wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 02:06 am GMT

PDB ID	:	4U4Y
Title	:	Crystal structure of Pactamycin 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:

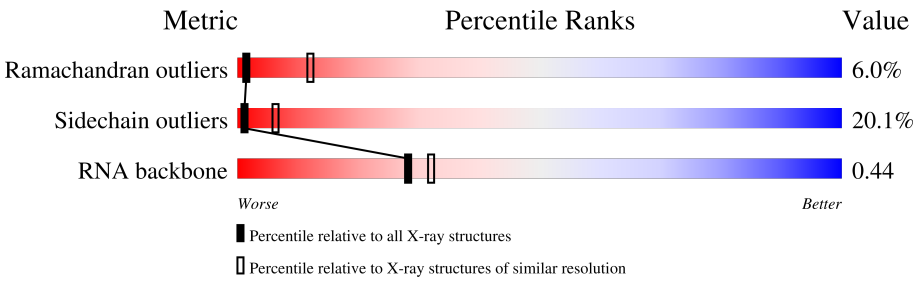
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et 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	62% 30% 5% •
1	6	1800	60% 33% 6%
2	S0	251	61% 20% • 18%
2	s0	251	62% 18% • 18%
3	S1	254	57% 24% • 16%
3	s1	254	63% 21% • 15%
4	S2	253	67% 18% • 14%
4	s2	253	62% 22% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	S3	239	74% 17% • 7%
5	s3	239	72% 19% • 7%
6	S4	260	73% 24% •
6	s4	260	77% 21% •
7	S5	224	70% 20% • 8%
7	s5	224	69% 22% • 8%
8	S6	236	76% 19% • •
8	s6	236	74% 17% • 8%
9	S7	189	72% 21% • •
9	s7	189	77% 20% • •
10	S8	200	76% 16% • 6%
10	s8	200	76% 17% • 6%
11	S9	196	71% 22% • 6%
11	s9	196	71% 22% • 6%
12	C0	105	69% 20% • 9%
12	c0	105	70% 17% • 9%
13	C1	155	79% 19% •
13	c1	155	74% 19% • 6%
14	C2	142	58% 27% • 13%
14	c2	142	60% 24% • • 13%
15	C3	150	79% 20% •
15	c3	150	79% 18% •
16	C4	136	71% 18% • 7%
16	c4	136	69% 22% • 6%
17	C5	141	67% 16% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	c5	141	68% 24%
18	C6	142	77% 21%
18	c6	142	81% 19%
19	C7	136	68% 16% 12%
19	c7	136	63% 21% 14%
20	C8	145	74% 22%
20	c8	145	77% 20%
21	C9	143	79% 20%
21	c9	143	82% 17%
22	D0	120	67% 22% 11%
22	d0	120	60% 30% 8%
23	D1	87	78% 18%
23	d1	87	77% 23%
24	D2	129	77% 22%
24	d2	129	85% 13%
25	D3	144	77% 22%
25	d3	144	82% 17%
26	D4	134	79% 20%
26	d4	134	80% 19%
27	D5	107	40% 24% 35%
27	d5	107	52% 11% 36%
28	D6	97	68% 26% 5%
28	d6	97	77% 22%
29	D7	81	88% 12%
29	d7	81	84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	D8	66	70% 24% 5%
30	d8	66	67% 26% 5%
31	D9	55	82% 13%
31	d9	55	69% 25%
32	E0	60	82% 15%
33	E1	76	49% 39% 5% 7%
33	e1	76	55% 41%
34	SR	318	82% 17%
34	sR	318	87% 12%
35	SM	273	45% 12% 42%
35	sM	273	27% 10% 62%
36	1	3396	47% 38% 8% 7%
36	5	3396	45% 40% 7% 7%
37	3	121	70% 27%
37	7	121	59% 32% 9%
38	4	158	49% 44% 7%
38	8	158	57% 35% 8%
39	L2	253	81% 18%
39	l2	253	83% 15%
40	L3	386	77% 22%
40	l3	386	81% 18%
41	L4	361	79% 19%
41	l4	361	80% 19%
42	L5	296	80% 19%
42	l5	296	79% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
43	L6	175	77% 12% • 11%
43	l6	175	75% 14% • 10%
44	L7	243	75% 14% • 9%
44	l7	243	79% 11% • 8%
45	L8	255	74% 17% 9%
45	l8	255	69% 21% • 9%
46	L9	191	81% 18% •
46	l9	191	77% 21% •
47	M0	220	77% 18% • •
47	m0	220	73% 22% • •
48	M1	173	72% 22% • •
48	m1	173	71% 24% • •
49	M3	198	80% 15% • •
49	m3	198	75% 22% • •
50	M4	137	81% 18% • •
50	m4	137	80% 18% •
51	M5	203	82% 17%
51	m5	203	82% 16% •
52	M6	198	85% 13% • • •
52	m6	198	76% 21% • • •
53	M7	183	80% 19% •
53	m7	183	70% 15% 15%
54	M8	185	83% 16% •
54	m8	185	78% 21% •
55	M9	188	82% 18% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	m9	188	80% 19% •
56	N0	172	80% 18% •
56	n0	172	75% 24% •
57	N1	159	77% 21% •
57	n1	159	82% 16% •
58	N2	120	65% 17% • 17%
58	n2	120	67% 13% • 18%
59	N3	136	83% 17%
59	n3	136	85% 15%
60	N4	155	55% 8% • 37%
60	n4	155	74% 13% • 13%
61	N5	141	65% 18% • 14%
61	n5	141	66% 18% • 15%
62	N6	126	77% 21% •
62	n6	126	78% 21% •
63	N7	135	79% 21% •
63	n7	135	77% 22% •
64	N8	148	84% 14% •
64	n8	148	79% 20% •
65	N9	58	78% 22%
65	n9	58	76% 17% 5% •
66	O0	104	76% 16% • 7%
66	o0	104	74% 22% •
67	O1	112	71% 24% • •
67	o1	112	72% 23% •• •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
68	O2	129	82% 15%
68	o2	129	73% 24%
69	O3	106	85% 15%
69	o3	106	84% 15%
70	O4	120	78% 13% 7%
70	o4	120	73% 18% 7%
71	O5	119	78% 20%
71	o5	119	76% 24%
72	O6	99	77% 19%
72	o6	99	70% 26%
73	O7	87	75% 23%
73	o7	87	78% 21%
74	O8	77	73% 26%
74	o8	77	81% 19%
75	O9	50	78% 22%
75	o9	50	82% 18%
76	Q0	52	81% 17%
76	q0	52	71% 29%
77	Q1	25	56% 44%
77	q1	25	72% 28%
78	Q2	105	73% 26%
78	q2	105	80% 19%
79	Q3	91	80% 19%
79	q3	91	81% 19%
80	e0	62	71% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
81	m2	160	93% • 6%
82	p0	311	39% 6% 54%
83	p1	47	100%
84	p2	46	100%

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 411223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C5	137	SER	ARG	conflict	UNP Q01855
c5	137	SER	ARG	conflict	UNP Q01855

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	159	1104	652	221	231	0	0	0
35	sM	104	679	402	140	137	0	0	0

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
71	O5	119	969	615	186	167	1	0	0	0
71	o5	119	965	612	185	167	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	2	124	124	124	0	0
85	S2	2	2	2	0	0
85	S8	1	1	1	0	0
85	D0	1	1	1	0	0
85	D3	1	1	1	0	0
85	SM	1	1	1	0	0
85	1	471	471	471	0	0
85	3	14	14	14	0	0
85	4	21	21	21	0	0
85	L2	1	1	1	0	0
85	L3	2	2	2	0	0
85	L4	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	L5	1	1	1	0	0
85	L7	3	3	3	0	0
85	L8	1	1	1	0	0
85	M0	2	2	2	0	0
85	M1	1	1	1	0	0
85	M3	3	3	3	0	0
85	M5	2	2	2	0	0
85	M6	2	2	2	0	0
85	M7	4	4	4	0	0
85	M9	3	3	3	0	0
85	N0	1	1	1	0	0
85	N3	2	2	2	0	0
85	N5	1	1	1	0	0
85	N6	1	1	1	0	0
85	N8	4	4	4	0	0
85	N9	1	1	1	0	0
85	O2	1	1	1	0	0
85	O3	1	1	1	0	0
85	O7	2	2	2	0	0
85	Q2	1	1	1	0	0
85	6	147	147	147	0	0

Continued on next page...

Continued from previous page...

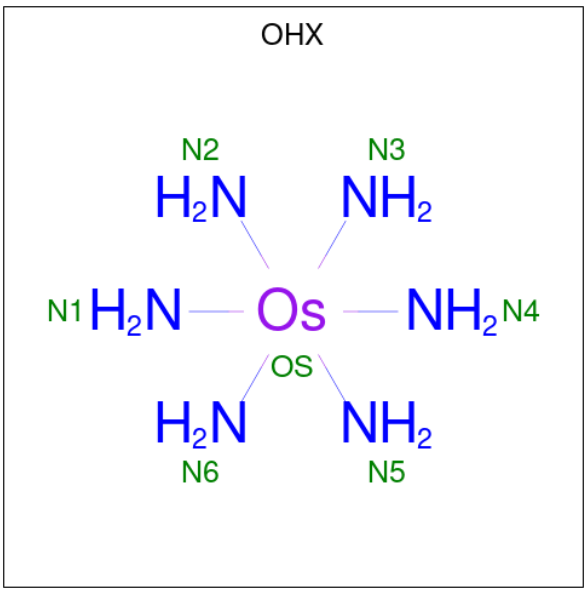
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	s1	1	1	1	0	0
85	s2	1	1	1	0	0
85	s8	2	2	2	0	0
85	c1	1	1	1	0	0
85	c7	1	1	1	0	0
85	c8	2	2	2	0	0
85	d3	2	2	2	0	0
85	d6	1	1	1	0	0
85	sM	2	2	2	0	0
85	5	504	504	504	0	0
85	7	14	14	14	0	0
85	8	16	16	16	0	0
85	l2	1	1	1	0	0
85	l3	2	2	2	0	0
85	l4	1	1	1	0	0
85	l5	2	2	2	0	0
85	l7	2	2	2	0	0
85	l8	1	1	1	0	0
85	m1	2	2	2	0	0
85	m5	4	4	4	0	0
85	m6	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	m7	5	Total Mg 5 5	0	0
85	n0	2	Total Mg 2 2	0	0
85	n3	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	o1	1	Total Mg 1 1	0	0
85	o3	1	Total Mg 1 1	0	0
85	o4	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
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	2	1	7	6	1	0	0
			Total	N	Os		
86	S6	1	7	6	1	0	0
			Total	N	Os		
86	S8	1	7	6	1	0	0
			Total	N	Os		
86	C3	1	7	6	1	0	0
			Total	N	Os		
86	C5	1	7	6	1	0	0
			Total	N	Os		
86	C8	1	7	6	1	0	0
			Total	N	Os		
86	D3	1	7	6	1	0	0
			Total	N	Os		
86	D9	1	7	6	1	0	0
			Total	N	Os		
86	SR	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0
			Total	N	Os		
86	1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	L3	1	7	6	1	0	0
86	L3	1	7	6	1	0	0
86	L3	1	7	6	1	0	0
86	L4	1	7	6	1	0	0
86	M0	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	M5	1	7	6	1	0	0
86	M7	1	7	6	1	0	0
86	M7	1	7	6	1	0	0
86	M9	1	7	6	1	0	0
86	N1	1	7	6	1	0	0
86	N9	1	7	6	1	0	0
86	O3	1	7	6	1	0	0
86	O7	1	7	6	1	0	0
86	Q2	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0
86	6	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	s1	1	7	6	1	0	0
86	s4	1	7	6	1	0	0
86	s8	1	7	6	1	0	0
86	s9	1	7	6	1	0	0
86	c3	1	7	6	1	0	0
86	c5	1	7	6	1	0	0
86	c8	1	7	6	1	0	0
86	d4	1	7	6	1	0	0
86	d9	1	7	6	1	0	0
86	sR	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0
86	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	5	1	7	6	1	0	0
			Total	N	Os		
86	5	1	7	6	1	0	0
			Total	N	Os		
86	5	1	7	6	1	0	0
			Total	N	Os		
86	5	1	7	6	1	0	0
			Total	N	Os		
86	5	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	7	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

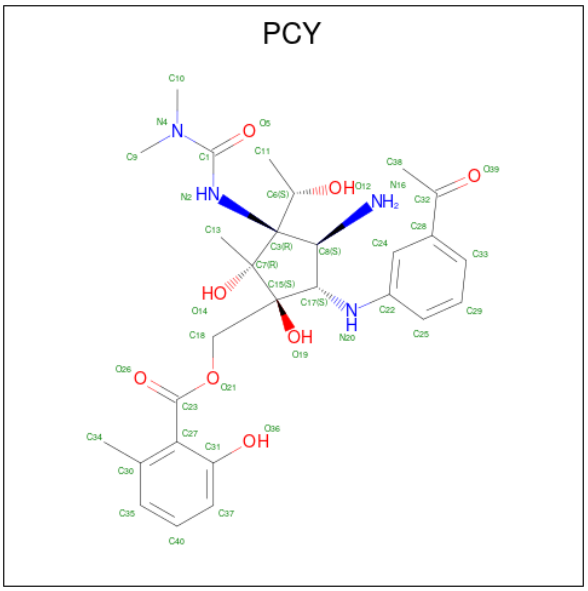
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6	1	0	0
			Total	N	Os		
86	8	1	7	6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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	m0	1	7	6	1	0	0
86	m1	1	7	6	1	0	0
86	m4	1	7	6	1	0	0
86	m5	1	7	6	1	0	0
86	m6	1	7	6	1	0	0
86	m7	1	7	6	1	0	0
86	m8	1	7	6	1	0	0
86	n3	1	7	6	1	0	0
86	n9	1	7	6	1	0	0
86	n9	1	7	6	1	0	0
86	o2	1	7	6	1	0	0
86	o3	1	7	6	1	0	0
86	o7	1	7	6	1	0	0
86	o7	1	7	6	1	0	0
86	q1	1	7	6	1	0	0
86	q2	1	7	6	1	0	0

- Molecule 87 is Pactamycin (three-letter code: PCY) (formula: $C_{28}H_{38}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
87	2	1	Total	C	N	O	0	0
			40	28	4	8		
87	6	1	Total	C	N	O	0	0
			40	28	4	8		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	D6	1	Total	Zn	0	0
			1	1		
88	D7	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		
88	O7	1	Total	Zn	0	0
			1	1		
88	Q0	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	Q3	1	Total	Zn	0	0
			1	1		
88	d6	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

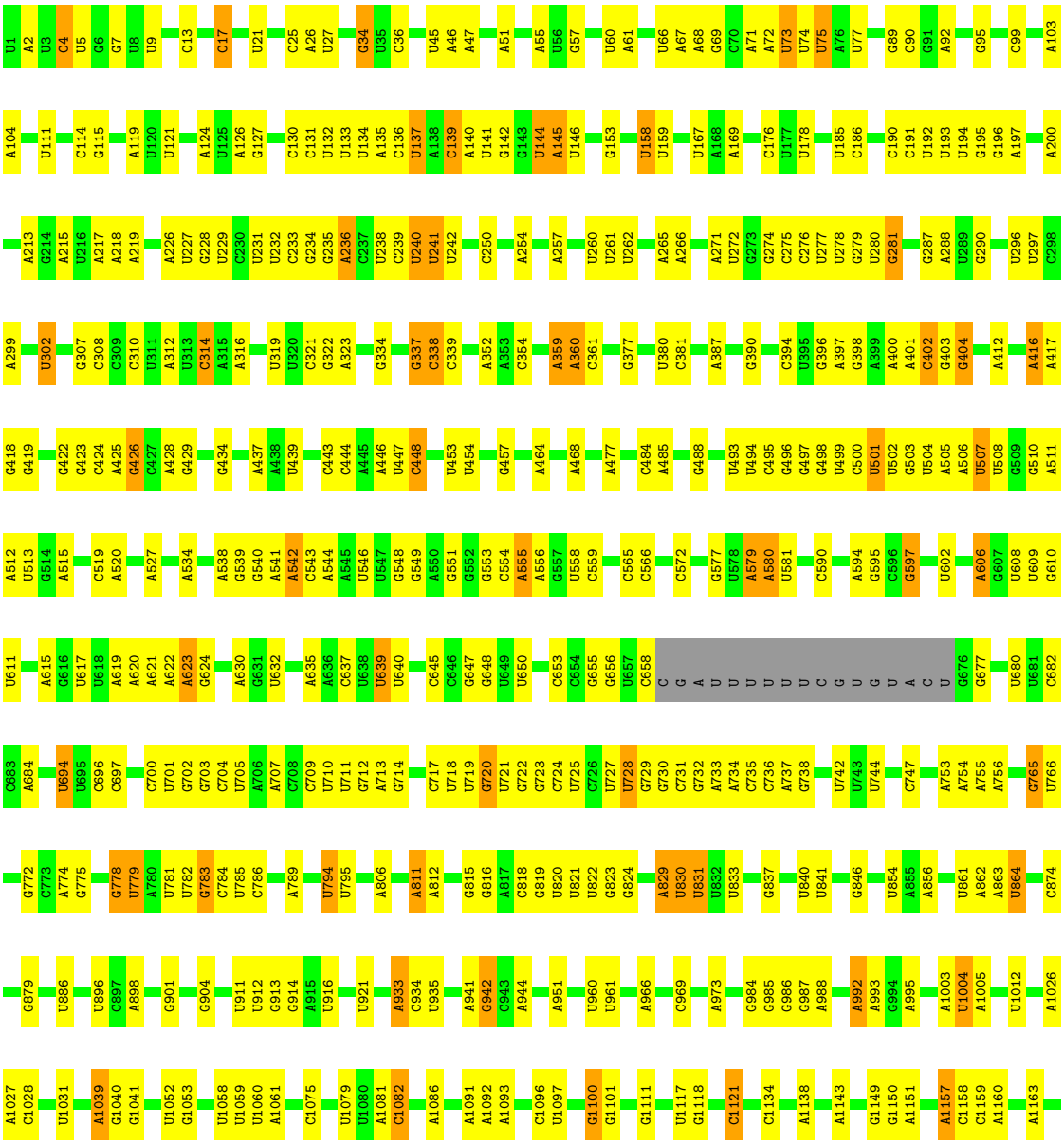
3 Residue-property plots (i)

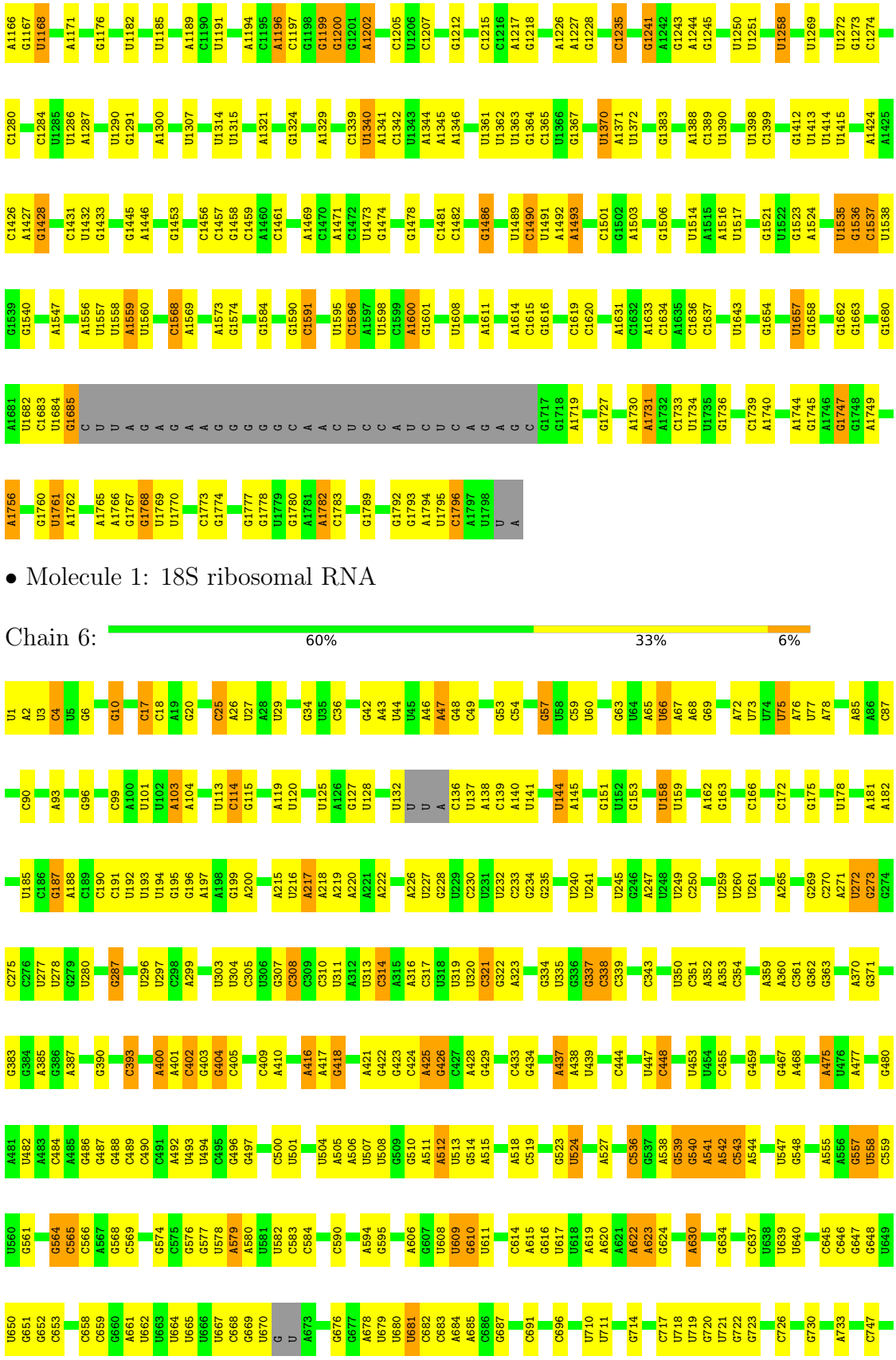
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

