wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 01:35 pm GMT

PDB ID	:	4U4U
Title	:	Crystal structure of Lycorine bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	3.00 Å(reported)

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

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

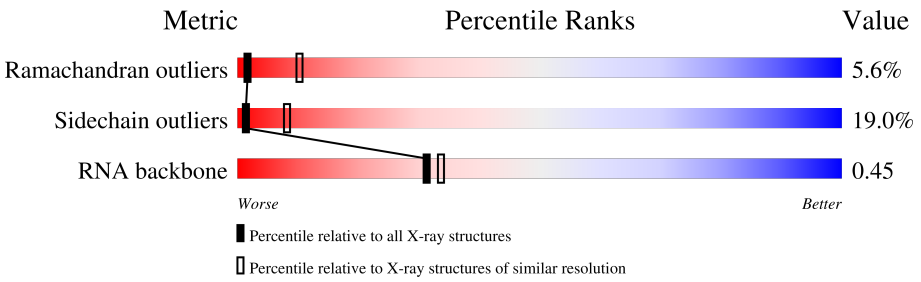
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et 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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	66% 27% • •
1	6	1800	65% 28% 6%
2	S0	251	62% 19% • 18%
2	s0	251	61% 18% • 18%
3	S1	254	61% 21% • 16%
3	s1	254	70% 15% 15%
4	S2	253	69% 16% • 14%
4	s2	253	64% 21% • 14%

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Mol	Chain	Length	Quality of chain
5	S3	239	74% 18% 7%
5	s3	239	75% 16% 7%
6	S4	260	82% 16%
6	s4	260	80% 19%
7	S5	224	73% 17% 8%
7	s5	224	68% 22% 8%
8	S6	236	74% 21%
8	s6	236	74% 17% 8%
9	S7	189	75% 20%
9	s7	189	78% 17%
10	S8	200	80% 14% 6%
10	s8	200	80% 13% 6%
11	S9	196	72% 21% 6%
11	s9	196	76% 16% 6%
12	C0	105	71% 19% 9%
12	c0	105	70% 18% 9%
13	C1	155	79% 20%
13	c1	155	74% 19% 6%
14	C2	142	55% 30% 13%
14	c2	142	59% 25% 13%
15	C3	150	79% 19%
15	c3	150	78% 21%
16	C4	136	71% 18% 7%
16	c4	136	74% 18% 6%
17	C5	141	70% 16% 12%

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Mol	Chain	Length	Quality of chain
17	c5	141	72% 20%
18	C6	142	78% 20%
18	c6	142	77% 21%
19	C7	136	66% 18% 12%
19	c7	136	71% 13% 14%
20	C8	145	72% 24%
20	c8	145	77% 21%
21	C9	143	81% 19%
21	c9	143	81% 17%
22	D0	120	68% 22% 11%
22	d0	120	63% 27% 8%
23	D1	87	76% 24%
23	d1	87	75% 24%
24	D2	129	86% 12%
24	d2	129	86% 13%
25	D3	144	81% 17%
25	d3	144	86% 13%
26	D4	134	81% 18%
26	d4	134	81% 18%
27	D5	107	40% 23% 35%
27	d5	107	50% 15% 36%
28	D6	97	72% 20% 8%
28	d6	97	80% 20%
29	D7	81	86% 14%
29	d7	81	80% 19%

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Mol	Chain	Length	Quality of chain
30	D8	66	73% 21% 5%
30	d8	66	73% 21% 5%
31	D9	55	78% 16%
31	d9	55	71% 25%
32	E0	60	82% 17%
33	E1	76	53% 38% 7%
33	e1	76	59% 34% 7%
34	SR	318	85% 14%
34	sR	318	88% 12%
35	SM	273	44% 13% 42%
36	1	3396	52% 34% 7% 7%
36	5	3396	49% 37% 7% 7%
37	3	121	67% 31%
37	7	121	56% 37% 7%
38	4	158	52% 41% 7%
38	8	158	64% 31% 5%
39	L2	253	80% 18%
39	l2	253	79% 19%
40	L3	386	81% 18%
40	l3	386	79% 20%
41	L4	361	78% 21%
41	l4	361	78% 20%
42	L5	296	78% 20%
42	l5	296	81% 17%
43	L6	175	74% 14% 11%

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Mol	Chain	Length	Quality of chain
43	l6	175	74% 15% • 10%
44	L7	243	79% 10% • 9%
44	l7	243	77% 13% • 8%
45	L8	255	74% 17% 9%
45	l8	255	72% 17% • 9%
46	L9	191	77% 23% •
46	l9	191	81% 18% •
47	M0	220	76% 18% • •
47	m0	220	74% 22% • •
48	M1	173	73% 20% 5% •
48	m1	173	77% 18% • •
49	M3	198	80% 17% • •
49	m3	198	78% 18% • •
50	M4	137	80% 18% ••
50	m4	137	84% 15% •
51	M5	203	78% 22%
51	m5	203	85% 14% •
52	M6	198	83% 15% • •
52	m6	198	79% 19% •••
53	M7	183	79% 20% •
53	m7	183	72% 13% 15%
54	M8	185	85% 14% •
54	m8	185	79% 19% •
55	M9	188	88% 12%
55	m9	188	82% 16% •

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Mol	Chain	Length	Quality of chain
56	N0	172	77% 20% •
56	n0	172	80% 19% •
57	N1	159	81% 17% •
57	n1	159	80% 19% •
58	N2	120	69% 13% • 17%
58	n2	120	68% 12% • 18%
59	N3	136	86% 14%
59	n3	136	91% 8% •
60	N4	155	54% 9% • 37%
60	n4	155	71% 15% • 13%
61	N5	141	70% 15% • 14%
61	n5	141	66% 17% • 15%
62	N6	126	75% 25% •
62	n6	126	75% 25% •
63	N7	135	81% 19% •
63	n7	135	80% 16% •
64	N8	148	79% 18% •
64	n8	148	80% 18% •
65	N9	58	78% 17% 5%
65	n9	58	79% 19% •
66	O0	104	80% 12% • 7%
66	o0	104	81% 13% • •
67	O1	112	76% 19% • •
67	o1	112	74% 22% • •
68	O2	129	79% 18% • •

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Mol	Chain	Length	Quality of chain
68	o2	129	78% 18%
69	O3	106	89% 10%
69	o3	106	84% 16%
70	O4	119	76% 16% 6%
70	o4	119	73% 20% 6%
71	O5	119	79% 20%
71	o5	119	80% 19%
72	O6	99	81% 17%
72	o6	99	72% 25%
73	O7	87	84% 15%
73	o7	87	84% 15%
74	O8	77	77% 23%
74	o8	77	78% 21%
75	O9	50	86% 14%
75	o9	50	82% 16%
76	Q0	52	75% 23%
76	q0	52	75% 23%
77	Q1	25	68% 28%
77	q1	25	64% 28% 8%
78	Q2	105	73% 24%
78	q2	105	83% 16%
79	Q3	91	81% 16%
79	q3	91	90% 10%
80	e0	62	74% 24%
81	sM	273	29% 8% 62%

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Mol	Chain	Length	Quality of chain
82	m2	160	94% 6%
83	p0	311	37% 9% 54%
84	p1	47	100%
85	p2	46	100%

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 411211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	2	1750	37283	16668	6591	12274	1750	0	0	0
1	6	1795	38238	17095	6758	12590	1795	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
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
			Total	C	N	O	S			
13	C1	155	1214	775	230	206	3	0	0	0
			Total	C	N	O	S			
13	c1	146	1168	747	221	197	3	0	0	0

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
			Total	C	N	O	S			
14	C2	124	892	562	156	172	2	0	0	0
14	c2	124	892	562	156	172	2	0	0	0

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
			Total	C	N	O	S			
15	C3	150	1192	759	224	207	2	0	0	0
15	c3	150	1192	759	224	207	2	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	C6	141	1105	708	203	194	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	c6	142	1111	711	204	196	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	159	1104	652	221	231	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 81 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
81	sM	104	681	404	140	137	0	0	0

- Molecule 82 is a protein called unknown protein chain m2.

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 84 is a protein called unknown protein chain p1.

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

- Molecule 85 is a protein called unknown protein chain p2.

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

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
86	2	123	123	123	0	0
86	S2	1	1	1	0	0
86	S8	1	1	1	0	0
86	D0	1	1	1	0	0
86	D3	1	1	1	0	0
86	D4	1	1	1	0	0
86	SM	1	1	1	0	0
86	1	477	477	477	0	0
86	3	14	14	14	0	0
86	4	21	21	21	0	0
86	L2	1	1	1	0	0
86	L3	2	2	2	0	0
86	L4	2	2	2	0	0
86	L5	2	2	2	0	0
86	L7	2	2	2	0	0
86	L8	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	M0	2	Total 2	Mg 2	0	0
86	M1	1	Total 1	Mg 1	0	0
86	M3	3	Total 3	Mg 3	0	0
86	M5	1	Total 1	Mg 1	0	0
86	M6	1	Total 1	Mg 1	0	0
86	M7	6	Total 6	Mg 6	0	0
86	M8	1	Total 1	Mg 1	0	0
86	M9	1	Total 1	Mg 1	0	0
86	N0	1	Total 1	Mg 1	0	0
86	N3	3	Total 3	Mg 3	0	0
86	N5	1	Total 1	Mg 1	0	0
86	N8	3	Total 3	Mg 3	0	0
86	O4	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	O8	1	Total 1	Mg 1	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	6	149	Total 149	Mg 149	0	0
86	s1	1	Total 1	Mg 1	0	0
86	s4	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	c1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
86	c7	1	1	1	0	0
86	d3	2	2	2	0	0
86	d4	1	1	1	0	0
86	sM	2	2	2	0	0
86	5	506	506	506	0	0
86	7	16	16	16	0	0
86	8	14	14	14	0	0
86	l2	2	2	2	0	0
86	l3	2	2	2	0	0
86	l4	1	1	1	0	0
86	l5	2	2	2	0	0
86	l7	2	2	2	0	0
86	l9	1	1	1	0	0
86	m1	1	1	1	0	0
86	m5	3	3	3	0	0
86	m6	1	1	1	0	0
86	m7	5	5	5	0	0
86	n0	1	1	1	0	0
86	n3	2	2	2	0	0
86	n6	1	1	1	0	0
86	n8	5	5	5	0	0

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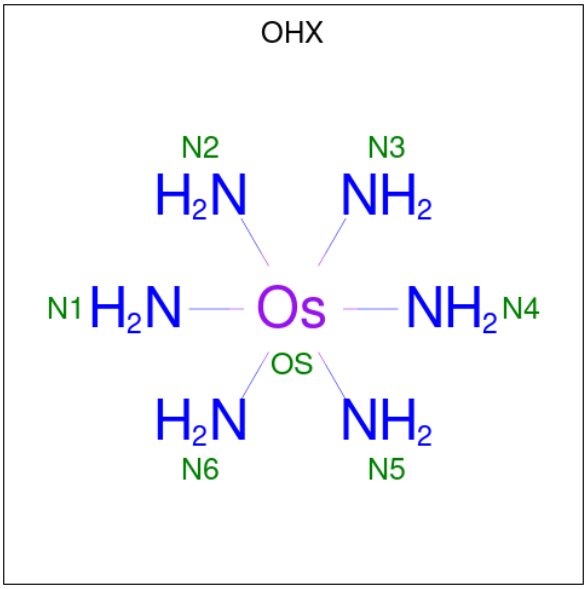
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	o1	2	Total	Mg		0	0
			2	2			
86	o3	2	Total	Mg		0	0
			2	2			
86	o4	1	Total	Mg		0	0
			1	1			
86	q0	1	Total	Mg		0	0
			1	1			
86	q1	1	Total	Mg		0	0
			1	1			
86	q3	1	Total	Mg		0	0
			1	1			

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	7	6	1	0	0
			Total	N	Os		
87	2	1	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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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
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87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	1	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
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87	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	7	6	1	0	0
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			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0
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87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0
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87	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
87	1	1	7	6	1	0	0
			Total	N	Os		
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87	4	1	7	6	1	0	0
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87	4	1	7	6	1	0	0
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87	4	1	7	6	1	0	0
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87	4	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	7	6	1	0	0
87	4	1	7	6	1	0	0
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87	4	1	7	6	1	0	0
87	4	1	7	6	1	0	0
87	4	1	7	6	1	0	0
87	L3	1	7	6	1	0	0
87	L3	1	7	6	1	0	0
87	L3	1	7	6	1	0	0
87	L4	1	7	6	1	0	0
87	M0	1	7	6	1	0	0
87	M5	1	7	6	1	0	0
87	M6	1	7	6	1	0	0
87	M7	1	7	6	1	0	0
87	M7	1	7	6	1	0	0
87	M8	1	7	6	1	0	0
87	M9	1	7	6	1	0	0
87	N1	1	7	6	1	0	0
87	N9	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	O2	1	7	6	1	0	0
87	O3	1	7	6	1	0	0
87	O7	1	7	6	1	0	0
87	O7	1	7	6	1	0	0
87	O9	1	7	6	1	0	0
87	Q2	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
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87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	7	6	1	0	0
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87	6	1	7	6	1	0	0
			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	6	1	7	6	1	0	0
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			Total	N	Os		
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			Total	N	Os		
87	6	1	7	6	1	0	0
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			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0
87	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	6	1	7	6	1	0	0
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87	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			Total	N	Os		
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			Total	N	Os		
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			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	6	1	7	6	1	0	0
			Total	N	Os		
87	s1	1	7	6	1	0	0
			Total	N	Os		
87	s1	1	7	6	1	0	0
			Total	N	Os		
87	s4	1	7	6	1	0	0
			Total	N	Os		
87	s8	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	s9	1	7	6	1	0	0
87	c1	1	7	6	1	0	0
87	c3	1	7	6	1	0	0
87	c5	1	7	6	1	0	0
87	c8	1	7	6	1	0	0
87	d4	1	7	6	1	0	0
87	d9	1	7	6	1	0	0
87	sR	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
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87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0
87	5	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	5	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	7	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	8	1	7	6	1	0	0
			Total	N	Os		
87	l3	1	7	6	1	0	0
			Total	N	Os		
87	l3	1	7	6	1	0	0
			Total	N	Os		
87	l4	1	7	6	1	0	0
			Total	N	Os		
87	l4	1	7	6	1	0	0
			Total	N	Os		
87	l5	1	7	6	1	0	0
			Total	N	Os		
87	l5	1	7	6	1	0	0
			Total	N	Os		
87	l5	1	7	6	1	0	0
			Total	N	Os		
87	l9	1	7	6	1	0	0
			Total	N	Os		
87	m0	1	7	6	1	0	0
			Total	N	Os		
87	m0	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
87	m1	1	7	6	1	0	0
87	m4	1	7	6	1	0	0
87	m5	1	7	6	1	0	0
87	m6	1	7	6	1	0	0
87	m7	1	7	6	1	0	0
87	m8	1	7	6	1	0	0
87	m9	1	7	6	1	0	0
87	n3	1	7	6	1	0	0
87	n6	1	7	6	1	0	0
87	n9	1	7	6	1	0	0
87	o2	1	7	6	1	0	0
87	o3	1	7	6	1	0	0
87	o7	1	7	6	1	0	0
87	o7	1	7	6	1	0	0
87	q2	1	7	6	1	0	0

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
88	D6	1	1	1	0	0
88	D7	1	1	1	0	0
88	D9	1	1	1	0	0
88	E1	1	1	1	0	0

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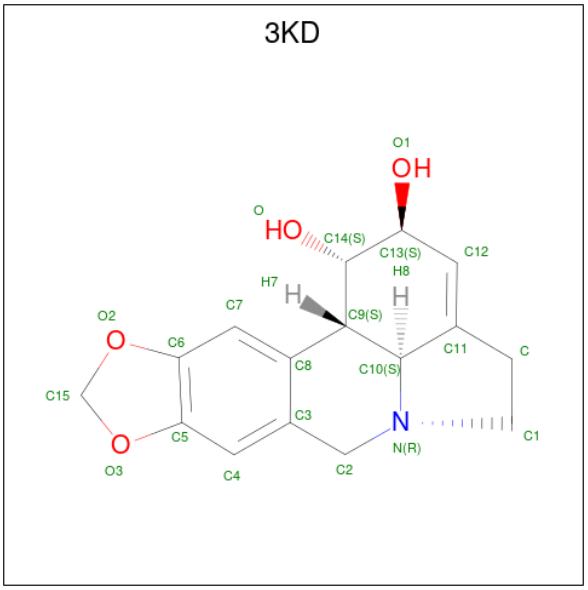
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	O7	1	Total Zn 1 1	0	0
88	Q0	1	Total Zn 1 1	0	0
88	Q2	1	Total Zn 1 1	0	0
88	Q3	1	Total Zn 1 1	0	0
88	d6	1	Total Zn 1 1	0	0
88	d7	1	Total Zn 1 1	0	0
88	d9	1	Total Zn 1 1	0	0
88	e1	1	Total Zn 1 1	0	0
88	o7	1	Total Zn 1 1	0	0
88	q0	1	Total Zn 1 1	0	0
88	q2	1	Total Zn 1 1	0	0
88	q3	1	Total Zn 1 1	0	0

- Molecule 89 is (1S,2S,12bS,12cS)-2,4,5,7,12b,12c-hexahydro-1H-[1,3]dioxolo[4,5-j]pyrrolo[3,2,1-de]phenanthridine-1,2-diol (three-letter code: 3KD) (formula: $C_{16}H_{17}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
89	1	1	21	16	1	4	0	0
			Total	C	N	O		
89	5	1	21	16	1	4	0	0

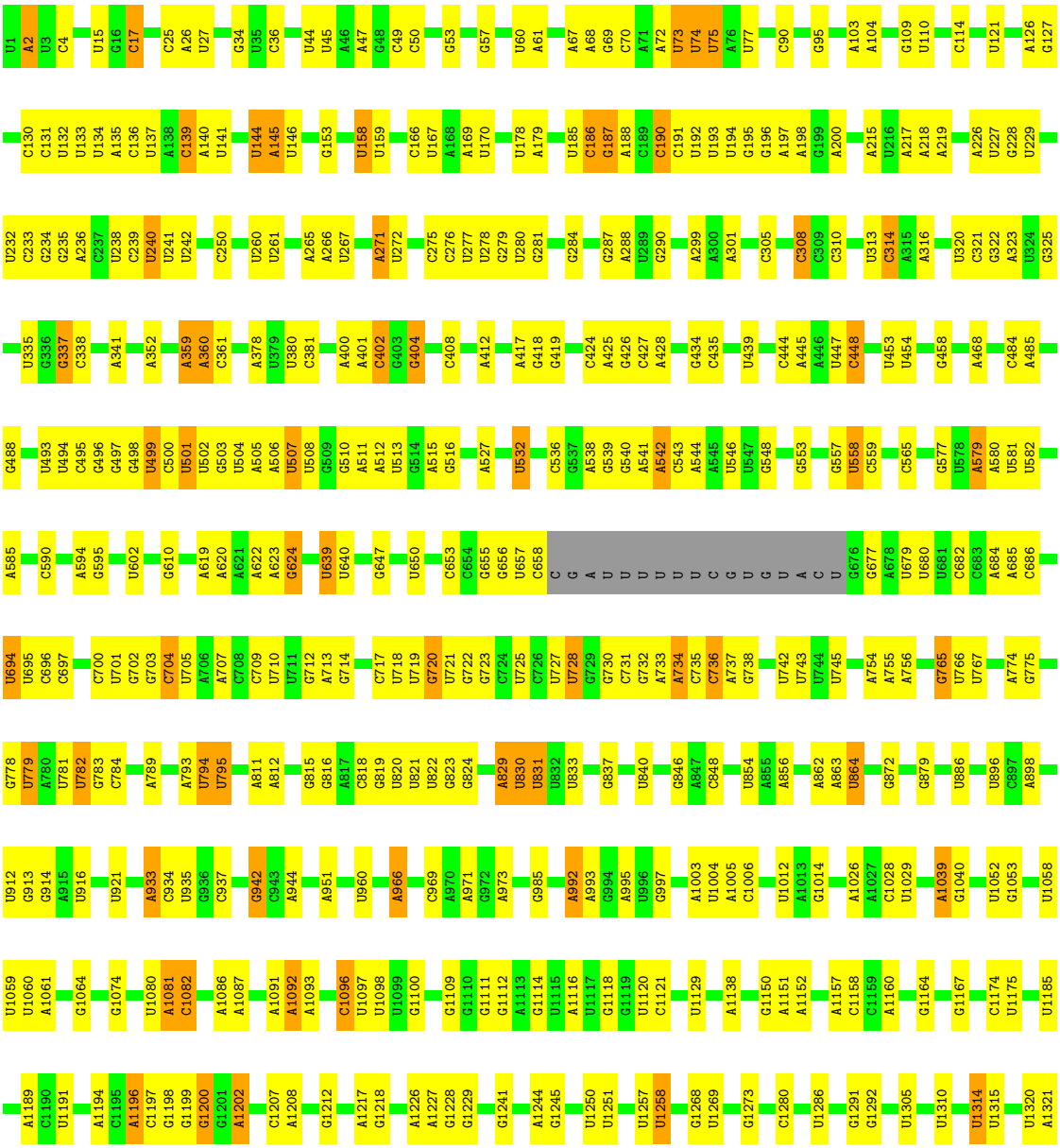
3 Residue-property plots (i)

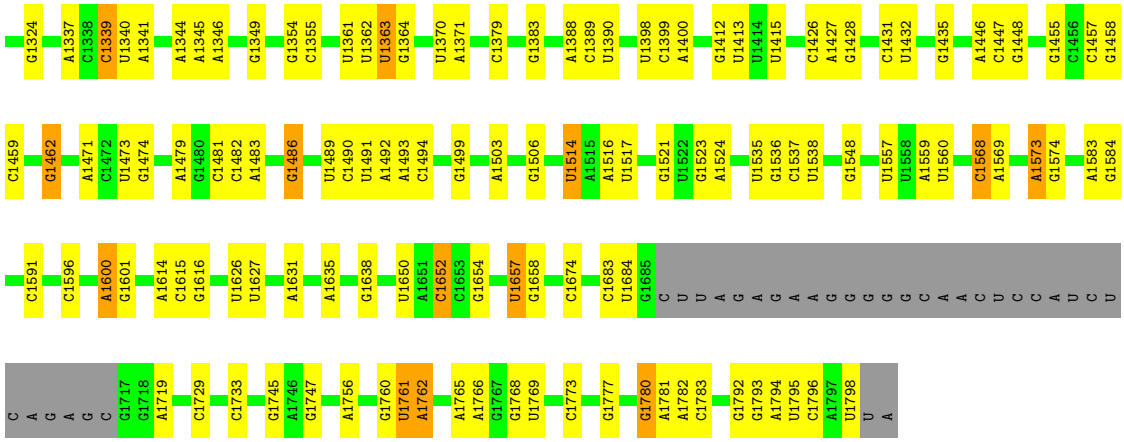
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

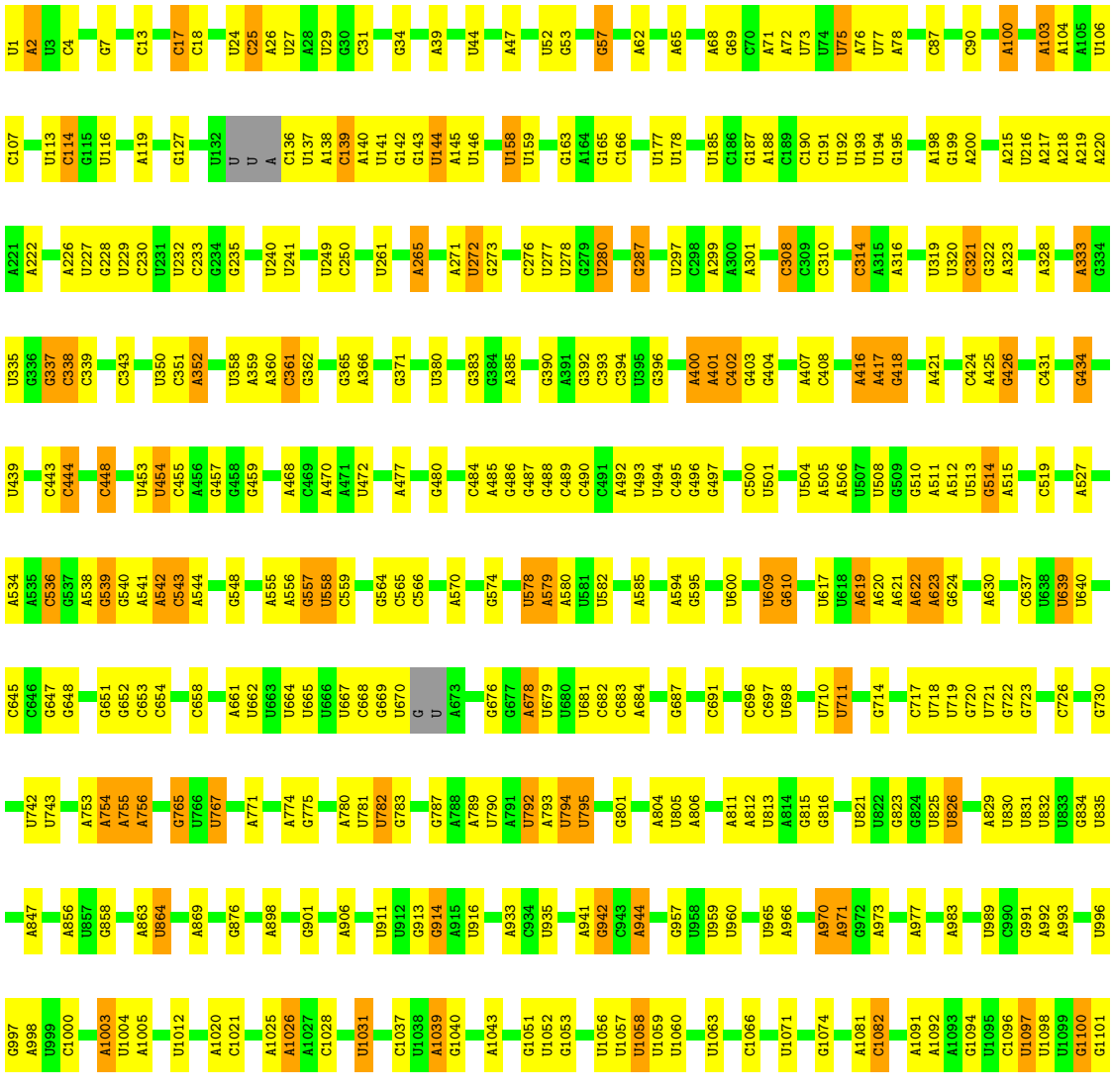
Chain 2: 66% 27%

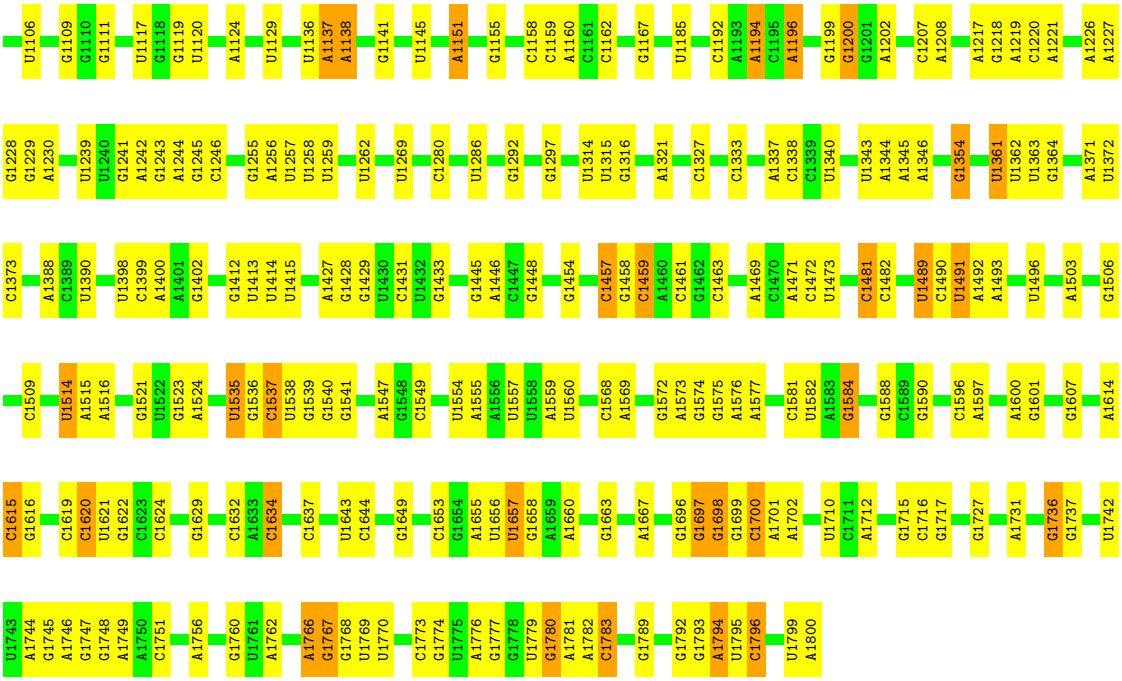




• Molecule 1: 18S ribosomal RNA

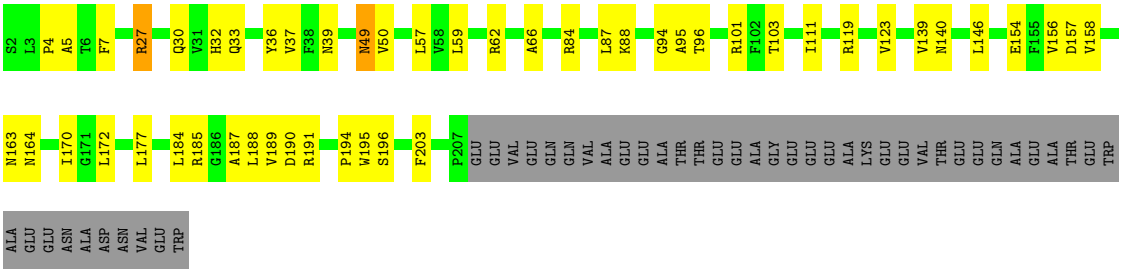
Chain 6:





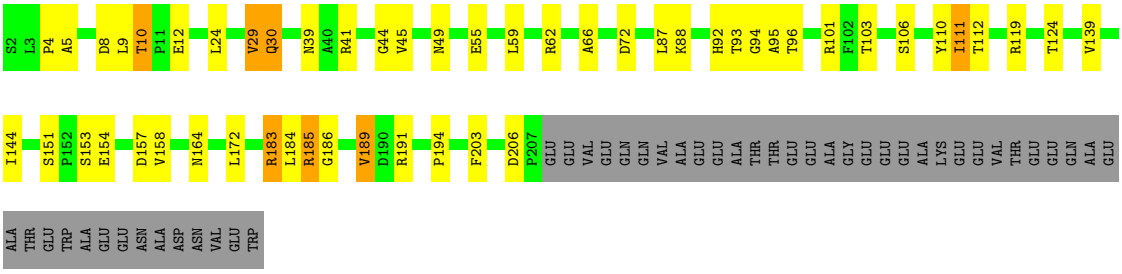
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



