



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 07:09 AM BST

PDB ID : 4U52
Title : Crystal structure of Nagilactone C bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), 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) : 2.13

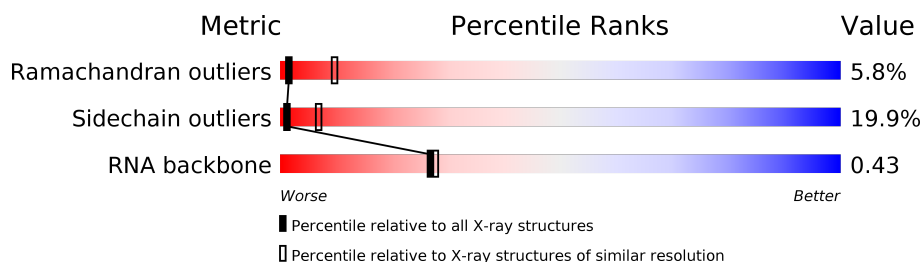
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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















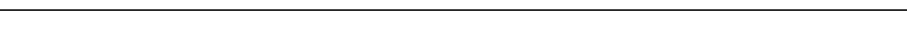




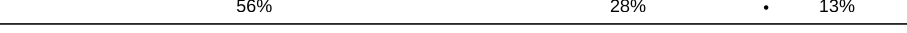





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	59% 32% 6% .
1	6	1800	59% 35% 6%
2	S0	251	61% 20% . 18%
2	s0	251	58% 20% . 18%
3	S1	254	59% 23% . 16%
3	s1	254	65% 18% . 15%
4	S2	253	69% 16% . 14%
4	s2	253	64% 19% . 14%




















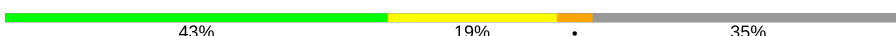





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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	







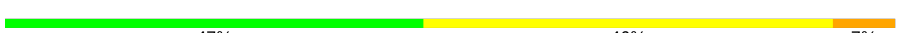




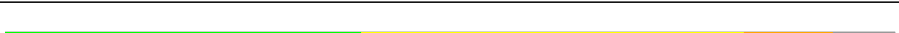


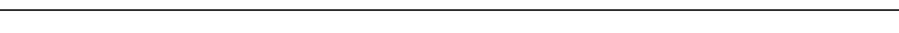




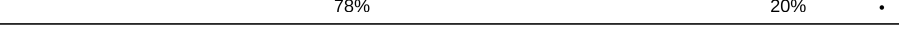





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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	


























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Mol	Chain	Length	Quality of chain
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	















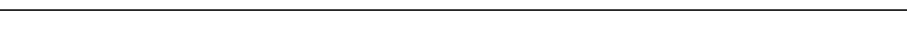




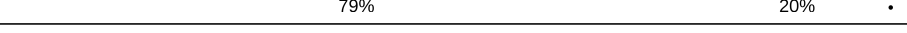





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6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















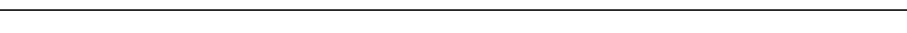




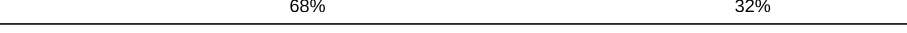





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Mol	Chain	Length	Quality of chain
55	m9	188	 84% 16% .
56	N0	172	 80% 19% .
56	n0	172	 81% 19% .
57	N1	159	 74% 23% .
57	n1	159	 79% 18% .
58	N2	120	 71% 13% 17%
58	n2	120	 71% 11% 18%
59	N3	136	 84% 15% .
59	n3	136	 88% 11% .
60	N4	155	 54% 9% 37%
60	n4	155	 71% 14% . 13%
61	N5	141	 67% 18% . 14%
61	n5	141	 67% 16% . 15%
62	N6	126	 74% 25% .
62	n6	126	 80% 18% .
63	N7	135	 73% 24% .
63	n7	135	 70% 27% .
64	N8	148	 81% 16% .
64	n8	148	 79% 20% .
65	N9	58	 79% 17% .
65	n9	58	 69% 24% 5% .
66	O0	104	 79% 13% . 7%
66	o0	104	 77% 19% .
67	O1	112	 73% 23% . .
67	o1	112	 72% 23% . .

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Mol	Chain	Length	Quality of chain
68	O2	129	 78% 21% .
68	o2	129	 77% 21% ..
69	O3	106	 86% 13% .
69	o3	106	 83% 17%
70	O4	119	 75% 18% . 6%
70	o4	119	 81% 12% . 6%
71	O5	119	 70% 29% .
71	o5	119	 78% 22%
72	O6	99	 72% 26% .
72	o6	99	 73% 27%
73	O7	87	 84% 11% 5%
73	o7	87	 84% 14% .
74	O8	77	 77% 22% .
74	o8	77	 73% 26% .
75	O9	50	 80% 18% .
75	o9	50	 72% 28%
76	Q0	52	 75% 21% .
76	q0	52	 79% 21%
77	Q1	25	 68% 32%
77	q1	25	 60% 32% 8%
78	Q2	105	 78% 17% 5%
78	q2	105	 84% 16%
79	Q3	91	 79% 20% .
79	q3	91	 82% 18%
80	e0	62	 74% 24% .

