wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 07:08 pm GMT

PDB ID	:	4U51
Title	:	Crystal structure of Narciclasine bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	3.20 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

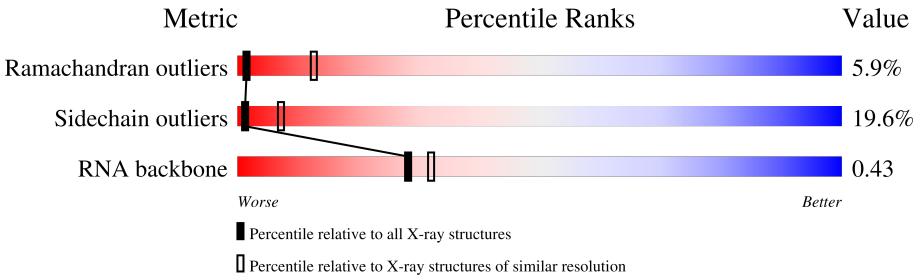
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	63% 30% • •
1	6	1800	65% 30% 5%
2	S0	251	61% 20% • 18%
2	s0	251	64% 16% • 18%
3	S1	254	58% 24% • 16%
3	s1	254	68% 16% • 15%
4	S2	253	68% 17% • 14%
4	s2	253	62% 23% • 14%

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Mol	Chain	Length	Quality of chain
5	S3	239	74% 18% • 7%
5	s3	239	71% 21% • 7%
6	S4	260	80% 18% •
6	s4	260	78% 20% •
7	S5	224	73% 19% 8%
7	s5	224	71% 21% • 8%
8	S6	236	75% 20% •
8	s6	236	77% 15% • 8%
9	S7	189	75% 21% • •
9	s7	189	74% 22% • •
10	S8	200	77% 15% • 6%
10	s8	200	78% 16% • 6%
11	S9	196	70% 22% • 6%
11	s9	196	70% 23% • 6%
12	C0	105	70% 21% • 9%
12	c0	105	66% 22% • 9%
13	C1	155	81% 18% •
13	c1	155	74% 19% • 6%
14	C2	142	64% 20% • 13%
14	c2	142	60% 25% • 13%
15	C3	150	79% 18% •
15	c3	150	79% 19% •
16	C4	136	71% 19% • 7%
16	c4	136	68% 22% • 6%
17	C5	141	69% 16% • 12%

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Mol	Chain	Length	Quality of chain
17	c5	141	71% 23%
18	C6	142	78% 19%
18	c6	142	80% 19%
19	C7	136	70% 12% 6% 12%
19	c7	136	65% 18% 14%
20	C8	145	70% 26%
20	c8	145	73% 26%
21	C9	143	77% 22%
21	c9	143	82% 17%
22	D0	120	72% 18% 11%
22	d0	120	62% 28% 8%
23	D1	87	74% 25%
23	d1	87	70% 28%
24	D2	129	78% 21%
24	d2	129	85% 14%
25	D3	144	83% 13%
25	d3	144	83% 15%
26	D4	134	86% 13%
26	d4	134	75% 24%
27	D5	107	39% 23% 35%
27	d5	107	50% 15% 36%
28	D6	97	66% 28% 6%
28	d6	97	76% 24%
29	D7	81	86% 12%
29	d7	81	77% 23%

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Mol	Chain	Length	Quality of chain
30	D8	66	67% 29% 5%
30	d8	66	74% 20% 5%
31	D9	55	69% 25%
31	d9	55	71% 25%
32	E0	60	82% 17%
33	E1	76	53% 34% 7% 7%
33	e1	76	59% 36% 5%
34	SR	318	86% 14%
34	sR	318	87% 13%
35	SM	273	44% 14% 42%
35	sM	273	29% 9% 62%
36	1	3396	49% 37% 7% 7%
36	5	3396	47% 39% 8% 7%
37	3	121	68% 27% 5%
37	7	121	62% 31% 7%
38	4	158	47% 48%
38	8	158	62% 32% 6%
39	L2	253	80% 19%
39	l2	253	79% 20%
40	L3	386	79% 20%
40	l3	386	78% 21%
41	L4	361	79% 20%
41	l4	361	78% 20%
42	L5	296	81% 18%
42	l5	296	82% 17%

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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	

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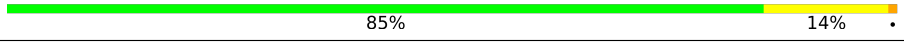
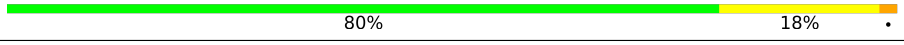
Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	

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Mol	Chain	Length	Quality of chain
68	O2	129	80% 19%
68	o2	129	78% 19%
69	O3	106	80% 19%
69	o3	106	84% 16%
70	O4	120	78% 13% 7%
70	o4	120	77% 17% 7%
71	O5	119	81% 17%
71	o5	119	75% 25%
72	O6	99	79% 17%
72	o6	99	74% 25%
73	O7	87	78% 21%
73	o7	87	87% 13%
74	O8	77	66% 34%
74	o8	77	79% 18%
75	O9	50	82% 18%
75	o9	50	76% 24%
76	Q0	52	81% 17%
76	q0	52	75% 21%
77	Q1	25	76% 24%
77	q1	25	64% 36%
78	Q2	105	73% 23%
78	q2	105	76% 21%
79	Q3	91	80% 19%
79	q3	91	85% 15%
80	e0	62	74% 24%

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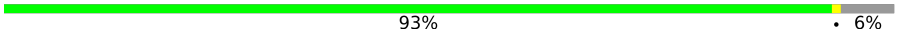
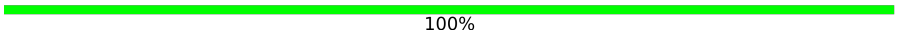
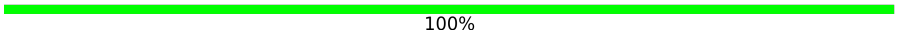
Mol	Chain	Length	Quality of chain
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 411178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	121	LYS	-	expression tag	UNP P87262
o4	121	LYS	-	expression tag	UNP P87262

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called unknown protein chain m2.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

- Molecule 83 is a protein called unknown protein chain p1.

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

- Molecule 84 is a protein called unknown protein chain p2.

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

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	125	Total 125	Mg 125	0	0
85	S2	1	Total 1	Mg 1	0	0
85	D0	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	1	472	Total 472	Mg 472	0	0
85	3	14	Total 14	Mg 14	0	0
85	4	20	Total 20	Mg 20	0	0
85	L2	1	Total 1	Mg 1	0	0
85	L3	1	Total 1	Mg 1	0	0
85	L4	1	Total 1	Mg 1	0	0
85	L5	1	Total 1	Mg 1	0	0
85	L7	4	Total 4	Mg 4	0	0
85	L8	1	Total 1	Mg 1	0	0
85	M0	2	Total 2	Mg 2	0	0
85	M1	1	Total 1	Mg 1	0	0
85	M3	3	Total 3	Mg 3	0	0
85	M5	2	Total 2	Mg 2	0	0
85	M6	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	M7	5	Total Mg 5 5	0	0
85	M9	1	Total Mg 1 1	0	0
85	N0	1	Total Mg 1 1	0	0
85	N3	3	Total Mg 3 3	0	0
85	N5	2	Total Mg 2 2	0	0
85	N6	1	Total Mg 1 1	0	0
85	N8	4	Total Mg 4 4	0	0
85	O2	1	Total Mg 1 1	0	0
85	O7	3	Total Mg 3 3	0	0
85	Q2	1	Total Mg 1 1	0	0
85	6	144	Total Mg 144 144	0	0
85	s1	1	Total Mg 1 1	0	0
85	s6	1	Total Mg 1 1	0	0
85	s8	3	Total Mg 3 3	0	0
85	c1	1	Total Mg 1 1	0	0
85	c4	1	Total Mg 1 1	0	0
85	c7	1	Total Mg 1 1	0	0
85	c8	2	Total Mg 2 2	0	0
85	d3	2	Total Mg 2 2	0	0
85	d4	1	Total Mg 1 1	0	0
85	d6	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	sM	2	Total Mg 2 2	0	0
85	5	501	Total Mg 501 501	0	0
85	7	17	Total Mg 17 17	0	0
85	8	13	Total Mg 13 13	0	0
85	l2	2	Total Mg 2 2	0	0
85	l3	2	Total Mg 2 2	0	0
85	l4	1	Total Mg 1 1	0	0
85	l5	1	Total Mg 1 1	0	0
85	l7	1	Total Mg 1 1	0	0
85	l9	1	Total Mg 1 1	0	0
85	m5	3	Total Mg 3 3	0	0
85	m6	3	Total Mg 3 3	0	0
85	m7	5	Total Mg 5 5	0	0
85	n0	3	Total Mg 3 3	0	0
85	n3	2	Total Mg 2 2	0	0
85	n6	2	Total Mg 2 2	0	0
85	n8	4	Total Mg 4 4	0	0
85	n9	1	Total Mg 1 1	0	0
85	o1	2	Total Mg 2 2	0	0
85	o3	1	Total Mg 1 1	0	0
85	o4	1	Total Mg 1 1	0	0

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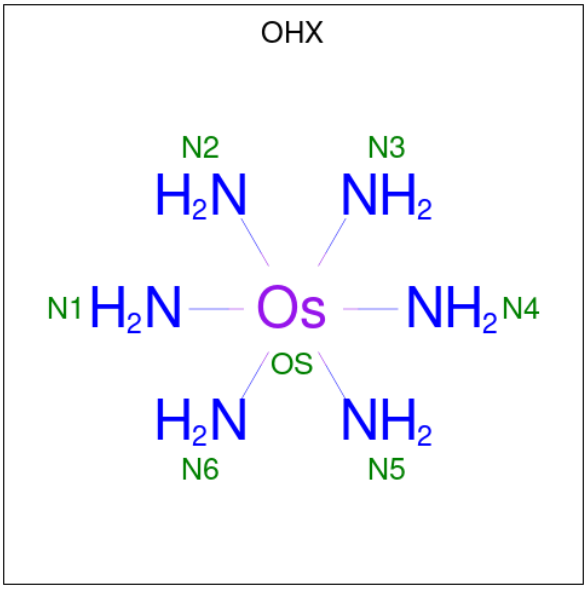
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	o7	1	Total Mg 1 1	0	0
85	o9	1	Total Mg 1 1	0	0
85	q0	1	Total Mg 1 1	0	0
85	q1	1	Total Mg 1 1	0	0
85	q3	2	Total Mg 2 2	0	0

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	1	1	Total N Os 7 6 1	0	0
86	3	1	Total N Os 7 6 1	0	0
86	3	1	Total N Os 7 6 1	0	0
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86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
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86	4	1	Total N Os 7 6 1	0	0
86	4	1	Total N Os 7 6 1	0	0
86	L3	1	Total N Os 7 6 1	0	0
86	L3	1	Total N Os 7 6 1	0	0
86	L4	1	Total N Os 7 6 1	0	0
86	M0	1	Total N Os 7 6 1	0	0
86	M5	1	Total N Os 7 6 1	0	0
86	M7	1	Total N Os 7 6 1	0	0
86	M7	1	Total N Os 7 6 1	0	0
86	M8	1	Total N Os 7 6 1	0	0
86	M9	1	Total N Os 7 6 1	0	0
86	N1	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	N9	1	Total N Os 7 6 1	0	0
86	O3	1	Total N Os 7 6 1	0	0
86	O7	1	Total N Os 7 6 1	0	0
86	O7	1	Total N Os 7 6 1	0	0
86	Q2	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
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86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	6	1	Total N Os 7 6 1	0	0
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86	6	1	Total N Os 7 6 1	0	0
86	s1	1	Total N Os 7 6 1	0	0
86	s1	1	Total N Os 7 6 1	0	0
86	s4	1	Total N Os 7 6 1	0	0
86	s8	1	Total N Os 7 6 1	0	0
86	s9	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	c3	1	Total N Os 7 6 1	0	0
86	c5	1	Total N Os 7 6 1	0	0
86	c8	1	Total N Os 7 6 1	0	0
86	d4	1	Total N Os 7 6 1	0	0
86	d9	1	Total N Os 7 6 1	0	0
86	sR	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	5	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	5	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	5	1	Total N Os 7 6 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
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86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0
86	5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	7	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	l3	1	Total N Os 7 6 1	0	0
86	l3	1	Total N Os 7 6 1	0	0
86	l4	1	Total N Os 7 6 1	0	0
86	l4	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l9	1	Total N Os 7 6 1	0	0
86	m0	1	Total N Os 7 6 1	0	0
86	m0	1	Total N Os 7 6 1	0	0
86	m1	1	Total N Os 7 6 1	0	0
86	m4	1	Total N Os 7 6 1	0	0
86	m5	1	Total N Os 7 6 1	0	0
86	m6	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	m7	1	Total N Os 7 6 1	0	0
86	m8	1	Total N Os 7 6 1	0	0
86	n3	1	Total N Os 7 6 1	0	0
86	n3	1	Total N Os 7 6 1	0	0
86	n5	1	Total N Os 7 6 1	0	0
86	n9	1	Total N Os 7 6 1	0	0
86	o2	1	Total N Os 7 6 1	0	0
86	o3	1	Total N Os 7 6 1	0	0
86	q1	1	Total N Os 7 6 1	0	0
86	q2	1	Total N Os 7 6 1	0	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	D6	1	Total Zn 1 1	0	0
87	D7	1	Total Zn 1 1	0	0
87	D9	1	Total Zn 1 1	0	0
87	E1	1	Total Zn 1 1	0	0
87	O7	1	Total Zn 1 1	0	0
87	Q0	1	Total Zn 1 1	0	0
87	Q2	1	Total Zn 1 1	0	0
87	Q3	1	Total Zn 1 1	0	0
87	d6	1	Total Zn 1 1	0	0

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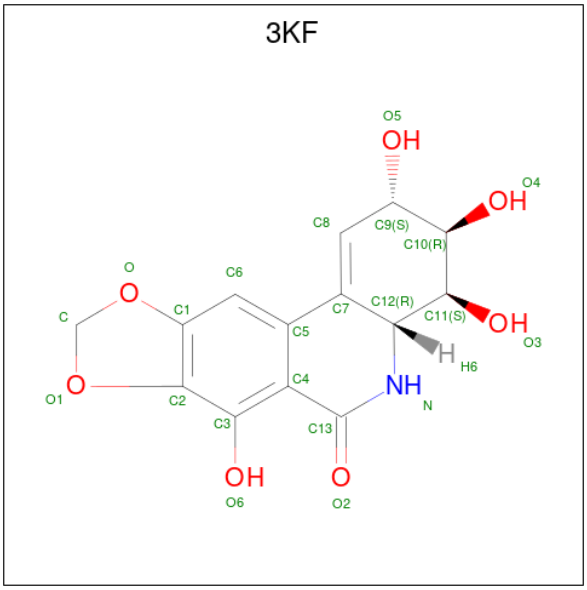
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	d7	1	Total Zn 1 1	0	0
87	d9	1	Total Zn 1 1	0	0
87	e1	1	Total Zn 1 1	0	0
87	o7	1	Total Zn 1 1	0	0
87	q0	1	Total Zn 1 1	0	0
87	q2	1	Total Zn 1 1	0	0
87	q3	1	Total Zn 1 1	0	0

- Molecule 88 is (2S,3R,4S,4aR)-2,3,4,7-tetrahydroxy-3,4,4a,5-tetrahydro[1,3]dioxolo[4,5-j]phenanthridin-6(2H)-one (three-letter code: 3KF) (formula: $C_{14}H_{13}NO_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	1	1	Total C N O 22 14 1 7	0	0
88	5	1	Total C N O 22 14 1 7	0	0

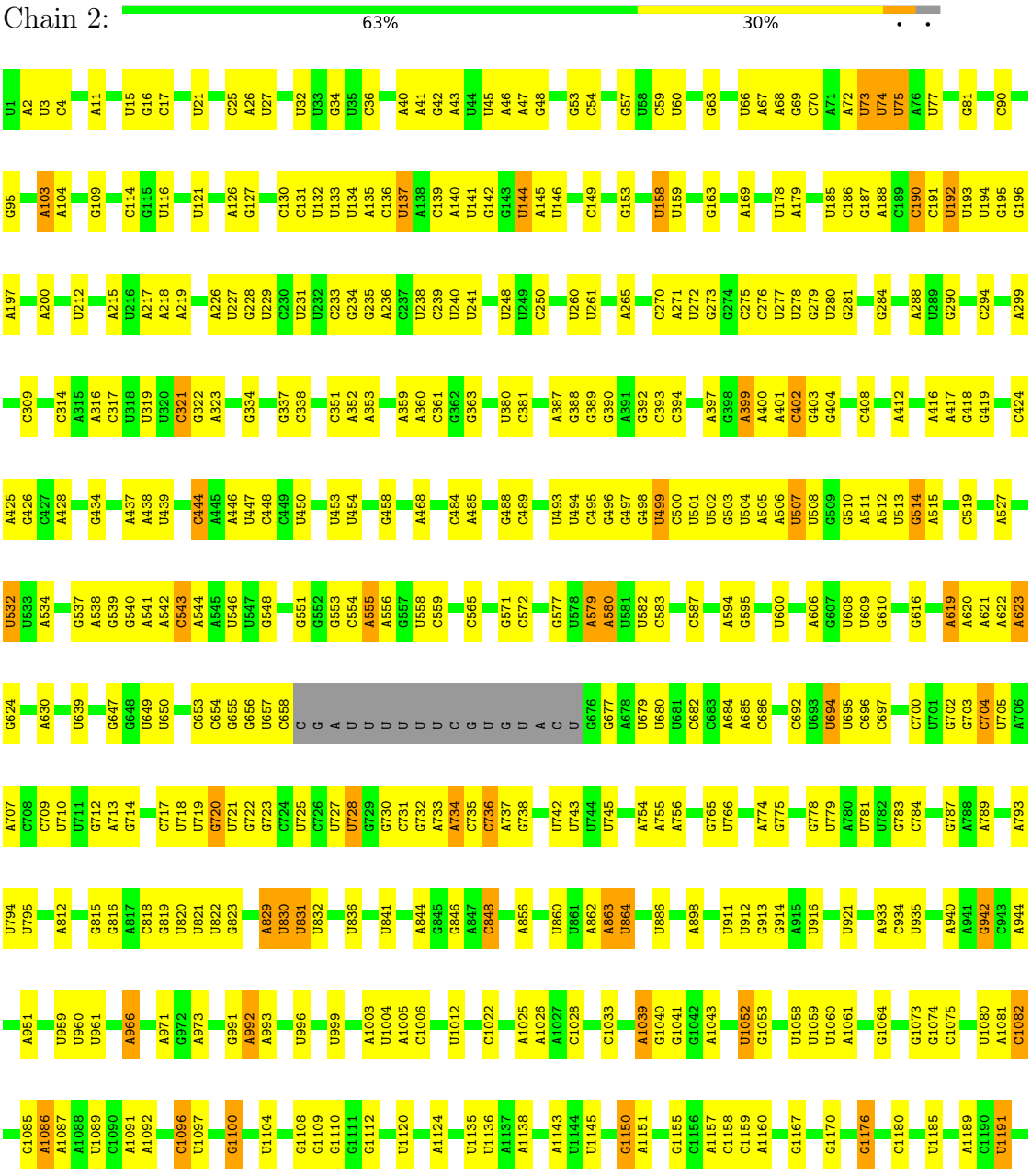
3 Residue-property plots (i)

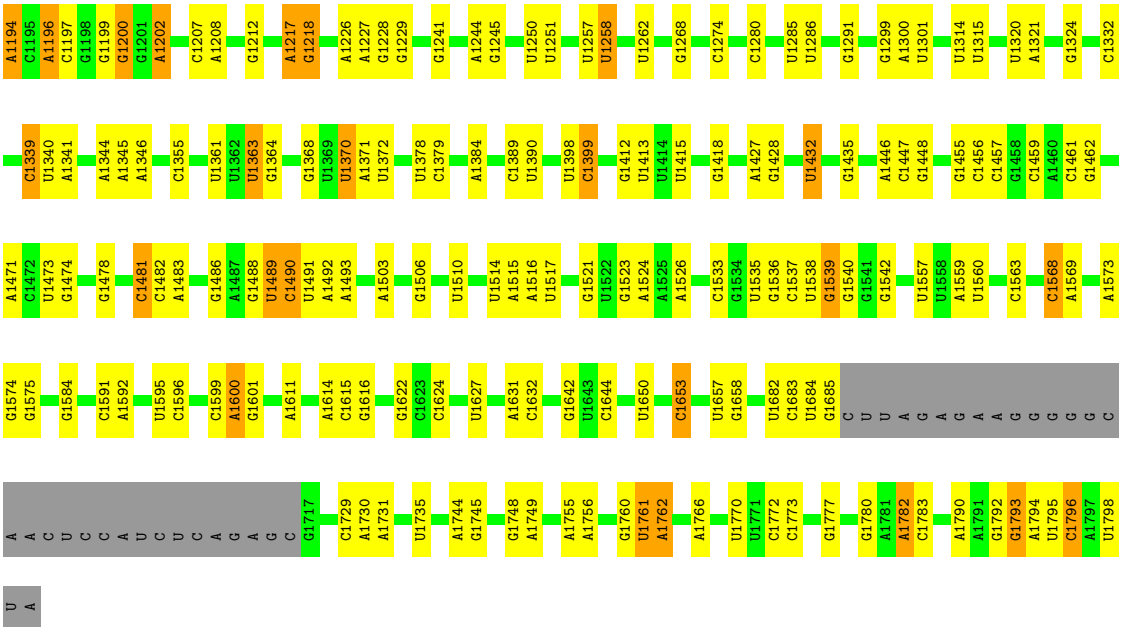
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