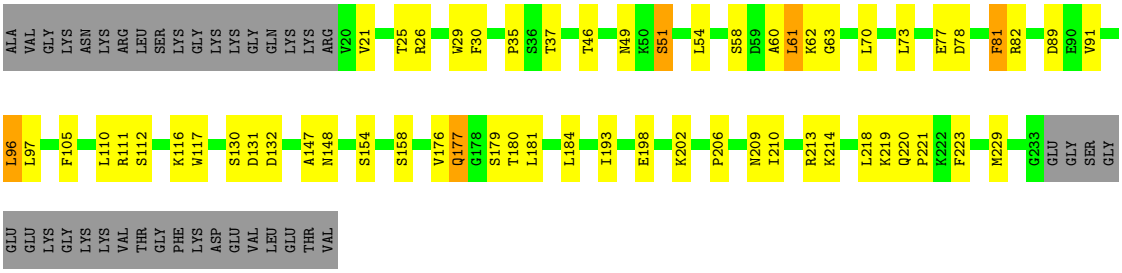
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



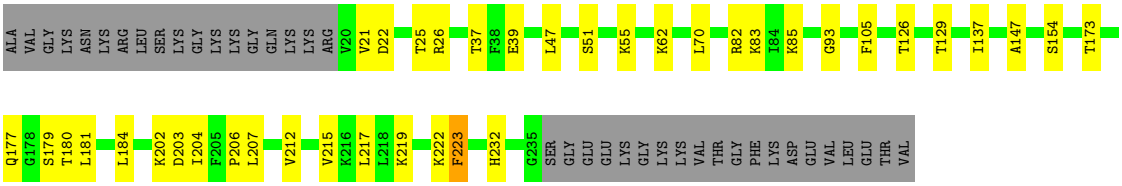
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



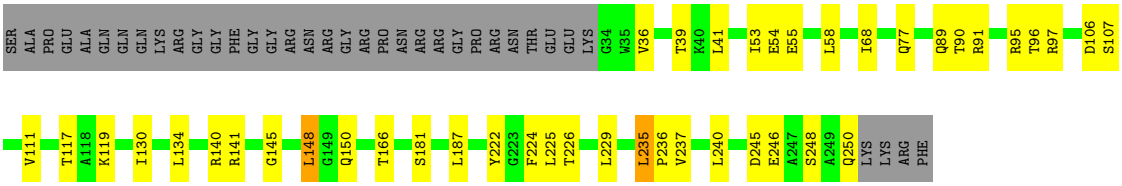
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



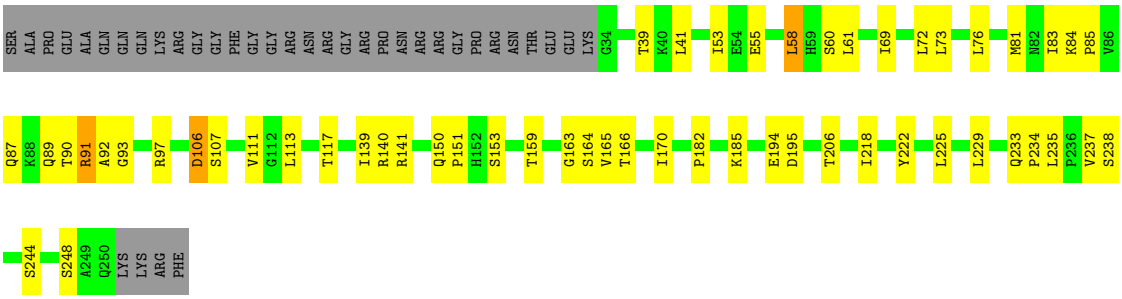
• Molecule 4: 40S ribosomal protein S2

Chain S2:



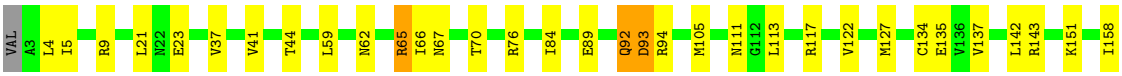
• Molecule 4: 40S ribosomal protein S2

Chain s2:



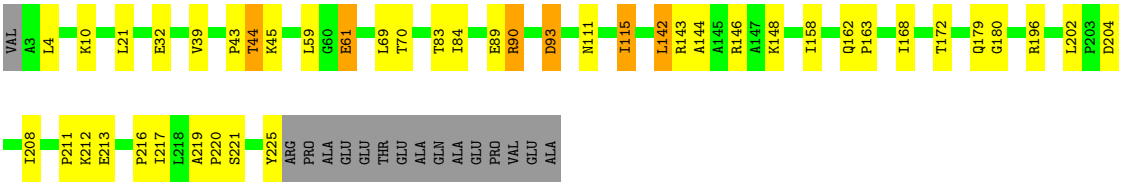
• Molecule 5: 40S ribosomal protein S3

Chain S3:



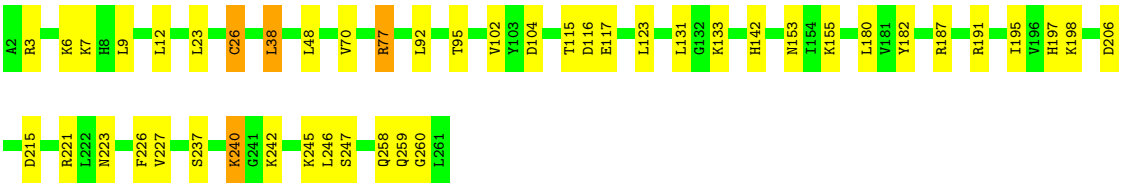
• Molecule 5: 40S ribosomal protein S3

Chain s3:



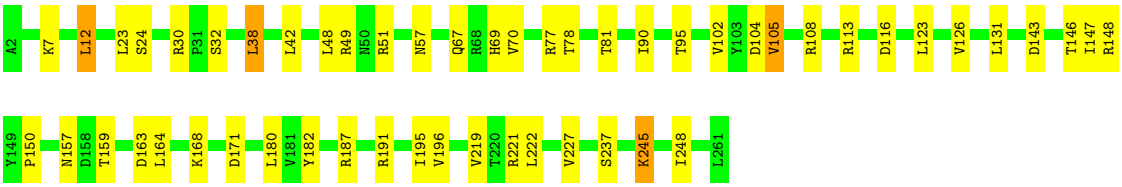
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



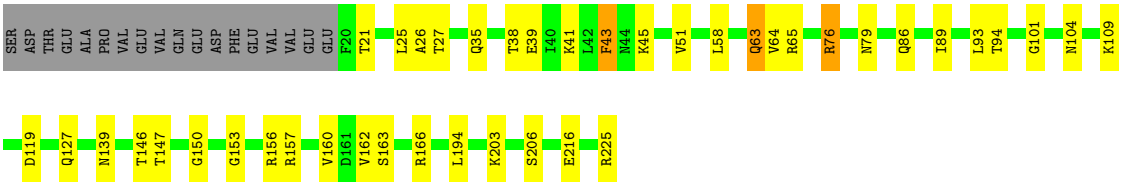
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



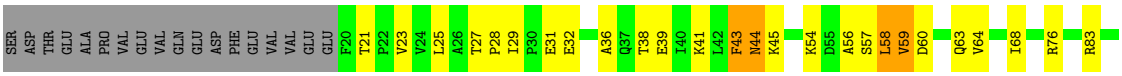
• Molecule 7: 40S ribosomal protein S5

Chain S5:



• Molecule 7: 40S ribosomal protein S5

Chain s5:



I89 L93 T94 M99 N100 G101 R102 K109 D119 N122 T125 N128 T140 T147 R148 R157 S163 R167 Q170 F184 R185 N186 L194 K203 G204 S208 K213 E216 R225

- Molecule 8: 40S ribosomal protein S6-A

Chain S6: 74% 21% • •

M1 V9 Q13 K14 R25 I32 F45 K51 K58 Q65 G66 V67 L68 L69 P70 L76 L77 T78 K79 N80 V81 S82 K93 R98 L109 E120 L121 E122 G123 L124 T125 D126 T127 T128 V129 R132 L133 K143 G146 L147 S148 K149 E150 D151

D152 V153 R154 D155 Y169 T170 P173 K174 I175 Q176 R177 R183 L211 L216 S217 K223 I226 ARG LYS ARG ARG ALA SER SER LEU LYS ALA

- Molecule 8: 40S ribosomal protein S6-A

Chain s6: 74% 17% • 8%

M1 E17 E21 R25 K30 Q34 D43 Q65 L68 L69 P70 T71 L76 L77 T78 K79 N80 V81 K93 V97 V108 L109 A110 L111 K115 E120 L121 D126 T127 T128 V129 P130 K131 K143 E150 D151 D152 V153 R154 D155 F156 G165

T170 P173 K174 L193 E203 L212 R215 E218 ARG LYS ALA GLU LYS ALA GLU ILE ARG LYS ARG ARG ALA SER SER LEU LYS ALA

- Molecule 9: 40S ribosomal protein S7-A

Chain S7: 75% 20% • •

SER ALA P4 L9 P13 N29 S30 S31 P32 L38 I46 D50 V51 V64 F70 V73 Q74 T75 K84 F85 Q86 D87 R97 I98 T105 S106 R107 K111 R112 P113 R114 S115 R116 D123 L126 V130 F131 P132 T133 E134 I135 V136 N147

D155 D158 D163 E167 N174 I185 P186 S187 GLU THR HIS

- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 78% 17% • •

S2 S10 Q11 A12 P13 E28 N29 S30 E33 Q42 K55 V64 P65 S66 L67 Q74 L77 T78 R79 E80 Q86 D87 R97 S103 R104 T105 S106 R107 Q108 K111 R114 S115 R116 T117 L118 L126 F131 P132 T133 V136 R139 L143

D155 V159 I185 P186 S187 GLU THR HIS

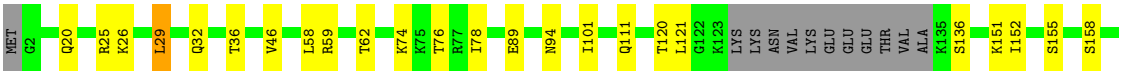
- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 80% 14% • 6%

MET G2 S7 R8 H9 K10 T14 F21 R22 K26 L29 T36 A40 V46 R49 N52 L58 S69 V82 D105 T120 K123 LYS LYS ASN VAL LYS GLU GLU GLU THR VAL ALA K135 N138 A147 A148 S149 A150 K151 I152 E153

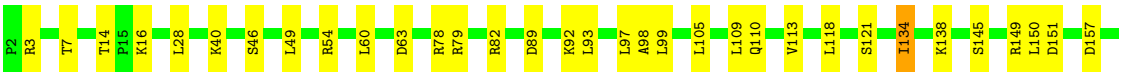
• Molecule 10: 40S ribosomal protein S8-A

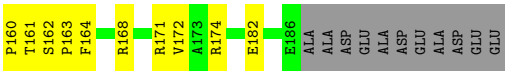
Chain s8:



• Molecule 11: 40S ribosomal protein S9-A

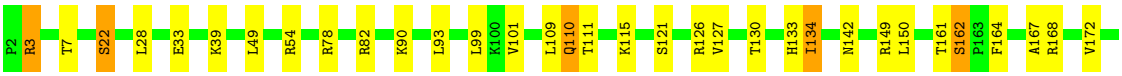
Chain S9:

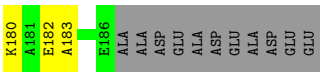




• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



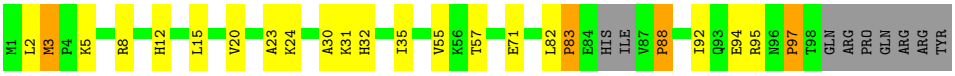


• Molecule 12: 40S ribosomal protein S10-A

Chain C0:

• Molecule 12: 40S ribosomal protein S10-A

Chain c0:



• Molecule 13: 40S ribosomal protein S11-A

Chain C1: 79% 20% •

S2 T3 E4 L5 T6 V7 Q8 N21 T27 S28 K29 R30 N37 L40 T44 D55 L63 R67 G68 K69 T72 G73 T74 K79 T83 V109 S112 P113 Q118 V123 Q127 I131 V140 S143 A144 A145 A146 A147 A154 K155

F156

• Molecule 13: 40S ribosomal protein S11-A

Chain c1: 74% 19% • 6%

S2 T3 E4 L5 T6 V7 E10 N21 K26 T27 R30 T31 K32 R33 L40 T44 F60 T61 R67 T74 V75 V76 M80 T83 I86 A114 D121 I122 V123 R129 K133 V139 V140 A144 A145 A146 A147 LYS ALA ASN LYS GLN

PHE ALA LYS PHE

• Molecule 14: 40S ribosomal protein S12

Chain C2: 55% 30% • 13%

SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU GLU THR VAL VAL GLU GLN THR A20 E21 V22 E25 L28 R33 V37 H38 D39 R43 R46 K50 A51 L52 I53 R54 G55 L58 V61 V66 A69 N70 I71 L74 D81 P82 E83 V86

P87 L88 I89 K90 V91 A92 D93 A101 G102 L103 I106 D107 A112 R113 K114 V115 S119 V120 V121 N125 W126 G127 A128 E129 T130 D131 E132 H139 F140 Q143

• Molecule 14: 40S ribosomal protein S12

Chain c2: 59% 25% • 13%

SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU GLU THR VAL VAL GLU GLN THR A20 E21 V22 L28 L36 D39 G40 R43 G44 L45 L52 L58 L59 L62 V63 V66 I71 L74 P82 E83 N84 K85 V86 P87 L88 I89 K90 V91 L97

A101 G102 L103 I106 D107 R108 E109 A110 V115 V116 G117 A118 S119 V120 V121 G127 A128 E129 T130 D131 E132 I136 F140 Q143

• Molecule 15: 40S ribosomal protein S13

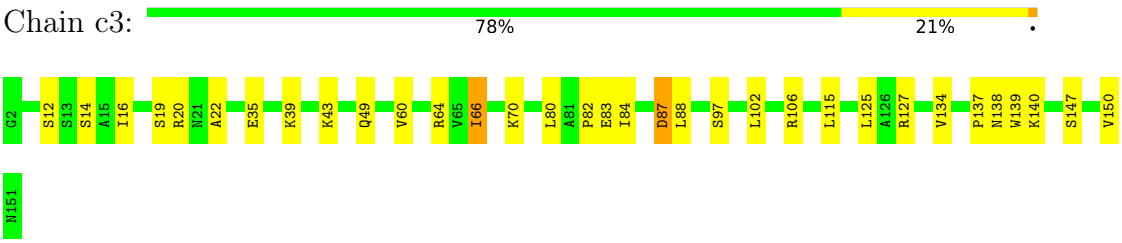
Chain C3: 79% 19% •

G2 R3 K9 G10 I11 S12 S13 I16 S19 A22 K27 S32 K39 R42 L45 I50 D56 A57 H58 R64 V65 I66 T67 G68 K76 E83 L88 L102 D110 R114 L115 L125 V134 P137 N138 E142 T145

N151

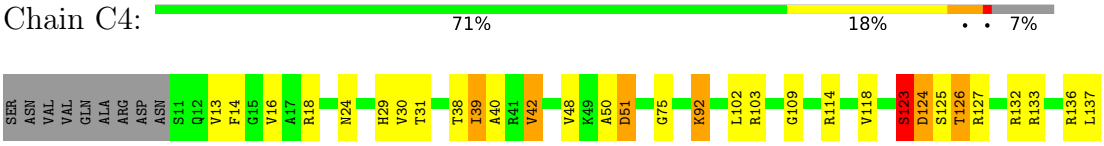
• Molecule 15: 40S ribosomal protein S13

Chain c3:



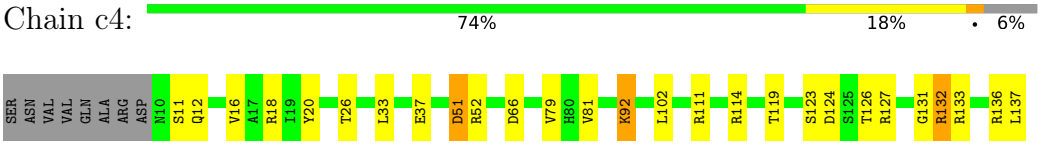
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



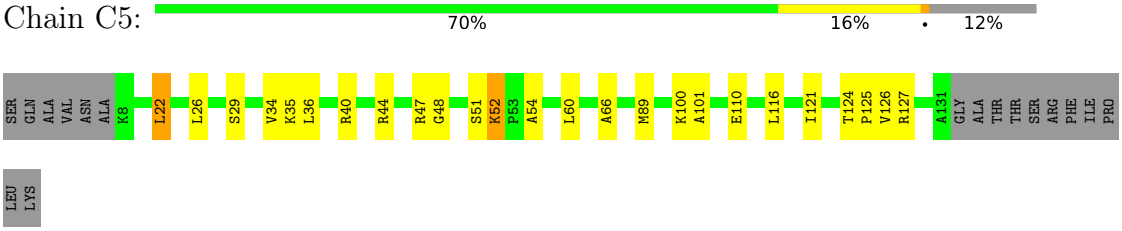
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



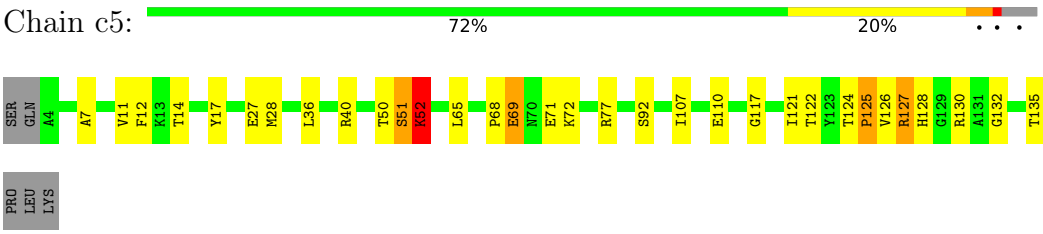
• Molecule 17: 40S ribosomal protein S15

Chain C5:



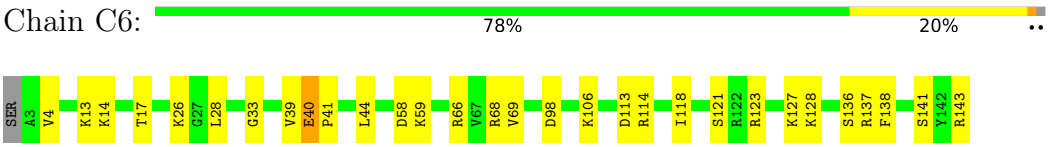
• Molecule 17: 40S ribosomal protein S15

Chain c5:



• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



• Molecule 18: 40S ribosomal protein S16-A

Chain c6: 77% 21% •

S2 A3 V4 T17 K23 L28 T37 L38 V39 E40 P41 E42 I43 V48 L53 L54 L57 R66 V67 R68 V69 T70 I81 Q94 V97 D98 K106 T110 D113 R114 T115 L116 R123 R137 Y142 R143

• Molecule 19: 40S ribosomal protein S17-A

Chain C7: 66% 18% • 12%

MET G2 R5 T6 P22 K23 L24 T25 Q29 T30 L34 I38 L46 K49 T54 I69 S70 F71 K72 R78 Q83 Y84 V85 P86 E87 V88 S89 ALA LEU ASP LEU SER R95 N104 Q105 T106 S107 L113 G114 L115 L119 N123 V124 S125 A126

GLN ARG ASP ARG ARG TYR ARG LYS ARG VAL

• Molecule 19: 40S ribosomal protein S17-A

Chain c7: 71% 13% • 14%

MET G2 R3 T8 Q29 L34 L46 K49 I50 R60 I61 Q62 K63 I69 V85 V88 S89 A90 LEU ASP LEU SER R95 G98 V99 N104 V110 L113 K116 S120 V121 I122 ASN VAL SER ALA GLN ARG ASP ARG ARG TYR ARG LYS ARG

VAL

• Molecule 20: 40S ribosomal protein S18-A

Chain C8: 72% 24% •

S2 L3 V4 V5 Q6 E7 Q8 F11 Q12 H13 I14 L17 I18 N19 T20 N25 I26 K27 I28 L32 R40 D53 L54 E60 L61 Q71 K80 I81 P82 A83 Q89 N90 D91 I92 D97 K108 R115 L116 R120 T125 R132 Q136

K139 T140 T141 G142 R143 R144 R145 A146

• Molecule 20: 40S ribosomal protein S18-A

Chain c8: 77% 21% •

S2 L3 V4 V5 Q6 S10 H13 I14 L15 L18 N25 I26 K27 I28 T33 V38 G39 R40 E60 L61 T62 Q63 L66 E67 R68 D91 I92 A102 L116 I119 R120 V133 R134 G135 T138 K139 R143 R144 R145 A146

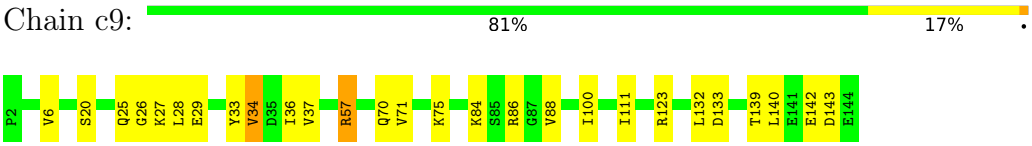
• Molecule 21: 40S ribosomal protein S19-A

Chain C9: 81% 19%

P2 G3 V4 S5 V6 Y18 L22 L28 E29 V30 P31 G32 Y33 V34 D35 I36 V37 A50 W53 R57 M67 R68 K69 Q70 K84 I94 I111 I116 S117 R130 D131 R134 L140 E144

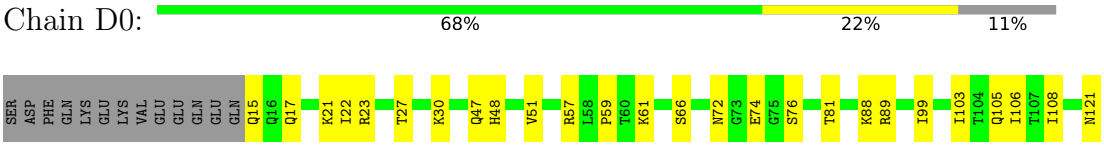
• Molecule 21: 40S ribosomal protein S19-A

Chain c9:



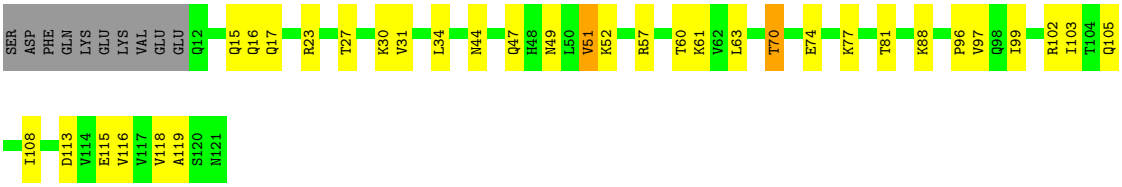
• Molecule 22: 40S ribosomal protein S20

Chain D0:



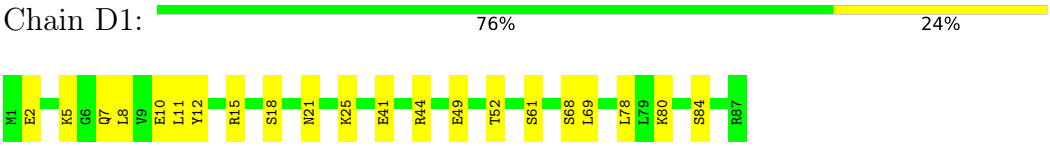
• Molecule 22: 40S ribosomal protein S20

Chain d0:



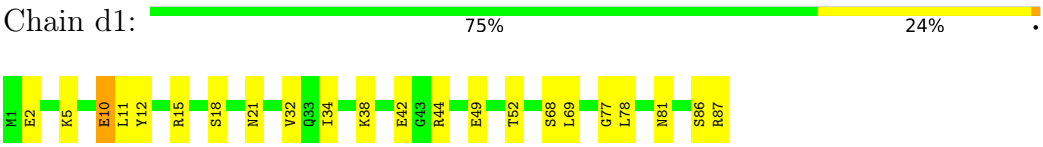
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



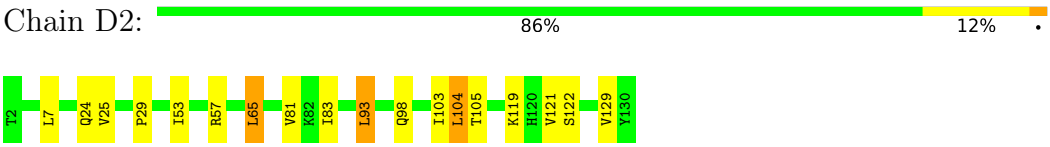
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



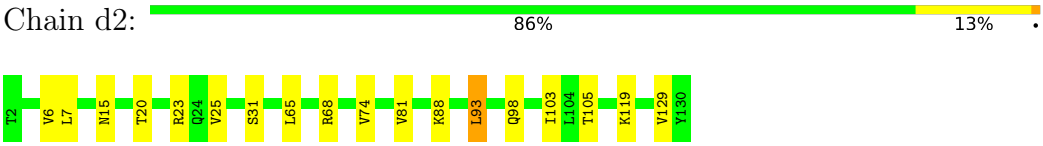
• Molecule 24: 40S ribosomal protein S22-A

Chain D2:



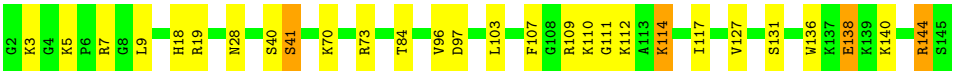
• Molecule 24: 40S ribosomal protein S22-A

Chain d2:



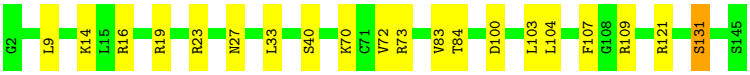
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



• Molecule 25: 40S ribosomal protein S23-A

Chain d3:

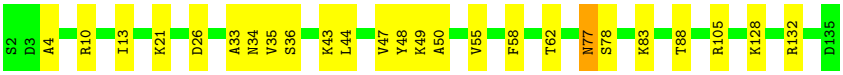


• Molecule 26: 40S ribosomal protein S24-A

Chain D4:

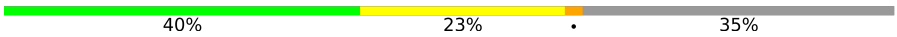
• Molecule 26: 40S ribosomal protein S24-A

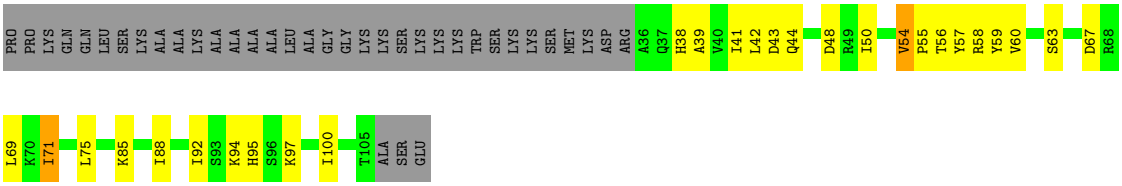
Chain d4:



• Molecule 27: 40S ribosomal protein S25-A

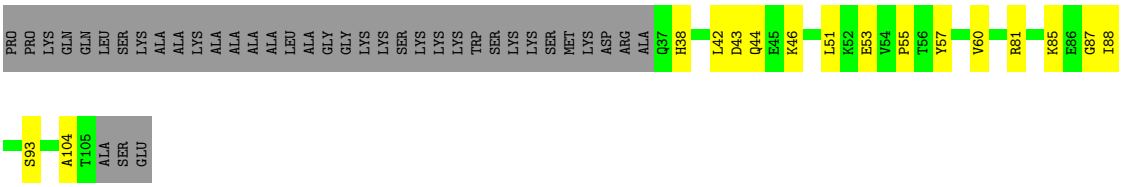
Chain D5:





• Molecule 27: 40S ribosomal protein S25-A

Chain d5:

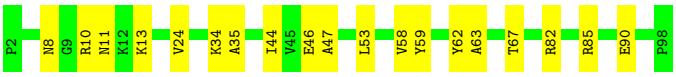


• Molecule 28: 40S ribosomal protein S26-B

Chain D6: 72% 20% 8%

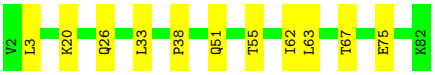
• Molecule 28: 40S ribosomal protein S26-B

Chain d6: 80% 20%



• Molecule 29: 40S ribosomal protein S27-A

Chain D7: 86% 14%



• Molecule 29: 40S ribosomal protein S27-A

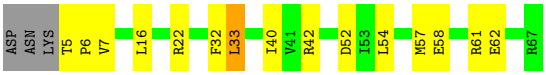
Chain d7: 80% 19%

• Molecule 30: 40S ribosomal protein S28-A

Chain D8: 73% 21% 5%

• Molecule 30: 40S ribosomal protein S28-A

Chain d8: 73% 21% 5%

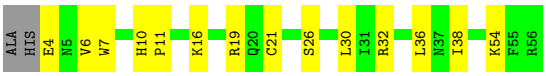


• Molecule 31: 40S ribosomal protein S29-A

Chain D9: 78% 16%

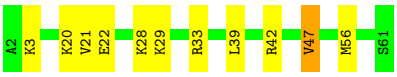
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



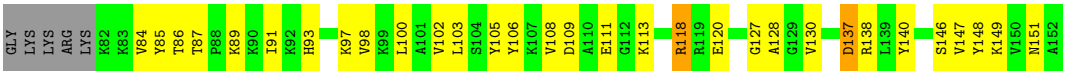
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



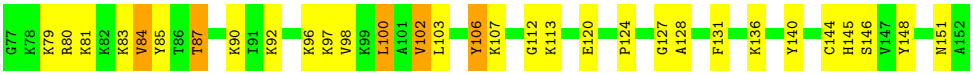
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



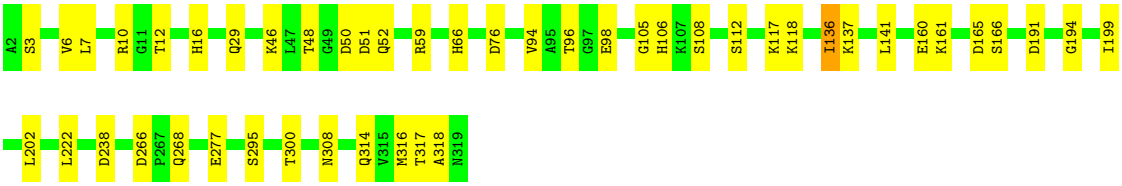
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



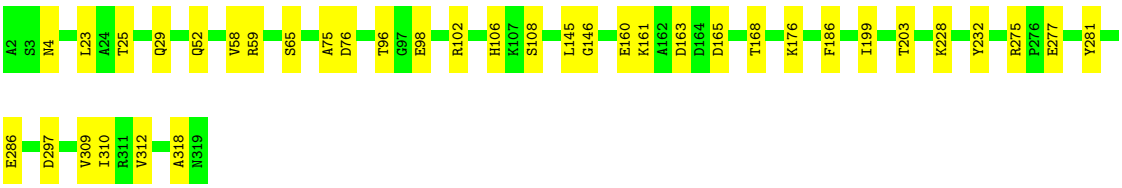
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



