88	OHX	5	4167	-	0,6,6	-	-	-		
88	OHX	6	2172	-	0,6,6	-	-	-		
88	OHX	2	2030	-	0,6,6	-	-	-		
88	OHX	5	3911	-	0,6,6	-	-	-		
88	OHX	1	4111	-	0,6,6	-	-	-		
88	OHX	5	4120	-	0,6,6	-	-	-		
88	OHX	1	3919	-	0,6,6	-	-	-		
88	OHX	1	3899	-	0,6,6	-	-	-		
88	OHX	1	4226	-	0,6,6	-	-	-		
88	OHX	5	4258	-	0,6,6	-	-	-		
88	OHX	1	4153	-	0,6,6	-	-	-		
88	OHX	5	4064	-	0,6,6	-	-	-		
88	OHX	1	4001	-	0,6,6	-	-	-		
88	OHX	5	3967	-	0,6,6	-	-	-		
88	OHX	2	2178	-	0,6,6	-	-	-		
88	OHX	m5	306	-	0,6,6	-	-	-		
88	OHX	5	4077	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	m4	201	-	0,6,6	-	-	-		
88	OHX	D3	202	-	0,6,6	-	-	-		
88	OHX	5	3906	-	0,6,6	-	-	-		
88	OHX	n9	101	-	0,6,6	-	-	-		
88	OHX	5	4161	-	0,6,6	-	-	-		
88	OHX	5	4135	-	0,6,6	-	-	-		
88	OHX	2	2080	-	0,6,6	-	-	-		
88	OHX	1	4174	-	0,6,6	-	-	-		
88	OHX	1	4075	-	0,6,6	-	-	-		
88	OHX	1	4082	-	0,6,6	-	-	-		
88	OHX	1	4118	-	0,6,6	-	-	-		
88	OHX	1	4197	-	0,6,6	-	-	-		
90	A	1	3401	-	18,24,25	0.72	0	18,35,38	0.96	2 (11%)
88	OHX	1	4044	-	0,6,6	-	-	-		
88	OHX	6	2045	-	0,6,6	-	-	-		
88	OHX	6	2156	-	0,6,6	-	-	-		
88	OHX	1	4030	-	0,6,6	-	-	-		
88	OHX	2	2130	-	0,6,6	-	-	-		
88	OHX	1	4072	-	0,6,6	-	-	-		
88	OHX	6	2051	-	0,6,6	-	-	-		
88	OHX	1	4190	-	0,6,6	-	-	-		
88	OHX	5	4193	-	0,6,6	-	-	-		
88	OHX	2	2164	-	0,6,6	-	-	-		
88	OHX	M5	303	-	0,6,6	-	-	-		
88	OHX	1	3893	-	0,6,6	-	-	-		
88	OHX	5	4214	-	0,6,6	-	-	-		
88	OHX	8	220	-	0,6,6	-	-	-		
88	OHX	5	4137	-	0,6,6	-	-	-		
88	OHX	5	4025	-	0,6,6	-	-	-		
88	OHX	2	2113	-	0,6,6	-	-	-		
88	OHX	2	2156	-	0,6,6	-	-	-		
88	OHX	5	3919	-	0,6,6	-	-	-		
88	OHX	5	4018	-	0,6,6	-	-	-		
88	OHX	5	3914	-	0,6,6	-	-	-		
88	OHX	5	4248	-	0,6,6	-	-	-		
88	OHX	2	2119	-	0,6,6	-	-	-		
88	OHX	1	4115	-	0,6,6	-	-	-		
88	OHX	4	224	-	0,6,6	-	-	-		
88	OHX	1	3891	-	0,6,6	-	-	-		
88	OHX	5	3918	-	0,6,6	-	-	-		
88	OHX	2	2092	-	0,6,6	-	-	-		
88	OHX	6	2126	-	0,6,6	-	-	-		
88	OHX	6	2128	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
88	OHX	5	4124	-	0,6,6	-	-	-		
88	OHX	5	4138	-	0,6,6	-	-	-		
88	OHX	1	3896	-	0,6,6	-	-	-		
88	OHX	5	4171	-	0,6,6	-	-	-		
88	OHX	2	2062	-	0,6,6	-	-	-		
88	OHX	2	2059	-	0,6,6	-	-	-		