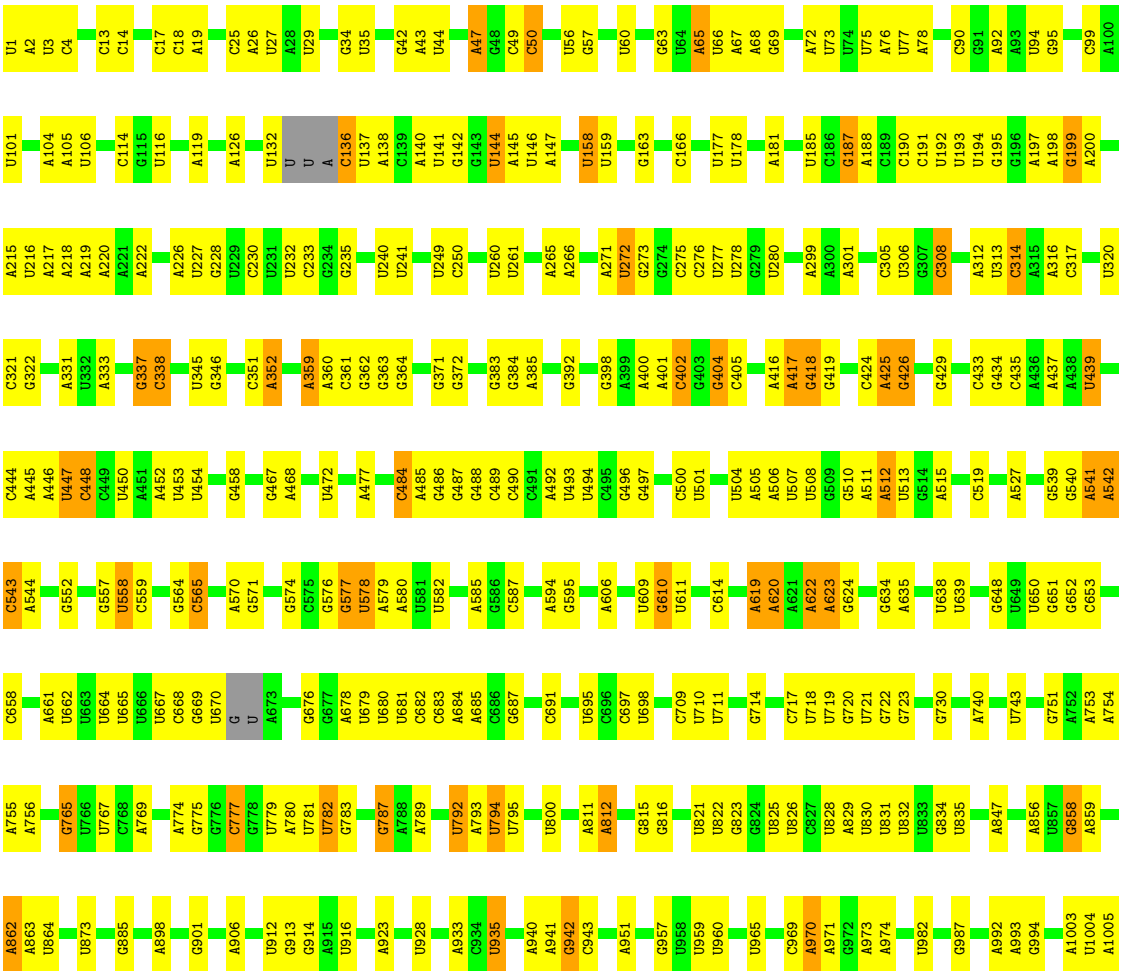
Chain 2:

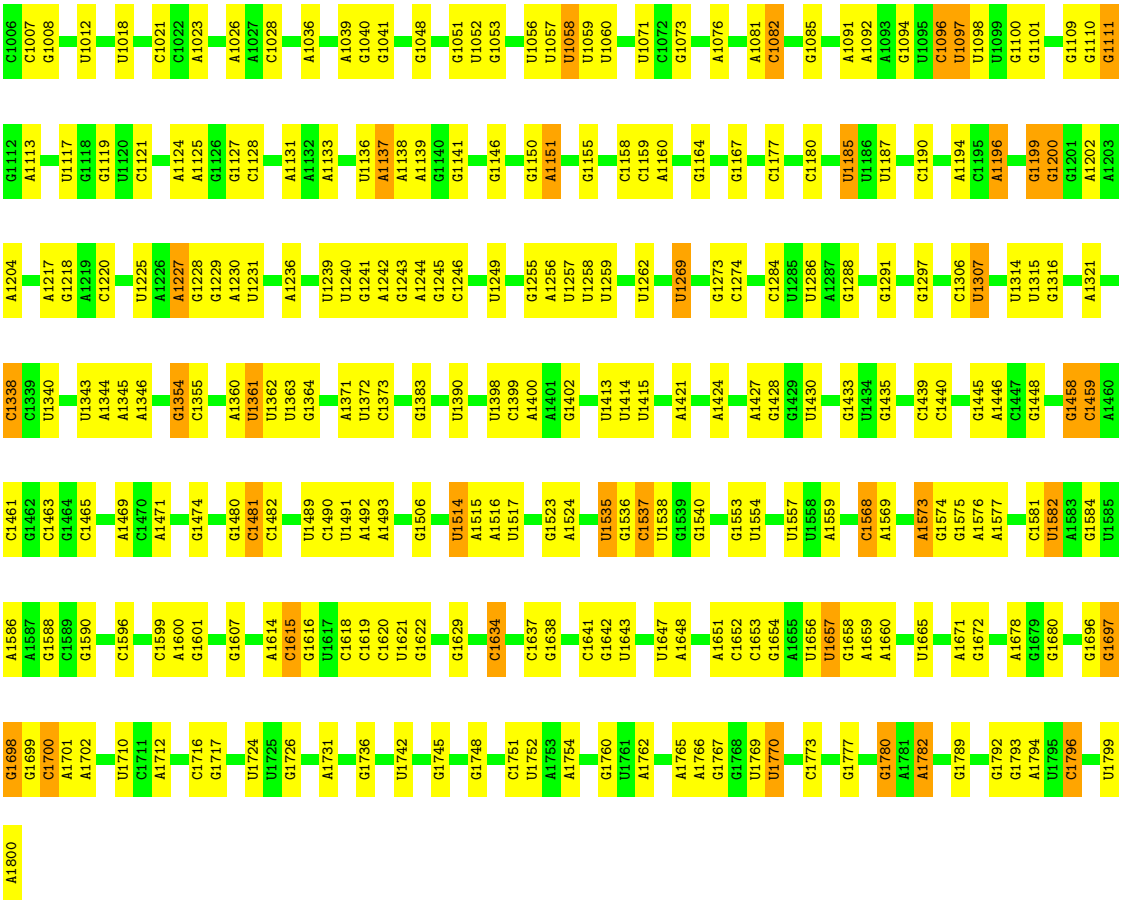




• Molecule 1: 18S ribosomal RNA

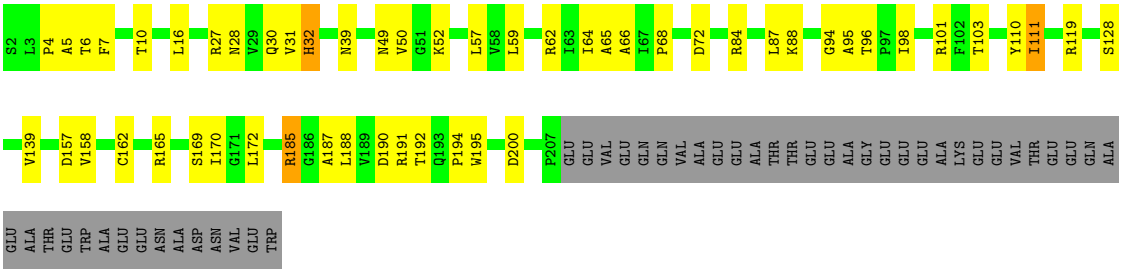
Chain 6:





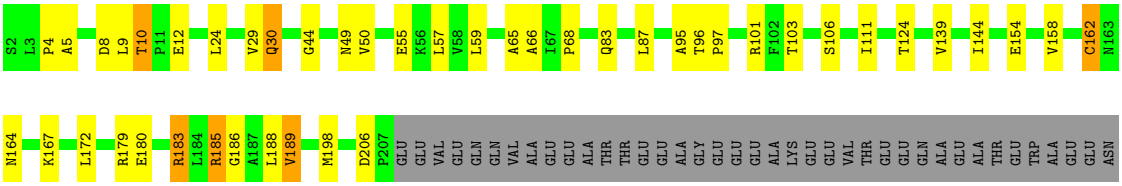
• Molecule 2: 40S ribosomal protein S0-A

Chain S0:



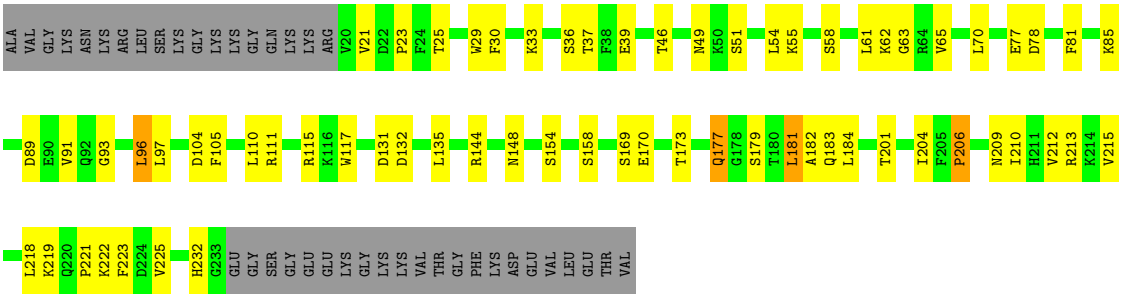
• Molecule 2: 40S ribosomal protein S0-A

Chain s0:



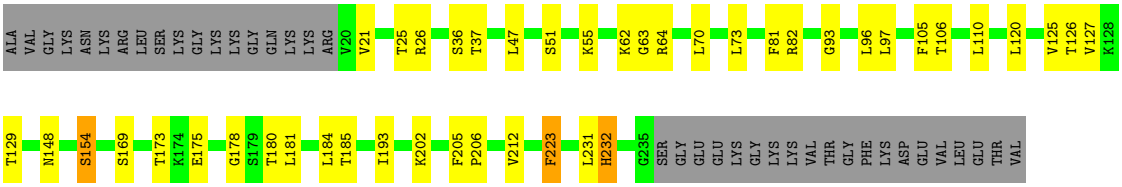
• Molecule 3: 40S ribosomal protein S1-A

Chain S1:



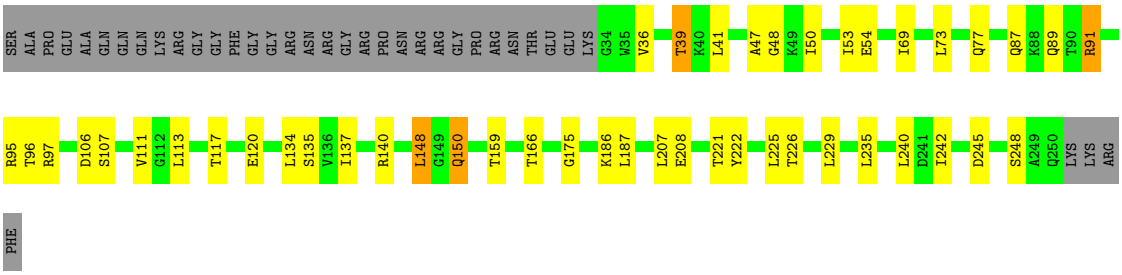
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



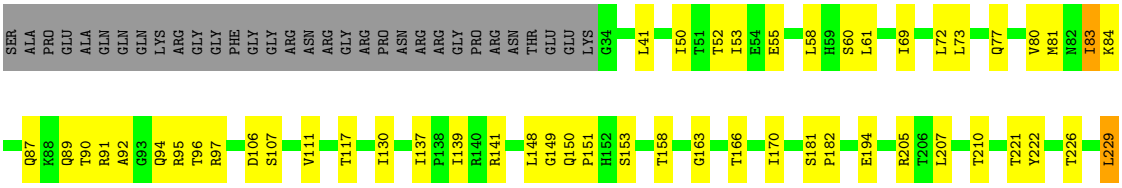
• Molecule 4: 40S ribosomal protein S2

Chain S2:



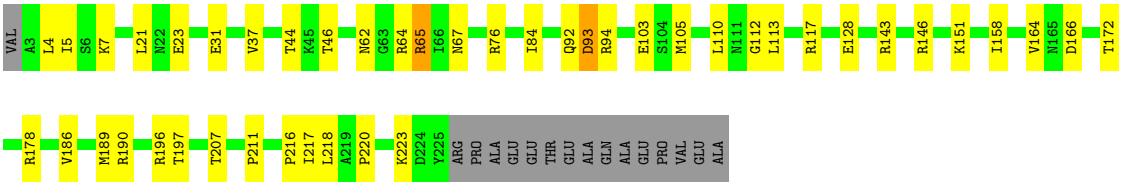
• Molecule 4: 40S ribosomal protein S2

Chain s2:



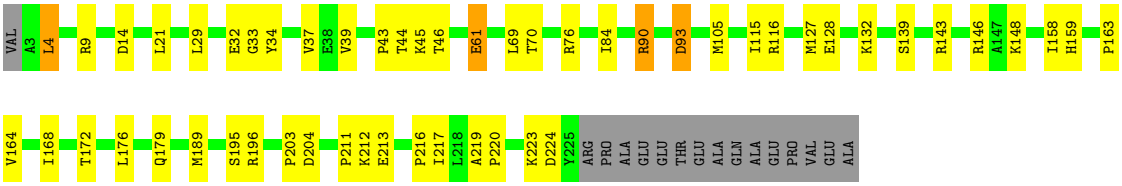
• Molecule 5: 40S ribosomal protein S3

Chain S3:



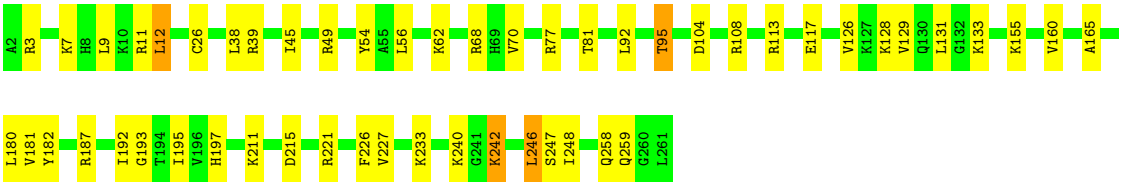
• Molecule 5: 40S ribosomal protein S3

Chain s3:



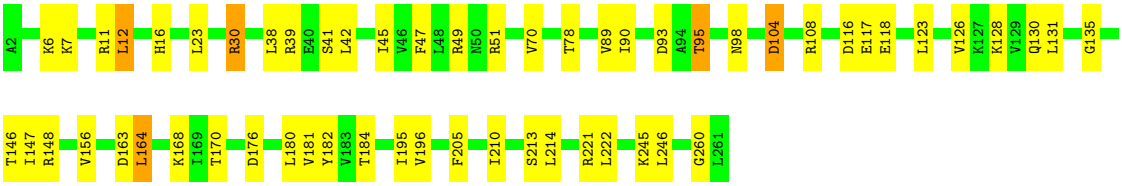
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



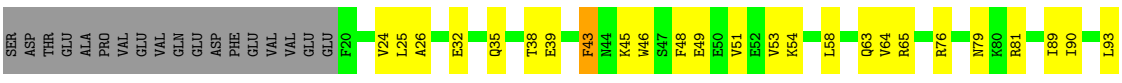
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



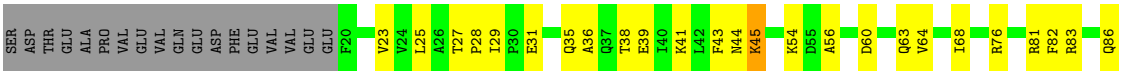
• Molecule 7: 40S ribosomal protein S5

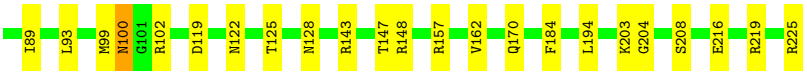
Chain S5:



• Molecule 7: 40S ribosomal protein S5

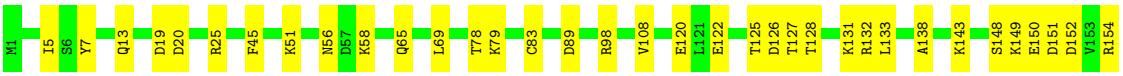
Chain s5:

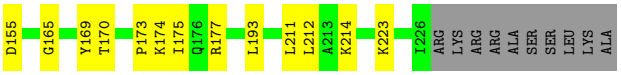




• Molecule 8: 40S ribosomal protein S6-A

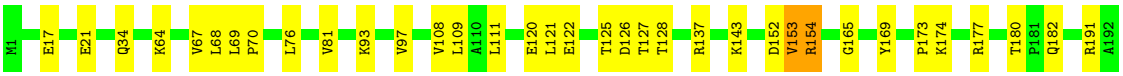
Chain S6:

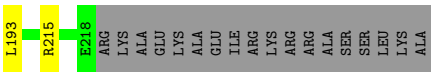




• Molecule 8: 40S ribosomal protein S6-A

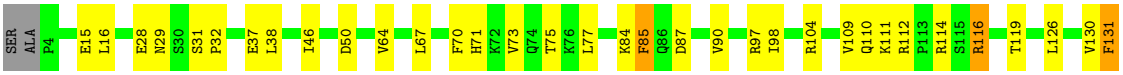
Chain s6:

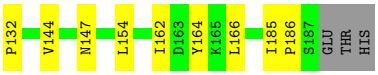




• Molecule 9: 40S ribosomal protein S7-A

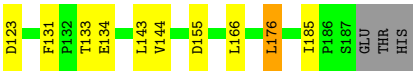
Chain S7:





• Molecule 9: 40S ribosomal protein S7-A

Chain s7:

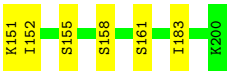


• Molecule 10: 40S ribosomal protein S8-A

Chain S8:

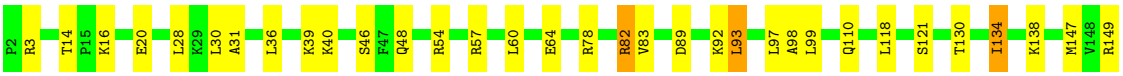
• Molecule 10: 40S ribosomal protein S8-A

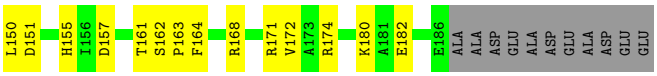
Chain s8:



• Molecule 11: 40S ribosomal protein S9-A

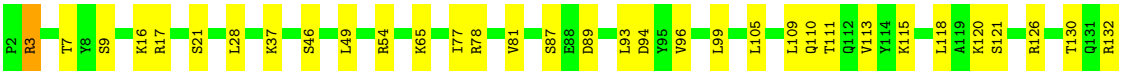
Chain S9:

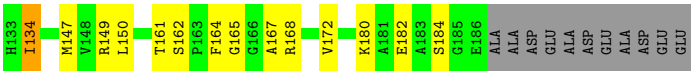




• Molecule 11: 40S ribosomal protein S9-A

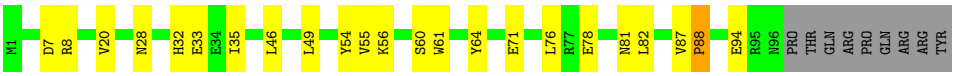
Chain s9:





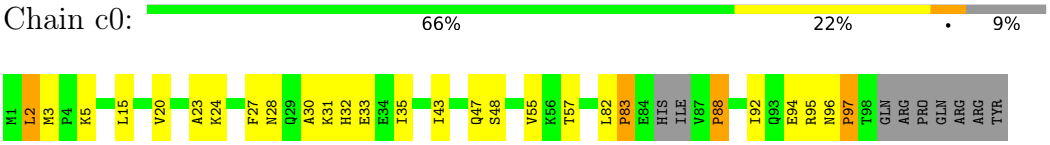
• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



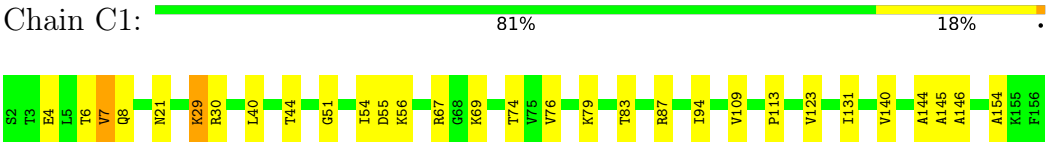
• Molecule 12: 40S ribosomal protein S10-A

Chain c0:



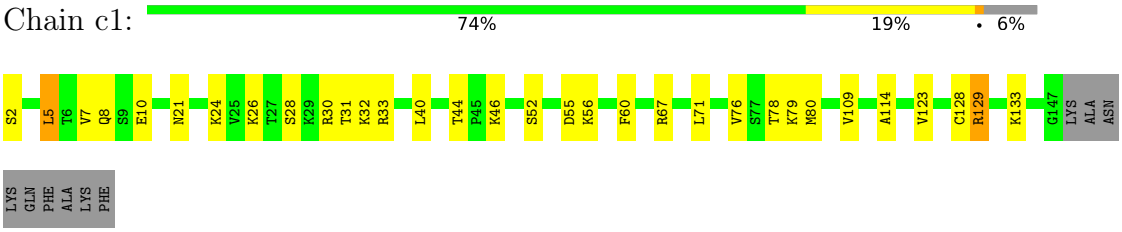
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