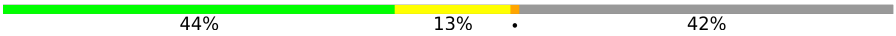
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

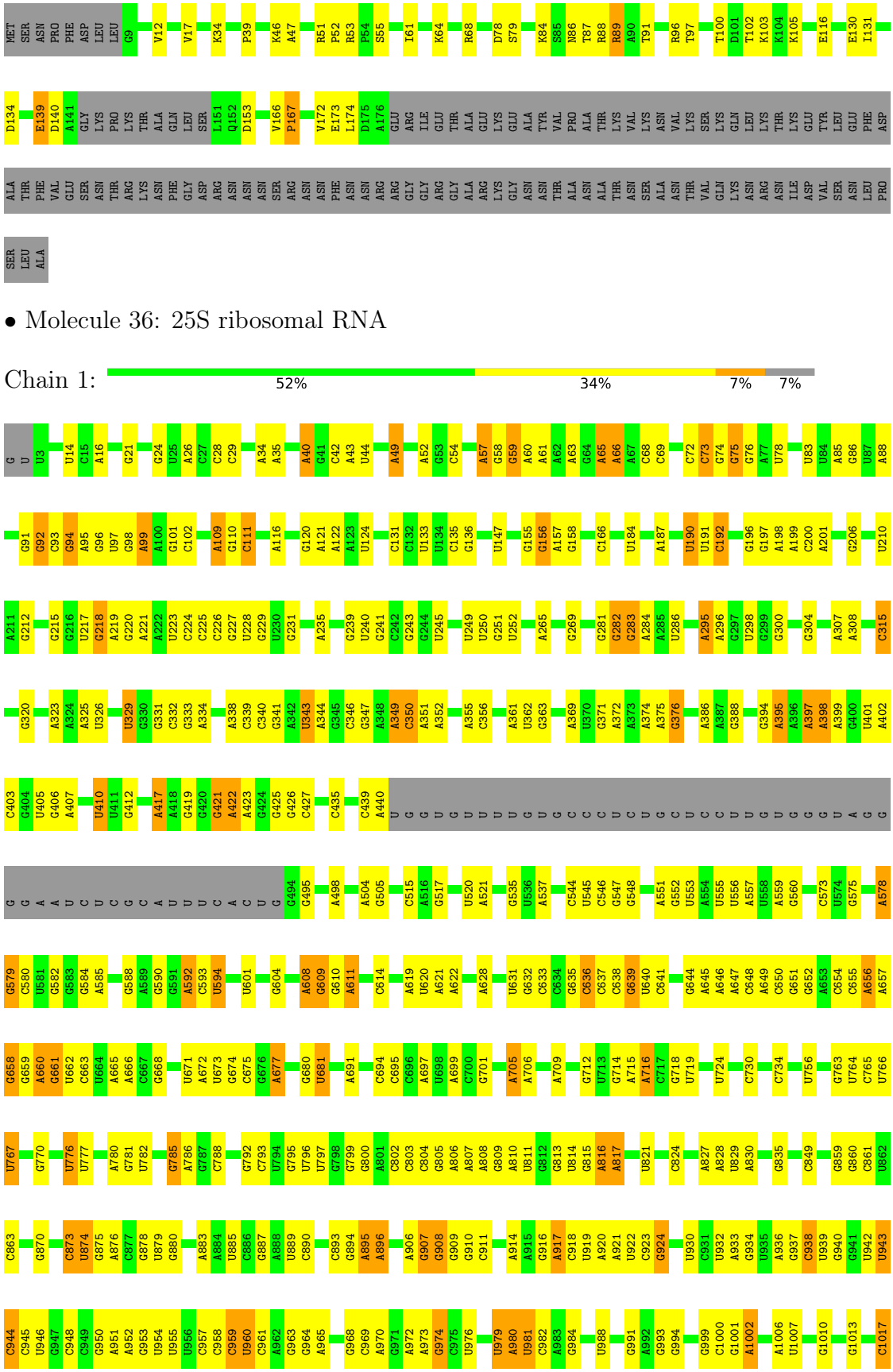
Chain sR:



• Molecule 35: Suppressor protein STM1

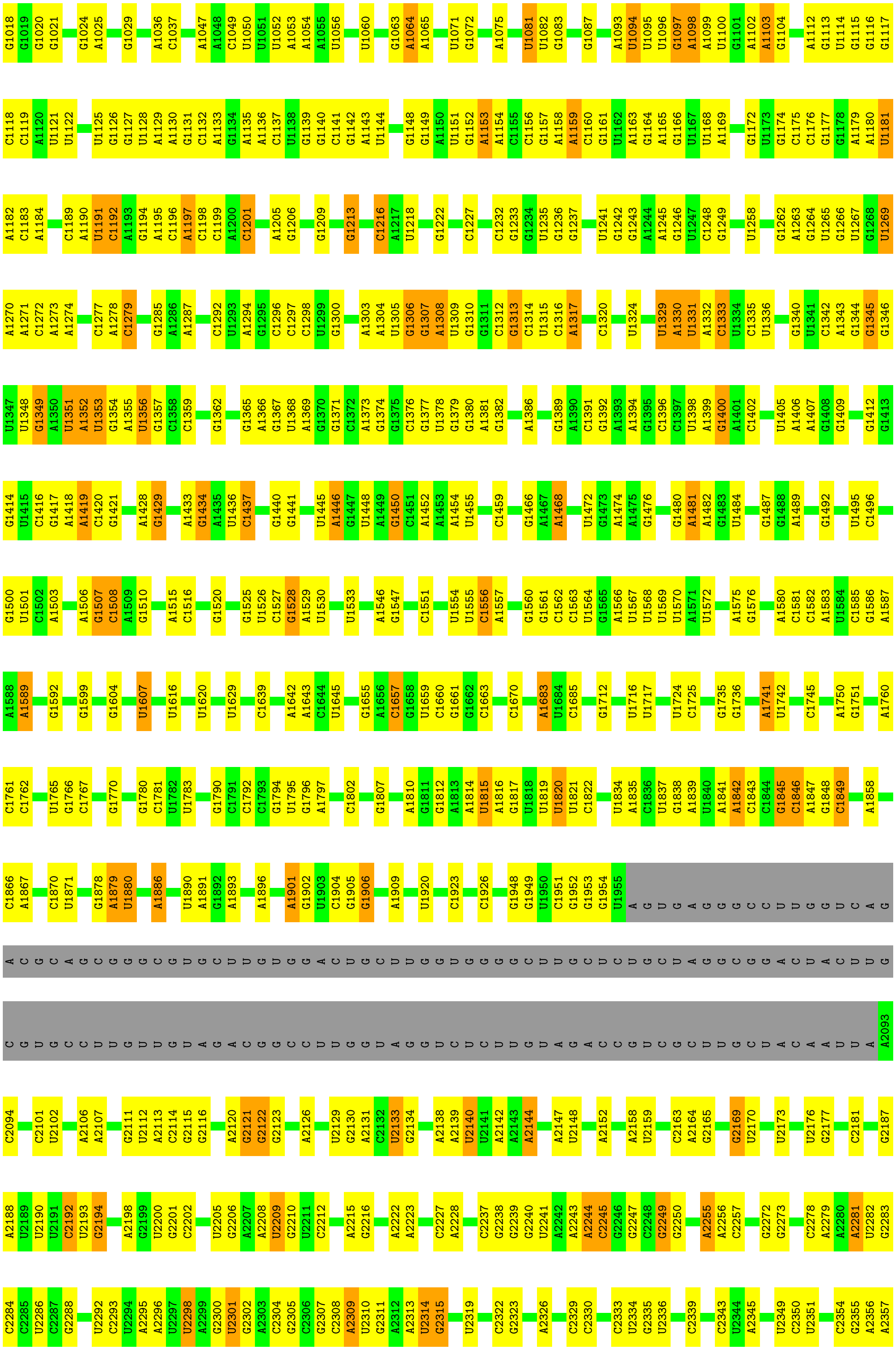
Chain SM:

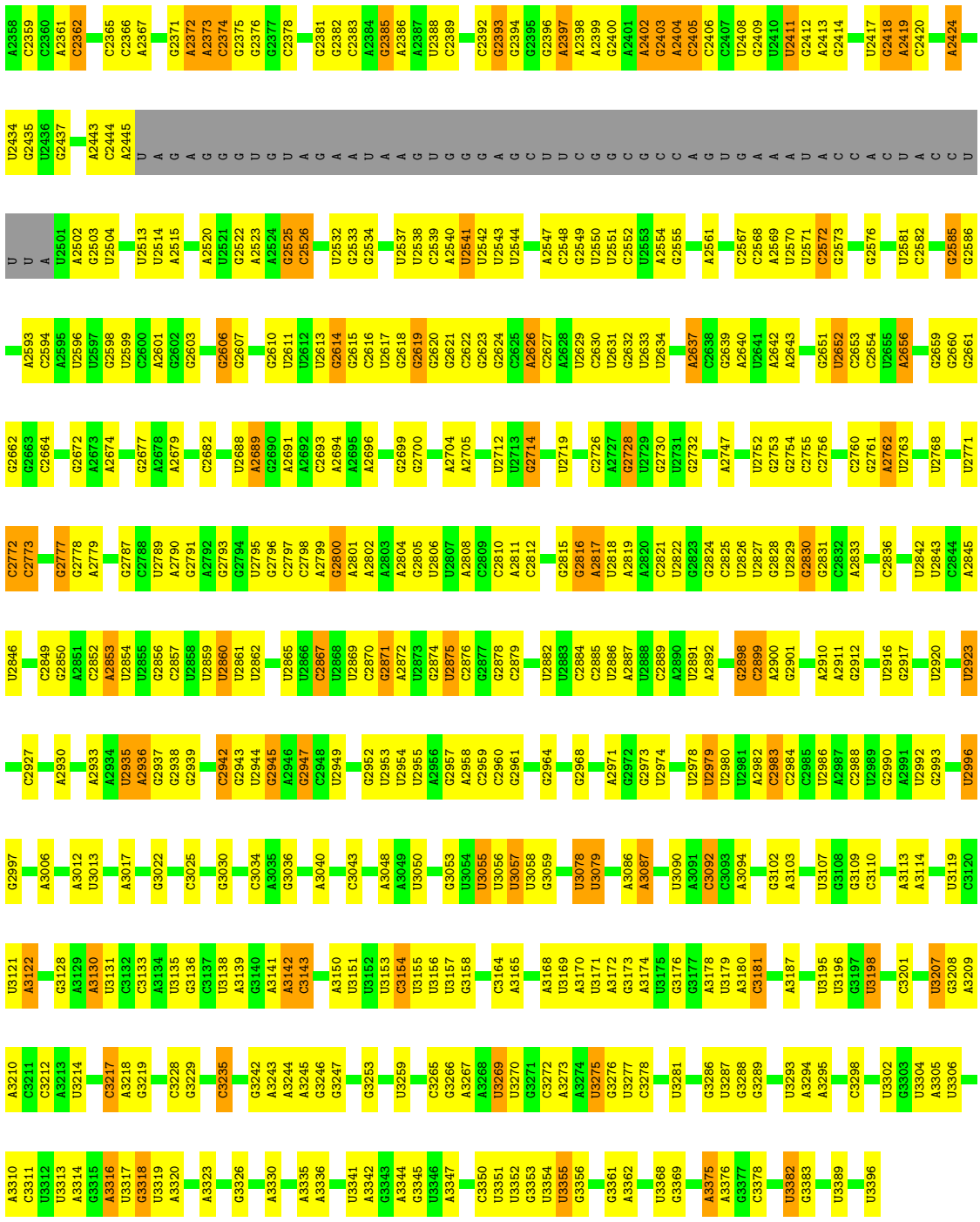




• Molecule 36: 25S ribosomal RNA

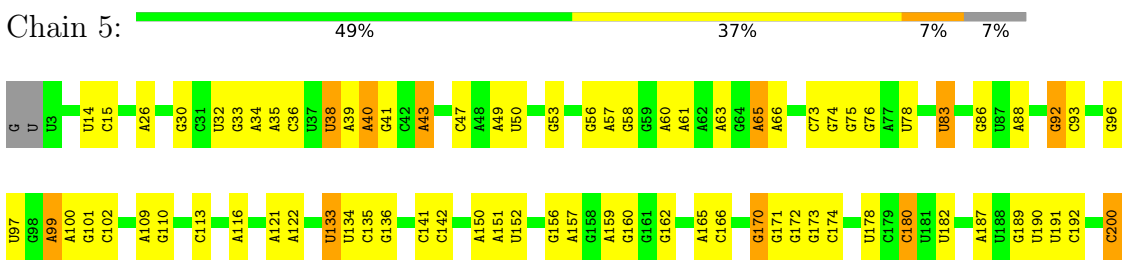
Chain 1: 52% 34% 7% 7%


G1018 G1019 G1020 G1021 G1024 A1025 G1029 A1036 C1037 A1047 A1048 C1049 U1050 U1051 U1052 A1053 A1054 A1055 U1056 U1060 G1063 A1064 A1065 U1071 G1072 A1075 U1081 U1082 G1083 G1087 A1093 U1094 U1095 U1096 G1097 A1098 A1099 U1100 G1101 A1102 A1103 G1104 A1112 G1113 U1114 G1115 G1116 G1117
C1118 C1119 A1120 U1121 U1122 U1125 G1126 G1127 U1128 A1129 A1130 G1131 C1132 A1133 G1134 A1135 A1136 C1137 U1138 G1139 G1140 C1141 G1142 A1143 U1144 G1148 G1149 A1150 U1151 G1152 A1153 A1154 C1155 C1156 G1157 A1158 A1159 C1160 G1161 U1162 A1163 G1164 A1165 G1166 U1167 U1168 A1169 G1172 U1173 G1174 C1175 C1176 G1177 G1178 A1179 A1180 U1181
A1182 C1183 A1184 C1189 A1190 U1191 C1192 A1193 G1194 A1195 C1196 A1197 C1198 C1199 A1200 C1201 A1205 G1206 G1209 G1213 C1216 A1217 U1218 G1222 C1227 C1232 G1233 G1234 U1235 G1236 G1237 U1241 G1242 G1243 A1244 A1245 G1246 U1247 C1248 G1249 U1258 G1262 A1263 G1264 U1265 G1266 U1267 G1268 U1269
A1270 A1271 C1272 A1273 A1274 C1277 A1278 C1279 G1285 A1286 A1287 C1292 U1293 A1294 G1295 C1296 C1297 C1298 U1299 G1300 A1303 A1304 U1305 G1306 G1307 A1308 U1309 G1310 G1311 C1312 G1313 C1314 U1315 C1316 A1317 C1320 U1324 U1329 A1330 U1331 A1332 C1333 U1334 C1335 U1336 G1340 U1341 C1342 A1343 G1344 G1345 G1346
U1347 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1358 C1359 G1362 G1365 A1366 G1367 U1368 A1369 G1370 C1371 C1372 A1373 G1374 G1375 C1376 G1377 U1378 C1379 G1380 A1381 G1382 A1386 G1389 A1390 C1391 G1392 A1393 A1394 G1395 C1396 C1397 U1398 A1399 G1400 A1401 C1402 U1405 A1406 A1407 G1408 G1409 G1412 G1413
G1414 U1415 C1416 G1417 A1418 A1419 C1420 G1421 A1428 G1429 A1433 G1434 A1435 U1436 C1437 G1440 G1441 U1445 A1446 G1447 U1448 A1449 G1450 C1451 A1452 A1453 A1454 U1455 C1459 G1466 A1467 A1468 U1472 G1473 A1474 A1475 G1476 G1480 A1481 A1482 G1483 U1484 G1487 G1488 A1489 G1492 U1495 C1496
G1500 U1501 C1502 A1503 A1506 G1507 C1508 A1509 G1510 A1515 C1516 G1520 G1525 U1526 C1527 G1528 A1529 U1530 U1533 A1546 G1547 C1551 U1554 U1555 C1556 A1557 G1560 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 A1575 G1576 A1580 C1581 C1582 A1583 U1584 C1585 G1586 A1587
A1588 A1589 G1592 G1599 G1604 U1607 U1616 U1620 U1629 C1639 A1642 A1643 C1644 U1645 G1655 A1656 C1657 G1658 U1659 C1660 G1661 G1662 C1663 C1670 A1683 U1684 C1685 G1712 U1716 U1717 U1724 C1725 G1735 G1736 A1741 U1742 C1745 A1750 G1751 A1760
C1761 C1762 U1765 G1766 C1767 G1770 G1780 C1781 U1782 U1783 G1790 C1791 C1792 C1793 G1794 U1795 G1796 A1797 C1802 G1807 A1810 G1811 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820 C1821 C1822 U1834 A1835 C1836 U1837 G1838 A1839 U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 A1858
C1866 A1867 C1870 U1871 G1878 A1879 U1880 A1886 U1890 A1891 G1892 A1893 A1896 A1901 G1902 U1903 C1904 G1905 G1906 A1909 U1920 C1923 C1926 G1948 G1949 U1950 C1951 G1952 G1953 G1954 U1955 A G U G A G G G C C U U G G U C A G
A C G C A G C G G G C G U G C U U G U G G A C U G C U U G G U G G G C U U G C U C U G C U A G G C G G A C U A C U U G
C G U G C C U U G U U G U A G A C G G C C U U G G U A G G U C U C U U G U A G A C C G U C G C U U G C U A C A A U U A A2093
C2094 C2101 U2102 A2106 A2107 G2111 U2112 A2113 C2114 G2115 G2116 A2120 G2121 G2122 G2123 A2126 U2129 G2130 A2131 C2132 U2133 G2134 A2138 A2139 U2140 U2141 A2142 A2143 A2144 A2147 U2148 A2152 A2158 U2159 C2163 A2164 G2165 G2169 U2170 U2173 U2176 G2177 C2181 G2187
A2188 U2189 U2190 U2191 C2192 U2193 G2194 A2198 G2199 U2200 G2201 C2202 U2205 G2206 A2207 A2208 U2209 G2210 U2211 C2212 A2215 G2216 A2222 A2223 C2227 A2228 C2237 G2238 G2239 G2240 U2241 A2242 A2243 A2244 C2245 G2246 G2247 C2248 G2249 G2250 A2255 A2256 C2257 G2272 G2273 C2278 A2279 A2280 A2281 U2282 G2283
C2284 C2285 U2286 C2287 G2288 U2292 C2293 U2294 A2295 A2296 U2297 U2298 A2299 G2300 U2301 G2302 A2303 C2304 G2305 C2306 G2307 C2308 A2309 U2310 G2311 A2312 A2313 U2314 G2315 U2319 C2322 G2323 A2326 C2329 C2330 C2333 U2334 G2335 U2336 C2339 C2343 U2344 A2345 U2349 C2350 U2351 C2354 G2355 A2356 A2357



• Molecule 36: 25S ribosomal RNA

Chain 5:



A201 A204 C205 A209 U210 A211 G212 A213 G214 G215 G216 U217 G218 A219 G220 A221 A222 U223 C224 U230 G231 G234 A235 G236 G237 A238 G239 U240 G244 U245 U246 C247 U248 U249 U250 G251 U252 A253 A254 C259 G264 G267 A268 G269 U278 U279 U280 G281 G282 G283 A284
A285 U286 A289 C293 U294 A295 A296 G297 G300 A308 A313 A323 U326 U329 G335 A338 C339 C340 G341 A342 U343 A344 G345 A348 A349 C350 A351 A352 G353 C356 A357 G358 U359 G360 A361 U362 G363 A367 G368 A369 U370 G376 A389 U393
G394 A395 A396 A397 A398 A399 G400 U401 A402 C403 G404 U405 G406 A407 U410 U411 G412 U413 U414 G415 A416 A417 A418 G419 G420 G421 A422 A423 G424 G425 G426 C427 A428 U429 U430 U431 G432 A433 A436 G437 A438 C439 A440 U441 G442 G443 U G U U U U G G U G C C C
U C U G C U C C U U G G U G G U A G G G G A A U C U U C C A C491 U492 G495 C496 C497 C500 A501 U502 C503 A504 G505 U506 U509 G513 G514 C515 A516 A519 U520 A521
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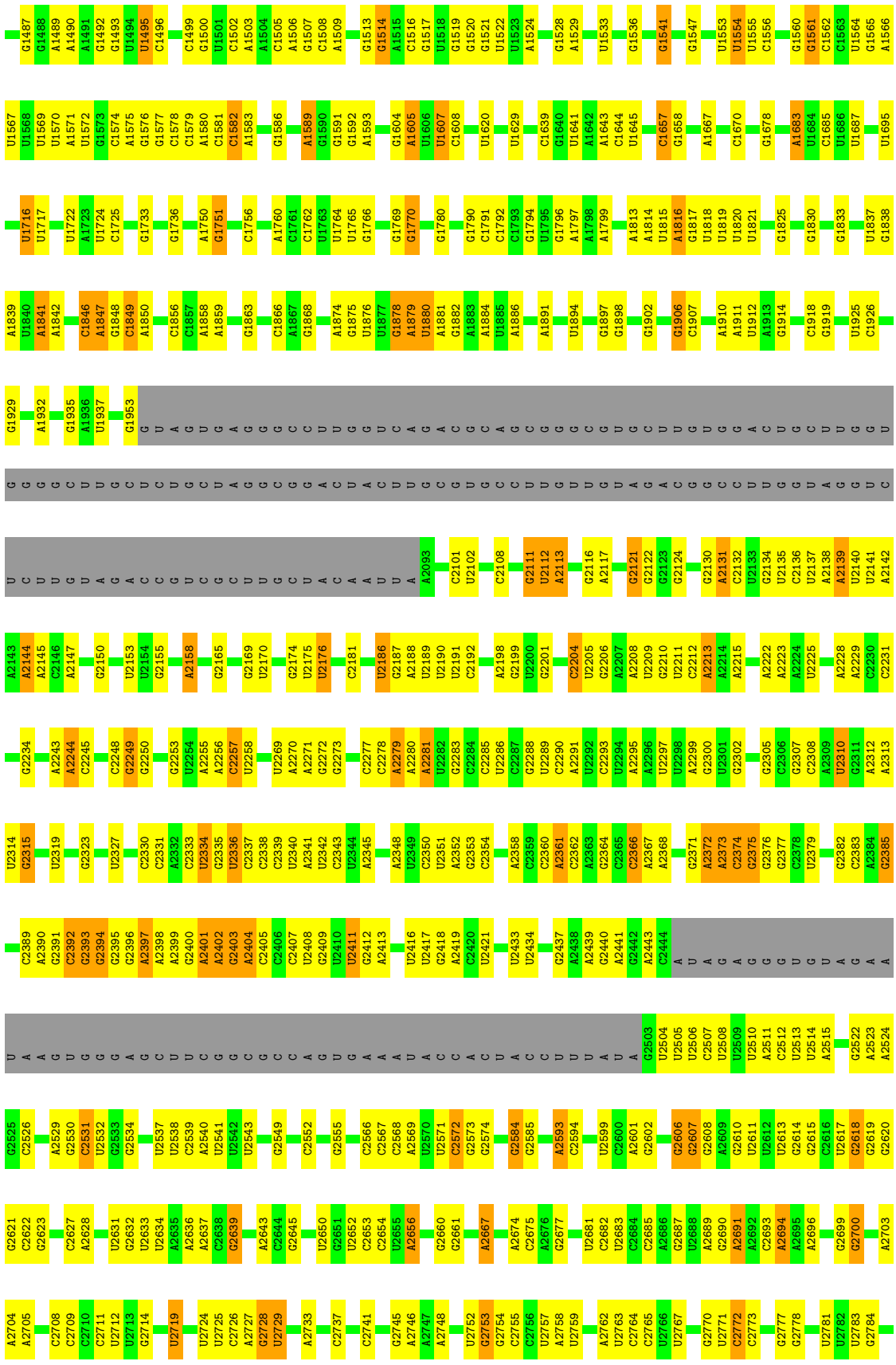
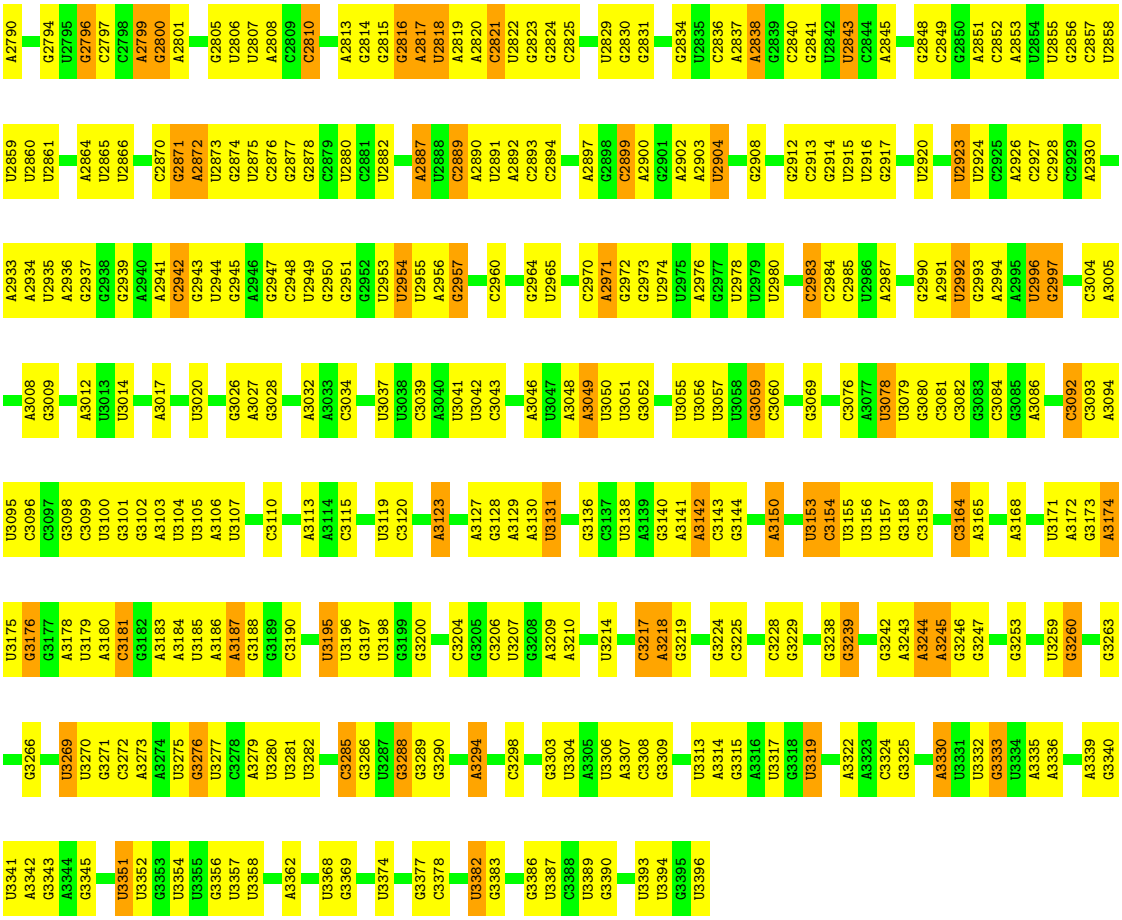
U704 A705 G708 A709 G712 U713 G714 A715 A716 C717 G718 U719 A720 G721 G725 G726 G727 A735 A736 C749 G750 A751 C758 C765 U766 U767 C768 G769 G770 A775 U776 U777 U778 G779 A780 G781 G785 A786 G787 C788 A789 U790 C793 U794 G795 U796 G799
C802 C803 C804 G805 A806 G809 A810 U811 A816 A817 G822 C823 C824 U825 G826 A830 G831 G832 G833 U834 G835 G838 C839 C840 A846 A847 A848 C851 G859 G860 C861 G864 U865 A866 G867 C868 G869 G870 U871 U872 C873 U874 C877 G878 U879 G880 C881 A882 A883 A884
G887 A888 U889 C890 G891 U892 C893 G894 A895 A896 U897 G901 G907 G908 G909 G910 C911 G912 A913 A914 A915 G916 A917 A921 U922 C923 G924 A925 A926 C927 U930 C931 U932 A933 G934 U935 A936 G937 C938 U939 G940 G941 U942 U943 C944 C945 U946 G947 C948 C949 G950 A951 A952 G953 U954
C958 C959 U960 C961 A962 G963 G964 A965 U966 C969 A970 G971 G974 C975 U979 A980 U981 C982 A983 A984 G993 G994 G999 C1000 G1001 A1002 A1003 U1004 G1005 A1006 U1007 U1008 A1009 G1010 U1014 U1015 C1016 C1017 G1018 G1019 G1020 G1021 G1024 A1025 A1026 A1027 U1028 G1029 G1035 U1041
U1044 A1047 A1048 C1049 U1052 A1053 A1054 U1060 A1064 A1065 G1066 G1072 A1075 U1081 U1082 A1085 A1093 U1094 U1095 U1096 G1097 A1098 A1099 U1100 G1101 A1102 A1103 G1104 U1108 U1109 U1110 U1111 A1112 G1113 U1114 G1115 G1116 G1117 C1118 C1119 A1120 U1121 U1124 U1125 G1126 G1127 U1128 A1129
A1130 G1131 C1132 A1133 G1134 A1135 U1138 A1143 G1147 G1148 G1149 A1150 U1151 G1152 A1153 A1154 C1155 C1156 G1157 A1158 A1159 C1160 G1161 U1162 G1166 U1167 U1168 A1169 A1170 G1171 C1175 C1176 A1180 U1181 A1182 C1183 A1184 C1187 U1188 C1189 A1190 U1191 C1192 A1193 G1194 A1197 C1198 C1199 A1200 C1201 A1202 A1203
A1204 A1205 U1208 G1209 A1212 G1213 G1222 G1226 C1232 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 A1252 U1253 C1254 U1258 G1262 A1263 G1264 U1265 G1266 G1295 C1296 C1297 C1298 U1299 G1300 A1301 A1302 A1303 A1304 U1305 G1306 G1307 A1308 U1309 G1310 G1311 C1312 G1313 C1314 U1315
C1316 A1317 A1318 G1319 C1320 G1321 U1322 G1323 U1329 A1330 U1331 A1332 C1335 U1336 A1337 C1338 C1339 G1340 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1358 C1359 G1362 A1363 C1364 G1365 A1366 A1369 G1370 G1371 C1372 A1373 G1374 G1375 C1376 G1380 C1385 A1386 G1387 A1390 C1391 G1392 A1393 A1394 G1395
U1398 A1399 G1400 A1406 A1407 U1410 C1411 G1412 C1416 A1419 G1422 C1423 C1424 G1429 U1430 G1431 C1432 A1433 G1434 A1435 U1436 C1437 G1440 U1445 A1446 G1447 U1448 A1449 G1450 C1451 A1452 U1455 A1456 A1460 A1461 G1464 A1465 A1468 G1473 G1476 G1480 A1481 A1482 G1483



