wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 08:59 pm GMT

PDB ID	:	4U4Z
Title	:	Crystal structure of Phyllanthoside bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	3.10 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:

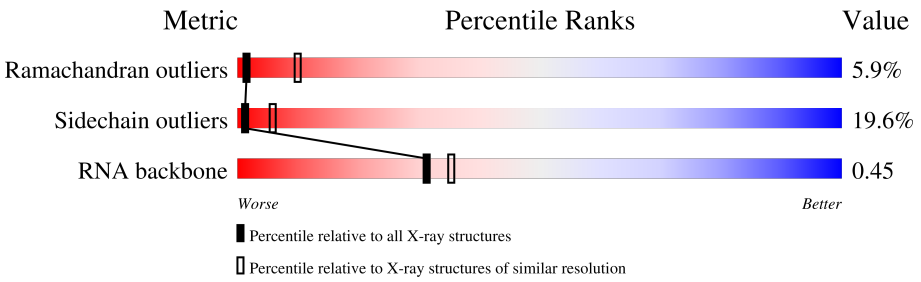
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et 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 3.10 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	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	64% 30% • •
1	6	1800	65% 30% 5%
2	S0	251	64% 16% • 18%
2	s0	251	61% 20% • 18%
3	S1	254	58% 22% • 16%
3	s1	254	65% 18% • 15%
4	S2	253	67% 17% • 14%
4	s2	253	64% 20% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	S3	239	69% 22% 7%
5	s3	239	72% 20% 7%
6	S4	260	77% 21%
6	s4	260	80% 18%
7	S5	224	70% 21% 8%
7	s5	224	69% 21% 8%
8	S6	236	76% 19%
8	s6	236	73% 18% 8%
9	S7	189	71% 25%
9	s7	189	78% 18%
10	S8	200	78% 14% 6%
10	s8	200	74% 20% 6%
11	S9	196	74% 19% 6%
11	s9	196	73% 20% 6%
12	C0	105	74% 14% 9%
12	c0	105	67% 20% 5% 9%
13	C1	155	86% 14%
13	c1	155	78% 15% 6%
14	C2	142	54% 31% 13%
14	c2	142	56% 28% 13%
15	C3	150	81% 17%
15	c3	150	79% 19%
16	C4	136	71% 19% 7%
16	c4	136	68% 24% 6%
17	C5	141	70% 16% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	c5	141	71% 23%
18	C6	142	77% 21%
18	c6	142	80% 18%
19	C7	136	66% 19% 12%
19	c7	136	67% 18% 14%
20	C8	145	79% 19%
20	c8	145	73% 25%
21	C9	143	80% 17%
21	c9	143	83% 15%
22	D0	120	63% 24% 11%
22	d0	120	62% 28% 8%
23	D1	87	80% 17%
23	d1	87	80% 18%
24	D2	129	83% 14%
24	d2	129	87% 11%
25	D3	144	80% 19%
25	d3	144	81% 18%
26	D4	134	84% 13%
26	d4	134	81% 18%
27	D5	107	40% 23% 35%
27	d5	107	50% 15% 36%
28	D6	97	67% 27% 6%
28	d6	97	71% 29%
29	D7	81	81% 16%
29	d7	81	83% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	D8	66	70% 23% 5%
30	d8	66	76% 17% 5%
31	D9	55	78% 18%
31	d9	55	73% 22%
32	E0	60	77% 22%
33	E1	76	51% 36% 7% 7%
33	e1	76	59% 36%
34	SR	318	79% 19%
34	sR	318	87% 13%
35	SM	273	46% 10% 42%
35	sM	273	28% 10% 62%
36	1	3396	50% 36% 7% 7%
36	5	3396	49% 37% 7% 7%
37	3	121	75% 22%
37	7	121	60% 34% 7%
38	4	158	56% 37% 7%
38	8	158	63% 29% 8%
39	L2	253	82% 17%
39	l2	253	81% 17%
40	L3	386	78% 21%
40	l3	386	79% 20%
41	L4	361	78% 19%
41	l4	361	80% 17%
42	L5	296	83% 15%
42	l5	296	80% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
43	L6	175	76% 12% • 11%
43	l6	175	75% 14% •• 10%
44	L7	243	77% 12% • 9%
44	l7	243	77% 13% • 8%
45	L8	255	76% 15% 9%
45	l8	255	67% 22% • 9%
46	L9	191	75% 24% •
46	l9	191	81% 19% •
47	M0	220	74% 20% • •
47	m0	220	76% 20% • •
48	M1	173	72% 20% 5% •
48	m1	173	73% 23% • •
49	M3	198	78% 18% • •
49	m3	198	79% 18% • •
50	M4	137	78% 20% •••
50	m4	137	85% 13% •
51	M5	203	80% 19% •
51	m5	203	83% 17%
52	M6	198	82% 15% •••
52	m6	198	81% 18% •••
53	M7	183	79% 20% •
53	m7	183	69% 15% 15%
54	M8	185	82% 16% ••
54	m8	185	78% 21% •
55	M9	188	86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	m9	188	80% 19%
56	N0	172	81% 19%
56	n0	172	78% 21%
57	N1	159	81% 16%
57	n1	159	80% 20%
58	N2	120	68% 14% 17%
58	n2	120	61% 20% 18%
59	N3	136	85% 15%
59	n3	136	88% 11%
60	N4	155	53% 8% 37%
60	n4	155	72% 14% 13%
61	N5	141	69% 16% 14%
61	n5	141	67% 17% 15%
62	N6	126	79% 21%
62	n6	126	80% 19%
63	N7	135	79% 20%
63	n7	135	78% 17%
64	N8	148	82% 16%
64	n8	148	84% 15%
65	N9	58	83% 17%
65	n9	58	69% 29%
66	O0	104	75% 18% 7%
66	o0	104	75% 19%
67	O1	112	79% 17%
67	o1	112	70% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
68	O2	129	80% 19%
68	o2	129	78% 19%
69	O3	106	90% 9%
69	o3	106	82% 16%
70	O4	119	77% 14% 6%
70	o4	119	76% 17% 6%
71	O5	119	75% 24%
71	o5	119	78% 21%
72	O6	99	76% 20%
72	o6	99	70% 28%
73	O7	87	76% 23%
73	o7	87	82% 16%
74	O8	77	73% 27%
74	o8	77	77% 23%
75	O9	50	80% 20%
75	o9	50	80% 20%
76	Q0	52	85% 15%
76	q0	52	85% 15%
77	Q1	25	64% 36%
77	q1	25	72% 20% 8%
78	Q2	105	80% 17%
78	q2	105	76% 22%
79	Q3	91	81% 19%
79	q3	91	82% 18%
80	e0	62	74% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
81	m2	160	94% 6%
82	p0	311	38% 8% 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 411276 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 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	110	GLU	-	expression tag	UNP P87262
O4	111	ALA	-	expression tag	UNP P87262
O4	112	ALA	-	expression tag	UNP P87262

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O4	113	LYS	-	expression tag	UNP P87262
O4	114	SER	-	expression tag	UNP P87262
O4	115	GLU	-	expression tag	UNP P87262
O4	116	LYS	-	expression tag	UNP P87262
O4	117	LYS	-	expression tag	UNP P87262
O4	118	ALA	-	expression tag	UNP P87262
O4	119	LYS	-	expression tag	UNP P87262
O4	120	LYS	-	expression tag	UNP P87262
o4	110	GLU	-	expression tag	UNP P87262
o4	111	ALA	-	expression tag	UNP P87262
o4	112	ALA	-	expression tag	UNP P87262
o4	113	LYS	-	expression tag	UNP P87262
o4	114	SER	-	expression tag	UNP P87262
o4	115	GLU	-	expression tag	UNP P87262
o4	116	LYS	-	expression tag	UNP P87262
o4	117	LYS	-	expression tag	UNP P87262
o4	118	ALA	-	expression tag	UNP P87262
o4	119	LYS	-	expression tag	UNP P87262
o4	120	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
			Total	C	N	O	S			
71	o5	119	965	612	185	167	1	0	0	0

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 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 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 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 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	121	121	121	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	S2	2	2	2	0	0
85	S4	1	1	1	0	0
85	S6	1	1	1	0	0
85	S8	1	1	1	0	0
85	D0	1	1	1	0	0
85	D3	1	1	1	0	0
85	1	471	471	471	0	0
85	3	13	13	13	0	0
85	4	23	23	23	0	0
85	L2	2	2	2	0	0
85	L3	3	3	3	0	0
85	L4	2	2	2	0	0
85	L5	1	1	1	0	0
85	L7	3	3	3	0	0
85	L8	1	1	1	0	0
85	M0	3	3	3	0	0
85	M1	2	2	2	0	0
85	M3	3	3	3	0	0
85	M5	1	1	1	0	0
85	M6	1	1	1	0	0
85	M7	4	4	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	M9	2	2	2	0	0
85	N0	1	1	1	0	0
85	N3	3	3	3	0	0
85	N5	1	1	1	0	0
85	N6	1	1	1	0	0
85	N8	3	3	3	0	0
85	O3	1	1	1	0	0
85	O4	1	1	1	0	0
85	O7	2	2	2	0	0
85	Q2	1	1	1	0	0
85	6	145	145	145	0	0
85	s1	1	1	1	0	0
85	s2	1	1	1	0	0
85	s4	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	c9	1	1	1	0	0
85	d3	2	2	2	0	0
85	d6	1	1	1	0	0

Continued on next page...

Continued from previous page...

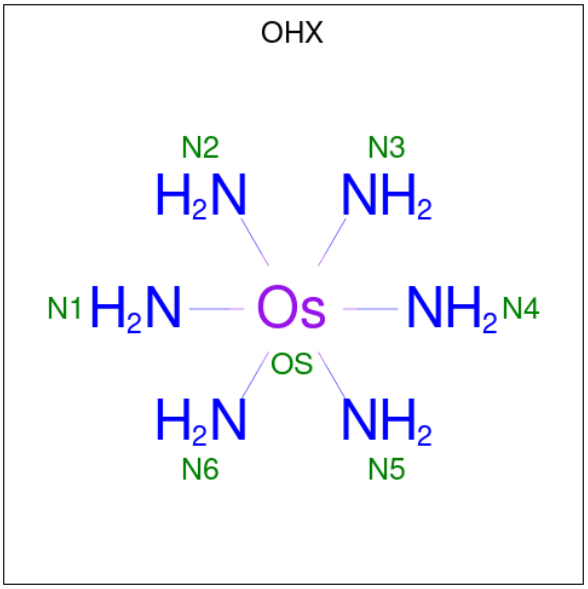
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
85	sM	2	2	2	0	0
85	5	497	497	497	0	0
85	7	16	16	16	0	0
85	8	15	15	15	0	0
85	l2	2	2	2	0	0
85	l3	3	3	3	0	0
85	l4	1	1	1	0	0
85	l5	2	2	2	0	0
85	l7	3	3	3	0	0
85	l8	1	1	1	0	0
85	l9	1	1	1	0	0
85	m1	1	1	1	0	0
85	m4	1	1	1	0	0
85	m5	3	3	3	0	0
85	m6	2	2	2	0	0
85	m7	5	5	5	0	0
85	n0	1	1	1	0	0
85	n3	2	2	2	0	0
85	n6	1	1	1	0	0
85	n8	5	5	5	0	0
85	o1	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	o3	2	Total Mg 2 2	0	0
85	o4	1	Total Mg 1 1	0	0
85	o7	1	Total Mg 1 1	0	0
85	q0	1	Total Mg 1 1	0	0
85	q1	1	Total Mg 1 1	0	0
85	q3	2	Total Mg 2 2	0	0

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



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

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
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	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
			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
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
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
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	1	7	6	1	0	0
86	3	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

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
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	1	7	6	1	0	0
			Total	N	Os		
86	4	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	L3	1	7	6	1	0	0
			Total	N	Os		
86	L4	1	7	6	1	0	0
			Total	N	Os		
86	M0	1	7	6	1	0	0
			Total	N	Os		
86	M5	1	7	6	1	0	0
			Total	N	Os		
86	M7	1	7	6	1	0	0
			Total	N	Os		
86	M7	1	7	6	1	0	0
			Total	N	Os		
86	M9	1	7	6	1	0	0
			Total	N	Os		
86	N1	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	N9	1	7	6	1	0	0
			Total	N	Os		
86	O1	1	7	6	1	0	0
			Total	N	Os		
86	O2	1	7	6	1	0	0
			Total	N	Os		
86	O3	1	7	6	1	0	0
			Total	N	Os		
86	O7	1	7	6	1	0	0
			Total	N	Os		
86	O7	1	7	6	1	0	0
			Total	N	Os		
86	Q2	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	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	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	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	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
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

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
			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
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	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
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	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
			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	l3	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	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	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	o2	1	7	6	1	0	0
86	o3	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 ZINC ION (three-letter code: ZN) (formula: Zn).

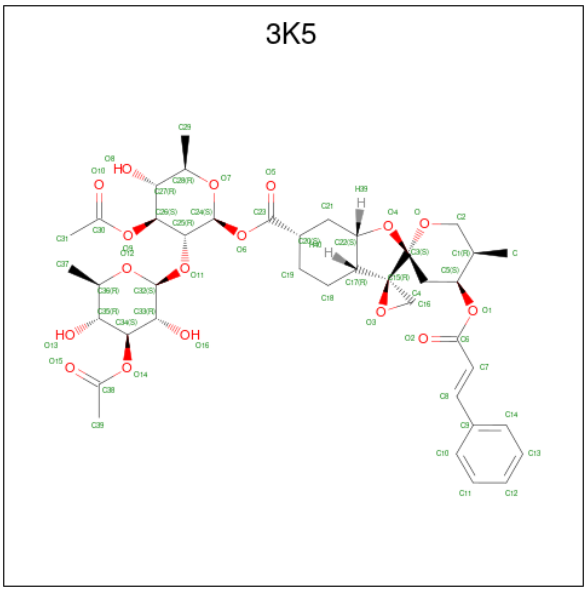
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
87	D6	1	1	1	0	0
87	D7	1	1	1	0	0
87	D9	1	1	1	0	0
87	E1	1	1	1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 88 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-{[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahydrodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose (three-letter code: 3K5) (formula: $C_{40}H_{52}O_{17}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
88	1	1	57	40	17	0	0
			Total	C	O		
88	5	1	57	40	17	0	0

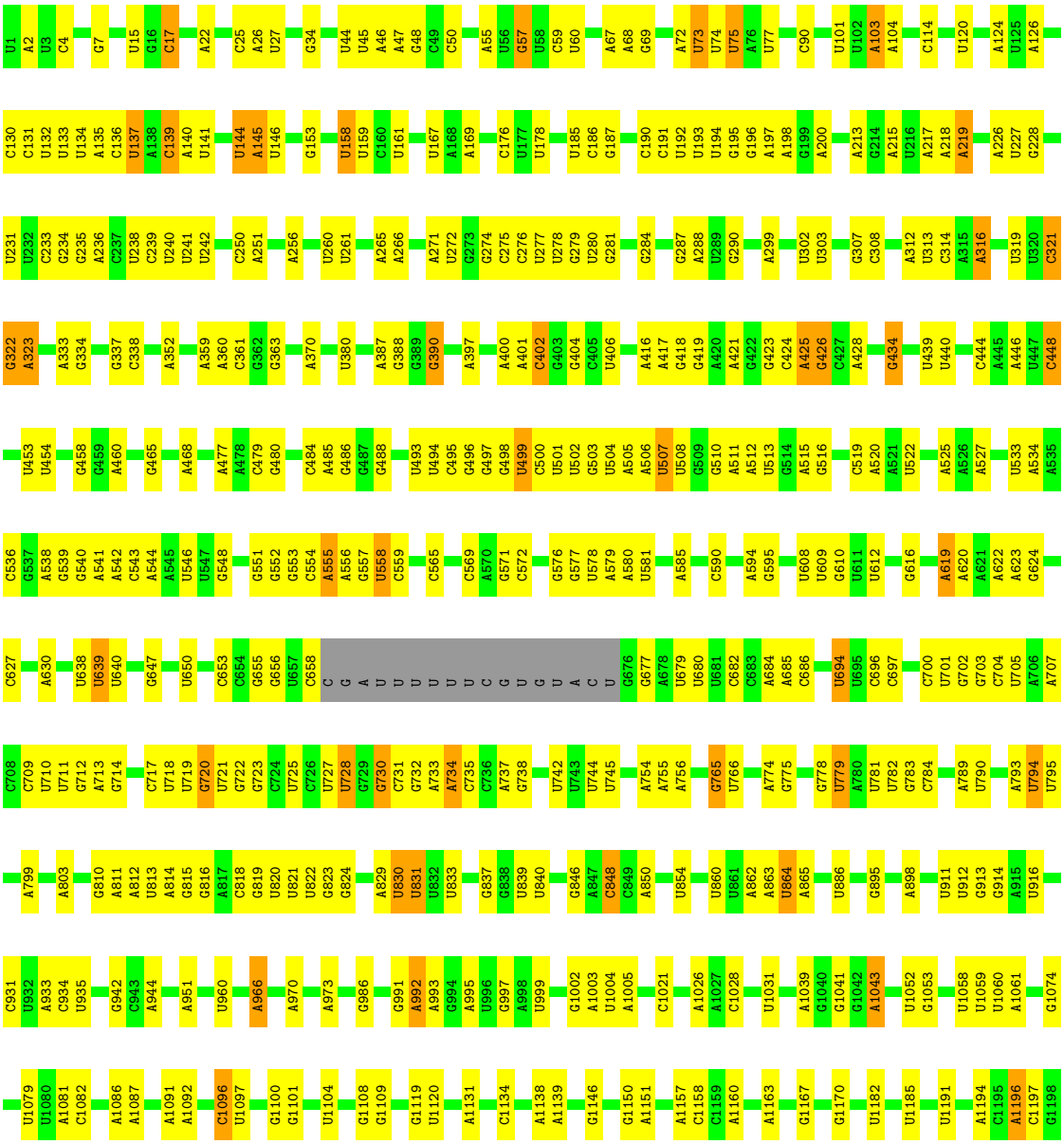
3 Residue-property plots (i)

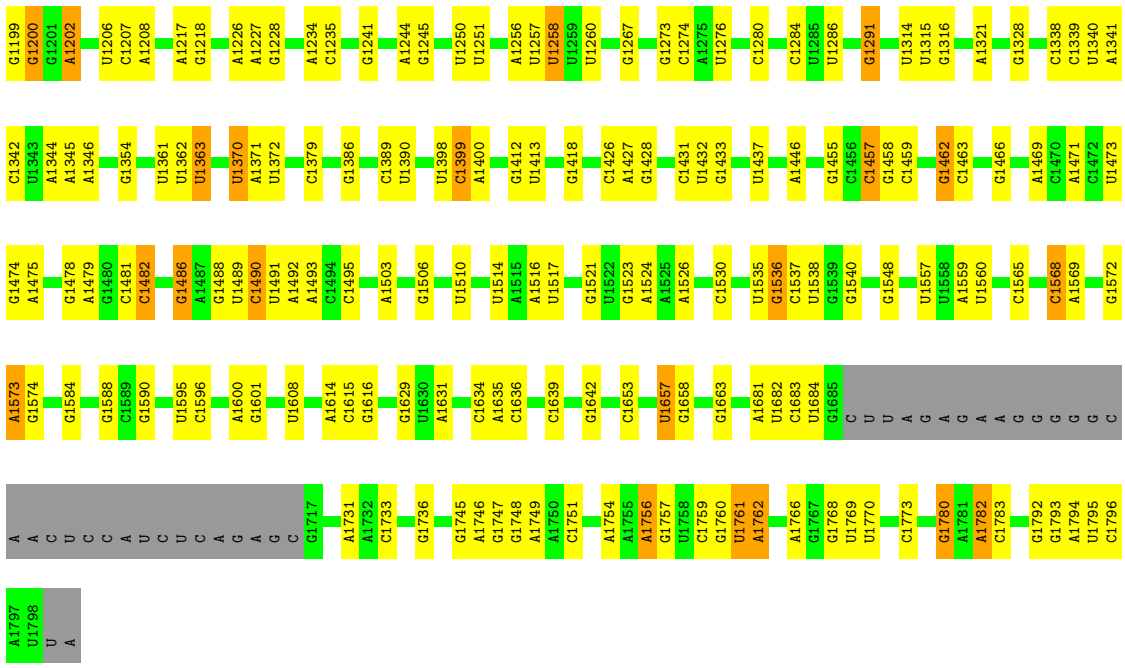
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