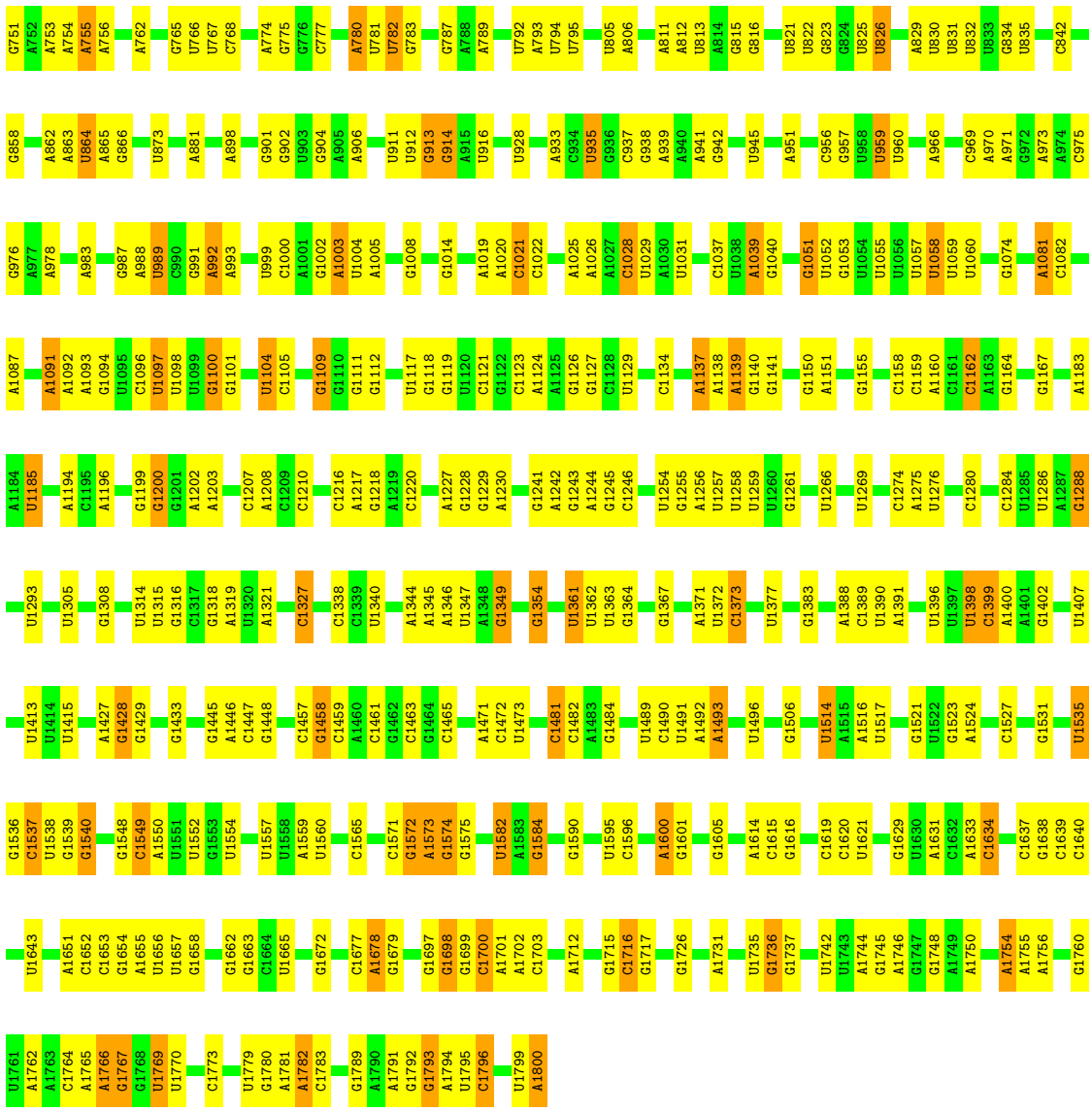
Chain 2: 62% 30% 5% •





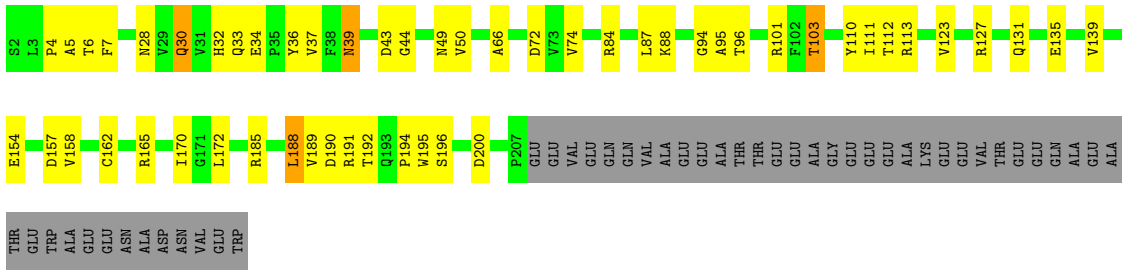
- Molecule 1: 18S ribosomal RNA

Chain 6: 60% 33% 6%



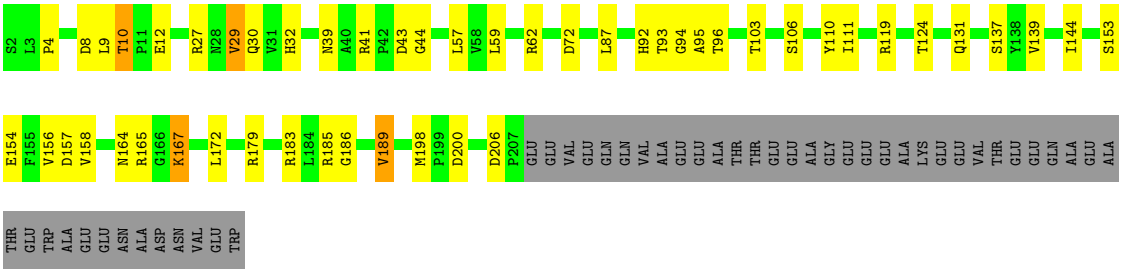
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



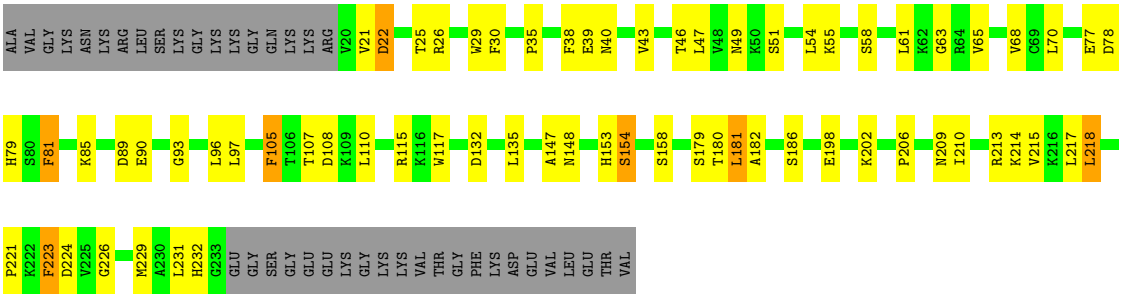
- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



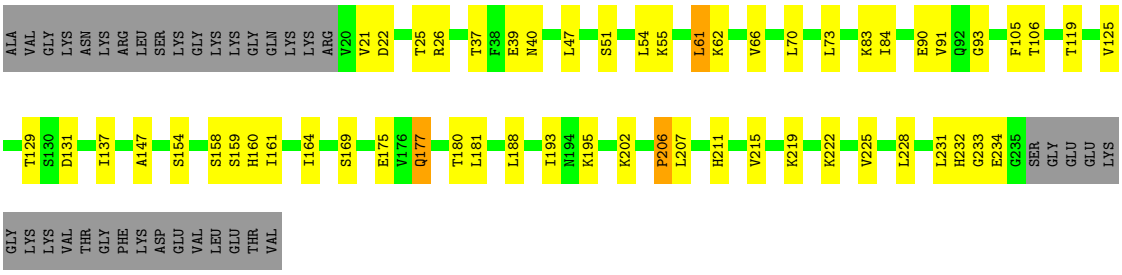
- Molecule 3: 40S ribosomal protein S1-A

Chain S1:



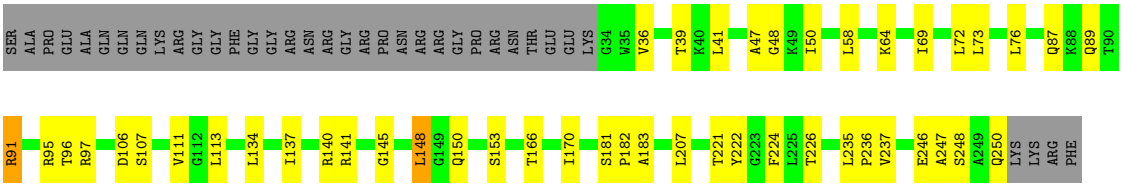
- Molecule 3: 40S ribosomal protein S1-A

Chain s1:



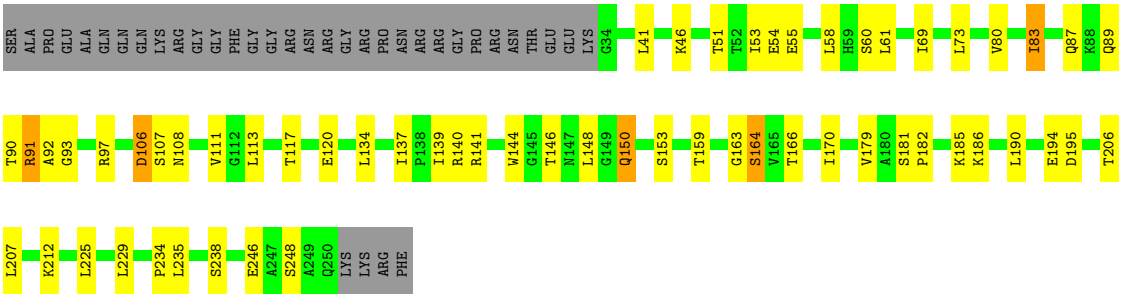
- Molecule 4: 40S ribosomal protein S2

Chain S2:



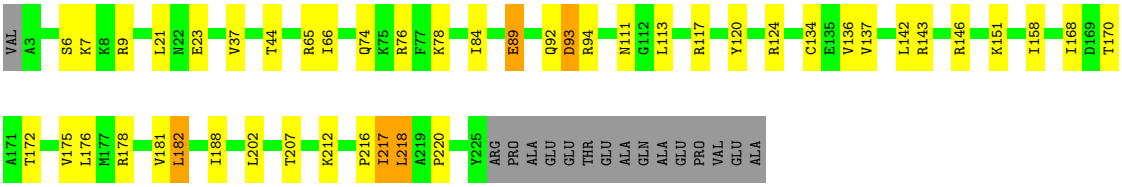
- Molecule 4: 40S ribosomal protein S2

Chain s2:



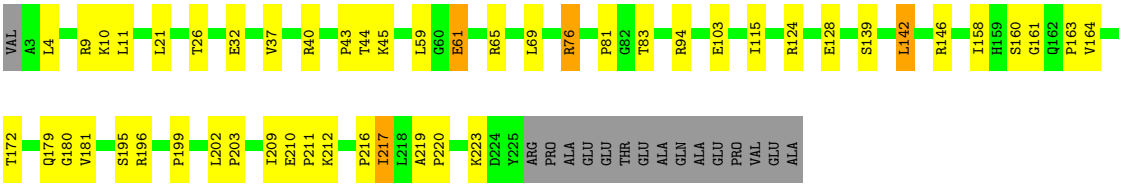
• Molecule 5: 40S ribosomal protein S3

Chain S3:



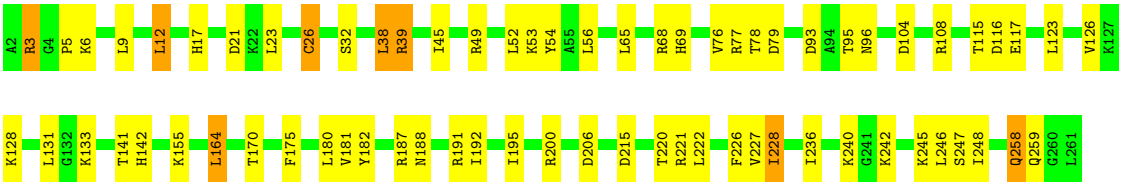
• Molecule 5: 40S ribosomal protein S3

Chain s3:



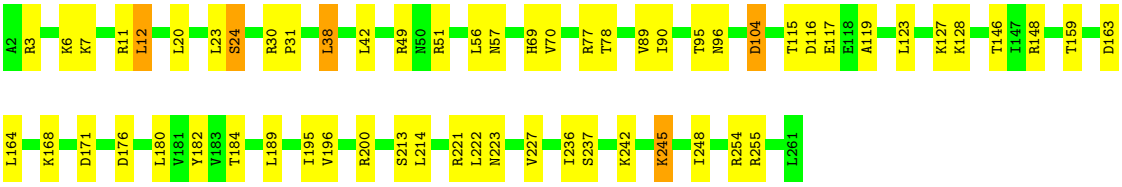
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



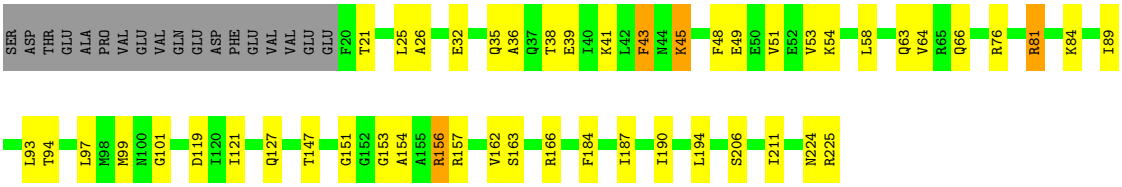
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



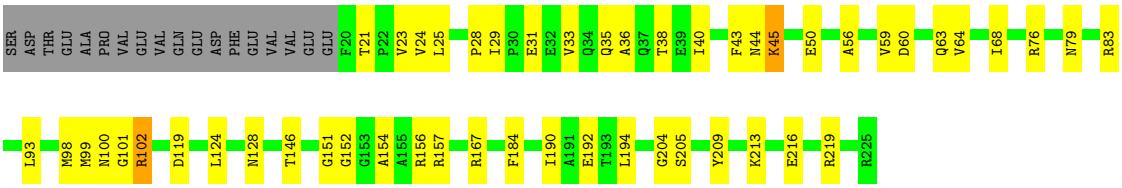
- Molecule 7: 40S ribosomal protein S5

Chain S5:



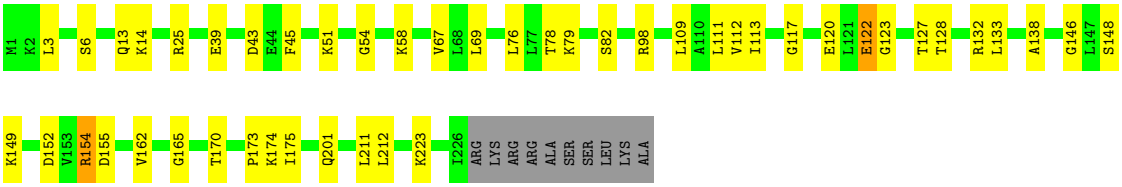
- Molecule 7: 40S ribosomal protein S5

Chain s5:



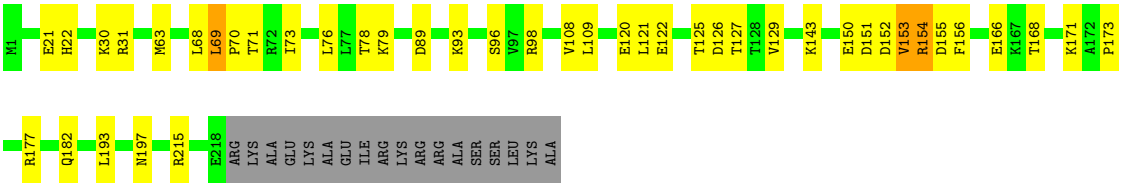
- Molecule 8: 40S ribosomal protein S6-A

Chain S6:



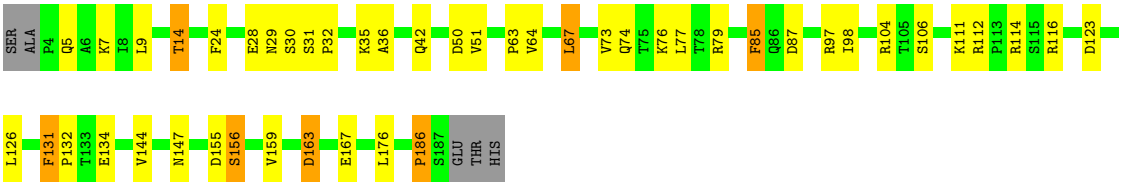
- Molecule 8: 40S ribosomal protein S6-A

Chain s6:



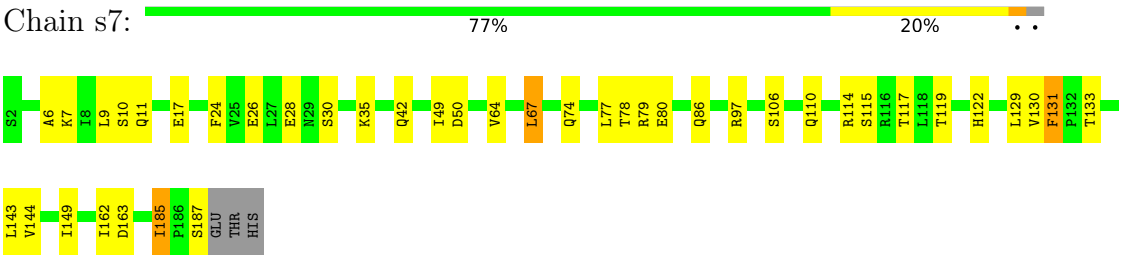
- Molecule 9: 40S ribosomal protein S7-A

Chain S7:



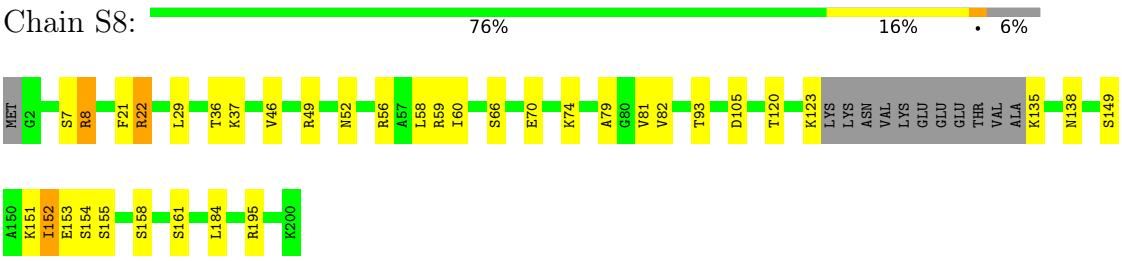
- Molecule 9: 40S ribosomal protein S7-A

Chain s7:



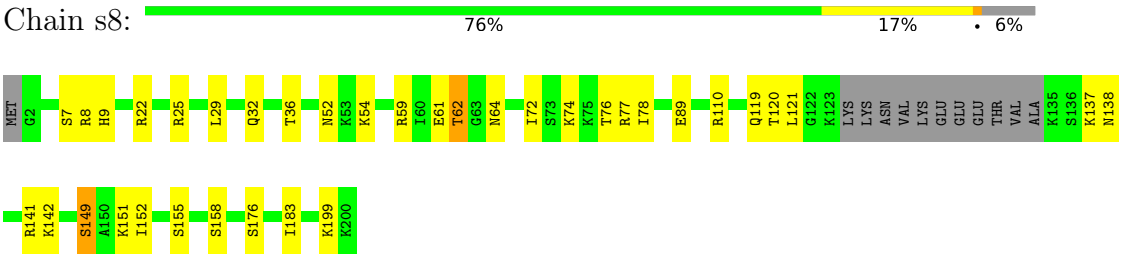
- Molecule 10: 40S ribosomal protein S8-A

Chain S8:



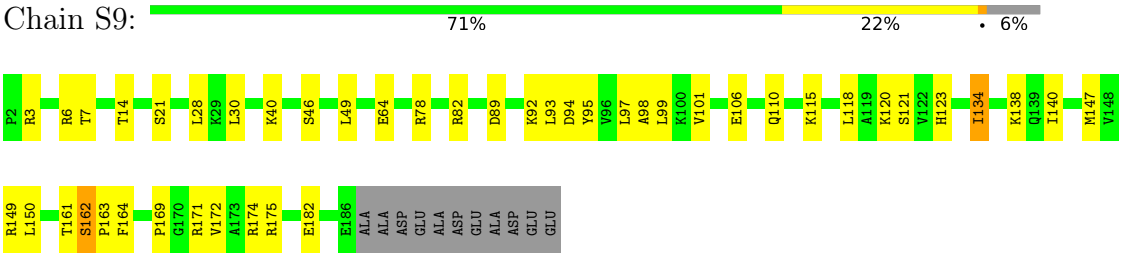
- Molecule 10: 40S ribosomal protein S8-A

Chain s8:



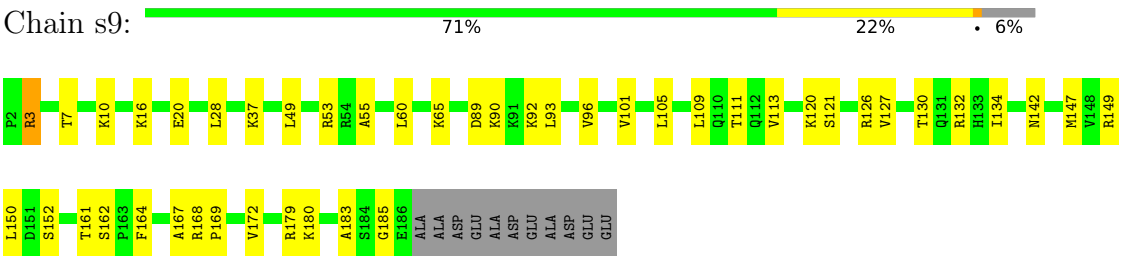
- Molecule 11: 40S ribosomal protein S9-A