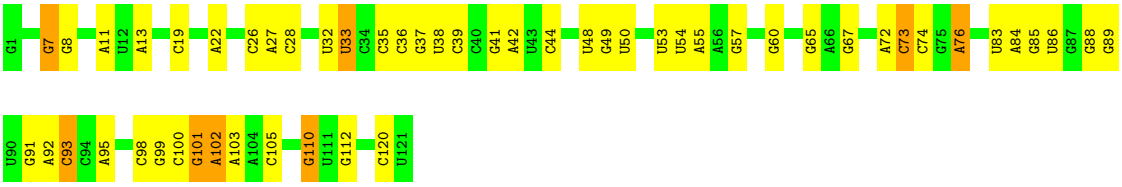


- Molecule 37: 5S ribosomal RNA

Chain 3:

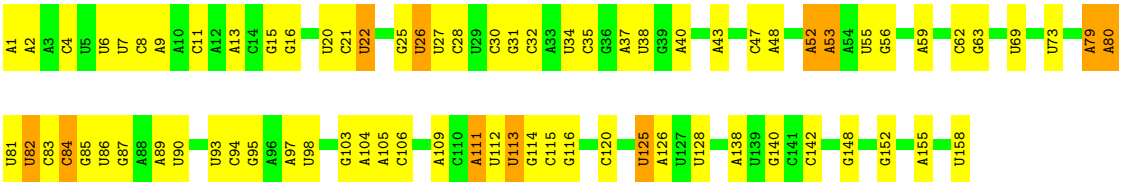
- Molecule 37: 5S ribosomal RNA

Chain 7:



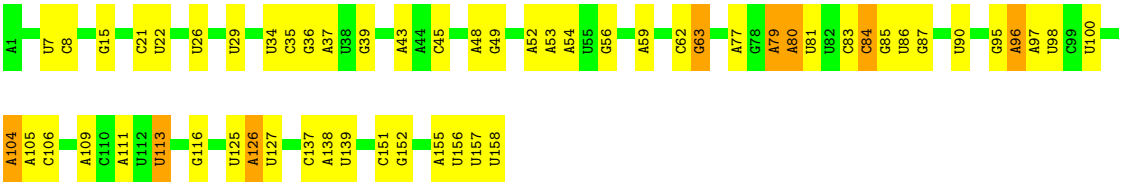
- Molecule 38: 5.8S ribosomal RNA

Chain 4:



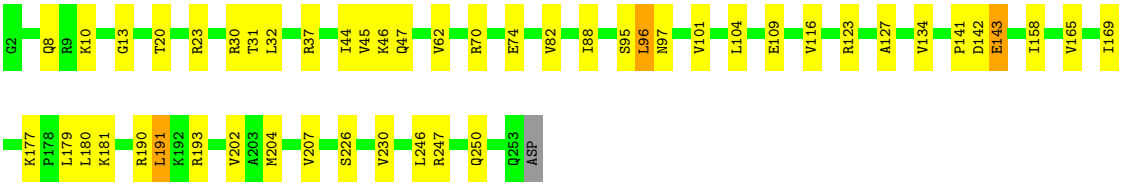
- Molecule 38: 5.8S ribosomal RNA

Chain 8:



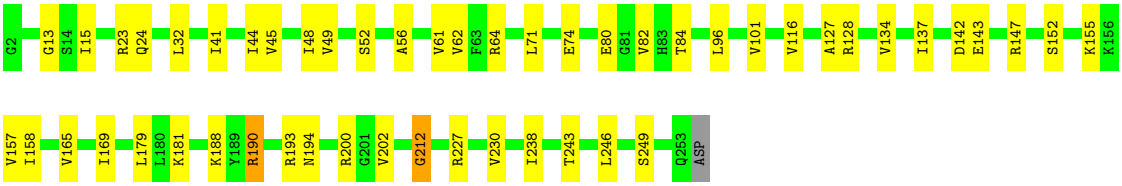
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



- Molecule 39: 60S ribosomal protein L2-A

Chain l2:

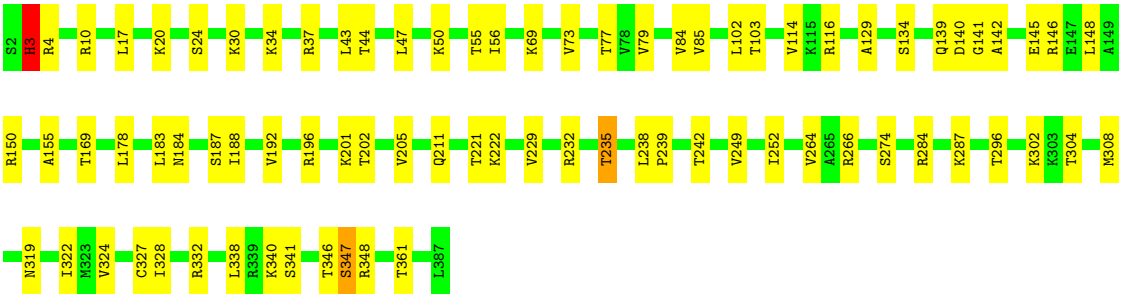


- Molecule 40: 60S ribosomal protein L3

Chain L3:

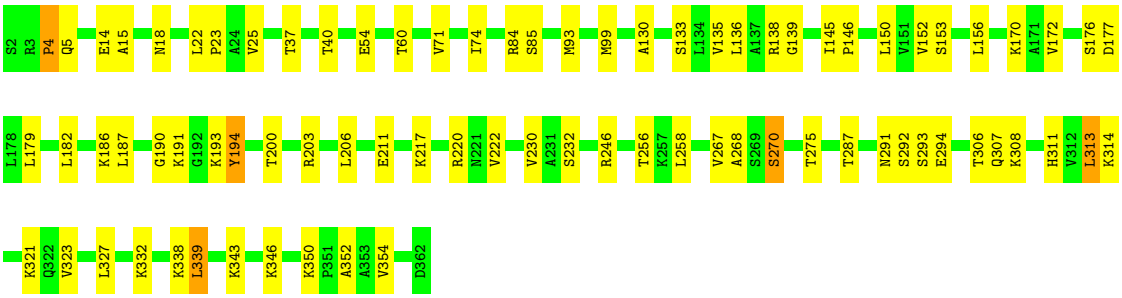
- Molecule 40: 60S ribosomal protein L3

Chain l3: 79% 20%



- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 78% 21%

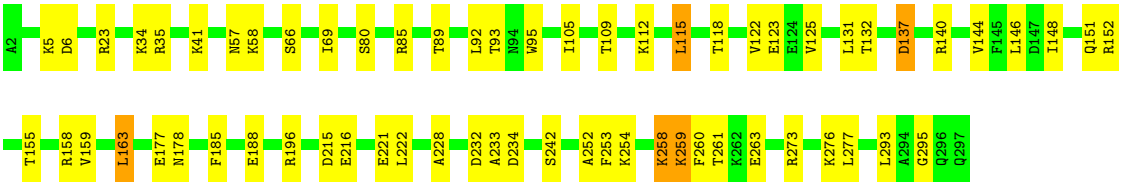


- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 78% 20%

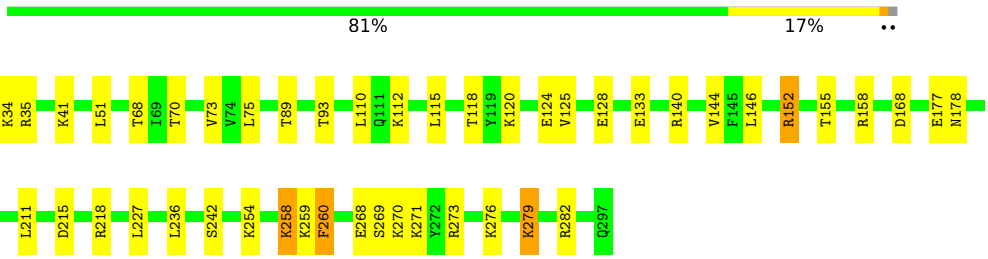
- Molecule 42: 60S ribosomal protein L5

Chain L5: 78% 20%



- Molecule 42: 60S ribosomal protein L5

Chain l5:

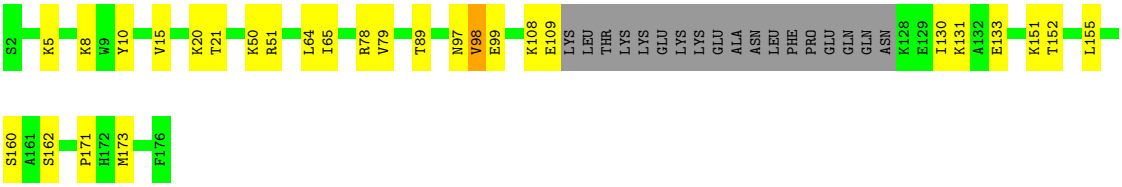


- Molecule 43: 60S ribosomal protein L6-A

Chain L6:

- Molecule 43: 60S ribosomal protein L6-A

Chain l6:

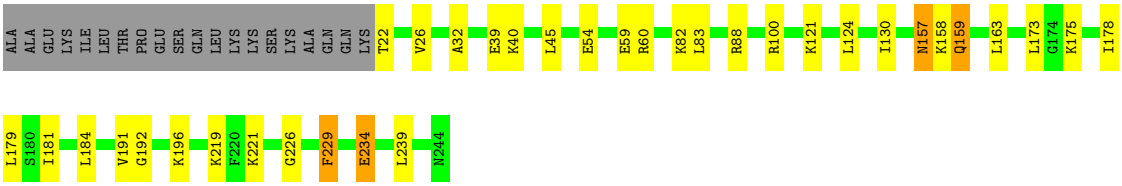


- Molecule 44: 60S ribosomal protein L7-A

Chain L7:

- Molecule 44: 60S ribosomal protein L7-A

Chain l7:



• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 74% 17% 9%

ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 L26 T27 T30 P31 I36 G37 G38 A39 V40 Q41 S47 K63 T74 Q79 Y80 T81 R84 E89 K92 N95 T101 K106 T110

V132 L136 N145 K149 L150 D156 V157 I160 L169 K172 R185 L189 V190 T194 V203 E206 D207 E208 L214 L238 K241 M246 D247 K248 D254 S255 A256

• Molecule 45: 60S ribosomal protein L8-A

Chain l8: 72% 17% • 9%

ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 L26 F34 A39 V40 Q41 L65 R68 L69 K70 V71 T74 Q79 Y80 T81 T90 N95 R98 L109 E112 A117 E118 G119 K120 S121

K122 K133 L136 K149 L150 I153 I160 V164 L169 K183 A184 R185 T188 N191 A196 V203 E208 K213 L214 T217 K230 I237 L238 G239 N240 K241 K245 K248 D254 SER ALA

• Molecule 46: 60S ribosomal protein L9-A

Chain L9: 77% 23% •

M1 K2 Y3 I4 Q5 T6 V12 V16 T17 V18 S19 I24 T33 L34 I41 V48 N49 N50 Q51 L52 R62 A66 A67 L68 R69 T70 T80 G81 V82 H96 D107 G108 A109 D120 I123 R124 T133 T134 E135 T138 N139 V151 E152

N157 L161 Q162 Q163 I164 C165 R166 I172 E189 D190 L191

• Molecule 46: 60S ribosomal protein L9-A

Chain l9: 81% 18% •

M1 K2 Q5 T6 V18 S22 T33 K39 V43 T44 L52 V55 R62 L68 R69 T70 V82 R91 Y92 E105 K106 D107 R129 V132 T133 T138 E143 I144 V151 N157 L161 Q162 R166 V167 L176 I179

L191

• Molecule 47: 60S ribosomal protein L10

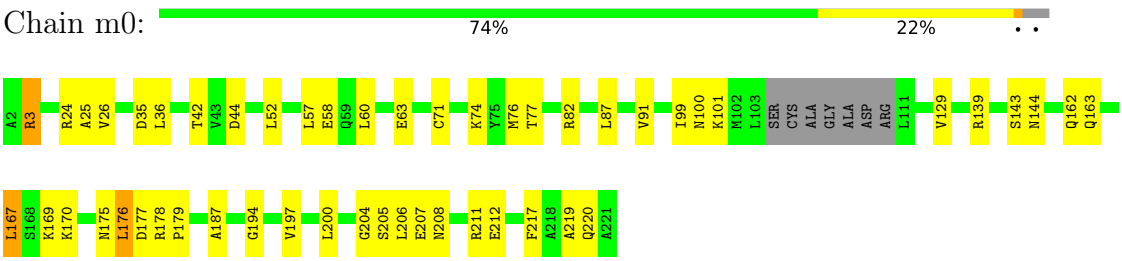
Chain M0: 76% 18% • •

A2 R3 R21 R24 K30 I31 R32 I33 L36 K39 K40 A41 T42 L48 L52 L57 E63 L87 V91 I99 M102 LEU SER CYS ALA GLY ALA ASP ARG LEU Q112 G117 V129 R139 T140 K141 D142 L152 Q162 Q163 K164 I165

I166 L167 S168 K169 T174 N175 L176 D177 K184 R185 E189 G194 L200 K203 E207 R211 A218 A219 Q220 A221

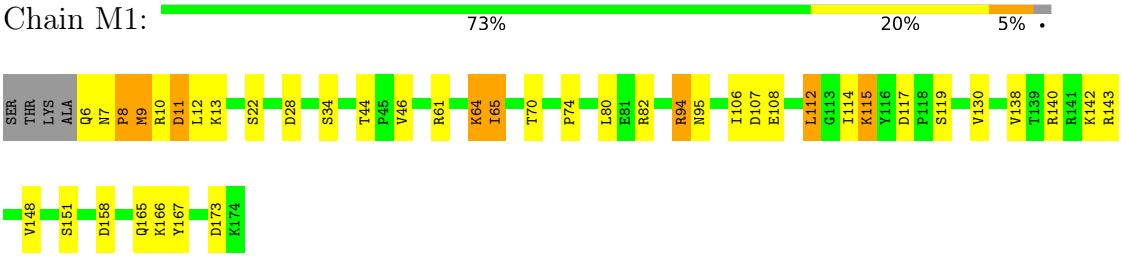
- Molecule 47: 60S ribosomal protein L10

Chain m0:



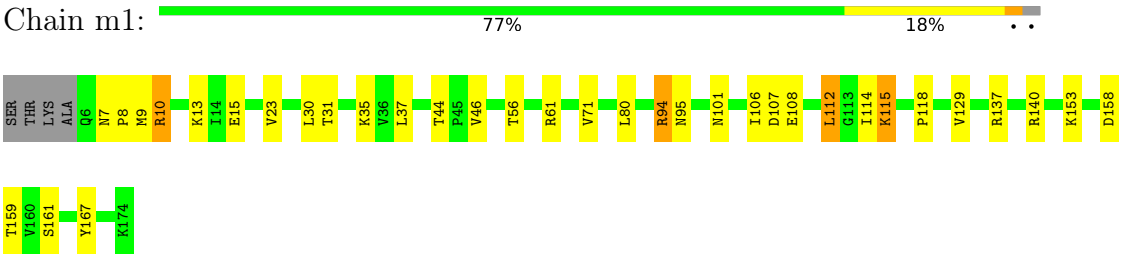
- Molecule 48: 60S ribosomal protein L11-B

Chain M1:



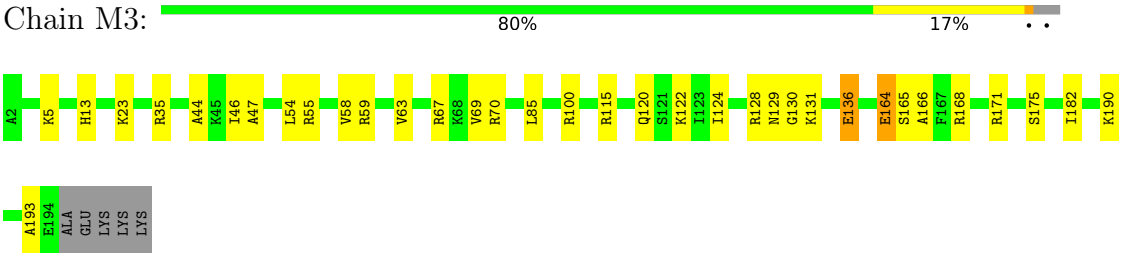
- Molecule 48: 60S ribosomal protein L11-B

Chain m1:



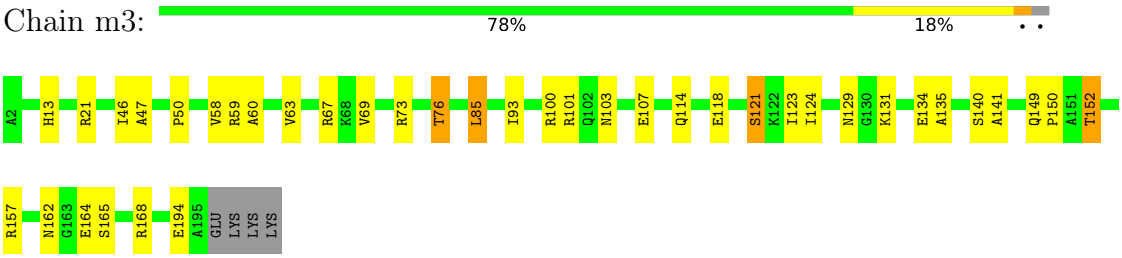
- Molecule 49: 60S ribosomal protein L13-A

Chain M3:



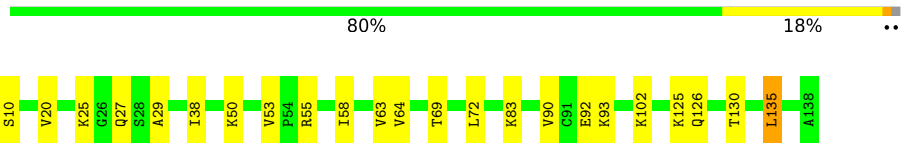
- Molecule 49: 60S ribosomal protein L13-A

Chain m3:



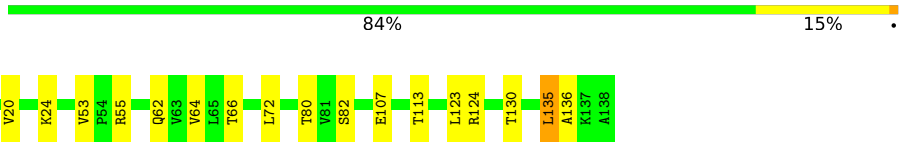
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



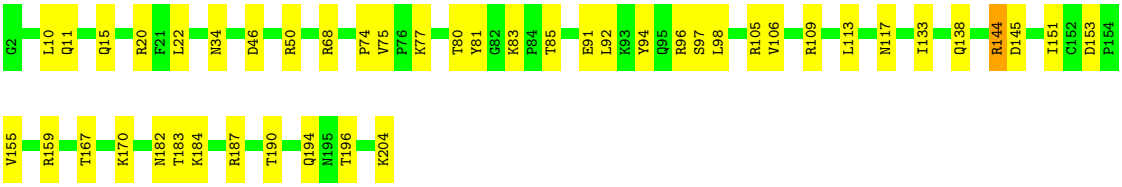
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

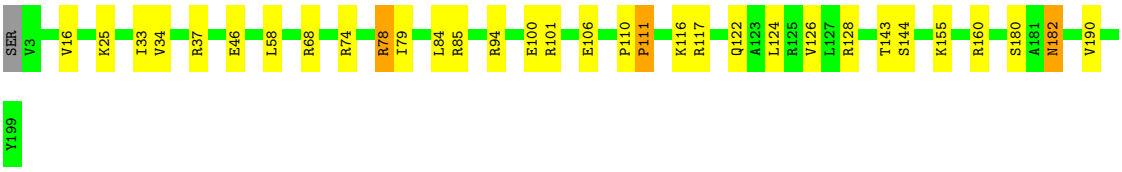


• Molecule 51: 60S ribosomal protein L15-A

Chain m5:

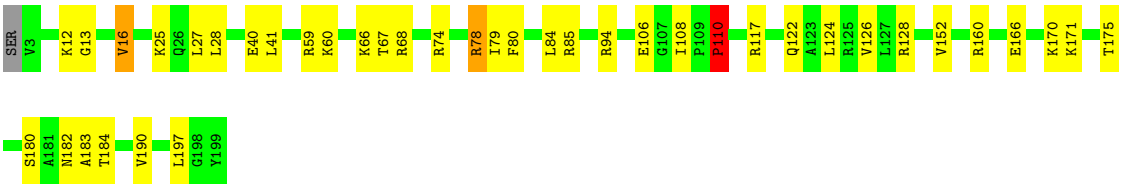
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



• Molecule 53: 60S ribosomal protein L17-A

Chain M7: 79% 20%

A2 S8 T9 G19 R23 V24 T29 T32 A33 Q34 A35 I36 L41 V51 L52 D53 S65 S66 I67 G68 R69 E75 V78 T79 L107 L112 Q118 V119 P123 R126 R127 I136 N137 K138 S142 P143 S144 V157 A160 A161 E162 K163 K164 L168 R171 K180 R181 A184

• Molecule 53: 60S ribosomal protein L17-A

Chain m7: 72% 13% 15%

A2 T9 V24 T29 T32 L41 L52 R56 S66 E75 T79 K80 K86 L94 L107 V114 Q118 V119 N120 R126 R127 I136 N137 K138 S144 E155 A156 VAL ALA LYS ALA ALA GLU LYS LYS VAL VAL ARG LEU THR SER ARG GLN ARG GLY ARG ILE ALA ALA GLN LYS ARG ILE ALA ALA

• Molecule 54: 60S ribosomal protein L18-A

Chain M8: 85% 14%

G2 I3 D4 T17 V24 Y25 L26 L32 Y33 T34 D41 K46 L49 I57 V64 Q73 E95 T99 R111 A112 K113 E120 Q135 L138 R141 V150 A162 P163 R164 R170 R178 R179 R180 V186

• Molecule 54: 60S ribosomal protein L18-A

Chain m8: 79% 19%

G2 I3 S7 R12 T17 K20 L26 K31 L32 Y33 T34 D41 L49 I57 S63 V64 S65 R66 R69 T80 T86 A91 R92 I93 K98 T99 T100 A112 K113 L127 Q135 L138 R147 V150 R151 K159 G160 K161 I165 R170 R176 G177 R178 R179 R180 V186

• Molecule 55: 60S ribosomal protein L19-A

Chain M9: 88% 12%

A2 T29 L44 V45 K46 V51 K52 K53 A54 V55 R71 R74 S91 R98 L99 R103 R104 L105 L106 I115 D116 K135 L138 K146 L164 R173 D182 A189

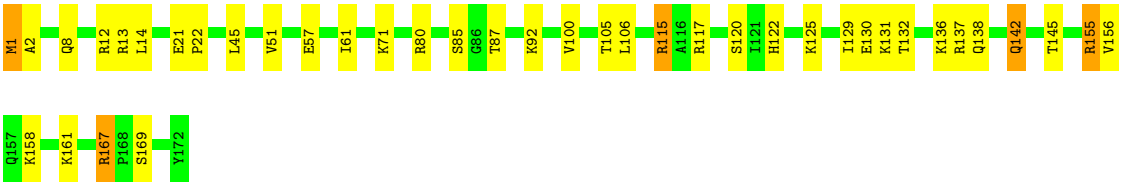
• Molecule 55: 60S ribosomal protein L19-A

Chain m9: 82% 16%

A2 Q7 K8 R9 L10 V17 R20 T29 S30 N36 K43 T49 K52 V55 T56 T63 R71 R74 H75 S76 R88 S91 L99 D116 K117 E126 L138 E152 K153 R162 R163 L164 R167 R170 R173 K180

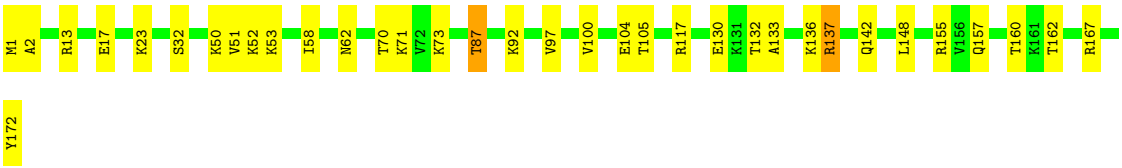
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

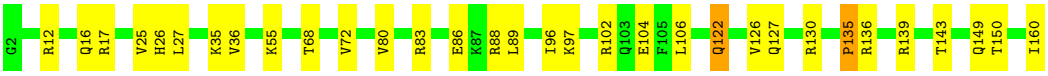


• Molecule 57: 60S ribosomal protein L21-A

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:

ALA PRO ASN THR SER ARG LYS GLN LYS I11 T16 T23 V27 L37 V43 N49 L50 G51 N52 A53 V54 T55 V63 T68 Y75 R90 D91 V96 T100 Y108 GLN VAL THR PRO GLU GLU ASP GLU GLU GLU GLU ASP GLU GLU

• Molecule 59: 60S ribosomal protein L23-A

Chain N3: 86% 14%

S2 I13 R32 R48 K63 L69 R70 K71 K72 V73 M74 V79 A82 K83 I102 M109 K110 T115 K120 L125 V135 V136 V137

• Molecule 59: 60S ribosomal protein L23-A

Chain n3: 91% 8% •

S2 Q7 I13 S14 L17 G41 S42 R45 R70 V73 R88 T115 V135 V136 V137

• Molecule 60: 60S ribosomal protein L24-A

Chain N4: 54% 9% • 37%

M1 E4 I5 R17 L39 R47 L54 T64 K69 V76 R80 P81 I82 S86 L89 K97 P98 GLU VAL ARG LYS ALA ASN ARG GLU GLU LYS LEU LYS ALA ASN LYS GLU LYS LYS LYS ALA GLU LYS ALA ALA ARG LYS ALA GLU LYS ALA LYS

SER ALA GLY THR GLN SER SER LYS PHE SER LYS GLN GLN ALA LYS GLY ALA PHE GLN LYS VAL ALA ALA THR SER ARG

• Molecule 60: 60S ribosomal protein L24-A

Chain n4: 71% 15% • 13%

M1 I5 T19 D25 S26 L39 R43 L54 K57 I63 R71 K74 T75 V76 K77 T83 L89 L96 K97 R105 E106 E107 E126 K127 G132 T133 Q134 S135 SER LYS PHE SER LYS GLN GLN ALA LYS GLY ALA PHE GLN LYS VAL ALA

ALA THR SER ARG

• Molecule 61: 60S ribosomal protein L25

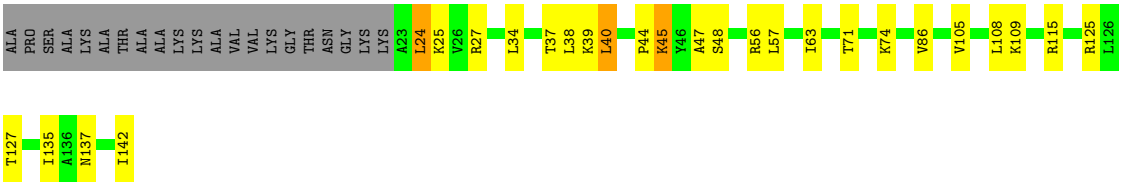
Chain N5: 70% 15% • 14%

ALA PRO SER ALA LYS ALA THR ALA ALA LYS LYS ALA VAL VAL LYS GLY THR ASN GLY LYS K22 R27 L34 T37 L38 K39 L40 P44 I63 T71 V86 K92 L108 R115 K120 R125 L126 T127 A128 D129 L133 D134 I135 R138 I139

I142

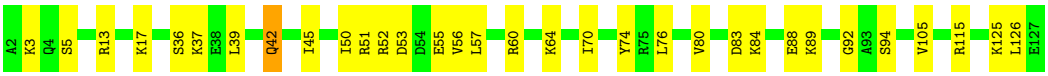
• Molecule 61: 60S ribosomal protein L25

Chain n5: 66% 17% • 15%



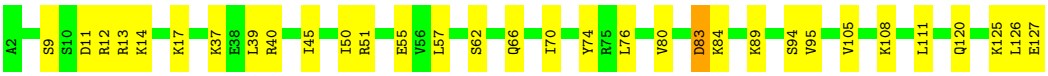
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



- Molecule 62: 60S ribosomal protein L26-A

Chain n6:

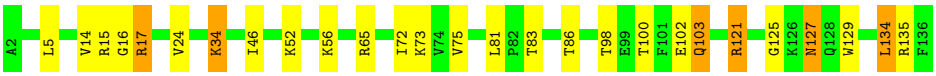


- Molecule 63: 60S ribosomal protein L27-A

Chain N7:

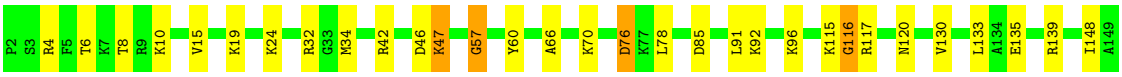
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



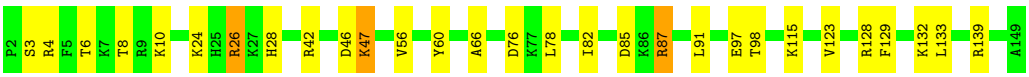
- Molecule 64: 60S ribosomal protein L28

Chain N8:



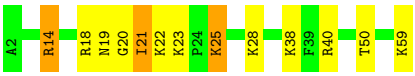
- Molecule 64: 60S ribosomal protein L28

Chain n8:



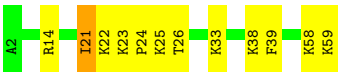
- Molecule 65: 60S ribosomal protein L29

Chain N9:



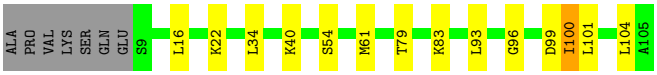
• Molecule 65: 60S ribosomal protein L29

Chain n9:



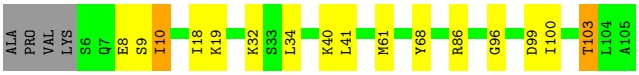
• Molecule 66: 60S ribosomal protein L30

Chain O0:



• Molecule 66: 60S ribosomal protein L30

Chain o0:

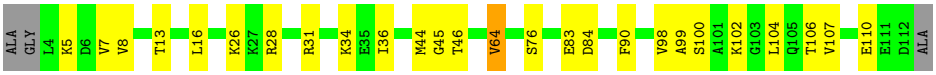


• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

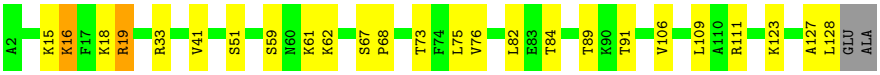
• Molecule 67: 60S ribosomal protein L31-A

Chain o1:



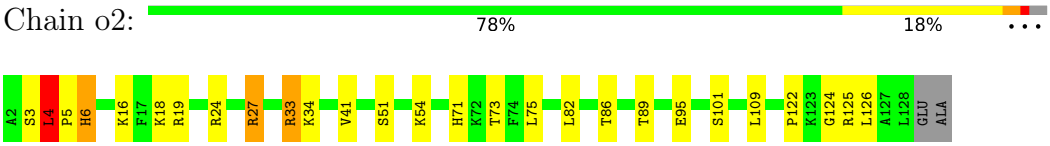
• Molecule 68: 60S ribosomal protein L32

Chain O2:



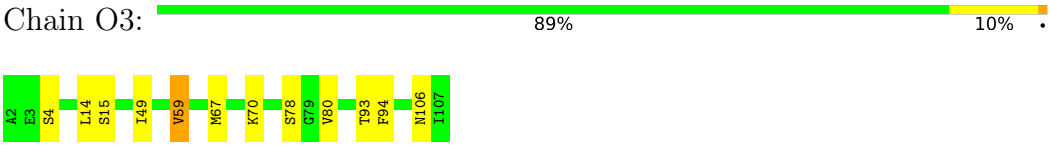
• Molecule 68: 60S ribosomal protein L32

Chain o2:



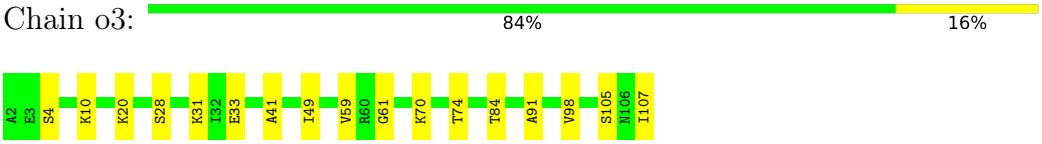
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



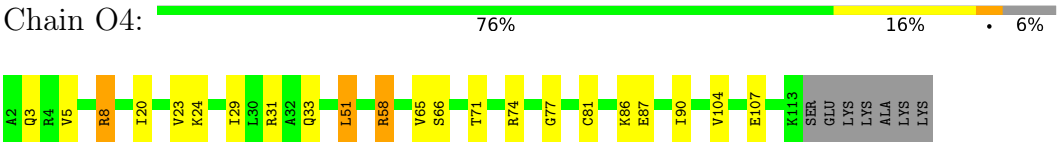
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



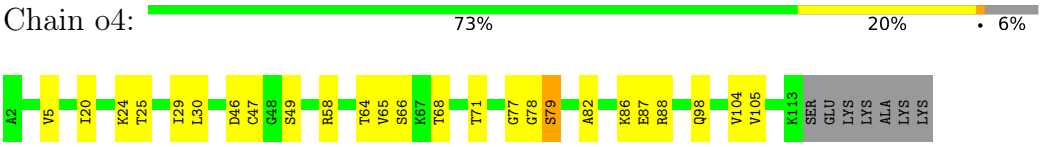
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



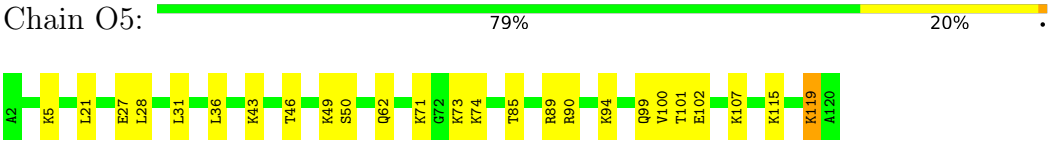
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



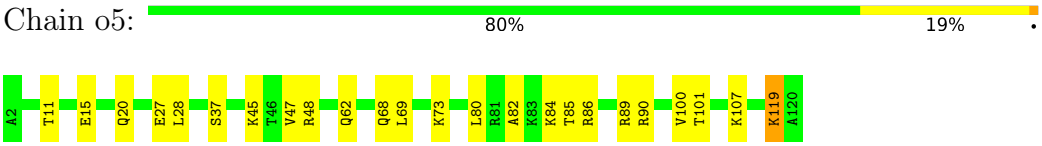
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



- Molecule 71: 60S ribosomal protein L35-A

Chain o5:

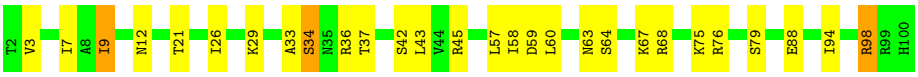


- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 81% 17%

• Molecule 72: 60S ribosomal protein L36-A

Chain o6: 72% 25%

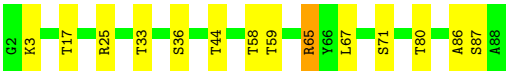


• Molecule 73: 60S ribosomal protein L37-A

Chain O7: 84% 15%

• Molecule 73: 60S ribosomal protein L37-A

Chain o7: 84% 15%



• Molecule 74: 60S ribosomal protein L38

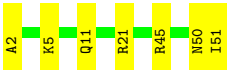
Chain O8: 77% 23%

• Molecule 74: 60S ribosomal protein L38

Chain o8: 78% 21%

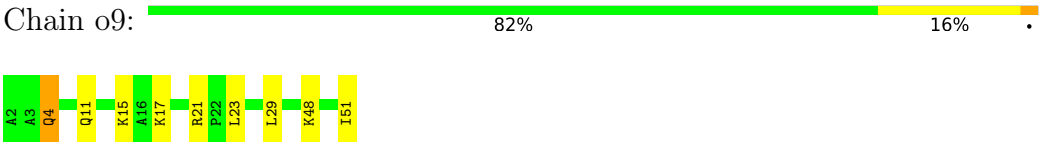
• Molecule 75: 60S ribosomal protein L39

Chain O9: 86% 14%



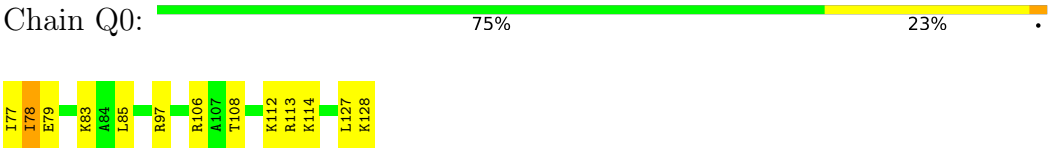
• Molecule 75: 60S ribosomal protein L39

Chain o9:



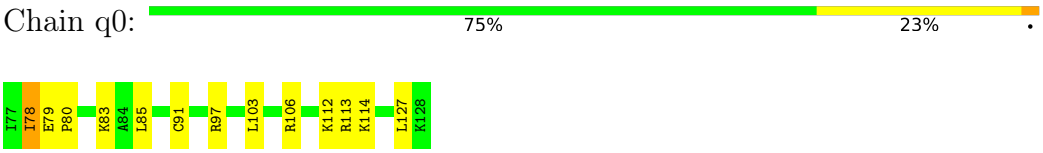
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



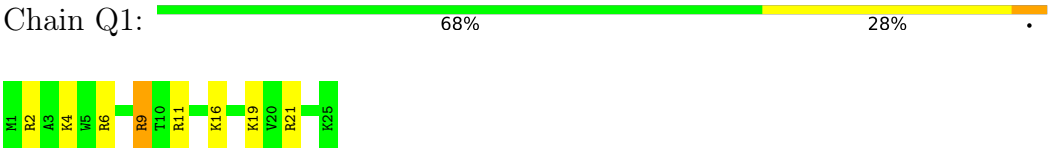
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



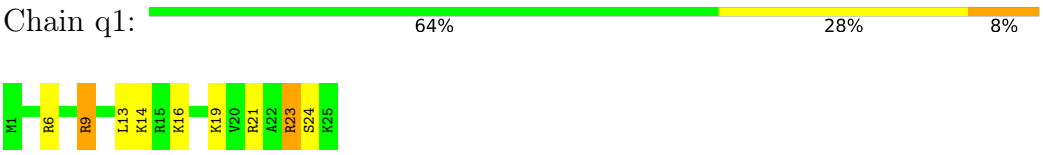
• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



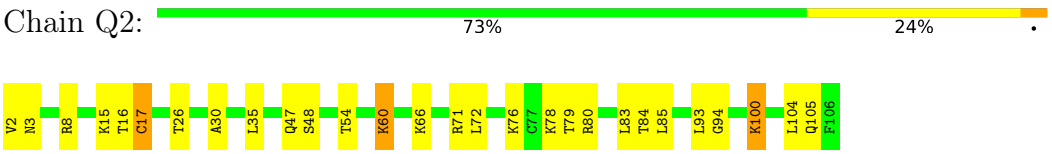
• Molecule 77: 60S ribosomal protein L41-A

Chain q1:



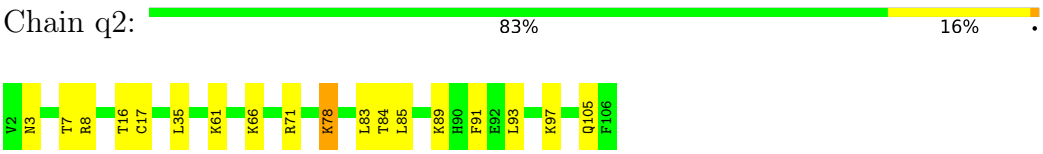
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



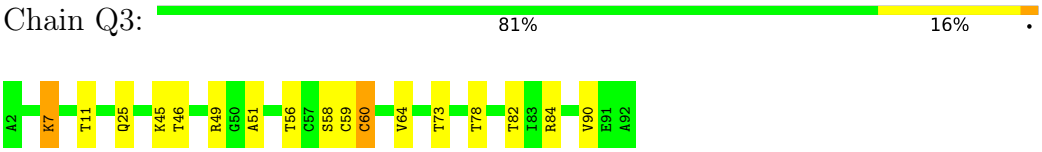
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



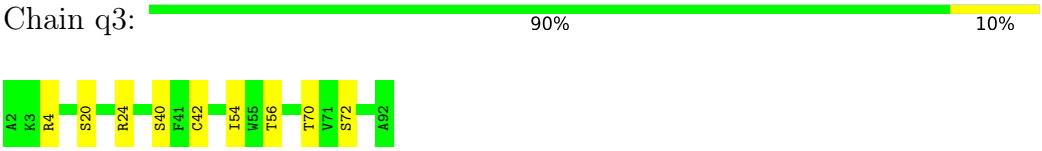
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



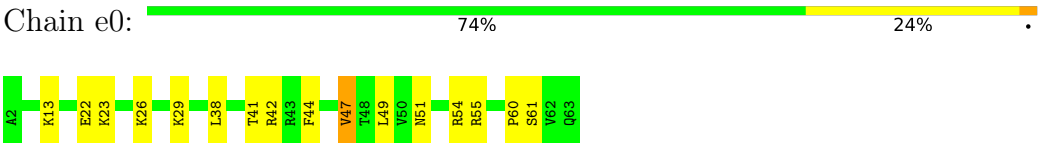
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



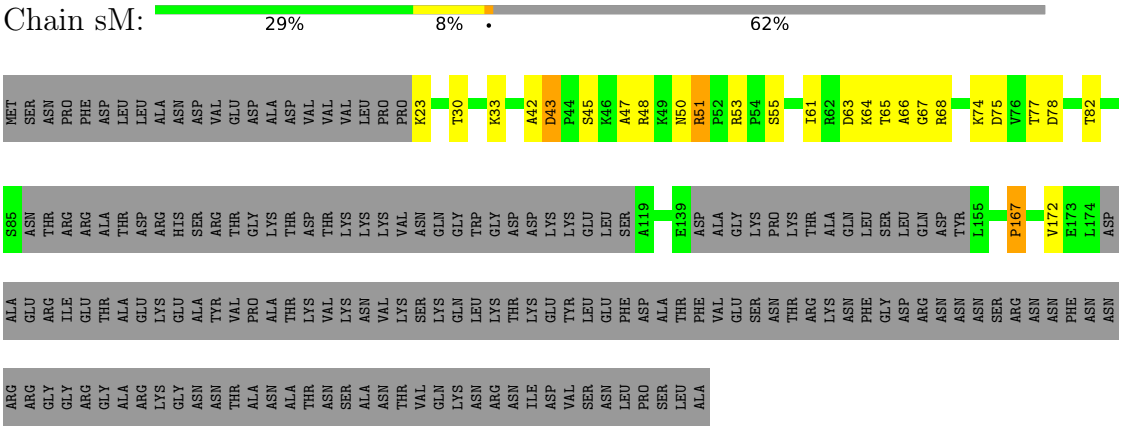
• Molecule 80: 40S ribosomal protein S30-A

Chain e0:



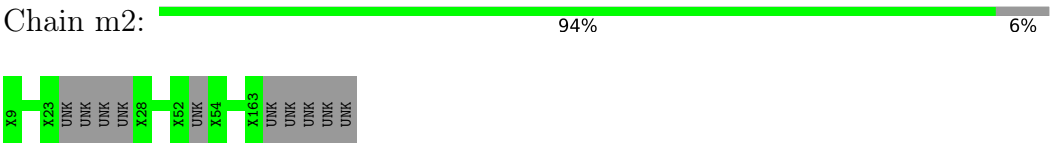
• Molecule 81: Suppressor protein STM1

Chain sM:



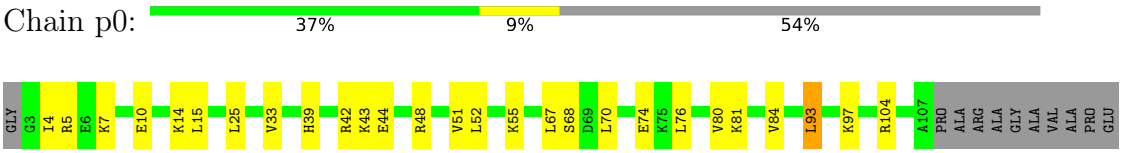
• Molecule 82: unknown protein chain m2

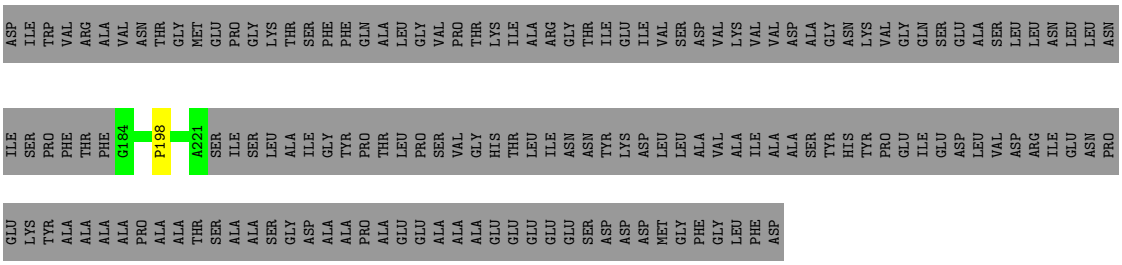
Chain m2:



• Molecule 83: 60S acidic ribosomal protein P0

Chain p0:





• Molecule 84: unknown protein chain p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

• Molecule 85: unknown protein chain p2

Chain p2: 100%

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	435.26Å 287.54Å 304.02Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	73.99 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (73.99-3.00)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.211 , 0.259	Depositor
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.199	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411211	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3KD, OHX, 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	0.71	1/41698 (0.0%)	1.27	275/64972 (0.4%)
1	6	0.88	13/42765 (0.0%)	1.38	436/66634 (0.7%)
2	S0	0.43	0/1617	0.66	0/2215
2	s0	0.49	0/1623	0.71	0/2222
3	S1	0.35	0/1735	0.63	1/2335 (0.0%)
3	s1	0.48	0/1748	0.66	0/2352
4	S2	0.49	0/1665	0.67	0/2263
4	s2	0.57	0/1665	0.75	2/2263 (0.1%)
5	S3	0.48	0/1759	0.66	1/2368 (0.0%)
5	s3	0.42	0/1759	0.60	0/2368
6	S4	0.46	0/2109	0.73	1/2839 (0.0%)
6	s4	0.55	0/2109	0.78	1/2839 (0.0%)
7	S5	0.36	0/1629	0.58	0/2202
7	s5	0.44	0/1629	0.64	0/2202
8	S6	0.44	0/1823	0.64	0/2439
8	s6	0.54	0/1779	0.70	0/2379
9	S7	0.42	0/1506	0.65	0/2028
9	s7	0.45	0/1516	0.67	1/2043 (0.0%)
10	S8	0.54	0/1514	0.72	1/2021 (0.0%)
10	s8	0.60	0/1514	0.76	1/2021 (0.0%)
11	S9	0.47	0/1519	0.64	0/2035
11	s9	0.55	0/1519	0.76	2/2035 (0.1%)
12	C0	0.42	0/790	0.70	1/1069 (0.1%)
12	c0	0.36	0/777	0.63	3/1049 (0.3%)
13	C1	0.55	0/1240	0.66	0/1675
13	c1	0.61	0/1194	0.77	0/1610
14	C2	0.38	0/900	0.62	0/1224
14	c2	0.28	0/900	0.56	0/1224
15	C3	0.47	0/1215	0.68	2/1638 (0.1%)
15	c3	0.56	0/1215	0.73	0/1638
16	C4	0.36	0/901	0.63	0/1217
16	c4	0.52	0/960	0.72	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.44	0/998	0.68	0/1341
17	c5	0.45	0/1060	0.66	0/1426
18	C6	0.41	0/1125	0.69	2/1510 (0.1%)
18	c6	0.49	0/1131	0.69	0/1518
19	C7	0.41	0/935	0.62	0/1254
19	c7	0.48	0/914	0.71	0/1224
20	C8	0.42	0/1211	0.63	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.41	0/1130	0.63	0/1517
21	c9	0.50	0/1130	0.70	2/1517 (0.1%)
22	D0	0.45	0/865	0.64	0/1169
22	d0	0.46	0/892	0.65	0/1205
23	D1	0.44	0/693	0.62	0/935
23	d1	0.54	0/693	0.71	0/935
24	D2	0.48	0/1038	0.73	3/1395 (0.2%)
24	d2	0.59	0/1038	0.74	1/1395 (0.1%)
25	D3	0.60	0/1139	0.77	1/1518 (0.1%)
25	d3	0.70	0/1139	0.89	3/1518 (0.2%)
26	D4	0.44	0/1087	0.63	0/1449
26	d4	0.53	0/1087	0.73	0/1449
27	D5	0.39	0/571	0.68	0/768
27	d5	0.41	0/566	0.63	0/761
28	D6	0.43	0/782	0.67	0/1047
28	d6	0.56	0/782	0.71	0/1047
29	D7	0.42	0/620	0.66	0/838
29	d7	0.46	0/620	0.66	0/838
30	D8	0.35	0/499	0.57	0/670
30	d8	0.44	0/499	0.64	0/670
31	D9	0.50	0/452	0.70	1/600 (0.2%)
31	d9	0.50	0/452	0.64	0/600
32	E0	0.46	0/483	0.63	0/643
33	E1	0.42	0/577	0.78	0/770
33	e1	0.39	0/619	0.72	0/822
34	SR	0.37	0/2494	0.57	0/3393
34	sR	0.38	0/2495	0.56	0/3395
35	SM	0.48	0/1113	0.70	2/1502 (0.1%)
36	1	1.16	153/75394 (0.2%)	1.66	1837/117545 (1.6%)
36	5	1.20	178/75414 (0.2%)	1.67	1863/117575 (1.6%)
37	3	0.95	2/2883 (0.1%)	1.47	39/4491 (0.9%)
37	7	1.16	5/2883 (0.2%)	1.62	57/4491 (1.3%)
38	4	1.13	5/3746 (0.1%)	1.66	86/5832 (1.5%)
38	8	0.98	2/3746 (0.1%)	1.48	42/5832 (0.7%)
39	L2	0.74	0/1948	0.84	3/2617 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	l2	0.71	0/1946	0.86	2/2614 (0.1%)
40	L3	0.74	1/3146 (0.0%)	0.82	1/4228 (0.0%)
40	l3	0.88	1/3146 (0.0%)	0.89	2/4228 (0.0%)
41	L4	0.84	1/2800 (0.0%)	0.94	7/3790 (0.2%)
41	l4	0.74	1/2800 (0.0%)	0.90	6/3790 (0.2%)
42	L5	0.57	0/2425	0.69	1/3271 (0.0%)
42	l5	0.73	0/2408	0.82	1/3248 (0.0%)
43	L6	0.76	0/1260	0.84	0/1694
43	l6	0.78	0/1269	0.84	1/1705 (0.1%)
44	L7	0.78	1/1821 (0.1%)	0.90	2/2451 (0.1%)
44	l7	0.85	1/1828 (0.1%)	0.90	4/2461 (0.2%)
45	L8	0.55	0/1836	0.70	1/2481 (0.0%)
45	l8	0.51	0/1795	0.65	1/2429 (0.0%)
46	L9	0.65	0/1539	0.77	1/2073 (0.0%)
46	l9	0.77	0/1539	0.85	0/2073
47	M0	0.71	0/1741	0.84	3/2335 (0.1%)
47	m0	0.75	0/1758	0.87	2/2358 (0.1%)
48	M1	0.54	0/1374	0.73	1/1842 (0.1%)
48	m1	0.65	0/1374	0.82	2/1842 (0.1%)
49	M3	0.75	0/1568	0.86	0/2106
49	m3	0.69	0/1573	0.85	3/2113 (0.1%)
50	M4	0.73	0/1068	0.80	1/1438 (0.1%)
50	m4	0.82	0/1074	0.85	0/1446
51	M5	0.77	0/1757	0.85	0/2354
51	m5	0.66	0/1757	0.79	0/2354
52	M6	0.86	1/1585 (0.1%)	0.92	3/2128 (0.1%)
52	m6	1.02	5/1585 (0.3%)	0.98	7/2128 (0.3%)
53	M7	0.80	0/1443	0.85	2/1944 (0.1%)
53	m7	0.89	0/1250	0.89	0/1683
54	M8	0.79	0/1465	0.92	3/1965 (0.2%)
54	m8	0.73	0/1465	0.95	2/1965 (0.1%)
55	M9	0.57	0/1538	0.69	0/2050
55	m9	0.61	0/1538	0.70	0/2050
56	N0	0.78	0/1481	0.87	4/1990 (0.2%)
56	n0	0.87	0/1481	0.91	2/1990 (0.1%)
57	N1	0.78	0/1300	0.82	0/1743
57	n1	0.85	1/1300 (0.1%)	0.86	1/1743 (0.1%)
58	N2	0.42	0/812	0.62	0/1099
58	n2	0.51	0/794	0.65	0/1076
59	N3	0.70	0/1018	0.81	0/1369
59	n3	0.87	0/1018	0.98	1/1369 (0.1%)
60	N4	0.56	0/712	0.68	0/958
60	n4	0.69	0/1052	0.75	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
61	N5	0.63	0/979	0.80	2/1321 (0.2%)
61	n5	0.65	0/974	0.77	0/1314
62	N6	0.68	0/1004	0.90	1/1341 (0.1%)
62	n6	0.71	1/1004 (0.1%)	0.84	0/1341
63	N7	0.52	0/1118	0.66	0/1497
63	n7	0.46	0/1118	0.63	0/1497
64	N8	0.82	0/1204	0.92	2/1612 (0.1%)
64	n8	0.79	0/1204	0.90	0/1612
65	N9	0.67	0/473	0.83	2/629 (0.3%)
65	n9	0.80	0/473	0.97	0/629
66	O0	0.48	0/751	0.66	0/1008
66	o0	0.49	0/775	0.65	0/1040
67	O1	0.60	0/890	0.72	0/1196
67	o1	0.76	0/897	0.86	0/1205
68	O2	0.85	0/1041	0.89	2/1394 (0.1%)
68	o2	0.82	0/1041	0.94	2/1394 (0.1%)
69	O3	0.95	0/868	0.91	1/1168 (0.1%)
69	o3	0.92	0/868	0.84	0/1168
70	O4	0.58	0/890	0.82	4/1189 (0.3%)
70	o4	0.59	0/890	0.78	0/1189
71	O5	0.70	0/978	0.81	1/1301 (0.1%)
71	o5	0.59	0/974	0.72	0/1297
72	O6	0.64	0/778	0.79	0/1034
72	o6	0.54	0/777	0.73	0/1033
73	O7	0.78	0/696	0.90	1/923 (0.1%)
73	o7	0.75	0/696	0.85	1/923 (0.1%)
74	O8	0.51	0/618	0.64	0/826
74	o8	0.42	0/614	0.61	0/822
75	O9	0.83	1/443 (0.2%)	0.90	0/588
75	o9	0.76	0/443	0.83	0/588
76	Q0	0.73	0/423	0.84	0/562
76	q0	0.95	0/423	1.03	1/562 (0.2%)
77	Q1	0.72	0/234	0.96	1/300 (0.3%)
77	q1	0.82	0/234	1.05	2/300 (0.7%)
78	Q2	0.93	1/860 (0.1%)	0.85	1/1136 (0.1%)
78	q2	0.82	1/860 (0.1%)	0.83	0/1136
79	Q3	0.74	0/701	0.85	0/934
79	q3	0.72	0/701	0.81	0/934
80	e0	0.56	0/499	0.74	0/665
81	sM	0.50	0/684	0.69	1/925 (0.1%)
83	p0	0.46	0/1092	0.61	0/1474
All	All	0.90	376/430075 (0.1%)	1.30	4764/631366 (0.8%)

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
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
18	c6	0	1
19	C7	0	2
22	d0	0	1
27	D5	0	2
28	D6	0	1
33	E1	0	1
39	l2	0	1
42	l5	0	2
43	L6	0	1
43	l6	0	1
44	l7	0	2
45	L8	0	1
48	M1	0	2
51	M5	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
55	m9	0	1
56	N0	0	2
56	n0	0	2
57	N1	0	1
62	n6	0	1
64	N8	0	1
64	n8	0	2
65	N9	0	1
67	O1	0	1
67	o1	0	2
All	All	0	43

The worst 5 of 376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	15.91	2.09	1.82
36	5	1152	G	N9-C4	-12.55	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	11.87	2.02	1.82
36	1	3181	C	N3-C4	-9.25	1.27	1.33
36	5	2138	A	N7-C5	-8.87	1.33	1.39

The worst 5 of 4764 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C4-C5	24.25	140.73	128.60
36	5	1152	G	N3-C4-N9	-22.33	112.60	126.00
36	5	1152	G	C2-N3-C4	-20.90	101.45	111.90
36	1	2945	G	O5'-P-OP2	-17.25	90.00	110.70
36	1	1308	A	O5'-P-OP2	-17.00	90.30	110.70