88	OHX	1	3902	-	0,6,6	-	-	-		
88	OHX	1	4004	-	0,6,6	-	-	-		
88	OHX	s1	302	-	0,6,6	-	-	-		
88	OHX	6	2149	-	0,6,6	-	-	-		
88	OHX	7	216	-	0,6,6	-	-	-		
88	OHX	1	4093	-	0,6,6	-	-	-		
88	OHX	5	4247	-	0,6,6	-	-	-		
88	OHX	5	4069	-	0,6,6	-	-	-		
88	OHX	5	4257	-	0,6,6	-	-	-		
88	OHX	5	4233	-	0,6,6	-	-	-		
88	OHX	5	4072	-	0,6,6	-	-	-		
88	OHX	5	3975	-	0,6,6	-	-	-		
88	OHX	5	4055	-	0,6,6	-	-	-		
88	OHX	1	4151	-	0,6,6	-	-	-		
88	OHX	c3	201	-	0,6,6	-	-	-		
88	OHX	7	225	-	0,6,6	-	-	-		
88	OHX	1	4188	-	0,6,6	-	-	-		
88	OHX	2	2168	-	0,6,6	-	-	-		
88	OHX	1	4077	-	0,6,6	-	-	-		
88	OHX	5	4048	-	0,6,6	-	-	-		
88	OHX	1	4126	-	0,6,6	-	-	-		
88	OHX	6	2073	-	0,6,6	-	-	-		
88	OHX	5	4053	-	0,6,6	-	-	-		
88	OHX	5	4234	-	0,6,6	-	-	-		
88	OHX	5	3973	-	0,6,6	-	-	-		
88	OHX	5	4108	-	0,6,6	-	-	-		
88	OHX	5	3904	-	0,6,6	-	-	-		
88	OHX	s8	304	-	0,6,6	-	-	-		
88	OHX	2	2086	-	0,6,6	-	-	-		
88	OHX	3	225	-	0,6,6	-	-	-		
88	OHX	1	4211	-	0,6,6	-	-	-		
88	OHX	5	4065	-	0,6,6	-	-	-		
88	OHX	4	221	-	0,6,6	-	-	-		
88	OHX	7	223	-	0,6,6	-	-	-		
88	OHX	6	2103	-	0,6,6	-	-	-		
88	OHX	2	2072	-	0,6,6	-	-	-		
88	OHX	5	4104	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4005	-	0,6,6	-	-	-		
88	OHX	5	3940	-	0,6,6	-	-	-		
88	OHX	1	4119	-	0,6,6	-	-	-		
88	OHX	2	2091	-	0,6,6	-	-	-		
88	OHX	1	3990	-	0,6,6	-	-	-		
88	OHX	1	4108	-	0,6,6	-	-	-		
88	OHX	1	4193	-	0,6,6	-	-	-		
88	OHX	6	2116	-	0,6,6	-	-	-		
88	OHX	2	2170	-	0,6,6	-	-	-		
88	OHX	6	2137	-	0,6,6	-	-	-		
88	OHX	1	3979	-	0,6,6	-	-	-		
88	OHX	6	2090	-	0,6,6	-	-	-		
88	OHX	1	3980	-	0,6,6	-	-	-		
88	OHX	5	3986	-	0,6,6	-	-	-		
88	OHX	2	2107	-	0,6,6	-	-	-		
88	OHX	6	2093	-	0,6,6	-	-	-		
88	OHX	1	3966	-	0,6,6	-	-	-		
88	OHX	1	3989	-	0,6,6	-	-	-		
88	OHX	6	2105	1	0,6,6	-	-	-		
88	OHX	5	4219	-	0,6,6	-	-	-		
88	OHX	5	4015	-	0,6,6	-	-	-		
88	OHX	1	3890	-	0,6,6	-	-	-		
88	OHX	2	2043	-	0,6,6	-	-	-		
88	OHX	1	4148	-	0,6,6	-	-	-		
88	OHX	5	4093	-	0,6,6	-	-	-		
88	OHX	O3	201	-	0,6,6	-	-	-		
88	OHX	5	4045	-	0,6,6	-	-	-		
88	OHX	1	3877	-	0,6,6	-	-	-		
88	OHX	1	3874	-	0,6,6	-	-	-		
88	OHX	6	2183	-	0,6,6	-	-	-		
88	OHX	m0	301	-	0,6,6	-	-	-		