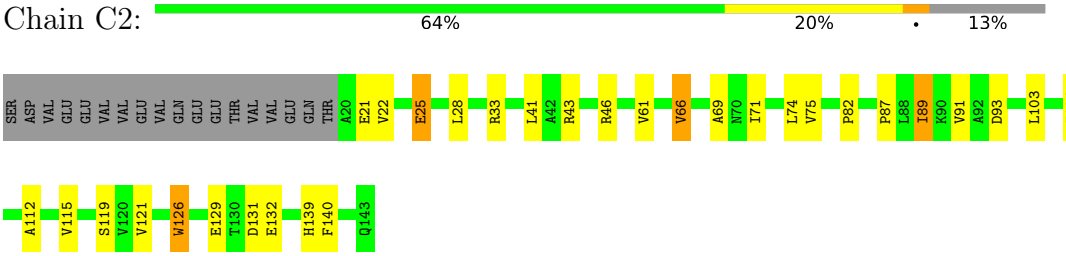
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



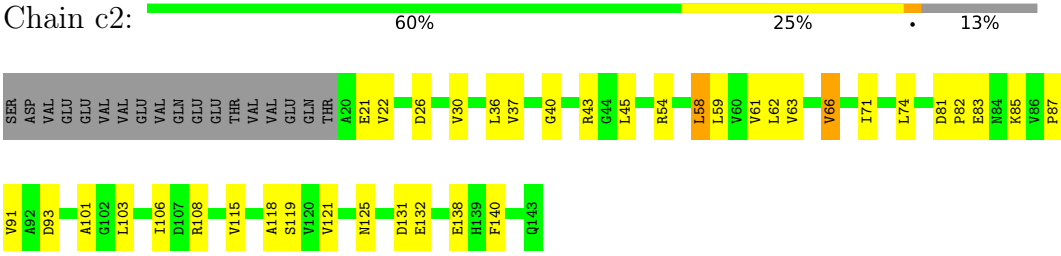
• Molecule 14: 40S ribosomal protein S12

Chain C2:



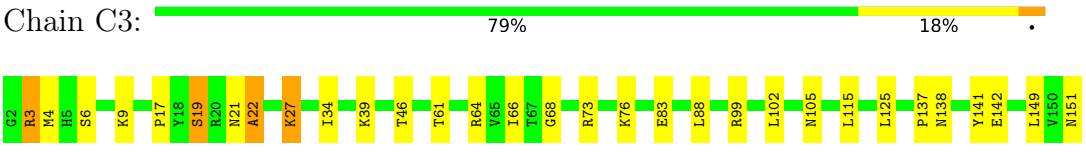
• Molecule 14: 40S ribosomal protein S12

Chain c2:



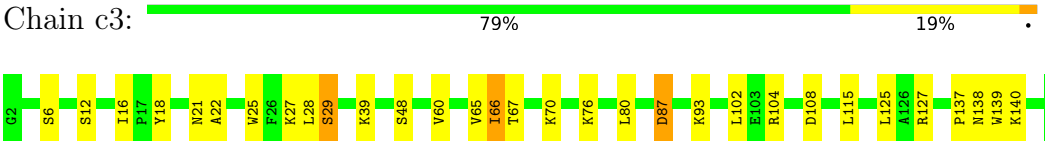
• Molecule 15: 40S ribosomal protein S13

Chain C3:



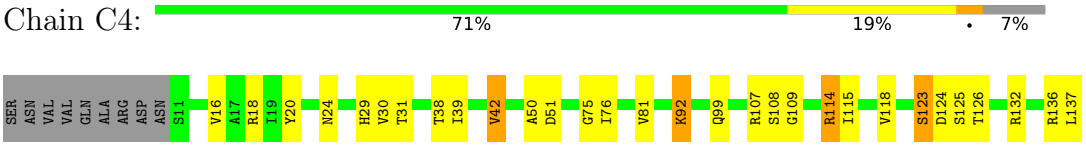
• Molecule 15: 40S ribosomal protein S13

Chain c3:



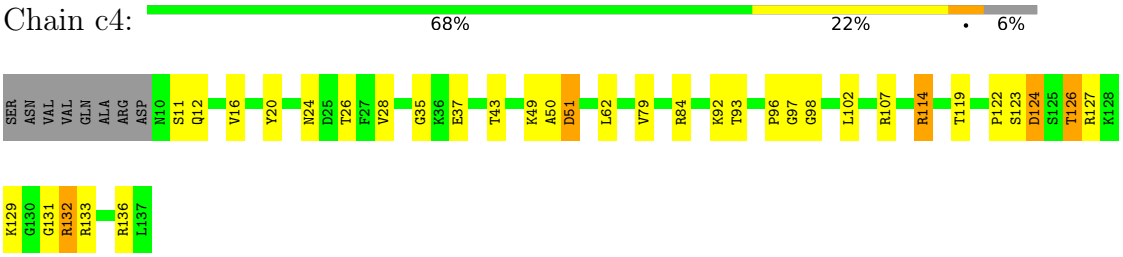
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



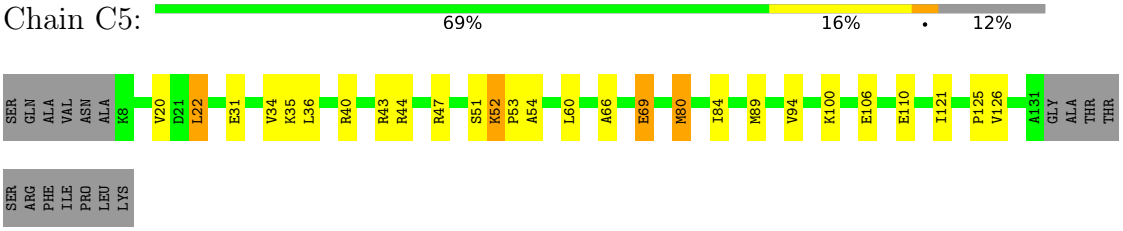
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



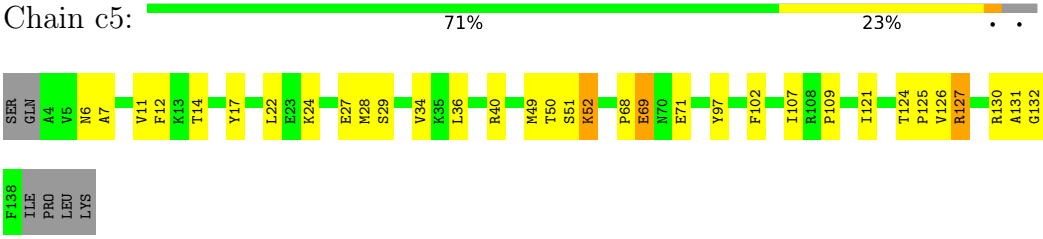
• Molecule 17: 40S ribosomal protein S15

Chain C5:



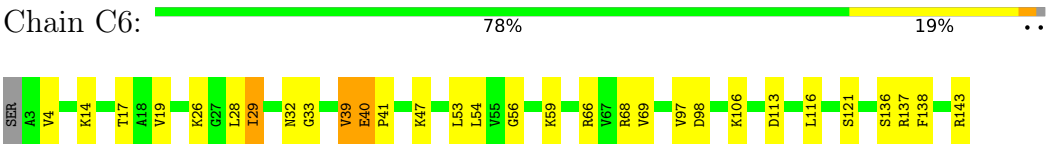
• Molecule 17: 40S ribosomal protein S15

Chain c5:



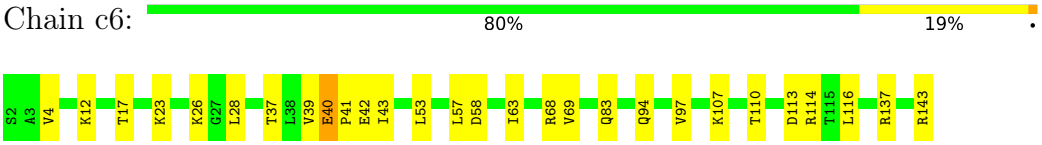
• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



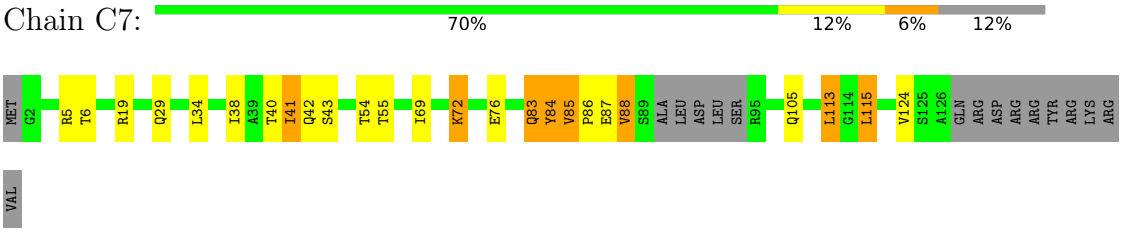
• Molecule 18: 40S ribosomal protein S16-A

Chain c6:



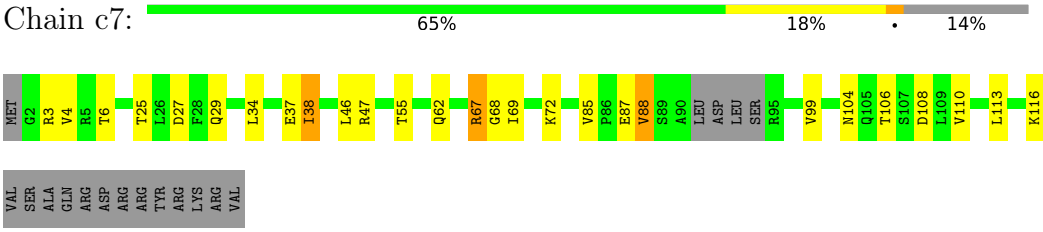
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



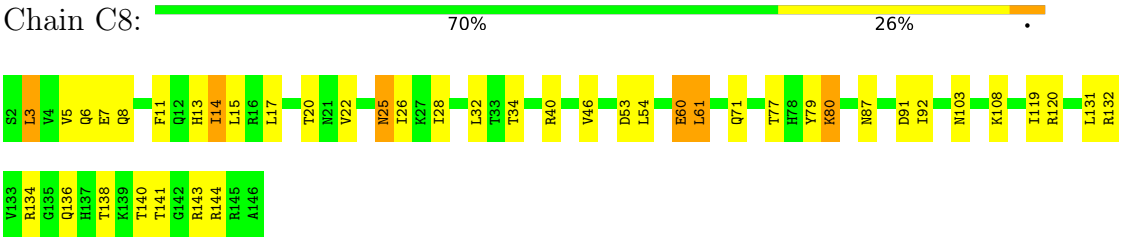
• Molecule 19: 40S ribosomal protein S17-A

Chain c7:



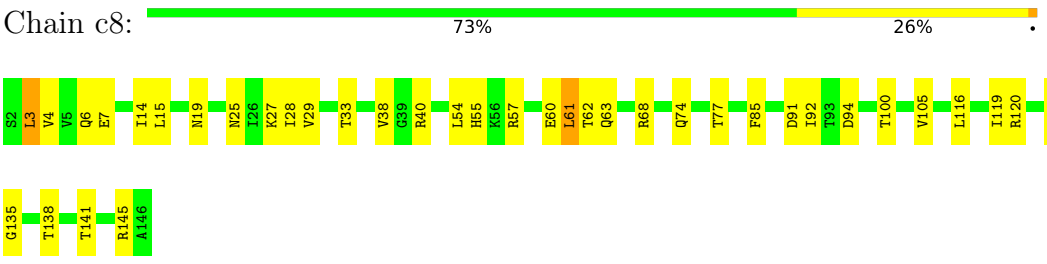
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



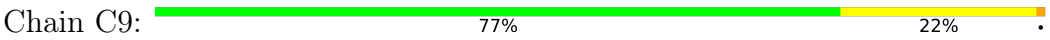
• Molecule 20: 40S ribosomal protein S18-A

Chain c8:



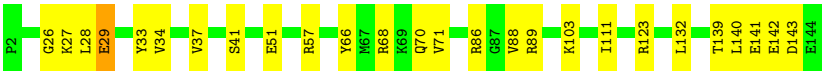
• Molecule 21: 40S ribosomal protein S19-A

Chain C9:



• Molecule 21: 40S ribosomal protein S19-A

Chain c9:

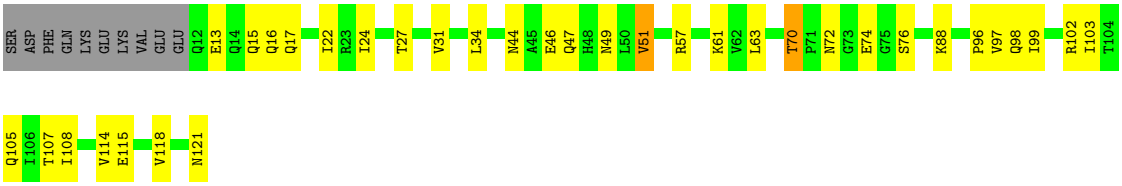


• Molecule 22: 40S ribosomal protein S20

Chain D0:

• Molecule 22: 40S ribosomal protein S20

Chain d0:



• Molecule 23: 40S ribosomal protein S21-A

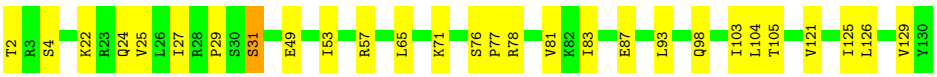
Chain D1:

• Molecule 23: 40S ribosomal protein S21-A

Chain d1:

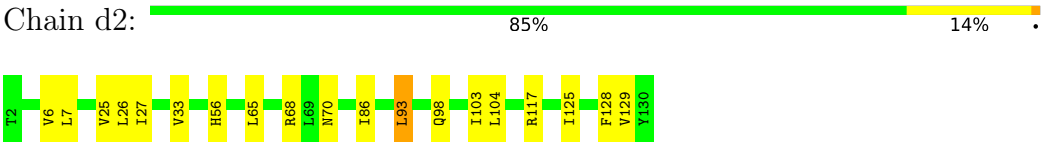
• Molecule 24: 40S ribosomal protein S22-A

Chain D2:



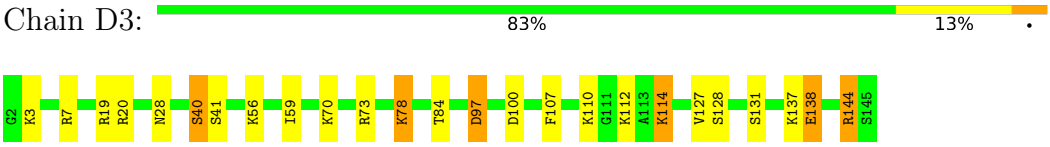
• Molecule 24: 40S ribosomal protein S22-A

Chain d2:



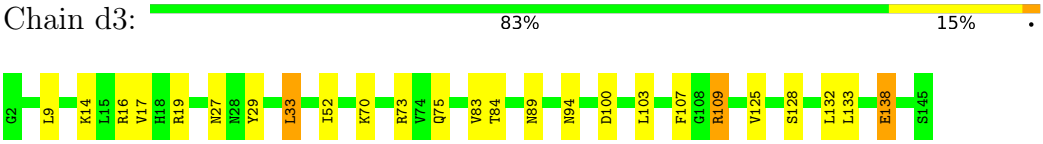
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



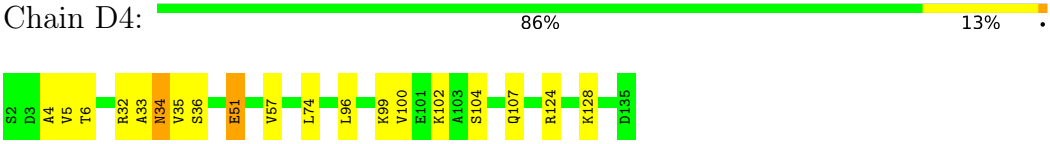
• Molecule 25: 40S ribosomal protein S23-A

Chain d3:



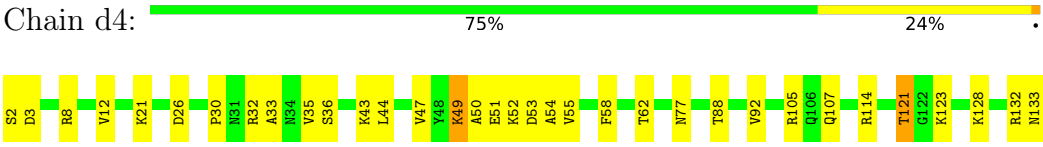
• Molecule 26: 40S ribosomal protein S24-A

Chain D4:



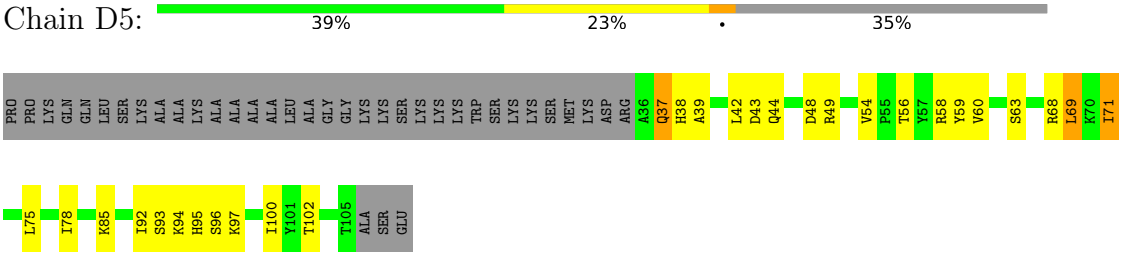
• Molecule 26: 40S ribosomal protein S24-A

Chain d4:



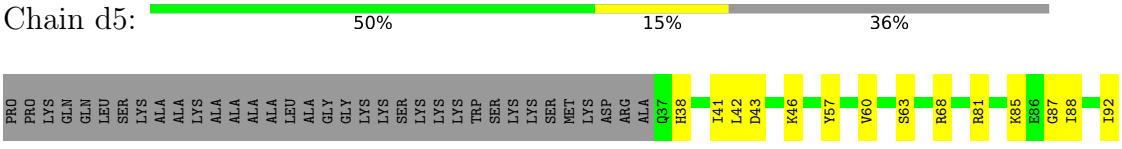
• Molecule 27: 40S ribosomal protein S25-A

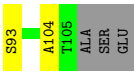
Chain D5:



• Molecule 27: 40S ribosomal protein S25-A

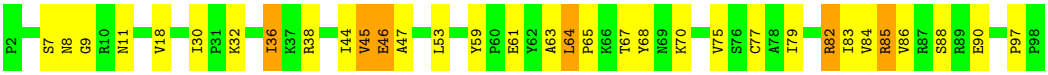
Chain d5:





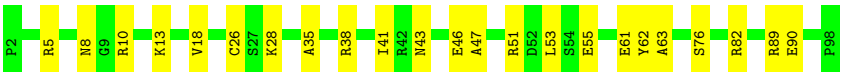
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



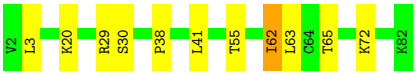
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



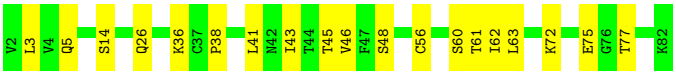
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



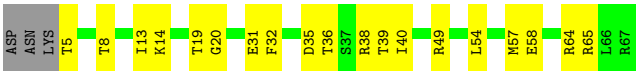
• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



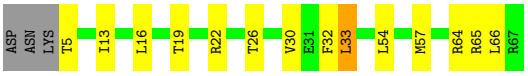
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



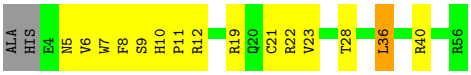
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



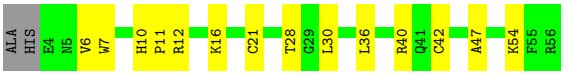
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



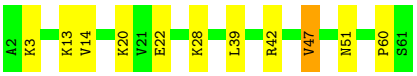
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



• Molecule 33: Ubiquitin-40S ribosomal protein S31

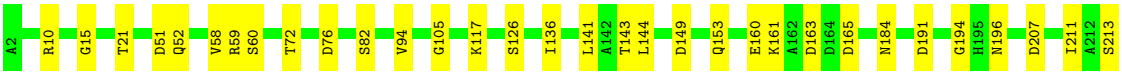
Chain E1:

• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:

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

Chain SR:

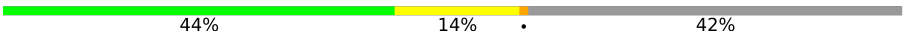


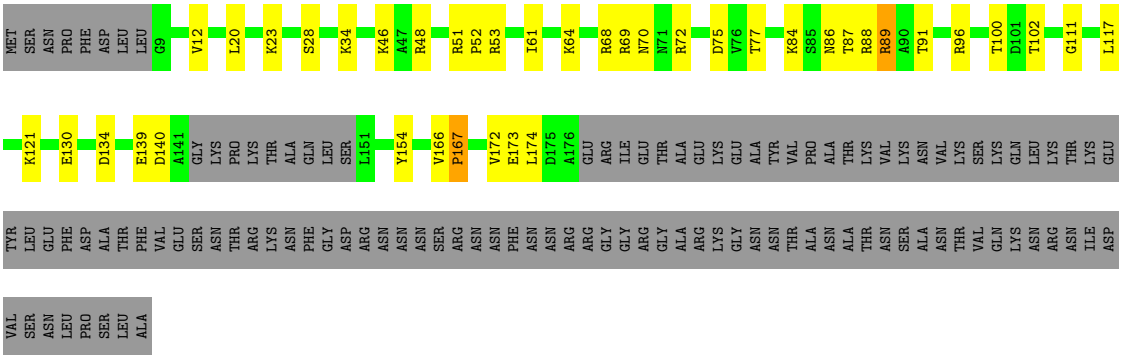
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:

• Molecule 35: Suppressor protein STM1

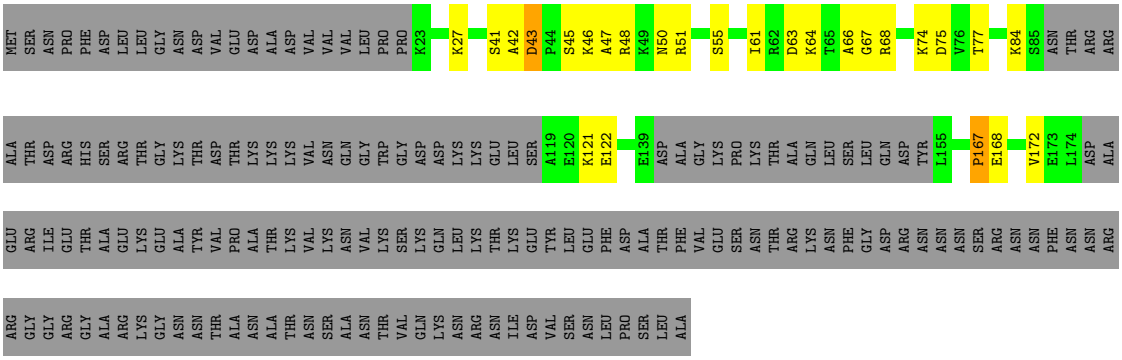
Chain SM:





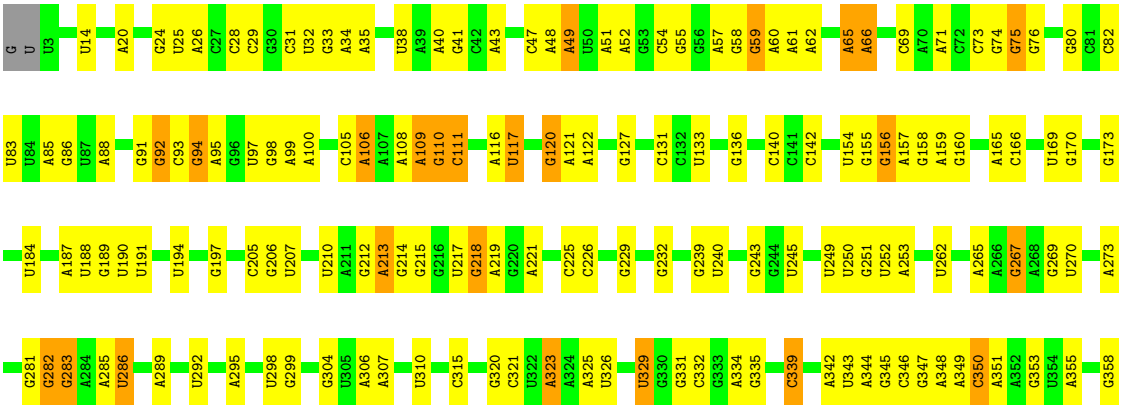
• Molecule 35: Suppressor protein STM1

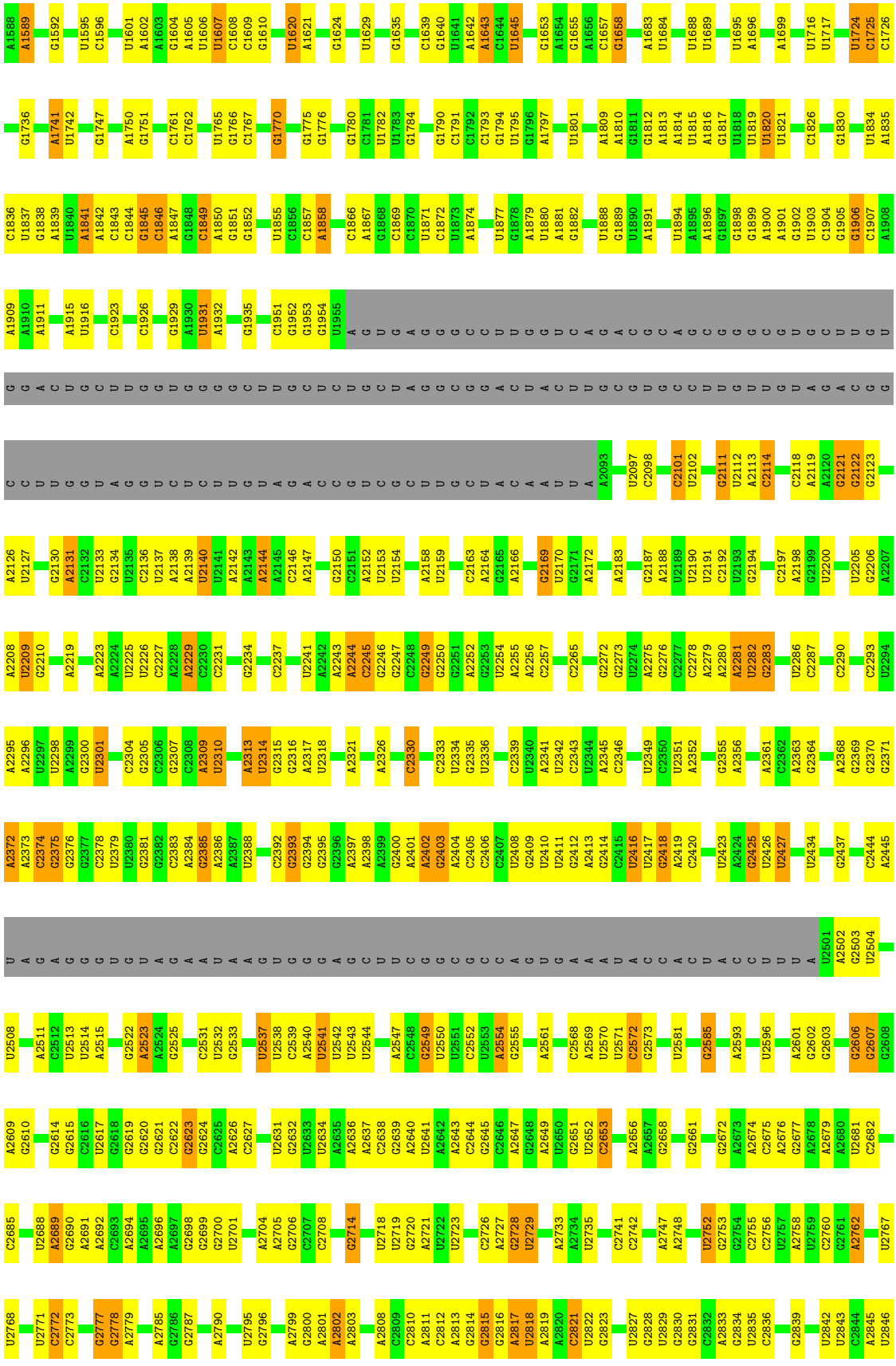
Chain sM:

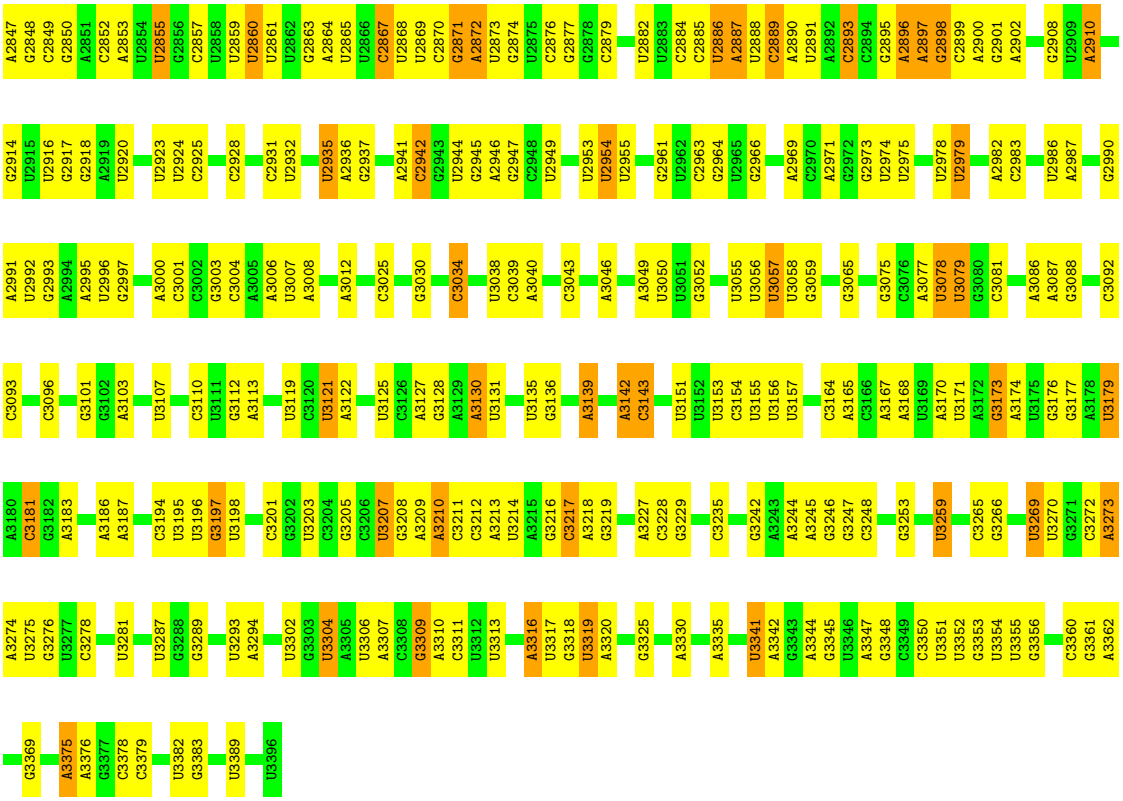


• Molecule 36: 25S ribosomal RNA

Chain 1:

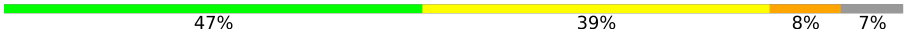


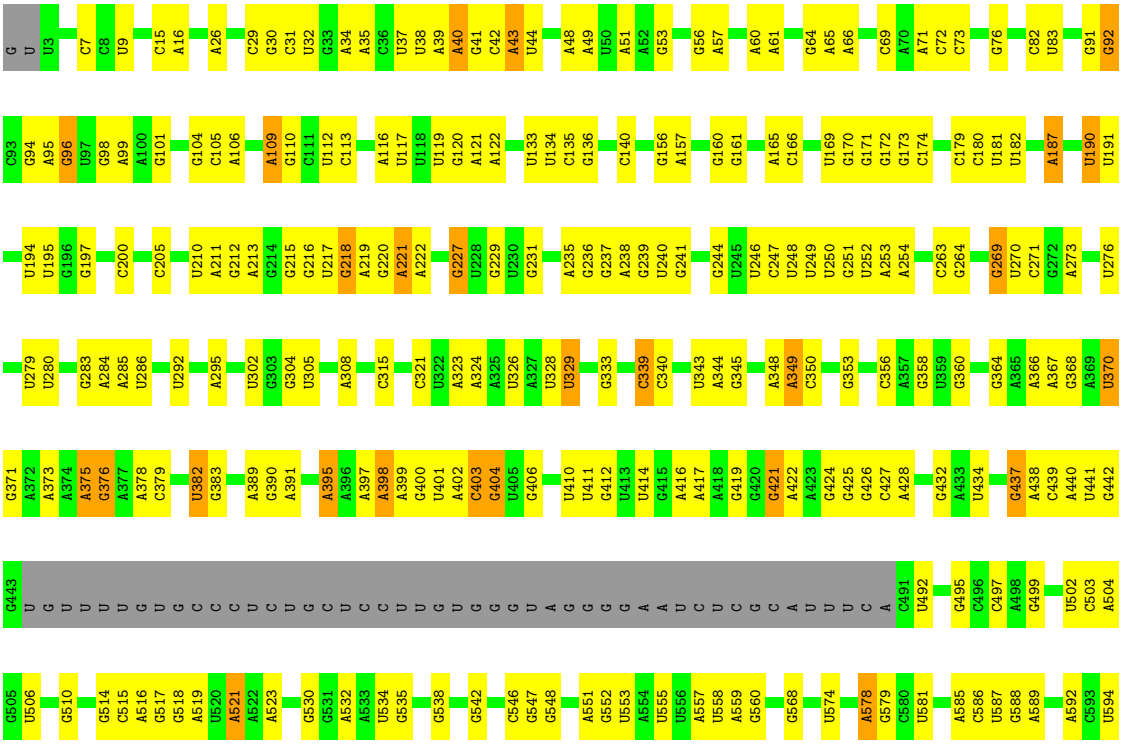




• Molecule 36: 25S ribosomal RNA

Chain 5:





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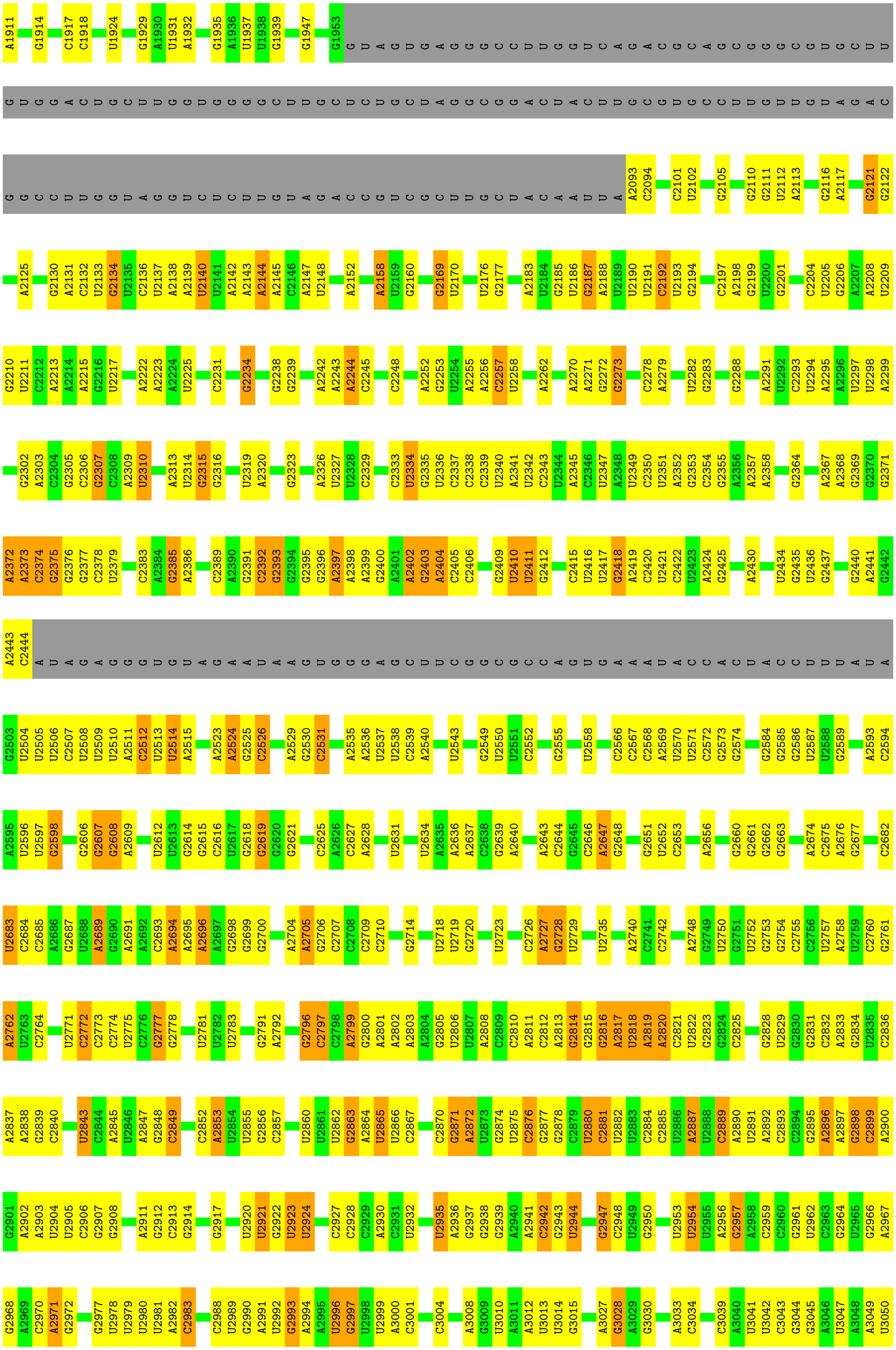
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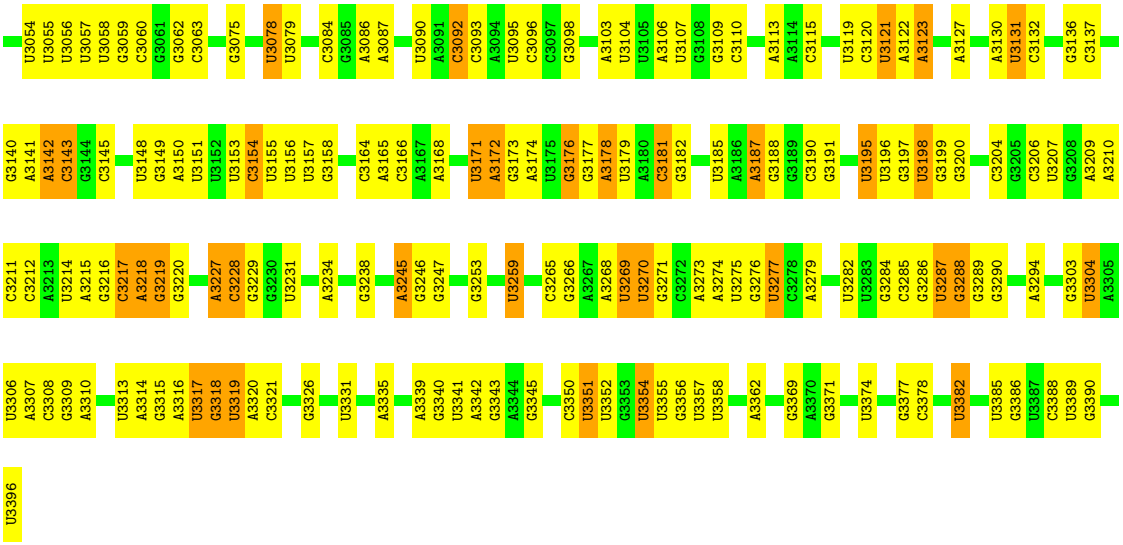
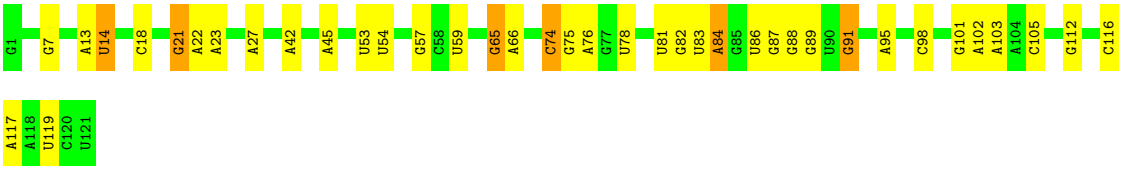


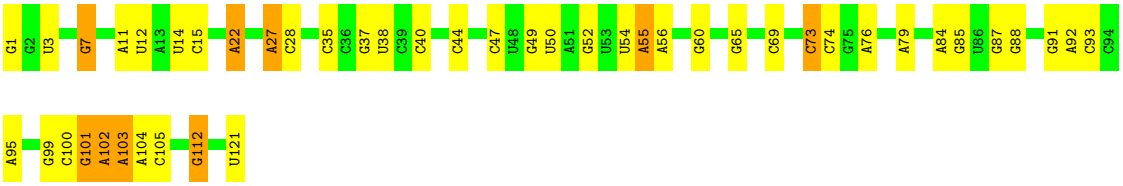
• Molecule 37: 5S ribosomal RNA

Chain 3:



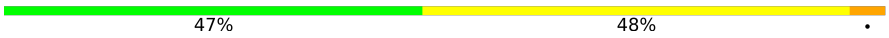
• Molecule 37: 5S ribosomal RNA

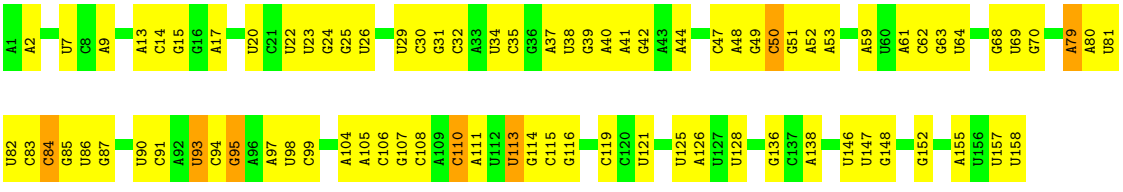
Chain 7:



• Molecule 38: 5.8S ribosomal RNA

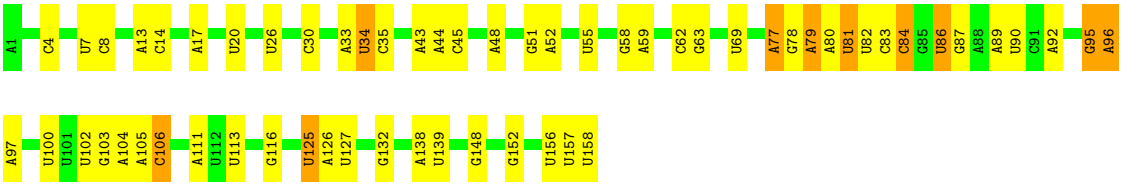
Chain 4:





• Molecule 38: 5.8S ribosomal RNA

Chain 8:



• Molecule 39: 60S ribosomal protein L2-A

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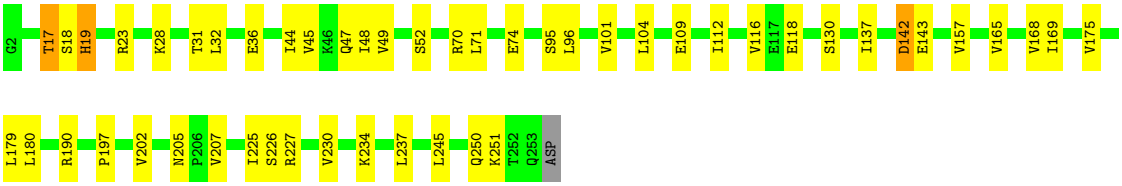
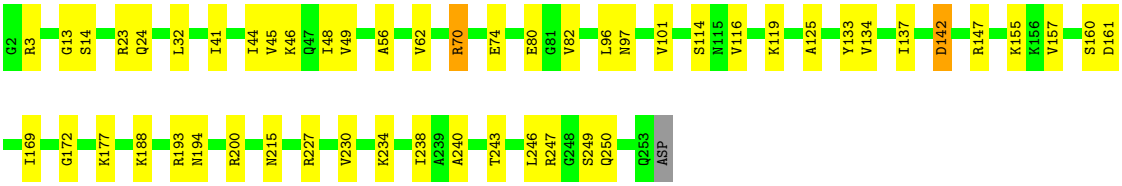


• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



• Molecule 40: 60S ribosomal protein L3

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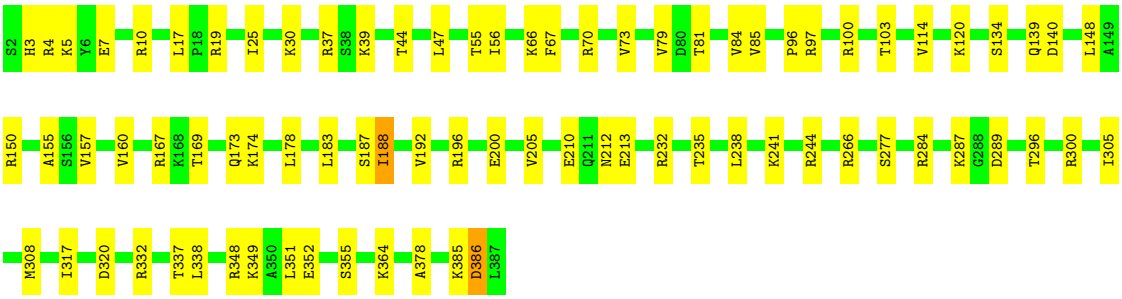
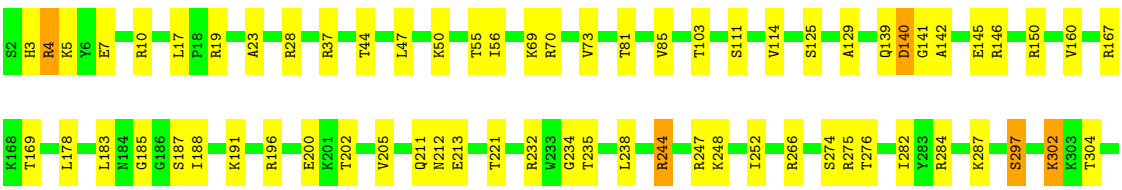
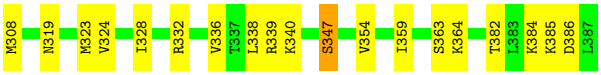


• Molecule 40: 60S ribosomal protein L3

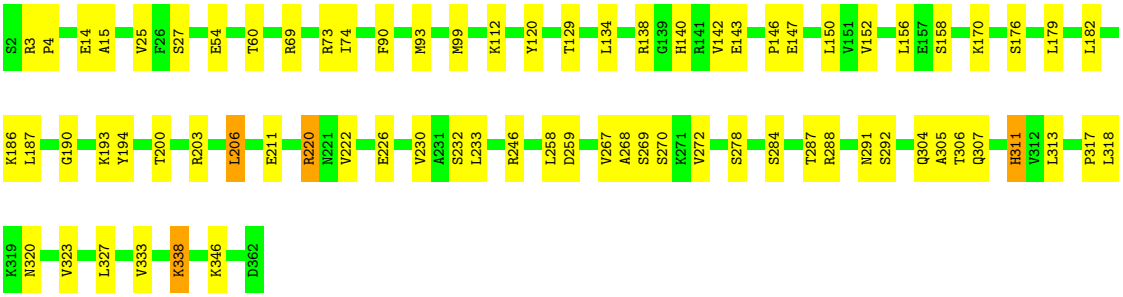
Chain l3:





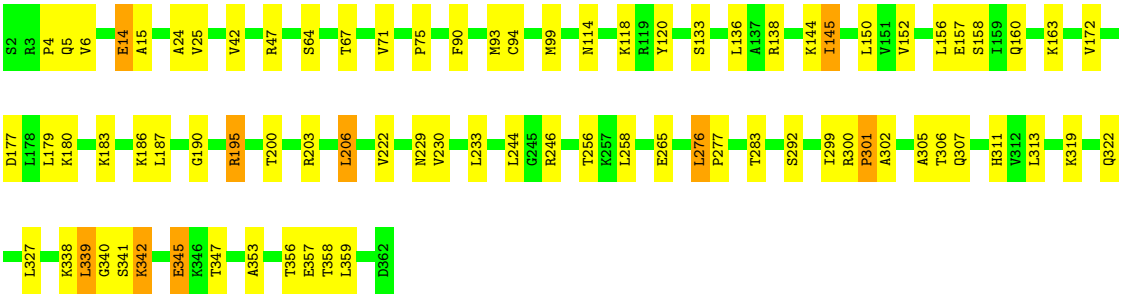
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



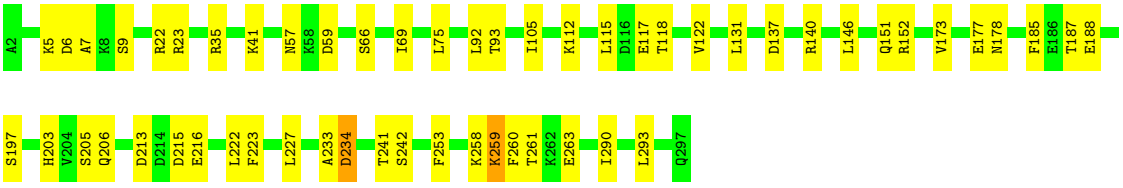
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:



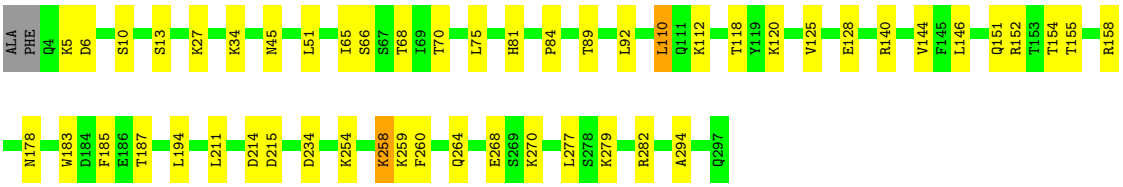
• Molecule 42: 60S ribosomal protein L5

Chain L5:



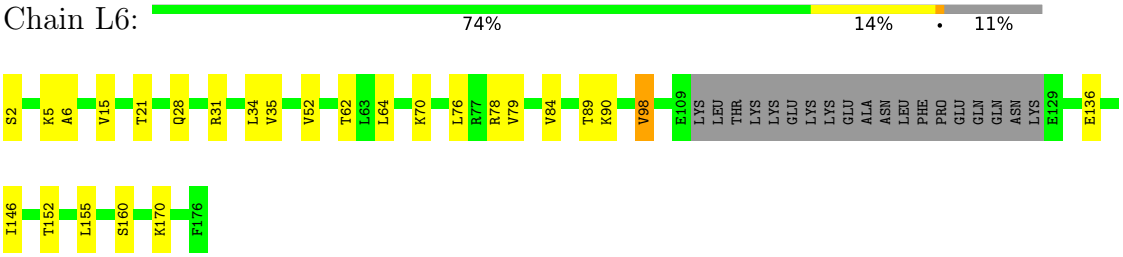
• Molecule 42: 60S ribosomal protein L5

Chain l5:



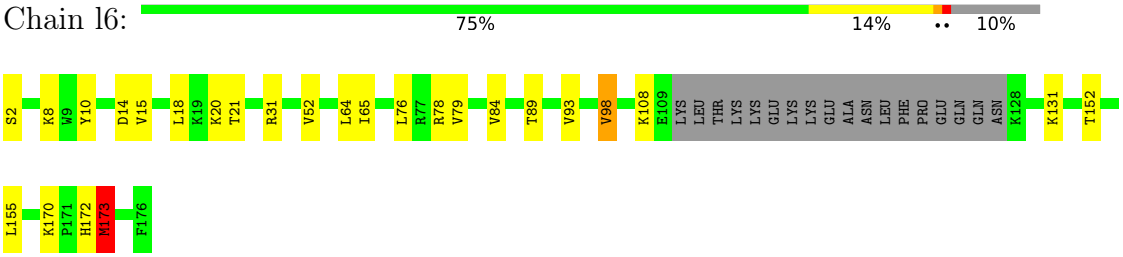
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



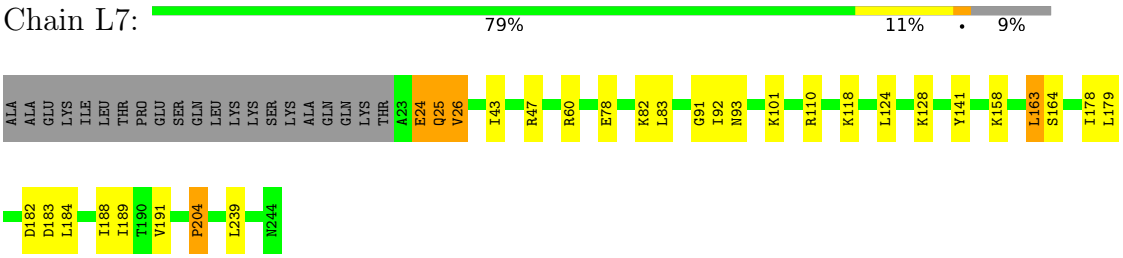
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



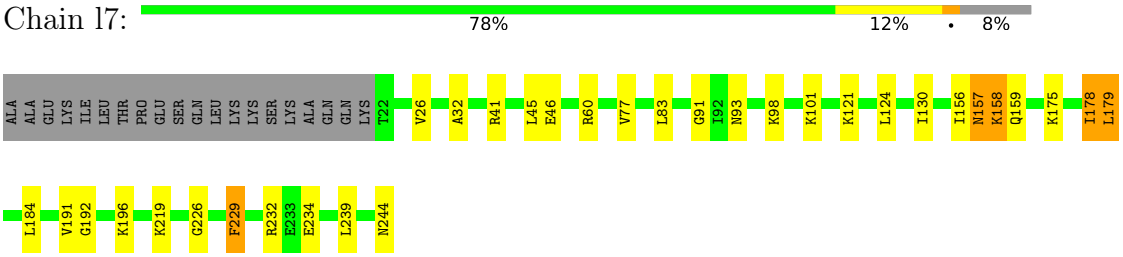
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



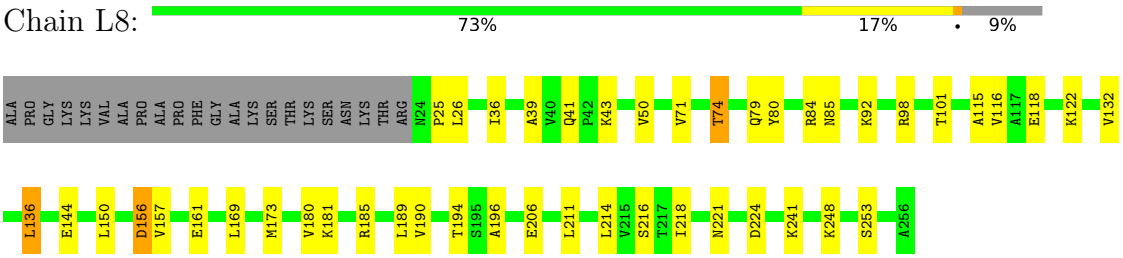
• Molecule 44: 60S ribosomal protein L7-A

Chain l7:



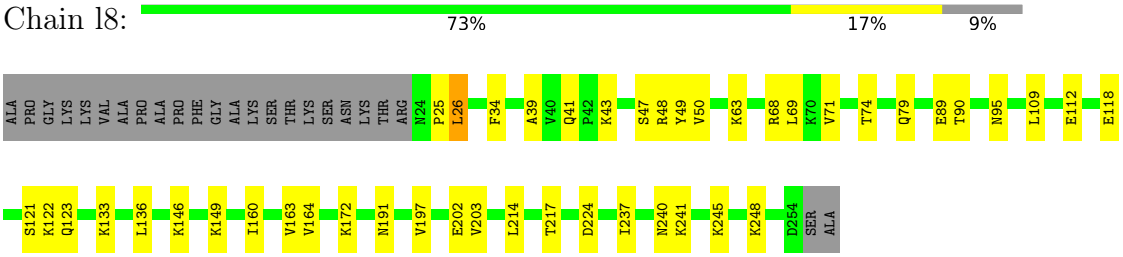
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



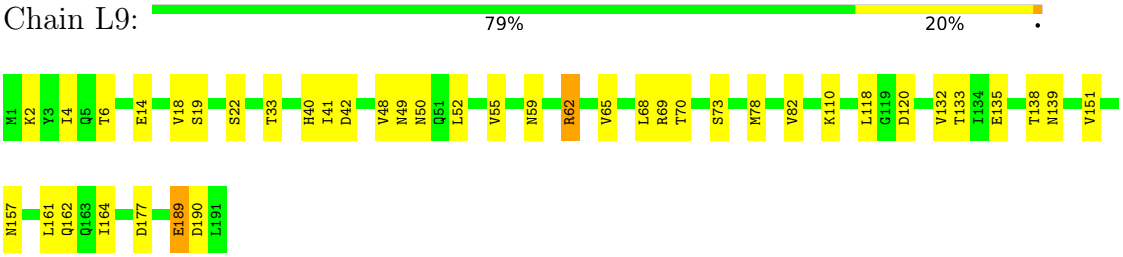
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



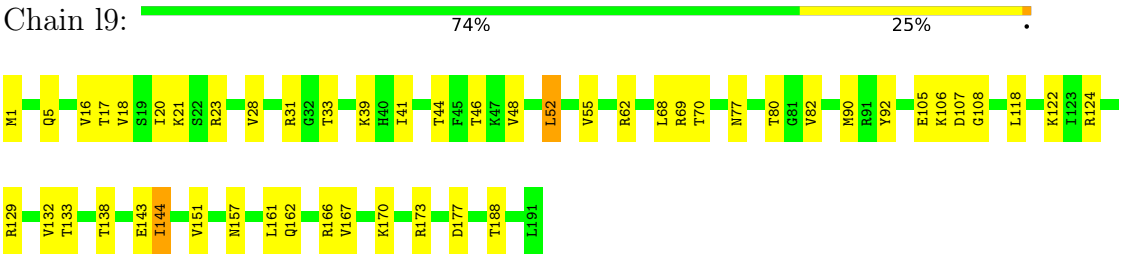
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



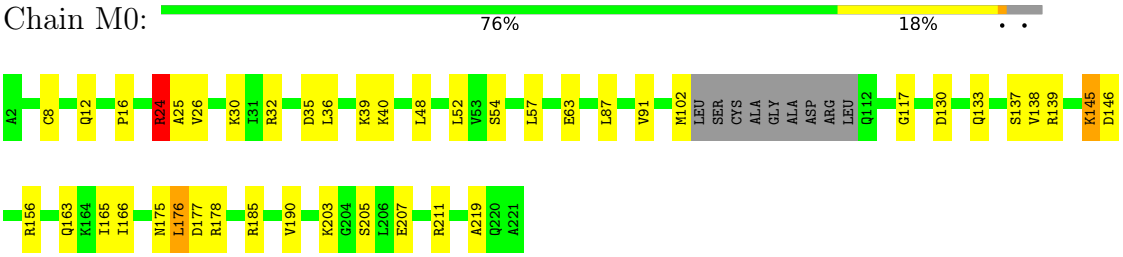
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



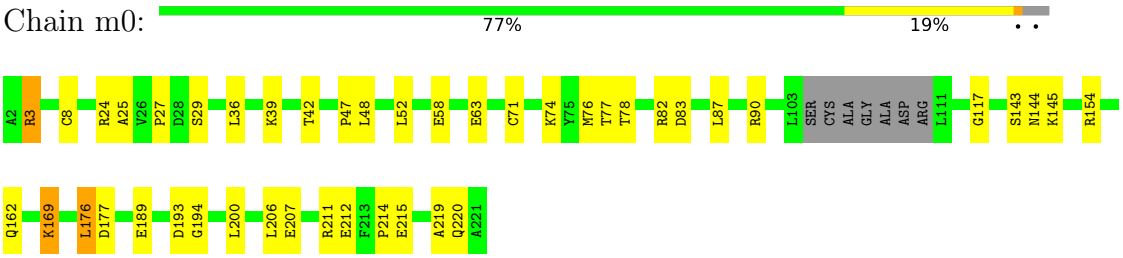
• Molecule 47: 60S ribosomal protein L10

Chain M0:



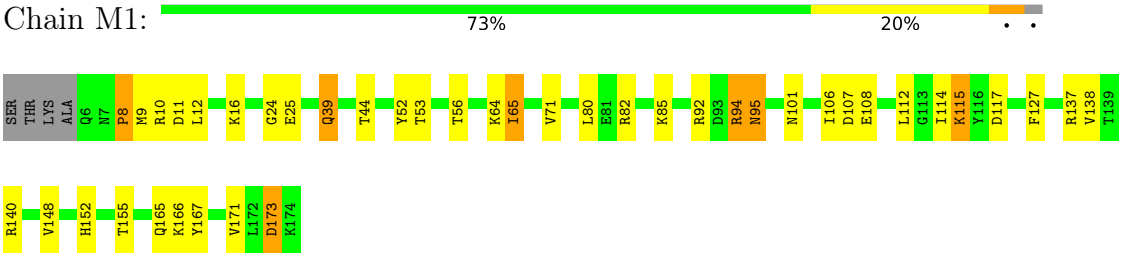
• Molecule 47: 60S ribosomal protein L10

Chain m0:



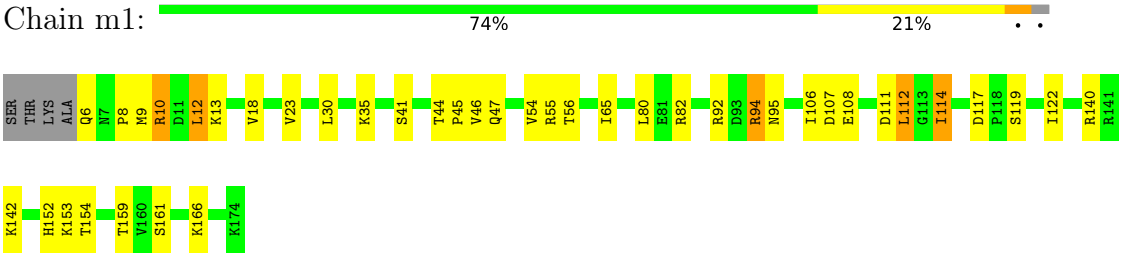
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



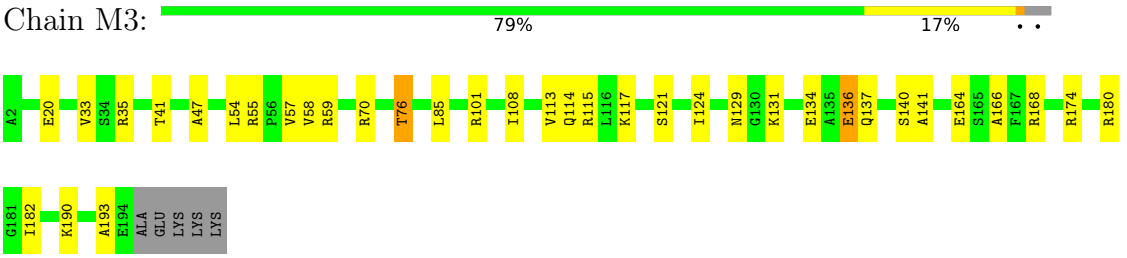
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



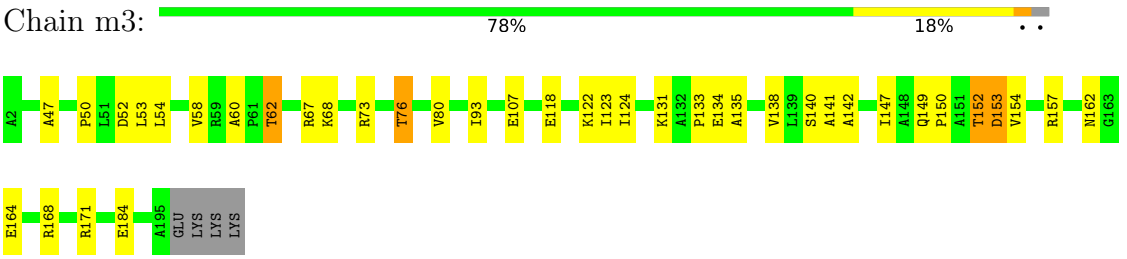
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



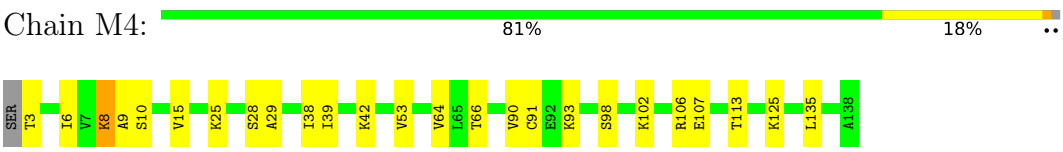
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



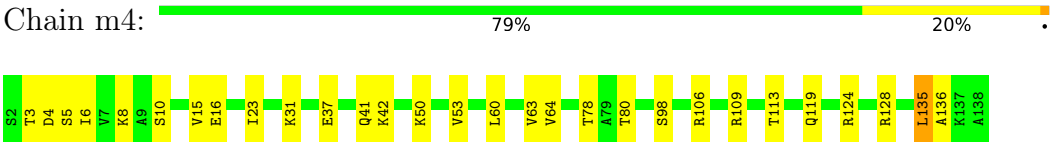
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