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	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%)	152 (74%)	31 (15%)	21 (10%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	s0	204/251 (81%)	153 (75%)	26 (13%)	25 (12%)	0	1
3	S1	212/254 (84%)	146 (69%)	39 (18%)	27 (13%)	0	1
3	s1	214/254 (84%)	177 (83%)	26 (12%)	11 (5%)	2	12
4	S2	215/253 (85%)	187 (87%)	17 (8%)	11 (5%)	2	12
4	s2	215/253 (85%)	186 (86%)	16 (7%)	13 (6%)	1	9
5	S3	221/239 (92%)	179 (81%)	29 (13%)	13 (6%)	1	9
5	s3	221/239 (92%)	183 (83%)	19 (9%)	19 (9%)	1	3
6	S4	258/260 (99%)	206 (80%)	41 (16%)	11 (4%)	2	15
6	s4	258/260 (99%)	216 (84%)	24 (9%)	18 (7%)	1	6
7	S5	204/224 (91%)	158 (78%)	32 (16%)	14 (7%)	1	6
7	s5	204/224 (91%)	164 (80%)	25 (12%)	15 (7%)	1	5
8	S6	224/236 (95%)	194 (87%)	17 (8%)	13 (6%)	1	10
8	s6	216/236 (92%)	189 (88%)	15 (7%)	12 (6%)	2	10
9	S7	182/189 (96%)	137 (75%)	25 (14%)	20 (11%)	0	2
9	s7	184/189 (97%)	148 (80%)	21 (11%)	15 (8%)	1	4
10	S8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	2	13
10	s8	184/200 (92%)	163 (89%)	16 (9%)	5 (3%)	5	26
11	S9	183/196 (93%)	151 (82%)	23 (13%)	9 (5%)	2	13
11	s9	183/196 (93%)	140 (76%)	34 (19%)	9 (5%)	2	13
12	C0	94/105 (90%)	68 (72%)	15 (16%)	11 (12%)	0	1
12	c0	92/105 (88%)	64 (70%)	14 (15%)	14 (15%)	0	1
13	C1	153/155 (99%)	126 (82%)	16 (10%)	11 (7%)	1	5
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	1	7
14	C2	122/142 (86%)	70 (57%)	25 (20%)	27 (22%)	0	0
14	c2	122/142 (86%)	68 (56%)	32 (26%)	22 (18%)	0	0
15	C3	148/150 (99%)	123 (83%)	18 (12%)	7 (5%)	2	14
15	c3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	5
16	C4	125/136 (92%)	94 (75%)	15 (12%)	16 (13%)	0	1
16	c4	126/136 (93%)	101 (80%)	16 (13%)	9 (7%)	1	5
17	C5	122/141 (86%)	88 (72%)	23 (19%)	11 (9%)	1	3
17	c5	133/141 (94%)	92 (69%)	22 (16%)	19 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	116 (84%)	16 (12%)	7 (5%)	2	12
18	c6	140/142 (99%)	116 (83%)	16 (11%)	8 (6%)	1	10
19	C7	116/136 (85%)	91 (78%)	13 (11%)	12 (10%)	0	2
19	c7	113/136 (83%)	87 (77%)	18 (16%)	8 (7%)	1	5
20	C8	143/145 (99%)	115 (80%)	16 (11%)	12 (8%)	1	4
20	c8	143/145 (99%)	114 (80%)	20 (14%)	9 (6%)	1	7
21	C9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	5	25
21	c9	141/143 (99%)	119 (84%)	16 (11%)	6 (4%)	2	15
22	D0	105/120 (88%)	88 (84%)	13 (12%)	4 (4%)	3	18
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	61 (72%)	16 (19%)	8 (9%)	0	3
23	d1	85/87 (98%)	72 (85%)	8 (9%)	5 (6%)	1	9
24	D2	127/129 (98%)	106 (84%)	19 (15%)	2 (2%)	9	40
24	d2	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	19	57
25	D3	142/144 (99%)	113 (80%)	19 (13%)	10 (7%)	1	6
25	d3	142/144 (99%)	123 (87%)	16 (11%)	3 (2%)	7	33
26	D4	132/134 (98%)	103 (78%)	20 (15%)	9 (7%)	1	6
26	d4	132/134 (98%)	103 (78%)	21 (16%)	8 (6%)	1	8
27	D5	68/107 (64%)	47 (69%)	9 (13%)	12 (18%)	0	0
27	d5	67/107 (63%)	52 (78%)	9 (13%)	6 (9%)	1	3
28	D6	95/97 (98%)	59 (62%)	18 (19%)	18 (19%)	0	0
28	d6	95/97 (98%)	74 (78%)	12 (13%)	9 (10%)	0	3
29	D7	79/81 (98%)	66 (84%)	8 (10%)	5 (6%)	1	7
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1	3
30	D8	61/66 (92%)	51 (84%)	6 (10%)	4 (7%)	1	6
30	d8	61/66 (92%)	42 (69%)	15 (25%)	4 (7%)	1	6
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	17
31	d9	51/55 (93%)	41 (80%)	6 (12%)	4 (8%)	1	4
32	E0	58/60 (97%)	44 (76%)	12 (21%)	2 (3%)	3	20
33	E1	69/76 (91%)	36 (52%)	17 (25%)	16 (23%)	0	0
33	e1	74/76 (97%)	36 (49%)	17 (23%)	21 (28%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	271 (86%)	35 (11%)	10 (3%)	4	22
34	sR	316/318 (99%)	270 (85%)	36 (11%)	10 (3%)	4	22
35	SM	155/273 (57%)	113 (73%)	23 (15%)	19 (12%)	0	1
39	L2	250/253 (99%)	223 (89%)	21 (8%)	6 (2%)	6	29
39	l2	250/253 (99%)	210 (84%)	30 (12%)	10 (4%)	3	17
40	L3	384/386 (100%)	326 (85%)	45 (12%)	13 (3%)	3	20
40	l3	384/386 (100%)	340 (88%)	32 (8%)	12 (3%)	4	23
41	L4	359/361 (99%)	299 (83%)	43 (12%)	17 (5%)	2	14
41	l4	359/361 (99%)	300 (84%)	39 (11%)	20 (6%)	2	10
42	L5	294/296 (99%)	242 (82%)	31 (10%)	21 (7%)	1	5
42	l5	292/296 (99%)	255 (87%)	30 (10%)	7 (2%)	6	29
43	L6	152/175 (87%)	132 (87%)	16 (10%)	4 (3%)	5	27
43	l6	153/175 (87%)	129 (84%)	20 (13%)	4 (3%)	5	27
44	L7	220/243 (90%)	198 (90%)	12 (6%)	10 (4%)	2	14
44	l7	221/243 (91%)	195 (88%)	20 (9%)	6 (3%)	5	26
45	L8	231/255 (91%)	188 (81%)	35 (15%)	8 (4%)	3	20
45	l8	229/255 (90%)	188 (82%)	21 (9%)	20 (9%)	1	3
46	L9	189/191 (99%)	167 (88%)	15 (8%)	7 (4%)	3	19
46	l9	189/191 (99%)	171 (90%)	15 (8%)	3 (2%)	9	40
47	M0	207/220 (94%)	178 (86%)	18 (9%)	11 (5%)	2	11
47	m0	209/220 (95%)	167 (80%)	27 (13%)	15 (7%)	1	5
48	M1	167/173 (96%)	131 (78%)	21 (13%)	15 (9%)	1	3
48	m1	167/173 (96%)	139 (83%)	16 (10%)	12 (7%)	1	5
49	M3	191/198 (96%)	164 (86%)	16 (8%)	11 (6%)	1	10
49	m3	192/198 (97%)	159 (83%)	17 (9%)	16 (8%)	1	4
50	M4	134/137 (98%)	117 (87%)	12 (9%)	5 (4%)	3	19
50	m4	135/137 (98%)	122 (90%)	10 (7%)	3 (2%)	6	31
51	M5	201/203 (99%)	181 (90%)	12 (6%)	8 (4%)	3	17
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	4	24
52	M6	195/198 (98%)	181 (93%)	11 (6%)	3 (2%)	10	42
52	m6	195/198 (98%)	179 (92%)	8 (4%)	8 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	M7	181/183 (99%)	152 (84%)	22 (12%)	7 (4%)	3	17
53	m7	153/183 (84%)	138 (90%)	13 (8%)	2 (1%)	12	45
54	M8	183/185 (99%)	165 (90%)	14 (8%)	4 (2%)	6	31
54	m8	183/185 (99%)	155 (85%)	22 (12%)	6 (3%)	4	21
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
55	m9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
56	N0	170/172 (99%)	150 (88%)	15 (9%)	5 (3%)	4	24
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	25	64
57	N1	157/159 (99%)	133 (85%)	18 (12%)	6 (4%)	3	18
57	n1	157/159 (99%)	141 (90%)	12 (8%)	4 (2%)	5	28
58	N2	98/120 (82%)	76 (78%)	17 (17%)	5 (5%)	2	12
58	n2	96/120 (80%)	77 (80%)	13 (14%)	6 (6%)	1	7
59	N3	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	22	60
59	n3	134/136 (98%)	121 (90%)	11 (8%)	2 (2%)	10	42
60	N4	96/155 (62%)	74 (77%)	13 (14%)	9 (9%)	0	3
60	n4	133/155 (86%)	107 (80%)	17 (13%)	9 (7%)	1	6
61	N5	119/141 (84%)	106 (89%)	12 (10%)	1 (1%)	19	57
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	5
62	N6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	2	13
62	n6	124/126 (98%)	113 (91%)	7 (6%)	4 (3%)	4	22
63	N7	133/135 (98%)	109 (82%)	18 (14%)	6 (4%)	2	14
63	n7	133/135 (98%)	104 (78%)	18 (14%)	11 (8%)	1	4
64	N8	146/148 (99%)	121 (83%)	15 (10%)	10 (7%)	1	6
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	3	20
65	N9	56/58 (97%)	48 (86%)	6 (11%)	2 (4%)	3	19
65	n9	56/58 (97%)	40 (71%)	12 (21%)	4 (7%)	1	5
66	O0	95/104 (91%)	89 (94%)	4 (4%)	2 (2%)	7	33
66	o0	98/104 (94%)	88 (90%)	6 (6%)	4 (4%)	3	16
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	14
67	o1	107/112 (96%)	90 (84%)	12 (11%)	5 (5%)	2	14
68	O2	125/129 (97%)	112 (90%)	10 (8%)	3 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	o2	125/129 (97%)	106 (85%)	13 (10%)	6 (5%)	2	13
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	4	24
69	o3	104/106 (98%)	92 (88%)	8 (8%)	4 (4%)	3	18
70	O4	110/119 (92%)	97 (88%)	12 (11%)	1 (1%)	17	55
70	o4	110/119 (92%)	93 (84%)	11 (10%)	6 (6%)	2	10
71	O5	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	17	55
71	o5	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	9	39
72	O6	97/99 (98%)	77 (79%)	15 (16%)	5 (5%)	2	12
72	o6	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	5
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	3	20
73	o7	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	6	29
74	O8	75/77 (97%)	62 (83%)	11 (15%)	2 (3%)	5	26
74	o8	75/77 (97%)	60 (80%)	11 (15%)	4 (5%)	2	11
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	33
75	o9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	33
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	17
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	34
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	15
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	1	10
78	q2	103/105 (98%)	92 (89%)	10 (10%)	1 (1%)	15	53
79	Q3	89/91 (98%)	77 (86%)	8 (9%)	4 (4%)	2	14
79	q3	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	14	50
80	e0	60/62 (97%)	43 (72%)	11 (18%)	6 (10%)	0	2
81	sM	98/273 (36%)	62 (63%)	22 (22%)	14 (14%)	0	1
83	p0	139/311 (45%)	120 (86%)	15 (11%)	4 (3%)	4	24
All	All	22333/24141 (92%)	18562 (83%)	2524 (11%)	1247 (6%)	2	10

5 of 1247 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN

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Mol	Chain	Res	Type
2	S0	66	ALA
2	S0	158	VAL
2	S0	191	ARG

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%)	133 (81%)	31 (19%)	1 8
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1 6
3	S1	191/223 (86%)	155 (81%)	36 (19%)	1 8
3	s1	192/223 (86%)	163 (85%)	29 (15%)	3 14
4	S2	176/204 (86%)	142 (81%)	34 (19%)	1 8
4	s2	176/204 (86%)	133 (76%)	43 (24%)	0 3
5	S3	182/194 (94%)	145 (80%)	37 (20%)	1 6
5	s3	182/194 (94%)	151 (83%)	31 (17%)	2 10
6	S4	221/221 (100%)	183 (83%)	38 (17%)	2 10
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2 10
7	S5	173/190 (91%)	142 (82%)	31 (18%)	2 9
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1 4
8	S6	188/201 (94%)	148 (79%)	40 (21%)	1 5
8	s6	187/201 (93%)	151 (81%)	36 (19%)	1 8
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3 14
9	s7	165/169 (98%)	138 (84%)	27 (16%)	2 11
10	S8	150/161 (93%)	130 (87%)	20 (13%)	4 17
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3 15
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1 4
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1 8
12	C0	77/98 (79%)	67 (87%)	10 (13%)	4 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c0	73/98 (74%)	63 (86%)	10 (14%)	3	17
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	10
13	c1	129/136 (95%)	106 (82%)	23 (18%)	2	9
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0	3
14	c2	88/118 (75%)	66 (75%)	22 (25%)	0	3
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%)	76 (78%)	21 (22%)	1	5
17	C5	101/117 (86%)	85 (84%)	16 (16%)	2	12
17	c5	103/117 (88%)	84 (82%)	19 (18%)	1	9
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	7
18	c6	118/118 (100%)	93 (79%)	25 (21%)	1	5
19	C7	94/124 (76%)	72 (77%)	22 (23%)	1	4
19	c7	92/124 (74%)	78 (85%)	14 (15%)	3	14
20	C8	128/128 (100%)	95 (74%)	33 (26%)	0	2
20	c8	128/128 (100%)	103 (80%)	25 (20%)	1	7
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	7
21	c9	115/115 (100%)	93 (81%)	22 (19%)	1	8
22	D0	100/113 (88%)	78 (78%)	22 (22%)	1	4
22	d0	103/113 (91%)	78 (76%)	25 (24%)	0	3
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	10
23	d1	74/74 (100%)	56 (76%)	18 (24%)	0	3
24	D2	110/110 (100%)	94 (86%)	16 (14%)	3	15
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2	13
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	10
25	d3	119/119 (100%)	104 (87%)	15 (13%)	4	20
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	10
26	d4	112/112 (100%)	94 (84%)	18 (16%)	2	12
27	D5	61/88 (69%)	46 (75%)	15 (25%)	0	3
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	D6	83/83 (100%)	67 (81%)	16 (19%)	1 8
28	d6	83/83 (100%)	73 (88%)	10 (12%)	5 22
29	D7	70/70 (100%)	64 (91%)	6 (9%)	10 37
29	d7	70/70 (100%)	60 (86%)	10 (14%)	3 15
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1 5
30	d8	56/59 (95%)	44 (79%)	12 (21%)	1 5
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2 10
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1 5
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1 7
33	E1	62/66 (94%)	46 (74%)	16 (26%)	0 2
33	e1	66/66 (100%)	51 (77%)	15 (23%)	1 4
34	SR	260/261 (100%)	222 (85%)	38 (15%)	3 15
34	sR	260/261 (100%)	233 (90%)	27 (10%)	7 27
35	SM	97/228 (42%)	76 (78%)	21 (22%)	1 5
39	L2	193/195 (99%)	150 (78%)	43 (22%)	1 4
39	l2	192/195 (98%)	152 (79%)	40 (21%)	1 5
40	L3	321/322 (100%)	257 (80%)	64 (20%)	1 7
40	l3	320/322 (99%)	251 (78%)	69 (22%)	1 5
41	L4	288/288 (100%)	228 (79%)	60 (21%)	1 5
41	l4	288/288 (100%)	229 (80%)	59 (20%)	1 6
42	L5	244/244 (100%)	197 (81%)	47 (19%)	1 8
42	l5	243/244 (100%)	196 (81%)	47 (19%)	1 8
43	L6	134/152 (88%)	112 (84%)	22 (16%)	2 11
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2 10
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4 19
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3 15
45	L8	187/207 (90%)	152 (81%)	35 (19%)	1 8
45	l8	177/207 (86%)	147 (83%)	30 (17%)	2 11
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1 5
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1 7
47	M0	177/186 (95%)	143 (81%)	34 (19%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	6
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	5
48	m1	147/150 (98%)	122 (83%)	25 (17%)	2	10
49	M3	154/158 (98%)	128 (83%)	26 (17%)	2	11
49	m3	154/158 (98%)	130 (84%)	24 (16%)	2	13
50	M4	107/108 (99%)	84 (78%)	23 (22%)	1	5
50	m4	108/108 (100%)	88 (82%)	20 (18%)	1	8
51	M5	175/175 (100%)	138 (79%)	37 (21%)	1	5
51	m5	175/175 (100%)	149 (85%)	26 (15%)	3	14
52	M6	160/161 (99%)	133 (83%)	27 (17%)	2	11
52	m6	160/161 (99%)	132 (82%)	28 (18%)	2	10
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	4
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	10
54	M8	150/150 (100%)	128 (85%)	22 (15%)	3	15
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	5
55	M9	153/153 (100%)	132 (86%)	21 (14%)	3	17
55	m9	153/153 (100%)	120 (78%)	33 (22%)	1	5
56	N0	156/156 (100%)	121 (78%)	35 (22%)	1	4
56	n0	156/156 (100%)	124 (80%)	32 (20%)	1	6
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	6
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	6
58	N2	87/106 (82%)	74 (85%)	13 (15%)	3	14
58	n2	85/106 (80%)	72 (85%)	13 (15%)	2	13
59	N3	104/104 (100%)	86 (83%)	18 (17%)	2	10
59	n3	104/104 (100%)	94 (90%)	10 (10%)	8	32
60	N4	57/129 (44%)	50 (88%)	7 (12%)	4	21
60	n4	100/129 (78%)	82 (82%)	18 (18%)	1	9
61	N5	104/117 (89%)	84 (81%)	20 (19%)	1	8
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	6
62	N6	109/109 (100%)	83 (76%)	26 (24%)	0	3
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	N7	115/115 (100%)	94 (82%)	21 (18%)	1	9
63	n7	115/115 (100%)	93 (81%)	22 (19%)	1	8
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1	8
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1	5
65	N9	46/46 (100%)	35 (76%)	11 (24%)	0	3
65	n9	46/46 (100%)	37 (80%)	9 (20%)	1	7
66	O0	81/87 (93%)	68 (84%)	13 (16%)	2	12
66	o0	84/87 (97%)	70 (83%)	14 (17%)	2	11
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	4
67	o1	94/96 (98%)	74 (79%)	20 (21%)	1	5
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	6
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	4
69	O3	90/90 (100%)	81 (90%)	9 (10%)	7	29
69	o3	90/90 (100%)	77 (86%)	13 (14%)	3	15
70	O4	95/101 (94%)	74 (78%)	21 (22%)	1	4
70	o4	95/101 (94%)	75 (79%)	20 (21%)	1	5
71	O5	104/104 (100%)	80 (77%)	24 (23%)	1	4
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1	4
72	O6	81/81 (100%)	65 (80%)	16 (20%)	1	7
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	10
73	o7	70/70 (100%)	58 (83%)	12 (17%)	2	10
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	3
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1	5
75	O9	45/45 (100%)	40 (89%)	5 (11%)	6	25
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1	7
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
76	q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	q2	90/90 (100%)	73 (81%)	17 (19%)	1 8
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1 5
79	q3	71/71 (100%)	63 (89%)	8 (11%)	6 24
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1 5
81	sM	54/228 (24%)	40 (74%)	14 (26%)	0 2
83	p0	105/253 (42%)	80 (76%)	25 (24%)	0 3
All	All	18729/20239 (92%)	15175 (81%)	3554 (19%)	1 8

5 of 3554 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	s2	69	ILE
83	p0	74	GLU
20	c8	143	ARG
78	q2	61	LYS
60	n4	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
74	O8	32	ASN
11	s9	142	ASN
64	n8	25	HIS
78	Q2	23	HIS
9	s7	71	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	451 (25%)	62 (3%)
1	6	1793/1800 (99%)	468 (26%)	56 (3%)
36	1	3145/3396 (92%)	662 (21%)	85 (2%)
36	5	3145/3396 (92%)	673 (21%)	84 (2%)
37	3	120/121 (99%)	16 (13%)	3 (2%)
37	7	120/121 (99%)	21 (17%)	0
38	4	157/158 (99%)	39 (24%)	3 (1%)
38	8	157/158 (99%)	36 (22%)	3 (1%)
All	All	10384/10950 (94%)	2366 (22%)	296 (2%)