88	OHX	5	4134	-	0,6,6	-	-	-		
88	OHX	5	4008	-	0,6,6	-	-	-		
88	OHX	5	4094	-	0,6,6	-	-	-		
88	OHX	1	4091	-	0,6,6	-	-	-		
88	OHX	6	2064	-	0,6,6	-	-	-		
88	OHX	5	4151	-	0,6,6	-	-	-		
88	OHX	o3	202	-	0,6,6	-	-	-		
88	OHX	1	3945	-	0,6,6	-	-	-		
88	OHX	1	3959	-	0,6,6	-	-	-		
88	OHX	1	4066	-	0,6,6	-	-	-		
88	OHX	5	4222	-	0,6,6	-	-	-		
88	OHX	5	3988	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4196	-	0,6,6	-	-	-		
88	OHX	6	2121	-	0,6,6	-	-	-		
88	OHX	1	4007	-	0,6,6	-	-	-		
88	OHX	1	4070	-	0,6,6	-	-	-		
88	OHX	6	2108	-	0,6,6	-	-	-		
88	OHX	4	220	-	0,6,6	-	-	-		
88	OHX	5	3902	-	0,6,6	-	-	-		
88	OHX	6	2170	-	0,6,6	-	-	-		
88	OHX	6	2184	-	0,6,6	-	-	-		
88	OHX	1	3961	-	0,6,6	-	-	-		
88	OHX	5	4010	-	0,6,6	-	-	-		
88	OHX	l3	405	-	0,6,6	-	-	-		
88	OHX	2	2126	-	0,6,6	-	-	-		
88	OHX	2	2040	-	0,6,6	-	-	-		
88	OHX	2	2082	-	0,6,6	-	-	-		
88	OHX	1	4053	-	0,6,6	-	-	-		
88	OHX	6	2198	-	0,6,6	-	-	-		
88	OHX	5	4030	-	0,6,6	-	-	-		
88	OHX	5	4051	-	0,6,6	-	-	-		
88	OHX	1	3987	-	0,6,6	-	-	-		
88	OHX	1	4027	-	0,6,6	-	-	-		
88	OHX	6	2071	-	0,6,6	-	-	-		
88	OHX	2	2136	-	0,6,6	-	-	-		
88	OHX	5	4228	-	0,6,6	-	-	-		
88	OHX	2	2031	-	0,6,6	-	-	-		
88	OHX	1	3930	-	0,6,6	-	-	-		
88	OHX	1	3956	-	0,6,6	-	-	-		
88	OHX	1	4130	-	0,6,6	-	-	-		
88	OHX	6	2099	-	0,6,6	-	-	-		
88	OHX	6	2125	-	0,6,6	-	-	-		
88	OHX	2	2094	-	0,6,6	-	-	-		
88	OHX	5	3977	-	0,6,6	-	-	-		
88	OHX	6	2124	-	0,6,6	-	-	-		
88	OHX	6	2166	-	0,6,6	-	-	-		
88	OHX	5	4014	-	0,6,6	-	-	-		
88	OHX	5	4043	-	0,6,6	-	-	-		
88	OHX	5	4086	-	0,6,6	-	-	-		
88	OHX	5	4098	-	0,6,6	-	-	-		
88	OHX	5	4255	-	0,6,6	-	-	-		
88	OHX	5	4250	-	0,6,6	-	-	-		
88	OHX	5	4075	-	0,6,6	-	-	-		
88	OHX	6	2067	-	0,6,6	-	-	-		
88	OHX	1	3954	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	4141	-	0,6,6	-	-	-		
88	OHX	6	2142	-	0,6,6	-	-	-		
88	OHX	5	4115	-	0,6,6	-	-	-		
88	OHX	1	4206	-	0,6,6	-	-	-		
88	OHX	1	3972	-	0,6,6	-	-	-		
88	OHX	1	4173	-	0,6,6	-	-	-		
88	OHX	5	3907	-	0,6,6	-	-	-		
88	OHX	1	4154	-	0,6,6	-	-	-		
88	OHX	5	4032	-	0,6,6	-	-	-		
88	OHX	5	4164	-	0,6,6	-	-	-		
88	OHX	2	2140	-	0,6,6	-	-	-		
88	OHX	6	2163	-	0,6,6	-	-	-		