Chain S9:



- Molecule 11: 40S ribosomal protein S9-A

Chain s9:



• Molecule 12: 40S ribosomal protein S10-A

Chain C0: 69% 20% • 9%

M1 K5 E6 Q13 F27 N28 E34 L40 L46 L49 V55 K56 S60 L76 R77 E78 Y79 L80 N81 L82 I86 V87 P88 I92 Q93 E94 R95 N96 PRO THR GLN ARG PRO GLN ARG ARG TYR

• Molecule 12: 40S ribosomal protein S10-A

Chain c0: 70% 17% • 9%

M1 L2 M3 P4 K5 V20 V21 V22 A23 K24 K25 A30 K31 H32 I35 L40 V55 K56 T57 V73 L76 L82 P83 E84 HIS ILE V87 P88 I92 Q93 E94 R95 N96 P97 T98 GLN ARG PRO GLN ARG ARG TYR

• Molecule 13: 40S ribosomal protein S11-A

Chain C1: 79% 19% •

S2 T3 E4 V7 N21 V25 K29 R30 T31 L40 K43 T44 D55 L63 V64 R67 G68 K69 I70 L71 T72 G73 T74 N80 L91 P95 K96 V107 P113 Q127 I131 N138 V139 V140 K141 A145 A146 A154 K155 F156

• Molecule 13: 40S ribosomal protein S11-A

Chain c1: 74% 19% • 6%

S2 L5 T6 V7 E10 N21 K24 T27 R30 T31 K32 L40 T44 D55 K56 F60 R67 G68 K69 T74 S77 M80 H81 R82 R87 V107 P113 V119 G120 D121 C128 R129 N138 V139 V140 S143 A144 A145 A146

A147 LYS ALA ASN LYS GLN PHE ALA LYS PHE

• Molecule 14: 40S ribosomal protein S12

Chain C2: 58% 27% • 13%

SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU GLU THR VAL VAL GLU GLN THR A20 E21 V22 E25 R33 V37 R43 G44 L45 R46 T49 K50 A51 L52 T53 R54 L59 L62 V66 I71 L74 E83 V86 P87 L88 I89 K90 V91 A92

A101 G102 L103 I106 D107 R108 A112 V115 S119 N125 W126 G127 A128 E129 T130 D131 E132 M135 H139 F140 Q143

• Molecule 14: 40S ribosomal protein S12

Chain c2: 60% 24% • • 13%

SER ASP VAL GLU GLU VAL VAL GLU VAL GLN GLU GLU THR VAL VAL GLU GLN THR A20 E21 V22 D26 A27 L28 K29 V30 L36 V37 H38 D39 G40 L45 L52 L53 V61 T67 I71 L74 P82 E83 N84 K85 V86 P87 L88 I89 K90 D93

L97 L103 I106 D107 R108 V115 A118 S119 V120 V121 E129 T130 D131 E132 I136 F140 S141 Q142 Q143

• Molecule 15: 40S ribosomal protein S13

Chain C3: 79% 20% •

G2 R3 S6 S12 I16 A22 P23 A24 K27 L28 S29 S30 E31 S32 K39 K43 G44 L45 T61 R64 V65 I66 T67 G68 M72 K76 L80 E83 V96 L102 N105 R114 L115 L125 T131 V134 T145 A146 S147

N151

• Molecule 15: 40S ribosomal protein S13

Chain c3: 79% 18% •

G2 R3 S6 S12 S13 S14 S19 R20 N21 A22 K27 L28 S29 E35 K43 V60 R64 V65 I66 K70 I84 D87 S97 L102 E103 R104 L115 L125 A126 R127 T131 V134 P137 N138 W139 K140 N151

• Molecule 16: 40S ribosomal protein S14-A

Chain C4: 71% 18% • 7%

SER ASN VAL VAL GLN ALA ARG ASP ASN S11 V16 N24 D25 T26 V30 T31 T38 I39 A40 R41 V42 N46 K47 V48 K49 A50 S55 G75 I76 V79 R84 T89 K92 T93 R103 R114 V118 T119 S123 D124 S125 T126 R132

L137

• Molecule 16: 40S ribosomal protein S14-A

Chain c4: 69% 22% • 6%

SER ASN VAL VAL GLN ALA ARG ASP N10 R18 I19 Y20 F23 T26 T31 D32 L33 S34 G35 T43 K49 A50 D51 R52 Y58 L62 K70 V81 T91 K92 G97 G98 Q99 A100 A101 L102 R107 S108 G109 R114 T119 S123 D124 S125

T126 R132 R133 R136 L137

• Molecule 17: 40S ribosomal protein S15

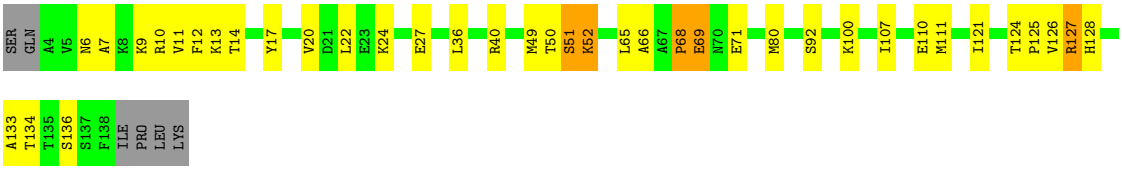
Chain C5: 67% 16% • 12%

SER GLN ALA VAL ASN ALA K8 V11 T14 L22 M28 S29 V34 K35 L36 R40 R44 S51 K52 P53 A54 P68 E69 M80 M89 S92 N98 A101 V105 E106 E110 L116 I121 T124 P125 V126 R130 A131 GLY ALA

THR THR SER SER PHE ILE PRO LEU LYS

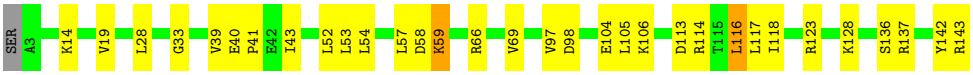
• Molecule 17: 40S ribosomal protein S15

Chain c5: 68% 24% • •



• Molecule 18: 40S ribosomal protein S16-A

Chain C6:

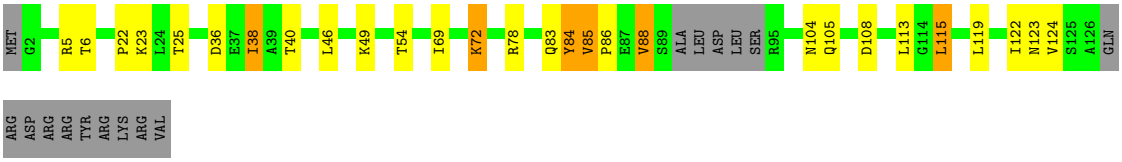


• Molecule 18: 40S ribosomal protein S16-A

Chain c6:

• Molecule 19: 40S ribosomal protein S17-A

Chain C7:

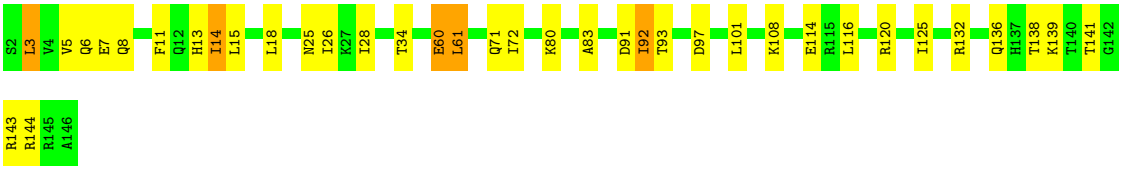


• Molecule 19: 40S ribosomal protein S17-A

Chain c7:

• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



• Molecule 20: 40S ribosomal protein S18-A

Chain c8: 77% 20% •

S2 L3 V4 V5 Q6 E7 Q8 G9 Q12 H13 I14 T20 N25 I28 V29 T33 T34 R40 V46 R57 E60 L61 T62 Q63 L66 K80 D91 I92 T93 D94 V105 L116 I119 G135 R143 R144 R145 A146

• Molecule 21: 40S ribosomal protein S19-A

Chain C9: 79% 20% •

P2 G3 V4 S5 V6 D13 Y18 L22 K27 L28 E29 V30 P31 G32 Y33 V34 D35 I36 V37 K38 T39 W53 R57 M67 R68 K69 Q70 V71 I94 I111 R122 R123 I124 S125 E126 R130 D131 L132 T139 E144

• Molecule 21: 40S ribosomal protein S19-A

Chain c9: 82% 17% •

P2 G3 V6 L28 E29 Y33 V34 V37 S41 E51 R57 R68 K69 Q70 V71 R86 Y91 R102 I116 S117 P118 K119 R123 E126 D131 L132 D133 T139 L140 E141 E142 D143 E144

• Molecule 22: 40S ribosomal protein S20

Chain D0: 67% 22% • 11%

SER ASP PHE GLN LYS GLU LYS VAL GLU GLU GLN GLU GLN Q15 Q16 Q17 Q18 I19 I20 R23 T27 V31 L34 S39 N40 I41 N49 L50 V51 R57 L58 K61 R68 E74 G75 S76 T81 R89 I99 I103 I106 N121

• Molecule 22: 40S ribosomal protein S20

Chain d0: 60% 30% • 8%

SER ASP PHE GLN LYS GLU LYS VAL GLU GLU Q12 E13 Q14 Q15 Q16 Q17 Q18 I19 R23 I24 T25 L26 T27 K30 V31 L34 N44 A45 N49 L50 V51 K52 R57 T60 K61 V62 L63 T70 P71 N72 G73 E74 K77 T81 K88 R89 P96 V97

Q98 I99 R102 I103 T104 Q105 I106 T107 D113 V114 E115 V118 N121

• Molecule 23: 40S ribosomal protein S21-A

Chain D1: 78% 18% •

M1 E2 N3 D4 Q7 L8 V9 E10 L11 Y12 S18 D27 V36 E41 E42 G43 T52 S68 L69 L78 V82 R87

• Molecule 23: 40S ribosomal protein S21-A

Chain d1: 77% 23%

M1 E2 N3 D4 K5 G6 E10 L11 Y12 K25 V32 K38 G43 R44 Y50 V51 T52 S68 L69 N75 L78 N81 R87

• Molecule 24: 40S ribosomal protein S22-A

Chain D2: 77% 22%

T2 L7 N12 K22 R23 Q24 V25 L26 S31 E49 I53 H56 R57 L65 N66 N70 S76 P77 R78 I83 L93 R97 Q98 F99 G100 I103 L104 V121 L126 G127 F128 V129 Y130

• Molecule 24: 40S ribosomal protein S22-A

Chain d2: 85% 13%

T2 L7 T20 R23 Q24 V25 L26 S31 F37 H56 L65 R68 L93 Q98 I103 L104 T105 R117 R118 K119 K124 V129 Y130

• Molecule 25: 40S ribosomal protein S23-A

Chain D3: 77% 22%

G2 K3 R7 G8 L9 N10 S11 R16 R19 N28 K31 T36 A37 S40 S41 S47 I52 V53 L54 Q63 K70 C71 V72 Q75 T84 L103 F107 G108 R109 K112 A113 K114 I117 V120 S128 S131 L132 E138

R144 S145

• Molecule 25: 40S ribosomal protein S23-A

Chain d3: 82% 17%

G2 L9 K14 L15 R16 R19 N28 Y29 L34 S40 G44 I52 S66 R73 K78 V83 T84 D100 E101 V102 L103 F107 G119 V120 R121 V125 S128 S131 L132 L133 A134 S145

• Molecule 26: 40S ribosomal protein S24-A

Chain D4: 79% 20%

S2 V5 T6 I13 K21 L28 H29 N34 V35 S36 L40 E51 K52 V57 F58 G59 F60 R61 T62 Q63 V70 V75 V79 L96 A97 K102 R124 K127 R131 R132 N133 A134 D135

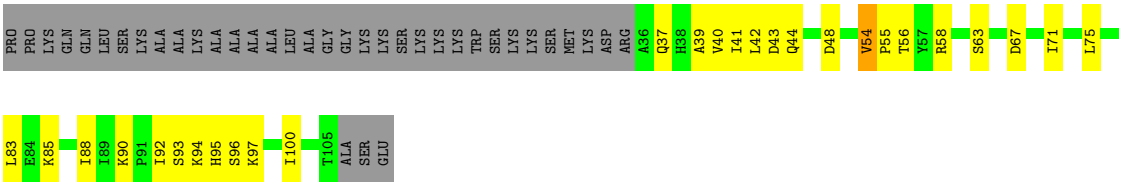
• Molecule 26: 40S ribosomal protein S24-A

Chain d4: 80% 19%

S2 T6 R10 K11 K21 H29 P30 A33 N34 V35 S36 K43 E46 V47 Y48 K49 K52 D53 F58 T62 S78 K83 T88 L91 V100 T121 L125 A126 K127 K128 N133 A134 D135

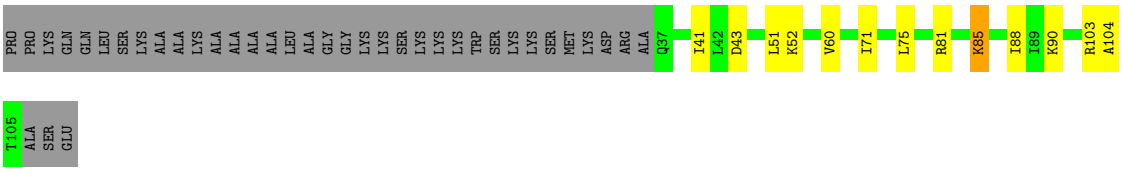
• Molecule 27: 40S ribosomal protein S25-A

Chain D5: 40% 24% 35%



• Molecule 27: 40S ribosomal protein S25-A

Chain d5: 52% 11% • 36%



• Molecule 28: 40S ribosomal protein S26-B

Chain D6: 68% 26% 5% •

• Molecule 28: 40S ribosomal protein S26-B

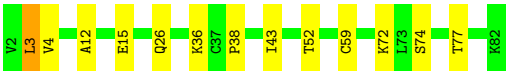
Chain d6: 77% 22% •

• Molecule 29: 40S ribosomal protein S27-A

Chain D7: 88% 12%

• Molecule 29: 40S ribosomal protein S27-A

Chain d7: 84% 15% •

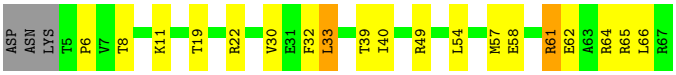


• Molecule 30: 40S ribosomal protein S28-A

Chain D8: 70% 24% • 5%

• Molecule 30: 40S ribosomal protein S28-A

Chain d8:

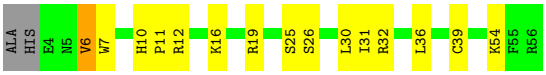


• Molecule 31: 40S ribosomal protein S29-A

Chain D9:

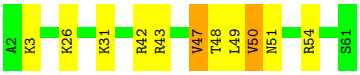
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



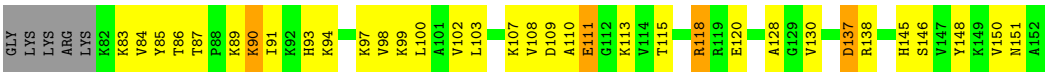
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:

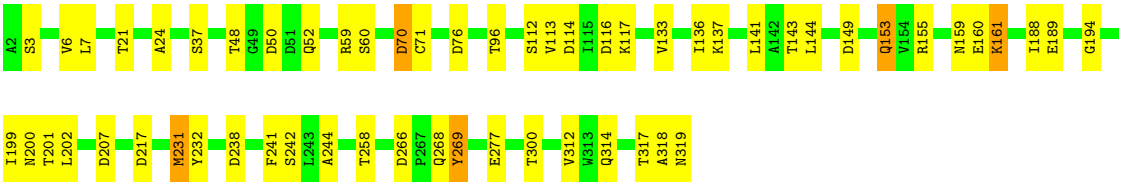


• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:

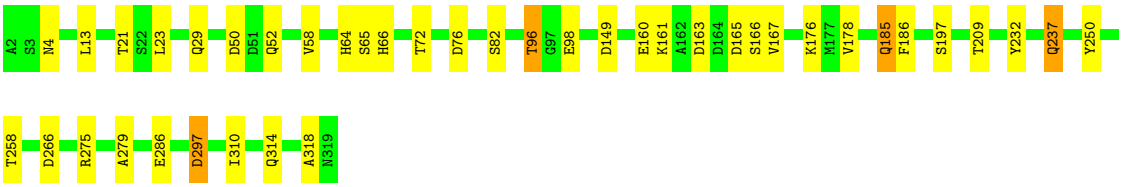
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



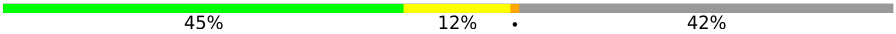
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

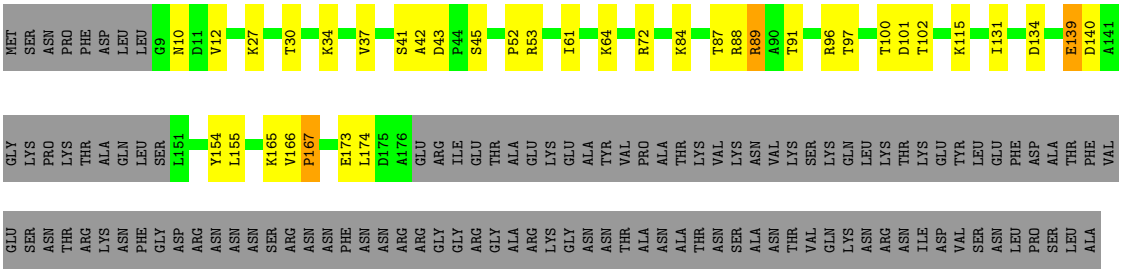
Chain sR:



• Molecule 35: Suppressor protein STM1

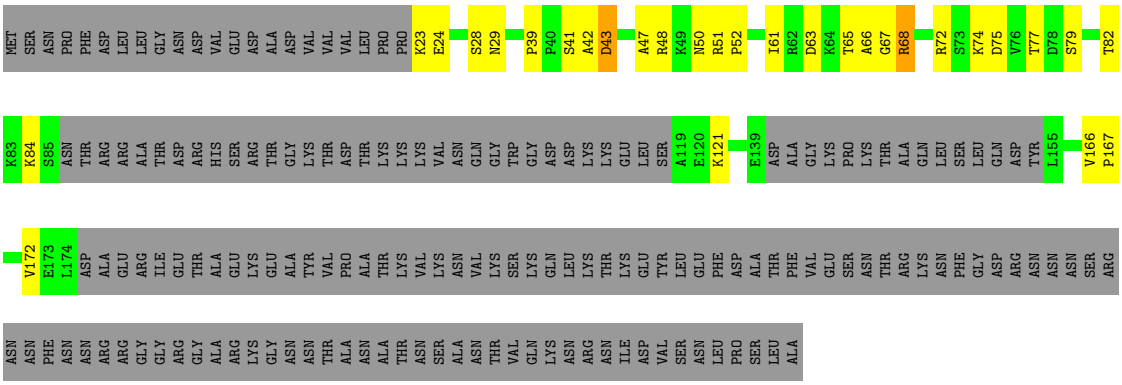
Chain SM:





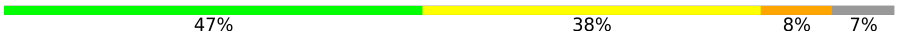
• Molecule 35: Suppressor protein STM1

Chain sM:

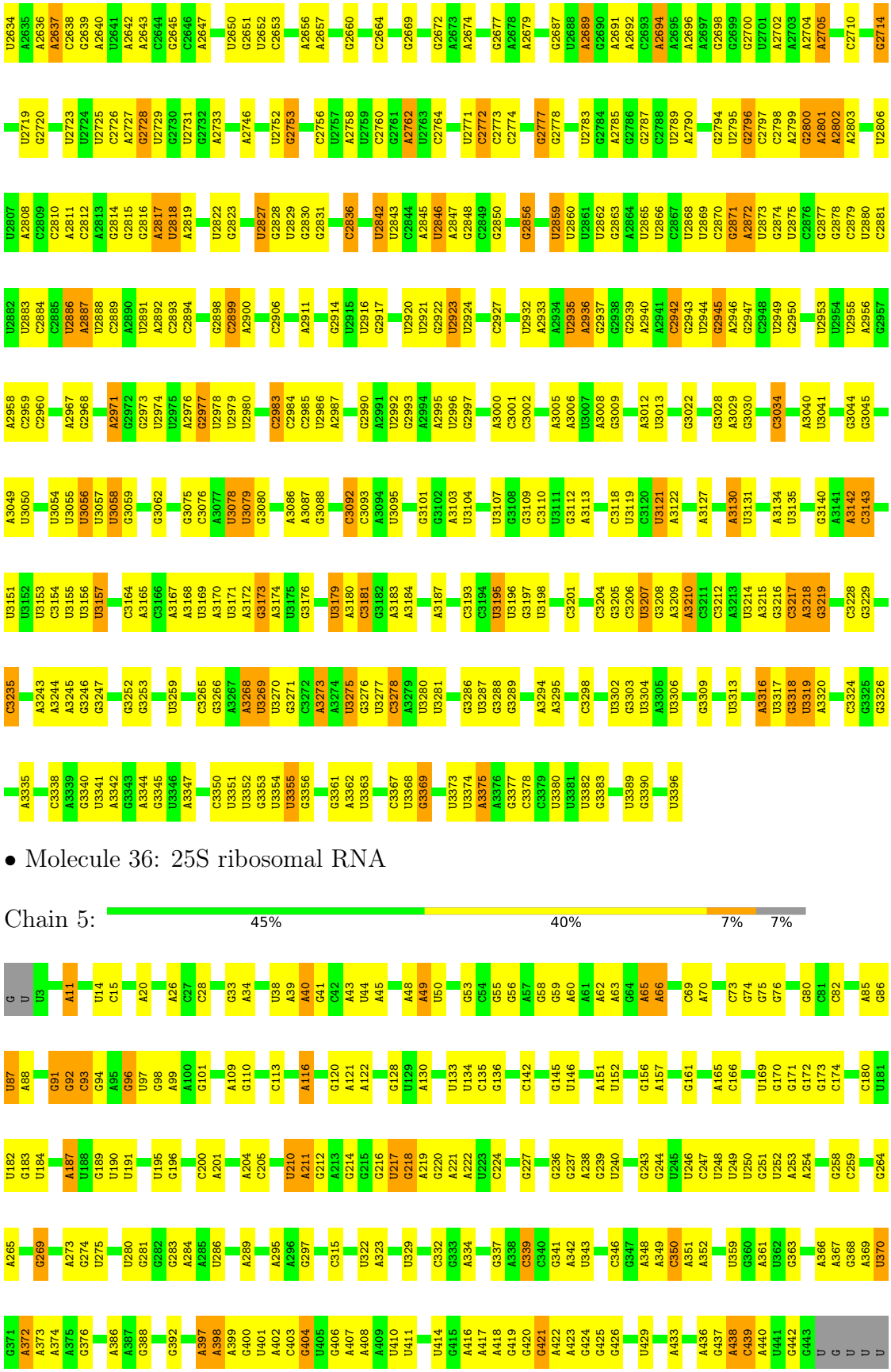


• Molecule 36: 25S ribosomal RNA

Chain 1:

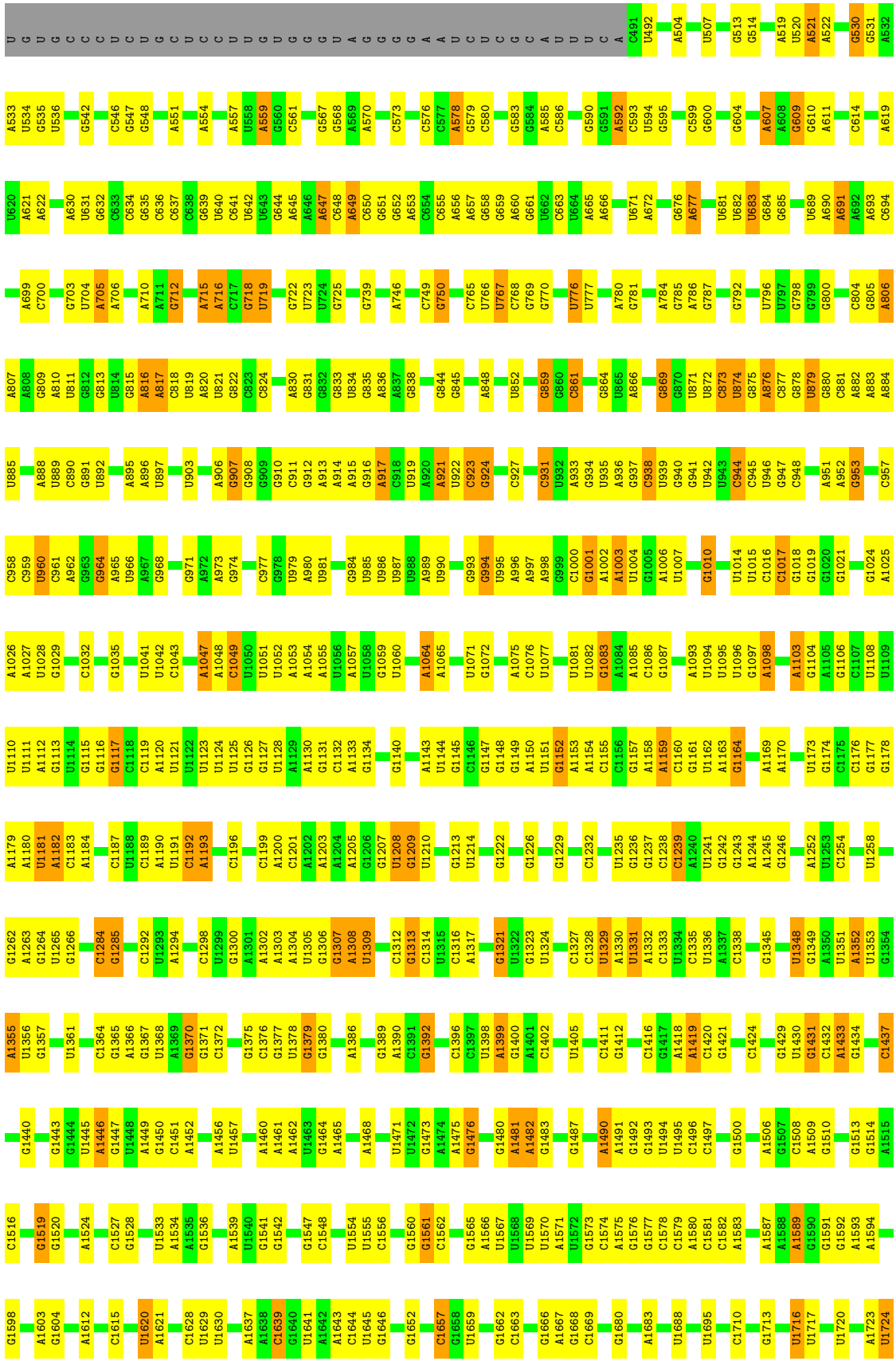


G U U3 A13 U14 C15 A16 G22 U25 A26 C27 C28 C29 G30 C31 U32 G33 A34 A35 C36 U37 U38 A39 A40 G41 C42 A43 U44 A45 U46 C47 A48 A49 U50 A51 A52 G53 C54 G55 G56 G59 A60 A61 G64 A65 A66 A67 C68 C69 A70 A71 C72 C73 G74 G75
G76 A77 U78 U79 G80 C81 C82 U83 U84 A85 G86 A89 C90 G91 G92 C93 G94 A95 G96 U97 G98 A99 A100 G101 G104 C105 A106 A107 A108 A109 G110 C111 U112 C113 A114 A115 A116 U117 A121 A122 A123 U124 G127 C131 C132 U133 U134 C135 G136 C142 G143 A144 G145 U146
U147 G148 U153 U154 G155 G156 A157 G158 A165 C166 U169 G170 G171 G176 A187 U188 G189 U190 U191 C192 G196 G197 A198 A199 C200 C205 G206 U207 U210 A211 G212 A213 G216 U217 G218 A219 G220 A221 A222 U223 C224 C225 U228 G229 G232 C233 G237 A238
G239 U240 G241 C242 G243 G244 U245 U246 C247 U248 U249 U250 U251 U252 G264 A265 G269 U270 U278 G282 G283 A284 A285 U286 G287 G290 C291 U292 A295 A296 G297 U298 G304 U305 C311 C315 U316 A317 A318 A319 G320 A323 A324 A325 U326 U329 G330 G331 C332
A336 G337 A338 C339 C340 U343 A344 G345 C346 A349 C350 C356 A357 G358 U359 G360 A361 U362 G363 G368 A369 U370 G371 A372 A373 G376 G388 G392 U393 G394 A395 A396 A397 A398 U401 A402 C403 G404 U405 G406 A407 A408 A409 U410 U411 G412 U413 A416 A417
G420 G421 A422 A423 G424 G425 G426 C427 A428 U429 C435 A438 C439 A440 U G G U U U U U G U G C C C C U U C C U C C U U G U G G G U A G G G G G C G C
A U U U C A C U G G494 G495 A498 G499 C500 A501 A504 G505 U506 U507 G511 A519 U520 A521 G535 U541 C544 U545 C546 C547 G548 U549 A550 A551 G552 U555 U556 A557 U558 A559 G560 C573 C577 A578 G579 C580 U581 G584 A585 C586
U587 G588 A589 G590 G591 A592 C593 U594 G600 U601 G604 A607 A608 G609 G610 A611 C614 A619 U620 A621 G624 U627 A628 U629 A630 U631 G632 C633 C634 G635 C636 C637 C638 G639 U640 C641 U642 U643 G644 A645 A646 A647 C648 A649 C650 G651 G652 A653 C654 C655 A656 A657 G658
G659 A660 G661 U662 C663 U664 A665 A666 C667 G668 U669 C670 U671 A672 U673 G674 C675 G676 A677 G678 U679 G680 U681 U682 U683 G684 G685 G686 U687 G688 A691 A692 A693 C694 C695 C696 A697 U698 A699 C700 G701 C702 A705 A706 U707 G708 A709 G712 A715 A716 C717 G718 U719 A720 G721
G725 G726 C730 C743 C758 G763 U764 C765 U766 U767 G770 U776 U777 U778 G779 A780 G781 G785 A786 G787 C788 A789 U790 A791 G792 C793 U794 G795 U796 U797 G798 G799 G800 A801 C802 C803 C804 C805 A806 A807 A808 G809 A810 U811 G815 A816 A817 A820 U821 G826
A830 G835 A836 A837 A843 C849 G857 A858 G859 C860 C861 U862 C863 G864 U865 G870 U871 U872 C873 U874 C877 G878 U879 G880 C881 A882 A883 A884 U885 C886 G887 A888 U889 C890 G894 A895 A896 G901 G902 A906 G907 G908 G909 G910 C911 G912 A913 A914 A915 G916
A917 C918 U919 A920 A921 U922 C923 G924 A925 C928 A929 U930 C931 U932 A933 G934 G937 C938 U939 G940 G941 U942 U943 C944 C945 U946 G947 C948 C949 A952 G953 U954 U955 U956 C957 C958 C959 U960 C961 G964 A965 U966 A967 G968 C969 A970 A973 U979 A980 U981 C982 A983 G984
G993 G994 A997 A998 G999 C1000 G1001 A1002 A1003 A1006 U1007 U1008 A1009 G1010 A1011 G1012 G1013 U1014 U1015 C1016 C1017 G1018 G1019 U1020 G1021 G1024 A1025 G1029 A1036 C1037 U1041 U1042 C1045 A1046 A1047 A1048 C1049 U1050 A1053 A1054 A1055 U1056 U1060 A1064 A1065 C1068 C1069 G1072
U1081 U1082 G1083 G1087 A1093 U1094 U1095 U1096 G1097 A1098 A1099 U1100 G1101 A1102 A1103 G1104 C1107 U1111 A1112 G1113 U1114 G1115 G1116 G1117 C1118 C1119 A1120 U1124 G1127 U1128 A1129 A1130 G1131 C1132 A1133 C1137 U1138 G1139 G1140 C1141 G1142 A1143 U1144 G1149 A1150 U1151 G1152 A1153 A1154 C1155 C1156
G1157 A1158 A1159 C1160 A1163 G1164 A1165 G1166 A1169 A1170 G1171 G1174 C1175 C1176 G1177 G1178 A1179 A1180 U1181 A1182 C1183 A1184 C1187 U1188 C1189 A1190 U1191 C1192 C1196 A1197 C1198 C1201 G1209 G1213 C1216 A1217 U1218 G1222 A1225 G1226 C1227 C1232 G1233 G1234 U1235 G1236 G1237
U1241 G1242 G1243 A1244 A1245 G1246 U1247 C1248 G1249 U1253 U1258 A1259 G1262 A1263 G1264 U1265 G1266 U1267 G1268 U1269 A1270 A1271 C1272 A1273 A1274 A1278 C1279 C1280 G1285 A1286 A1287 A1294 G1295 C1296 C1297 C1298 U1299 G1300 A1304 U1305 G1306 G1307 A1308 U1309 G1310 G1313 C1314 U1315 C1316 A1317 C1320



• Molecule 36: 25S ribosomal RNA

Chain 5: 45% 40% 7% 7%


U G U G C C C U C U G C U C C U U G U G G G U A A U C U A C491 U492 A504 U507 G513 G514 A519 U520 A521 A522 G530 G531 A532
A533 U534 G535 U536 G542 C546 G547 G548 A551 A554 A557 U558 A559 G560 C561 G567 G568 A569 A570 C573 C576 C577 A578 G579 C580 G583 G584 A585 C586 G590 G591 A592 C593 U594 G595 C599 G600 G604 A607 A608 G609 G610 A611 C614 A619
U620 A621 A622 A630 U631 G632 C633 C634 G635 C636 C637 C638 G639 U640 C641 U642 U643 G644 A645 A646 A647 C648 A649 C650 G651 G652 A653 C654 C655 A656 A657 G658 G659 A660 G661 U662 C663 U664 A665 A666 U671 A672 G676 A677 U681 U682 U683 G684 G685 U689 A690 A691 A692 A693 C694
A699 C700 G703 U704 A705 A706 A710 A711 G712 A715 A716 C717 G718 U719 G722 U723 U724 G725 G739 A746 C749 G750 C765 U766 U767 C768 G769 G770 U776 U777 A780 G781 A784 G785 A786 G787 G792 U796 U797 G798 G799 G800 C804 G805 A806
A807 A808 G809 A810 U811 G812 G813 U814 G815 A816 A817 C818 U819 A820 U821 G822 C823 C824 A830 G831 G832 G833 U834 G835 A836 A837 G838 G844 G845 A848 U852 G859 G860 C861 G864 U865 A866 G869 G870 U871 U872 C873 U874 G875 A876 C877 G878 U879 G880 C881 A882 A883 A884
U885 A888 U889 C890 G891 U892 A895 A896 U897 U903 A906 G907 G908 C909 C910 C911 G912 A913 A914 A915 G916 A917 C918 U919 A920 A921 U922 C923 G924 C927 C931 U932 A933 G934 U935 A936 G937 C938 U939 G940 G941 U942 U943 C944 C945 U946 G947 C948 A951 A952 G953 C957
C958 C959 U960 C961 A962 G963 G964 A965 U966 A967 G968 G971 A972 A973 G974 C977 G978 U979 A980 U981 G984 U985 U986 U987 U988 A989 U990 G993 G994 U995 A996 A997 A998 G999 C1000 G1001 A1002 A1003 U1004 G1005 A1006 U1007 G1010 U1014 U1015 C1016 C1017 G1018 G1019 G1020 G1021 G1024 A1025
A1026 A1027 U1028 G1029 C1032 G1035 U1041 U1042 C1043 A1047 A1048 C1049 U1050 U1051 U1052 A1053 A1054 A1055 U1056 A1057 U1058 G1059 U1060 A1064 A1065 U1071 G1072 A1075 C1076 U1077 U1081 U1082 G1083 A1084 A1085 C1086 G1087 A1093 U1094 U1095 U1096 G1097 A1098 A1103 G1104 A1105 G1106 C1107 U1108 U1109
U1110 U1111 A1112 G1113 U1114 G1115 G1116 G1117 C1118 C1119 A1120 U1121 U1122 U1123 U1124 U1125 G1126 G1127 U1128 A1129 A1130 G1131 C1132 A1133 G1134 G1140 A1143 U1144 G1145 C1146 G1147 G1148 G1149 A1150 U1151 G1152 A1153 A1154 C1155 C1156 G1157 A1158 A1159 C1160 G1161 U1162 A1163 G1164 A1169 A1170 U1173 G1174 C1175 C1176 G1177 G1178
A1179 A1180 U1181 A1182 C1183 A1184 C1187 U1188 C1189 A1190 U1191 C1192 A1193 C1196 C1199 A1200 C1201 A1202 A1203 A1204 A1205 G1206 G1207 U1208 G1209 U1210 G1213 U1214 G1222 G1226 G1229 C1232 U1235 G1236 G1237 C1238 C1239 A1240 U1241 G1242 G1243 A1244 A1245 G1246 A1252 U1253 C1254 U1258
G1262 A1263 G1264 U1265 G1266 C1284 G1285 C1292 U1293 A1294 C1298 U1299 G1300 A1301 A1302 A1303 A1304 U1305 G1306 G1307 A1308 U1309 C1312 G1313 C1314 U1315 C1316 A1317 G1321 U1322 G1323 U1324 C1327 C1328 U1329 A1330 U1331 A1332 C1333 U1334 C1335 U1336 A1337 C1338 G1345 U1348 G1349 A1350 U1351 A1352 U1353 G1354
A1355 U1356 G1357 U1361 C1364 G1365 A1366 G1367 U1368 A1369 G1370 G1371 C1372 G1375 C1376 G1377 U1378 G1379 G1380 A1386 G1389 A1390 C1391 G1392 C1396 C1397 U1398 A1399 G1400 A1401 C1402 U1405 C1411 G1412 C1416 G1417 A1418 A1419 C1420 G1421 C1424 G1429 U1430 G1431 C1432 A1433 G1434 C1437
G1440 G1443 G1444 U1445 A1446 G1447 U1448 A1449 G1450 C1451 A1452 A1456 U1457 A1460 A1461 A1462 U1463 G1464 A1465 A1468 U1471 U1472 G1473 A1474 A1475 G1476 G1480 A1481 A1482 G1483 G1487 A1490 A1491 G1492 G1493 U1494 U1495 C1496 C1497 G1500 A1506 G1507 C1508 A1509 G1510 G1513 G1514 A1515
C1516 G1519 G1520 A1524 C1527 G1528 U1533 A1534 A1535 G1536 A1539 U1540 G1541 G1542 G1547 C1548 U1554 U1555 C1556 G1560 G1561 C1562 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 G1573 C1574 A1575 G1576 G1577 C1578 C1579 A1580 C1581 C1582 A1583 A1587 A1588 A1589 G1590 G1591 G1592 A1593 A1594
G1598 A1603 G1604 A1612 C1615 U1620 A1621 C1628 U1629 U1630 A1637 A1638 C1639 G1640 U1641 A1642 A1643 C1644 U1645 G1646 G1652 C1657 G1658 U1659 G1662 C1663 G1666 A1667 G1668 C1669 G1680 A1683 U1688 U1695 C1710 G1713 U1716 U1717 U1720 A1723 U1724

C1725 A1741 A1749 A1750 G1751 C1756 C1759 A1760 C1761 C1762 U1763 U1764 U1765 G1766 G1770 G1775 G1778 C1779 G1780 G1786 A1787 C1788 G1789 G1790 C1791 C1792 C1793 A1797 C1803 A1810 G1811 G1812 A1813 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 G1825 U1834 U1837 G1838 A1839

U1840 A1841 A1842 C1843 C1844 G1845 C1846 A1847 G1848 C1849 A1850 G1851 C1852 U1853 C1854 U1855 C1856 C1857 A1858 A1859 U1862 G1863 A1864 A1865 C1866 C1869 C1870 U1871 C1872 U1873 A1874 G1875 U1876 U1877 G1878 A1879 U1880 A1881 A1884 U1885 A1886 A1887 U1888 G1889 U1890 A1891 G1892 A1893 U1894 G1897 A1900 A1901 G1902 U1903

G1906 C1907 A1908 A1909 A1910 A1911 U1912 A1913 G1914 A1915 U1925 G1929 A1930 U1931 A1932 G1935 A1936 U1937 U1938 G1939 G1940 C1941 G1947 G1952 G1953 G U A G U G A G G G C C U U G G U C A G A C G C A G C G G G

C G U G C U U G U G G A C U G C U U G G U G G G G C U U G C U C U G C U A G G C G G A C U A C U U G C G U G C C U U G U

U G U A G A C G G C C U U G G G U A G G U C U C U U G U A G A C C G U C G C U U G C U A C A A U U A A2093 U2097 A2100 C2101 U2102 U2103 A2107 C2108

U2109 G2110 G2111 U2112 A2113 C2114 G2115 G2116 A2117 C2118 A2119 A2120 G2121 G2122 G2123 C2128 U2129 G2130 A2131 C2132 U2133 G2134 U2135 C2136 U2137 A2138 A2139 U2140 U2141 A2142 A2143 A2144 A2145 C2146 A2147 U2148 C2151 C2156 G2157 A2158 U2159 C2163 A2164 G2165 A2166 A2167 A2168 G2169 U2170 G2171 A2172 U2173 G2174 U2175 U2176 G2177

A2178 A2183 U2186 U2189 U2190 U2191 C2192 U2193 G2194 C2195 C2196 C2197 A2198 C2204 U2205 G2206 A2207 A2208 U2209 G2210 U2211 A2215 A2220 G2221 A2222 A2223 A2228 A2229 G2230 C2231 G2234 A2244 C2245 G2246 G2247 C2248 G2253 U2254 A2255 A2256 C2257 U2258 C2267 U2268 U2269 A2270 A2271 G2272 G2273

C2277 C2278 A2279 A2280 A2281 U2282 G2283 C2284 C2285 U2286 C2287 G2288 U2289 C2290 A2291 U2292 C2293 U2294 A2295 A2296 U2297 U2298 A2299 A2303 C2304 G2305 C2306 G2307 C2308 A2309 U2310 A2313 U2314 G2315 G2316 A2317 U2318 U2319 A2320 G2323 A2324 G2325 A2326 U2327 U2328 C2329 C2330 C2331 A2332 C2333 U2334 G2335 U2336 C2337 C2338 C2339

U2340 A2341 U2342 C2343 U2344 A2345 C2346 U2349 C2350 U2351 A2352 G2353 C2354 G2355 A2356 A2357 A2358 C2359 C2360 A2361 C2362 A2363 G2364 C2365 C2366 A2367 G2371 A2372 A2373 C2374 G2375 G2376 G2377 C2378 U2379 G2382 C2383 A2384 G2385 A2386 A2387 U2388 G2391 C2392 G2393 G2394 G2395 G2396 A2397 A2398 A2399 G2400 A2401 A2402 G2403 A2404

C2405 C2406 C2407 U2410 U2411 G2412 U2416 U2417 G2418 A2419 C2420 G2425 U2426 G2429 U2434 G2435 U2436 G2437 A2438 A2439 G2440 A2441 G2442 A2443 C2444 A U A G A G G G U G U A G A A U A A G U G G G A G C U U C G