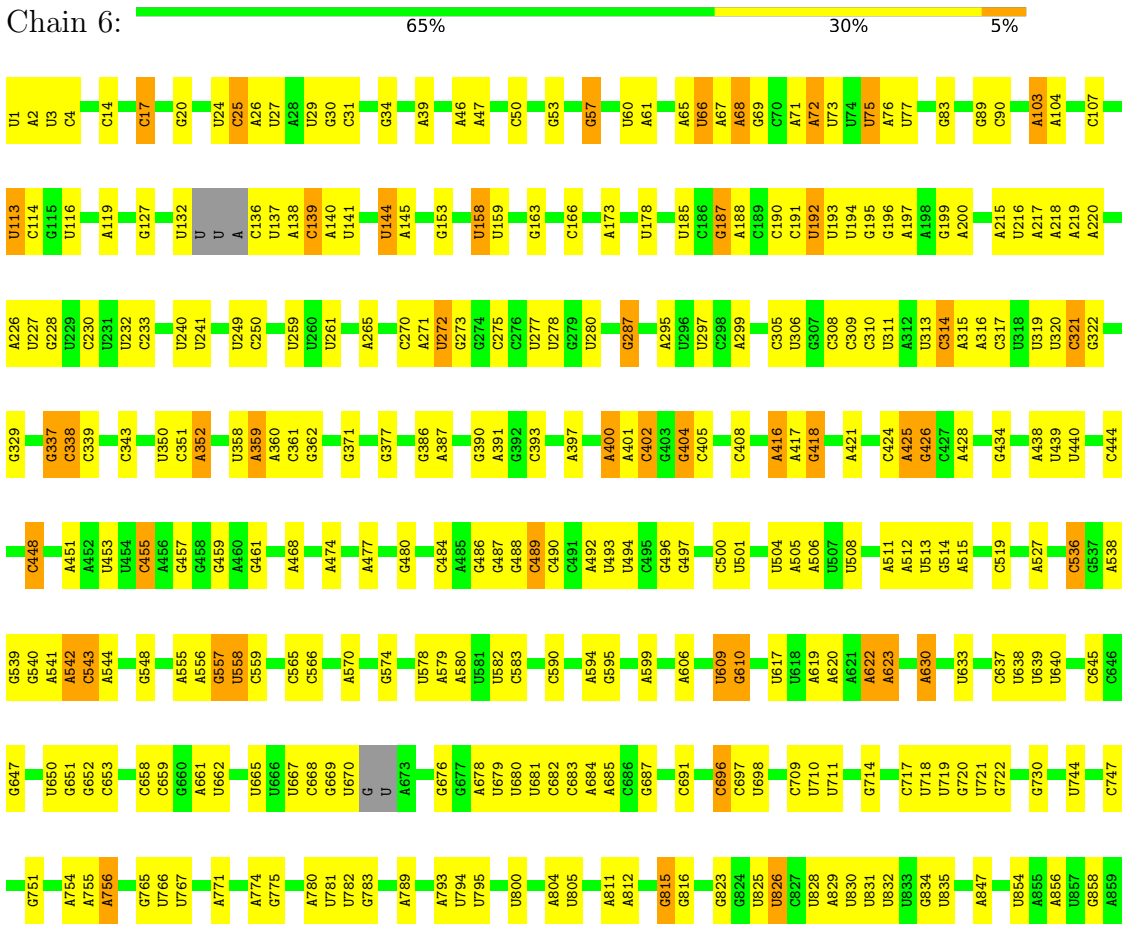
Chain 2: 64% 30%

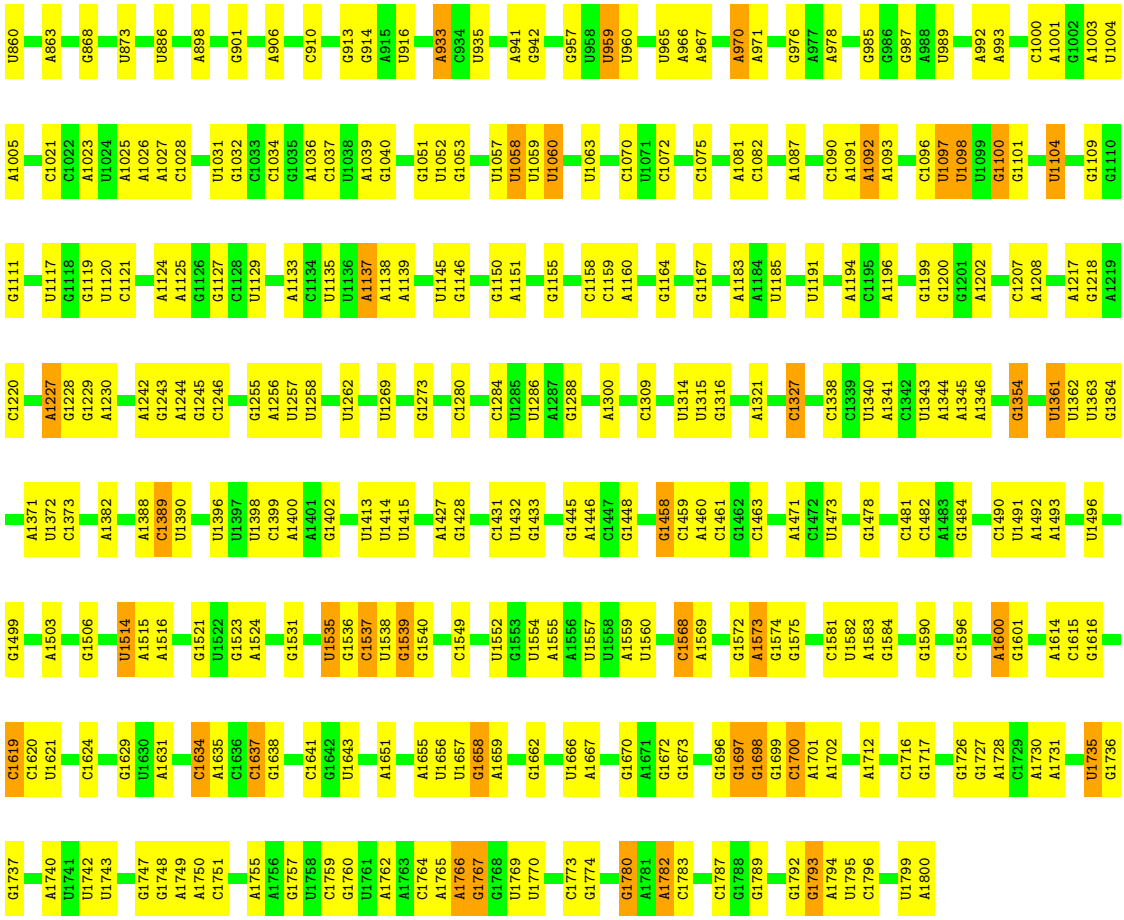




- Molecule 1: 18S ribosomal RNA

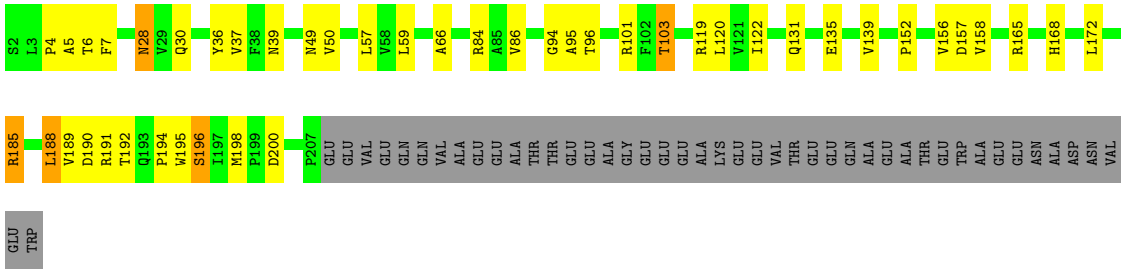
Chain 6:





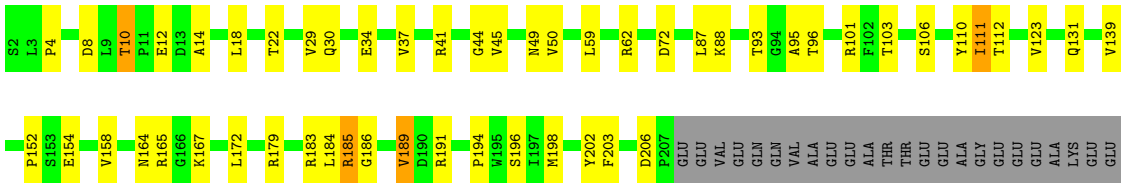
- Molecule 2: 40S ribosomal protein S0-A

Chain S0:



- Molecule 2: 40S ribosomal protein S0-A

Chain s0:



VAL THR GLU GLU GLN ALA GLU ALA THR GLU TRP ALA GLU GLU ASN ALA ASP ASN VAL GLU TRP

- Molecule 3: 40S ribosomal protein S1-A

Chain S1:

ALA VAL GLY LYS ASN LYS ARG LEU SER LYS GLY LYS LYS GLY GLN LYS LYS ARG V20 V21 T25 W29 F30 P35 N42 T46 L47 V48 N49 K50 S51 L54 K55 S58 D59 A60 L61 K62 G63 R64 V65 L70 E77 D78 F81 R82 K85 D89

G93 L97 D104 F105 D108 R111 W117 V125 T126 D131 D132 I137 R144 K145 Q146 A147 N148 S154 S158 S169 V176 Q177 G178 S179 T180 L181 A182 I193 T201 K202 D203 I204 F205 P206 N209 I210 R213 K214 L217 L218 K219

Q220 P221 K222 F223 D224 V225 G226 G233 GLU GLY SER GLY GLU GLU LYS GLY LYS LYS VAL THR GLY PHE LYS ASP GLU VAL LEU GLU THR VAL

- Molecule 3: 40S ribosomal protein S1-A

Chain s1:

ALA VAL GLY LYS ASN LYS ARG LEU SER LYS GLY LYS LYS GLY GLN LYS LYS ARG V20 V21 D22 T25 T37 L47 D59 K62 L70 L73 Q74 D78 F81 R82 K83 D89 E90 G93 K94 L97 F105 D108 V114 L120 T129

S130 D131 I137 Q146 R152 S159 S169 T173 Q177 L181 A182 Q183 L184 I193 N194 K195 E196 I197 K202 P206 L207 Q208 N209 V212 R213 K214 L218 K219 K222 F223 L228 L231 H232 G235 SER GLY GLU GLU LYS GLY LYS LYS VAL

THR GLY PHE LYS ASP GLU VAL LEU GLU THR VAL

- Molecule 4: 40S ribosomal protein S2

Chain S2:

SER ALA PRO GLU ALA GLN GLN GLN LYS ARG GLY GLY PHE GLY GLY ARG ASN ARG GLY ARG PRO ASN ARG ARG GLY PRO ARG ASN THR GLU GLU LYS G34 W35 V36 L41 I53 E54 I69 D70 L76 Q77 I83 Q87 K88 Q89 T90 R91 Q94 R95 T96 R97

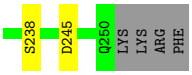
S107 V111 G112 L113 T117 A118 K119 I130 L134 I137 P138 I139 R140 R141 G145 T146 N147 L148 G149 Q150 S153 L154 T166 P182 L187 N201 L207 E208 Y222 L225 T226 L235 P236 D245 E246 Q250 LYS LYS ARG PHE

- Molecule 4: 40S ribosomal protein S2

Chain s2:

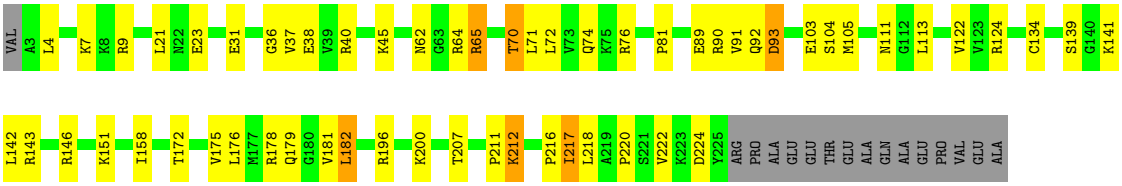
SER ALA PRO GLU ALA GLN GLN GLN LYS ARG GLY GLY PHE GLY GLY ARG ASN ARG GLY ARG PRO ASN ARG ARG GLY PRO ARG ASN THR GLU GLU LYS G34 L41 K46 T51 T52 I53 L58 H59 S60 L61 I69 L73 Q77 D78 E79 V80 M81 N82 I83 K84 P85

V86 Q87 K88 Q89 T90 R91 A92 G93 Q94 R95 T96 D106 S107 V111 G112 L113 T117 A118 K119 E120 V121 R141 T146 N147 L148 G149 Q150 T159 G163 S164 V165 T166 I170 V179 K185 K186 Q199 T206 L207 Y222 L225 L229 P234 L235



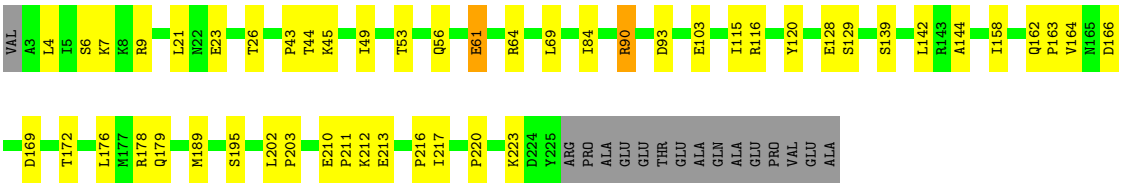
- Molecule 5: 40S ribosomal protein S3

Chain S3:



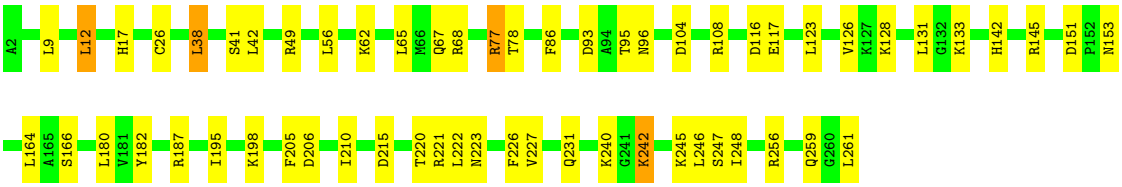
- Molecule 5: 40S ribosomal protein S3

Chain s3:



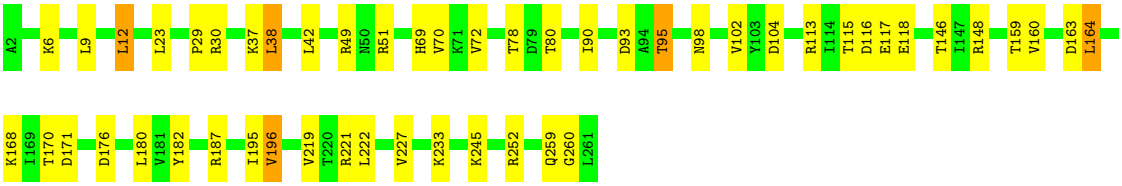
- Molecule 6: 40S ribosomal protein S4-A

Chain S4:



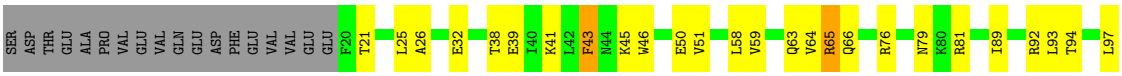
- Molecule 6: 40S ribosomal protein S4-A

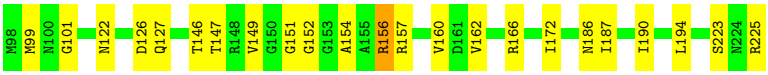
Chain s4:



- Molecule 7: 40S ribosomal protein S5

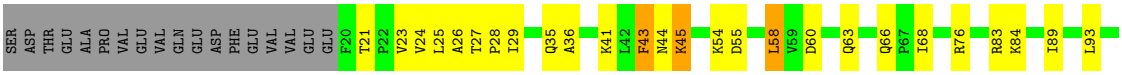
Chain S5:

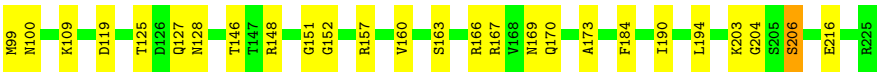




• Molecule 7: 40S ribosomal protein S5

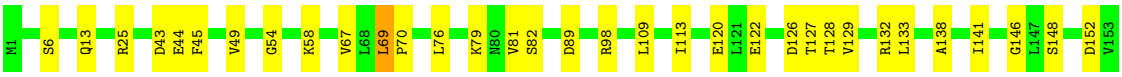
Chain s5:





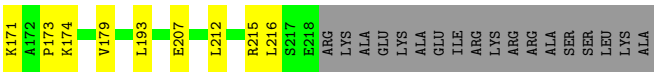
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



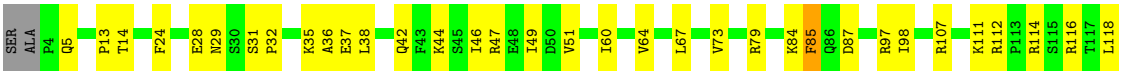
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



• Molecule 9: 40S ribosomal protein S7-A

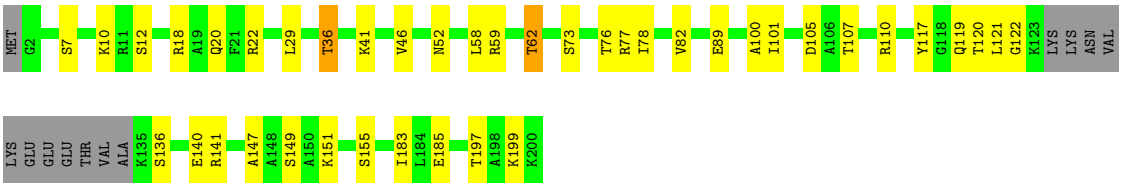
Chain s7:

• Molecule 10: 40S ribosomal protein S8-A

Chain S8:

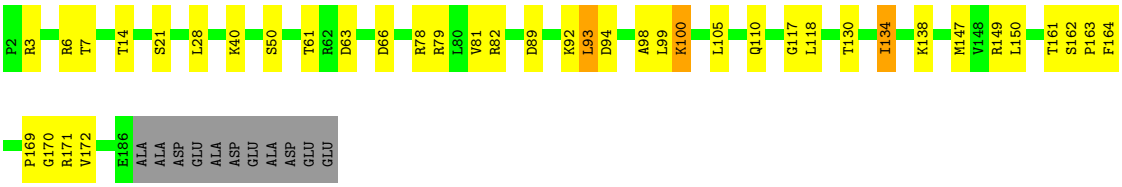
• Molecule 10: 40S ribosomal protein S8-A

Chain s8:



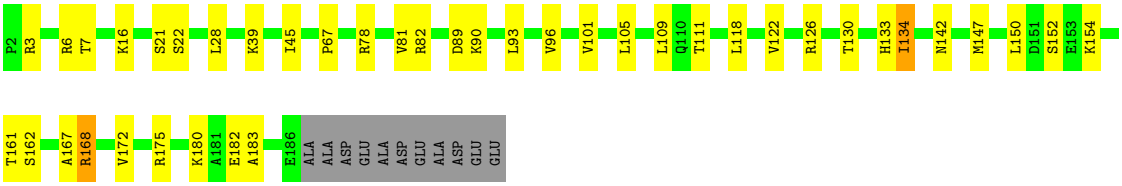
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



• Molecule 11: 40S ribosomal protein S9-A

Chain s9:

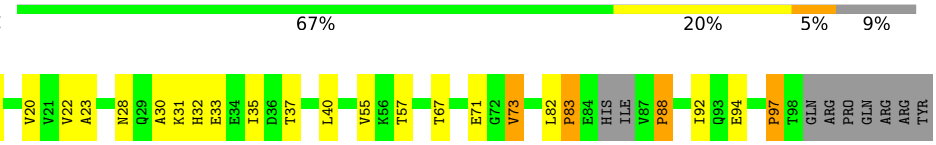


• Molecule 12: 40S ribosomal protein S10-A

Chain C0:

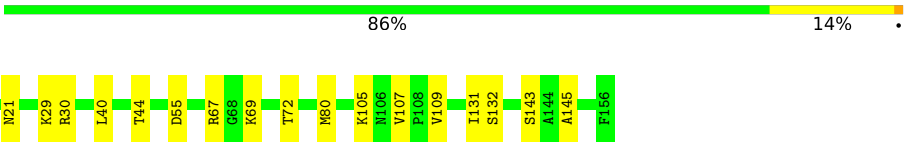
- Molecule 12: 40S ribosomal protein S10-A

Chain c0:



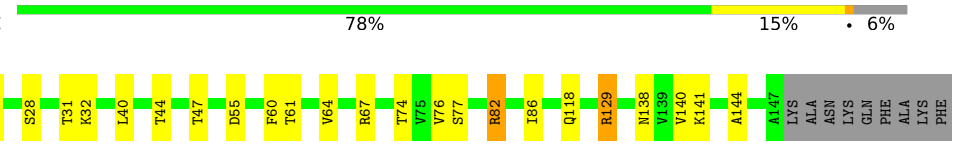
- Molecule 13: 40S ribosomal protein S11-A

Chain C1:



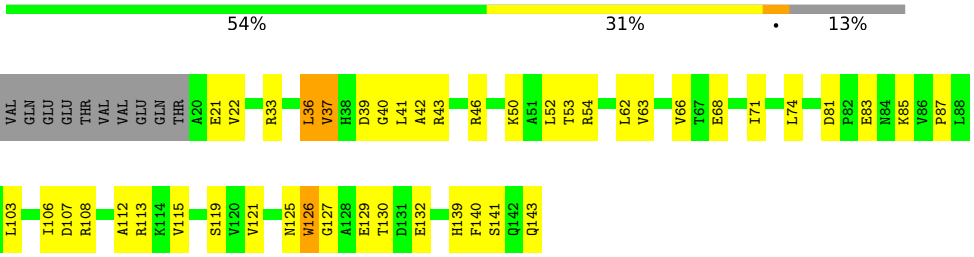
- Molecule 13: 40S ribosomal protein S11-A

Chain c1:



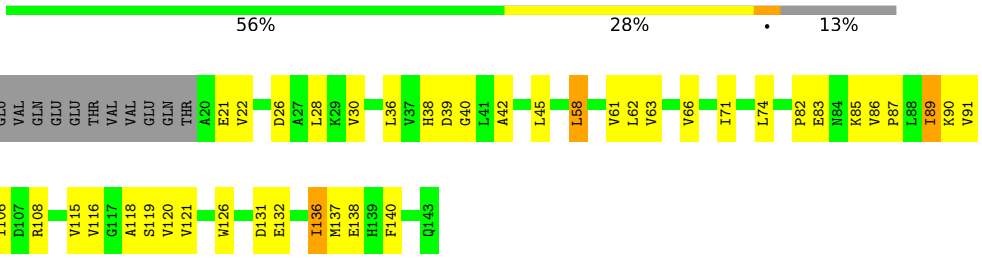
- Molecule 14: 40S ribosomal protein S12

Chain C2:



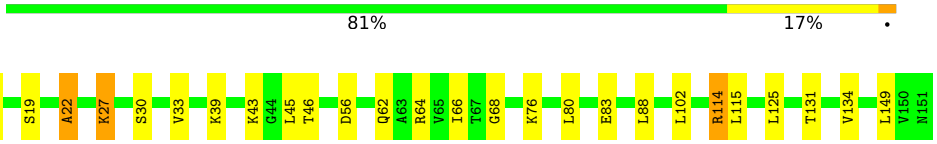
- Molecule 14: 40S ribosomal protein S12

Chain c2:



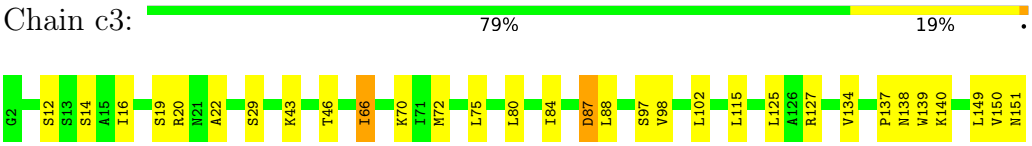
- Molecule 15: 40S ribosomal protein S13

Chain C3:



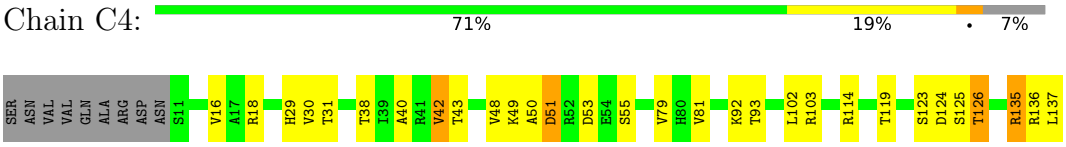
- Molecule 15: 40S ribosomal protein S13

Chain c3:



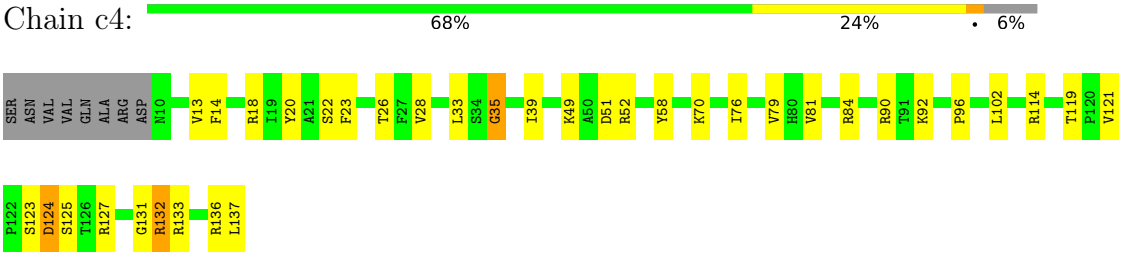
- Molecule 16: 40S ribosomal protein S14-A

Chain C4:



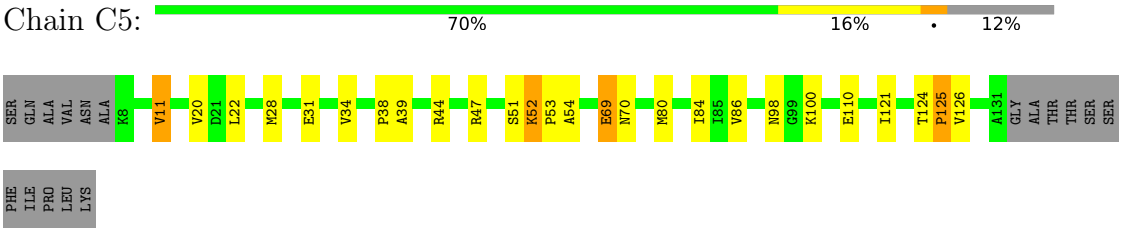
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:



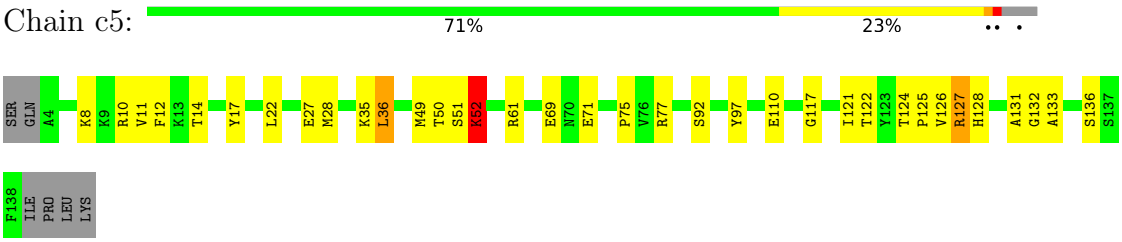
- Molecule 17: 40S ribosomal protein S15

Chain C5:



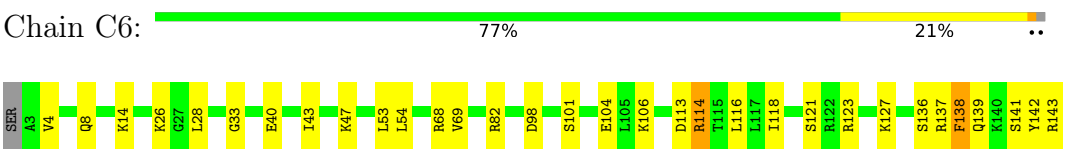
- Molecule 17: 40S ribosomal protein S15

Chain c5:



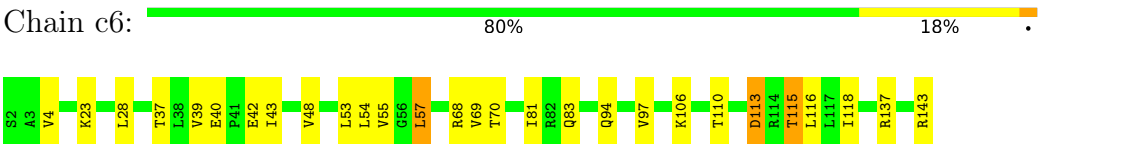
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



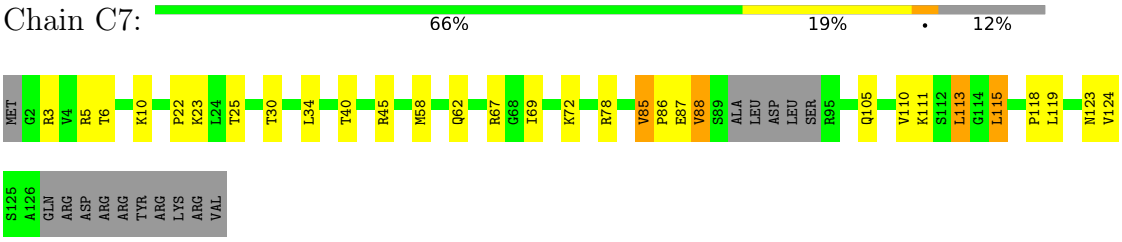
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:



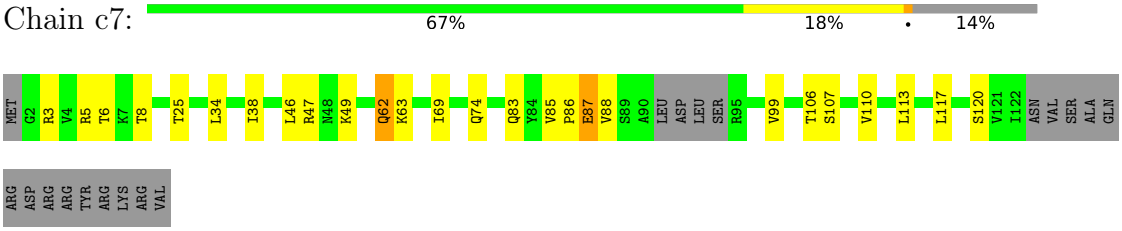
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:



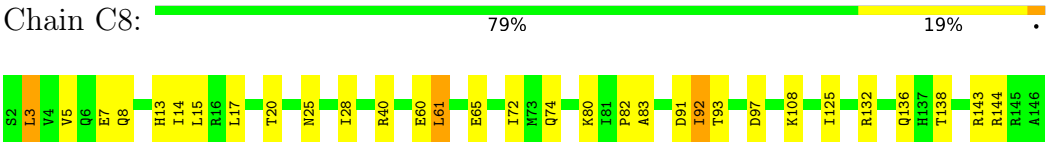
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:



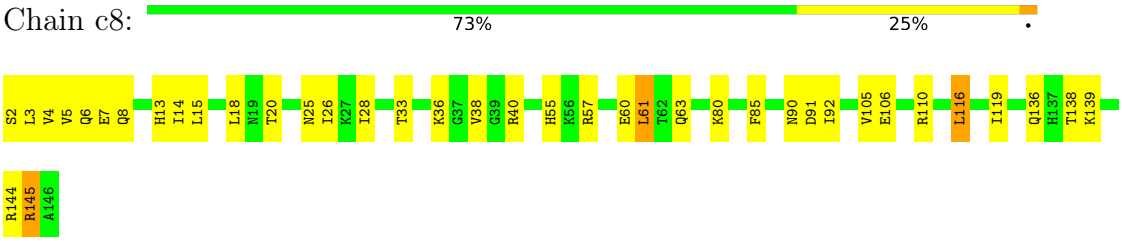
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:



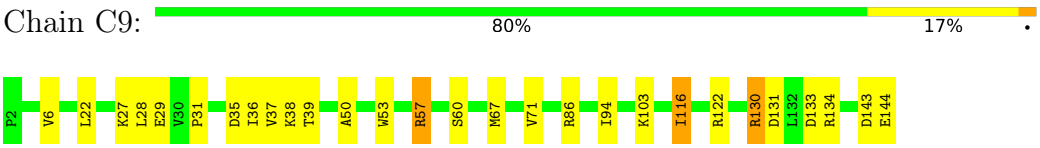
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



- Molecule 21: 40S ribosomal protein S19-A

Chain C9:

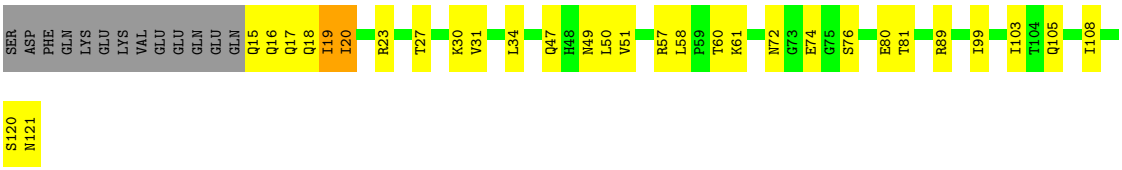


- Molecule 21: 40S ribosomal protein S19-A

Chain c9:

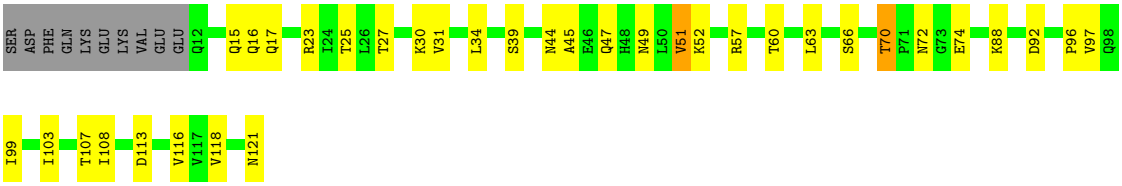
• Molecule 22: 40S ribosomal protein S20

Chain D0:



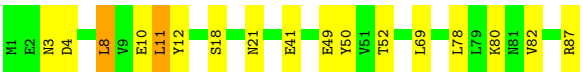
• Molecule 22: 40S ribosomal protein S20

Chain d0:



• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



• Molecule 23: 40S ribosomal protein S21-A

Chain d1:

• Molecule 24: 40S ribosomal protein S22-A

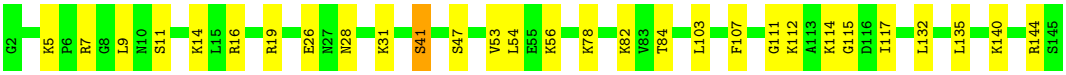
Chain D2:

• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

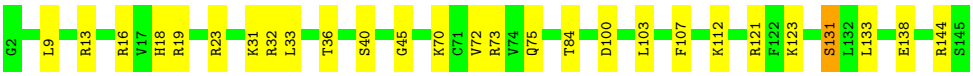
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



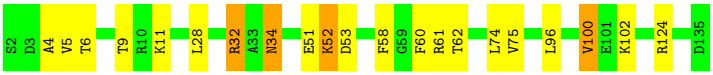
• Molecule 25: 40S ribosomal protein S23-A

Chain d3:



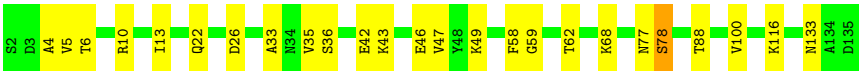
• Molecule 26: 40S ribosomal protein S24-A

Chain D4:



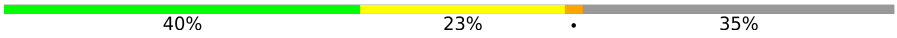
• Molecule 26: 40S ribosomal protein S24-A

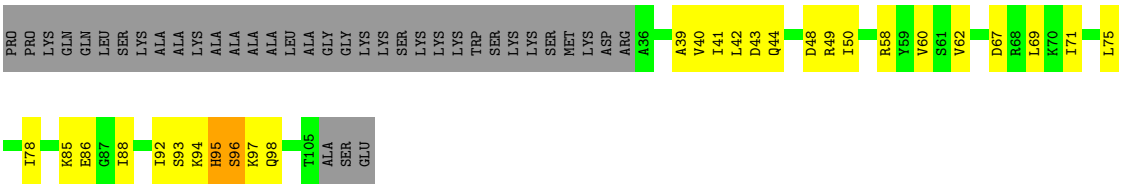
Chain d4:



• Molecule 27: 40S ribosomal protein S25-A

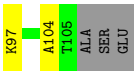
Chain D5:





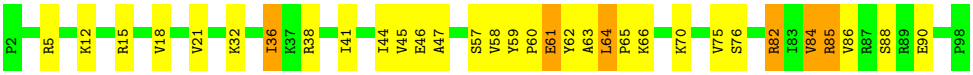
• Molecule 27: 40S ribosomal protein S25-A

Chain d5:



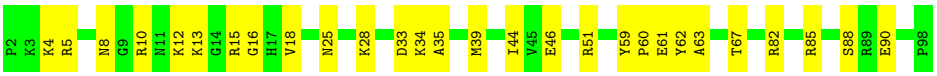
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



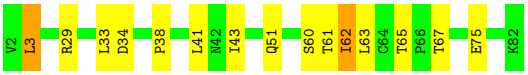
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



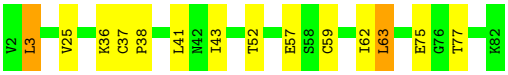
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



• Molecule 29: 40S ribosomal protein S27-A

Chain d7:

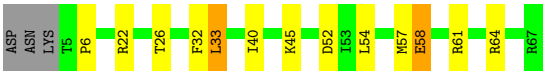


• Molecule 30: 40S ribosomal protein S28-A

Chain D8:

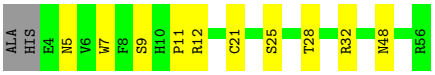
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



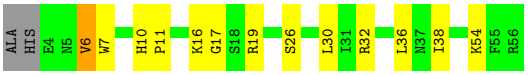
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



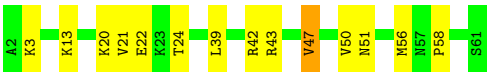
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:



• Molecule 32: 40S ribosomal protein S30-A

Chain E0:

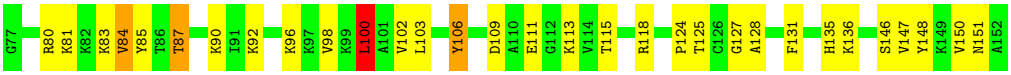


• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:

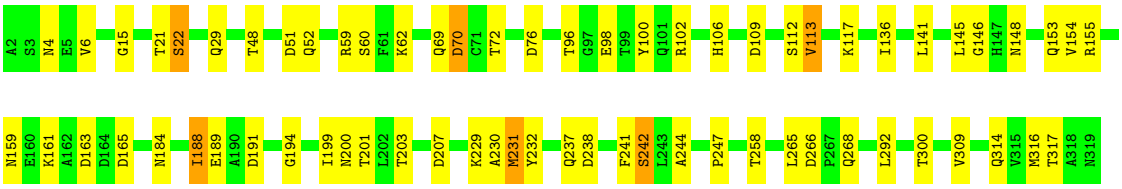
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



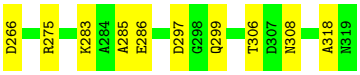
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



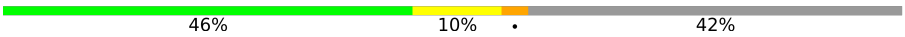
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

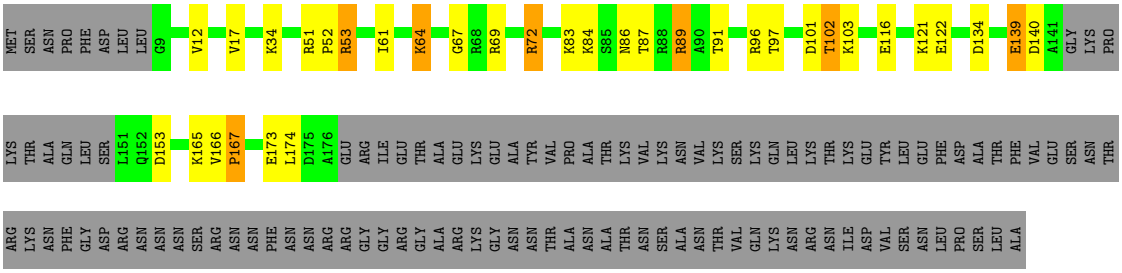
Chain sR:



• Molecule 35: Suppressor protein STM1

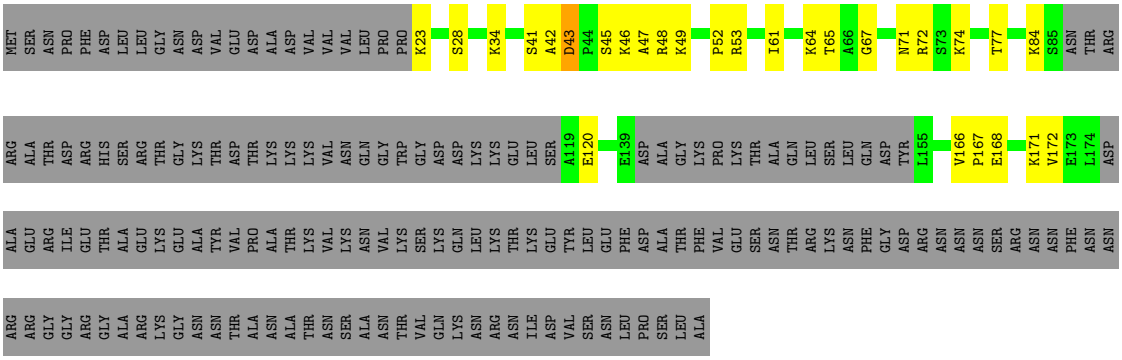
Chain SM:





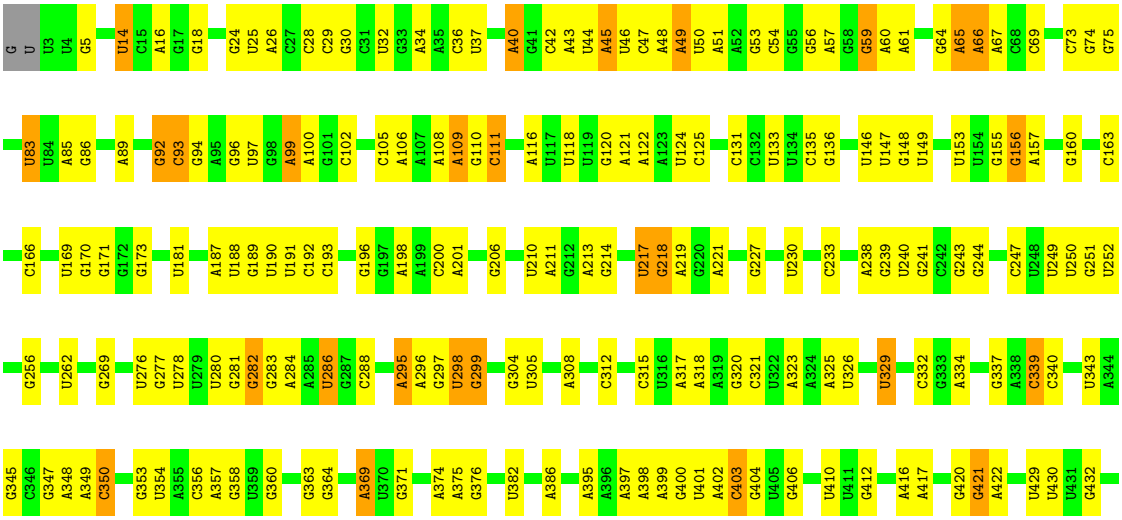
• Molecule 35: Suppressor protein STM1

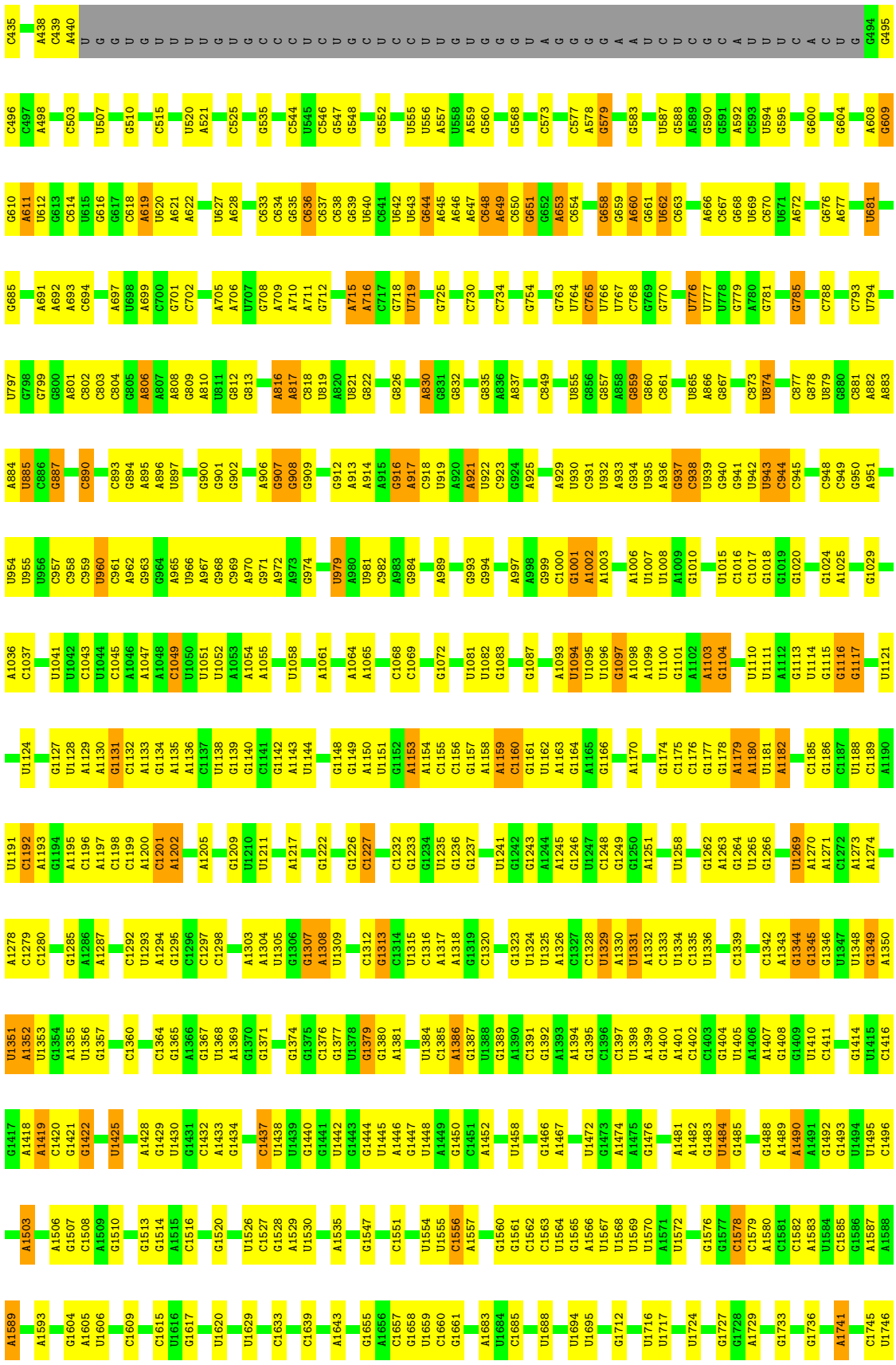
Chain sM:

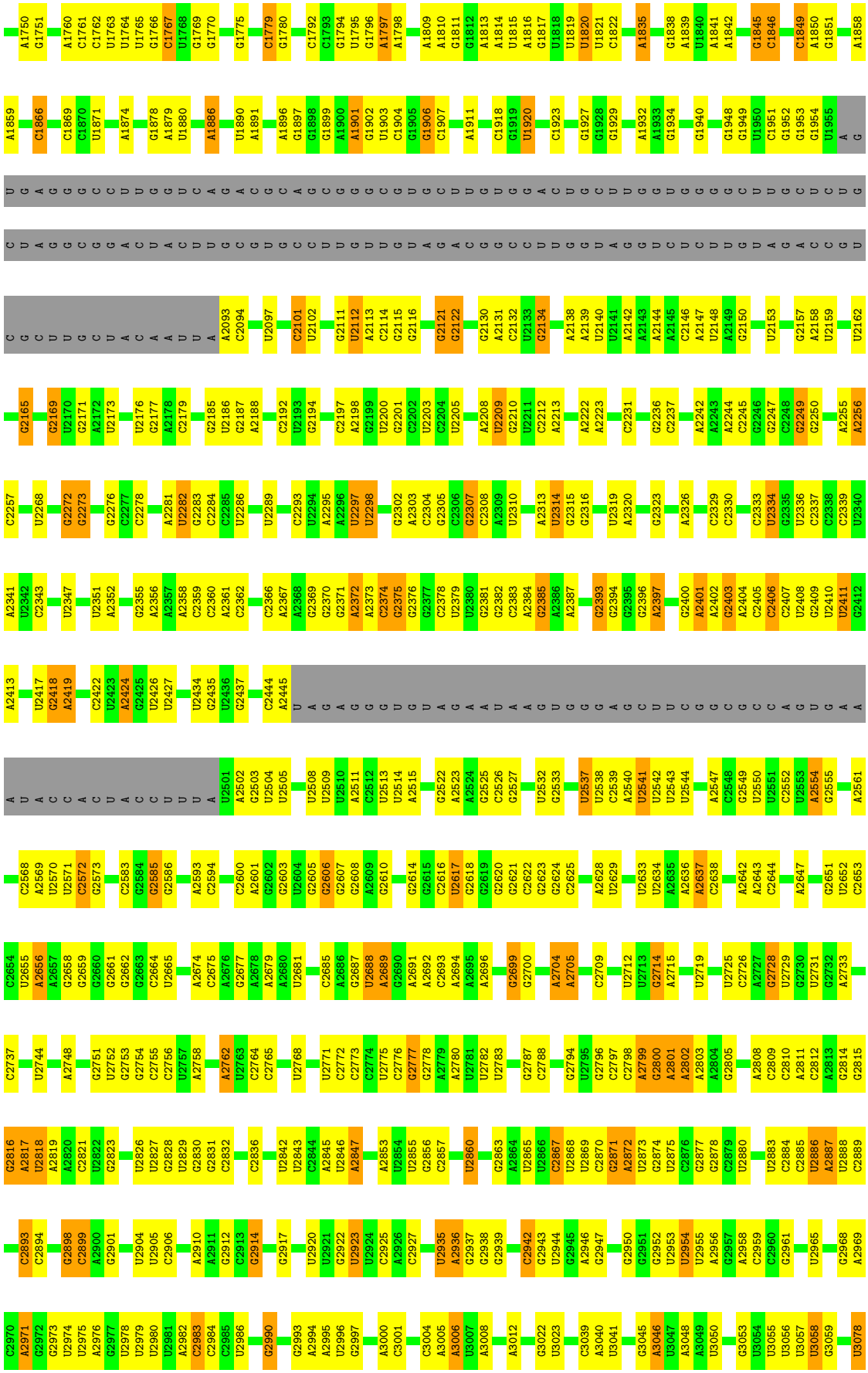


• Molecule 36: 25S ribosomal RNA

Chain 1:

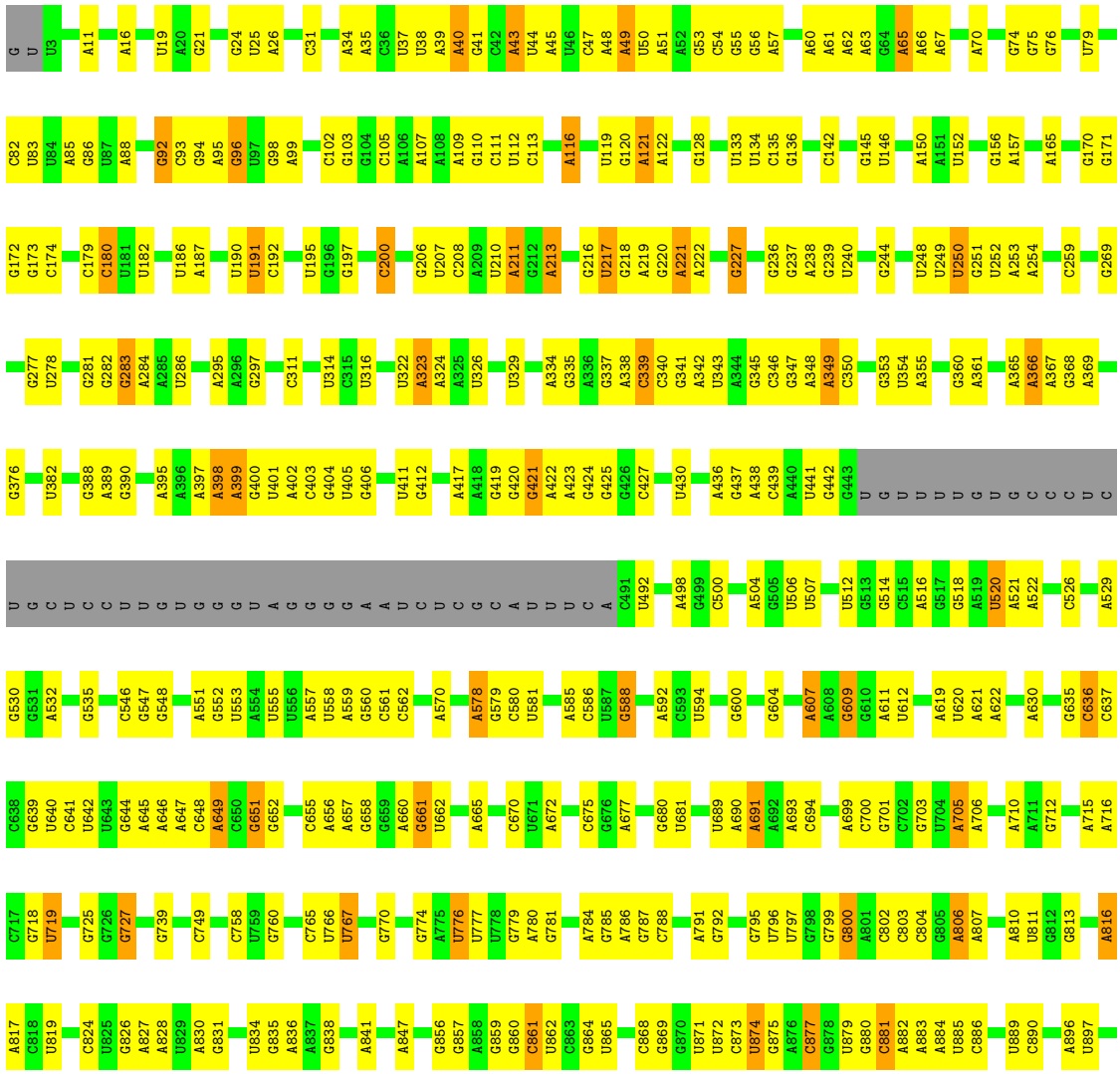


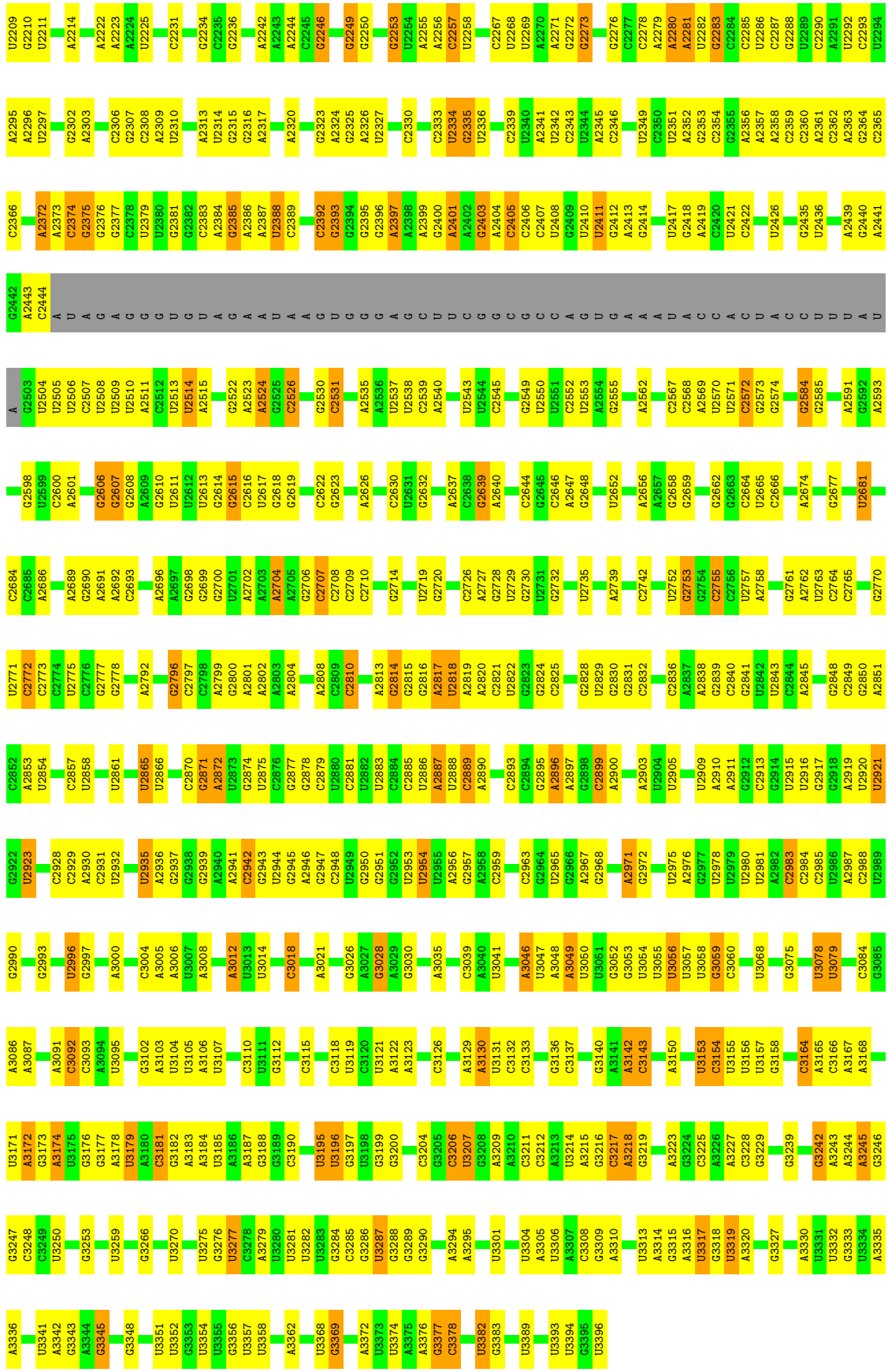

C435 A438 C439 A440 U G G U G U U U U G U G C C C U C U G C U U C C U U G U G G G U A G G G G A A U U C U U C C G C A U U U C A C U G G494 G495
C496 C497 A498 C503 U507 G510 C515 U520 A521 C525 G535 C544 U545 C546 C547 G548 G552 U555 U556 A557 U558 A559 G560 G568 C573 C577 A578 G579 G583 U587 G588 A589 G590 G591 A592 C593 U594 G595 G600 G604 A608 G609
G610 A611 U612 G613 C614 U615 G616 G617 C618 A619 U620 A621 A622 U627 A628 C633 C634 G635 C636 C637 C638 G639 U640 C641 U642 U643 G644 A645 A646 A647 C648 A649 C650 G651 G652 A653 C654 G658 G659 A660 G661 U662 C663 A666 C667 G668 U669 C670 U671 A672 G676 A677 U681
G685 A691 A692 A693 C694 A697 U698 A699 C700 G701 C702 A705 A706 U707 G708 A709 A710 A711 G712 A715 A716 C717 A718 U719 G725 C730 C734 G754 G763 U764 C765 U766 U767 C768 G769 G770 U776 U777 U778 G779 A780 G781 G785 C788 C793 U794
U797 G798 G799 G800 A801 C802 C803 C804 G805 A806 A807 A808 G809 A810 U811 G812 G813 A816 A817 C818 U819 A820 U821 G822 G826 A830 G831 G832 G835 A836 A837 C849 U855 G856 G857 A858 G859 G860 C861 U865 A866 G867 C873 U874 C877 G878 U879 G880 C881 A882 A883
A884 U885 C886 G887 C890 C893 G894 A895 A896 U897 G900 G901 G902 A906 G907 G908 G909 G912 A913 A914 A915 G916 A917 C918 U919 A920 A921 U922 C923 G924 A925 A929 U930 C931 U932 A933 G934 U935 A936 G937 C938 U939 G940 G941 U942 U943 C944 C945 C948 C949 G950 A951
U954 U955 U956 C957 C958 C959 U960 C961 A962 G963 G964 A965 U966 A967 G968 C969 A970 G971 A972 A973 G974 U979 A980 U981 C982 A983 G984 A989 G993 G994 A997 A998 G999 C1000 G1001 A1002 A1003 A1006 U1007 U1008 A1009 G1010 U1015 C1016 C1017 G1018 G1019 G1020 G1024 A1025 G1029
A1036 C1037 U1041 U1042 C1043 U1044 C1045 A1046 A1047 A1048 C1049 U1050 U1051 U1052 A1053 A1054 A1055 U1058 A1061 A1064 A1065 C1068 C1069 G1072 U1081 U1082 G1083 G1087 A1093 U1094 U1095 U1096 G1097 A1098 A1099 U1100 G1101 A1102 A1103 G1104 U1110 U1111 A1112 G1113 U1114 G1115 G1116 G1117 U1121
U1124 G1127 U1128 A1129 A1130 G1131 C1132 A1133 G1134 A1135 A1136 C1137 U1138 G1139 G1140 C1141 G1142 A1143 U1144 G1148 G1149 A1150 U1151 C1152 A1153 A1154 C1155 C1156 G1157 A1158 A1159 C1160 G1161 U1162 A1163 G1164 A1165 G1166 A1170 G1174 C1175 C1176 G1177 G1178 A1179 A1180 U1181 A1182 C1185 G1186 C1187 U1188 C1189 A1190
U1191 C1192 A1193 G1194 A1195 C1196 A1197 C1198 C1199 A1200 C1201 A1202 A1205 G1209 U1210 U1211 A1217 G1222 G1226 C1227 C1232 G1233 G1234 U1235 G1236 G1237 U1241 G1242 G1243 A1244 A1245 G1246 U1247 C1248 G1249 G1250 A1251 U1258 G1262 A1263 G1264 U1265 G1266 U1269 A1270 A1271 C1272 A1273 A1274
A1278 C1279 C1280 G1285 A1286 A1287 C1292 U1293 A1294 G1295 C1296 C1297 C1298 A1303 A1304 U1305 G1306 G1307 A1308 U1309 C1312 G1313 C1314 U1315 C1316 A1317 A1318 G1319 C1320 G1323 U1324 U1325 A1326 C1327 C1328 U1329 A1330 U1331 A1332 C1333 U1334 C1335 U1336 C1339 C1342 A1343 G1344 G1345 G1346 U1347 U1348 G1349 A1350
U1351 A1352 U1353 G1354 A1355 U1356 G1357 C1360 C1364 G1365 A1366 G1367 U1368 A1369 G1370 G1371 G1374 G1375 C1376 G1377 U1378 G1379 G1380 A1381 U1384 C1385 A1386 G1387 U1388 G1389 A1390 C1391 G1392 A1393 A1394 G1395 C1396 C1397 U1398 A1399 G1400 A1401 C1402 G1403 G1404 U1405 A1406 A1407 G1408 G1409 U1410 C1411 G1414 U1415 C1416
G1417 A1418 A1419 C1420 G1421 G1422 U1425 A1428 G1429 U1430 G1431 C1432 A1433 G1434 C1437 U1438 U1439 G1440 G1441 U1442 G1443 G1444 U1445 A1446 G1447 U1448 A1449 G1450 C1451 A1452 U1458 G1466 A1467 U1472 G1473 A1474 A1475 G1476 A1481 A1482 G1483 U1484 G1485 G1488 A1489 A1490 A1491 G1492 G1493 U1494 U1495 C1496
A1503 A1506 G1507 C1508 A1509 G1510 G1513 G1514 A1515 C1516 G1520 U1526 C1527 G1528 A1529 U1530 A1535 G1547 C1551 U1554 U1555 C1556 A1557 G1560 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 G1576 G1577 C1578 C1579 A1580 C1581 C1582 A1583 U1584 C1585 G1586 A1587 A1588
A1589 A1593 G1604 A1605 U1606 C1609 C1615 U1616 G1617 U1620 U1629 C1633 C1639 A1643 G1655 A1656 C1657 G1658 U1659 C1660 G1661 A1683 U1684 C1685 U1688 U1694 U1695 G1712 U1716 U1717 U1724 G1727 G1728 A1729 G1733 G1736 A1741 C1745 U1746



- Molecule 36: 25S ribosomal RNA

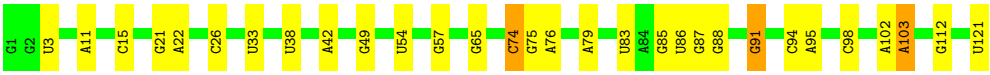
Chain 5:




U2209 G2210 U2211 A2214 A2222 A2223 A2224 U2225 C2231 G2234 C2235 G2236 A2242 A2243 A2244 C2245 G2246 G2249 G2250 G2253 U2254 A2255 A2256 C2257 U2258 C2267 U2268 U2269 A2270 A2271 G2272 G2273 G2276 C2277 C2278 A2279 A2280 A2281 U2282 G2283 C2284 C2285 U2286 C2287 G2288 U2289 C2290 A2291 U2292 C2293 U2294
A2295 A2296 U2297 G2302 A2303 C2306 G2307 C2308 A2309 U2310 A2313 U2314 G2315 G2316 A2317 A2320 G2323 A2324 G2325 A2326 U2327 C2330 C2333 U2334 G2335 U2336 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 A2372 A2373 C2374 G2375 G2376 G2377 C2378 U2379 U2380 G2381 G2382 C2383 A2384 G2385 A2386 A2387 U2388 C2389 C2392 G2393 G2394 G2395 G2396 A2397 A2398 A2399 G2400 A2401 A2402 G2403 A2404 C2405 C2406 C2407 U2408 G2409 U2410 U2411 G2412 A2413 G2414 U2417 G2418 A2419 C2420 U2421 C2422 U2426 G2435 U2436 A2439 G2440 A2441
G2442 A2443 C2444 A U A G A G G G U G U A G A A G U G G G G A G C U U C G G G C G C C A G U G A A A U U A C C 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 U2544 C2545 G2549 U2550 U2551 C2552 U2553 A2554 G2555 A2562 C2567 C2568 A2569 U2570 U2571 C2572 G2573 G2574 G2584 G2585 A2591 G2592 A2593
G2598 U2599 C2600 A2601 G2606 G2607 G2608 A2609 G2610 U2611 U2612 U2613 G2614 G2615 C2616 U2617 G2618 G2619 C2622 G2623 A2626 C2630 U2631 G2632 A2637 C2638 G2639 A2640 C2644 G2645 C2646 A2647 G2648 U2652 A2656 A2657 G2658 G2659 G2662 G2663 C2664 U2665 C2666 A2674 G2677 U2681
C2684 C2685 A2686 A2689 G2690 A2691 A2692 C2693 A2696 A2697 G2698 G2699 G2700 U2701 A2702 A2703 A2704 A2705 G2706 C2707 C2708 C2709 C2710 G2714 U2719 G2720 C2726 A2727 G2728 U2729 G2730 U2731 G2732 U2735 A2739 C2742 U2752 G2753 G2754 C2755 C2756 U2757 A2758 G2761 A2762 U2763 C2764 C2765 G2770
U2771 C2772 C2773 C2774 U2775 C2776 G2777 G2778 A2792 G2796 C2797 C2798 A2799 G2800 A2801 A2802 A2803 A2804 A2808 C2809 C2810 A2813 G2814 G2815 G2816 A2817 U2818 A2819 A2820 C2821 U2822 G2823 G2824 C2825 G2828 U2829 G2830 G2831 C2832 C2836 A2837 A2838 G2839 C2840 G2841 U2842 U2843 C2844 A2845 G2848 C2849 G2850 A2851
C2852 A2853 U2854 C2857 U2858 U2861 U2865 U2866 C2870 G2871 A2872 U2873 G2874 U2875 C2876 G2877 G2878 C2879 U2880 C2881 U2882 U2883 C2884 C2885 U2886 A2887 U2888 C2889 A2890 C2893 C2894 G2895 A2896 A2897 G2898 C2899 A2900 A2903 U2904 U2905 U2909 A2910 A2911 G2912 C2913 G2914 U2915 U2916 G2917 G2918 A2919 U2920 U2921
G2922 U2923 C2928 C2929 A2930 C2931 U2932 U2935 A2936 G2937 G2938 G2939 A2940 A2941 C2942 G2943 U2944 G2945 A2946 G2947 C2948 U2949 G2950 G2951 G2952 U2953 U2954 U2955 A2956 G2957 A2958 C2959 C2963 G2964 U2965 G2966 A2967 G2968 A2971 G2972 U2975 A2976 G2977 U2978 U2979 U2980 U2981 A2982 C2983 C2984 C2985 U2986 A2987 C2988 U2989
G2990 G2993 U2996 G2997 A3000 C3004 A3005 A3006 U3007 A3008 A3012 U3013 U3014 C3018 A3021 G3026 A3027 G3028 A3029 G3030 A3035 C3039 A3040 U3041 A3046 U3047 A3048 A3049 U3050 U3051 G3052 G3053 U3054 U3055 U3056 U3057 U3058 G3059 C3060 U3068 G3075 U3078 U3079 C3084 G3085
A3086 A3087 A3091 C3092 C3093 A3094 U3095 G3102 A3103 U3104 U3105 A3106 U3107 C3110 U3111 G3112 C3115 C3118 U3119 C3120 U3121 A3122 A3123 C3126 A3129 A3130 U3131 C3132 C3133 G3136 C3137 G3140 A3141 A3142 C3143 A3150 U3153 C3154 U3155 U3156 U3157 G3158 C3164 A3165 C3166 A3167 A3168
U3171 A3172 G3173 A3174 U3175 G3176 G3177 A3178 U3179 A3180 C3181 G3182 A3183 A3184 U3185 A3186 A3187 G3188 G3189 C3190 U3195 U3196 G3197 U3198 G3199 G3200 C3204 G3205 C3206 U3207 G3208 A3209 A3210 C3211 C3212 A3213 U3214 A3215 G3216 C3217 A3218 G3219 A3223 G3224 C3225 A3226 A3227 C3228 G3229 G3239 G3242 A3243 A3244 A3245 G3246
G3247 C3248 C3249 U3250 G3253 U3259 G3266 U3270 U3275 G3276 U3277 C3278 A3279 U3280 U3281 U3282 U3283 G3284 C3285 G3286 U3287 G3288 G3289 G3290 A3294 A3295 U3301 U3304 A3305 U3306 A3307 C3308 G3309 A3310 U3313 A3314 G3315 A3316 U3317 G3318 U3319 A3320 G3327 A3330 U3331 U3332 G3333 U3334 A3335
A3336 U3341 A3342 G3343 A3344 G3345 G3348 U3351 U3352 G3353 U3354 U3355 G3356 U3357 U3358 A3362 U3368 G3369 A3372 U3373 U3374 A3375 A3376 G3377 C3378 U3382 G3383 U3389 U3393 U3394 G3395 U3396

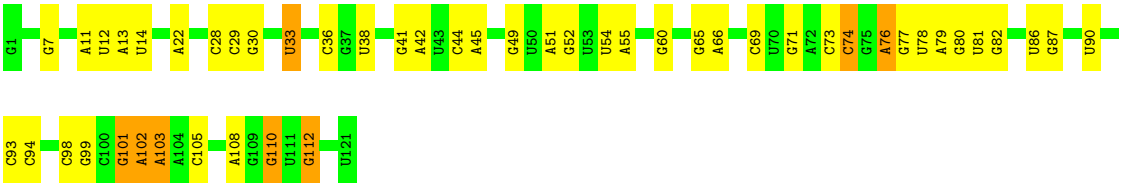
• Molecule 37: 5S ribosomal RNA

Chain 3:



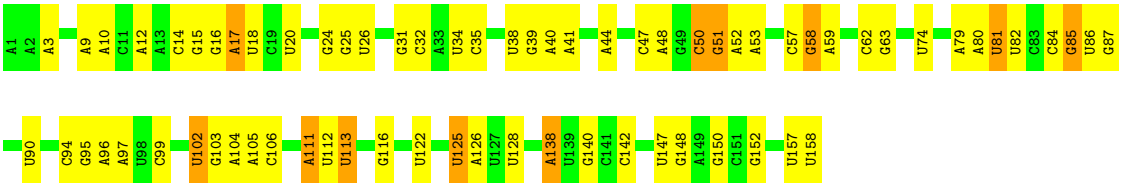
• Molecule 37: 5S ribosomal RNA

Chain 7:



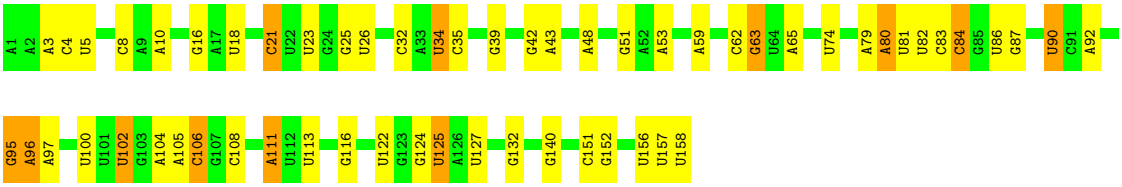
• Molecule 38: 5.8S ribosomal RNA

Chain 4:



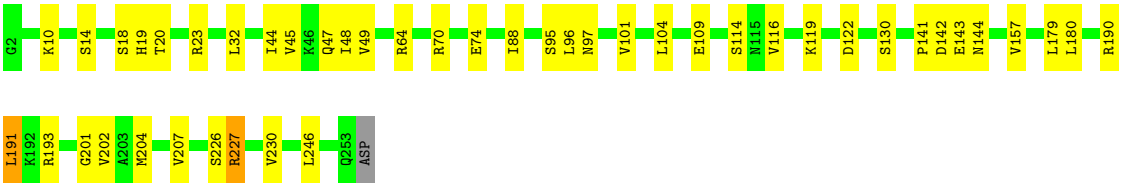
• Molecule 38: 5.8S ribosomal RNA

Chain 8:



• Molecule 39: 60S ribosomal protein L2-A

Chain L2:



• Molecule 39: 60S ribosomal protein L2-A

Chain l2:

G2 G13 S14 I15 R23 Q24 L29 R30 T31 L32 I44 I48 V49 A56 V61 V62 R70 E74 E80 G81 V82 L96 V101 L104 I112 S130 G131 N132 I137 D142 I158 V168 I169 L179 L180 R193 N194 R200

M204 N205 P206 G213 G214 N215 H216 V230 L237 T243 L246 R247 G248 S249 Q250 K251 T252 Q253 ASP

• Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 21%

S2 H3 R4 K5 Y6 E7 L17 P18 R19 K20 R21 S24 I25 K30 P33 R37 T44 L47 T55 I56 R70 T81 V84 V85 V93 T103 D112 E113 V114 K115 R116 S134 Q139 D140 G141 A142 R146 E147 L148 A149 R150 A155

S156 V157 Q165 I166 Q173 N184 G185 G186 S187 I188 V192 R196 T202 V208 T221 V229 R232 T235 K236 K237 L238 K241 R244 I252 V264 A265 R266 R270 S274 I278 R284 K287 G288 D289 T296 T304 I305 T306

P307 M308 V312 I317 V324 K325 R332 T337 S341 N345 T346 S347 R348 L351 E352 E353 V354 S355 K385 D386 L387

• Molecule 40: 60S ribosomal protein L3

Chain l3: 79% 20%

S2 H3 R4 R10 L17 P18 R19 K20 R21 A22 I25 K30 R37 T44 L47 T55 I56 K69 R70 T77 T81 V85 V90 T103 E113 V114 K120 S125 K128 A129 Q139 D140 G141 A142 E145 R146 E147 L148 A149 R150

V157 V160 R167 K168 T169 L183 S187 V192 R196 T202 V205 V208 E213 M214 I215 K222 R232 T235 L238 K248 V249 I252 H256 R266 S274 R275 R284 K287 N293 S297 T301 T304 M308

I328 R332 K333 L338 R339 K340 S341 T346 S347 R348 S363 F370 A378 F379 M380 G381 T382 D386 L387

• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 78% 19%

S2 R3 P4 Q5 A15 L20 P21 L22 T37 T40 S41 R47 E63 I74 F90 M93 C94 G97 R98 M99 K108 S124 A130 V131 A132 S133 R138 I145 P146 E147 L150 V151 V152 L156 V172 L179 L182 K185 K186

L187 R188 A189 G190 K193 Y194 T200 R203 L206 R220 N221 V222 V230 A231 S232 R246 L258 D259 V267 A268 S269 S270 T283 I289 I290 N291 S292 S293 E294 I295 Q296 S297 T306 Q307 K308 H311 V312 L313 P317 L318 K319 N320 V323 L327

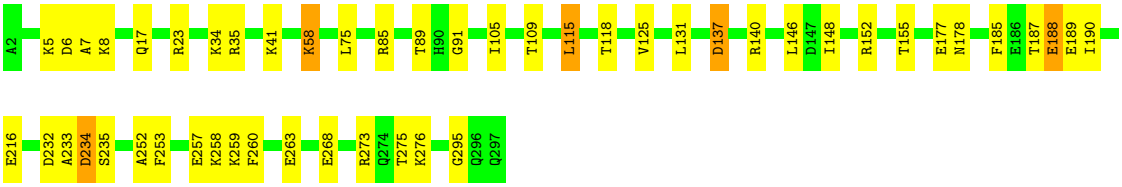
K332 V333 K338 K343 K346 T349 K350 V354 F355 T356 D362

• Molecule 41: 60S ribosomal protein L4-A

Chain l4: 80% 17%

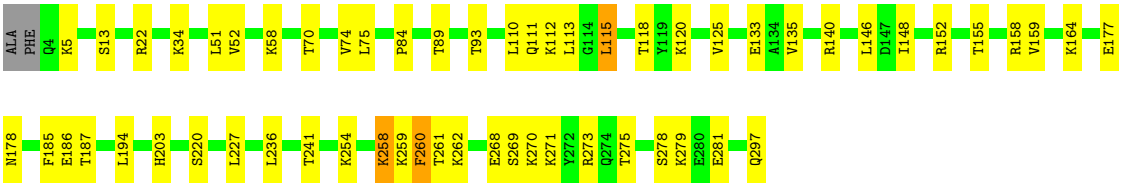
- Molecule 42: 60S ribosomal protein L5

Chain L5:



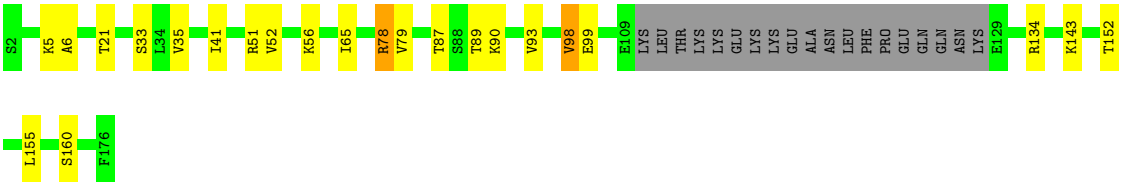
- Molecule 42: 60S ribosomal protein L5

Chain l5:



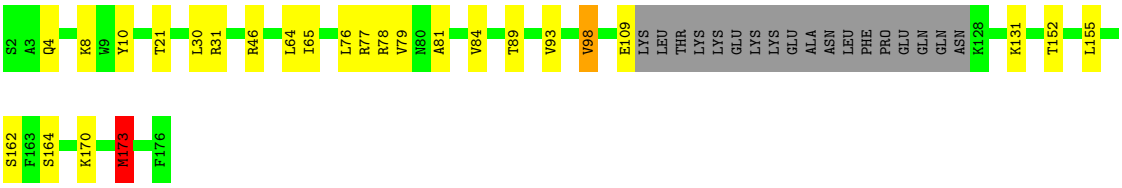
- Molecule 43: 60S ribosomal protein L6-A

Chain L6:



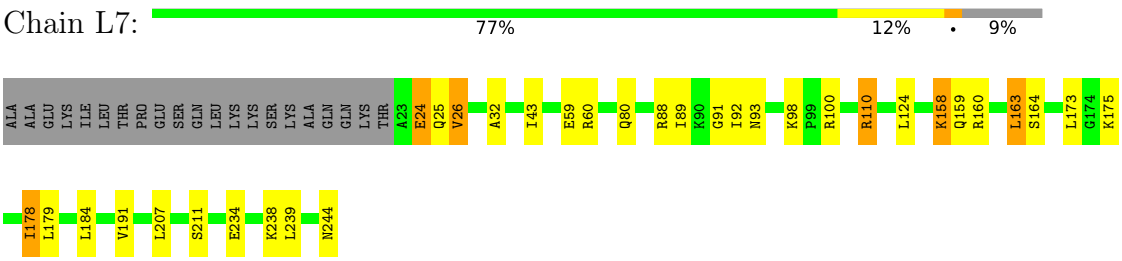
- Molecule 43: 60S ribosomal protein L6-A

Chain l6:



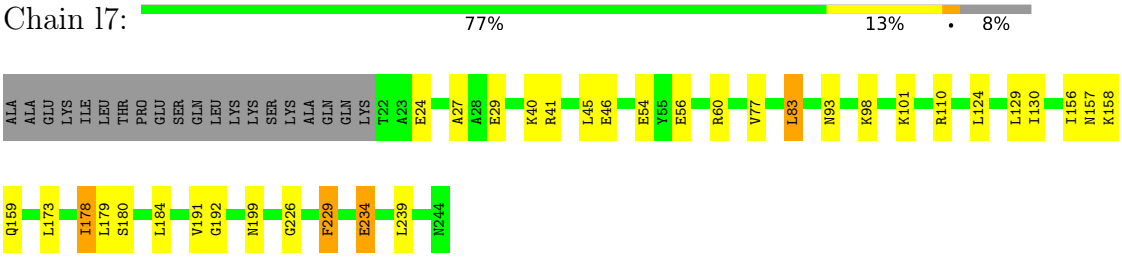
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:



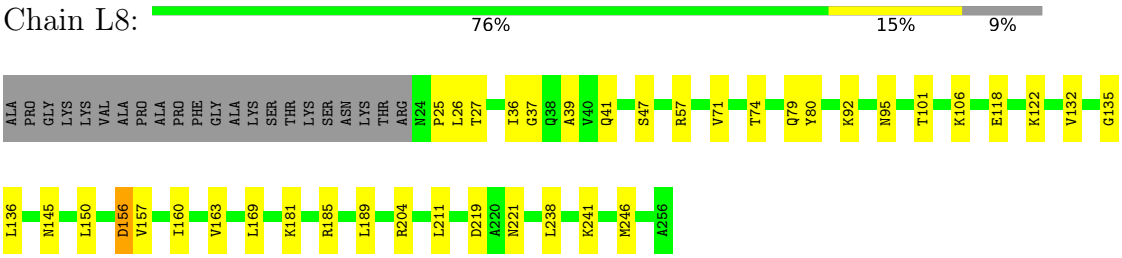
- Molecule 44: 60S ribosomal protein L7-A

Chain l7:



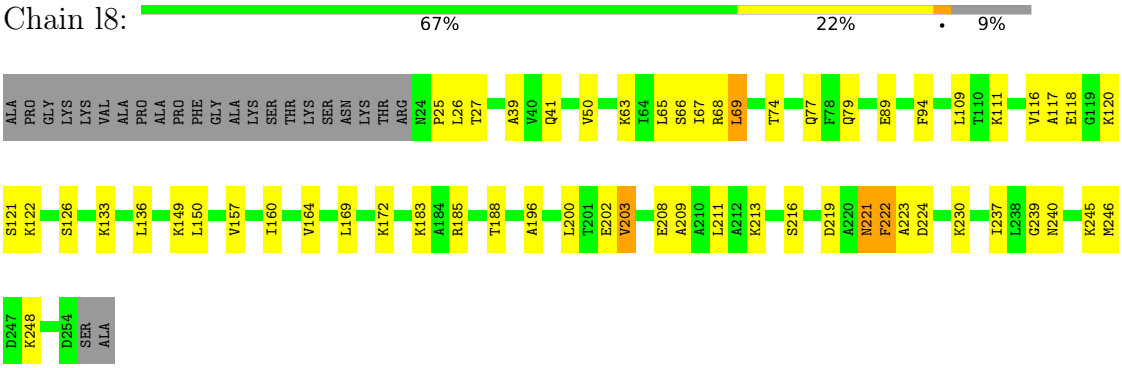
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:



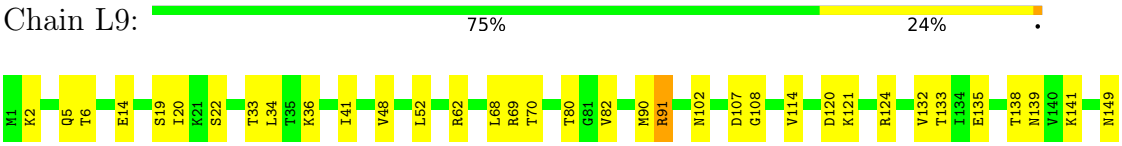
- Molecule 45: 60S ribosomal protein L8-A

Chain l8:



- Molecule 46: 60S ribosomal protein L9-A

Chain L9:



S150 V151 S155 Q156 N157 L161 Q162 Q163 I164 R168 I172 R173 T188 E189 D190 L191

- Molecule 46: 60S ribosomal protein L9-A

Chain l9: 81% 19%

M1 K2 Y3 I4 Q5 T6 S19 R31 G32 T33 K39 V43 T44 V48 L52 V55 R62 L68 R69 T70 T80 E105 K106 D107 R115 K122 I123 R129 D130 G131 V132 T133 T138 I144 V151 N157 L161 Q162 Q163 V167

D177 G178 I179 L191

- Molecule 47: 60S ribosomal protein L10

Chain M0: 74% 20%

A2 R3 R7 C8 P16 R21 R24 A25 V26 P27 D28 S29 K30 I31 R32 I33 K39 T42 L48 L52 L57 E63 K74 L87 M102 LEU SER CYS ALA GLY ALA ASP ARG LEU Q112 G117 A127 R128 V129 D130 V138 R139 S143

N144 K145 D146 V147 R156 Q163 K164 I165 K169 G172 F173 T174 N175 L176 D177 R178 G188 E189 D192 K203 G204 S205 L206 E207 A219 Q220 A221

- Molecule 47: 60S ribosomal protein L10

Chain m0: 76% 20%

A2 R3 R4 R7 C8 Y9 R10 R21 R24 A25 D28 L36 T42 E45 L48 L52 E58 Q59 L60 E63 T77 L87 R90 K101 M102 L103 SER CYS ALA GLY ALA ASP ARG L111 G117 D130 R139 N144 K145 R156

K169 L176 D177 L182 K191 D192 D193 F196 V197 L200 K203 G204 S205 L206 E207 R211 E212 F217 Q220 A221

- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 72% 20% 5%

SER THR LYS ALA Q6 N7 P8 M9 R10 D11 L12 K13 L19 N20 I21 S22 V23 T31 S34 L40 T44 P45 V46 Y52 T56 E63 T70 L80 E81 R82 R94 T99 I106 D107 E108 L112 G113 I114 K115 Y116 D117 V130 R137