88	OHX	1	4221	-	0,6,6	-	-	-		
88	OHX	5	4005	-	0,6,6	-	-	-		
88	OHX	2	2116	-	0,6,6	-	-	-		
88	OHX	5	4184	-	0,6,6	-	-	-		
88	OHX	5	4036	-	0,6,6	-	-	-		
88	OHX	5	4136	-	0,6,6	-	-	-		
88	OHX	1	4207	-	0,6,6	-	-	-		
88	OHX	2	2083	-	0,6,6	-	-	-		
88	OHX	1	4202	-	0,6,6	-	-	-		
88	OHX	n3	203	-	0,6,6	-	-	-		
88	OHX	1	4168	-	0,6,6	-	-	-		
88	OHX	1	4059	-	0,6,6	-	-	-		
88	OHX	2	2024	-	0,6,6	-	-	-		
88	OHX	1	3889	-	0,6,6	-	-	-		
88	OHX	3	219	-	0,6,6	-	-	-		
88	OHX	5	3929	-	0,6,6	-	-	-		
88	OHX	5	4256	-	0,6,6	-	-	-		
88	OHX	1	3914	-	0,6,6	-	-	-		
88	OHX	1	3953	-	0,6,6	-	-	-		
88	OHX	2	2078	-	0,6,6	-	-	-		
88	OHX	2	2167	-	0,6,6	-	-	-		
88	OHX	6	2046	-	0,6,6	-	-	-		
88	OHX	5	4109	-	0,6,6	-	-	-		
88	OHX	1	4087	-	0,6,6	-	-	-		
88	OHX	1	3947	-	0,6,6	-	-	-		
88	OHX	1	4212	-	0,6,6	-	-	-		
88	OHX	6	2171	-	0,6,6	-	-	-		
88	OHX	1	4045	-	0,6,6	-	-	-		
88	OHX	1	4113	-	0,6,6	-	-	-		
88	OHX	1	3922	-	0,6,6	-	-	-		
88	OHX	2	2032	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	6	2086	-	0,6,6	-	-	-		
88	OHX	6	2134	-	0,6,6	-	-	-		
88	OHX	6	2151	-	0,6,6	-	-	-		
88	OHX	2	2131	-	0,6,6	-	-	-		
88	OHX	6	2146	-	0,6,6	-	-	-		
88	OHX	1	4081	-	0,6,6	-	-	-		
88	OHX	4	223	-	0,6,6	-	-	-		
88	OHX	1	4210	-	0,6,6	-	-	-		
88	OHX	4	233	-	0,6,6	-	-	-		
88	OHX	7	221	-	0,6,6	-	-	-		
88	OHX	6	2200	-	0,6,6	-	-	-		
88	OHX	5	4091	-	0,6,6	-	-	-		
88	OHX	6	2048	-	0,6,6	-	-	-		
88	OHX	5	4097	-	0,6,6	-	-	-		
88	OHX	6	2072	-	0,6,6	-	-	-		
88	OHX	1	4051	-	0,6,6	-	-	-		
88	OHX	2	2058	-	0,6,6	-	-	-		
88	OHX	2	2068	-	0,6,6	-	-	-		
88	OHX	1	3875	-	0,6,6	-	-	-		
88	OHX	1	4020	-	0,6,6	-	-	-		
88	OHX	1	4086	-	0,6,6	-	-	-		
88	OHX	6	2112	-	0,6,6	-	-	-		
88	OHX	1	4063	-	0,6,6	-	-	-		
88	OHX	1	3904	-	0,6,6	-	-	-		
88	OHX	5	3997	-	0,6,6	-	-	-		
88	OHX	2	2101	-	0,6,6	-	-	-		
88	OHX	6	2148	-	0,6,6	-	-	-		
88	OHX	1	4125	-	0,6,6	-	-	-		
88	OHX	1	4011	-	0,6,6	-	-	-		
88	OHX	6	2145	-	0,6,6	-	-	-		
88	OHX	7	224	-	0,6,6	-	-	-		
88	OHX	5	4011	-	0,6,6	-	-	-		
88	OHX	l5	306	-	0,6,6	-	-	-		
88	OHX	6	2122	-	0,6,6	-	-	-		
88	OHX	5	4071	-	0,6,6	-	-	-		
88	OHX	1	4017	-	0,6,6	-	-	-		
88	OHX	5	4213	-	0,6,6	-	-	-		