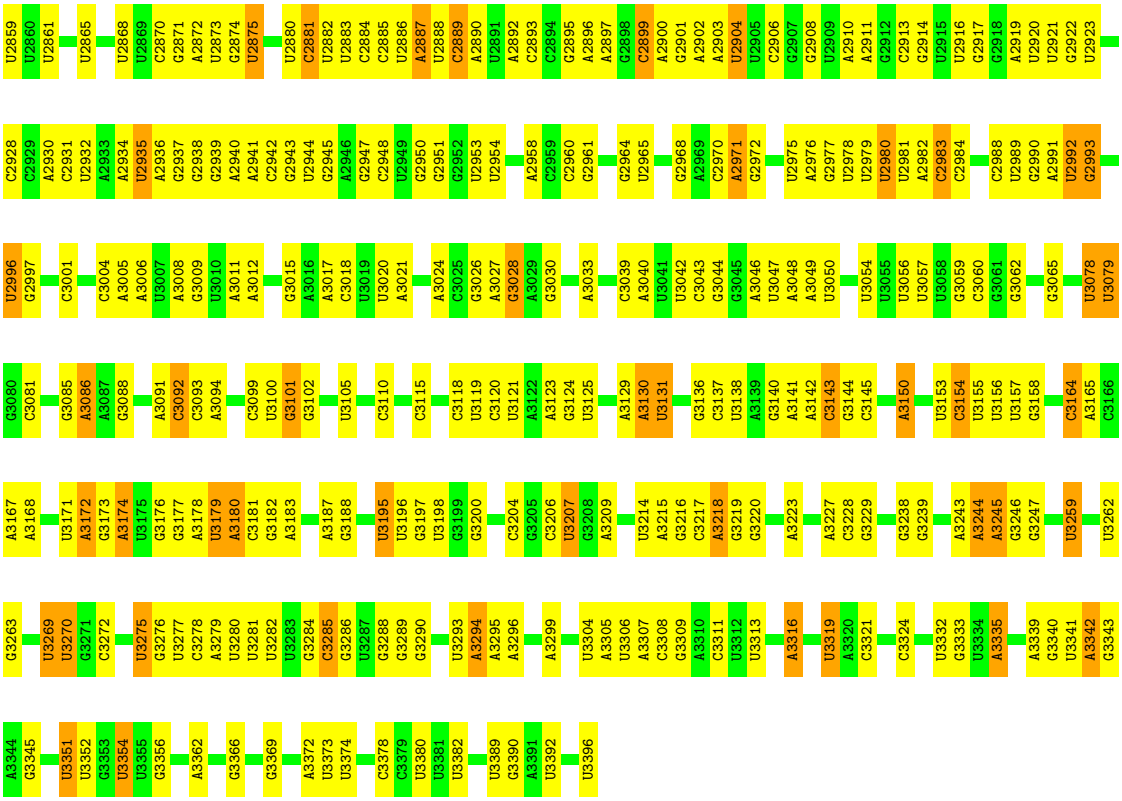
G C G C C A G U G A A A U A C C A C U A C C U U U U A U A G2503 U2504 U2505 U2506 C2507 U2508 U2509 U2510 A2511 C2512 U2513 U2514 A2515 G2522 A2523 A2524 G2525 C2526 G2530 C2531 A2535 A2536 U2537 U2538 C2539 A2540 U2543

G2549 U2550 U2551 C2552 G2555 A2562 C2567 C2568 A2569 U2570 U2571 C2572 G2573 G2574 A2580 G2584 G2585 U2588 G2589 A2593 C2594 G2598 U2599 C2600 G2606 C2607 G2608 A2609 G2610 U2611 G2614 G2615 C2616 U2617 G2618 G2619 G2620 C2621 C2622 G2623 G2624 C2625 A2626 C2627 A2628 U2629 C2630 U2631 G2632 U2633

U2634 A2635 A2636 A2637 C2638 G2639 A2640 A2643 C2644 G2645 C2646 A2647 G2648 A2649 U2650 G2651 U2652 A2656 G2659 G2660 G2661 G2662 G2663 C2664 U2665 C2666 A2674 C2675 A2676 G2677 A2678 A2679 A2680 U2681 C2682 U2683 C2684 G2685 A2686 G2687 U2688 A2689 G2690 A2691 A2692 C2693 A2694 A2695 A2696 G2699 G2700 U2701 A2702 A2703 A2704

C2707 C2708 C2709 C2710 U2713 G2714 A2715 U2716 U2717 U2718 U2719 G2720 U2723 U2724 U2725 C2726 A2727 G2728 U2729 G2730 U2735 A2739 C2742 A2743 U2744 U2750 G2751 U2752 G2753 G2754 C2755 C2756 U2757 A2758 U2759 C2760 G2761 A2762 U2763 C2764 C2765 U2766 U2767 U2771 C2772 C2773 C2774 G2777 G2778 A2779 A2780

G2787 A2790 G2794 U2795 G2796 C2797 C2798 A2799 G2800 A2801 A2808 C2809 C2810 A2811 G2814 G2815 G2816 A2817 U2818 A2819 A2820 C2821 U2822 G2823 G2824 C2825 U2826 U2827 G2828 U2829 G2830 G2831 C2832 A2833 C2836 A2837 A2838 G2839 C2840 G2841 U2842 U2843 C2844 A2845 G2848 C2849 G2850 A2851 C2852 A2853 C2857 U2858

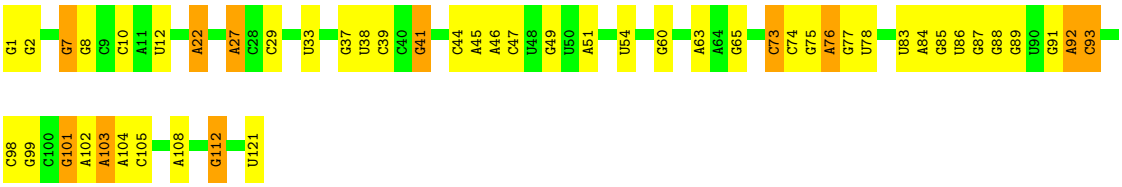


- Molecule 37: 5S ribosomal RNA

Chain 3:

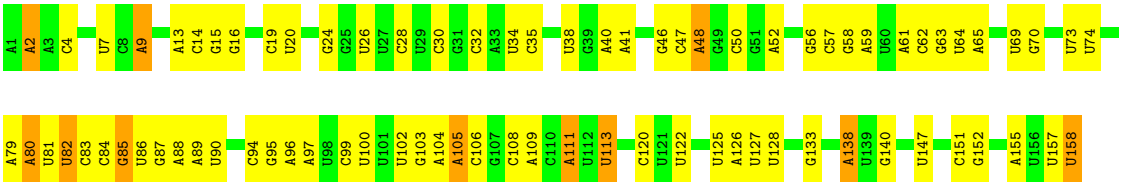
- Molecule 37: 5S ribosomal RNA

Chain 7:



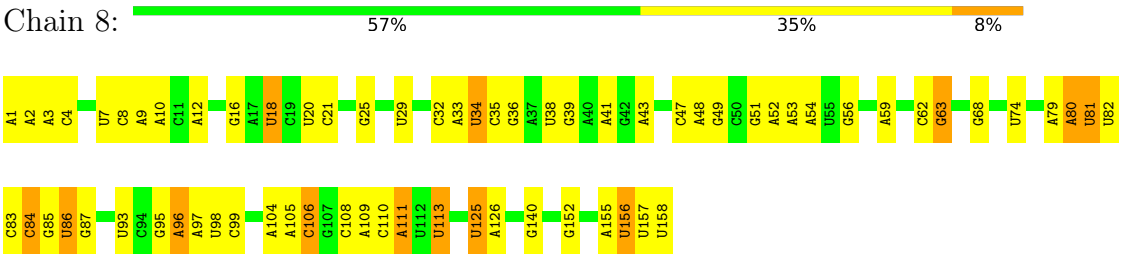
- Molecule 38: 5.8S ribosomal RNA

Chain 4:



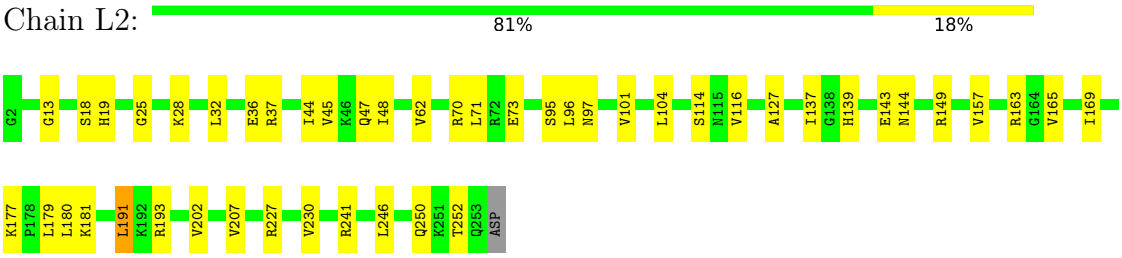
- Molecule 38: 5.8S ribosomal RNA

Chain 8:



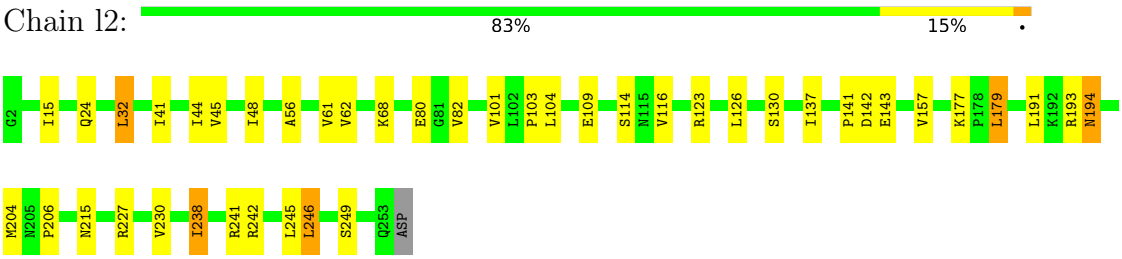
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



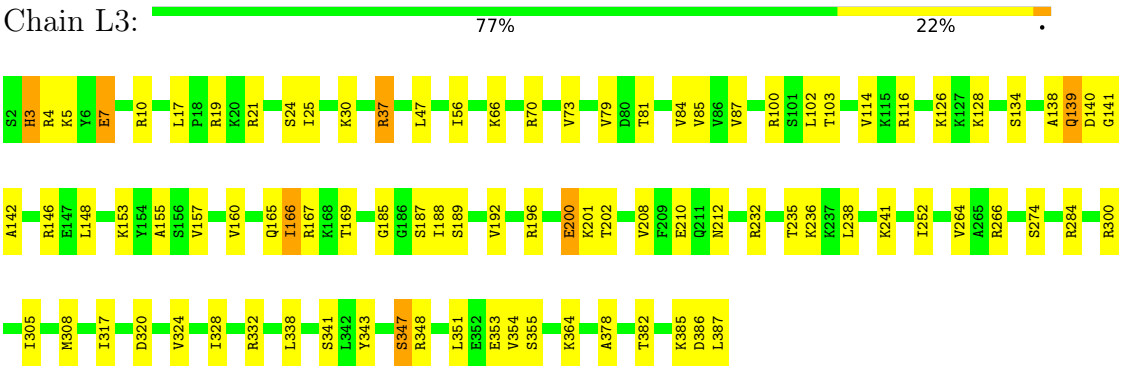
- Molecule 39: 60S ribosomal protein L2-A

Chain l2:



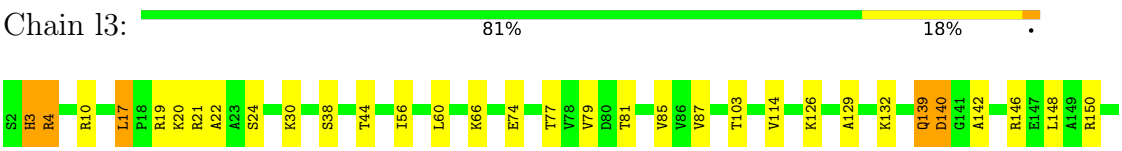
- Molecule 40: 60S ribosomal protein L3

Chain L3:



- Molecule 40: 60S ribosomal protein L3

Chain l3:



A155 S156 V157 T169 Q173 G185 I188 V192 R196 E200 K201 T202 V208 Q211 T221 R232 T235 K236 K237 L238 P239 T242 H243 R244 C251 I252 V264 A265 R266 S274 R284 D289 S297 T304 M308 I317 I328

R332 K333 R334 L338 T346 S347 I359 A362 S363 T382 L387

• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 79% 19% •

S2 R3 P4 Q5 V6 E14 A15 T16 L20 T37 T40 K46 S64 V71 A72 R73 I74 G79 F90 M93 M99 K112 E117 Y120 S124 A130 V131 A132 S133 L136 G139 H140 P146 E147 I148 P149 L150 V151 V152 L156

L179 K186 L187 R188 A189 G190 K193 Y194 W199 T200 R203 L206 E211 D212 R220 N221 V222 P223 V230 A231 S232 L233 L258 D259 V267 S270 S284 T287 R288 I289 I290 N291 S292 I295 T306 Q307 K308 H311 V312 L313 V323

L327 V333 K338 K343 K346 T349 K350 L359 D362

• Molecule 41: 60S ribosomal protein L4-A

Chain l4: 80% 19% •

S2 R3 P4 Q5 V6 E14 A15 V25 N43 R47 V52 S53 E54 K55 R69 R73 F90 M93 C94 R98 K112 Y120 A121 T122 T129 A132 S133 L134 K144 L156 V172 S176 D177 L178 L179 L182 K186 L187 G190

R203 L206 I215 V222 E226 V230 A231 S232 L233 K257 L258 V272 T287 N291 I299 R300 P301 A302 G303 Q304 A305 T306 Q307 T310 H311 V312 L313 K319 V323 L327 N328 P329 Y330 V333 K338 L339 K342 E345 K346 T347 G348

T349 T356 E357 T358 L359 D362

• Molecule 42: 60S ribosomal protein L5

Chain L5: 80% 19% •

A2 F3 Q4 A7 R22 R23 K27 K34 K41 A42 K43 N57 K58 C62 I65 S66 T70 L75 I105 T109 K112 L115 T118 V125 L131 T132 D137 R140 L146 D147 I148 Q151 R152 T155 R158 V159

L163 N178 F185 E186 T187 E188 R196 D214 D215 E216 E217 R218 F219 S220 E221 L222 L227 D232 A233 D234 S242 F253 E257 K258 K259 F260 E263 R273 Q274 T275 T290 G295 Q296 Q297

• Molecule 42: 60S ribosomal protein L5

Chain l5: 79% 19% • •

ALA PHE Q4 S9 S10 R15 K34 R35 K41 L51 I61 T68 I69 T70 V73 V74 L75 T109 L110 Q111 K112 L113 G114 L115 T118 Y119 K120 V125 L131 T132 E133 A134 V135 R140 V144 F145 L146 D147 I148 R152 T155 K164

S176 E177 N178 W183 D184 F185 E186 T187 L194 L211 R218 L227 D230 L236 E237 D238 I239 K254 K258 K259 F260 T261 K262 Y265 A266 A267 E268 S269 K270 K271 T275 K276 L277 S278 K279 V286 L293 Q297

• Molecule 43: 60S ribosomal protein L6-A

Chain L6: 77% 12% • 11%

S2 K5 A6 P7 V15 L18 T21 R48 R51 V52 L64 I65 V79 V84 T89 K90 E94 V98 K108 E109 LYS LEU THR LYS LYS GLU LYS LYS GLU ALA ASN LEU PHE PRO GLU GLN GLN ASN LYS E129 R134 L155 S162

K166 F176

• Molecule 43: 60S ribosomal protein L6-A

Chain l6: 75% 14% • 10%

S2 K8 W9 Y10 D14 V15 K20 T21 L30 R31 R46 L64 I65 R78 R82 T89 K90 V91 N97 V98 E99 E109 LYS LEU THR LYS LYS GLU LYS LYS GLU ALA ASN LEU PHE PRO GLU GLN GLN ASN K128 K131 A132 E133 K150 K151 T152

L155 K170 M173 L174 K175 F176

• Molecule 44: 60S ribosomal protein L7-A

Chain L7: 75% 14% • 9%

ALA ALA GLU LYS ILE LEU THR PRO GLU SER GLN LEU LYS LYS SER LYS ALA GLN GLN LYS THR A23 E24 Q25 V26 A32 R33 K38 E39 K40 E59 R60 V77 K82 I89 K90 G91 I92 N93 K98 R110 K118 V119 T120 L124 K128 L129 K158

Q159 R160 V161 P162 L163 S164 K175 I178 L179 D182 D183 L184 K206 L207 P217 I224 S228 L239 N244

• Molecule 44: 60S ribosomal protein L7-A

Chain l7: 79% 11% • 8%

ALA ALA GLU LYS ILE LEU THR PRO GLU SER GLN LEU LYS LYS SER LYS ALA GLN GLN LYS T22 A23 E24 R30 R41 L45 E54 R60 K82 L83 R88 K94 R100 K121 L124 L129 T130 I156 N157 K158 Q159 L173 T178 L179 S180

I181 L184 V191 G192 P193 K219 G226 F229 L239 S242 M243 N244

• Molecule 45: 60S ribosomal protein L8-A

Chain L8: 74% 17% 9%

ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 L26 T27 I36 A39 V40 Q41 S47 V50 K63 V71 T74 Q79 Y80 T81 L82 D83 R84 N95 T101 K106 E118 K122

V132 G135 L136 N137 H138 K149 L150 D156 V157 V163 L169 K172 K181 R185 L189 V197 V203 E206 L211 D219 A220 N221 H232 L238 K241 M246 D247 K248 A256

- Molecule 45: 60S ribosomal protein L8-A

Chain l8: 69% 21% • 9%

ALA PRO GLY LYS LYS VAL ALA PRO ALA PRO PHE GLY ALA LYS SER THR LYS SER ASN LYS THR ARG N24 P25 S29 A39 V40 Q41 L46 L65 R68 L69 K70 V71 T74 I75 A76 Q79 Y80 T81 L82 D83 R84 N85 L93 F94 N95 L109 T110 K111

A117 K120 S121 K122 Q123 D124 K128 V132 K133 L136 K147 A148 K149 I153 I160 V163 V164 L169 K183 A196 L200 T201 E202 V203 E208 A209 A210 L211 A212 K213 L214 A223 D224 K231 I237 L238 G239 N240 K245 K248 D254

SER ALA

- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 81% 18% •

M1 K2 Q5 T6 E14 V18 S19 I20 K21 S22 L34 T35 K36 I41 V48 L52 L68 R69 T70 V71 K72 M78 V82 P98 G108 R115 I123 R124 E135 T138 N139 S147 V151 E152 N157 L161 Q162 Q163 I164

R173 D177 E189 D190 L191

- Molecule 46: 60S ribosomal protein L9-A

Chain l9: 77% 21% •

M1 Q5 T6 V16 T17 V18 S19 R31 G32 T33 N37 V43 T44 Q51 L52 V55 R62 L68 R69 T70 T80 G81 V82 G85 Y92 A109 K110 R115 L118 K121 K122 I123 R129 V132 T133 T138 E143 I144 V151

N157 Q162 Q163 R166 V167 R173 I179 L191

- Molecule 47: 60S ribosomal protein L10

Chain M0: 77% 18% • •

A2 R3 R21 R24 A25 V26 K30 I31 R32 I33 K39 T42 L48 L52 L57 E63 L87 M102 LEU SER CYS ALA GLY ALA ASP ARG LEU Q112 G117 A127 R128 V129 D130 Q133 V138 R139 K145 D146 Q163 K164 I165 I166

T174 N175 L176 D177 R178 P179 E180 K184 E189 V190 K191 K203 G204 S205 L206 E207 N208 A219 Q220 A221

- Molecule 47: 60S ribosomal protein L10

Chain m0: 73% 22% • •

A2 R3 R4 R24 A25 D28 L36 T42 V43 D44 L48 C49 V50 H51 L52 L57 E58 E63 C71 T77 T78 R82 D83 L87 R88 V91 I99 N100 K101 M102 L103 SER CYS ALA GLY ALA ASP ARG L111 V129 I135 R139 S143

N144 K145 R156 S168 K169 K170 L176 D177 L182 R185 D193 G194 V197 L200 S201 K202 K203 G204 S205 L206 E207 I210 R211 E212 A219 Q220 A221

• Molecule 48: 60S ribosomal protein L11-B

Chain M1: 72% 22%

SER THR LYS ALA Q6 N7 P8 M9 R10 D11 L12 K13 S26 G27 D28 S34 E38 Q39 L40 T44 P45 V46 Y52 E63 K64 I65 V71 E77 L80 E81 R82 R94 N95 I106 D107 E108 L112 G113 I114 K115 Y116 D117 V130 R137 R140

R141 K142 K145 S151 T155 D158 S161 Q165 K166 Y167 V171 L172 D173 K174

• Molecule 48: 60S ribosomal protein L11-B

Chain m1: 71% 24%

SER THR LYS ALA Q6 N7 P8 M9 R10 D11 L12 K13 K16 V23 L37 E38 Q39 T44 P45 V46 K49 R60 I65 E78 I79 L80 K87 R94 T99 I106 D107 E108 L112 G113 I114 K115 Y116 D117 I122 V129 V130 R137 V138 T139

R140 R141 K142 T147 H152 K153 T154 D158 T159 Y167 V171 K174

• Molecule 49: 60S ribosomal protein L13-A

Chain M3: 80% 15%

A2 H13 K23 R35 A47 L54 R55 P56 V57 V58 R59 T62 R67 K68 V69 R70 T76 V80 L85 E107 Q114 K122 I123 I124 N129 G130 K131 E136 A141 T144 I147 G163 E164 S165 R168 T169 L170 R171 K190

A191 E192 A193 E194 ALA GLU LYS LYS LYS

• Molecule 49: 60S ribosomal protein L13-A

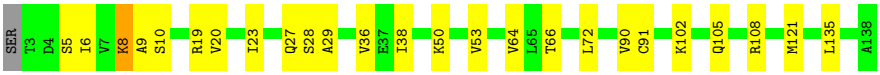
Chain m3: 75% 22%

A2 H13 R21 Q28 K31 R36 A44 K45 I46 A47 P50 L51 L54 R55 R59 A60 V63 R67 K68 V69 R73 T76 L85 I93 N103 R104 E107 I124 N129 G130 K131 E134 A135 S140 A141 Q149 P150 A151