R140 R141 K142 S151 T155 D158 Q165 K166 Y167 D168 V171 L172 D173 K174

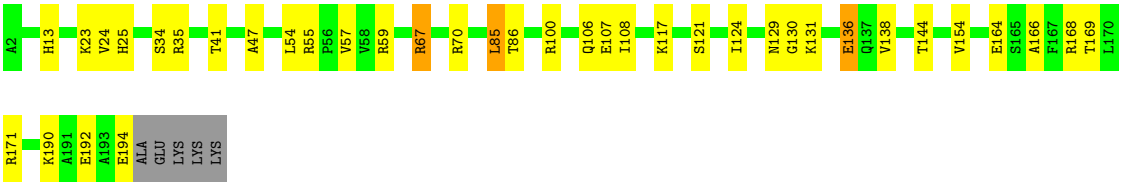
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 73% 23%

SER THR LYS ALA Q6 N7 P8 M9 R10 D11 L12 K13 K16 V23 D28 T31 Q39 L40 T44 P45 V46 V54 R55 T56 I59 K87 R94 N95 D107 E108 I114 D117 P118 S119 I120 G121 I122 V129 V130 R137 R140 K145

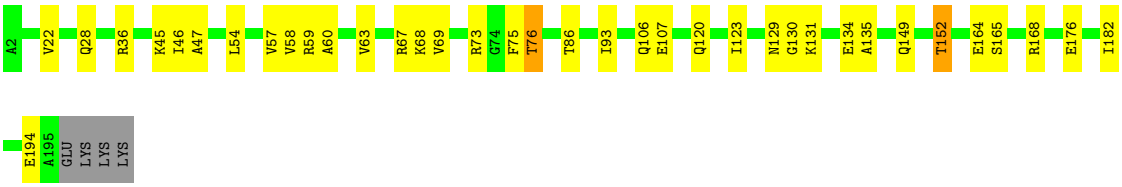
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



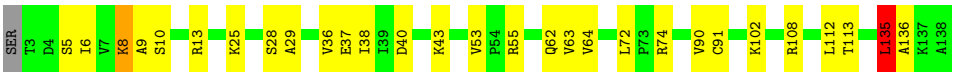
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



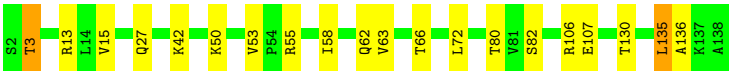
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



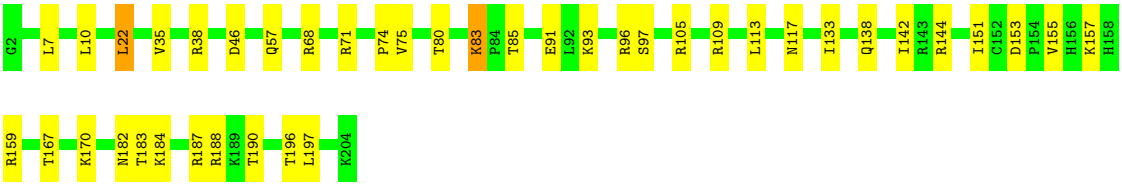
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



• Molecule 51: 60S ribosomal protein L15-A

Chain M5:

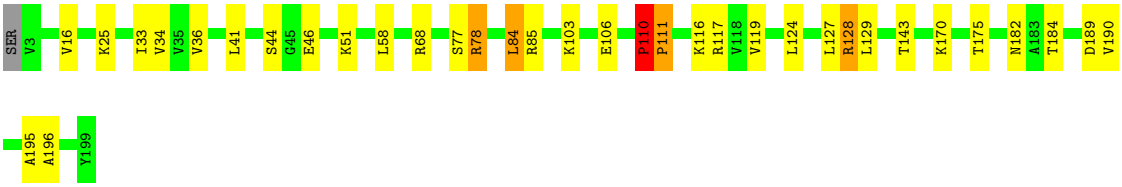


• Molecule 51: 60S ribosomal protein L15-A

Chain m5: 83% 17%

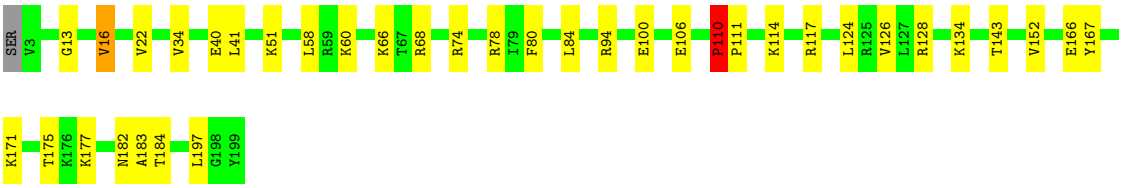
- Molecule 52: 60S ribosomal protein L16-A

Chain M6: 82% 15%



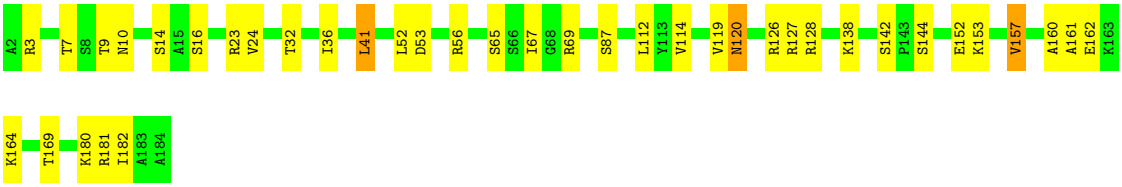
- Molecule 52: 60S ribosomal protein L16-A

Chain m6: 81% 18%



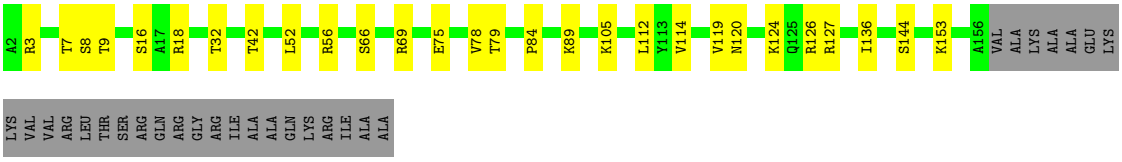
- Molecule 53: 60S ribosomal protein L17-A

Chain M7: 79% 20%



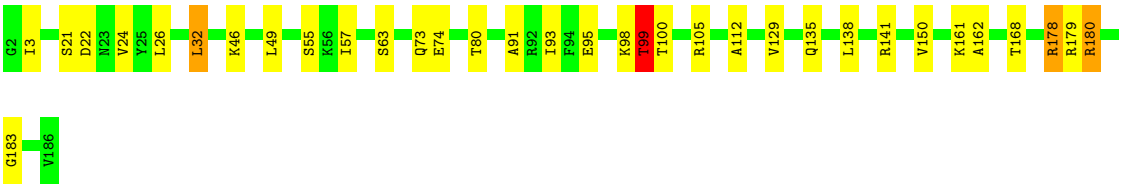
- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 69% 15% 15%



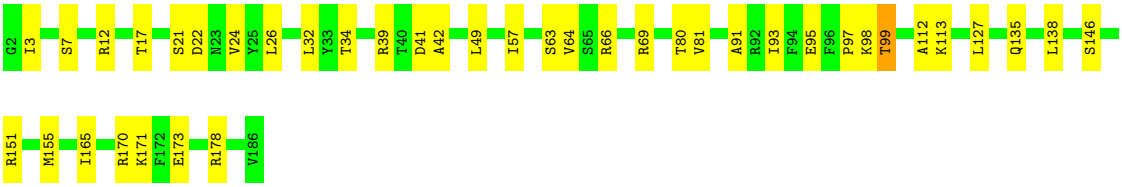
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



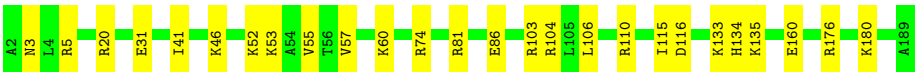
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



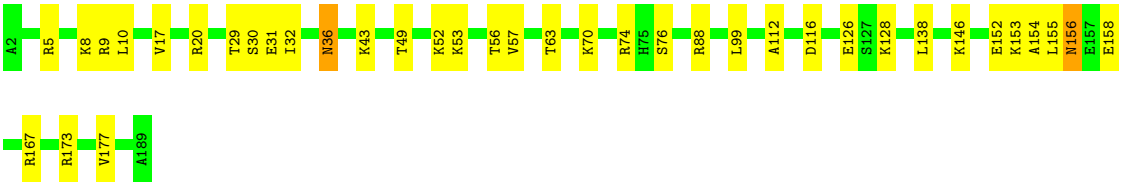
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



- Molecule 55: 60S ribosomal protein L19-A

Chain m9:



- Molecule 56: 60S ribosomal protein L20-A

Chain N0:

- Molecule 56: 60S ribosomal protein L20-A

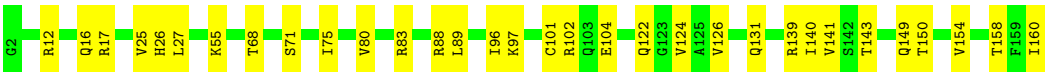
Chain n0:

• Molecule 57: 60S ribosomal protein L21-A

Chain N1:

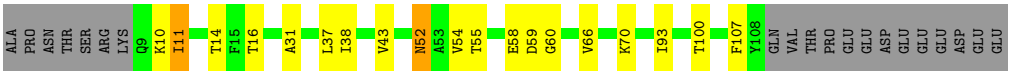
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



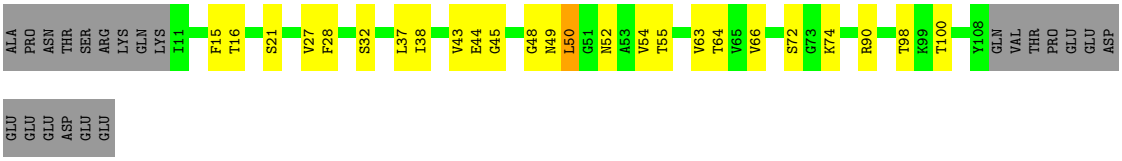
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



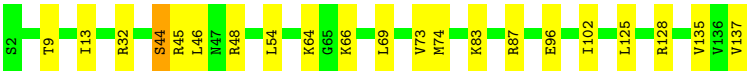
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



• Molecule 59: 60S ribosomal protein L23-A

Chain n3:

• Molecule 60: 60S ribosomal protein L24-A

Chain N4: 53% 8% • 37%

M1 E4 I5 G10 T19 K27 L39 P46 R47 T64 K69 V76 K77 P81 S86 L96 K97 P98 GLU VAL ARG LYS ALA ASN ARG GLU GLU LYS LEU LYS ALA ASN LYS GLU LYS LYS LYS ALA GLU LYS ALA ALA ARG LYS ALA GLU LYS ALA

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

• Molecule 60: 60S ribosomal protein L24-A

Chain n4: 72% 14% • 13%

M1 T19 D25 S26 S34 L39 L54 K57 I63 V76 K77 T83 L89 I90 K91 L96 K97 P98 R105 E106 E107 E119 E126 G132 S135 SER LYS PHE SER LYS GLN GLN ALA LYS GLY ALA PHE GLN LYS VAL ALA ALA THR SER

ARG

• Molecule 61: 60S ribosomal protein L25

Chain N5: 69% 16% • 14%

ALA PRO SER ALA LYS ALA THR ALA ALA LYS LYS ALA VAL VAL LYS GLY THR ASN GLY LYS K22 R27 R33 L34 T37 L38 K39 K45 S59 I63 K74 V86 K92 K96 V105 L108 K109 L113 V114 R115 R125 L126 T127 D134 I135

I139 I142

• Molecule 61: 60S ribosomal protein L25

Chain n5: 67% 17% • 15%

ALA PRO SER ALA LYS ALA THR ALA ALA LYS LYS ALA VAL VAL LYS GLY THR ASN GLY LYS LYS A23 L24 K25 V26 R27 T37 L38 K39 L40 P44 K45 Y46 A47 N55 R56 L57 I63 E64 V86 K96 E104 L108 K109 R115 P116 N117 R125 L133

D134 I135 A136 N137 I142

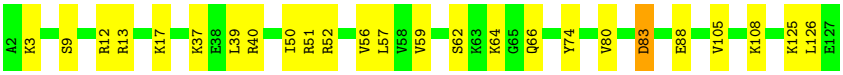
• Molecule 62: 60S ribosomal protein L26-A

Chain N6: 79% 21%

A2 K3 Q4 S5 S10 R13 S36 K37 E38 I50 R51 R52 D53 D54 E55 V56 L57 K63 I70 Y74 R75 L76 V80 D83 K84 G92 A93 S94 V105 R115 L126 E127

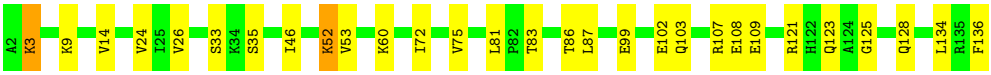
• Molecule 62: 60S ribosomal protein L26-A

Chain n6: 80% 19% •



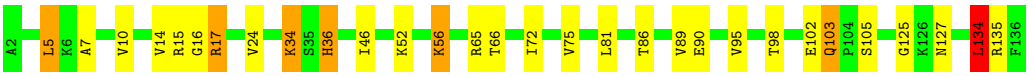
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



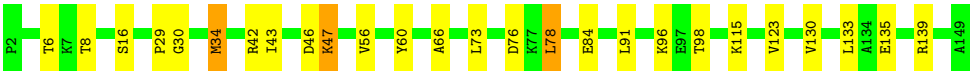
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



• Molecule 64: 60S ribosomal protein L28

Chain N8:

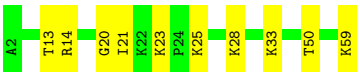


• Molecule 64: 60S ribosomal protein L28

Chain n8:

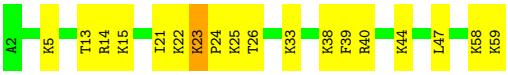
• Molecule 65: 60S ribosomal protein L29

Chain N9:



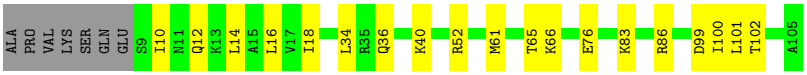
• Molecule 65: 60S ribosomal protein L29

Chain n9:



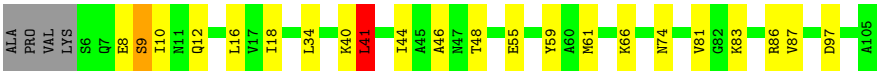
• Molecule 66: 60S ribosomal protein L30

Chain O0:



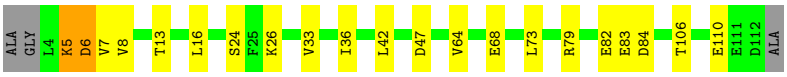
• Molecule 66: 60S ribosomal protein L30

Chain o0:



• Molecule 67: 60S ribosomal protein L31-A

Chain O1:



• Molecule 67: 60S ribosomal protein L31-A

Chain o1:

• Molecule 68: 60S ribosomal protein L32

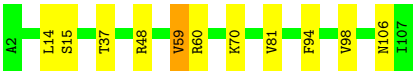
Chain O2:

• Molecule 68: 60S ribosomal protein L32

Chain o2:

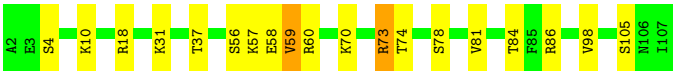
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



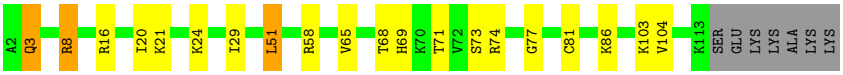
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



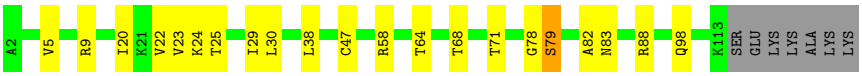
• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



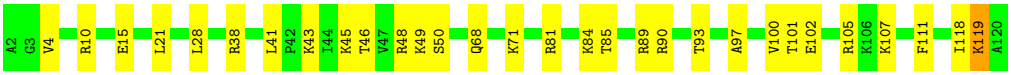
• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



• Molecule 71: 60S ribosomal protein L35-A

Chain O5:

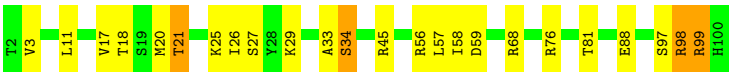


• Molecule 71: 60S ribosomal protein L35-A

Chain o5:

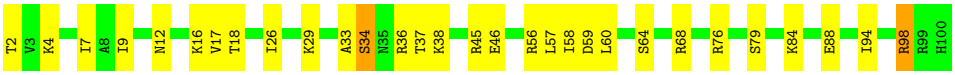
• Molecule 72: 60S ribosomal protein L36-A

Chain O6:



• Molecule 72: 60S ribosomal protein L36-A

Chain o6:

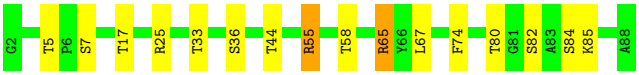


• Molecule 73: 60S ribosomal protein L37-A

Chain O7:

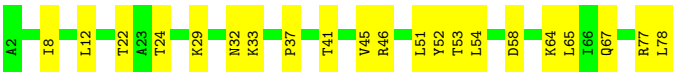
• Molecule 73: 60S ribosomal protein L37-A

Chain o7:



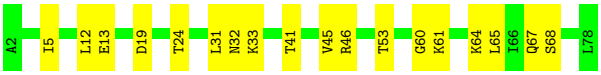
• Molecule 74: 60S ribosomal protein L38

Chain O8:



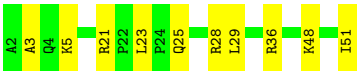
• Molecule 74: 60S ribosomal protein L38

Chain o8:



• Molecule 75: 60S ribosomal protein L39

Chain O9:

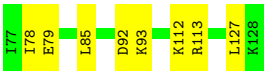


• Molecule 75: 60S ribosomal protein L39

Chain o9:

• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



• Molecule 76: Ubiquitin-60S ribosomal protein L40

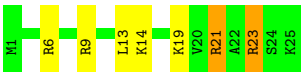
Chain q0:

• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:

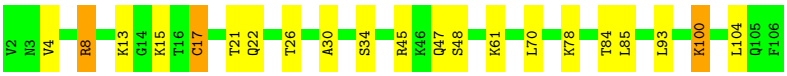
• Molecule 77: 60S ribosomal protein L41-A

Chain q1:



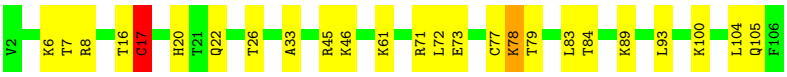
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



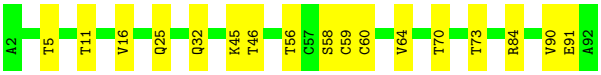
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:

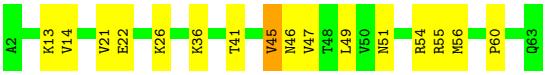


• Molecule 79: 60S ribosomal protein L43-A

Chain q3:

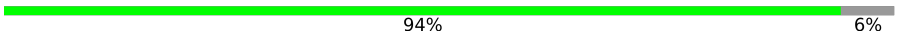
• Molecule 80: 40S ribosomal protein S30-A

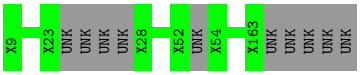
Chain e0:



• Molecule 81: Unknown protein m2

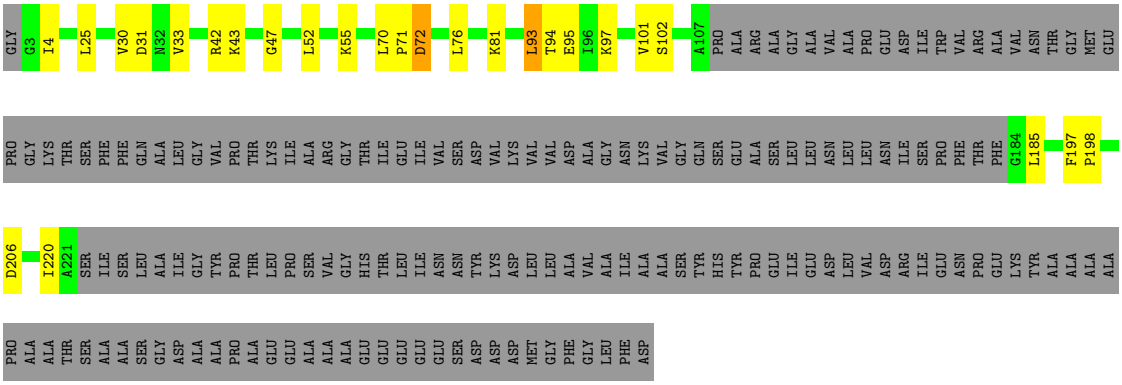
Chain m2:





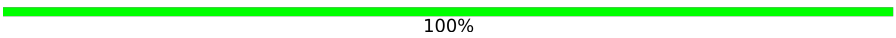
• Molecule 82: 60S acidic ribosomal protein P0

Chain p0:



• Molecule 83: Unknown protein p1

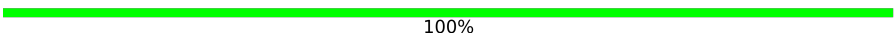
Chain p1:



There are no outlier residues recorded for this chain.