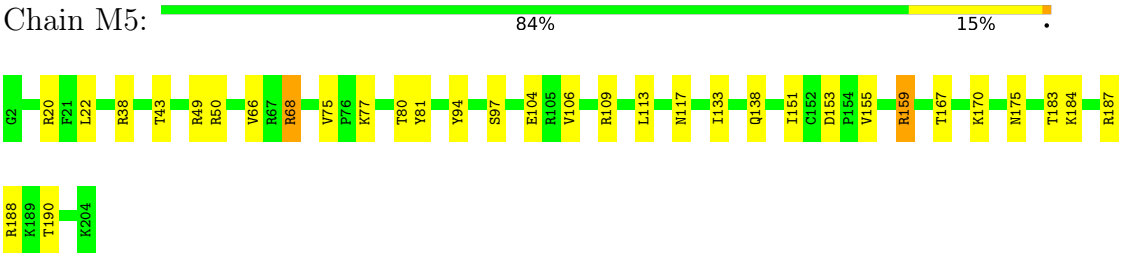
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



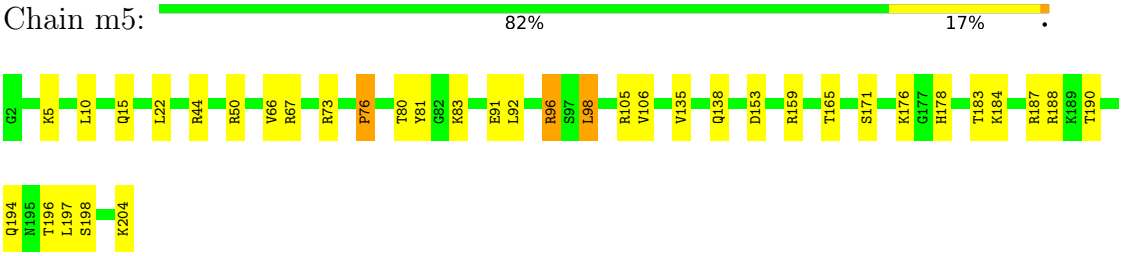
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



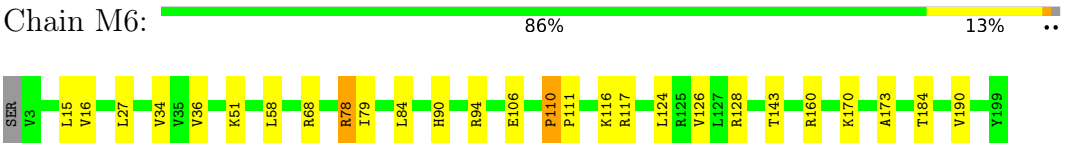
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



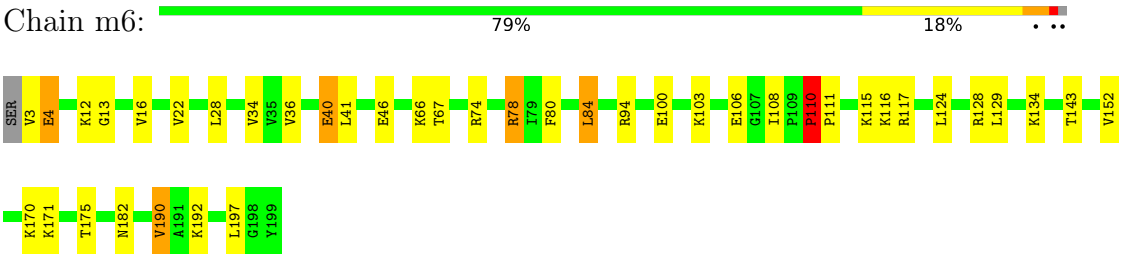
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



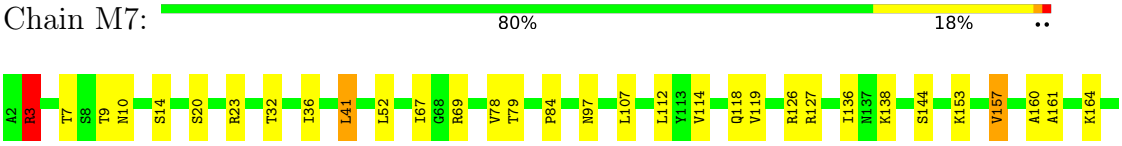
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



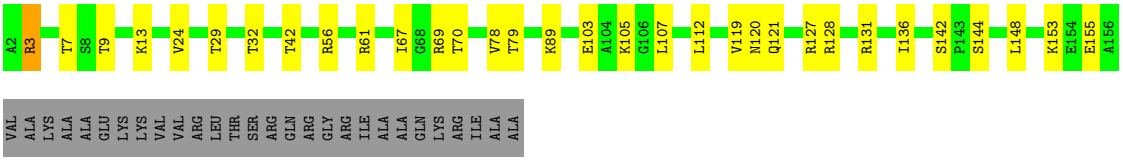
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



• Molecule 54: 60S ribosomal protein L18-A

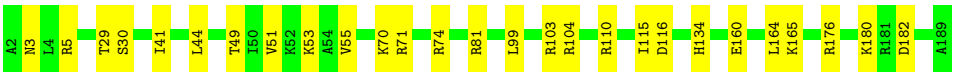
Chain M8:

• Molecule 54: 60S ribosomal protein L18-A

Chain m8:

• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



• Molecule 55: 60S ribosomal protein L19-A

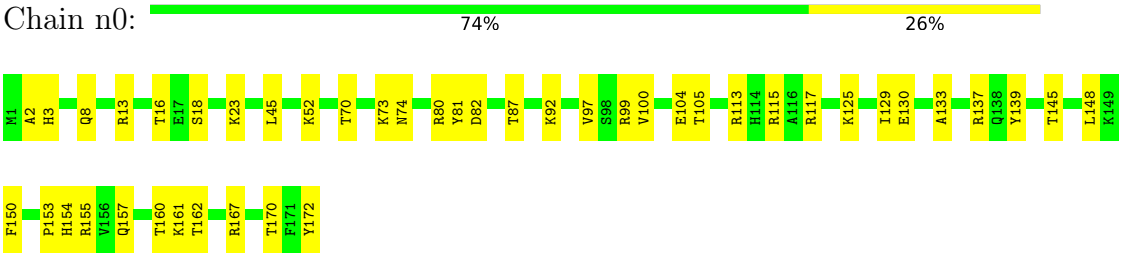
Chain m9:

• Molecule 56: 60S ribosomal protein L20-A

Chain N0:

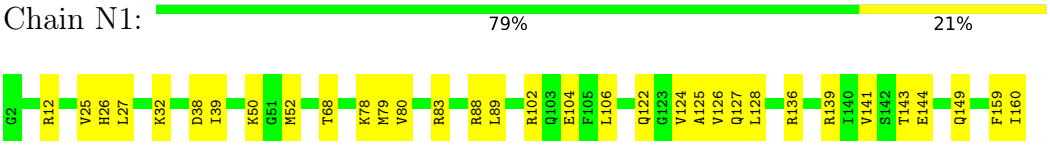
• Molecule 56: 60S ribosomal protein L20-A

Chain n0:



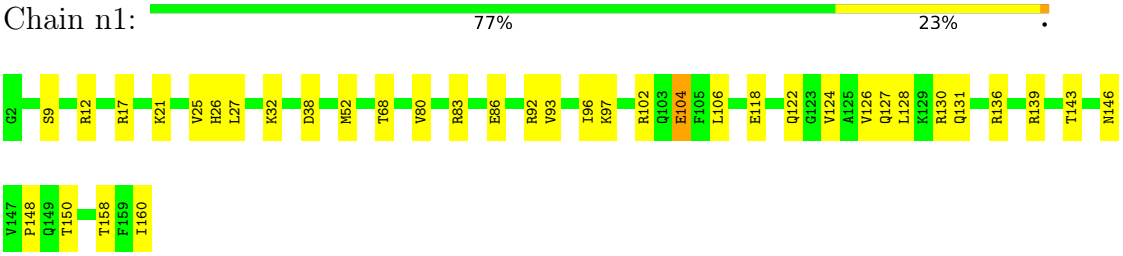
• Molecule 57: 60S ribosomal protein L21-A

Chain N1:



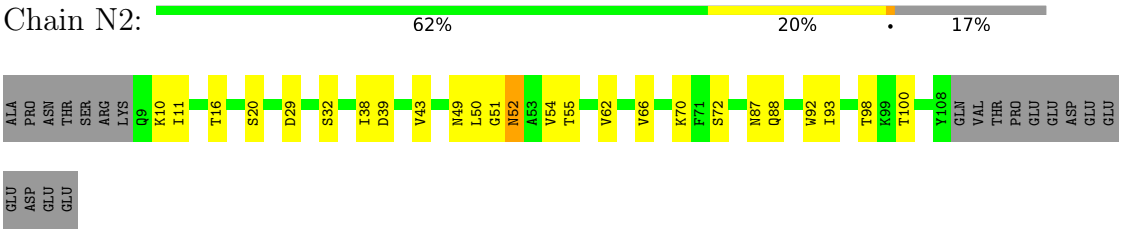
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



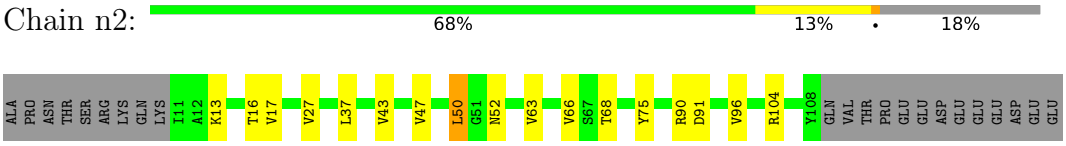
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



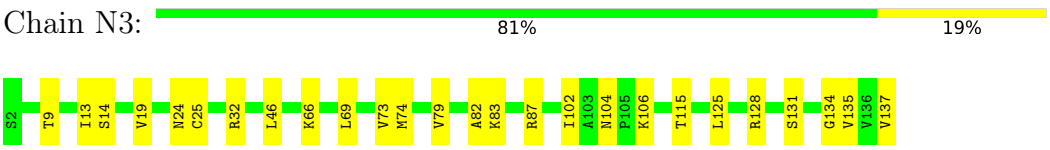
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



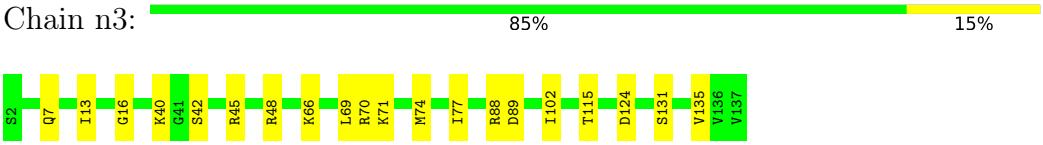
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



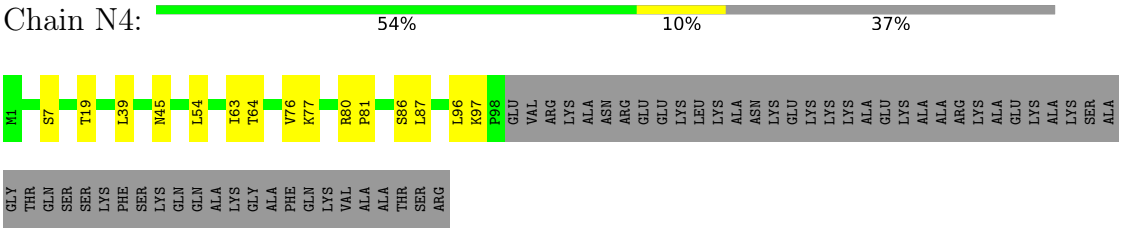
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



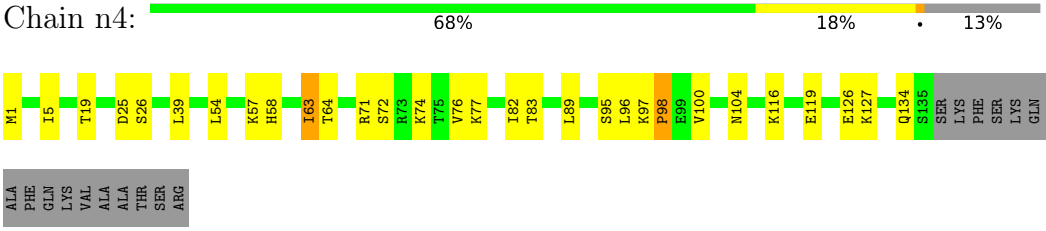
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



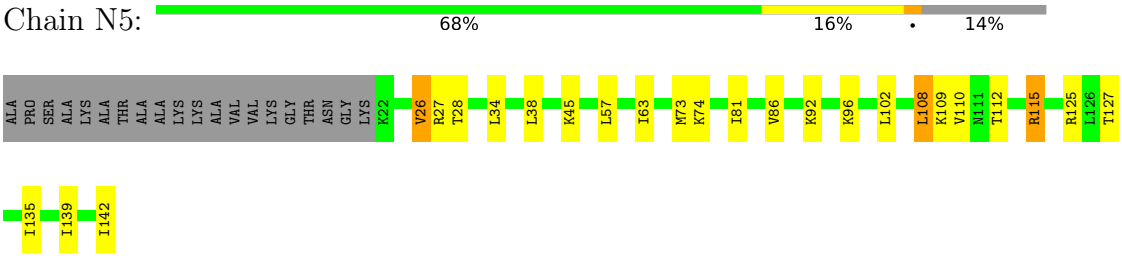
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



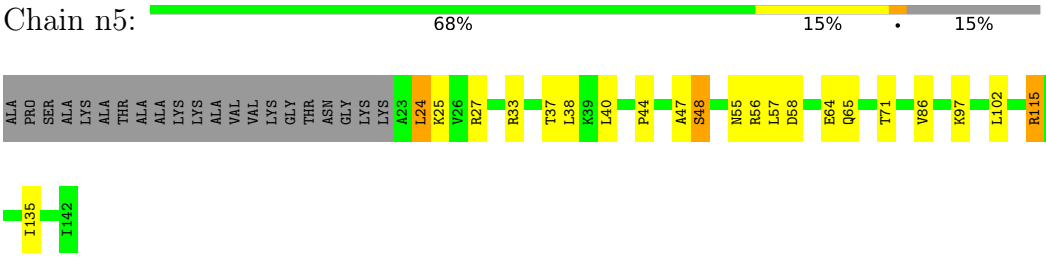
• Molecule 61: 60S ribosomal protein L25

Chain N5:



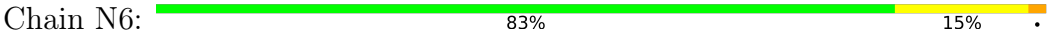
• Molecule 61: 60S ribosomal protein L25

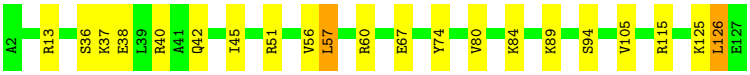
Chain n5:



• Molecule 62: 60S ribosomal protein L26-A

Chain N6:



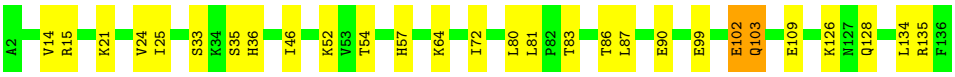


• Molecule 62: 60S ribosomal protein L26-A

Chain n6:

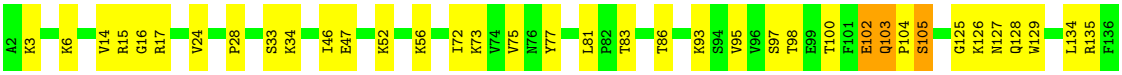
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



• Molecule 64: 60S ribosomal protein L28

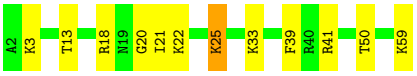
Chain N8:

• Molecule 64: 60S ribosomal protein L28

Chain n8:

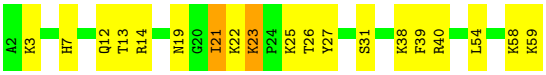
• Molecule 65: 60S ribosomal protein L29

Chain N9:



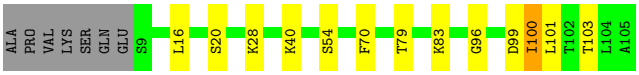
• Molecule 65: 60S ribosomal protein L29

Chain n9:



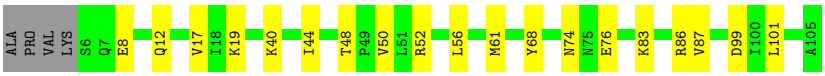
• Molecule 66: 60S ribosomal protein L30

Chain O0:



• Molecule 66: 60S ribosomal protein L30

Chain o0:



• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

• Molecule 67: 60S ribosomal protein L31-A

Chain o1:

• Molecule 68: 60S ribosomal protein L32

Chain O2:

• Molecule 68: 60S ribosomal protein L32

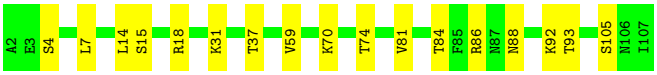
Chain o2:

• Molecule 69: 60S ribosomal protein L33-A

Chain O3:

• Molecule 69: 60S ribosomal protein L33-A

Chain o3:

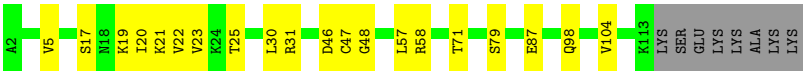


• Molecule 70: 60S ribosomal protein L34-A

Chain O4:

• Molecule 70: 60S ribosomal protein L34-A

Chain o4:

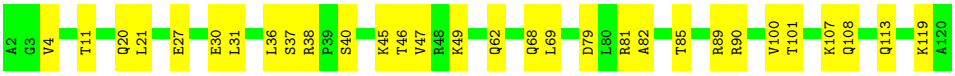


• Molecule 71: 60S ribosomal protein L35-A

Chain O5:

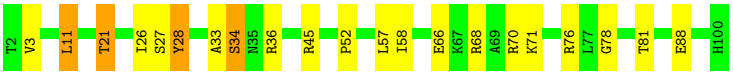
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



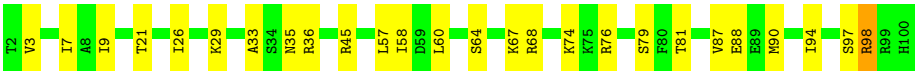
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



• Molecule 72: 60S ribosomal protein L36-A

Chain o6:

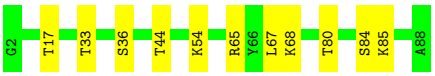


• Molecule 73: 60S ribosomal protein L37-A

Chain O7:

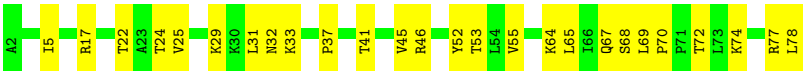
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



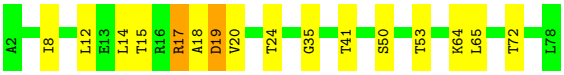
• Molecule 74: 60S ribosomal protein L38

Chain O8:



• Molecule 74: 60S ribosomal protein L38

Chain o8:



• Molecule 75: 60S ribosomal protein L39

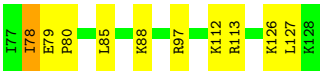
Chain O9:

• Molecule 75: 60S ribosomal protein L39

Chain o9:

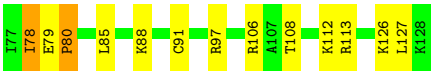
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



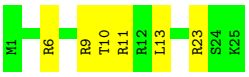
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



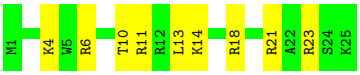
• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



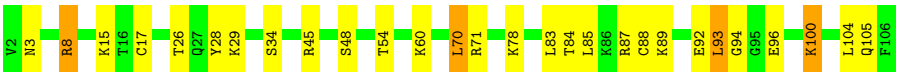
• Molecule 77: 60S ribosomal protein L41-A

Chain q1:



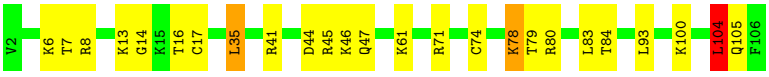
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



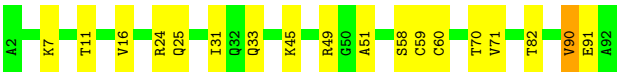
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



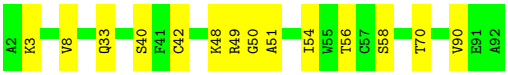
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



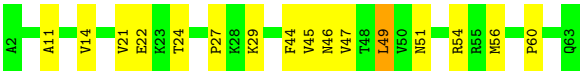
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



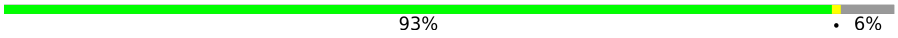
• Molecule 80: 40S ribosomal protein S30-A

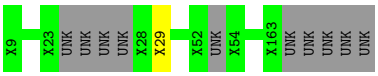
Chain e0:



• Molecule 81: unknown protein chain m2

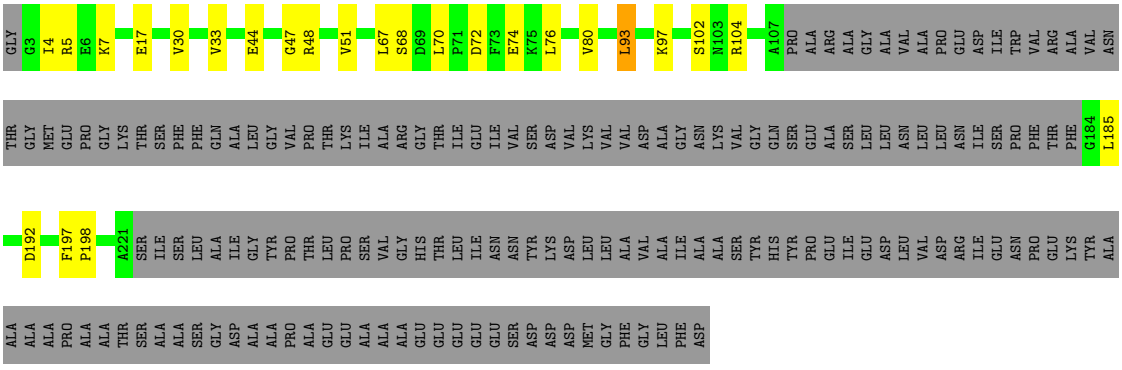
Chain m2:





• Molecule 82: 60S acidic ribosomal protein P0

Chain p0:



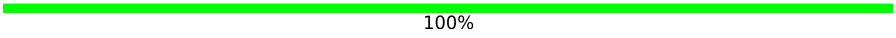
• Molecule 83: unknown protein chain p1

Chain p1:

There are no outlier residues recorded for this chain.