5 of 2366 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 296 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	1241	U
36	5	3269	U
36	5	1434	G
36	5	2281	A
36	1	1507	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, 1428 are monoatomic - leaving 1135 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	$\#\|Z\| > 2$
87	OHX	2	2166	-	0,6,6	-	-	-		
87	OHX	2	2132	-	0,6,6	-	-	-		
87	OHX	1	4085	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	2	2171	-	0,6,6	-	-	-		
87	OHX	1	4163	-	0,6,6	-	-	-		
87	OHX	5	4113	-	0,6,6	-	-	-		
87	OHX	1	3912	-	0,6,6	-	-	-		
87	OHX	5	4010	-	0,6,6	-	-	-		
87	OHX	1	4065	-	0,6,6	-	-	-		
87	OHX	5	4025	-	0,6,6	-	-	-		
87	OHX	1	3988	-	0,6,6	-	-	-		
87	OHX	5	3982	-	0,6,6	-	-	-		
87	OHX	2	2025	-	0,6,6	-	-	-		
87	OHX	1	4192	-	0,6,6	-	-	-		
87	OHX	1	3944	-	0,6,6	-	-	-		
87	OHX	1	4088	-	0,6,6	-	-	-		
87	OHX	6	2148	-	0,6,6	-	-	-		
87	OHX	5	4221	-	0,6,6	-	-	-		
87	OHX	4	231	-	0,6,6	-	-	-		
87	OHX	6	2076	-	0,6,6	-	-	-		
87	OHX	1	4152	-	0,6,6	-	-	-		
87	OHX	1	3933	-	0,6,6	-	-	-		
87	OHX	s9	201	-	0,6,6	-	-	-		
87	OHX	5	3963	-	0,6,6	-	-	-		
87	OHX	5	4074	-	0,6,6	-	-	-		
87	OHX	4	232	-	0,6,6	-	-	-		
87	OHX	5	4240	-	0,6,6	-	-	-		
87	OHX	6	2165	-	0,6,6	-	-	-		
87	OHX	5	4120	-	0,6,6	-	-	-		
87	OHX	1	4175	-	0,6,6	-	-	-		
87	OHX	5	4053	-	0,6,6	-	-	-		
87	OHX	1	4180	-	0,6,6	-	-	-		
87	OHX	1	4171	-	0,6,6	-	-	-		
87	OHX	6	2158	-	0,6,6	-	-	-		
87	OHX	5	4032	-	0,6,6	-	-	-		
87	OHX	1	3891	-	0,6,6	-	-	-		
87	OHX	1	4104	-	0,6,6	-	-	-		
87	OHX	5	3972	-	0,6,6	-	-	-		
87	OHX	5	4003	-	0,6,6	-	-	-		
87	OHX	5	3974	-	0,6,6	-	-	-		
87	OHX	1	3872	-	0,6,6	-	-	-		
87	OHX	6	2171	-	0,6,6	-	-	-		
87	OHX	5	4157	-	0,6,6	-	-	-		
87	OHX	2	2172	-	0,6,6	-	-	-		
87	OHX	l3	404	-	0,6,6	-	-	-		
87	OHX	5	4173	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4017	-	0,6,6	-	-	-		
87	OHX	2	2110	-	0,6,6	-	-	-		
87	OHX	1	3960	-	0,6,6	-	-	-		
87	OHX	5	4135	-	0,6,6	-	-	-		
87	OHX	2	2068	-	0,6,6	-	-	-		
87	OHX	6	2099	-	0,6,6	-	-	-		
87	OHX	6	2107	-	0,6,6	-	-	-		
87	OHX	1	3982	-	0,6,6	-	-	-		
87	OHX	1	4179	-	0,6,6	-	-	-		
87	OHX	m7	206	-	0,6,6	-	-	-		
87	OHX	5	4045	-	0,6,6	-	-	-		
87	OHX	5	4047	-	0,6,6	-	-	-		
87	OHX	6	2108	-	0,6,6	-	-	-		
87	OHX	5	4196	-	0,6,6	-	-	-		
87	OHX	5	3983	-	0,6,6	-	-	-		
87	OHX	5	4022	-	0,6,6	-	-	-		
87	OHX	m9	201	-	0,6,6	-	-	-		
87	OHX	2	2038	-	0,6,6	-	-	-		
87	OHX	5	3904	-	0,6,6	-	-	-		
87	OHX	5	3993	-	0,6,6	-	-	-		
87	OHX	5	3999	-	0,6,6	-	-	-		
87	OHX	6	2085	-	0,6,6	-	-	-		
87	OHX	5	4180	-	0,6,6	-	-	-		
87	OHX	1	4129	-	0,6,6	-	-	-		
87	OHX	1	4121	-	0,6,6	-	-	-		
87	OHX	1	4055	-	0,6,6	-	-	-		
87	OHX	1	4190	-	0,6,6	-	-	-		
87	OHX	2	2153	-	0,6,6	-	-	-		
87	OHX	1	4114	-	0,6,6	-	-	-		
87	OHX	1	4021	-	0,6,6	-	-	-		
87	OHX	8	227	-	0,6,6	-	-	-		
87	OHX	5	4178	-	0,6,6	-	-	-		
87	OHX	1	3991	-	0,6,6	-	-	-		
87	OHX	1	3917	-	0,6,6	-	-	-		
87	OHX	1	3896	-	0,6,6	-	-	-		
87	OHX	2	2120	-	0,6,6	-	-	-		
87	OHX	1	4134	-	0,6,6	-	-	-		
87	OHX	6	2191	-	0,6,6	-	-	-		
87	OHX	6	2086	-	0,6,6	-	-	-		
87	OHX	1	4156	-	0,6,6	-	-	-		
87	OHX	6	2065	-	0,6,6	-	-	-		
87	OHX	5	3910	-	0,6,6	-	-	-		
87	OHX	2	2026	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4169	-	0,6,6	-	-	-		
87	OHX	2	2090	-	0,6,6	-	-	-		
87	OHX	2	2107	-	0,6,6	-	-	-		
87	OHX	5	3976	-	0,6,6	-	-	-		
87	OHX	1	3964	-	0,6,6	-	-	-		
87	OHX	1	3970	-	0,6,6	-	-	-		
87	OHX	1	3877	-	0,6,6	-	-	-		
87	OHX	5	4202	-	0,6,6	-	-	-		
87	OHX	6	2195	-	0,6,6	-	-	-		
87	OHX	5	3961	-	0,6,6	-	-	-		
87	OHX	5	4161	-	0,6,6	-	-	-		
87	OHX	5	3909	-	0,6,6	-	-	-		
87	OHX	2	2030	-	0,6,6	-	-	-		
87	OHX	5	4041	-	0,6,6	-	-	-		
87	OHX	5	4241	-	0,6,6	-	-	-		
87	OHX	5	3911	-	0,6,6	-	-	-		
87	OHX	1	3998	-	0,6,6	-	-	-		
87	OHX	1	3929	-	0,6,6	-	-	-		
87	OHX	2	2168	-	0,6,6	-	-	-		
87	OHX	1	3873	-	0,6,6	-	-	-		
87	OHX	1	4146	-	0,6,6	-	-	-		
87	OHX	1	4133	-	0,6,6	-	-	-		
87	OHX	6	2152	-	0,6,6	-	-	-		
87	OHX	5	4182	-	0,6,6	-	-	-		
87	OHX	5	4198	-	0,6,6	-	-	-		
87	OHX	5	4215	-	0,6,6	-	-	-		
87	OHX	6	2178	-	0,6,6	-	-	-		
87	OHX	1	4144	-	0,6,6	-	-	-		
87	OHX	2	2118	-	0,6,6	-	-	-		
87	OHX	5	4070	-	0,6,6	-	-	-		
87	OHX	2	2159	-	0,6,6	-	-	-		
87	OHX	8	221	-	0,6,6	-	-	-		
87	OHX	5	3948	-	0,6,6	-	-	-		
87	OHX	1	3907	-	0,6,6	-	-	-		
87	OHX	1	3949	-	0,6,6	-	-	-		
87	OHX	6	2114	-	0,6,6	-	-	-		
87	OHX	5	4229	-	0,6,6	-	-	-		
87	OHX	5	3921	-	0,6,6	-	-	-		
87	OHX	1	4072	-	0,6,6	-	-	-		
87	OHX	1	3950	-	0,6,6	-	-	-		
87	OHX	4	233	-	0,6,6	-	-	-		
87	OHX	M9	202	-	0,6,6	-	-	-		
87	OHX	6	2140	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4199	-	0,6,6	-	-	-		
87	OHX	1	3981	-	0,6,6	-	-	-		
87	OHX	5	4149	-	0,6,6	-	-	-		
87	OHX	6	2194	-	0,6,6	-	-	-		
87	OHX	3	219	-	0,6,6	-	-	-		
87	OHX	1	3992	-	0,6,6	-	-	-		
87	OHX	6	2115	-	0,6,6	-	-	-		
87	OHX	5	4083	-	0,6,6	-	-	-		
87	OHX	5	4093	-	0,6,6	-	-	-		
87	OHX	1	3966	-	0,6,6	-	-	-		
87	OHX	2	2079	-	0,6,6	-	-	-		
87	OHX	1	4150	-	0,6,6	-	-	-		
87	OHX	5	4036	-	0,6,6	-	-	-		
87	OHX	1	4166	-	0,6,6	-	-	-		
87	OHX	1	4044	-	0,6,6	-	-	-		
87	OHX	6	2153	-	0,6,6	-	-	-		
87	OHX	2	2176	-	0,6,6	-	-	-		
87	OHX	3	221	-	0,6,6	-	-	-		
87	OHX	6	2117	-	0,6,6	-	-	-		
87	OHX	2	2145	-	0,6,6	-	-	-		
87	OHX	5	3995	-	0,6,6	-	-	-		
87	OHX	6	2192	-	0,6,6	-	-	-		
87	OHX	1	4023	-	0,6,6	-	-	-		
87	OHX	5	4094	-	0,6,6	-	-	-		
87	OHX	1	4029	-	0,6,6	-	-	-		
87	OHX	6	2101	-	0,6,6	-	-	-		
87	OHX	5	4082	-	0,6,6	-	-	-		
87	OHX	5	4243	-	0,6,6	-	-	-		
89	3KD	1	4218	-	24,25,25	0.80	0	30,39,39	1.10	1 (3%)
87	OHX	8	228	-	0,6,6	-	-	-		
87	OHX	2	2103	-	0,6,6	-	-	-		
87	OHX	1	3875	-	0,6,6	-	-	-		
87	OHX	1	4008	-	0,6,6	-	-	-		
87	OHX	2	2128	-	0,6,6	-	-	-		
87	OHX	1	3884	-	0,6,6	-	-	-		
87	OHX	1	4168	-	0,6,6	-	-	-		
87	OHX	6	2066	-	0,6,6	-	-	-		
87	OHX	6	2162	-	0,6,6	-	-	-		
87	OHX	1	3926	-	0,6,6	-	-	-		
87	OHX	5	4037	-	0,6,6	-	-	-		
87	OHX	1	4153	-	0,6,6	-	-	-		
87	OHX	1	4174	-	0,6,6	-	-	-		
87	OHX	1	4099	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	6	2111	-	0,6,6	-	-	-		
87	OHX	6	2200	-	0,6,6	-	-	-		
87	OHX	1	4024	-	0,6,6	-	-	-		
87	OHX	6	2182	-	0,6,6	-	-	-		
87	OHX	5	4181	-	0,6,6	-	-	-		
87	OHX	5	4191	-	0,6,6	-	-	-		
87	OHX	6	2146	-	0,6,6	-	-	-		
87	OHX	5	4183	-	0,6,6	-	-	-		
87	OHX	1	4108	-	0,6,6	-	-	-		
87	OHX	3	223	-	0,6,6	-	-	-		
87	OHX	2	2096	-	0,6,6	-	-	-		
87	OHX	2	2054	-	0,6,6	-	-	-		
87	OHX	1	3898	-	0,6,6	-	-	-		
87	OHX	1	3962	-	0,6,6	-	-	-		
87	OHX	5	4081	-	0,6,6	-	-	-		
87	OHX	1	4195	-	0,6,6	-	-	-		
87	OHX	6	2052	-	0,6,6	-	-	-		
87	OHX	1	4017	-	0,6,6	-	-	-		
87	OHX	5	4040	-	0,6,6	-	-	-		
87	OHX	5	4085	-	0,6,6	-	-	-		
87	OHX	1	4100	-	0,6,6	-	-	-		
87	OHX	2	2100	-	0,6,6	-	-	-		
87	OHX	1	3957	-	0,6,6	-	-	-		
87	OHX	6	2128	-	0,6,6	-	-	-		
87	OHX	1	4000	-	0,6,6	-	-	-		
87	OHX	5	3942	-	0,6,6	-	-	-		
87	OHX	1	4112	-	0,6,6	-	-	-		
87	OHX	2	2043	-	0,6,6	-	-	-		
87	OHX	1	3963	-	0,6,6	-	-	-		
87	OHX	5	3998	-	0,6,6	-	-	-		
87	OHX	L3	404	-	0,6,6	-	-	-		
87	OHX	5	4133	-	0,6,6	-	-	-		
87	OHX	5	4023	-	0,6,6	-	-	-		
87	OHX	6	2119	-	0,6,6	-	-	-		
87	OHX	1	4038	-	0,6,6	-	-	-		
87	OHX	6	2087	-	0,6,6	-	-	-		
87	OHX	5	4190	-	0,6,6	-	-	-		
87	OHX	1	3990	-	0,6,6	-	-	-		
87	OHX	6	2142	-	0,6,6	-	-	-		
87	OHX	6	2188	-	0,6,6	-	-	-		
87	OHX	1	3888	-	0,6,6	-	-	-		
87	OHX	2	2137	-	0,6,6	-	-	-		
87	OHX	5	4142	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	2	2065	-	0,6,6	-	-	-		
87	OHX	2	2126	-	0,6,6	-	-	-		
87	OHX	1	3972	-	0,6,6	-	-	-		
87	OHX	m5	304	-	0,6,6	-	-	-		
87	OHX	5	4247	-	0,6,6	-	-	-		
87	OHX	2	2124	-	0,6,6	-	-	-		
87	OHX	6	2123	-	0,6,6	-	-	-		
87	OHX	5	4130	-	0,6,6	-	-	-		
87	OHX	5	4197	-	0,6,6	-	-	-		
87	OHX	8	223	-	0,6,6	-	-	-		
87	OHX	5	4072	-	0,6,6	-	-	-		
87	OHX	7	227	-	0,6,6	-	-	-		
87	OHX	1	4096	-	0,6,6	-	-	-		
87	OHX	1	3986	-	0,6,6	-	-	-		
87	OHX	6	2109	-	0,6,6	-	-	-		
87	OHX	d9	102	-	0,6,6	-	-	-		
87	OHX	5	4131	-	0,6,6	-	-	-		
87	OHX	1	3883	-	0,6,6	-	-	-		
87	OHX	5	3992	-	0,6,6	-	-	-		
87	OHX	5	3920	-	0,6,6	-	-	-		
87	OHX	1	4058	-	0,6,6	-	-	-		
87	OHX	1	4071	-	0,6,6	-	-	-		
87	OHX	5	4107	-	0,6,6	-	-	-		
87	OHX	1	4013	-	0,6,6	-	-	-		
87	OHX	4	225	-	0,6,6	-	-	-		
87	OHX	5	4077	-	0,6,6	-	-	-		
87	OHX	2	2069	-	0,6,6	-	-	-		
87	OHX	5	4203	-	0,6,6	-	-	-		
87	OHX	2	2144	-	0,6,6	-	-	-		
87	OHX	1	3989	-	0,6,6	-	-	-		
87	OHX	1	4006	-	0,6,6	-	-	-		
87	OHX	1	4212	-	0,6,6	-	-	-		
87	OHX	1	4002	-	0,6,6	-	-	-		
87	OHX	5	3981	-	0,6,6	-	-	-		
87	OHX	6	2127	-	0,6,6	-	-	-		
87	OHX	5	3937	-	0,6,6	-	-	-		
87	OHX	5	4224	-	0,6,6	-	-	-		
87	OHX	1	3939	-	0,6,6	-	-	-		
87	OHX	1	3971	-	0,6,6	-	-	-		
87	OHX	1	4207	-	0,6,6	-	-	-		
87	OHX	2	2160	-	0,6,6	-	-	-		
87	OHX	1	4007	-	0,6,6	-	-	-		
87	OHX	1	3975	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	3918	-	0,6,6	-	-	-		
87	OHX	1	3928	-	0,6,6	-	-	-		
87	OHX	1	4043	-	0,6,6	-	-	-		
87	OHX	1	4057	-	0,6,6	-	-	-		
87	OHX	6	2163	-	0,6,6	-	-	-		
87	OHX	5	4199	-	0,6,6	-	-	-		
87	OHX	N1	201	-	0,6,6	-	-	-		
87	OHX	5	4008	-	0,6,6	-	-	-		
87	OHX	2	2063	-	0,6,6	-	-	-		
87	OHX	1	3895	-	0,6,6	-	-	-		
87	OHX	8	229	-	0,6,6	-	-	-		
87	OHX	2	2022	-	0,6,6	-	-	-		
87	OHX	1	4025	-	0,6,6	-	-	-		
87	OHX	2	2051	-	0,6,6	-	-	-		
87	OHX	C8	201	-	0,6,6	-	-	-		
87	OHX	1	3909	-	0,6,6	-	-	-		
87	OHX	1	3977	-	0,6,6	-	-	-		
87	OHX	2	2042	-	0,6,6	-	-	-		
87	OHX	5	4066	-	0,6,6	-	-	-		
87	OHX	5	4111	-	0,6,6	-	-	-		
87	OHX	5	4168	-	0,6,6	-	-	-		
87	OHX	6	2173	-	0,6,6	-	-	-		
87	OHX	5	4096	-	0,6,6	-	-	-		
87	OHX	5	4119	-	0,6,6	-	-	-		
87	OHX	1	4046	-	0,6,6	-	-	-		
87	OHX	1	3874	-	0,6,6	-	-	-		
87	OHX	5	4031	-	0,6,6	-	-	-		
87	OHX	2	2046	-	0,6,6	-	-	-		
87	OHX	2	2152	-	0,6,6	-	-	-		
87	OHX	6	2106	-	0,6,6	-	-	-		
87	OHX	6	2190	-	0,6,6	-	-	-		
87	OHX	5	4251	-	0,6,6	-	-	-		
87	OHX	O7	103	-	0,6,6	-	-	-		
87	OHX	1	4032	-	0,6,6	-	-	-		
87	OHX	1	4035	-	0,6,6	-	-	-		
87	OHX	2	2154	-	0,6,6	-	-	-		
87	OHX	5	3978	-	0,6,6	-	-	-		
87	OHX	o3	203	-	0,6,6	-	-	-		
87	OHX	5	4216	-	0,6,6	-	-	-		
87	OHX	5	4026	-	0,6,6	-	-	-		
87	OHX	5	4228	-	0,6,6	-	-	-		
87	OHX	6	2135	-	0,6,6	-	-	-		
87	OHX	7	221	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4034	-	0,6,6	-	-	-		
87	OHX	1	4081	-	0,6,6	-	-	-		
87	OHX	6	2063	-	0,6,6	-	-	-		
87	OHX	5	3955	-	0,6,6	-	-	-		
87	OHX	5	4245	-	0,6,6	-	-	-		
87	OHX	1	3974	-	0,6,6	-	-	-		
87	OHX	5	4027	-	0,6,6	-	-	-		
87	OHX	5	3954	-	0,6,6	-	-	-		
87	OHX	2	2134	-	0,6,6	-	-	-		
87	OHX	6	2139	-	0,6,6	-	-	-		
87	OHX	8	222	-	0,6,6	-	-	-		
87	OHX	o7	503	-	0,6,6	-	-	-		
87	OHX	1	4142	-	0,6,6	-	-	-		
87	OHX	6	2121	-	0,6,6	-	-	-		
87	OHX	1	4193	-	0,6,6	-	-	-		
87	OHX	2	2099	-	0,6,6	-	-	-		
87	OHX	1	3901	-	0,6,6	-	-	-		
87	OHX	6	2133	-	0,6,6	-	-	-		
87	OHX	sR	401	-	0,6,6	-	-	-		
87	OHX	5	4009	-	0,6,6	-	-	-		
87	OHX	2	2086	-	0,6,6	-	-	-		
87	OHX	2	2083	-	0,6,6	-	-	-		
87	OHX	6	2179	-	0,6,6	-	-	-		
87	OHX	1	4155	-	0,6,6	-	-	-		
87	OHX	1	4170	-	0,6,6	-	-	-		
87	OHX	1	4067	-	0,6,6	-	-	-		
87	OHX	5	4156	-	0,6,6	-	-	-		
87	OHX	5	3979	-	0,6,6	-	-	-		
87	OHX	1	3996	-	0,6,6	-	-	-		
87	OHX	5	4150	-	0,6,6	-	-	-		
87	OHX	1	4084	-	0,6,6	-	-	-		
87	OHX	5	4116	-	0,6,6	-	-	-		
87	OHX	1	4136	-	0,6,6	-	-	-		
87	OHX	6	2079	-	0,6,6	-	-	-		
87	OHX	1	4083	-	0,6,6	-	-	-		
87	OHX	5	4105	-	0,6,6	-	-	-		
87	OHX	2	2034	-	0,6,6	-	-	-		
87	OHX	l5	305	-	0,6,6	-	-	-		
87	OHX	6	2150	-	0,6,6	-	-	-		
87	OHX	1	3923	-	0,6,6	-	-	-		
87	OHX	1	4068	-	0,6,6	-	-	-		
87	OHX	5	4038	-	0,6,6	-	-	-		
87	OHX	1	4145	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4191	-	0,6,6	-	-	-		
87	OHX	4	223	-	0,6,6	-	-	-		
87	OHX	5	3971	-	0,6,6	-	-	-		
87	OHX	1	4196	-	0,6,6	-	-	-		
87	OHX	1	4183	-	0,6,6	-	-	-		
87	OHX	1	4200	-	0,6,6	-	-	-		
87	OHX	5	3905	-	0,6,6	-	-	-		
87	OHX	2	2178	-	0,6,6	-	-	-		
87	OHX	5	3913	-	0,6,6	-	-	-		
87	OHX	5	3932	-	0,6,6	-	-	-		
87	OHX	5	4063	-	0,6,6	-	-	-		
87	OHX	5	4233	-	0,6,6	-	-	-		
87	OHX	1	4194	-	0,6,6	-	-	-		
87	OHX	5	4125	-	0,6,6	-	-	-		
87	OHX	2	2158	-	0,6,6	-	-	-		
87	OHX	5	3901	-	0,6,6	-	-	-		
87	OHX	1	4139	-	0,6,6	-	-	-		
87	OHX	5	3965	-	0,6,6	-	-	-		
87	OHX	5	4162	-	0,6,6	-	-	-		
87	OHX	5	4019	-	0,6,6	-	-	-		
87	OHX	5	4153	-	0,6,6	-	-	-		
87	OHX	1	4045	-	0,6,6	-	-	-		
87	OHX	6	2197	-	0,6,6	-	-	-		
87	OHX	3	225	-	0,6,6	-	-	-		
87	OHX	1	3945	-	0,6,6	-	-	-		
87	OHX	1	4138	-	0,6,6	-	-	-		
87	OHX	7	224	-	0,6,6	-	-	-		
87	OHX	5	4067	-	0,6,6	-	-	-		
87	OHX	5	4115	-	0,6,6	-	-	-		
87	OHX	5	4189	-	0,6,6	-	-	-		
87	OHX	1	3921	-	0,6,6	-	-	-		
87	OHX	2	2066	-	0,6,6	-	-	-		
87	OHX	5	3975	-	0,6,6	-	-	-		
87	OHX	5	3996	-	0,6,6	-	-	-		
87	OHX	5	4237	-	0,6,6	-	-	-		
87	OHX	6	2072	-	0,6,6	-	-	-		
87	OHX	5	3906	-	0,6,6	-	-	-		
87	OHX	M5	302	-	0,6,6	-	-	-		
87	OHX	5	3923	-	0,6,6	-	-	-		
87	OHX	2	2040	-	0,6,6	-	-	-		
87	OHX	1	3890	-	0,6,6	-	-	-		
87	OHX	6	2198	-	0,6,6	-	-	-		
87	OHX	5	4118	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4059	-	0,6,6	-	-	-		
87	OHX	1	4165	-	0,6,6	-	-	-		
87	OHX	1	3915	-	0,6,6	-	-	-		
87	OHX	1	4069	-	0,6,6	-	-	-		
87	OHX	d4	202	-	0,6,6	-	-	-		
87	OHX	5	4016	-	0,6,6	-	-	-		
87	OHX	5	3936	-	0,6,6	-	-	-		
87	OHX	1	4076	-	0,6,6	-	-	-		
87	OHX	1	4135	-	0,6,6	-	-	-		
87	OHX	s1	303	-	0,6,6	-	-	-		
87	OHX	2	2087	-	0,6,6	-	-	-		
87	OHX	6	2122	-	0,6,6	-	-	-		
87	OHX	1	4111	-	0,6,6	-	-	-		
87	OHX	1	4211	-	0,6,6	-	-	-		
87	OHX	5	4137	-	0,6,6	-	-	-		
87	OHX	2	2157	-	0,6,6	-	-	-		
87	OHX	1	4060	-	0,6,6	-	-	-		
87	OHX	1	3968	-	0,6,6	-	-	-		
87	OHX	5	4011	-	0,6,6	-	-	-		
87	OHX	1	4036	-	0,6,6	-	-	-		
87	OHX	3	220	-	0,6,6	-	-	-		
87	OHX	1	4208	-	0,6,6	-	-	-		
87	OHX	6	2102	-	0,6,6	-	-	-		
87	OHX	2	2131	-	0,6,6	-	-	-		
87	OHX	5	4246	-	0,6,6	-	-	-		
87	OHX	1	4092	-	0,6,6	-	-	-		
87	OHX	1	3983	-	0,6,6	-	-	-		
87	OHX	1	4107	-	0,6,6	-	-	-		
87	OHX	o7	502	-	0,6,6	-	-	-		
87	OHX	2	2119	-	0,6,6	-	-	-		
87	OHX	2	2044	-	0,6,6	-	-	-		
87	OHX	1	4186	-	0,6,6	-	-	-		
87	OHX	1	4037	-	0,6,6	-	-	-		
87	OHX	5	3926	-	0,6,6	-	-	-		
87	OHX	6	2130	-	0,6,6	-	-	-		
87	OHX	6	2177	-	0,6,6	-	-	-		
87	OHX	3	224	-	0,6,6	-	-	-		
87	OHX	5	4101	-	0,6,6	-	-	-		
87	OHX	2	2072	-	0,6,6	-	-	-		
87	OHX	2	2055	-	0,6,6	-	-	-		
87	OHX	1	3946	-	0,6,6	-	-	-		
87	OHX	5	4167	-	0,6,6	-	-	-		
87	OHX	5	4201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4065	-	0,6,6	-	-	-		
87	OHX	5	3997	-	0,6,6	-	-	-		
87	OHX	1	4169	-	0,6,6	-	-	-		
87	OHX	6	2180	-	0,6,6	-	-	-		
87	OHX	6	2187	-	0,6,6	-	-	-		
87	OHX	5	4152	-	0,6,6	-	-	-		
87	OHX	5	3933	-	0,6,6	-	-	-		
87	OHX	4	222	-	0,6,6	-	-	-		
87	OHX	5	4033	-	0,6,6	-	-	-		
87	OHX	2	2088	-	0,6,6	-	-	-		
87	OHX	1	4102	-	0,6,6	-	-	-		
87	OHX	5	4172	-	0,6,6	-	-	-		
87	OHX	6	2056	-	0,6,6	-	-	-		
87	OHX	5	4232	-	0,6,6	-	-	-		
87	OHX	2	2175	-	0,6,6	-	-	-		
87	OHX	s1	302	-	0,6,6	-	-	-		
87	OHX	5	4024	-	0,6,6	-	-	-		
87	OHX	4	228	-	0,6,6	-	-	-		
87	OHX	5	4164	-	0,6,6	-	-	-		
87	OHX	m6	202	-	0,6,6	-	-	-		
87	OHX	2	2130	-	0,6,6	-	-	-		
87	OHX	M7	207	-	0,6,6	-	-	-		
87	OHX	2	2115	-	0,6,6	-	-	-		
87	OHX	2	2052	-	0,6,6	-	-	-		
87	OHX	5	4112	-	0,6,6	-	-	-		
87	OHX	2	2102	-	0,6,6	-	-	-		
87	OHX	2	2125	-	0,6,6	-	-	-		
87	OHX	1	3870	-	0,6,6	-	-	-		
87	OHX	2	2021	-	0,6,6	-	-	-		
87	OHX	1	4090	-	0,6,6	-	-	-		
87	OHX	1	4019	-	0,6,6	-	-	-		
87	OHX	1	4119	-	0,6,6	-	-	-		
87	OHX	L4	403	-	0,6,6	-	-	-		
87	OHX	1	3967	-	0,6,6	-	-	-		
87	OHX	1	3934	-	0,6,6	-	-	-		
87	OHX	1	4028	-	0,6,6	-	-	-		
87	OHX	5	4122	-	0,6,6	-	-	-		
87	OHX	5	4141	-	0,6,6	-	-	-		
87	OHX	6	2154	-	0,6,6	-	-	-		
87	OHX	6	2113	-	0,6,6	-	-	-		
87	OHX	5	3950	-	0,6,6	-	-	-		
87	OHX	1	3994	-	0,6,6	-	-	-		
87	OHX	2	2045	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	6	2074	-	0,6,6	-	-	-		
87	OHX	1	3969	-	0,6,6	-	-	-		
87	OHX	6	2161	-	0,6,6	-	-	-		
87	OHX	8	226	-	0,6,6	-	-	-		
87	OHX	2	2143	-	0,6,6	-	-	-		
87	OHX	2	2141	-	0,6,6	-	-	-		
87	OHX	2	2150	-	0,6,6	-	-	-		
87	OHX	1	3905	-	0,6,6	-	-	-		
87	OHX	2	2039	-	0,6,6	-	-	-		
87	OHX	2	2167	-	0,6,6	-	-	-		
87	OHX	6	2175	-	0,6,6	-	-	-		
87	OHX	2	2036	-	0,6,6	-	-	-		
87	OHX	1	4015	-	0,6,6	-	-	-		
87	OHX	5	3945	-	0,6,6	-	-	-		
87	OHX	5	4075	-	0,6,6	-	-	-		
87	OHX	M7	208	-	0,6,6	-	-	-		
87	OHX	s8	303	-	0,6,6	-	-	-		
87	OHX	5	4014	-	0,6,6	-	-	-		
87	OHX	5	4176	-	0,6,6	-	-	-		
87	OHX	q2	502	-	0,6,6	-	-	-		
87	OHX	5	4055	-	0,6,6	-	-	-		
87	OHX	5	3938	-	0,6,6	-	-	-		
87	OHX	5	4138	-	0,6,6	-	-	-		
87	OHX	1	4079	-	0,6,6	-	-	-		
87	OHX	2	2098	-	0,6,6	-	-	-		
87	OHX	1	4009	-	0,6,6	-	-	-		
87	OHX	1	4082	-	0,6,6	-	-	-		
87	OHX	5	4060	-	0,6,6	-	-	-		
87	OHX	5	4160	-	0,6,6	-	-	-		
87	OHX	5	4163	-	0,6,6	-	-	-		
87	OHX	1	4056	-	0,6,6	-	-	-		
87	OHX	7	222	-	0,6,6	-	-	-		
87	OHX	6	2064	-	0,6,6	-	-	-		
87	OHX	2	2101	-	0,6,6	-	-	-		
87	OHX	1	4062	-	0,6,6	-	-	-		
87	OHX	5	4192	-	0,6,6	-	-	-		
87	OHX	5	3934	-	0,6,6	-	-	-		
87	OHX	1	4051	-	0,6,6	-	-	-		
87	OHX	5	4195	-	0,6,6	-	-	-		
87	OHX	1	4047	-	0,6,6	-	-	-		
87	OHX	n6	202	-	0,6,6	-	-	-		
87	OHX	5	4043	-	0,6,6	-	-	-		
87	OHX	1	3937	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	6	2164	-	0,6,6	-	-	-		
87	OHX	5	4073	-	0,6,6	-	-	-		
87	OHX	2	2113	-	0,6,6	-	-	-		
87	OHX	1	4137	-	0,6,6	-	-	-		
87	OHX	6	2060	-	0,6,6	-	-	-		
87	OHX	5	4089	-	0,6,6	-	-	-		
87	OHX	2	2121	-	0,6,6	-	-	-		
87	OHX	6	2131	-	0,6,6	-	-	-		
87	OHX	C5	201	-	0,6,6	-	-	-		
87	OHX	2	2023	-	0,6,6	-	-	-		
87	OHX	1	4063	-	0,6,6	-	-	-		
87	OHX	2	2047	-	0,6,6	-	-	-		
87	OHX	5	3907	-	0,6,6	-	-	-		
87	OHX	5	3927	-	0,6,6	-	-	-		
87	OHX	5	3941	-	0,6,6	-	-	-		
87	OHX	6	2181	-	0,6,6	-	-	-		
87	OHX	5	4159	-	0,6,6	-	-	-		
87	OHX	1	3953	-	0,6,6	-	-	-		
87	OHX	1	4197	-	0,6,6	-	-	-		
87	OHX	5	4091	-	0,6,6	-	-	-		
87	OHX	6	2206	-	0,6,6	-	-	-		
87	OHX	5	4147	-	0,6,6	-	-	-		
87	OHX	2	2032	-	0,6,6	-	-	-		
87	OHX	8	220	-	0,6,6	-	-	-		
87	OHX	1	3978	-	0,6,6	-	-	-		
87	OHX	1	4101	-	0,6,6	-	-	-		
87	OHX	6	2082	-	0,6,6	-	-	-		
87	OHX	1	4061	-	0,6,6	-	-	-		
87	OHX	1	4185	-	0,6,6	-	-	-		
87	OHX	5	4248	-	0,6,6	-	-	-		
87	OHX	5	4231	-	0,6,6	-	-	-		
87	OHX	1	4167	-	0,6,6	-	-	-		
87	OHX	5	4044	-	0,6,6	-	-	-		
87	OHX	5	4175	-	0,6,6	-	-	-		
87	OHX	5	3917	-	0,6,6	-	-	-		
87	OHX	2	2106	-	0,6,6	-	-	-		
87	OHX	3	222	-	0,6,6	-	-	-		
87	OHX	1	4198	-	0,6,6	-	-	-		
87	OHX	8	217	-	0,6,6	-	-	-		
87	OHX	M0	303	-	0,6,6	-	-	-		
87	OHX	6	2169	-	0,6,6	-	-	-		
87	OHX	2	2077	-	0,6,6	-	-	-		
87	OHX	1	4026	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4033	-	0,6,6	-	-	-		
87	OHX	1	4054	-	0,6,6	-	-	-		
87	OHX	1	4130	-	0,6,6	-	-	-		
87	OHX	5	3988	-	0,6,6	-	-	-		
87	OHX	5	4029	-	0,6,6	-	-	-		
87	OHX	6	2059	-	0,6,6	-	-	-		
87	OHX	5	4188	-	0,6,6	-	-	-		
87	OHX	1	3900	-	0,6,6	-	-	-		
87	OHX	6	2144	-	0,6,6	-	-	-		
87	OHX	1	4078	-	0,6,6	-	-	-		
87	OHX	5	4211	-	0,6,6	-	-	-		
87	OHX	2	2122	-	0,6,6	-	-	-		
87	OHX	1	3954	-	0,6,6	-	-	-		
87	OHX	1	3931	-	0,6,6	-	-	-		
87	OHX	2	2105	-	0,6,6	-	-	-		
87	OHX	6	2183	-	0,6,6	-	-	-		
87	OHX	6	2207	-	0,6,6	-	-	-		
87	OHX	5	4123	-	0,6,6	-	-	-		
87	OHX	5	4092	-	0,6,6	-	-	-		
87	OHX	7	220	-	0,6,6	-	-	-		
87	OHX	1	4203	-	0,6,6	-	-	-		
87	OHX	6	2149	-	0,6,6	-	-	-		
87	OHX	5	3924	-	0,6,6	-	-	-		
87	OHX	1	4178	-	0,6,6	-	-	-		
87	OHX	m8	201	-	0,6,6	-	-	-		
87	OHX	1	3916	-	0,6,6	-	-	-		
87	OHX	2	2082	-	0,6,6	-	-	-		
87	OHX	6	2147	-	0,6,6	-	-	-		
87	OHX	N9	101	-	0,6,6	-	-	-		
87	OHX	1	3878	-	0,6,6	-	-	-		
87	OHX	m0	301	-	0,6,6	-	-	-		
87	OHX	5	4039	-	0,6,6	-	-	-		
87	OHX	5	4015	-	0,6,6	-	-	-		
87	OHX	1	4080	-	0,6,6	-	-	-		
87	OHX	2	2177	-	0,6,6	-	-	-		
87	OHX	6	2051	-	0,6,6	-	-	-		
87	OHX	5	4100	-	0,6,6	-	-	-		
87	OHX	6	2145	-	0,6,6	-	-	-		
87	OHX	1	3913	-	0,6,6	-	-	-		
87	OHX	1	3918	-	0,6,6	-	-	-		
87	OHX	5	4187	-	0,6,6	-	-	-		
87	OHX	5	3951	-	0,6,6	-	-	-		
87	OHX	1	3961	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	3997	-	0,6,6	-	-	-		
87	OHX	6	2129	-	0,6,6	-	-	-		
87	OHX	m4	201	-	0,6,6	-	-	-		
87	OHX	2	2057	-	0,6,6	-	-	-		
87	OHX	6	2088	-	0,6,6	-	-	-		
87	OHX	D9	102	-	0,6,6	-	-	-		
87	OHX	7	226	-	0,6,6	-	-	-		
87	OHX	6	2136	-	0,6,6	-	-	-		
87	OHX	M6	202	-	0,6,6	-	-	-		
87	OHX	1	4172	-	0,6,6	-	-	-		
87	OHX	1	3880	-	0,6,6	-	-	-		
87	OHX	2	2117	-	0,6,6	-	-	-		
87	OHX	1	3980	-	0,6,6	-	-	-		
87	OHX	5	3944	-	0,6,6	-	-	-		
87	OHX	1	4116	-	0,6,6	-	-	-		
87	OHX	7	217	-	0,6,6	-	-	-		
87	OHX	1	4066	-	0,6,6	-	-	-		
87	OHX	5	4184	-	0,6,6	-	-	-		
87	OHX	2	2112	-	0,6,6	-	-	-		
87	OHX	4	221	-	0,6,6	-	-	-		
87	OHX	5	4012	-	0,6,6	-	-	-		
87	OHX	2	2142	-	0,6,6	-	-	-		
87	OHX	6	2203	-	0,6,6	-	-	-		
87	OHX	1	4173	-	0,6,6	-	-	-		
87	OHX	6	2096	-	0,6,6	-	-	-		
87	OHX	6	2054	-	0,6,6	-	-	-		
87	OHX	5	4193	-	0,6,6	-	-	-		
87	OHX	1	3919	-	0,6,6	-	-	-		
87	OHX	1	4027	-	0,6,6	-	-	-		
87	OHX	6	2092	-	0,6,6	-	-	-		
87	OHX	6	2143	-	0,6,6	-	-	-		
87	OHX	6	2071	-	0,6,6	-	-	-		
87	OHX	6	2053	-	0,6,6	-	-	-		
87	OHX	6	2155	-	0,6,6	-	-	-		
87	OHX	5	3986	-	0,6,6	-	-	-		
87	OHX	1	4118	-	0,6,6	-	-	-		
87	OHX	c3	201	-	0,6,6	-	-	-		
87	OHX	2	2094	-	0,6,6	-	-	-		
87	OHX	5	3947	-	0,6,6	-	-	-		
87	OHX	6	2055	-	0,6,6	-	-	-		
87	OHX	C3	201	-	0,6,6	-	-	-		
87	OHX	1	4034	-	0,6,6	-	-	-		
87	OHX	5	4005	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	2	2041	-	0,6,6	-	-	-		
87	OHX	1	4113	-	0,6,6	-	-	-		
87	OHX	5	4128	-	0,6,6	-	-	-		
87	OHX	1	3927	-	0,6,6	-	-	-		
87	OHX	2	2129	-	0,6,6	-	-	-		
87	OHX	5	3930	-	0,6,6	-	-	-		
87	OHX	5	4220	-	0,6,6	-	-	-		
87	OHX	5	3959	-	0,6,6	-	-	-		
87	OHX	5	4250	-	0,6,6	-	-	-		
87	OHX	1	4031	-	0,6,6	-	-	-		
87	OHX	1	4094	-	0,6,6	-	-	-		
87	OHX	1	4181	-	0,6,6	-	-	-		
87	OHX	1	3911	-	0,6,6	-	-	-		
87	OHX	1	4074	-	0,6,6	-	-	-		
87	OHX	5	4108	-	0,6,6	-	-	-		
87	OHX	1	4049	-	0,6,6	-	-	-		
87	OHX	5	4165	-	0,6,6	-	-	-		
87	OHX	5	4143	-	0,6,6	-	-	-		
87	OHX	5	4207	-	0,6,6	-	-	-		
87	OHX	3	226	-	0,6,6	-	-	-		
87	OHX	5	4218	-	0,6,6	-	-	-		
87	OHX	8	216	-	0,6,6	-	-	-		
87	OHX	1	4188	-	0,6,6	-	-	-		
87	OHX	5	4095	-	0,6,6	-	-	-		
87	OHX	5	4057	-	0,6,6	-	-	-		
87	OHX	m1	202	-	0,6,6	-	-	-		
87	OHX	5	4121	-	0,6,6	-	-	-		
87	OHX	1	3897	-	0,6,6	-	-	-		
87	OHX	6	2170	-	0,6,6	-	-	-		
87	OHX	3	217	-	0,6,6	-	-	-		
87	OHX	5	4021	-	0,6,6	-	-	-		
87	OHX	2	2161	-	0,6,6	-	-	-		
87	OHX	5	4114	-	0,6,6	-	-	-		
87	OHX	8	215	-	0,6,6	-	-	-		
87	OHX	5	3946	-	0,6,6	-	-	-		
87	OHX	5	4217	-	0,6,6	-	-	-		
87	OHX	1	3973	-	0,6,6	-	-	-		
87	OHX	1	3965	-	0,6,6	-	-	-		
87	OHX	5	4204	-	0,6,6	-	-	-		
87	OHX	5	3900	-	0,6,6	-	-	-		
87	OHX	1	4105	-	0,6,6	-	-	-		
87	OHX	5	3908	-	0,6,6	-	-	-		
87	OHX	5	4227	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	l4	403	-	0,6,6	-	-	-		
87	OHX	1	4087	-	0,6,6	-	-	-		
87	OHX	5	4235	-	0,6,6	-	-	-		
87	OHX	1	3956	-	0,6,6	-	-	-		
87	OHX	4	229	-	0,6,6	-	-	-		
87	OHX	6	2069	-	0,6,6	-	-	-		
87	OHX	5	4225	-	0,6,6	-	-	-		
87	OHX	2	2027	-	0,6,6	-	-	-		
87	OHX	O7	104	-	0,6,6	-	-	-		
87	OHX	5	4209	-	0,6,6	-	-	-		
87	OHX	1	4187	-	0,6,6	-	-	-		
87	OHX	1	3894	-	0,6,6	-	-	-		
87	OHX	1	3903	-	0,6,6	-	-	-		
87	OHX	2	2147	-	0,6,6	-	-	-		
87	OHX	6	2201	-	0,6,6	-	-	-		
87	OHX	5	3922	-	0,6,6	-	-	-		
87	OHX	5	4004	-	0,6,6	-	-	-		
87	OHX	5	4124	-	0,6,6	-	-	-		
87	OHX	1	3904	-	0,6,6	-	-	-		
87	OHX	5	4205	-	0,6,6	-	-	-		
87	OHX	c5	201	-	0,6,6	-	-	-		
87	OHX	1	4042	-	0,6,6	-	-	-		
87	OHX	5	4242	-	0,6,6	-	-	-		
87	OHX	5	4013	-	0,6,6	-	-	-		
87	OHX	5	4144	-	0,6,6	-	-	-		
87	OHX	5	4179	-	0,6,6	-	-	-		
87	OHX	5	3915	-	0,6,6	-	-	-		
87	OHX	1	4189	-	0,6,6	-	-	-		
87	OHX	5	4002	-	0,6,6	-	-	-		
87	OHX	5	4086	-	0,6,6	-	-	-		
87	OHX	6	2083	-	0,6,6	-	-	-		
87	OHX	2	2031	-	0,6,6	-	-	-		
87	OHX	2	2085	-	0,6,6	-	-	-		
87	OHX	1	3871	-	0,6,6	-	-	-		
87	OHX	1	4064	-	0,6,6	-	-	-		
87	OHX	2	2070	-	0,6,6	-	-	-		
87	OHX	5	4253	-	0,6,6	-	-	-		
87	OHX	O9	101	-	0,6,6	-	-	-		
87	OHX	5	4087	-	0,6,6	-	-	-		
87	OHX	1	4059	-	0,6,6	-	-	-		
87	OHX	7	219	-	0,6,6	-	-	-		
87	OHX	2	2097	-	0,6,6	-	-	-		
87	OHX	1	3936	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	6	2062	-	0,6,6	-	-	-		
87	OHX	6	2080	-	0,6,6	-	-	-		
87	OHX	1	4157	-	0,6,6	-	-	-		
87	OHX	2	2049	-	0,6,6	-	-	-		
87	OHX	1	4184	-	0,6,6	-	-	-		
87	OHX	2	2064	-	0,6,6	-	-	-		
87	OHX	5	4042	-	0,6,6	-	-	-		
87	OHX	1	4005	-	0,6,6	-	-	-		
87	OHX	1	4077	-	0,6,6	-	-	-		
87	OHX	5	4103	-	0,6,6	-	-	-		
87	OHX	7	223	-	0,6,6	-	-	-		
87	OHX	1	3902	-	0,6,6	-	-	-		
87	OHX	2	2174	-	0,6,6	-	-	-		
87	OHX	1	3892	-	0,6,6	-	-	-		
87	OHX	5	3952	-	0,6,6	-	-	-		
87	OHX	5	4127	-	0,6,6	-	-	-		
87	OHX	5	4158	-	0,6,6	-	-	-		
87	OHX	5	3956	-	0,6,6	-	-	-		
87	OHX	6	2132	-	0,6,6	-	-	-		
87	OHX	5	3931	-	0,6,6	-	-	-		
87	OHX	8	225	-	0,6,6	-	-	-		
87	OHX	6	2091	-	0,6,6	-	-	-		
87	OHX	2	2035	-	0,6,6	-	-	-		
87	OHX	3	216	-	0,6,6	-	-	-		
87	OHX	1	3924	-	0,6,6	-	-	-		
87	OHX	1	4148	-	0,6,6	-	-	-		
87	OHX	1	3999	-	0,6,6	-	-	-		
87	OHX	2	2092	-	0,6,6	-	-	-		
87	OHX	1	4206	-	0,6,6	-	-	-		
87	OHX	2	2071	-	0,6,6	-	-	-		
87	OHX	5	4154	-	0,6,6	-	-	-		
87	OHX	2	2140	-	0,6,6	-	-	-		
87	OHX	5	3919	-	0,6,6	-	-	-		
87	OHX	1	4201	-	0,6,6	-	-	-		
87	OHX	1	3879	-	0,6,6	-	-	-		
87	OHX	5	4126	-	0,6,6	-	-	-		
87	OHX	2	2073	-	0,6,6	-	-	-		
87	OHX	1	3941	-	0,6,6	-	-	-		
87	OHX	5	3973	-	0,6,6	-	-	-		
87	OHX	2	2109	-	0,6,6	-	-	-		
87	OHX	1	3935	-	0,6,6	-	-	-		
87	OHX	1	3881	-	0,6,6	-	-	-		
87	OHX	5	4249	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	4164	-	0,6,6	-	-	-		
87	OHX	2	2162	-	0,6,6	-	-	-		
87	OHX	4	227	-	0,6,6	-	-	-		
87	OHX	5	4050	-	0,6,6	-	-	-		
87	OHX	1	4205	-	0,6,6	-	-	-		
87	OHX	6	2084	-	0,6,6	-	-	-		
87	OHX	1	4091	-	0,6,6	-	-	-		
87	OHX	5	4170	-	0,6,6	-	-	-		
87	OHX	1	4160	-	0,6,6	-	-	-		
87	OHX	5	4206	-	0,6,6	-	-	-		
87	OHX	6	2151	-	0,6,6	-	-	-		
87	OHX	1	3987	-	0,6,6	-	-	-		
87	OHX	2	2059	-	0,6,6	-	-	-		
87	OHX	1	4141	-	0,6,6	-	-	-		
87	OHX	M8	202	-	0,6,6	-	-	-		
87	OHX	5	3916	-	0,6,6	-	-	-		
87	OHX	1	4122	-	0,6,6	-	-	-		
87	OHX	5	3960	-	0,6,6	-	-	-		
87	OHX	n3	203	-	0,6,6	-	-	-		
87	OHX	5	3943	-	0,6,6	-	-	-		
87	OHX	5	3968	-	0,6,6	-	-	-		
87	OHX	1	3955	-	0,6,6	-	-	-		
87	OHX	5	4068	-	0,6,6	-	-	-		
87	OHX	5	4145	-	0,6,6	-	-	-		
87	OHX	5	4051	-	0,6,6	-	-	-		
87	OHX	2	2146	-	0,6,6	-	-	-		
87	OHX	5	4236	-	0,6,6	-	-	-		
87	OHX	1	4147	-	0,6,6	-	-	-		
87	OHX	5	4177	-	0,6,6	-	-	-		
87	OHX	S8	302	-	0,6,6	-	-	-		
87	OHX	1	3886	-	0,6,6	-	-	-		
87	OHX	2	2058	-	0,6,6	-	-	-		
87	OHX	1	3984	-	0,6,6	-	-	-		
87	OHX	1	4093	-	0,6,6	-	-	-		
87	OHX	5	4054	-	0,6,6	-	-	-		
87	OHX	2	2164	-	0,6,6	-	-	-		
87	OHX	1	4014	-	0,6,6	-	-	-		
87	OHX	1	4176	-	0,6,6	-	-	-		
87	OHX	6	2070	-	0,6,6	-	-	-		
87	OHX	5	4110	-	0,6,6	-	-	-		
87	OHX	5	4129	-	0,6,6	-	-	-		
87	OHX	1	4217	-	0,6,6	-	-	-		
87	OHX	6	2104	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	3903	-	0,6,6	-	-	-		
87	OHX	1	4016	-	0,6,6	-	-	-		
87	OHX	4	226	-	0,6,6	-	-	-		
87	OHX	5	4064	-	0,6,6	-	-	-		
87	OHX	5	4106	-	0,6,6	-	-	-		
87	OHX	6	2050	-	0,6,6	-	-	-		
87	OHX	5	4194	-	0,6,6	-	-	-		
87	OHX	5	4223	-	0,6,6	-	-	-		
87	OHX	1	3995	-	0,6,6	-	-	-		
87	OHX	5	3991	-	0,6,6	-	-	-		
87	OHX	1	3914	-	0,6,6	-	-	-		
87	OHX	5	3925	-	0,6,6	-	-	-		
87	OHX	2	2053	-	0,6,6	-	-	-		
87	OHX	1	4140	-	0,6,6	-	-	-		
87	OHX	2	2084	-	0,6,6	-	-	-		
87	OHX	2	2076	-	0,6,6	-	-	-		
87	OHX	5	4102	-	0,6,6	-	-	-		
87	OHX	2	2170	-	0,6,6	-	-	-		
87	OHX	6	2184	-	0,6,6	-	-	-		
87	OHX	2	2135	-	0,6,6	-	-	-		
87	OHX	2	2111	-	0,6,6	-	-	-		
87	OHX	1	3925	-	0,6,6	-	-	-		
87	OHX	1	3882	-	0,6,6	-	-	-		
87	OHX	1	3940	-	0,6,6	-	-	-		
87	OHX	2	2037	-	0,6,6	-	-	-		
87	OHX	1	4073	-	0,6,6	-	-	-		
87	OHX	1	4125	-	0,6,6	-	-	-		
87	OHX	c8	201	-	0,6,6	-	-	-		
87	OHX	1	4089	-	0,6,6	-	-	-		
87	OHX	5	4069	-	0,6,6	-	-	-		
87	OHX	1	4020	-	0,6,6	-	-	-		
87	OHX	5	4088	-	0,6,6	-	-	-		
87	OHX	5	4076	-	0,6,6	-	-	-		
87	OHX	n9	101	-	0,6,6	-	-	-		
87	OHX	2	2050	-	0,6,6	-	-	-		
87	OHX	5	3929	-	0,6,6	-	-	-		
87	OHX	1	4162	-	0,6,6	-	-	-		
87	OHX	1	4010	-	0,6,6	-	-	-		
87	OHX	2	2123	-	0,6,6	-	-	-		
87	OHX	1	4052	-	0,6,6	-	-	-		
87	OHX	s4	302	-	0,6,6	-	-	-		
87	OHX	2	2075	-	0,6,6	-	-	-		
87	OHX	5	3990	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	6	2186	-	0,6,6	-	-	-		
87	OHX	l5	304	-	0,6,6	-	-	-		
87	OHX	6	2077	-	0,6,6	-	-	-		
87	OHX	1	4095	-	0,6,6	-	-	-		
87	OHX	1	4159	-	0,6,6	-	-	-		
87	OHX	L3	403	-	0,6,6	-	-	-		
87	OHX	2	2169	-	0,6,6	-	-	-		
87	OHX	5	4208	-	0,6,6	-	-	-		
87	OHX	5	3914	-	0,6,6	-	-	-		
87	OHX	1	4040	-	0,6,6	-	-	-		
87	OHX	8	218	-	0,6,6	-	-	-		
87	OHX	6	2172	-	0,6,6	-	-	-		
87	OHX	5	4018	-	0,6,6	-	-	-		
87	OHX	2	2091	-	0,6,6	-	-	-		
87	OHX	6	2110	-	0,6,6	-	-	-		
87	OHX	6	2073	-	0,6,6	-	-	-		
87	OHX	5	3970	-	0,6,6	-	-	-		
87	OHX	5	4001	-	0,6,6	-	-	-		
87	OHX	5	4171	-	0,6,6	-	-	-		
87	OHX	8	224	-	0,6,6	-	-	-		
87	OHX	2	2078	-	0,6,6	-	-	-		
87	OHX	2	2029	-	0,6,6	-	-	-		
87	OHX	2	2114	-	0,6,6	-	-	-		
87	OHX	1	4151	-	0,6,6	-	-	-		
87	OHX	5	4035	-	0,6,6	-	-	-		
87	OHX	6	2157	-	0,6,6	-	-	-		
87	OHX	6	2168	-	0,6,6	-	-	-		
87	OHX	5	3966	-	0,6,6	-	-	-		
87	OHX	2	2127	-	0,6,6	-	-	-		
87	OHX	5	4214	-	0,6,6	-	-	-		
87	OHX	1	4075	-	0,6,6	-	-	-		
87	OHX	5	4166	-	0,6,6	-	-	-		
87	OHX	6	2067	-	0,6,6	-	-	-		
87	OHX	5	4238	-	0,6,6	-	-	-		
87	OHX	5	4134	-	0,6,6	-	-	-		
87	OHX	8	219	-	0,6,6	-	-	-		
87	OHX	6	2137	-	0,6,6	-	-	-		
87	OHX	2	2149	-	0,6,6	-	-	-		
87	OHX	2	2155	-	0,6,6	-	-	-		
87	OHX	m0	302	-	0,6,6	-	-	-		
87	OHX	2	2024	-	0,6,6	-	-	-		
87	OHX	1	3932	-	0,6,6	-	-	-		
87	OHX	6	2125	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	1	3943	-	0,6,6	-	-	-		
87	OHX	2	2156	-	0,6,6	-	-	-		
87	OHX	2	2163	-	0,6,6	-	-	-		
87	OHX	6	2126	-	0,6,6	-	-	-		
87	OHX	5	3935	-	0,6,6	-	-	-		
87	OHX	5	4056	-	0,6,6	-	-	-		
87	OHX	1	3958	-	0,6,6	-	-	-		
87	OHX	l4	402	-	0,6,6	-	-	-		
87	OHX	6	2095	-	0,6,6	-	-	-		
87	OHX	1	4216	-	0,6,6	-	-	-		
87	OHX	6	2124	-	0,6,6	-	-	-		
87	OHX	1	4109	-	0,6,6	-	-	-		
87	OHX	3	218	-	0,6,6	-	-	-		
87	OHX	1	4022	-	0,6,6	-	-	-		
87	OHX	1	3930	-	0,6,6	-	-	-		
87	OHX	1	4103	-	0,6,6	-	-	-		
87	OHX	6	2078	-	0,6,6	-	-	-		
87	OHX	1	4131	-	0,6,6	-	-	-		
87	OHX	2	2139	-	0,6,6	-	-	-		
87	OHX	1	3920	-	0,6,6	-	-	-		
87	OHX	6	2061	-	0,6,6	-	-	-		
87	OHX	1	4123	-	0,6,6	-	-	-		
87	OHX	7	218	-	0,6,6	-	-	-		
87	OHX	2	2173	-	0,6,6	-	-	-		
87	OHX	1	3947	-	0,6,6	-	-	-		
87	OHX	5	3987	-	0,6,6	-	-	-		
87	OHX	8	230	-	0,6,6	-	-	-		
87	OHX	1	4050	-	0,6,6	-	-	-		
87	OHX	5	3964	-	0,6,6	-	-	-		
87	OHX	2	2165	-	0,6,6	-	-	-		
87	OHX	5	4030	-	0,6,6	-	-	-		
87	OHX	1	4041	-	0,6,6	-	-	-		
87	OHX	1	4128	-	0,6,6	-	-	-		
87	OHX	5	4052	-	0,6,6	-	-	-		
87	OHX	6	2081	-	0,6,6	-	-	-		
87	OHX	1	3910	-	0,6,6	-	-	-		
87	OHX	5	3994	-	0,6,6	-	-	-		
87	OHX	5	4136	-	0,6,6	-	-	-		
87	OHX	6	2118	-	0,6,6	-	-	-		
87	OHX	5	3969	-	0,6,6	-	-	-		
87	OHX	5	3962	-	0,6,6	-	-	-		
87	OHX	5	4148	-	0,6,6	-	-	-		
87	OHX	6	2189	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	2	2095	-	0,6,6	-	-	-		
87	OHX	1	4039	-	0,6,6	-	-	-		
87	OHX	6	2156	-	0,6,6	-	-	-		
87	OHX	6	2205	-	0,6,6	-	-	-		
87	OHX	5	3902	-	0,6,6	-	-	-		
87	OHX	5	3984	-	0,6,6	-	-	-		
87	OHX	1	4048	-	0,6,6	-	-	-		
87	OHX	1	4097	-	0,6,6	-	-	-		
87	OHX	1	3893	-	0,6,6	-	-	-		
87	OHX	1	3951	-	0,6,6	-	-	-		
87	OHX	6	2068	-	0,6,6	-	-	-		
87	OHX	1	4126	-	0,6,6	-	-	-		
87	OHX	5	3957	-	0,6,6	-	-	-		
87	OHX	2	2089	-	0,6,6	-	-	-		
87	OHX	1	4115	-	0,6,6	-	-	-		
87	OHX	6	2193	-	0,6,6	-	-	-		
87	OHX	6	2090	-	0,6,6	-	-	-		
87	OHX	5	4151	-	0,6,6	-	-	-		
87	OHX	5	4061	-	0,6,6	-	-	-		
87	OHX	1	4215	-	0,6,6	-	-	-		
87	OHX	5	4185	-	0,6,6	-	-	-		
87	OHX	2	2116	-	0,6,6	-	-	-		
87	OHX	1	4120	-	0,6,6	-	-	-		
87	OHX	5	4079	-	0,6,6	-	-	-		
87	OHX	1	4106	-	0,6,6	-	-	-		
87	OHX	1	4209	-	0,6,6	-	-	-		
87	OHX	6	2141	-	0,6,6	-	-	-		
87	OHX	5	4099	-	0,6,6	-	-	-		
87	OHX	2	2104	-	0,6,6	-	-	-		
87	OHX	5	4140	-	0,6,6	-	-	-		
87	OHX	1	3948	-	0,6,6	-	-	-		
87	OHX	1	4182	-	0,6,6	-	-	-		
87	OHX	7	225	-	0,6,6	-	-	-		
87	OHX	5	4244	-	0,6,6	-	-	-		
87	OHX	1	4012	-	0,6,6	-	-	-		
87	OHX	5	4109	-	0,6,6	-	-	-		
87	OHX	2	2062	-	0,6,6	-	-	-		
87	OHX	6	2199	-	0,6,6	-	-	-		
87	OHX	2	2061	-	0,6,6	-	-	-		
87	OHX	1	3942	-	0,6,6	-	-	-		
87	OHX	5	4020	-	0,6,6	-	-	-		
87	OHX	6	2159	-	0,6,6	-	-	-		
87	OHX	5	4062	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	3967	-	0,6,6	-	-	-		
87	OHX	3	215	-	0,6,6	-	-	-		
87	OHX	5	4097	-	0,6,6	-	-	-		
87	OHX	5	4078	-	0,6,6	-	-	-		
87	OHX	6	2196	-	0,6,6	-	-	-		
87	OHX	1	4213	-	0,6,6	-	-	-		
87	OHX	6	2166	-	0,6,6	-	-	-		
87	OHX	5	4155	-	0,6,6	-	-	-		
87	OHX	o2	201	-	0,6,6	-	-	-		
87	OHX	6	2098	-	0,6,6	-	-	-		
87	OHX	1	4117	-	0,6,6	-	-	-		
87	OHX	5	4058	-	0,6,6	-	-	-		
87	OHX	2	2151	-	0,6,6	-	-	-		
87	OHX	2	2056	-	0,6,6	-	-	-		
87	OHX	5	3940	-	0,6,6	-	-	-		
87	OHX	5	4000	-	0,6,6	-	-	-		
87	OHX	1	3959	-	0,6,6	-	-	-		
87	OHX	6	2058	-	0,6,6	-	-	-		
87	OHX	6	2120	-	0,6,6	-	-	-		
87	OHX	D3	202	-	0,6,6	-	-	-		
87	OHX	1	4086	-	0,6,6	-	-	-		
87	OHX	1	4070	-	0,6,6	-	-	-		
87	OHX	1	4177	-	0,6,6	-	-	-		
87	OHX	5	3953	-	0,6,6	-	-	-		
87	OHX	5	4212	-	0,6,6	-	-	-		
87	OHX	6	2097	-	0,6,6	-	-	-		
87	OHX	6	2138	-	0,6,6	-	-	-		
87	OHX	5	4146	-	0,6,6	-	-	-		
87	OHX	1	4143	-	0,6,6	-	-	-		
87	OHX	1	4132	-	0,6,6	-	-	-		
87	OHX	1	3906	-	0,6,6	-	-	-		
87	OHX	6	2176	-	0,6,6	-	-	-		
87	OHX	6	2204	-	0,6,6	-	-	-		
87	OHX	5	3958	-	0,6,6	-	-	-		
87	OHX	5	4139	-	0,6,6	-	-	-		
87	OHX	5	4186	-	0,6,6	-	-	-		
87	OHX	6	2174	-	0,6,6	-	-	-		
87	OHX	4	224	-	0,6,6	-	-	-		
87	OHX	Q2	503	-	0,6,6	-	-	-		
87	OHX	O3	201	-	0,6,6	-	-	-		
87	OHX	2	2074	-	0,6,6	-	-	-		
87	OHX	1	3899	-	0,6,6	-	-	-		
87	OHX	5	4213	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4234	-	0,6,6	-	-	-		
87	OHX	5	4006	-	0,6,6	-	-	-		
87	OHX	1	3922	-	0,6,6	-	-	-		
87	OHX	5	3912	-	0,6,6	-	-	-		
87	OHX	L3	405	-	0,6,6	-	-	-		
87	OHX	6	2167	-	0,6,6	-	-	-		
87	OHX	1	4204	-	0,6,6	-	-	-		
87	OHX	1	4161	-	0,6,6	-	-	-		
87	OHX	6	2202	-	0,6,6	-	-	-		
87	OHX	1	3908	-	0,6,6	-	-	-		
87	OHX	1	3985	-	0,6,6	-	-	-		
87	OHX	6	2075	-	0,6,6	-	-	-		
87	OHX	2	2028	-	0,6,6	-	-	-		
87	OHX	5	4252	-	0,6,6	-	-	-		
87	OHX	5	4222	-	0,6,6	-	-	-		
87	OHX	5	3977	-	0,6,6	-	-	-		
87	OHX	1	4210	-	0,6,6	-	-	-		
87	OHX	5	4239	-	0,6,6	-	-	-		
87	OHX	1	3889	-	0,6,6	-	-	-		
87	OHX	O2	201	-	0,6,6	-	-	-		
87	OHX	l5	303	-	0,6,6	-	-	-		
87	OHX	c1	202	-	0,6,6	-	-	-		
87	OHX	5	4226	-	0,6,6	-	-	-		
87	OHX	5	4048	-	0,6,6	-	-	-		
87	OHX	1	4003	-	0,6,6	-	-	-		
87	OHX	l9	202	-	0,6,6	-	-	-		
87	OHX	2	2048	-	0,6,6	-	-	-		
87	OHX	1	3938	-	0,6,6	-	-	-		
87	OHX	1	4004	-	0,6,6	-	-	-		
87	OHX	1	4124	-	0,6,6	-	-	-		
87	OHX	5	3949	-	0,6,6	-	-	-		
87	OHX	5	4132	-	0,6,6	-	-	-		
87	OHX	1	4030	-	0,6,6	-	-	-		
87	OHX	SR	401	-	0,6,6	-	-	-		
87	OHX	2	2080	-	0,6,6	-	-	-		
87	OHX	2	2108	-	0,6,6	-	-	-		
87	OHX	4	230	-	0,6,6	-	-	-		
87	OHX	1	4018	-	0,6,6	-	-	-		
87	OHX	1	4149	-	0,6,6	-	-	-		
87	OHX	5	4028	-	0,6,6	-	-	-		
87	OHX	1	4001	-	0,6,6	-	-	-		
87	OHX	1	4098	-	0,6,6	-	-	-		
87	OHX	5	3989	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	6	2089	-	0,6,6	-	-	-		
87	OHX	1	3887	-	0,6,6	-	-	-		
87	OHX	6	2103	-	0,6,6	-	-	-		
87	OHX	2	2081	-	0,6,6	-	-	-		
87	OHX	l3	403	-	0,6,6	-	-	-		
87	OHX	5	3985	-	0,6,6	-	-	-		
87	OHX	5	4080	-	0,6,6	-	-	-		
87	OHX	1	4214	-	0,6,6	-	-	-		
87	OHX	6	2116	-	0,6,6	-	-	-		
87	OHX	5	4049	-	0,6,6	-	-	-		
87	OHX	5	4071	-	0,6,6	-	-	-		
87	OHX	2	2093	-	0,6,6	-	-	-		
87	OHX	1	4053	-	0,6,6	-	-	-		
87	OHX	6	2105	-	0,6,6	-	-	-		
87	OHX	1	4158	-	0,6,6	-	-	-		
87	OHX	5	4090	-	0,6,6	-	-	-		
87	OHX	1	3993	-	0,6,6	-	-	-		
87	OHX	5	3928	-	0,6,6	-	-	-		
87	OHX	1	3976	-	0,6,6	-	-	-		
87	OHX	6	2112	-	0,6,6	-	-	-		
87	OHX	2	2033	-	0,6,6	-	-	-		
87	OHX	1	4110	-	0,6,6	-	-	-		
87	OHX	6	2057	-	0,6,6	-	-	-		
87	OHX	5	4098	-	0,6,6	-	-	-		
87	OHX	5	4117	-	0,6,6	-	-	-		
87	OHX	2	2060	-	0,6,6	-	-	-		
87	OHX	6	2100	-	0,6,6	-	-	-		
87	OHX	1	3876	-	0,6,6	-	-	-		
87	OHX	2	2067	-	0,6,6	-	-	-		
89	3KD	5	4254	-	24,25,25	1.04	2 (8%)	30,39,39	1.06	1 (3%)
87	OHX	6	2160	-	0,6,6	-	-	-		
87	OHX	5	3980	-	0,6,6	-	-	-		
87	OHX	2	2148	-	0,6,6	-	-	-		
87	OHX	5	4084	-	0,6,6	-	-	-		
87	OHX	1	3952	-	0,6,6	-	-	-		
87	OHX	1	4127	-	0,6,6	-	-	-		
87	OHX	2	2133	-	0,6,6	-	-	-		
87	OHX	6	2094	-	0,6,6	-	-	-		
87	OHX	1	4011	-	0,6,6	-	-	-		
87	OHX	5	4174	-	0,6,6	-	-	-		
87	OHX	6	2134	-	0,6,6	-	-	-		
87	OHX	2	2136	-	0,6,6	-	-	-		
87	OHX	5	3939	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	OHX	5	4210	-	0,6,6	-	-	-		
87	OHX	5	4219	-	0,6,6	-	-	-		
87	OHX	5	4046	-	0,6,6	-	-	-		
87	OHX	1	4202	-	0,6,6	-	-	-		
87	OHX	6	2185	-	0,6,6	-	-	-		
87	OHX	6	2093	-	0,6,6	-	-	-		
87	OHX	1	3885	-	0,6,6	-	-	-		
87	OHX	5	4200	-	0,6,6	-	-	-		
87	OHX	5	4104	-	0,6,6	-	-	-		
87	OHX	5	4230	-	0,6,6	-	-	-		
87	OHX	2	2138	-	0,6,6	-	-	-		
87	OHX	1	4154	-	0,6,6	-	-	-		
87	OHX	5	4007	-	0,6,6	-	-	-		
87	OHX	1	3979	-	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
89	3KD	1	4218	-	-	-	0/5/5/5
89	3KD	5	4254	-	-	-	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4254	3KD	C13-C12	3.04	1.54	1.50
89	5	4254	3KD	C8-C9	-2.40	1.47	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
89	5	4254	3KD	O-C14-C9	-3.44	101.86	109.57
89	1	4218	3KD	O-C14-C9	-2.91	103.05	109.57