• Molecule 84: Unknown protein p2

Chain p2:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	434.98Å 287.50Å 303.22Å 90.00° 98.85° 90.00°	Depositor
Resolution (Å)	299.60 – 3.10	Depositor
% Data completeness (in resolution range)	100.0 (299.60-3.10)	Depositor
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.202 , 0.252	Depositor
Wilson B-factor (Å^2)	76.9	Xtriage
Anisotropy	0.178	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	411276	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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, 3K5, OHX, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	2	0.73	5/41698 (0.0%)	1.28	279/64972 (0.4%)
1	6	0.89	29/42765 (0.1%)	1.39	455/66634 (0.7%)
2	S0	0.48	0/1617	0.67	0/2215
2	s0	0.50	0/1623	0.68	0/2222
3	S1	0.37	0/1735	0.68	1/2335 (0.0%)
3	s1	0.53	0/1748	0.70	0/2352
4	S2	0.51	0/1665	0.66	0/2263
4	s2	0.59	0/1665	0.77	0/2263
5	S3	0.51	0/1759	0.70	1/2368 (0.0%)
5	s3	0.47	0/1759	0.61	0/2368
6	S4	0.50	0/2109	0.72	0/2839
6	s4	0.56	0/2109	0.76	1/2839 (0.0%)
7	S5	0.41	0/1629	0.61	0/2202
7	s5	0.47	0/1629	0.66	0/2202
8	S6	0.49	0/1823	0.67	0/2439
8	s6	0.57	0/1779	0.71	0/2379
9	S7	0.44	0/1506	0.67	0/2028
9	s7	0.49	0/1516	0.72	1/2043 (0.0%)
10	S8	0.56	0/1514	0.74	2/2021 (0.1%)
10	s8	0.65	0/1514	0.78	0/2021
11	S9	0.49	0/1519	0.68	1/2035 (0.0%)
11	s9	0.59	0/1519	0.74	0/2035
12	C0	0.42	0/790	0.64	1/1069 (0.1%)
12	c0	0.40	0/777	0.64	3/1049 (0.3%)
13	C1	0.61	0/1240	0.75	0/1675
13	c1	0.65	0/1194	0.77	0/1610
14	C2	0.38	0/900	0.64	0/1224
14	c2	0.30	0/900	0.59	1/1224 (0.1%)
15	C3	0.51	0/1215	0.72	3/1638 (0.2%)
15	c3	0.60	0/1215	0.73	0/1638
16	C4	0.38	0/901	0.63	0/1217
16	c4	0.54	0/960	0.78	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.46	0/998	0.71	0/1341
17	c5	0.52	0/1060	0.69	1/1426 (0.1%)
18	C6	0.46	0/1125	0.67	0/1510
18	c6	0.50	0/1131	0.72	1/1518 (0.1%)
19	C7	0.44	0/935	0.63	0/1254
19	c7	0.50	0/914	0.71	0/1224
20	C8	0.45	0/1211	0.65	1/1628 (0.1%)
20	c8	0.50	0/1211	0.70	1/1628 (0.1%)
21	C9	0.46	0/1130	0.68	1/1517 (0.1%)
21	c9	0.50	0/1130	0.67	1/1517 (0.1%)
22	D0	0.48	0/865	0.66	0/1169
22	d0	0.50	0/892	0.66	0/1205
23	D1	0.45	0/693	0.62	1/935 (0.1%)
23	d1	0.57	0/693	0.73	0/935
24	D2	0.52	0/1038	0.73	1/1395 (0.1%)
24	d2	0.63	0/1038	0.75	1/1395 (0.1%)
25	D3	0.62	0/1139	0.76	1/1518 (0.1%)
25	d3	0.74	0/1139	0.87	3/1518 (0.2%)
26	D4	0.46	0/1087	0.62	0/1449
26	d4	0.57	0/1087	0.74	0/1449
27	D5	0.40	0/571	0.73	1/768 (0.1%)
27	d5	0.41	0/566	0.64	0/761
28	D6	0.47	0/782	0.68	0/1047
28	d6	0.57	0/782	0.70	0/1047
29	D7	0.43	0/620	0.67	0/838
29	d7	0.49	0/620	0.71	0/838
30	D8	0.36	0/499	0.59	0/670
30	d8	0.45	0/499	0.66	0/670
31	D9	0.55	0/452	0.74	0/600
31	d9	0.57	0/452	0.69	0/600
32	E0	0.48	0/483	0.62	0/643
33	E1	0.46	0/577	0.78	0/770
33	e1	0.42	0/619	0.73	1/822 (0.1%)
34	SR	0.41	0/2494	0.64	0/3393
34	sR	0.40	0/2495	0.60	0/3395
35	SM	0.52	0/1113	0.73	2/1502 (0.1%)
35	sM	0.48	0/682	0.68	1/921 (0.1%)
36	1	1.17	163/75394 (0.2%)	1.66	1841/117545 (1.6%)
36	5	1.20	181/75414 (0.2%)	1.67	1895/117575 (1.6%)
37	3	0.96	1/2883 (0.0%)	1.41	24/4491 (0.5%)
37	7	1.17	3/2883 (0.1%)	1.66	57/4491 (1.3%)
38	4	1.15	2/3746 (0.1%)	1.64	82/5832 (1.4%)
38	8	1.04	3/3746 (0.1%)	1.50	53/5832 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	0.74	0/1948	0.86	3/2617 (0.1%)
39	l2	0.74	0/1946	0.89	3/2614 (0.1%)
40	L3	0.72	0/3146	0.81	0/4228
40	l3	0.86	0/3146	0.90	5/4228 (0.1%)
41	L4	0.84	2/2800 (0.1%)	0.95	6/3790 (0.2%)
41	l4	0.75	1/2800 (0.0%)	0.92	6/3790 (0.2%)
42	L5	0.60	0/2425	0.71	1/3271 (0.0%)
42	l5	0.70	0/2408	0.79	1/3248 (0.0%)
43	L6	0.76	0/1260	0.84	1/1694 (0.1%)
43	l6	0.78	0/1269	0.85	3/1705 (0.2%)
44	L7	0.82	0/1821	0.94	3/2451 (0.1%)
44	l7	0.85	1/1828 (0.1%)	0.89	2/2461 (0.1%)
45	L8	0.60	0/1836	0.69	1/2481 (0.0%)
45	l8	0.57	0/1795	0.70	1/2429 (0.0%)
46	L9	0.67	0/1539	0.78	1/2073 (0.0%)
46	l9	0.79	0/1539	0.81	0/2073
47	M0	0.77	2/1741 (0.1%)	0.87	2/2335 (0.1%)
47	m0	0.78	1/1758 (0.1%)	0.87	3/2358 (0.1%)
48	M1	0.55	0/1374	0.74	1/1842 (0.1%)
48	m1	0.65	0/1374	0.78	1/1842 (0.1%)
49	M3	0.77	0/1568	0.88	2/2106 (0.1%)
49	m3	0.67	0/1573	0.79	1/2113 (0.0%)
50	M4	0.72	0/1068	0.80	1/1438 (0.1%)
50	m4	0.85	0/1074	0.87	2/1446 (0.1%)
51	M5	0.80	0/1757	0.87	3/2354 (0.1%)
51	m5	0.69	0/1757	0.82	2/2354 (0.1%)
52	M6	0.85	0/1585	0.91	5/2128 (0.2%)
52	m6	1.03	4/1585 (0.3%)	0.98	3/2128 (0.1%)
53	M7	0.77	0/1443	0.86	2/1944 (0.1%)
53	m7	0.90	0/1250	0.84	0/1683
54	M8	0.79	0/1465	0.90	4/1965 (0.2%)
54	m8	0.76	0/1465	0.91	2/1965 (0.1%)
55	M9	0.55	0/1538	0.69	0/2050
55	m9	0.63	0/1538	0.71	0/2050
56	N0	0.82	0/1481	0.87	0/1990
56	n0	0.88	0/1481	0.88	2/1990 (0.1%)
57	N1	0.77	0/1300	0.84	2/1743 (0.1%)
57	n1	0.83	1/1300 (0.1%)	0.81	0/1743
58	N2	0.48	0/812	0.64	0/1099
58	n2	0.51	0/794	0.69	0/1076
59	N3	0.73	0/1018	0.81	0/1369
59	n3	0.88	0/1018	0.90	3/1369 (0.2%)
60	N4	0.57	0/712	0.71	1/958 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	n4	0.71	0/1052	0.76	0/1398
61	N5	0.64	0/979	0.81	1/1321 (0.1%)
61	n5	0.68	0/974	0.85	1/1314 (0.1%)
62	N6	0.73	0/1004	0.91	0/1341
62	n6	0.68	0/1004	0.84	0/1341
63	N7	0.52	0/1118	0.66	0/1497
63	n7	0.49	0/1118	0.72	3/1497 (0.2%)
64	N8	0.80	0/1204	0.90	2/1612 (0.1%)
64	n8	0.78	0/1204	0.87	0/1612
65	N9	0.72	0/473	0.79	0/629
65	n9	0.80	0/473	0.87	0/629
66	O0	0.50	0/751	0.72	0/1008
66	o0	0.52	0/775	0.68	1/1040 (0.1%)
67	O1	0.63	0/890	0.78	0/1196
67	o1	0.79	0/897	0.89	0/1205
68	O2	0.86	0/1041	0.90	1/1394 (0.1%)
68	o2	0.85	0/1041	0.92	2/1394 (0.1%)
69	O3	0.90	0/868	0.89	0/1168
69	o3	0.92	0/868	0.90	3/1168 (0.3%)
70	O4	0.63	0/890	0.83	2/1189 (0.2%)
70	o4	0.65	0/890	0.83	0/1189
71	O5	0.73	0/978	0.76	1/1301 (0.1%)
71	o5	0.62	0/974	0.74	1/1297 (0.1%)
72	O6	0.67	0/778	0.78	0/1034
72	o6	0.63	0/777	0.71	0/1033
73	O7	0.80	0/696	0.93	2/923 (0.2%)
73	o7	0.77	0/696	0.88	1/923 (0.1%)
74	O8	0.53	0/618	0.64	0/826
74	o8	0.50	0/614	0.66	0/822
75	O9	0.76	0/443	0.98	1/588 (0.2%)
75	o9	0.71	0/443	0.79	0/588
76	Q0	0.71	0/423	0.80	0/562
76	q0	0.94	0/423	0.94	0/562
77	Q1	0.74	0/234	0.89	0/300
77	q1	0.76	0/234	0.94	1/300 (0.3%)
78	Q2	0.89	1/860 (0.1%)	0.88	1/1136 (0.1%)
78	q2	0.80	1/860 (0.1%)	0.82	0/1136
79	Q3	0.76	0/701	0.83	0/934
79	q3	0.75	0/701	0.80	1/934 (0.1%)
80	e0	0.56	0/499	0.81	0/665
82	p0	0.47	0/1091	0.63	0/1472
All	All	0.92	401/430072 (0.1%)	1.31	4824/631360 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	s0	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
12	c0	0	1
16	c4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	1
22	d0	0	1
25	D3	0	1
26	d4	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	2
41	L4	0	1
43	L6	0	1
44	l7	0	2
45	l8	0	1
48	M1	0	1
49	M3	0	1
50	M4	0	1
52	M6	0	2
52	m6	0	1
53	M7	0	1
56	n0	0	2
57	N1	0	1
63	N7	0	1
64	N8	0	1
64	n8	0	3
65	N9	0	1
67	O1	0	1
All	All	0	43

The worst 5 of 401 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-12.58	1.27	1.38
78	Q2	17	CYS	CB-SG	11.86	2.02	1.82
36	5	960	U	N1-C2	10.74	1.48	1.38
36	5	2971	A	N9-C4	9.52	1.43	1.37
78	q2	17	CYS	CB-SG	8.98	1.97	1.82

The worst 5 of 4824 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1152	G	C2-N3-C4	-23.10	100.35	111.90
36	5	1152	G	N3-C4-C5	23.05	140.12	128.60
36	5	1152	G	N3-C4-N9	-22.76	112.34	126.00
36	1	2714	G	N3-C4-C5	15.18	136.19	128.60
36	1	1308	A	O5'-P-OP2	-14.90	92.29	105.70

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	C6	113	ASP	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
25	D3	78	LYS	Peptide
9	S7	131	PHE	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	142 (70%)	40 (20%)	22 (11%)	0	2
2	s0	204/251 (81%)	155 (76%)	28 (14%)	21 (10%)	0	3
3	S1	212/254 (84%)	144 (68%)	35 (16%)	33 (16%)	0	0
3	s1	214/254 (84%)	174 (81%)	27 (13%)	13 (6%)	1	9
4	S2	215/253 (85%)	182 (85%)	22 (10%)	11 (5%)	2	13
4	s2	215/253 (85%)	178 (83%)	22 (10%)	15 (7%)	1	7
5	S3	221/239 (92%)	177 (80%)	25 (11%)	19 (9%)	1	4
5	s3	221/239 (92%)	179 (81%)	28 (13%)	14 (6%)	1	8
6	S4	258/260 (99%)	205 (80%)	36 (14%)	17 (7%)	1	7
6	s4	258/260 (99%)	212 (82%)	29 (11%)	17 (7%)	1	7
7	S5	204/224 (91%)	155 (76%)	33 (16%)	16 (8%)	1	5
7	s5	204/224 (91%)	160 (78%)	23 (11%)	21 (10%)	0	3
8	S6	224/236 (95%)	195 (87%)	17 (8%)	12 (5%)	2	12
8	s6	216/236 (92%)	181 (84%)	22 (10%)	13 (6%)	1	9
9	S7	182/189 (96%)	128 (70%)	28 (15%)	26 (14%)	0	1
9	s7	184/189 (97%)	148 (80%)	26 (14%)	10 (5%)	2	12
10	S8	184/200 (92%)	152 (83%)	21 (11%)	11 (6%)	1	9
10	s8	184/200 (92%)	155 (84%)	17 (9%)	12 (6%)	1	8
11	S9	183/196 (93%)	149 (81%)	24 (13%)	10 (6%)	2	11
11	s9	183/196 (93%)	152 (83%)	22 (12%)	9 (5%)	2	14
12	C0	94/105 (90%)	77 (82%)	10 (11%)	7 (7%)	1	6
12	c0	92/105 (88%)	58 (63%)	19 (21%)	15 (16%)	0	0
13	C1	153/155 (99%)	121 (79%)	23 (15%)	9 (6%)	1	10
13	c1	144/155 (93%)	122 (85%)	15 (10%)	7 (5%)	2	14
14	C2	122/142 (86%)	66 (54%)	30 (25%)	26 (21%)	0	0
14	c2	122/142 (86%)	62 (51%)	37 (30%)	23 (19%)	0	0
15	C3	148/150 (99%)	124 (84%)	19 (13%)	5 (3%)	3	21
15	c3	148/150 (99%)	116 (78%)	22 (15%)	10 (7%)	1	7
16	C4	125/136 (92%)	90 (72%)	25 (20%)	10 (8%)	1	5
16	c4	126/136 (93%)	100 (79%)	16 (13%)	10 (8%)	1	5
17	C5	122/141 (86%)	85 (70%)	26 (21%)	11 (9%)	1	4
17	c5	133/141 (94%)	93 (70%)	23 (17%)	17 (13%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	114 (82%)	19 (14%)	6 (4%)	2	16
18	c6	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	2	13
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	0	3
19	c7	113/136 (83%)	89 (79%)	17 (15%)	7 (6%)	1	9
20	C8	143/145 (99%)	106 (74%)	25 (18%)	12 (8%)	1	5
20	c8	143/145 (99%)	116 (81%)	16 (11%)	11 (8%)	1	5
21	C9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	2	13
21	c9	141/143 (99%)	119 (84%)	18 (13%)	4 (3%)	5	25
22	D0	105/120 (88%)	84 (80%)	16 (15%)	5 (5%)	2	14
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	1	10
23	d1	85/87 (98%)	70 (82%)	9 (11%)	6 (7%)	1	6
24	D2	127/129 (98%)	102 (80%)	19 (15%)	6 (5%)	2	14
24	d2	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	6	27
25	D3	142/144 (99%)	114 (80%)	22 (16%)	6 (4%)	3	16
25	d3	142/144 (99%)	125 (88%)	13 (9%)	4 (3%)	5	25
26	D4	132/134 (98%)	104 (79%)	17 (13%)	11 (8%)	1	5
26	d4	132/134 (98%)	111 (84%)	15 (11%)	6 (4%)	2	15
27	D5	68/107 (64%)	48 (71%)	12 (18%)	8 (12%)	0	1
27	d5	67/107 (63%)	51 (76%)	10 (15%)	6 (9%)	1	4
28	D6	95/97 (98%)	59 (62%)	18 (19%)	18 (19%)	0	0
28	d6	95/97 (98%)	74 (78%)	10 (10%)	11 (12%)	0	2
29	D7	79/81 (98%)	65 (82%)	8 (10%)	6 (8%)	1	5
29	d7	79/81 (98%)	59 (75%)	14 (18%)	6 (8%)	1	5
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	0	3
30	d8	61/66 (92%)	42 (69%)	14 (23%)	5 (8%)	1	5
31	D9	51/55 (93%)	40 (78%)	9 (18%)	2 (4%)	3	18
31	d9	51/55 (93%)	40 (78%)	6 (12%)	5 (10%)	0	3
32	E0	58/60 (97%)	43 (74%)	12 (21%)	3 (5%)	2	12
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
33	e1	74/76 (97%)	35 (47%)	20 (27%)	19 (26%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	242 (77%)	50 (16%)	24 (8%)	1	5
34	sR	316/318 (99%)	253 (80%)	48 (15%)	15 (5%)	2	14
35	SM	155/273 (57%)	103 (66%)	30 (19%)	22 (14%)	0	1
35	sM	98/273 (36%)	65 (66%)	18 (18%)	15 (15%)	0	0
39	L2	250/253 (99%)	224 (90%)	20 (8%)	6 (2%)	6	27
39	l2	250/253 (99%)	215 (86%)	24 (10%)	11 (4%)	2	15
40	L3	384/386 (100%)	328 (85%)	38 (10%)	18 (5%)	2	14
40	l3	384/386 (100%)	338 (88%)	35 (9%)	11 (3%)	4	24
41	L4	359/361 (99%)	299 (83%)	36 (10%)	24 (7%)	1	7
41	l4	359/361 (99%)	287 (80%)	51 (14%)	21 (6%)	1	10
42	L5	294/296 (99%)	241 (82%)	37 (13%)	16 (5%)	2	12
42	l5	292/296 (99%)	247 (85%)	37 (13%)	8 (3%)	5	25
43	L6	152/175 (87%)	128 (84%)	21 (14%)	3 (2%)	7	31
43	l6	153/175 (87%)	131 (86%)	17 (11%)	5 (3%)	4	21
44	L7	220/243 (90%)	186 (84%)	23 (10%)	11 (5%)	2	13
44	l7	221/243 (91%)	194 (88%)	23 (10%)	4 (2%)	8	34
45	L8	231/255 (91%)	190 (82%)	32 (14%)	9 (4%)	3	18
45	l8	229/255 (90%)	177 (77%)	30 (13%)	22 (10%)	0	3
46	L9	189/191 (99%)	164 (87%)	21 (11%)	4 (2%)	7	30
46	l9	189/191 (99%)	172 (91%)	14 (7%)	3 (2%)	9	37
47	M0	207/220 (94%)	172 (83%)	24 (12%)	11 (5%)	2	12
47	m0	209/220 (95%)	168 (80%)	28 (13%)	13 (6%)	1	9
48	M1	167/173 (96%)	126 (75%)	28 (17%)	13 (8%)	1	5
48	m1	167/173 (96%)	137 (82%)	16 (10%)	14 (8%)	1	5
49	M3	191/198 (96%)	161 (84%)	22 (12%)	8 (4%)	3	16
49	m3	192/198 (97%)	162 (84%)	21 (11%)	9 (5%)	2	14
50	M4	134/137 (98%)	113 (84%)	11 (8%)	10 (8%)	1	6
50	m4	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	6	29
51	M5	201/203 (99%)	182 (90%)	15 (8%)	4 (2%)	7	31
51	m5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	5	27
52	M6	195/198 (98%)	173 (89%)	14 (7%)	8 (4%)	3	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m6	195/198 (98%)	178 (91%)	11 (6%)	6 (3%)	4	23
53	M7	181/183 (99%)	146 (81%)	30 (17%)	5 (3%)	5	25
53	m7	153/183 (84%)	138 (90%)	11 (7%)	4 (3%)	5	26
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	4	21
54	m8	183/185 (99%)	154 (84%)	19 (10%)	10 (6%)	2	11
55	M9	186/188 (99%)	164 (88%)	18 (10%)	4 (2%)	6	29
55	m9	186/188 (99%)	162 (87%)	18 (10%)	6 (3%)	4	22
56	N0	170/172 (99%)	149 (88%)	16 (9%)	5 (3%)	4	24
56	n0	170/172 (99%)	156 (92%)	13 (8%)	1 (1%)	25	59
57	N1	157/159 (99%)	134 (85%)	16 (10%)	7 (4%)	2	15
57	n1	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	12	42
58	N2	98/120 (82%)	77 (79%)	15 (15%)	6 (6%)	1	9
58	n2	96/120 (80%)	76 (79%)	14 (15%)	6 (6%)	1	8
59	N3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	39
59	n3	134/136 (98%)	125 (93%)	6 (4%)	3 (2%)	6	29
60	N4	96/155 (62%)	65 (68%)	20 (21%)	11 (12%)	0	2
60	n4	133/155 (86%)	108 (81%)	17 (13%)	8 (6%)	1	9
61	N5	119/141 (84%)	103 (87%)	15 (13%)	1 (1%)	19	54
61	n5	118/141 (84%)	99 (84%)	10 (8%)	9 (8%)	1	5
62	N6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	3	17
62	n6	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	6	27
63	N7	133/135 (98%)	114 (86%)	12 (9%)	7 (5%)	2	12
63	n7	133/135 (98%)	109 (82%)	13 (10%)	11 (8%)	1	5
64	N8	146/148 (99%)	125 (86%)	16 (11%)	5 (3%)	3	21
64	n8	146/148 (99%)	121 (83%)	19 (13%)	6 (4%)	3	16
65	N9	56/58 (97%)	48 (86%)	7 (12%)	1 (2%)	8	34
65	n9	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	4
66	O0	95/104 (91%)	82 (86%)	12 (13%)	1 (1%)	14	46
66	o0	98/104 (94%)	81 (83%)	14 (14%)	3 (3%)	4	23
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	2	11
67	o1	107/112 (96%)	88 (82%)	12 (11%)	7 (6%)	1	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O2	125/129 (97%)	114 (91%)	10 (8%)	1 (1%)	19	54
68	o2	125/129 (97%)	101 (81%)	18 (14%)	6 (5%)	2	14
69	O3	104/106 (98%)	93 (89%)	9 (9%)	2 (2%)	8	33
69	o3	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	15	49
70	O4	110/119 (92%)	91 (83%)	16 (14%)	3 (3%)	5	25
70	o4	110/119 (92%)	92 (84%)	15 (14%)	3 (3%)	5	25
71	O5	117/119 (98%)	96 (82%)	17 (14%)	4 (3%)	3	21
71	o5	117/119 (98%)	96 (82%)	14 (12%)	7 (6%)	1	9
72	O6	97/99 (98%)	77 (79%)	12 (12%)	8 (8%)	1	5
72	o6	97/99 (98%)	77 (79%)	14 (14%)	6 (6%)	1	9
73	O7	85/87 (98%)	76 (89%)	7 (8%)	2 (2%)	6	27
73	o7	85/87 (98%)	73 (86%)	9 (11%)	3 (4%)	3	20
74	O8	75/77 (97%)	63 (84%)	10 (13%)	2 (3%)	5	25
74	o8	75/77 (97%)	62 (83%)	11 (15%)	2 (3%)	5	25
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	30
75	o9	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	3	16
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	17
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	31
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	3 (13%)	1 (4%)	2	16
78	Q2	103/105 (98%)	82 (80%)	15 (15%)	6 (6%)	1	10
78	q2	103/105 (98%)	92 (89%)	7 (7%)	4 (4%)	3	18
79	Q3	89/91 (98%)	73 (82%)	15 (17%)	1 (1%)	14	46
79	q3	89/91 (98%)	78 (88%)	10 (11%)	1 (1%)	14	46
80	e0	60/62 (97%)	46 (77%)	9 (15%)	5 (8%)	1	5
82	p0	139/311 (45%)	109 (78%)	20 (14%)	10 (7%)	1	6
All	All	22333/24141 (92%)	18272 (82%)	2751 (12%)	1310 (6%)	1	10