88	OHX	5	4128	-	0,6,6	-	-	-		
88	OHX	6	2069	-	0,6,6	-	-	-		
88	OHX	1	4122	-	0,6,6	-	-	-		
88	OHX	6	2088	-	0,6,6	-	-	-		
88	OHX	1	3969	-	0,6,6	-	-	-		
88	OHX	6	2085	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	5	3954	-	0,6,6	-	-	-		
88	OHX	1	4201	-	0,6,6	-	-	-		
88	OHX	6	2098	-	0,6,6	-	-	-		
88	OHX	5	3972	-	0,6,6	-	-	-		
88	OHX	5	4117	-	0,6,6	-	-	-		
88	OHX	2	2143	-	0,6,6	-	-	-		
88	OHX	1	4076	-	0,6,6	-	-	-		
88	OHX	5	4150	-	0,6,6	-	-	-		
88	OHX	5	4217	-	0,6,6	-	-	-		
88	OHX	1	3994	-	0,6,6	-	-	-		
88	OHX	1	3929	-	0,6,6	-	-	-		
88	OHX	5	4178	-	0,6,6	-	-	-		
88	OHX	5	4186	-	0,6,6	-	-	-		
88	OHX	6	2191	-	0,6,6	-	-	-		
88	OHX	5	4207	-	0,6,6	-	-	-		
88	OHX	1	4147	-	0,6,6	-	-	-		
88	OHX	1	4215	-	0,6,6	-	-	-		
88	OHX	5	4132	-	0,6,6	-	-	-		
88	OHX	1	4039	-	0,6,6	-	-	-		
88	OHX	6	2082	-	0,6,6	-	-	-		
88	OHX	5	3987	-	0,6,6	-	-	-		
88	OHX	5	4081	-	0,6,6	-	-	-		
88	OHX	1	4182	-	0,6,6	-	-	-		
88	OHX	5	4160	-	0,6,6	-	-	-		
88	OHX	5	4087	-	0,6,6	-	-	-		
88	OHX	5	3959	-	0,6,6	-	-	-		
88	OHX	5	4066	-	0,6,6	-	-	-		
88	OHX	6	2158	-	0,6,6	-	-	-		
88	OHX	1	3883	-	0,6,6	-	-	-		
88	OHX	1	4094	-	0,6,6	-	-	-		
88	OHX	5	3974	-	0,6,6	-	-	-		
88	OHX	6	2197	-	0,6,6	-	-	-		
88	OHX	5	4007	-	0,6,6	-	-	-		
88	OHX	1	3984	-	0,6,6	-	-	-		
88	OHX	1	4218	-	0,6,6	-	-	-		
88	OHX	6	2186	-	0,6,6	-	-	-		
88	OHX	5	4113	-	0,6,6	-	-	-		
88	OHX	1	3963	-	0,6,6	-	-	-		
88	OHX	4	232	-	0,6,6	-	-	-		
88	OHX	3	220	-	0,6,6	-	-	-		
88	OHX	5	4170	-	0,6,6	-	-	-		
88	OHX	1	4103	-	0,6,6	-	-	-		
88	OHX	1	4169	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
88	OHX	1	3920	-	0,6,6	-	-	-		
88	OHX	1	4000	-	0,6,6	-	-	-		
88	OHX	1	4047	-	0,6,6	-	-	-		
88	OHX	1	4135	-	0,6,6	-	-	-		
88	OHX	6	2129	-	0,6,6	-	-	-		
88	OHX	1	4056	-	0,6,6	-	-	-		
88	OHX	2	2104	-	0,6,6	-	-	-		
88	OHX	5	4169	-	0,6,6	-	-	-		
88	OHX	5	4229	-	0,6,6	-	-	-		
88	OHX	2	2048	-	0,6,6	-	-	-		
88	OHX	5	4040	-	0,6,6	-	-	-		
88	OHX	5	3996	-	0,6,6	-	-	-		
88	OHX	1	3916	-	0,6,6	-	-	-		
88	OHX	6	2167	-	0,6,6	-	-	-		
88	OHX	5	4119	-	0,6,6	-	-	-		
88	OHX	2	2103	-	0,6,6	-	-	-		
88	OHX	1	3934	-	0,6,6	-	-	-		
88	OHX	2	2070	-	0,6,6	-	-	-		