• Molecule 84: unknown protein chain p2

Chain p2:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	435.34Å 287.00Å 303.36Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	49.18 – 3.20	Depositor
% Data completeness (in resolution range)	99.9 (49.18-3.20)	Depositor
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.204 , 0.253	Depositor
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.212	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411178	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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: MG, ZN, 3KF, OHX

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	5/41698 (0.0%)	1.31	312/64972 (0.5%)
1	6	0.78	12/42765 (0.0%)	1.35	404/66634 (0.6%)
2	S0	0.44	0/1617	0.66	0/2215
2	s0	0.44	0/1623	0.65	0/2222
3	S1	0.39	0/1735	0.66	2/2335 (0.1%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.51	1/1665 (0.1%)	0.66	0/2263
4	s2	0.56	0/1665	0.75	1/2263 (0.0%)
5	S3	0.49	0/1759	0.68	0/2368
5	s3	0.41	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.72	2/2839 (0.1%)
6	s4	0.49	0/2109	0.72	0/2839
7	S5	0.38	0/1629	0.60	0/2202
7	s5	0.41	0/1629	0.61	0/2202
8	S6	0.47	0/1823	0.66	0/2439
8	s6	0.53	0/1779	0.69	0/2379
9	S7	0.43	0/1506	0.64	0/2028
9	s7	0.44	0/1516	0.63	0/2043
10	S8	0.54	0/1514	0.70	0/2021
10	s8	0.59	0/1514	0.75	3/2021 (0.1%)
11	S9	0.49	0/1519	0.69	1/2035 (0.0%)
11	s9	0.52	0/1519	0.72	2/2035 (0.1%)
12	C0	0.45	0/790	0.71	1/1069 (0.1%)
12	c0	0.36	0/777	0.64	3/1049 (0.3%)
13	C1	0.56	0/1239	0.66	0/1673
13	c1	0.57	0/1194	0.74	1/1610 (0.1%)
14	C2	0.37	0/900	0.66	0/1224
14	c2	0.31	0/900	0.58	0/1224
15	C3	0.50	0/1215	0.66	2/1638 (0.1%)
15	c3	0.53	0/1215	0.70	0/1638
16	C4	0.40	0/901	0.66	0/1217
16	c4	0.51	0/960	0.73	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.46	0/998	0.66	0/1341
17	c5	0.47	0/1060	0.69	0/1426
18	C6	0.44	0/1125	0.68	2/1510 (0.1%)
18	c6	0.44	0/1131	0.65	0/1518
19	C7	0.43	0/935	0.65	0/1254
19	c7	0.45	0/914	0.68	0/1224
20	C8	0.43	0/1211	0.65	1/1628 (0.1%)
20	c8	0.45	0/1211	0.66	1/1628 (0.1%)
21	C9	0.41	0/1130	0.60	0/1517
21	c9	0.46	0/1130	0.66	0/1517
22	D0	0.43	0/865	0.65	0/1169
22	d0	0.43	0/892	0.65	0/1205
23	D1	0.42	0/693	0.63	0/935
23	d1	0.50	0/693	0.70	0/935
24	D2	0.53	0/1038	0.72	0/1395
24	d2	0.56	0/1038	0.73	1/1395 (0.1%)
25	D3	0.60	0/1139	0.77	0/1518
25	d3	0.66	0/1139	0.81	2/1518 (0.1%)
26	D4	0.45	0/1087	0.61	0/1449
26	d4	0.51	0/1087	0.71	0/1449
27	D5	0.39	0/571	0.72	0/768
27	d5	0.41	0/566	0.65	0/761
28	D6	0.46	0/782	0.71	0/1047
28	d6	0.57	0/782	0.73	0/1047
29	D7	0.44	0/620	0.66	0/838
29	d7	0.47	0/620	0.74	0/838
30	D8	0.37	0/499	0.60	0/670
30	d8	0.40	0/499	0.64	0/670
31	D9	0.53	0/452	0.70	1/600 (0.2%)
31	d9	0.46	0/452	0.61	0/600
32	E0	0.47	0/483	0.62	0/643
33	E1	0.47	0/577	0.79	0/770
33	e1	0.39	0/619	0.71	0/822
34	SR	0.36	0/2494	0.57	0/3393
34	sR	0.35	0/2495	0.56	0/3395
35	SM	0.51	0/1113	0.71	2/1502 (0.1%)
35	sM	0.46	0/683	0.68	1/923 (0.1%)
36	1	1.08	102/75394 (0.1%)	1.68	1977/117545 (1.7%)
36	5	1.10	107/75414 (0.1%)	1.70	2076/117575 (1.8%)
37	3	0.91	3/2883 (0.1%)	1.45	38/4491 (0.8%)
37	7	1.04	3/2883 (0.1%)	1.64	63/4491 (1.4%)
38	4	1.03	0/3746	1.64	78/5832 (1.3%)
38	8	0.95	0/3746	1.54	62/5832 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	0.70	0/1948	0.84	1/2617 (0.0%)
39	l2	0.65	0/1946	0.85	1/2614 (0.0%)
40	L3	0.72	1/3146 (0.0%)	0.80	0/4228
40	l3	0.78	0/3146	0.86	2/4228 (0.0%)
41	L4	0.76	0/2800	0.90	3/3790 (0.1%)
41	l4	0.75	1/2800 (0.0%)	0.92	5/3790 (0.1%)
42	L5	0.56	0/2425	0.69	0/3271
42	l5	0.70	0/2408	0.80	1/3248 (0.0%)
43	L6	0.72	0/1260	0.81	1/1694 (0.1%)
43	l6	0.77	0/1269	0.82	2/1705 (0.1%)
44	L7	0.79	0/1821	0.87	2/2451 (0.1%)
44	l7	0.83	0/1828	0.91	4/2461 (0.2%)
45	L8	0.54	0/1836	0.68	0/2481
45	l8	0.49	0/1795	0.65	0/2429
46	L9	0.68	0/1539	0.79	0/2073
46	l9	0.77	0/1539	0.83	1/2073 (0.0%)
47	M0	0.71	1/1741 (0.1%)	0.84	3/2335 (0.1%)
47	m0	0.72	1/1758 (0.1%)	0.81	1/2358 (0.0%)
48	M1	0.50	0/1374	0.72	0/1842
48	m1	0.63	0/1374	0.80	2/1842 (0.1%)
49	M3	0.74	0/1568	0.84	0/2106
49	m3	0.69	0/1573	0.79	0/2113
50	M4	0.74	0/1068	0.83	0/1438
50	m4	0.78	0/1074	0.81	1/1446 (0.1%)
51	M5	0.73	0/1757	0.90	2/2354 (0.1%)
51	m5	0.65	0/1757	0.83	3/2354 (0.1%)
52	M6	0.84	0/1585	0.88	3/2128 (0.1%)
52	m6	0.95	2/1585 (0.1%)	0.94	4/2128 (0.2%)
53	M7	0.77	0/1443	0.86	2/1944 (0.1%)
53	m7	0.91	0/1250	0.88	0/1683
54	M8	0.75	0/1465	0.88	1/1965 (0.1%)
54	m8	0.75	0/1465	0.88	1/1965 (0.1%)
55	M9	0.56	0/1538	0.65	0/2050
55	m9	0.56	0/1538	0.67	0/2050
56	N0	0.75	0/1481	0.81	0/1990
56	n0	0.86	0/1481	0.89	1/1990 (0.1%)
57	N1	0.72	0/1300	0.78	0/1743
57	n1	0.79	1/1300 (0.1%)	0.84	1/1743 (0.1%)
58	N2	0.45	0/812	0.59	0/1099
58	n2	0.46	0/794	0.69	0/1076
59	N3	0.69	0/1018	0.82	0/1369
59	n3	0.78	0/1018	0.85	1/1369 (0.1%)
60	N4	0.56	0/712	0.68	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	n4	0.62	0/1052	0.73	0/1398
61	N5	0.65	0/979	0.82	1/1321 (0.1%)
61	n5	0.64	0/974	0.80	1/1314 (0.1%)
62	N6	0.68	0/1004	0.87	1/1341 (0.1%)
62	n6	0.67	0/1004	0.84	0/1341
63	N7	0.53	0/1118	0.65	0/1497
63	n7	0.53	0/1118	0.68	0/1497
64	N8	0.76	0/1204	0.90	2/1612 (0.1%)
64	n8	0.77	0/1204	0.86	1/1612 (0.1%)
65	N9	0.66	0/473	0.75	0/629
65	n9	0.71	0/473	0.96	1/629 (0.2%)
66	O0	0.50	0/751	0.69	0/1008
66	o0	0.49	0/775	0.66	0/1040
67	O1	0.63	0/890	0.72	0/1196
67	o1	0.73	0/897	0.86	0/1205
68	O2	0.82	0/1041	0.90	0/1394
68	o2	0.81	0/1041	0.90	1/1394 (0.1%)
69	O3	0.87	0/868	0.94	2/1168 (0.2%)
69	o3	0.87	0/868	0.91	2/1168 (0.2%)
70	O4	0.60	0/890	0.77	2/1189 (0.2%)
70	o4	0.58	0/890	0.79	0/1189
71	O5	0.71	0/978	0.81	1/1301 (0.1%)
71	o5	0.58	0/974	0.72	1/1297 (0.1%)
72	O6	0.63	0/778	0.77	0/1034
72	o6	0.56	0/777	0.68	0/1033
73	O7	0.76	0/696	0.95	2/923 (0.2%)
73	o7	0.68	0/696	0.84	0/923
74	O8	0.55	0/618	0.67	0/826
74	o8	0.53	0/614	0.66	0/822
75	O9	0.77	0/443	0.91	0/588
75	o9	0.67	0/443	0.85	0/588
76	Q0	0.72	0/423	0.82	0/562
76	q0	0.86	0/423	0.93	0/562
77	Q1	0.62	0/234	0.81	0/300
77	q1	0.80	0/234	1.02	0/300
78	Q2	0.80	1/860 (0.1%)	0.84	2/1136 (0.2%)
78	q2	0.75	1/860 (0.1%)	0.82	2/1136 (0.2%)
79	Q3	0.70	0/701	0.80	0/934
79	q3	0.70	0/701	0.82	1/934 (0.1%)
80	e0	0.53	0/499	0.74	0/665
82	p0	0.45	0/1091	0.60	0/1472
All	All	0.84	242/430072 (0.1%)	1.32	5111/631360 (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
5	s3	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
11	s9	0	1
16	C4	0	2
18	c6	0	1
19	C7	0	1
19	c7	0	1
22	d0	0	1
25	D3	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	2
40	l3	0	1
41	L4	0	1
44	l7	0	2
45	L8	0	1
48	M1	0	1
50	m4	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
56	n0	0	3
64	n8	0	1
65	N9	0	1
69	o3	0	1
72	O6	0	1
75	O9	0	1
81	m2	0	1
All	All	0	37

The worst 5 of 242 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	12.79	2.04	1.82
36	5	1152	G	N9-C4	-11.94	1.28	1.38
36	1	3181	C	N3-C4	-9.75	1.27	1.33
36	1	895	A	C5-C6	-9.41	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	9.34	1.98	1.82

The worst 5 of 5111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	N3-C4-N9	-26.30	110.22	126.00
36	5	1152	G	N3-C4-C5	25.75	141.47	128.60
36	5	1152	G	C2-N3-C4	-18.79	102.51	111.90
36	5	929	A	O5'-P-OP2	-14.22	92.90	105.70
36	1	2420	C	O5'-P-OP1	-13.73	93.34	105.70

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	38	THR	Peptide
19	C7	85	VAL	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%)	140 (69%)	38 (19%)	26 (13%)	0 1
2	s0	204/251 (81%)	148 (72%)	33 (16%)	23 (11%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	S1	212/254 (84%)	149 (70%)	39 (18%)	24 (11%)	0 2
3	s1	214/254 (84%)	173 (81%)	32 (15%)	9 (4%)	3 20
4	S2	215/253 (85%)	175 (81%)	27 (13%)	13 (6%)	1 12
4	s2	215/253 (85%)	176 (82%)	26 (12%)	13 (6%)	1 12
5	S3	221/239 (92%)	177 (80%)	30 (14%)	14 (6%)	1 10
5	s3	221/239 (92%)	168 (76%)	35 (16%)	18 (8%)	1 5
6	S4	258/260 (99%)	206 (80%)	42 (16%)	10 (4%)	3 22
6	s4	258/260 (99%)	212 (82%)	26 (10%)	20 (8%)	1 6
7	S5	204/224 (91%)	158 (78%)	30 (15%)	16 (8%)	1 6
7	s5	204/224 (91%)	144 (71%)	45 (22%)	15 (7%)	1 7
8	S6	224/236 (95%)	194 (87%)	18 (8%)	12 (5%)	2 14
8	s6	216/236 (92%)	189 (88%)	17 (8%)	10 (5%)	2 18
9	S7	182/189 (96%)	142 (78%)	25 (14%)	15 (8%)	1 5
9	s7	184/189 (97%)	144 (78%)	23 (12%)	17 (9%)	1 3
10	S8	184/200 (92%)	155 (84%)	19 (10%)	10 (5%)	2 14
10	s8	184/200 (92%)	158 (86%)	18 (10%)	8 (4%)	2 20
11	S9	183/196 (93%)	135 (74%)	36 (20%)	12 (7%)	1 9
11	s9	183/196 (93%)	149 (81%)	25 (14%)	9 (5%)	2 17
12	C0	94/105 (90%)	66 (70%)	20 (21%)	8 (8%)	1 4
12	c0	92/105 (88%)	64 (70%)	12 (13%)	16 (17%)	0 0
13	C1	153/155 (99%)	124 (81%)	18 (12%)	11 (7%)	1 7
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	1 10
14	C2	122/142 (86%)	71 (58%)	32 (26%)	19 (16%)	0 1
14	c2	122/142 (86%)	69 (57%)	31 (25%)	22 (18%)	0 0
15	C3	148/150 (99%)	119 (80%)	21 (14%)	8 (5%)	2 14
15	c3	148/150 (99%)	110 (74%)	27 (18%)	11 (7%)	1 7
16	C4	125/136 (92%)	87 (70%)	24 (19%)	14 (11%)	0 2
16	c4	126/136 (93%)	95 (75%)	16 (13%)	15 (12%)	0 2
17	C5	122/141 (86%)	86 (70%)	26 (21%)	10 (8%)	1 5
17	c5	133/141 (94%)	88 (66%)	25 (19%)	20 (15%)	0 1
18	C6	139/142 (98%)	114 (82%)	14 (10%)	11 (8%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	c6	140/142 (99%)	113 (81%)	21 (15%)	6 (4%)	2 20
19	C7	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0 3
19	c7	113/136 (83%)	89 (79%)	15 (13%)	9 (8%)	1 6
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1 5
20	c8	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1 6
21	C9	141/143 (99%)	109 (77%)	23 (16%)	9 (6%)	1 10
21	c9	141/143 (99%)	117 (83%)	17 (12%)	7 (5%)	2 16
22	D0	105/120 (88%)	78 (74%)	23 (22%)	4 (4%)	3 22
22	d0	108/120 (90%)	82 (76%)	19 (18%)	7 (6%)	1 10
23	D1	85/87 (98%)	59 (69%)	19 (22%)	7 (8%)	1 5
23	d1	85/87 (98%)	65 (76%)	13 (15%)	7 (8%)	1 5
24	D2	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	3 22
24	d2	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19 58
25	D3	142/144 (99%)	108 (76%)	20 (14%)	14 (10%)	0 3
25	d3	142/144 (99%)	121 (85%)	16 (11%)	5 (4%)	3 24
26	D4	132/134 (98%)	108 (82%)	14 (11%)	10 (8%)	1 7
26	d4	132/134 (98%)	101 (76%)	17 (13%)	14 (11%)	0 2
27	D5	68/107 (64%)	46 (68%)	12 (18%)	10 (15%)	0 1
27	d5	67/107 (63%)	50 (75%)	13 (19%)	4 (6%)	1 12
28	D6	95/97 (98%)	55 (58%)	21 (22%)	19 (20%)	0 0
28	d6	95/97 (98%)	69 (73%)	19 (20%)	7 (7%)	1 7
29	D7	79/81 (98%)	59 (75%)	17 (22%)	3 (4%)	3 22
29	d7	79/81 (98%)	58 (73%)	14 (18%)	7 (9%)	1 4
30	D8	61/66 (92%)	46 (75%)	12 (20%)	3 (5%)	2 17
30	d8	61/66 (92%)	44 (72%)	15 (25%)	2 (3%)	4 25
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1 12
31	d9	51/55 (93%)	38 (74%)	8 (16%)	5 (10%)	0 3
32	E0	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1 4
33	E1	69/76 (91%)	32 (46%)	17 (25%)	20 (29%)	0 0
33	e1	74/76 (97%)	39 (53%)	17 (23%)	18 (24%)	0 0
34	SR	316/318 (99%)	265 (84%)	43 (14%)	8 (2%)	5 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	sR	316/318 (99%)	263 (83%)	40 (13%)	13 (4%)	3 21
35	SM	155/273 (57%)	105 (68%)	32 (21%)	18 (12%)	0 2
35	sM	98/273 (36%)	60 (61%)	21 (21%)	17 (17%)	0 0
39	L2	250/253 (99%)	222 (89%)	21 (8%)	7 (3%)	5 29
39	l2	250/253 (99%)	205 (82%)	27 (11%)	18 (7%)	1 7
40	L3	384/386 (100%)	316 (82%)	52 (14%)	16 (4%)	3 20
40	l3	384/386 (100%)	334 (87%)	32 (8%)	18 (5%)	2 17
41	L4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	1 12
41	l4	359/361 (99%)	299 (83%)	37 (10%)	23 (6%)	1 10
42	L5	294/296 (99%)	243 (83%)	35 (12%)	16 (5%)	2 14
42	l5	292/296 (99%)	255 (87%)	28 (10%)	9 (3%)	4 26
43	L6	152/175 (87%)	142 (93%)	8 (5%)	2 (1%)	12 47
43	l6	153/175 (87%)	136 (89%)	13 (8%)	4 (3%)	5 31
44	L7	220/243 (90%)	189 (86%)	22 (10%)	9 (4%)	3 21
44	l7	221/243 (91%)	190 (86%)	25 (11%)	6 (3%)	5 30
45	L8	231/255 (91%)	182 (79%)	34 (15%)	15 (6%)	1 10
45	l8	229/255 (90%)	180 (79%)	32 (14%)	17 (7%)	1 7
46	L9	189/191 (99%)	158 (84%)	20 (11%)	11 (6%)	1 13
46	l9	189/191 (99%)	166 (88%)	18 (10%)	5 (3%)	5 31
47	M0	207/220 (94%)	177 (86%)	21 (10%)	9 (4%)	2 20
47	m0	209/220 (95%)	160 (77%)	31 (15%)	18 (9%)	1 4
48	M1	167/173 (96%)	127 (76%)	23 (14%)	17 (10%)	0 3
48	m1	167/173 (96%)	136 (81%)	21 (13%)	10 (6%)	1 12
49	M3	191/198 (96%)	156 (82%)	28 (15%)	7 (4%)	3 22
49	m3	192/198 (97%)	153 (80%)	23 (12%)	16 (8%)	1 5
50	M4	134/137 (98%)	118 (88%)	10 (8%)	6 (4%)	2 18
50	m4	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	6 35
51	M5	201/203 (99%)	178 (89%)	20 (10%)	3 (2%)	10 44
51	m5	201/203 (99%)	171 (85%)	24 (12%)	6 (3%)	4 28
52	M6	195/198 (98%)	174 (89%)	17 (9%)	4 (2%)	7 37
52	m6	195/198 (98%)	170 (87%)	19 (10%)	6 (3%)	4 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	M7	181/183 (99%)	151 (83%)	23 (13%)	7 (4%)	3 22
53	m7	153/183 (84%)	135 (88%)	16 (10%)	2 (1%)	12 47
54	M8	183/185 (99%)	153 (84%)	22 (12%)	8 (4%)	2 19
54	m8	183/185 (99%)	152 (83%)	25 (14%)	6 (3%)	4 25
55	M9	186/188 (99%)	162 (87%)	22 (12%)	2 (1%)	14 51
55	m9	186/188 (99%)	159 (86%)	24 (13%)	3 (2%)	9 43
56	N0	170/172 (99%)	149 (88%)	15 (9%)	6 (4%)	3 24
56	n0	170/172 (99%)	153 (90%)	13 (8%)	4 (2%)	6 34
57	N1	157/159 (99%)	136 (87%)	18 (12%)	3 (2%)	8 39
57	n1	157/159 (99%)	137 (87%)	15 (10%)	5 (3%)	4 26
58	N2	98/120 (82%)	82 (84%)	11 (11%)	5 (5%)	2 15
58	n2	96/120 (80%)	79 (82%)	13 (14%)	4 (4%)	3 20
59	N3	134/136 (98%)	119 (89%)	12 (9%)	3 (2%)	6 35
59	n3	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	6 35
60	N4	96/155 (62%)	73 (76%)	14 (15%)	9 (9%)	0 3
60	n4	133/155 (86%)	106 (80%)	15 (11%)	12 (9%)	1 4
61	N5	119/141 (84%)	105 (88%)	12 (10%)	2 (2%)	9 42
61	n5	118/141 (84%)	92 (78%)	15 (13%)	11 (9%)	0 3
62	N6	124/126 (98%)	113 (91%)	9 (7%)	2 (2%)	9 43
62	n6	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	3 21
63	N7	133/135 (98%)	112 (84%)	16 (12%)	5 (4%)	3 22
63	n7	133/135 (98%)	109 (82%)	13 (10%)	11 (8%)	1 5
64	N8	146/148 (99%)	118 (81%)	21 (14%)	7 (5%)	2 17
64	n8	146/148 (99%)	119 (82%)	21 (14%)	6 (4%)	3 21
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	3 23
65	n9	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0 2
66	O0	95/104 (91%)	83 (87%)	9 (10%)	3 (3%)	4 26
66	o0	98/104 (94%)	84 (86%)	14 (14%)	0	100 100
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	2 14
67	o1	107/112 (96%)	93 (87%)	9 (8%)	5 (5%)	2 17
68	O2	125/129 (97%)	111 (89%)	10 (8%)	4 (3%)	4 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
68	o2	125/129 (97%)	100 (80%)	18 (14%)	7 (6%)	2 14
69	O3	104/106 (98%)	90 (86%)	10 (10%)	4 (4%)	3 22
69	o3	104/106 (98%)	92 (88%)	10 (10%)	2 (2%)	8 39
70	O4	110/120 (92%)	88 (80%)	18 (16%)	4 (4%)	3 23
70	o4	110/120 (92%)	97 (88%)	10 (9%)	3 (3%)	5 30
71	O5	117/119 (98%)	100 (86%)	11 (9%)	6 (5%)	2 15
71	o5	117/119 (98%)	97 (83%)	17 (14%)	3 (3%)	5 31
72	O6	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1 7
72	o6	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	3 21
73	O7	85/87 (98%)	70 (82%)	13 (15%)	2 (2%)	6 34
73	o7	85/87 (98%)	65 (76%)	17 (20%)	3 (4%)	3 24
74	O8	75/77 (97%)	59 (79%)	12 (16%)	4 (5%)	2 15
74	o8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2 15
75	O9	48/50 (96%)	42 (88%)	6 (12%)	0	100 100
75	o9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	7 37
76	Q0	50/52 (96%)	46 (92%)	1 (2%)	3 (6%)	1 12
76	q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3 21
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100 100
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100 100
78	Q2	103/105 (98%)	82 (80%)	15 (15%)	6 (6%)	1 13
78	q2	103/105 (98%)	90 (87%)	9 (9%)	4 (4%)	3 22
79	Q3	89/91 (98%)	76 (85%)	9 (10%)	4 (4%)	2 18
79	q3	89/91 (98%)	77 (86%)	11 (12%)	1 (1%)	14 51
80	e0	60/62 (97%)	42 (70%)	11 (18%)	7 (12%)	0 2
82	p0	139/311 (45%)	117 (84%)	15 (11%)	7 (5%)	2 16
All	All	22333/24143 (92%)	18126 (81%)	2889 (13%)	1318 (6%)	1 12