5 of 1310 Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S0	164/209 (78%)	136 (83%)	28 (17%)	2 9
2	s0	165/209 (79%)	130 (79%)	35 (21%)	1 5
3	S1	191/223 (86%)	150 (78%)	41 (22%)	1 4
3	s1	192/223 (86%)	151 (79%)	41 (21%)	1 4
4	S2	176/204 (86%)	137 (78%)	39 (22%)	1 4
4	s2	176/204 (86%)	133 (76%)	43 (24%)	0 2
5	S3	182/194 (94%)	138 (76%)	44 (24%)	0 2
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1 5
6	S4	221/221 (100%)	175 (79%)	46 (21%)	1 5
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2 9
7	S5	173/190 (91%)	137 (79%)	36 (21%)	1 5
7	s5	173/190 (91%)	140 (81%)	33 (19%)	1 6
8	S6	188/201 (94%)	152 (81%)	36 (19%)	1 6
8	s6	187/201 (93%)	152 (81%)	35 (19%)	1 7
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3 12
9	s7	165/169 (98%)	135 (82%)	30 (18%)	1 7
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3 13
10	s8	150/161 (93%)	119 (79%)	31 (21%)	1 5
11	S9	158/165 (96%)	126 (80%)	32 (20%)	1 5
11	s9	158/165 (96%)	124 (78%)	34 (22%)	1 4
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c0	73/98 (74%)	61 (84%)	12 (16%)	2	10
13	C1	129/136 (95%)	115 (89%)	14 (11%)	6	25
13	c1	129/136 (95%)	109 (84%)	20 (16%)	2	11
14	C2	88/118 (75%)	62 (70%)	26 (30%)	0	1
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	1
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	6
15	c3	127/127 (100%)	104 (82%)	23 (18%)	1	7
16	C4	81/104 (78%)	57 (70%)	24 (30%)	0	1
16	c4	97/104 (93%)	70 (72%)	27 (28%)	0	1
17	C5	101/117 (86%)	82 (81%)	19 (19%)	1	6
17	c5	103/117 (88%)	83 (81%)	20 (19%)	1	6
18	C6	117/118 (99%)	90 (77%)	27 (23%)	1	3
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1	7
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1	4
19	c7	92/124 (74%)	72 (78%)	20 (22%)	1	4
20	C8	128/128 (100%)	107 (84%)	21 (16%)	2	10
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	3
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	5
21	c9	115/115 (100%)	94 (82%)	21 (18%)	1	7
22	D0	100/113 (88%)	72 (72%)	28 (28%)	0	1
22	d0	103/113 (91%)	77 (75%)	26 (25%)	0	1
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	8
23	d1	74/74 (100%)	62 (84%)	12 (16%)	2	10
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	9
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3	13
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	7
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2	8
26	D4	112/112 (100%)	98 (88%)	14 (12%)	4	18
26	d4	112/112 (100%)	93 (83%)	19 (17%)	2	9
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0	1
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	2
28	d6	83/83 (100%)	66 (80%)	17 (20%)	1	5
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	11
29	d7	70/70 (100%)	60 (86%)	10 (14%)	3	14
30	D8	56/59 (95%)	43 (77%)	13 (23%)	1	3
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2	8
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	9
31	d9	47/48 (98%)	38 (81%)	9 (19%)	1	6
32	E0	51/51 (100%)	39 (76%)	12 (24%)	1	3
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1
33	e1	66/66 (100%)	50 (76%)	16 (24%)	0	2
34	SR	260/261 (100%)	211 (81%)	49 (19%)	1	6
34	sR	260/261 (100%)	231 (89%)	29 (11%)	6	24
35	SM	97/228 (42%)	80 (82%)	17 (18%)	2	8
35	sM	54/228 (24%)	41 (76%)	13 (24%)	0	2
39	L2	193/195 (99%)	157 (81%)	36 (19%)	1	7
39	l2	192/195 (98%)	158 (82%)	34 (18%)	2	8
40	L3	320/322 (99%)	252 (79%)	68 (21%)	1	4
40	l3	321/322 (100%)	252 (78%)	69 (22%)	1	4
41	L4	288/288 (100%)	230 (80%)	58 (20%)	1	5
41	l4	288/288 (100%)	231 (80%)	57 (20%)	1	5
42	L5	244/244 (100%)	206 (84%)	38 (16%)	2	11
42	l5	243/244 (100%)	191 (79%)	52 (21%)	1	4
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	13
43	l6	135/152 (89%)	114 (84%)	21 (16%)	2	11
44	L7	186/204 (91%)	160 (86%)	26 (14%)	3	15
44	l7	187/204 (92%)	157 (84%)	30 (16%)	2	11
45	L8	187/207 (90%)	157 (84%)	30 (16%)	2	11
45	l8	177/207 (86%)	138 (78%)	39 (22%)	1	4
46	L9	171/171 (100%)	128 (75%)	43 (25%)	0	1
46	l9	171/171 (100%)	136 (80%)	35 (20%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	4
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	9
48	M1	147/150 (98%)	109 (74%)	38 (26%)	0	1
48	m1	147/150 (98%)	117 (80%)	30 (20%)	1	5
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1	6
49	m3	154/158 (98%)	125 (81%)	29 (19%)	1	6
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	7
50	m4	108/108 (100%)	91 (84%)	17 (16%)	2	11
51	M5	175/175 (100%)	139 (79%)	36 (21%)	1	5
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2	9
52	M6	160/161 (99%)	132 (82%)	28 (18%)	2	8
52	m6	160/161 (99%)	134 (84%)	26 (16%)	2	10
53	M7	140/145 (97%)	106 (76%)	34 (24%)	0	2
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	6
54	M8	150/150 (100%)	121 (81%)	29 (19%)	1	6
54	m8	150/150 (100%)	121 (81%)	29 (19%)	1	6
55	M9	153/153 (100%)	131 (86%)	22 (14%)	3	14
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	4
56	N0	156/156 (100%)	127 (81%)	29 (19%)	1	7
56	n0	156/156 (100%)	123 (79%)	33 (21%)	1	5
57	N1	136/136 (100%)	111 (82%)	25 (18%)	1	7
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	4
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2	9
58	n2	85/106 (80%)	65 (76%)	20 (24%)	1	3
59	N3	104/104 (100%)	84 (81%)	20 (19%)	1	6
59	n3	104/104 (100%)	91 (88%)	13 (12%)	4	18
60	N4	57/129 (44%)	50 (88%)	7 (12%)	4	19
60	n4	100/129 (78%)	84 (84%)	16 (16%)	2	11
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	4
61	n5	104/117 (89%)	86 (83%)	18 (17%)	2	9
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	n6	109/109 (100%)	86 (79%)	23 (21%)	1	5
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1	5
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1	4
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	8
64	n8	118/118 (100%)	103 (87%)	15 (13%)	4	18
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	9
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	0
66	O0	81/87 (93%)	63 (78%)	18 (22%)	1	4
66	o0	84/87 (97%)	63 (75%)	21 (25%)	0	2
67	O1	92/96 (96%)	76 (83%)	16 (17%)	2	9
67	o1	94/96 (98%)	68 (72%)	26 (28%)	0	1
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	5
68	o2	109/110 (99%)	87 (80%)	22 (20%)	1	5
69	O3	90/90 (100%)	80 (89%)	10 (11%)	6	24
69	o3	90/90 (100%)	72 (80%)	18 (20%)	1	5
70	O4	95/101 (94%)	77 (81%)	18 (19%)	1	6
70	o4	95/101 (94%)	76 (80%)	19 (20%)	1	5
71	O5	104/104 (100%)	78 (75%)	26 (25%)	0	2
71	o5	103/104 (99%)	84 (82%)	19 (18%)	1	7
72	O6	81/81 (100%)	61 (75%)	20 (25%)	0	2
72	o6	80/81 (99%)	54 (68%)	26 (32%)	0	0
73	O7	70/70 (100%)	52 (74%)	18 (26%)	0	1
73	o7	70/70 (100%)	56 (80%)	14 (20%)	1	5
74	O8	68/68 (100%)	49 (72%)	19 (28%)	0	1
74	o8	67/68 (98%)	51 (76%)	16 (24%)	0	2
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	8
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	8
76	Q0	47/47 (100%)	41 (87%)	6 (13%)	4	18
76	q0	47/47 (100%)	40 (85%)	7 (15%)	3	13
77	Q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2 8
78	q2	90/90 (100%)	67 (74%)	23 (26%)	0 1
79	Q3	71/71 (100%)	55 (78%)	16 (22%)	1 3
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1 6
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1 3
82	p0	105/253 (42%)	87 (83%)	18 (17%)	2 9
All	All	18729/20239 (92%)	15053 (80%)	3676 (20%)	1 6

5 of 3676 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	s0	123	VAL
72	o6	16	LYS
16	c4	136	ARG
70	o4	23	VAL
55	m9	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
69	O3	106	ASN
8	s6	139	ASN
82	p0	37	GLN
46	l9	169	ASN
70	O4	69	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	488 (27%)	54 (3%)
1	6	1792/1800 (99%)	440 (24%)	49 (2%)
36	1	3145/3396 (92%)	696 (22%)	89 (2%)
36	5	3145/3396 (92%)	666 (21%)	74 (2%)
37	3	120/121 (99%)	15 (12%)	0
37	7	120/121 (99%)	20 (16%)	0
38	4	157/158 (99%)	39 (24%)	2 (1%)
38	8	157/158 (99%)	36 (22%)	1 (0%)
All	All	10383/10950 (94%)	2400 (23%)	269 (2%)

5 of 2400 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 269 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	1716	U
36	5	2249	G
36	5	3218	A
36	1	1716	U
36	1	1562	C

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 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	6	2205	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	O3	202	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	Q2	503	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	1	4219	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	c8	203	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	m1	202	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	l9	202	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	1	4212	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	l5	303	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	O7	105	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	o7	503	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	l3	406	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	m6	203	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	4	238	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	1	4218	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	3	214	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	M9	203	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	1	4214	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	8	232	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	M0	304	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	l4	403	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	L3	406	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	2	2179	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	q1	102	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	1	4215	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	4211	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	1	4217	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	6	2204	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	1	4220	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	4	237	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	4	239	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	n9	101	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	D3	202	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	M7	206	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	m0	301	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	M7	205	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
88	3K5	5	4249	-	62,63,63	0.62	1 (1%)	82,95,95	1.38	11 (13%)
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	2	2022	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	m5	305	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	o3	203	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	L4	403	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	N1	201	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	4	236	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	1	4213	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	O7	104	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	M5	302	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	O2	201	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	l5	305	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	m5	304	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	1	4216	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		
86	OHX	m4	202	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
88	3K5	1	4221	-	62,63,63	1.22	2 (3%)	82,95,95	1.47	11 (13%)
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	l3	405	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	l5	306	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	o2	201	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	s4	302	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	3K5	5	4249	-	-	7/29/121/121	0/7/7/7
88	3K5	1	4221	-	-	2/29/121/121	0/7/7/7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4221	3K5	O3-C15	8.97	1.60	1.44
88	5	4249	3K5	O3-C15	-3.50	1.38	1.44
88	1	4221	3K5	C17-C22	-2.16	1.49	1.53

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	1	4221	3K5	O3-C16-C15	7.82	67.35	59.35
88	5	4249	3K5	O14-C34-C35	5.62	120.52	107.70
88	5	4249	3K5	C3-C15-C17	4.49	111.30	103.01
88	1	4221	3K5	O3-C15-C16	-4.41	55.88	59.74
88	5	4249	3K5	O3-C15-C16	3.88	63.14	59.74

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

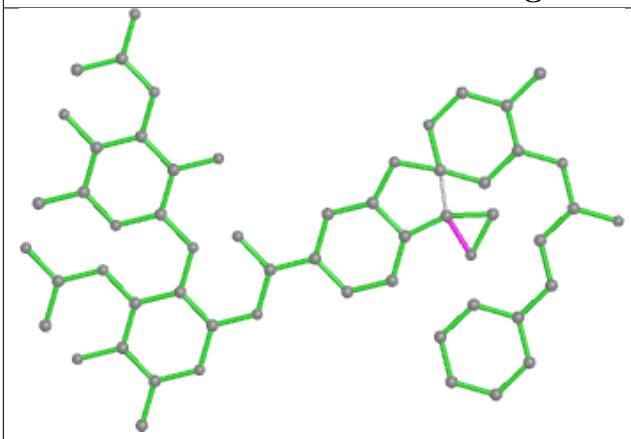
Mol	Chain	Res	Type	Atoms
88	5	4249	3K5	C6-C7-C8-C9
88	5	4249	3K5	C35-C34-O14-C38
88	5	4249	3K5	C39-C38-O14-C34
88	5	4249	3K5	C33-C34-O14-C38
88	5	4249	3K5	O15-C38-O14-C34

There are no ring outliers.

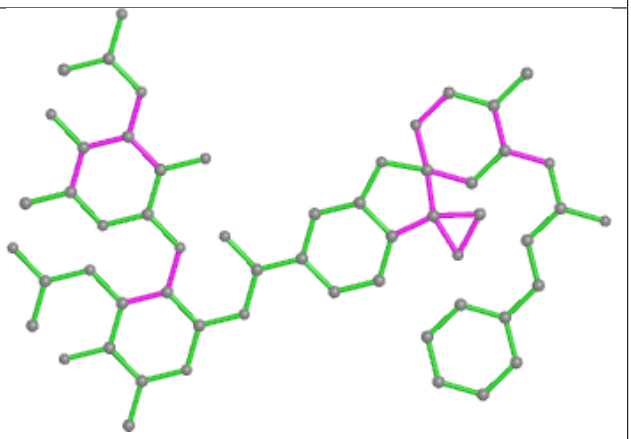
No monomer is involved in short contacts.

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.

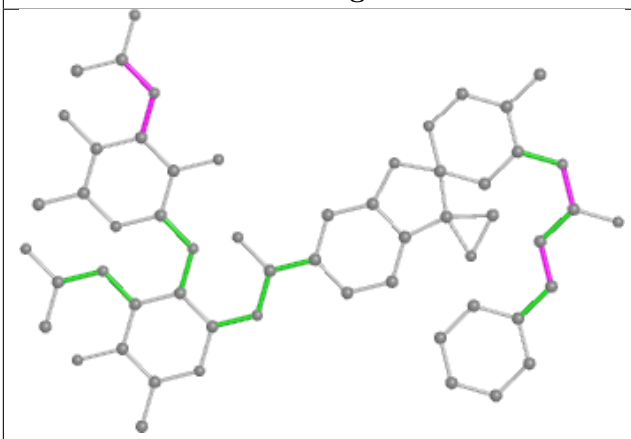
Ligand 3K5 5 4249



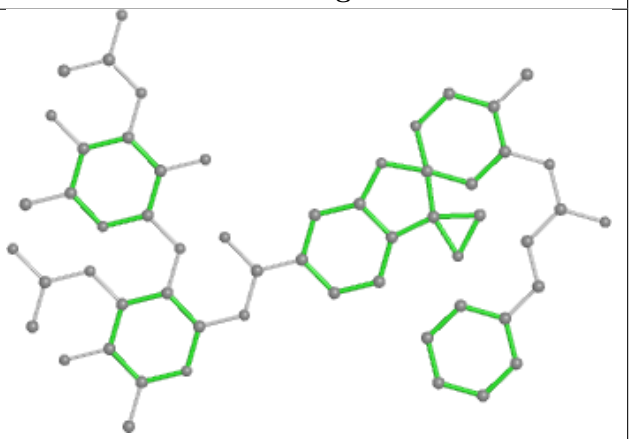
Bond lengths



Bond angles

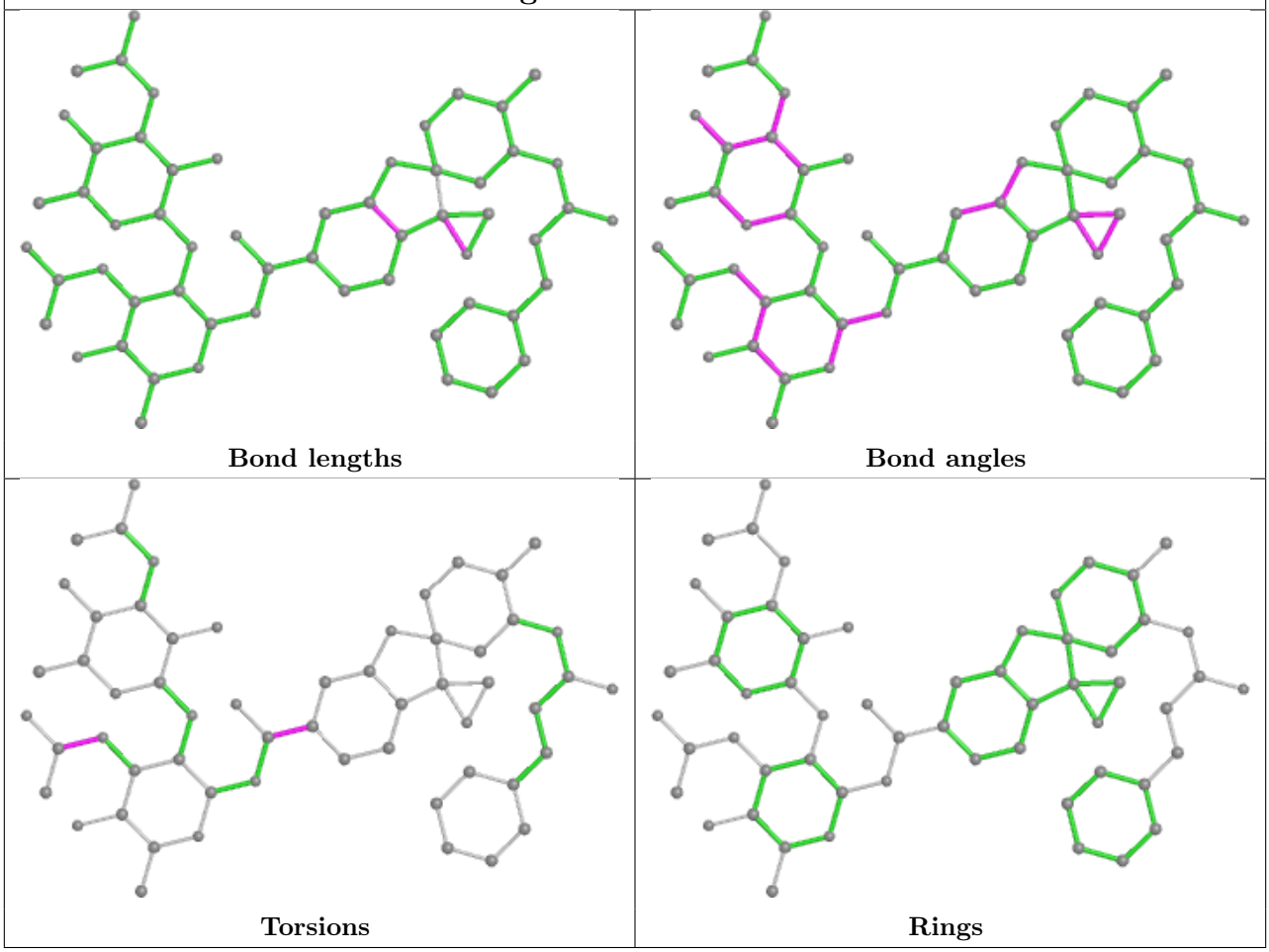


Torsions



Rings

Ligand 3K5 1 4221



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.