T152 R157 N162 S165 R171 S175 E176 E184 A193 E194 A195 GLU LYS LYS LYS

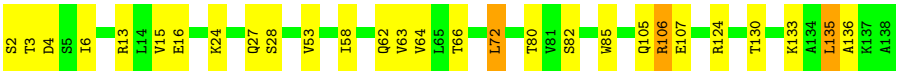
• Molecule 50: 60S ribosomal protein L14-A

Chain M4: 81% 18%



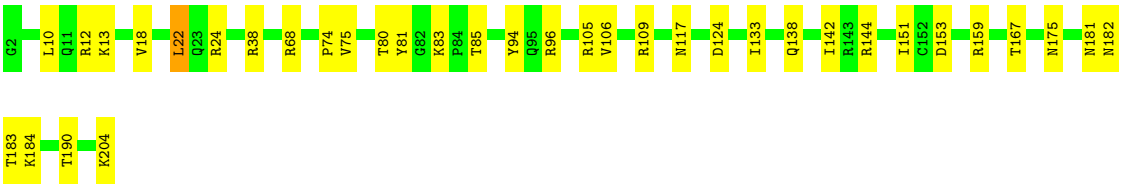
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



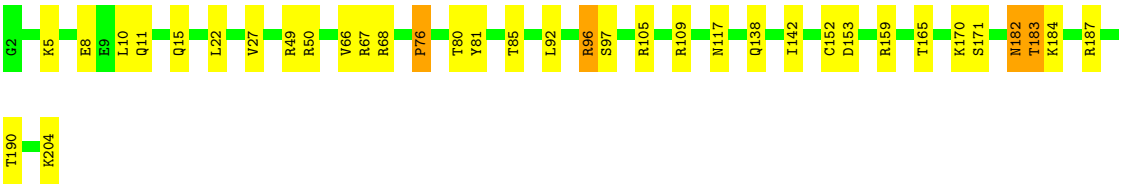
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



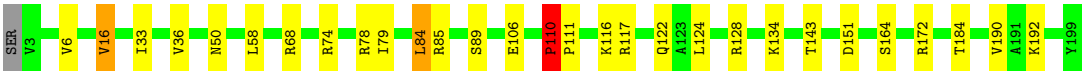
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



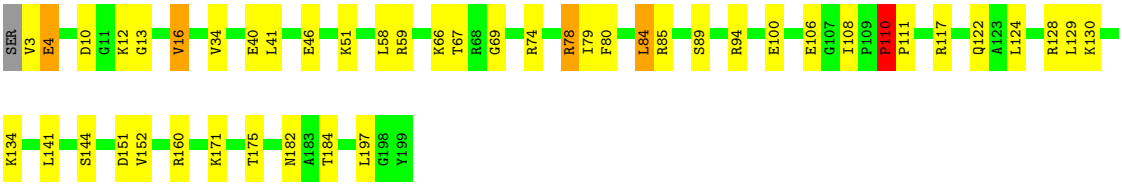
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



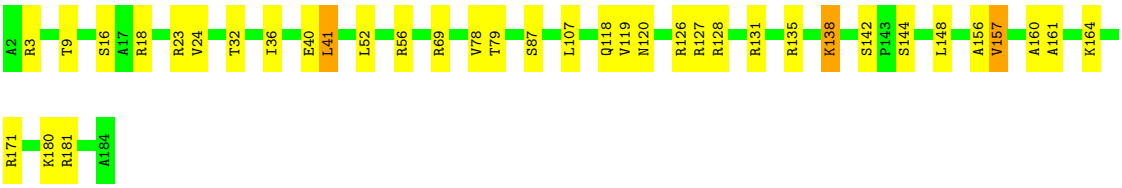
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



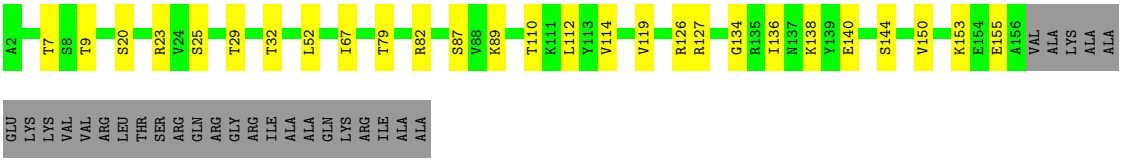
• Molecule 53: 60S ribosomal protein L17-A

Chain M7: 80% 19%



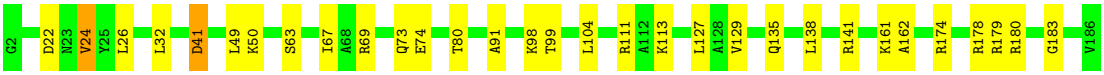
- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 70% 15% 15%



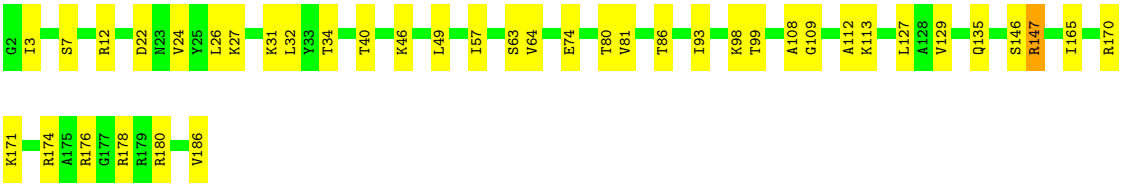
- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 83% 16%



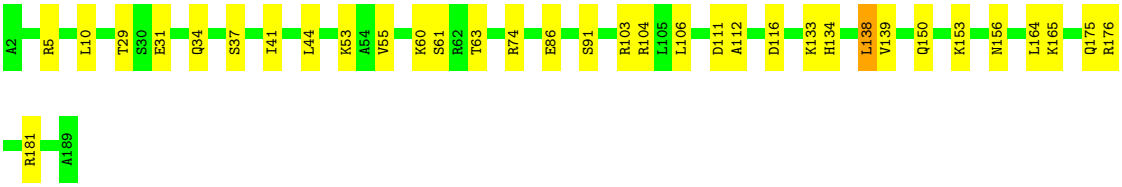
- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 78% 21%



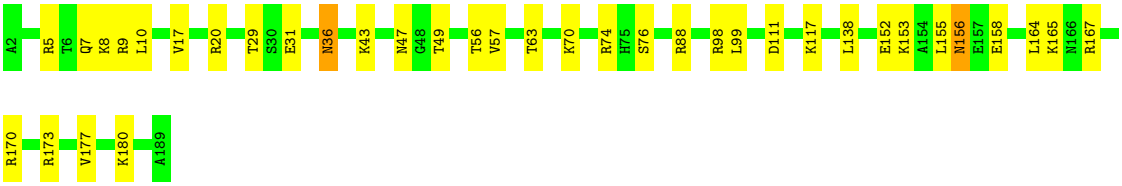
- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 82% 18%



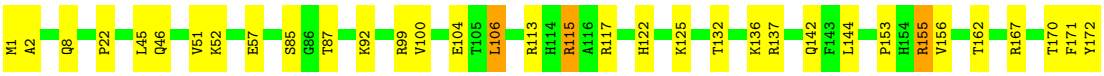
- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 80% 19%



• Molecule 56: 60S ribosomal protein L20-A

Chain N0:

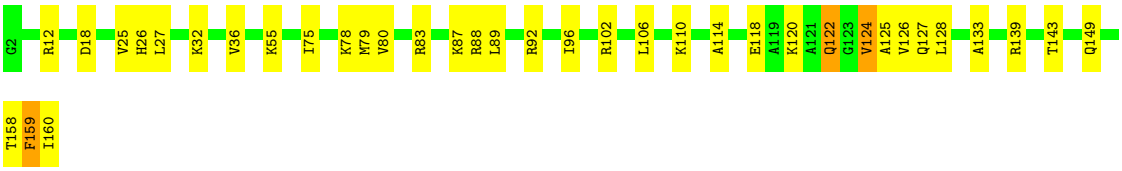


• Molecule 56: 60S ribosomal protein L20-A

Chain n0:

• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

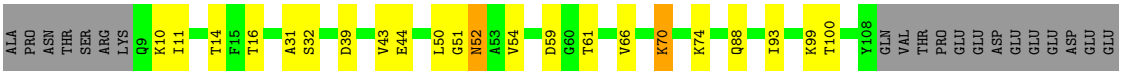


• Molecule 57: 60S ribosomal protein L21-A

Chain n1:

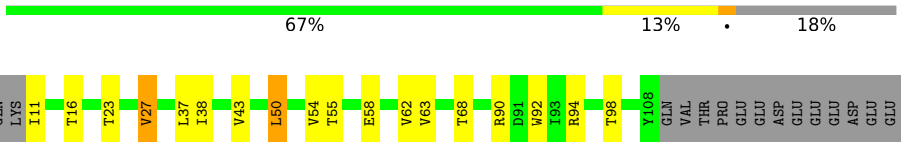
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



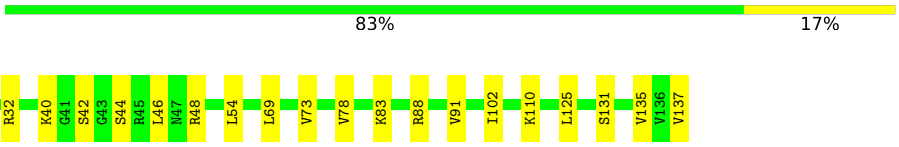
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



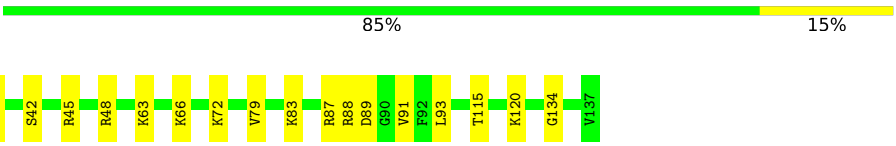
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



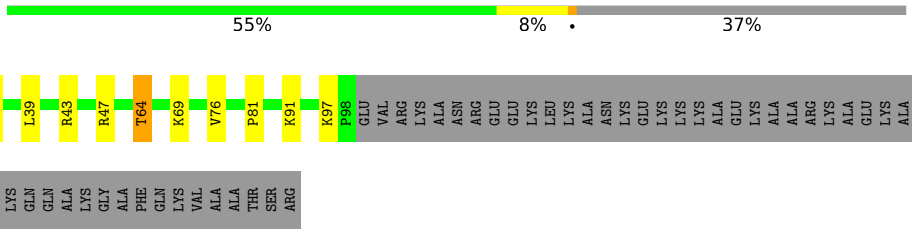
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



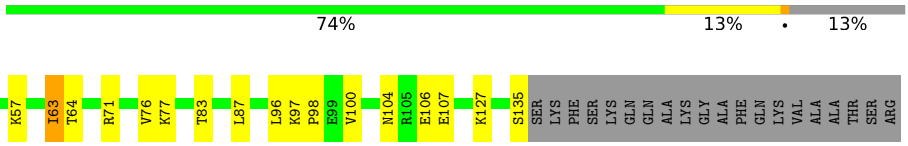
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



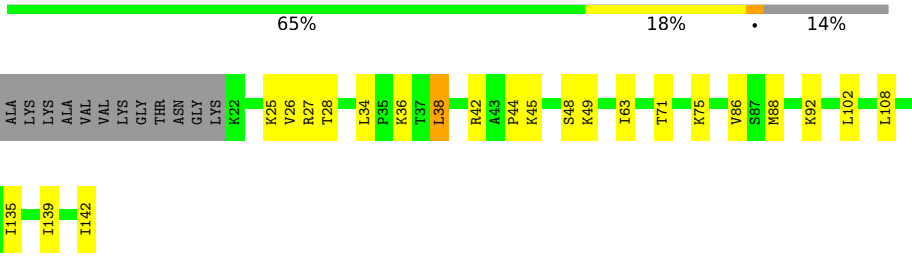
• Molecule 60: 60S ribosomal protein L24-A

Chain n4:



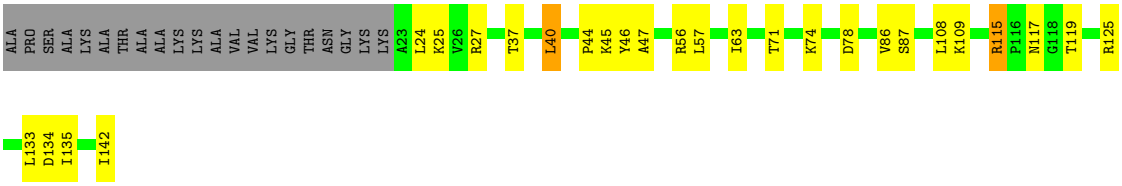
• Molecule 61: 60S ribosomal protein L25

Chain N5:



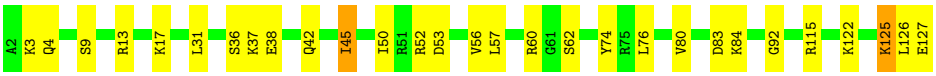
• Molecule 61: 60S ribosomal protein L25

Chain n5:



- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 77% 21%

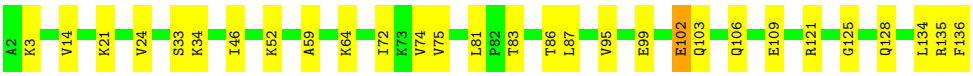


- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 78% 21%

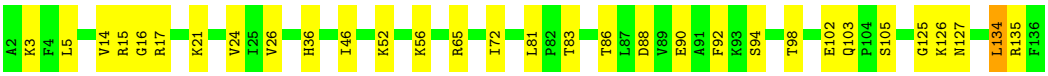
- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 79% 21%



- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 77% 22%

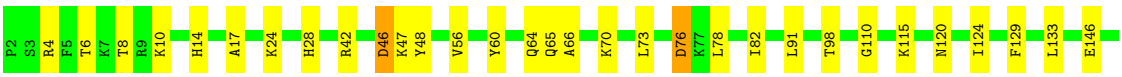


- Molecule 64: 60S ribosomal protein L28

Chain N8: 84% 14%

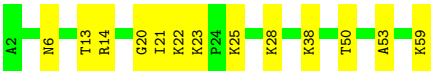
- Molecule 64: 60S ribosomal protein L28

Chain n8: 79% 20%



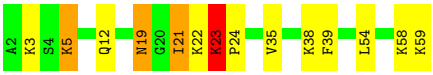
• Molecule 65: 60S ribosomal protein L29

Chain N9:



• Molecule 65: 60S ribosomal protein L29

Chain n9:

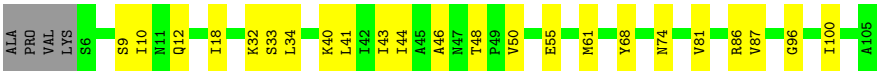


• Molecule 66: 60S ribosomal protein L30

Chain O0:

• Molecule 66: 60S ribosomal protein L30

Chain o0:

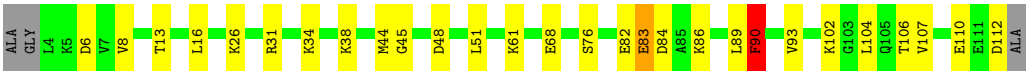


• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

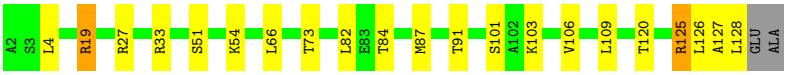
• Molecule 67: 60S ribosomal protein L31-A

Chain o1:



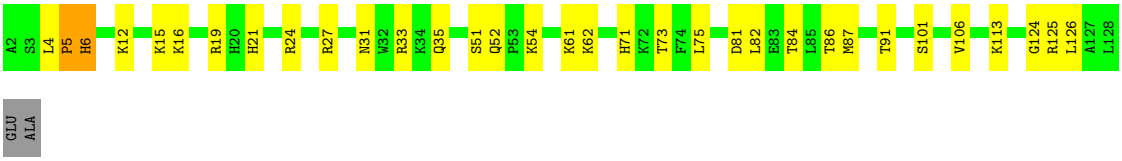
• Molecule 68: 60S ribosomal protein L32

Chain O2:



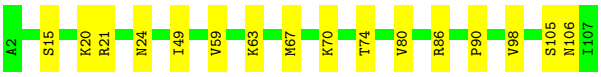
• Molecule 68: 60S ribosomal protein L32

Chain o2:



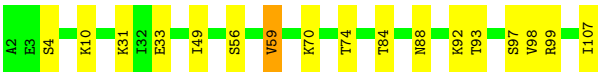
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



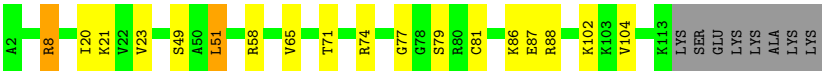
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



• Molecule 70: 60S ribosomal protein L34-A

Chain O4:

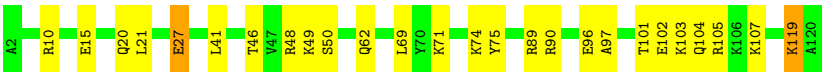


• Molecule 70: 60S ribosomal protein L34-A

Chain o4:

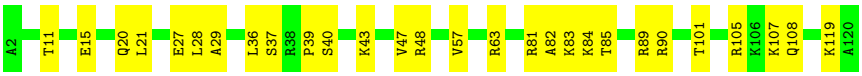
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



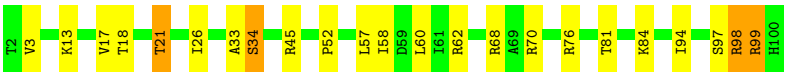
• Molecule 71: 60S ribosomal protein L35-A

Chain o5: 76% 24%



• Molecule 72: 60S ribosomal protein L36-A

Chain O6: 77% 19%



• Molecule 72: 60S ribosomal protein L36-A

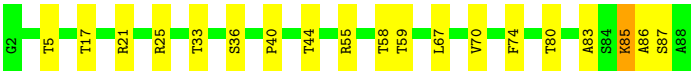
Chain o6: 70% 26%

• Molecule 73: 60S ribosomal protein L37-A

Chain O7: 75% 23%

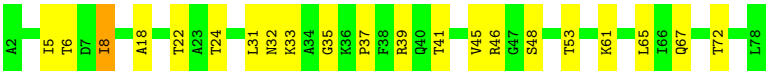
• Molecule 73: 60S ribosomal protein L37-A

Chain o7: 78% 21%



• Molecule 74: 60S ribosomal protein L38

Chain O8: 73% 26%

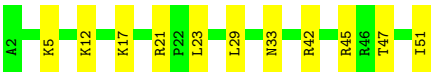


• Molecule 74: 60S ribosomal protein L38

Chain o8: 81% 19%

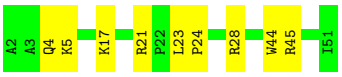
• Molecule 75: 60S ribosomal protein L39

Chain O9: 78% 22%



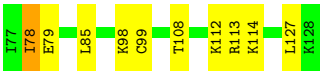
- Molecule 75: 60S ribosomal protein L39

Chain o9: 82% 18%



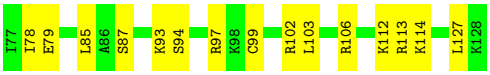
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 81% 17%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 71% 29%

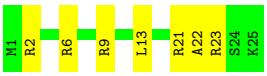


- Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 56% 44%

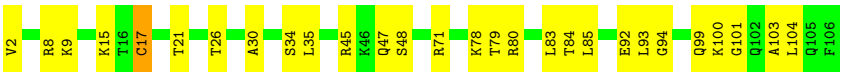
- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 72% 28%



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 73% 26%



- Molecule 78: 60S ribosomal protein L42-A

Chain q2: 80% 19%

• Molecule 79: 60S ribosomal protein L43-A

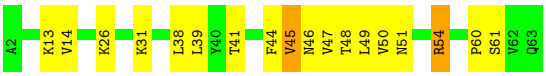
Chain Q3: 80% 19%

• Molecule 79: 60S ribosomal protein L43-A

Chain q3: 81% 19%

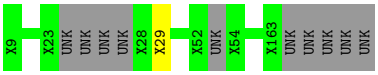
• Molecule 80: 40S ribosomal protein S30-A

Chain e0: 71% 26%



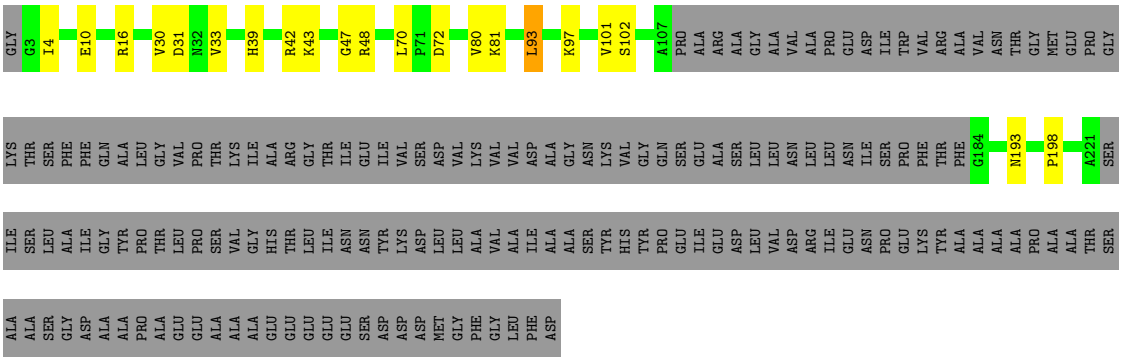
• Molecule 81: unknown protein chain m2

Chain m2: 93% 6%



• Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 39% 6% 54%



• Molecule 83: unknown protein chain p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