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Mol	Chain	Length	Quality of chain
81	m2	160	<div><div></div><div>94%6%</div></div>
82	p0	311	<div><div></div><div>38%8%54%</div></div>
83	p1	47	<div><div></div><div>100%</div></div>
84	p2	46	<div><div></div><div>100%</div></div>

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e0	62	VAL	-	expression tag	UNP P0CX33
e0	63	GLN	-	expression tag	UNP P0CX33

- Molecule 81 is a protein called Unknown Protein m2.

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

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

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

- Molecule 83 is a protein called Unknown Protein p1.

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

- Molecule 84 is a protein called Unknown Protein p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	3	Total	Mg	0	0
			3	3		
85	N9	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	n8	5	Total 5	Mg 5	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	150	Total 150	Mg 150	0	0
85	sM	2	Total 2	Mg 2	0	0
85	O4	1	Total 1	Mg 1	0	0
85	m5	4	Total 4	Mg 4	0	0
85	l3	2	Total 2	Mg 2	0	0
85	M1	1	Total 1	Mg 1	0	0
85	n0	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	125	Total 125	Mg 125	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	3	Total 3	Mg 3	0	0
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	5	502	Total 502	Mg 502	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	M4	1	Total 1	Mg 1	0	0
85	n9	1	Total 1	Mg 1	0	0
85	1	469	Total 469	Mg 469	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	3	Total 3	Mg 3	0	0
85	M8	1	Total 1	Mg 1	0	0
85	q3	1	Total 1	Mg 1	0	0
85	o3	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	22	Total 22	Mg 22	0	0
85	n6	1	Total 1	Mg 1	0	0

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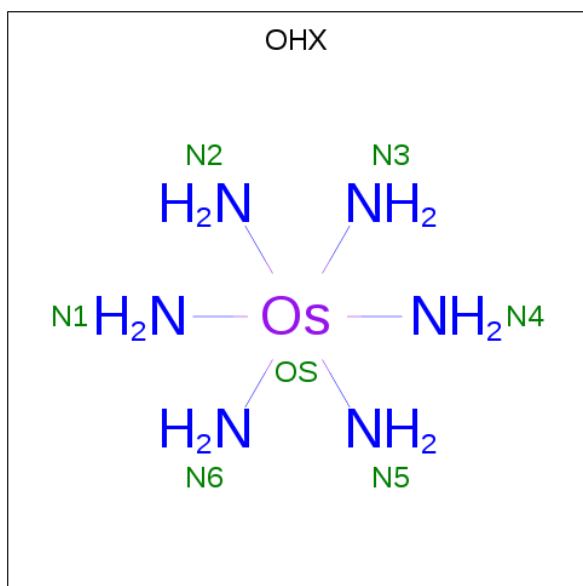
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L2	3	Total 3	Mg 3	0	0
85	m1	2	Total 2	Mg 2	0	0
85	l5	1	Total 1	Mg 1	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	3	Total 3	Mg 3	0	0
85	N8	5	Total 5	Mg 5	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	O1	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	l8	1	Total 1	Mg 1	0	0
85	c7	2	Total 2	Mg 2	0	0
85	7	17	Total 17	Mg 17	0	0
85	n3	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	m6	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	8	15	Total 15	Mg 15	0	0
85	m0	1	Total 1	Mg 1	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	3	14	Total	Mg	0	0
			14	14		

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	S9	1	Total	N	Os	0	0
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86	C3	1	Total	N	Os	0	0
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86	C5	1	Total	N	Os	0	0
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86	C8	1	Total	N	Os	0	0
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86	D9	1	Total	N	Os	0	0
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86	SR	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	L3	1	Total	N	Os	0	0
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86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
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86	M5	1	Total	N	Os	0	0
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86	M6	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M7	1	Total	N	Os	0	0
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86	M8	1	Total	N	Os	0	0
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86	M9	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
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86	O2	1	Total	N	Os	0	0
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86	O3	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O7	1	Total	N	Os	0	0
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86	O9	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	d4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	19	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m9	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n6	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q1	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