There are no chirality outliers.

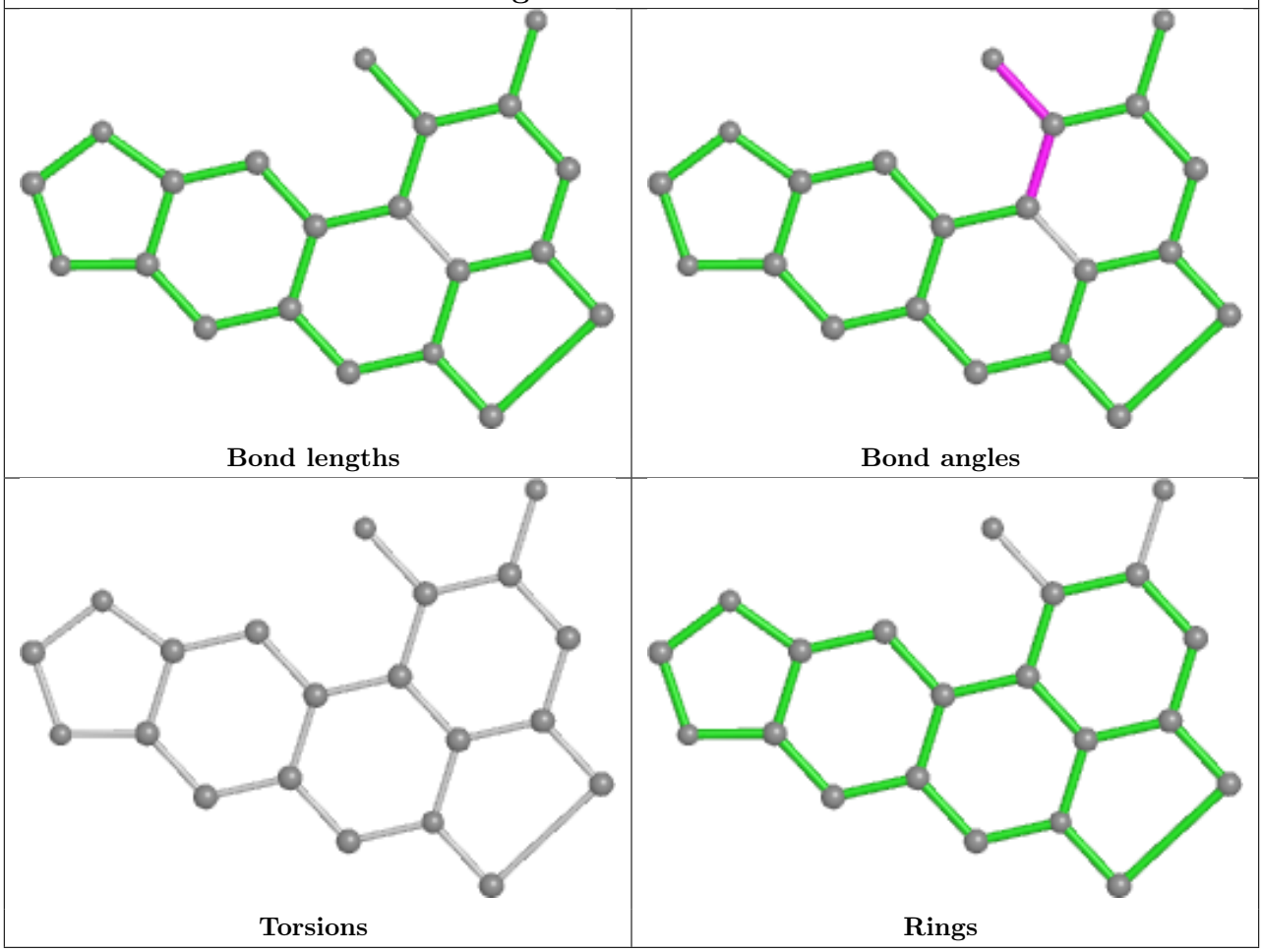
There are no torsion outliers.

There are no ring outliers.

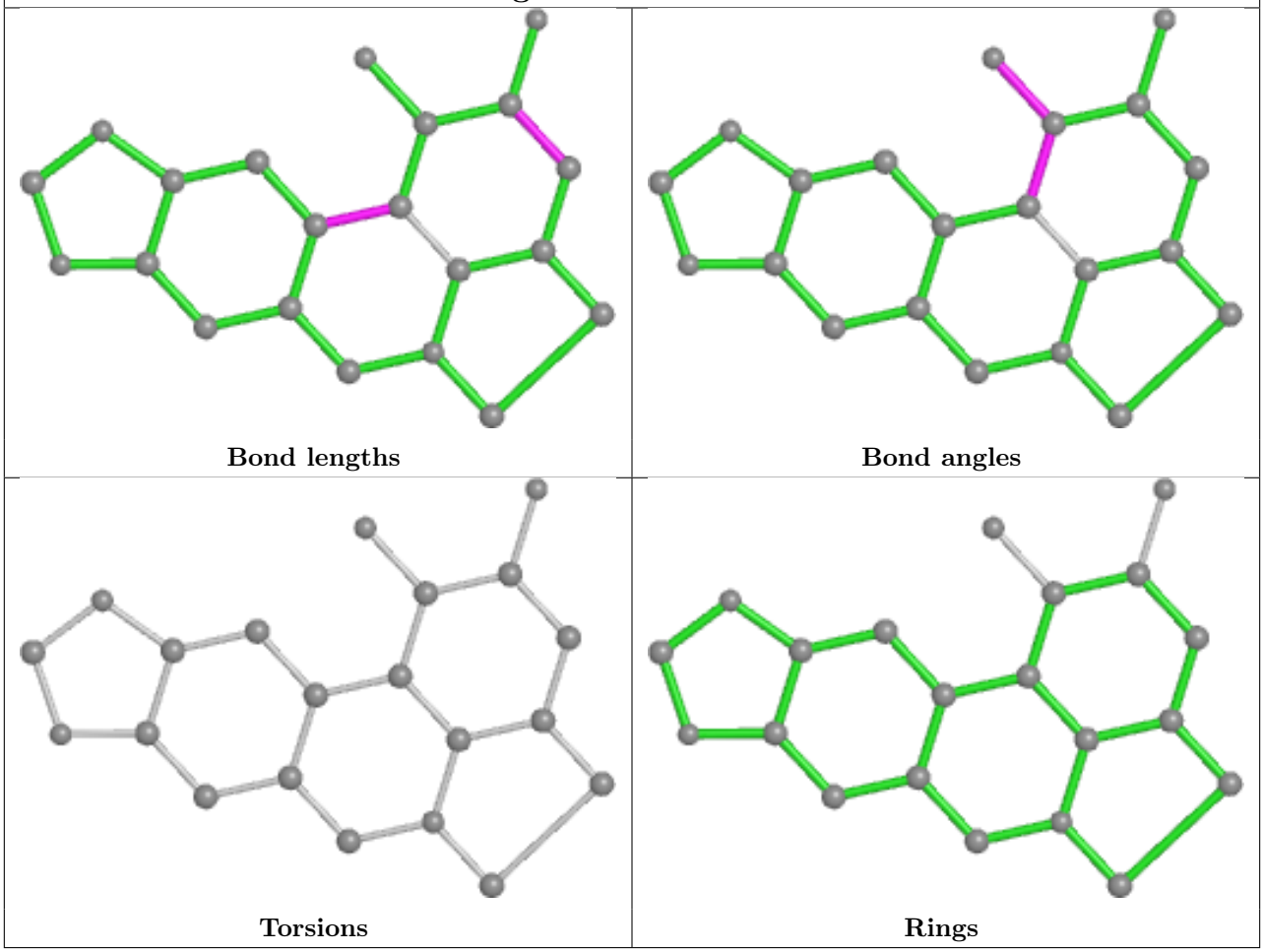
No monomer is involved in short contacts.

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 3KD 1 4218



Ligand 3KD 5 4254



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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