• Molecule 84: unknown protein chain p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.92Å 288.52Å 305.75Å 90.00° 99.04° 90.00°	Depositor
Resolution (Å)	267.96 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (267.96-3.20)	Depositor
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.193 , 0.245	Depositor
Wilson B-factor (Å^2)	81.5	Xtriage
Anisotropy	0.087	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411223	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PCY, 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	0.79	6/41698 (0.0%)	1.36	368/64972 (0.6%)
1	6	0.95	31/42765 (0.1%)	1.47	608/66634 (0.9%)
2	S0	0.48	0/1617	0.69	0/2215
2	s0	0.53	0/1623	0.71	0/2222
3	S1	0.42	0/1735	0.70	1/2335 (0.0%)
3	s1	0.51	0/1748	0.70	1/2352 (0.0%)
4	S2	0.54	0/1665	0.69	0/2263
4	s2	0.64	0/1665	0.82	0/2263
5	S3	0.51	0/1759	0.71	1/2368 (0.0%)
5	s3	0.48	0/1759	0.63	0/2368
6	S4	0.51	0/2109	0.74	1/2839 (0.0%)
6	s4	0.60	0/2109	0.82	2/2839 (0.1%)
7	S5	0.43	0/1629	0.62	0/2202
7	s5	0.49	0/1629	0.67	0/2202
8	S6	0.49	0/1823	0.68	0/2439
8	s6	0.62	0/1779	0.74	0/2379
9	S7	0.46	0/1506	0.67	0/2028
9	s7	0.51	0/1516	0.71	2/2043 (0.1%)
10	S8	0.58	0/1514	0.77	1/2021 (0.0%)
10	s8	0.67	0/1514	0.80	1/2021 (0.0%)
11	S9	0.51	0/1519	0.68	0/2035
11	s9	0.62	0/1519	0.80	1/2035 (0.0%)
12	C0	0.45	0/790	0.65	1/1069 (0.1%)
12	c0	0.40	0/777	0.66	3/1049 (0.3%)
13	C1	0.64	0/1240	0.78	1/1675 (0.1%)
13	c1	0.70	1/1194 (0.1%)	0.81	0/1610
14	C2	0.38	0/900	0.61	0/1224
14	c2	0.29	0/900	0.58	1/1224 (0.1%)
15	C3	0.54	0/1215	0.71	1/1638 (0.1%)
15	c3	0.60	0/1215	0.74	0/1638
16	C4	0.46	0/901	0.69	0/1217
16	c4	0.55	0/960	0.77	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.48	0/998	0.69	0/1341
17	c5	0.51	0/1060	0.68	0/1426
18	C6	0.47	0/1125	0.71	2/1510 (0.1%)
18	c6	0.52	0/1131	0.73	0/1518
19	C7	0.46	0/935	0.67	0/1254
19	c7	0.53	0/914	0.73	0/1224
20	C8	0.48	0/1211	0.71	1/1628 (0.1%)
20	c8	0.52	0/1211	0.73	1/1628 (0.1%)
21	C9	0.47	0/1130	0.68	1/1517 (0.1%)
21	c9	0.56	0/1130	0.69	1/1517 (0.1%)
22	D0	0.48	0/865	0.68	0/1169
22	d0	0.53	0/892	0.68	0/1205
23	D1	0.51	0/693	0.67	0/935
23	d1	0.59	0/693	0.70	0/935
24	D2	0.53	0/1038	0.76	2/1395 (0.1%)
24	d2	0.66	0/1038	0.76	1/1395 (0.1%)
25	D3	0.65	0/1139	0.80	0/1518
25	d3	0.75	0/1139	0.87	1/1518 (0.1%)
26	D4	0.48	0/1087	0.67	0/1449
26	d4	0.59	0/1087	0.75	0/1449
27	D5	0.43	0/571	0.72	0/768
27	d5	0.49	0/566	0.75	0/761
28	D6	0.53	0/782	0.75	0/1047
28	d6	0.63	0/782	0.75	2/1047 (0.2%)
29	D7	0.47	0/620	0.71	0/838
29	d7	0.48	0/620	0.70	0/838
30	D8	0.40	0/499	0.64	0/670
30	d8	0.46	0/499	0.67	0/670
31	D9	0.55	0/452	0.80	1/600 (0.2%)
31	d9	0.57	0/452	0.68	0/600
32	E0	0.47	0/483	0.63	0/643
33	E1	0.47	0/577	0.76	0/770
33	e1	0.42	0/619	0.68	0/822
34	SR	0.44	0/2494	0.67	1/3393 (0.0%)
34	sR	0.42	0/2495	0.60	0/3395
35	SM	0.54	0/1113	0.76	2/1502 (0.1%)
35	sM	0.50	0/682	0.73	1/921 (0.1%)
36	1	1.21	245/75394 (0.3%)	1.71	2098/117545 (1.8%)
36	5	1.24	244/75414 (0.3%)	1.72	2161/117575 (1.8%)
37	3	1.00	5/2883 (0.2%)	1.48	35/4491 (0.8%)
37	7	1.20	3/2883 (0.1%)	1.74	84/4491 (1.9%)
38	4	1.17	3/3746 (0.1%)	1.66	91/5832 (1.6%)
38	8	1.05	3/3746 (0.1%)	1.57	70/5832 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	0.77	0/1948	0.86	2/2617 (0.1%)
39	l2	0.76	0/1946	0.91	4/2614 (0.2%)
40	L3	0.78	2/3146 (0.1%)	0.84	1/4228 (0.0%)
40	l3	0.90	1/3146 (0.0%)	0.94	5/4228 (0.1%)
41	L4	0.86	2/2800 (0.1%)	0.95	6/3790 (0.2%)
41	l4	0.77	1/2800 (0.0%)	0.89	3/3790 (0.1%)
42	L5	0.62	1/2425 (0.0%)	0.72	1/3271 (0.0%)
42	l5	0.77	0/2408	0.83	2/3248 (0.1%)
43	L6	0.79	0/1260	0.86	0/1694
43	l6	0.81	0/1269	0.88	1/1705 (0.1%)
44	L7	0.81	0/1821	0.91	4/2451 (0.2%)
44	l7	0.88	0/1828	0.91	3/2461 (0.1%)
45	L8	0.59	0/1836	0.68	0/2481
45	l8	0.55	0/1795	0.72	1/2429 (0.0%)
46	L9	0.66	0/1539	0.75	0/2073
46	l9	0.84	0/1539	0.83	0/2073
47	M0	0.77	1/1741 (0.1%)	0.82	2/2335 (0.1%)
47	m0	0.81	0/1758	0.88	2/2358 (0.1%)
48	M1	0.52	0/1374	0.73	1/1842 (0.1%)
48	m1	0.68	0/1374	0.85	3/1842 (0.2%)
49	M3	0.79	0/1568	0.91	4/2106 (0.2%)
49	m3	0.70	0/1573	0.87	2/2113 (0.1%)
50	M4	0.80	0/1068	0.81	0/1438
50	m4	0.88	0/1074	0.90	2/1446 (0.1%)
51	M5	0.79	0/1757	0.87	2/2354 (0.1%)
51	m5	0.67	0/1757	0.83	3/2354 (0.1%)
52	M6	0.86	0/1585	0.94	4/2128 (0.2%)
52	m6	1.08	3/1585 (0.2%)	1.03	7/2128 (0.3%)
53	M7	0.82	0/1443	0.86	4/1944 (0.2%)
53	m7	0.94	0/1250	0.89	0/1683
54	M8	0.81	0/1465	0.93	2/1965 (0.1%)
54	m8	0.77	0/1465	0.90	0/1965
55	M9	0.58	0/1538	0.72	1/2050 (0.0%)
55	m9	0.65	0/1538	0.71	1/2050 (0.0%)
56	N0	0.77	0/1481	0.86	5/1990 (0.3%)
56	n0	0.94	0/1481	0.96	4/1990 (0.2%)
57	N1	0.87	0/1300	0.85	0/1743
57	n1	0.87	1/1300 (0.1%)	0.88	4/1743 (0.2%)
58	N2	0.46	0/812	0.63	0/1099
58	n2	0.53	0/794	0.70	0/1076
59	N3	0.73	0/1018	0.80	0/1369
59	n3	0.90	0/1018	0.94	3/1369 (0.2%)
60	N4	0.61	0/712	0.70	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	n4	0.76	0/1052	0.77	0/1398
61	N5	0.67	0/979	0.88	4/1321 (0.3%)
61	n5	0.69	0/974	0.82	1/1314 (0.1%)
62	N6	0.73	0/1004	0.87	0/1341
62	n6	0.68	0/1004	0.84	0/1341
63	N7	0.56	0/1118	0.70	0/1497
63	n7	0.53	0/1118	0.66	0/1497
64	N8	0.86	0/1204	0.97	1/1612 (0.1%)
64	n8	0.78	0/1204	0.91	1/1612 (0.1%)
65	N9	0.75	0/473	0.84	0/629
65	n9	0.80	0/473	1.02	1/629 (0.2%)
66	O0	0.52	0/751	0.70	0/1008
66	o0	0.50	0/775	0.67	1/1040 (0.1%)
67	O1	0.69	0/890	0.78	0/1196
67	o1	0.83	0/897	0.89	2/1205 (0.2%)
68	O2	0.87	0/1041	0.94	1/1394 (0.1%)
68	o2	0.83	0/1041	0.91	0/1394
69	O3	0.91	0/868	0.87	1/1168 (0.1%)
69	o3	0.93	0/868	0.98	1/1168 (0.1%)
70	O4	0.72	1/890 (0.1%)	0.90	3/1189 (0.3%)
70	o4	0.61	0/890	0.84	1/1189 (0.1%)
71	O5	0.74	0/978	0.82	0/1301
71	o5	0.63	0/974	0.72	0/1297
72	O6	0.67	0/778	0.78	0/1034
72	o6	0.59	0/777	0.73	0/1033
73	O7	0.84	0/696	1.08	6/923 (0.7%)
73	o7	0.74	0/696	0.81	0/923
74	O8	0.51	0/618	0.70	0/826
74	o8	0.49	0/614	0.67	0/822
75	O9	0.82	0/443	0.87	0/588
75	o9	0.68	0/443	0.81	0/588
76	Q0	0.67	0/423	0.79	0/562
76	q0	0.96	1/423 (0.2%)	0.97	3/562 (0.5%)
77	Q1	0.66	0/234	0.81	0/300
77	q1	0.77	0/234	0.91	0/300
78	Q2	0.88	1/860 (0.1%)	0.86	0/1136
78	q2	0.80	1/860 (0.1%)	0.77	0/1136
79	Q3	0.75	0/701	0.86	1/934 (0.1%)
79	q3	0.72	0/701	0.80	0/934
80	e0	0.59	0/499	0.77	0/665
82	p0	0.49	0/1091	0.67	0/1472
All	All	0.95	557/430072 (0.1%)	1.36	5668/631360 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	2
9	S7	0	1
9	s7	0	2
10	S8	0	2
16	C4	0	2
16	c4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	2
22	d0	0	1
25	d3	0	1
26	d4	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	1
31	D9	0	1
34	SR	0	1
39	L2	0	1
39	l2	0	2
43	L6	0	1
44	l7	0	2
47	m0	0	1
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
68	o2	0	2
73	o7	0	1
81	m2	0	1
All	All	0	46

The worst 5 of 557 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	13.06	2.04	1.82
36	5	1152	G	N9-C4	-11.97	1.28	1.38
78	q2	17	CYS	CB-SG	11.57	2.02	1.82
36	5	1152	G	N3-C4	-10.20	1.28	1.35
36	5	2971	A	N9-C4	9.62	1.43	1.37

The worst 5 of 5668 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	C2-N3-C4	-24.18	99.81	111.90
36	5	1152	G	N3-C4-C5	20.67	138.94	128.60
36	5	1152	G	N3-C4-N9	-18.57	114.86	126.00
36	1	1902	G	N1-C6-O6	17.91	130.65	119.90
36	5	2893	C	N3-C4-C5	-17.30	114.98	121.90

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
9	S7	131	PHE	Peptide
10	S8	79	ALA	Peptide
10	S8	8	ARG	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%)	148 (72%)	34 (17%)	22 (11%)	0	2
2	s0	204/251 (81%)	155 (76%)	31 (15%)	18 (9%)	1	4
3	S1	212/254 (84%)	143 (68%)	36 (17%)	33 (16%)	0	1
3	s1	214/254 (84%)	168 (78%)	30 (14%)	16 (8%)	1	7
4	S2	215/253 (85%)	176 (82%)	24 (11%)	15 (7%)	1	8
4	s2	215/253 (85%)	178 (83%)	24 (11%)	13 (6%)	1	12
5	S3	221/239 (92%)	182 (82%)	31 (14%)	8 (4%)	3	23
5	s3	221/239 (92%)	172 (78%)	31 (14%)	18 (8%)	1	5
6	S4	258/260 (99%)	208 (81%)	27 (10%)	23 (9%)	1	4
6	s4	258/260 (99%)	200 (78%)	36 (14%)	22 (8%)	1	4
7	S5	204/224 (91%)	154 (76%)	29 (14%)	21 (10%)	0	3
7	s5	204/224 (91%)	158 (78%)	26 (13%)	20 (10%)	0	3
8	S6	224/236 (95%)	185 (83%)	22 (10%)	17 (8%)	1	7
8	s6	216/236 (92%)	187 (87%)	19 (9%)	10 (5%)	2	18
9	S7	182/189 (96%)	134 (74%)	23 (13%)	25 (14%)	0	1
9	s7	184/189 (97%)	145 (79%)	27 (15%)	12 (6%)	1	10
10	S8	184/200 (92%)	149 (81%)	24 (13%)	11 (6%)	1	12
10	s8	184/200 (92%)	159 (86%)	19 (10%)	6 (3%)	4	25
11	S9	183/196 (93%)	143 (78%)	29 (16%)	11 (6%)	1	12
11	s9	183/196 (93%)	148 (81%)	25 (14%)	10 (6%)	2	14
12	C0	94/105 (90%)	74 (79%)	10 (11%)	10 (11%)	0	2
12	c0	92/105 (88%)	63 (68%)	15 (16%)	14 (15%)	0	1
13	C1	153/155 (99%)	118 (77%)	20 (13%)	15 (10%)	0	3
13	c1	144/155 (93%)	117 (81%)	19 (13%)	8 (6%)	2	14
14	C2	122/142 (86%)	75 (62%)	26 (21%)	21 (17%)	0	0
14	c2	122/142 (86%)	69 (57%)	34 (28%)	19 (16%)	0	1
15	C3	148/150 (99%)	120 (81%)	20 (14%)	8 (5%)	2	14
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	1	9
16	C4	125/136 (92%)	94 (75%)	21 (17%)	10 (8%)	1	6
16	c4	126/136 (93%)	92 (73%)	22 (18%)	12 (10%)	0	3
17	C5	122/141 (86%)	90 (74%)	18 (15%)	14 (12%)	0	2
17	c5	133/141 (94%)	86 (65%)	23 (17%)	24 (18%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	116 (84%)	13 (9%)	10 (7%)	1	7
18	c6	140/142 (99%)	115 (82%)	18 (13%)	7 (5%)	2	16
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	0	3
19	c7	113/136 (83%)	87 (77%)	12 (11%)	14 (12%)	0	2
20	C8	143/145 (99%)	110 (77%)	22 (15%)	11 (8%)	1	6
20	c8	143/145 (99%)	111 (78%)	22 (15%)	10 (7%)	1	8
21	C9	141/143 (99%)	113 (80%)	25 (18%)	3 (2%)	7	37
21	c9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	2	16
22	D0	105/120 (88%)	83 (79%)	19 (18%)	3 (3%)	4	28
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	65 (76%)	14 (16%)	6 (7%)	1	8
23	d1	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	2	17
24	D2	127/129 (98%)	108 (85%)	12 (9%)	7 (6%)	2	14
24	d2	127/129 (98%)	114 (90%)	9 (7%)	4 (3%)	4	26
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	1	3
25	d3	142/144 (99%)	116 (82%)	19 (13%)	7 (5%)	2	17
26	D4	132/134 (98%)	102 (77%)	23 (17%)	7 (5%)	2	15
26	d4	132/134 (98%)	101 (76%)	21 (16%)	10 (8%)	1	7
27	D5	68/107 (64%)	43 (63%)	14 (21%)	11 (16%)	0	0
27	d5	67/107 (63%)	50 (75%)	14 (21%)	3 (4%)	2	18
28	D6	95/97 (98%)	56 (59%)	19 (20%)	20 (21%)	0	0
28	d6	95/97 (98%)	73 (77%)	13 (14%)	9 (10%)	0	3
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	3	22
29	d7	79/81 (98%)	60 (76%)	15 (19%)	4 (5%)	2	15
30	D8	61/66 (92%)	50 (82%)	7 (12%)	4 (7%)	1	9
30	d8	61/66 (92%)	44 (72%)	10 (16%)	7 (12%)	0	2
31	D9	51/55 (93%)	43 (84%)	7 (14%)	1 (2%)	7	38
31	d9	51/55 (93%)	39 (76%)	8 (16%)	4 (8%)	1	6
32	E0	58/60 (97%)	49 (84%)	6 (10%)	3 (5%)	2	15
33	E1	69/76 (91%)	33 (48%)	15 (22%)	21 (30%)	0	0
33	e1	74/76 (97%)	33 (45%)	24 (32%)	17 (23%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	244 (77%)	52 (16%)	20 (6%)	1	10
34	sR	316/318 (99%)	259 (82%)	43 (14%)	14 (4%)	2	19
35	SM	155/273 (57%)	114 (74%)	23 (15%)	18 (12%)	0	2
35	sM	98/273 (36%)	61 (62%)	21 (21%)	16 (16%)	0	0
39	L2	250/253 (99%)	218 (87%)	26 (10%)	6 (2%)	6	34
39	l2	250/253 (99%)	203 (81%)	36 (14%)	11 (4%)	2	19
40	L3	384/386 (100%)	336 (88%)	30 (8%)	18 (5%)	2	17
40	l3	384/386 (100%)	329 (86%)	42 (11%)	13 (3%)	3	24
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	2	15
41	l4	359/361 (99%)	297 (83%)	43 (12%)	19 (5%)	2	15
42	L5	294/296 (99%)	244 (83%)	31 (10%)	19 (6%)	1	10
42	l5	292/296 (99%)	250 (86%)	30 (10%)	12 (4%)	3	21
43	L6	152/175 (87%)	129 (85%)	19 (12%)	4 (3%)	5	31
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	5	31
44	L7	220/243 (90%)	183 (83%)	28 (13%)	9 (4%)	3	21
44	l7	221/243 (91%)	191 (86%)	24 (11%)	6 (3%)	5	30
45	L8	231/255 (91%)	185 (80%)	37 (16%)	9 (4%)	3	22
45	l8	229/255 (90%)	175 (76%)	32 (14%)	22 (10%)	0	3
46	L9	189/191 (99%)	161 (85%)	24 (13%)	4 (2%)	7	37
46	l9	189/191 (99%)	165 (87%)	18 (10%)	6 (3%)	4	26
47	M0	207/220 (94%)	168 (81%)	33 (16%)	6 (3%)	4	28
47	m0	209/220 (95%)	175 (84%)	20 (10%)	14 (7%)	1	9
48	M1	167/173 (96%)	135 (81%)	18 (11%)	14 (8%)	1	5
48	m1	167/173 (96%)	132 (79%)	20 (12%)	15 (9%)	1	4
49	M3	191/198 (96%)	161 (84%)	21 (11%)	9 (5%)	2	17
49	m3	192/198 (97%)	154 (80%)	19 (10%)	19 (10%)	0	3
50	M4	134/137 (98%)	119 (89%)	8 (6%)	7 (5%)	2	15
50	m4	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	10	44
51	M5	201/203 (99%)	184 (92%)	11 (6%)	6 (3%)	4	28
51	m5	201/203 (99%)	181 (90%)	15 (8%)	5 (2%)	5	32
52	M6	195/198 (98%)	176 (90%)	16 (8%)	3 (2%)	10	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m6	195/198 (98%)	175 (90%)	15 (8%)	5 (3%)	5	31
53	M7	181/183 (99%)	154 (85%)	22 (12%)	5 (3%)	5	29
53	m7	153/183 (84%)	131 (86%)	19 (12%)	3 (2%)	7	38
54	M8	183/185 (99%)	157 (86%)	19 (10%)	7 (4%)	3	22
54	m8	183/185 (99%)	148 (81%)	29 (16%)	6 (3%)	4	25
55	M9	186/188 (99%)	165 (89%)	17 (9%)	4 (2%)	6	35
55	m9	186/188 (99%)	162 (87%)	20 (11%)	4 (2%)	6	35
56	N0	170/172 (99%)	152 (89%)	15 (9%)	3 (2%)	8	41
56	n0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	8	41
57	N1	157/159 (99%)	136 (87%)	13 (8%)	8 (5%)	2	15
57	n1	157/159 (99%)	139 (88%)	16 (10%)	2 (1%)	12	47
58	N2	98/120 (82%)	77 (79%)	15 (15%)	6 (6%)	1	12
58	n2	96/120 (80%)	75 (78%)	19 (20%)	2 (2%)	7	37
59	N3	134/136 (98%)	119 (89%)	15 (11%)	0	100	100
59	n3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	44
60	N4	96/155 (62%)	72 (75%)	18 (19%)	6 (6%)	1	10
60	n4	133/155 (86%)	111 (84%)	15 (11%)	7 (5%)	2	15
61	N5	119/141 (84%)	106 (89%)	9 (8%)	4 (3%)	3	24
61	n5	118/141 (84%)	96 (81%)	15 (13%)	7 (6%)	1	12
62	N6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	2	17
62	n6	124/126 (98%)	108 (87%)	11 (9%)	5 (4%)	3	21
63	N7	133/135 (98%)	112 (84%)	14 (10%)	7 (5%)	2	15
63	n7	133/135 (98%)	108 (81%)	20 (15%)	5 (4%)	3	22
64	N8	146/148 (99%)	124 (85%)	18 (12%)	4 (3%)	5	30
64	n8	146/148 (99%)	120 (82%)	16 (11%)	10 (7%)	1	9
65	N9	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	3	23
65	n9	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	4
66	O0	95/104 (91%)	83 (87%)	10 (10%)	2 (2%)	7	37
66	o0	98/104 (94%)	86 (88%)	9 (9%)	3 (3%)	4	26
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	17
67	o1	107/112 (96%)	91 (85%)	12 (11%)	4 (4%)	3	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O2	125/129 (97%)	109 (87%)	13 (10%)	3 (2%)	6	34
68	o2	125/129 (97%)	102 (82%)	18 (14%)	5 (4%)	3	21
69	O3	104/106 (98%)	93 (89%)	10 (10%)	1 (1%)	15	54
69	o3	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	4	28
70	O4	110/120 (92%)	92 (84%)	16 (14%)	2 (2%)	8	41
70	o4	110/120 (92%)	92 (84%)	12 (11%)	6 (6%)	2	14
71	O5	117/119 (98%)	103 (88%)	8 (7%)	6 (5%)	2	15
71	o5	117/119 (98%)	97 (83%)	13 (11%)	7 (6%)	1	12
72	O6	97/99 (98%)	76 (78%)	11 (11%)	10 (10%)	0	3
72	o6	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	7
73	O7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	6	34
73	o7	85/87 (98%)	69 (81%)	13 (15%)	3 (4%)	3	24
74	O8	75/77 (97%)	61 (81%)	9 (12%)	5 (7%)	1	9
74	o8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	1	9
75	O9	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
75	o9	48/50 (96%)	41 (85%)	5 (10%)	2 (4%)	3	20
76	Q0	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	3	21
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	7	38
77	Q1	23/25 (92%)	23 (100%)	0	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	20
78	Q2	103/105 (98%)	78 (76%)	16 (16%)	9 (9%)	1	4
78	q2	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	8	39
79	Q3	89/91 (98%)	75 (84%)	10 (11%)	4 (4%)	2	18
79	q3	89/91 (98%)	76 (85%)	12 (14%)	1 (1%)	14	51
80	e0	60/62 (97%)	48 (80%)	5 (8%)	7 (12%)	0	2
82	p0	139/311 (45%)	111 (80%)	23 (16%)	5 (4%)	3	23
All	All	22333/24143 (92%)	18179 (81%)	2816 (13%)	1338 (6%)	1	12