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
91	C	q2	502	-	-	0/7/25/26	0/2/2/2
91	C	Q2	502	-	-	5/7/25/26	0/2/2/2
91	C	q2	503	-	-	2/7/25/26	0/2/2/2
90	A	5	3401	-	-	2/3/25/26	0/3/3/3
91	C	Q2	503	-	-	2/7/25/26	0/2/2/2
90	A	1	3401	-	-	2/3/25/26	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	Q2	503	C	O2-C2-N1	-2.93	112.84	118.89
91	Q2	503	C	C1'-N1-C6	2.63	126.58	120.84
90	5	3401	A	C5-C6-N6	2.29	123.84	120.35
91	Q2	503	C	N1-C2-N3	2.29	122.97	118.81
91	q2	503	C	C5-C4-N4	-2.22	117.08	120.57

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

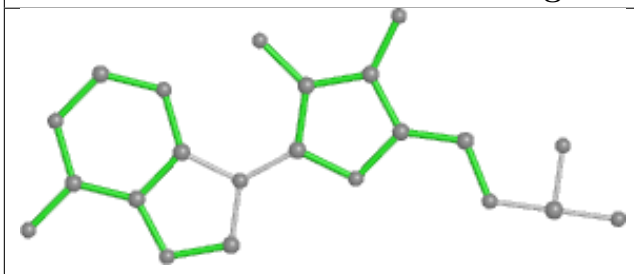
Mol	Chain	Res	Type	Atoms
91	Q2	502	C	C2'-C1'-N1-C2
91	Q2	502	C	C2'-C1'-N1-C6
91	Q2	503	C	O4'-C4'-C5'-O5'
91	q2	503	C	O4'-C4'-C5'-O5'
91	q2	503	C	C3'-C4'-C5'-O5'

There are no ring outliers.

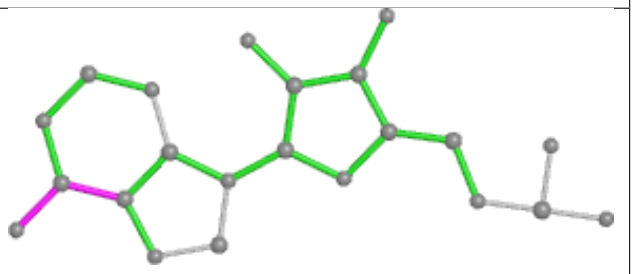
No monomer is involved in short contacts.

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.