5 of 1318 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	32	HIS
2	S0	66	ALA

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Mol	Chain	Res	Type
2	S0	68	PRO
2	S0	111	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S0	164/209 (78%)	134 (82%)	30 (18%)	1 8
2	s0	165/209 (79%)	137 (83%)	28 (17%)	2 10
3	S1	191/223 (86%)	147 (77%)	44 (23%)	1 3
3	s1	192/223 (86%)	154 (80%)	38 (20%)	1 7
4	S2	176/204 (86%)	140 (80%)	36 (20%)	1 6
4	s2	176/204 (86%)	127 (72%)	49 (28%)	0 1
5	S3	182/194 (94%)	149 (82%)	33 (18%)	1 8
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1 6
6	S4	221/221 (100%)	177 (80%)	44 (20%)	1 6
6	s4	221/221 (100%)	179 (81%)	42 (19%)	1 8
7	S5	173/190 (91%)	145 (84%)	28 (16%)	2 11
7	s5	173/190 (91%)	140 (81%)	33 (19%)	1 8
8	S6	188/201 (94%)	152 (81%)	36 (19%)	1 8
8	s6	187/201 (93%)	158 (84%)	29 (16%)	2 12
9	S7	165/169 (98%)	135 (82%)	30 (18%)	1 8
9	s7	165/169 (98%)	131 (79%)	34 (21%)	1 6
10	S8	150/161 (93%)	123 (82%)	27 (18%)	1 9
10	s8	150/161 (93%)	125 (83%)	25 (17%)	2 10
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1 3
11	s9	158/165 (96%)	121 (77%)	37 (23%)	1 3
12	C0	77/98 (79%)	62 (80%)	15 (20%)	1 7
12	c0	73/98 (74%)	61 (84%)	12 (16%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	C1	129/136 (95%)	108 (84%)	21 (16%)	2 11
13	c1	129/136 (95%)	105 (81%)	24 (19%)	1 8
14	C2	88/118 (75%)	70 (80%)	18 (20%)	1 6
14	c2	88/118 (75%)	68 (77%)	20 (23%)	1 4
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1 6
15	c3	127/127 (100%)	104 (82%)	23 (18%)	1 8
16	C4	81/104 (78%)	63 (78%)	18 (22%)	1 4
16	c4	97/104 (93%)	72 (74%)	25 (26%)	0 2
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1 6
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2 9
18	C6	117/118 (99%)	96 (82%)	21 (18%)	2 9
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1 8
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1 5
19	c7	92/124 (74%)	71 (77%)	21 (23%)	1 4
20	C8	128/128 (100%)	92 (72%)	36 (28%)	0 1
20	c8	128/128 (100%)	99 (77%)	29 (23%)	1 4
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1 4
21	c9	115/115 (100%)	95 (83%)	20 (17%)	2 10
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2 10
22	d0	103/113 (91%)	74 (72%)	29 (28%)	0 1
23	D1	74/74 (100%)	57 (77%)	17 (23%)	1 3
23	d1	74/74 (100%)	53 (72%)	21 (28%)	0 1
24	D2	110/110 (100%)	86 (78%)	24 (22%)	1 5
24	d2	110/110 (100%)	92 (84%)	18 (16%)	2 11
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4 18
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2 9
26	D4	112/112 (100%)	101 (90%)	11 (10%)	8 31
26	d4	112/112 (100%)	90 (80%)	22 (20%)	1 7
27	D5	61/88 (69%)	42 (69%)	19 (31%)	0 0
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1 7
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	d6	83/83 (100%)	67 (81%)	16 (19%)	1 8
29	D7	70/70 (100%)	61 (87%)	9 (13%)	4 19
29	d7	70/70 (100%)	58 (83%)	12 (17%)	2 10
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0 1
30	d8	56/59 (95%)	43 (77%)	13 (23%)	1 3
31	D9	47/48 (98%)	35 (74%)	12 (26%)	0 2
31	d9	47/48 (98%)	38 (81%)	9 (19%)	1 8
32	E0	51/51 (100%)	44 (86%)	7 (14%)	3 17
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0 2
33	e1	66/66 (100%)	49 (74%)	17 (26%)	0 2
34	SR	260/261 (100%)	225 (86%)	35 (14%)	4 18
34	sR	260/261 (100%)	229 (88%)	31 (12%)	5 22
35	SM	97/228 (42%)	75 (77%)	22 (23%)	1 4
35	sM	54/228 (24%)	44 (82%)	10 (18%)	1 8
39	L2	193/195 (99%)	150 (78%)	43 (22%)	1 4
39	l2	192/195 (98%)	157 (82%)	35 (18%)	1 8
40	L3	319/322 (99%)	254 (80%)	65 (20%)	1 6
40	l3	320/322 (99%)	249 (78%)	71 (22%)	1 4
41	L4	288/288 (100%)	235 (82%)	53 (18%)	1 8
41	l4	288/288 (100%)	227 (79%)	61 (21%)	1 5
42	L5	244/244 (100%)	203 (83%)	41 (17%)	2 10
42	l5	243/244 (100%)	200 (82%)	43 (18%)	2 9
43	L6	134/152 (88%)	110 (82%)	24 (18%)	2 9
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2 10
44	L7	186/204 (91%)	161 (87%)	25 (13%)	4 18
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3 15
45	L8	187/207 (90%)	154 (82%)	33 (18%)	2 9
45	l8	177/207 (86%)	148 (84%)	29 (16%)	2 11
46	L9	171/171 (100%)	139 (81%)	32 (19%)	1 8
46	l9	171/171 (100%)	125 (73%)	46 (27%)	0 2
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%)	152 (85%)	27 (15%)	3 14
48	M1	147/150 (98%)	116 (79%)	31 (21%)	1 6
48	m1	147/150 (98%)	113 (77%)	34 (23%)	1 3
49	M3	154/158 (98%)	123 (80%)	31 (20%)	1 6
49	m3	154/158 (98%)	127 (82%)	27 (18%)	2 9
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1 8
50	m4	108/108 (100%)	83 (77%)	25 (23%)	1 3
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2 10
51	m5	175/175 (100%)	144 (82%)	31 (18%)	2 9
52	M6	160/161 (99%)	139 (87%)	21 (13%)	4 19
52	m6	160/161 (99%)	125 (78%)	35 (22%)	1 5
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1 4
53	m7	125/145 (86%)	94 (75%)	31 (25%)	0 2
54	M8	150/150 (100%)	129 (86%)	21 (14%)	3 16
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1 5
55	M9	153/153 (100%)	128 (84%)	25 (16%)	2 11
55	m9	153/153 (100%)	127 (83%)	26 (17%)	2 10
56	N0	156/156 (100%)	126 (81%)	30 (19%)	1 8
56	n0	156/156 (100%)	120 (77%)	36 (23%)	1 3
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1 4
57	n1	136/136 (100%)	105 (77%)	31 (23%)	1 4
58	N2	87/106 (82%)	66 (76%)	21 (24%)	0 3
58	n2	85/106 (80%)	71 (84%)	14 (16%)	2 10
59	N3	104/104 (100%)	81 (78%)	23 (22%)	1 4
59	n3	104/104 (100%)	88 (85%)	16 (15%)	2 13
60	N4	57/129 (44%)	51 (90%)	6 (10%)	7 28
60	n4	100/129 (78%)	80 (80%)	20 (20%)	1 6
61	N5	104/117 (89%)	79 (76%)	25 (24%)	0 3
61	n5	104/117 (89%)	89 (86%)	15 (14%)	3 15
62	N6	109/109 (100%)	89 (82%)	20 (18%)	1 8
62	n6	109/109 (100%)	89 (82%)	20 (18%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
63	N7	115/115 (100%)	90 (78%)	25 (22%)	1 5
63	n7	115/115 (100%)	86 (75%)	29 (25%)	0 2
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2 10
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1 5
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1 5
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0 0
66	O0	81/87 (93%)	70 (86%)	11 (14%)	3 17
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1 4
67	O1	92/96 (96%)	76 (83%)	16 (17%)	2 10
67	o1	94/96 (98%)	66 (70%)	28 (30%)	0 1
68	O2	109/110 (99%)	89 (82%)	20 (18%)	1 8
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1 8
69	O3	90/90 (100%)	74 (82%)	16 (18%)	2 9
69	o3	90/90 (100%)	78 (87%)	12 (13%)	4 18
70	O4	95/102 (93%)	81 (85%)	14 (15%)	3 14
70	o4	95/102 (93%)	78 (82%)	17 (18%)	2 9
71	O5	104/104 (100%)	85 (82%)	19 (18%)	1 8
71	o5	103/104 (99%)	77 (75%)	26 (25%)	0 2
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1 6
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0 1
73	O7	70/70 (100%)	53 (76%)	17 (24%)	0 2
73	o7	70/70 (100%)	62 (89%)	8 (11%)	5 24
74	O8	68/68 (100%)	46 (68%)	22 (32%)	0 0
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1 6
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2 9
75	o9	45/45 (100%)	34 (76%)	11 (24%)	0 2
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2 10
76	q0	47/47 (100%)	34 (72%)	13 (28%)	0 1
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0 2
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0 0
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	q2	90/90 (100%)	68 (76%)	22 (24%)	0 2
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1 6
79	q3	71/71 (100%)	59 (83%)	12 (17%)	2 10
80	e0	53/53 (100%)	43 (81%)	10 (19%)	1 8
82	p0	105/253 (42%)	86 (82%)	19 (18%)	1 8
All	All	18727/20241 (92%)	15053 (80%)	3674 (20%)	1 7

5 of 3674 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	s1	223	PHE
72	o6	21	THR
19	c7	34	LEU
70	o4	31	ARG
55	m9	177	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
78	Q2	82	GLN
55	m9	7	GLN
11	s9	133	HIS
52	m6	31	GLN
64	n8	49	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	487 (27%)	58 (3%)
1	6	1793/1800 (99%)	477 (26%)	48 (2%)
36	1	3145/3396 (92%)	709 (22%)	82 (2%)
36	5	3146/3396 (92%)	741 (23%)	85 (2%)
37	3	120/121 (99%)	21 (17%)	1 (0%)
37	7	120/121 (99%)	20 (16%)	1 (0%)
38	4	157/158 (99%)	41 (26%)	2 (1%)
38	8	157/158 (99%)	34 (21%)	2 (1%)
All	All	10385/10950 (94%)	2530 (24%)	279 (2%)

5 of 2530 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 279 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	1792	C
36	5	2093	A
36	5	2896	A
36	1	1751	G
36	1	1607	U

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 2555 ligands modelled in this entry, 1424 are monoatomic - leaving 1131 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	$\#\|Z\| > 2$
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	4	221	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	4	237	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	S8	301	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	2	2179	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	6	2045	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	N1	201	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	n3	204	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	O7	105	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	n5	201	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	3	214	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	l5	302	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	L3	402	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	O7	106	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	m1	201	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	2	2180	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	m5	304	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	2	2181	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	M7	206	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	6	2043	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	7	228	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	1	4211	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	M8	201	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	q1	102	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	4	238	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	l4	403	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	d4	202	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	s8	304	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	l5	303	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	M7	207	-	0,6,6	-	-	-		
88	3KF	1	4212	85	25,25,25	0.85	0	30,39,39	0.93	1 (3%)
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
88	3KF	5	4248	85	25,25,25	0.60	0	30,39,39	0.98	2 (6%)
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	6	2044	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	5	3897	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	L4	402	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	m6	204	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	l9	202	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	2	2125	-	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
88	3KF	5	4248	85	-	-	0/4/4/4
88	3KF	1	4212	85	-	-	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	1	4212	3KF	O3-C11-C12	-2.66	103.48	109.01
88	5	4248	3KF	C5-C4-C13	2.26	122.00	119.22
88	5	4248	3KF	O4-C10-C11	-2.09	105.53	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

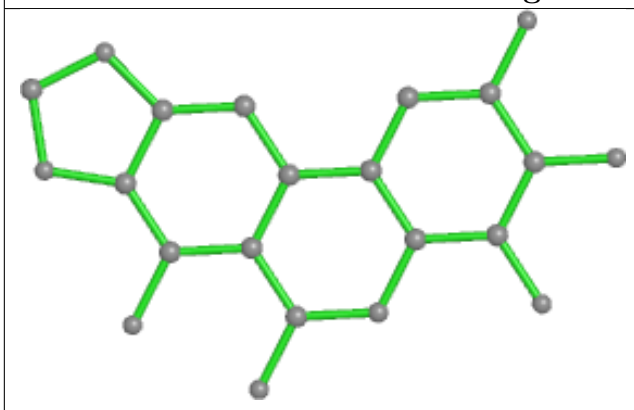
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2162	OHX	0	1
86	5	3939	OHX	0	1

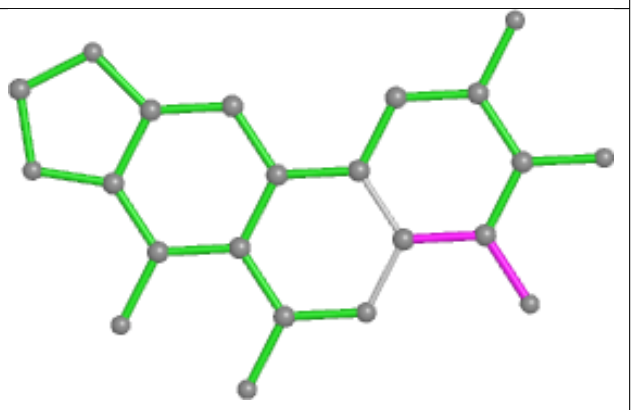
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

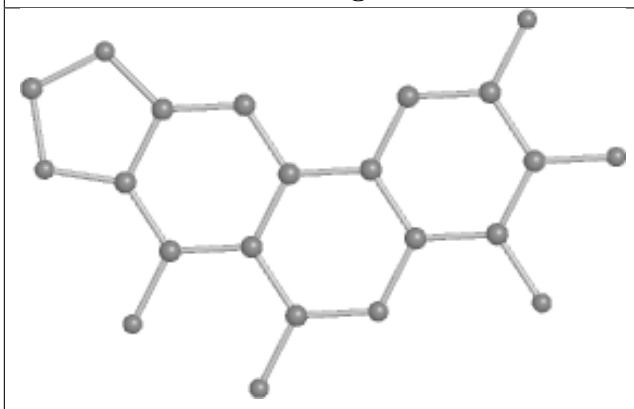
Ligand 3KF 1 4212



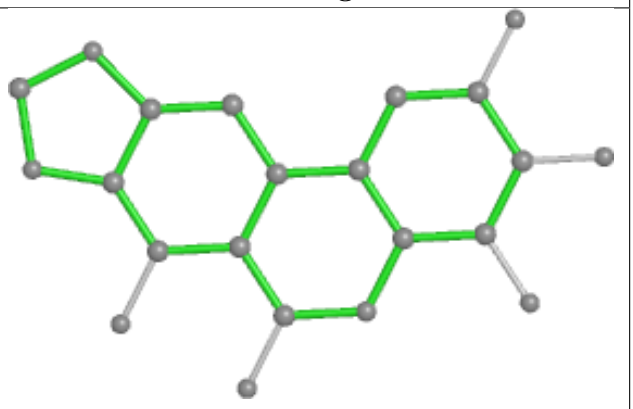
Bond lengths



Bond angles

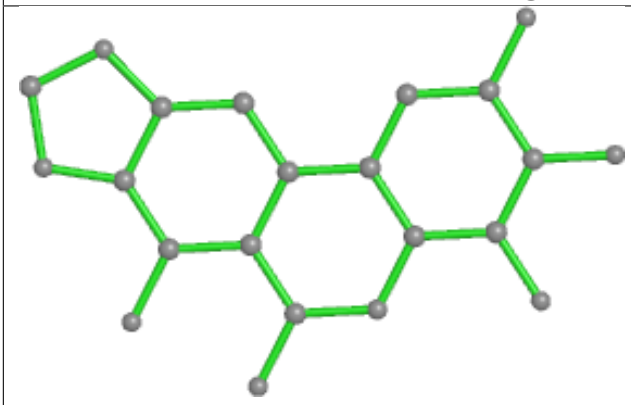


Torsions

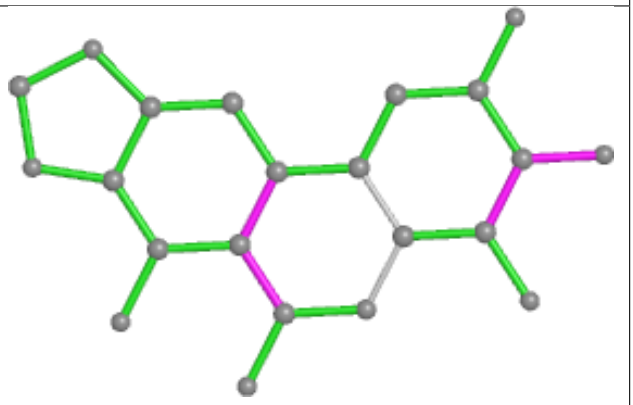


Rings

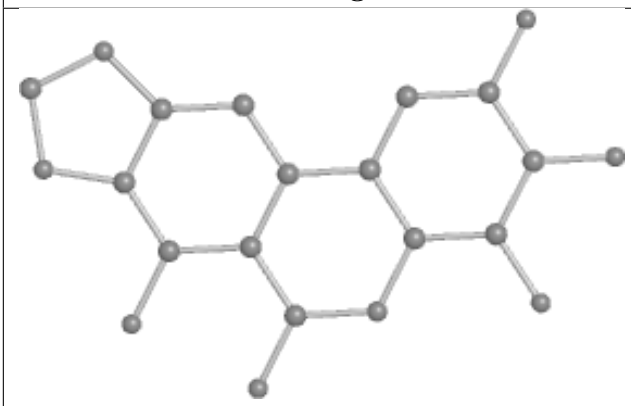
Ligand 3KF 5 4248



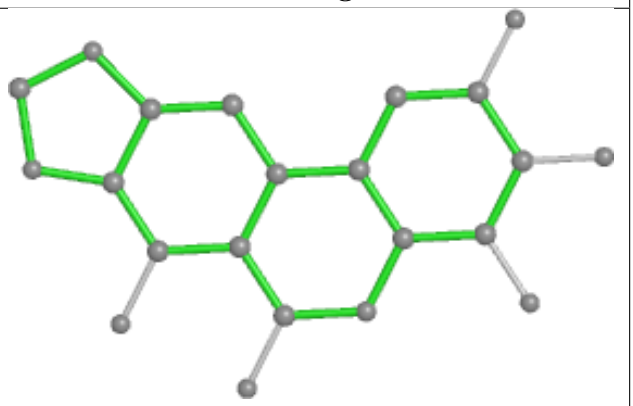
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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