5 of 1338 Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S0	191	ARG
2	S0	194	PRO
3	S1	40	ASN

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%)	129 (79%)	35 (21%)	1 5
2	s0	165/209 (79%)	129 (78%)	36 (22%)	1 5
3	S1	191/223 (86%)	150 (78%)	41 (22%)	1 5
3	s1	192/223 (86%)	150 (78%)	42 (22%)	1 5
4	S2	176/204 (86%)	142 (81%)	34 (19%)	1 8
4	s2	176/204 (86%)	124 (70%)	52 (30%)	0 1
5	S3	182/194 (94%)	140 (77%)	42 (23%)	1 3
5	s3	182/194 (94%)	146 (80%)	36 (20%)	1 7
6	S4	221/221 (100%)	167 (76%)	54 (24%)	0 2
6	s4	221/221 (100%)	180 (81%)	41 (19%)	1 8
7	S5	173/190 (91%)	141 (82%)	32 (18%)	1 8
7	s5	173/190 (91%)	142 (82%)	31 (18%)	2 9
8	S6	188/201 (94%)	156 (83%)	32 (17%)	2 10
8	s6	187/201 (93%)	151 (81%)	36 (19%)	1 8
9	S7	165/169 (98%)	137 (83%)	28 (17%)	2 10
9	s7	165/169 (98%)	137 (83%)	28 (17%)	2 10
10	S8	150/161 (93%)	125 (83%)	25 (17%)	2 10
10	s8	150/161 (93%)	119 (79%)	31 (21%)	1 6
11	S9	158/165 (96%)	122 (77%)	36 (23%)	1 4
11	s9	158/165 (96%)	123 (78%)	35 (22%)	1 4
12	C0	77/98 (79%)	61 (79%)	16 (21%)	1 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c0	73/98 (74%)	64 (88%)	9 (12%)	4	21
13	C1	129/136 (95%)	108 (84%)	21 (16%)	2	11
13	c1	129/136 (95%)	104 (81%)	25 (19%)	1	7
14	C2	88/118 (75%)	64 (73%)	24 (27%)	0	1
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	1
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	7
15	c3	127/127 (100%)	102 (80%)	25 (20%)	1	7
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	1
16	c4	97/104 (93%)	73 (75%)	24 (25%)	0	2
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	6
17	c5	103/117 (88%)	84 (82%)	19 (18%)	1	8
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	7
18	c6	118/118 (100%)	99 (84%)	19 (16%)	2	11
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1	5
19	c7	92/124 (74%)	73 (79%)	19 (21%)	1	6
20	C8	128/128 (100%)	98 (77%)	30 (23%)	1	3
20	c8	128/128 (100%)	102 (80%)	26 (20%)	1	6
21	C9	115/115 (100%)	88 (76%)	27 (24%)	1	3
21	c9	115/115 (100%)	95 (83%)	20 (17%)	2	10
22	D0	100/113 (88%)	75 (75%)	25 (25%)	0	2
22	d0	103/113 (91%)	74 (72%)	29 (28%)	0	1
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	5
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	5
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	6
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3	15
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	9
25	d3	119/119 (100%)	100 (84%)	19 (16%)	2	11
26	D4	112/112 (100%)	90 (80%)	22 (20%)	1	7
26	d4	112/112 (100%)	94 (84%)	18 (16%)	2	11
27	D5	61/88 (69%)	46 (75%)	15 (25%)	0	2
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	6
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2	12
29	D7	70/70 (100%)	63 (90%)	7 (10%)	7	30
29	d7	70/70 (100%)	60 (86%)	10 (14%)	3	15
30	D8	56/59 (95%)	42 (75%)	14 (25%)	0	2
30	d8	56/59 (95%)	42 (75%)	14 (25%)	0	2
31	D9	47/48 (98%)	41 (87%)	6 (13%)	4	20
31	d9	47/48 (98%)	35 (74%)	12 (26%)	0	2
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	7
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1
33	e1	66/66 (100%)	46 (70%)	20 (30%)	0	0
34	SR	260/261 (100%)	219 (84%)	41 (16%)	2	12
34	sR	260/261 (100%)	229 (88%)	31 (12%)	5	22
35	SM	97/228 (42%)	77 (79%)	20 (21%)	1	6
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	1
39	L2	193/195 (99%)	154 (80%)	39 (20%)	1	6
39	l2	192/195 (98%)	161 (84%)	31 (16%)	2	11
40	L3	321/322 (100%)	245 (76%)	76 (24%)	1	3
40	l3	321/322 (100%)	257 (80%)	64 (20%)	1	6
41	L4	288/288 (100%)	231 (80%)	57 (20%)	1	7
41	l4	288/288 (100%)	232 (81%)	56 (19%)	1	7
42	L5	244/244 (100%)	199 (82%)	45 (18%)	1	8
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	6
43	L6	134/152 (88%)	116 (87%)	18 (13%)	4	18
43	l6	135/152 (89%)	113 (84%)	22 (16%)	2	11
44	L7	186/204 (91%)	156 (84%)	30 (16%)	2	11
44	l7	187/204 (92%)	159 (85%)	28 (15%)	3	14
45	L8	187/207 (90%)	150 (80%)	37 (20%)	1	7
45	l8	177/207 (86%)	141 (80%)	36 (20%)	1	6
46	L9	171/171 (100%)	138 (81%)	33 (19%)	1	8
46	l9	171/171 (100%)	131 (77%)	40 (23%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	M0	177/186 (95%)	142 (80%)	35 (20%)	1	7
47	m0	179/186 (96%)	138 (77%)	41 (23%)	1	4
48	M1	147/150 (98%)	112 (76%)	35 (24%)	0	3
48	m1	147/150 (98%)	114 (78%)	33 (22%)	1	4
49	M3	154/158 (98%)	129 (84%)	25 (16%)	2	11
49	m3	154/158 (98%)	128 (83%)	26 (17%)	2	10
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	9
50	m4	108/108 (100%)	81 (75%)	27 (25%)	0	2
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	10
51	m5	175/175 (100%)	144 (82%)	31 (18%)	2	9
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2	11
52	m6	160/161 (99%)	123 (77%)	37 (23%)	1	3
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	4
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	8
54	M8	150/150 (100%)	126 (84%)	24 (16%)	2	11
54	m8	150/150 (100%)	115 (77%)	35 (23%)	1	3
55	M9	153/153 (100%)	123 (80%)	30 (20%)	1	7
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	4
56	N0	156/156 (100%)	127 (81%)	29 (19%)	1	8
56	n0	156/156 (100%)	118 (76%)	38 (24%)	0	2
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	3
57	n1	136/136 (100%)	110 (81%)	26 (19%)	1	8
58	N2	87/106 (82%)	69 (79%)	18 (21%)	1	6
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1	5
59	N3	104/104 (100%)	81 (78%)	23 (22%)	1	4
59	n3	104/104 (100%)	87 (84%)	17 (16%)	2	11
60	N4	57/129 (44%)	49 (86%)	8 (14%)	3	16
60	n4	100/129 (78%)	86 (86%)	14 (14%)	3	16
61	N5	104/117 (89%)	79 (76%)	25 (24%)	0	3
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	6
62	N6	109/109 (100%)	84 (77%)	25 (23%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1 5
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1 6
63	n7	115/115 (100%)	88 (76%)	27 (24%)	1 3
64	N8	118/118 (100%)	98 (83%)	20 (17%)	2 10
64	n8	118/118 (100%)	98 (83%)	20 (17%)	2 10
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1 5
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0 2
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1 6
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1 4
67	O1	92/96 (96%)	65 (71%)	27 (29%)	0 1
67	o1	94/96 (98%)	70 (74%)	24 (26%)	0 2
68	O2	109/110 (99%)	90 (83%)	19 (17%)	2 10
68	o2	109/110 (99%)	81 (74%)	28 (26%)	0 2
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2 12
69	o3	90/90 (100%)	76 (84%)	14 (16%)	2 12
70	O4	95/102 (93%)	80 (84%)	15 (16%)	2 12
70	o4	95/102 (93%)	76 (80%)	19 (20%)	1 6
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1 5
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1 6
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1 6
72	o6	80/81 (99%)	53 (66%)	27 (34%)	0 0
73	O7	70/70 (100%)	53 (76%)	17 (24%)	0 2
73	o7	70/70 (100%)	54 (77%)	16 (23%)	1 4
74	O8	68/68 (100%)	51 (75%)	17 (25%)	0 2
74	o8	67/68 (98%)	57 (85%)	10 (15%)	3 14
75	O9	45/45 (100%)	34 (76%)	11 (24%)	0 2
75	o9	45/45 (100%)	38 (84%)	7 (16%)	2 12
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	1 8
76	q0	47/47 (100%)	37 (79%)	10 (21%)	1 5
77	Q1	23/23 (100%)	12 (52%)	11 (48%)	0 0
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	Q2	90/90 (100%)	71 (79%)	19 (21%)	1 6
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1 6
79	Q3	71/71 (100%)	57 (80%)	14 (20%)	1 7
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1 4
80	e0	53/53 (100%)	40 (76%)	13 (24%)	0 2
82	p0	105/253 (42%)	89 (85%)	16 (15%)	3 13
All	All	18730/20241 (92%)	14956 (80%)	3774 (20%)	1 6

5 of 3774 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
78	Q2	80	ARG
67	o1	31	ARG
14	c2	89	ILE
64	n8	146	GLU
52	m6	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
55	M9	34	GLN
75	o9	38	ASN
78	Q2	99	GLN
75	o9	4	GLN
54	m8	58	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	480 (27%)	50 (2%)
1	6	1792/1800 (99%)	484 (27%)	49 (2%)
36	1	3145/3396 (92%)	690 (21%)	93 (2%)
36	5	3145/3396 (92%)	693 (22%)	78 (2%)
37	3	120/121 (99%)	17 (14%)	1 (0%)
37	7	120/121 (99%)	20 (16%)	1 (0%)
38	4	157/158 (99%)	40 (25%)	6 (3%)
38	8	157/158 (99%)	38 (24%)	1 (0%)
All	All	10383/10950 (94%)	2462 (23%)	279 (2%)

5 of 2462 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	1355	A
36	5	1580	A
36	5	2682	C
36	1	1751	G
36	1	1589	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2558 ligands modelled in this entry, 1426 are monoatomic - leaving 1132 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	4197	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	7	215	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	M7	206	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	1	4211	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3943	86	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	o7	503	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	4233	86	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	5	4250	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	L4	403	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	l5	303	-	0,6,6	-	-	-		
86	OHX	l9	600	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	N1	201	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	5	4249	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	7	216	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	D3	202	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	M7	205	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	q1	102	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	5	4251	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	n9	101	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	m5	305	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	PCY	2	2178	-	36,42,42	0.45	0	41,65,65	0.86	2 (4%)
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	M9	204	-	0,6,6	-	-	-		
86	OHX	1	4212	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	m1	203	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	8	232	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	S6	301	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
87	PCY	6	2204	-	36,42,42	0.60	1 (2%)	41,65,65	0.91	1 (2%)
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	l5	305	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	m6	203	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	3	226	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	1	4213	-	0,6,6	-	-	-		
86	OHX	4	238	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	4	237	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	N9	102	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	l4	403	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	1	4043	-	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
87	PCY	6	2204	-	-	10/33/67/67	0/3/3/3
87	PCY	2	2178	-	-	6/33/67/67	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	6	2204	PCY	C24-C28	2.12	1.42	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	2	2178	PCY	O14-C7-C13	-2.92	102.82	109.09
87	2	2178	PCY	O5-C1-N2	2.62	126.12	121.05
87	6	2204	PCY	O5-C1-N2	2.58	126.04	121.05

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	2	2178	PCY	N2-C3-C6-C11
87	2	2178	PCY	N2-C3-C6-O12
87	2	2178	PCY	C7-C3-C6-C11
87	2	2178	PCY	C8-C3-C6-C11

Continued on next page...

Continued from previous page...

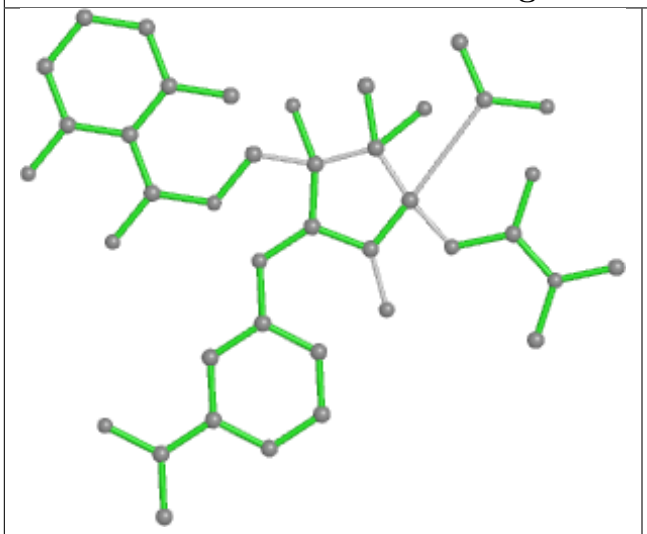
Mol	Chain	Res	Type	Atoms
87	6	2204	PCY	N2-C3-C6-C11

There are no ring outliers.

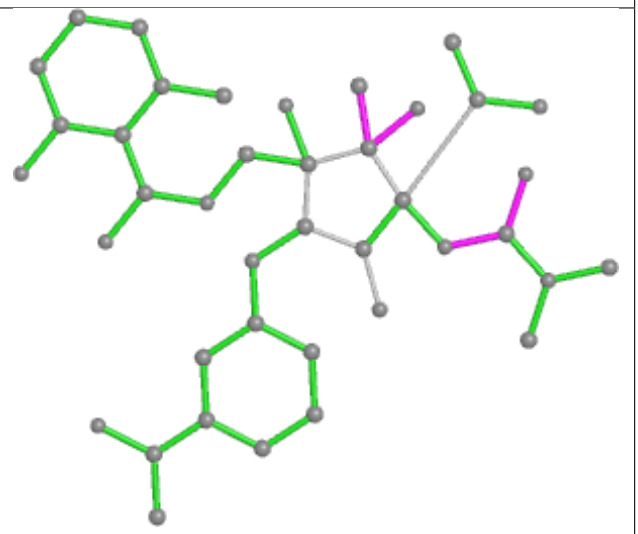
No monomer is involved in short contacts.

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

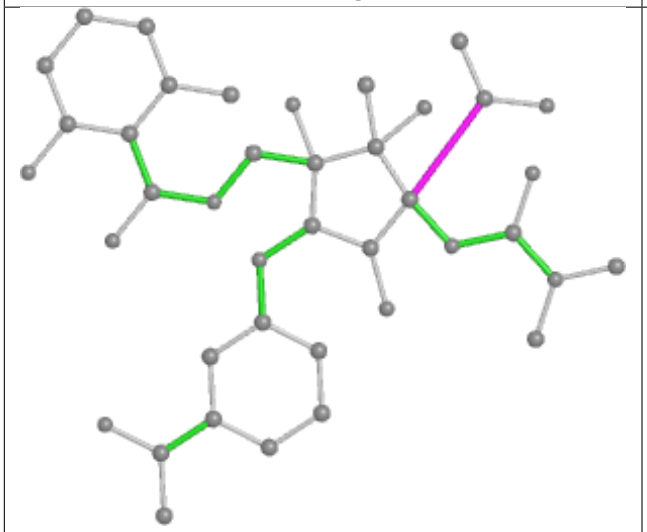
Ligand PCY 2 2178



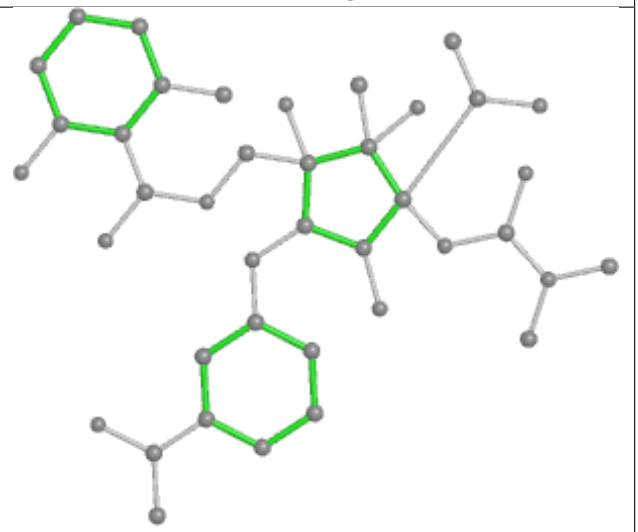
Bond lengths



Bond angles

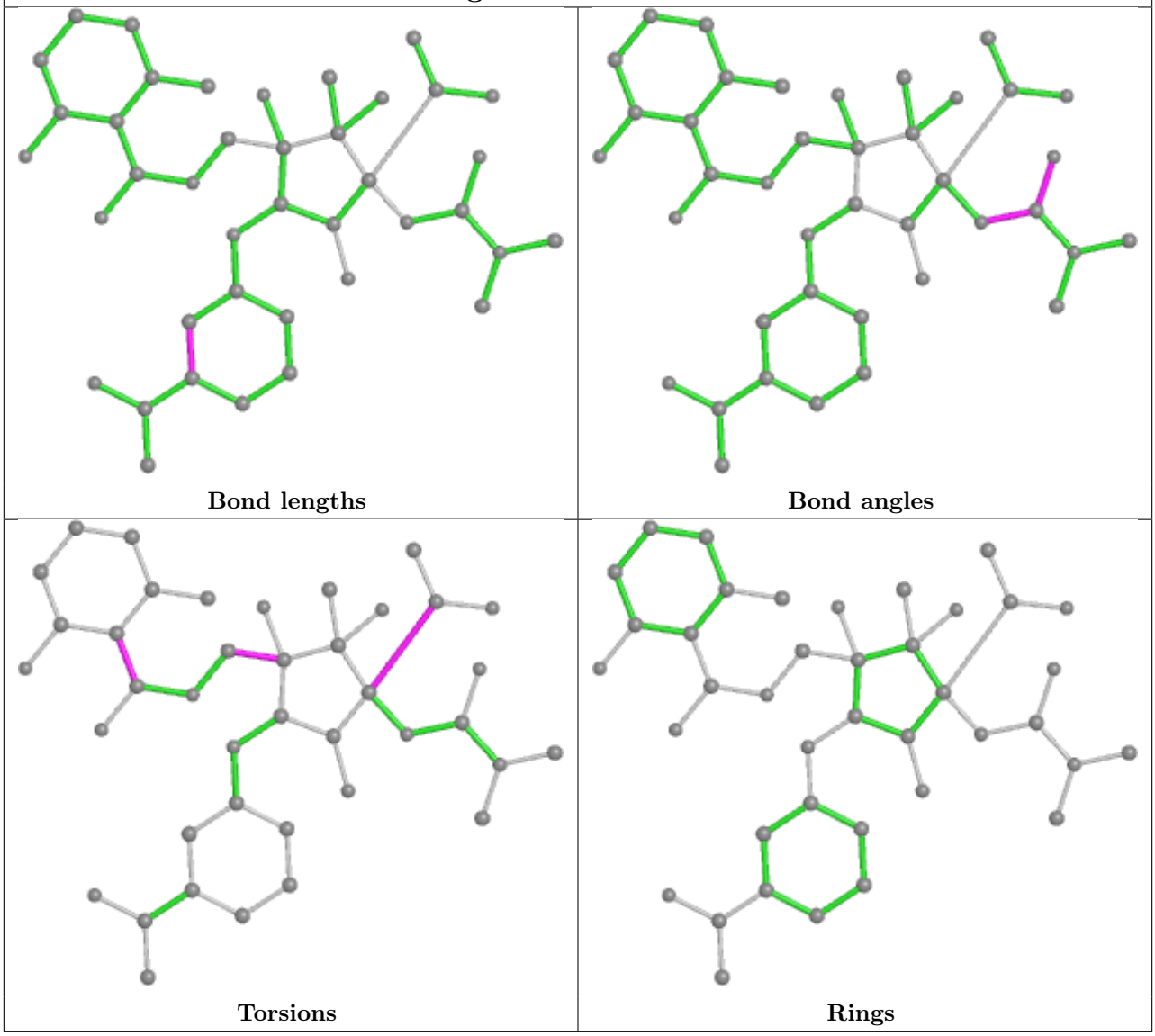


Torsions



Rings

Ligand PCY 6 2204



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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