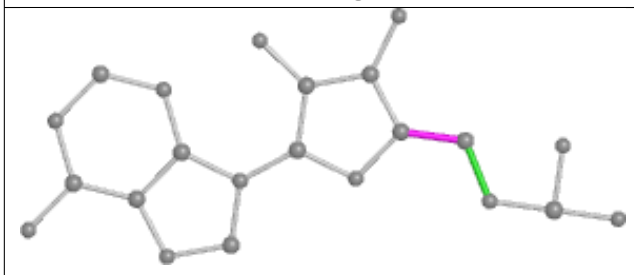
Ligand A 5 3401



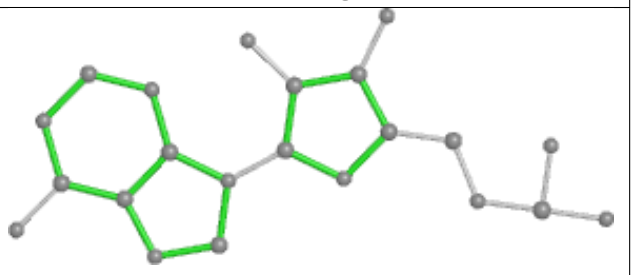
Bond lengths



Bond angles

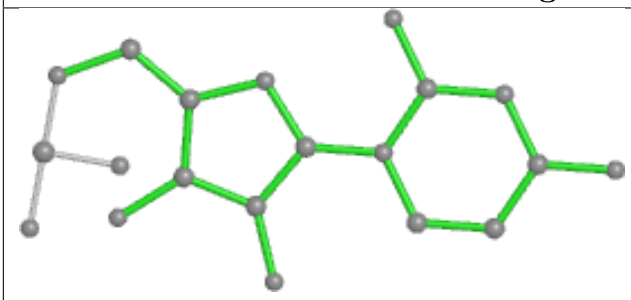


Torsions

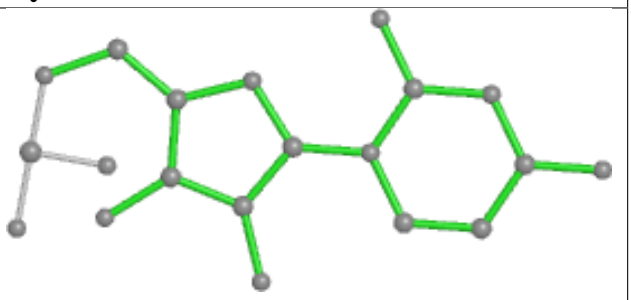


Rings

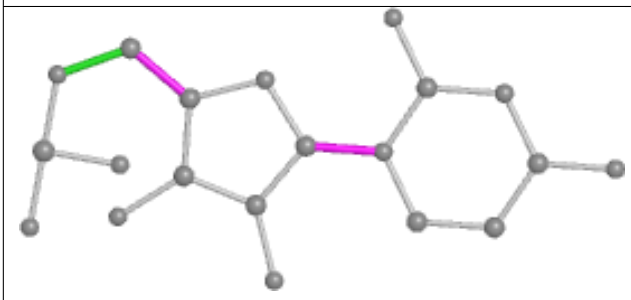
Ligand C Q2 502



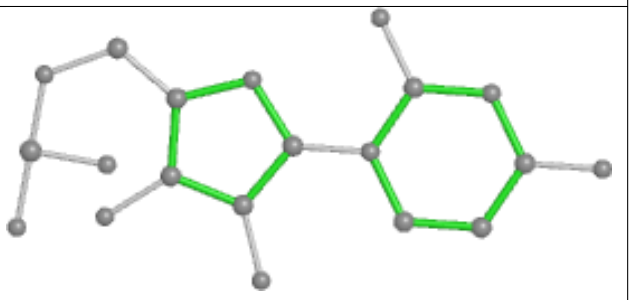
Bond lengths



Bond angles

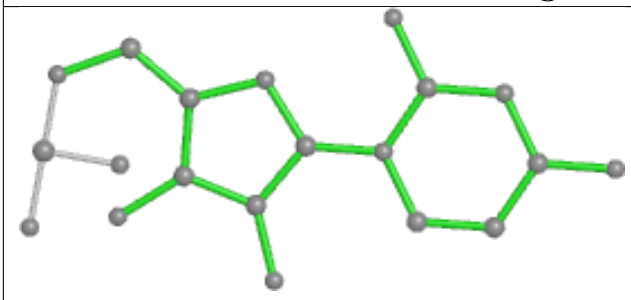


Torsions

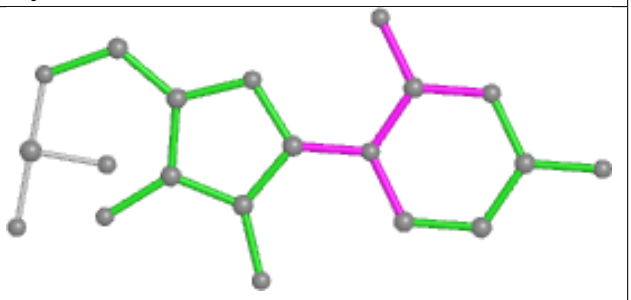


Rings

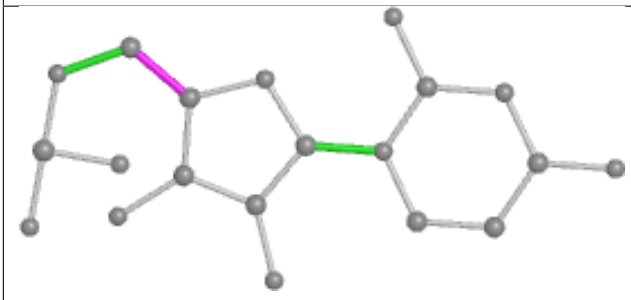
Ligand C Q2 503



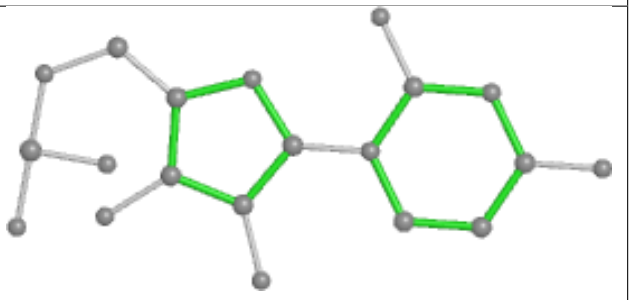
Bond lengths



Bond angles

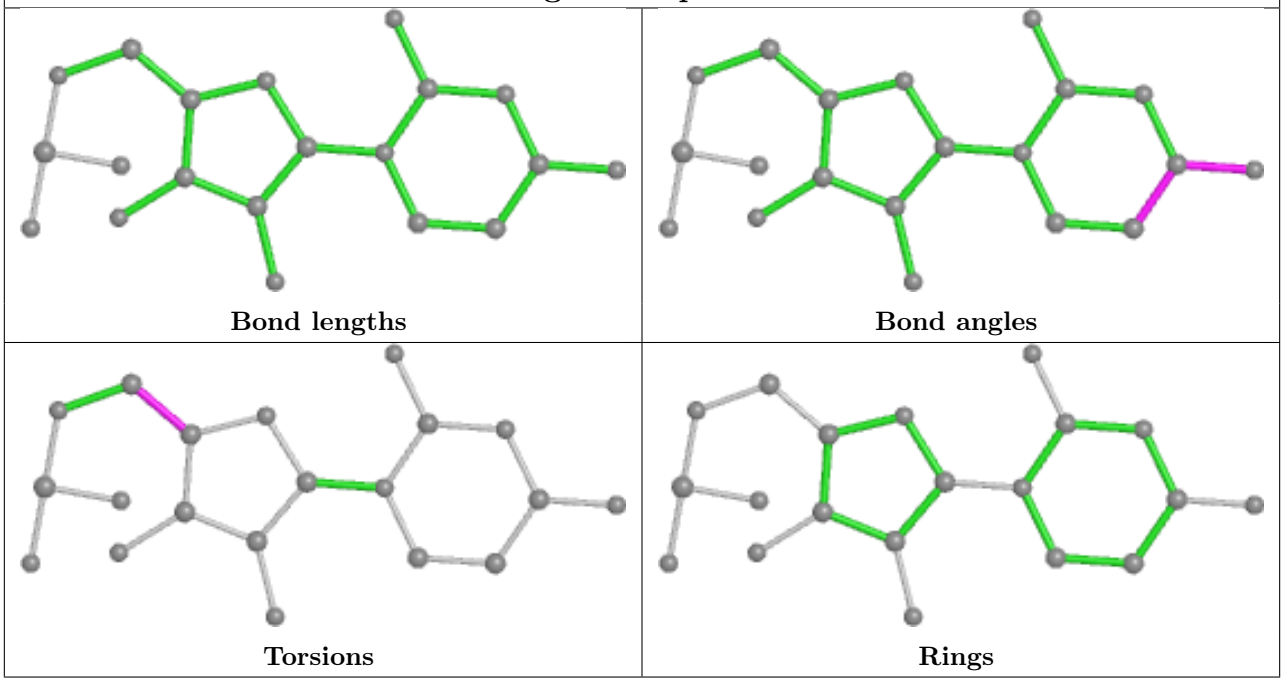


Torsions

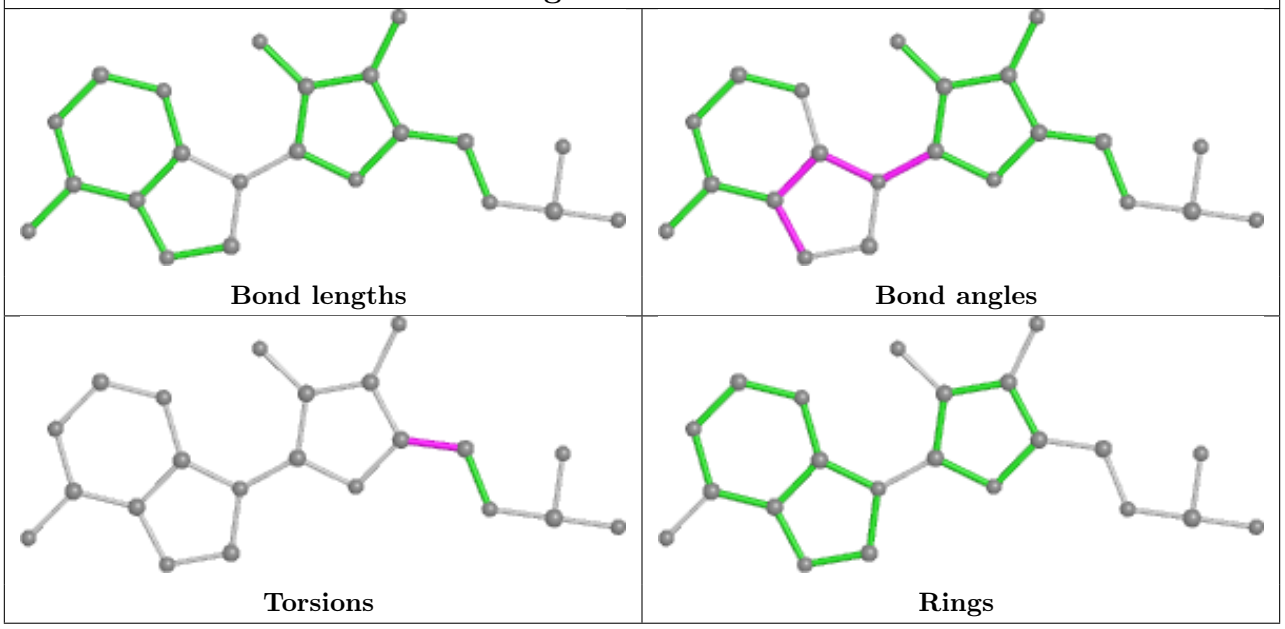


Rings

Ligand C q2 503



Ligand A 1 3401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.