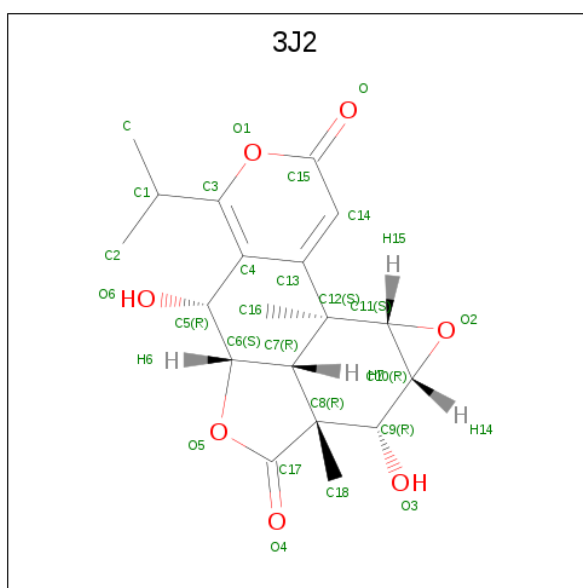
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	D7	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		

- Molecule 88 is Nagilactone C (three-letter code: 3J2) (formula: $C_{19}H_{22}O_7$).



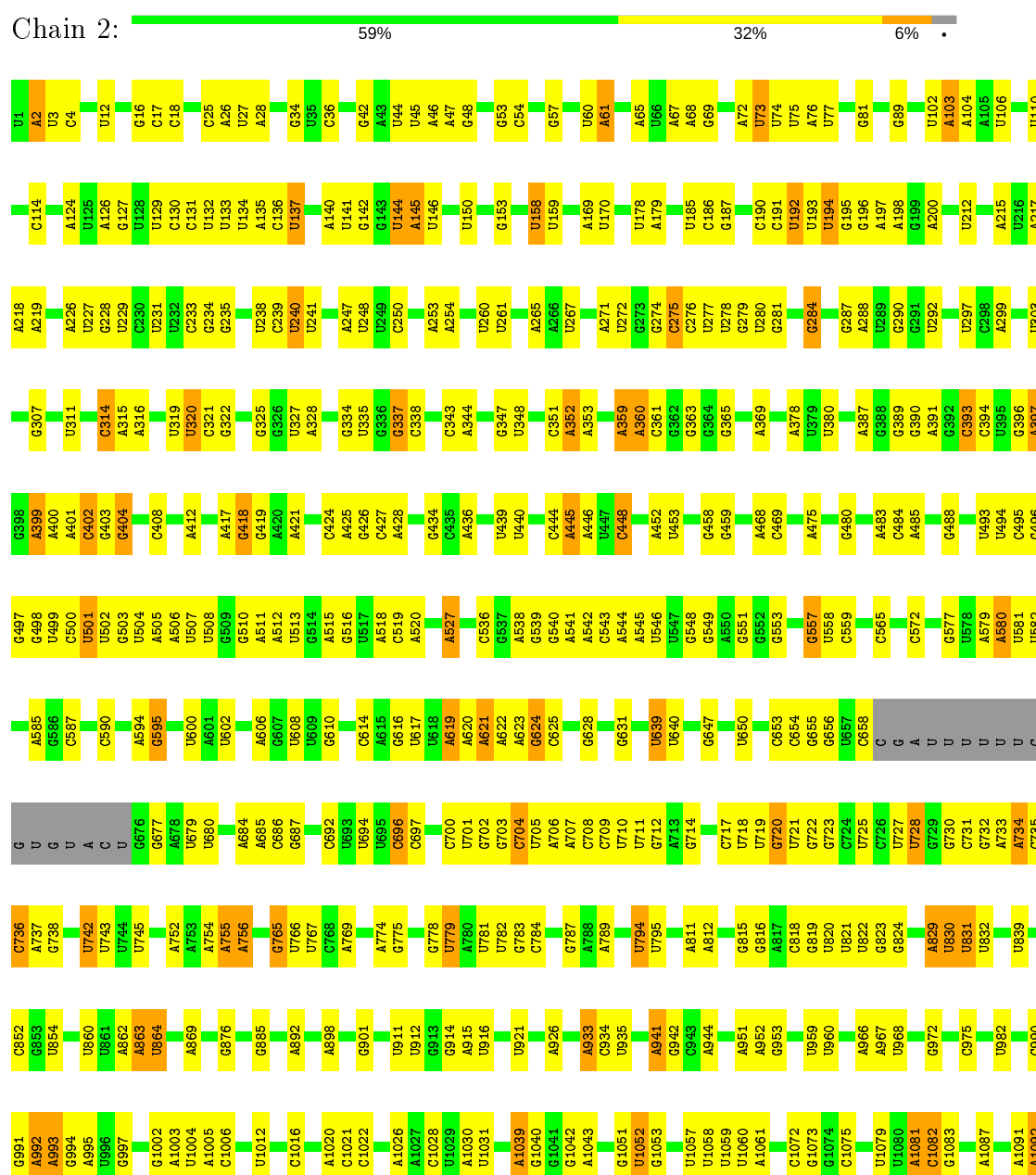
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			26	19	7		
88	5	1	Total	C	O	0	0
			26	19	7		

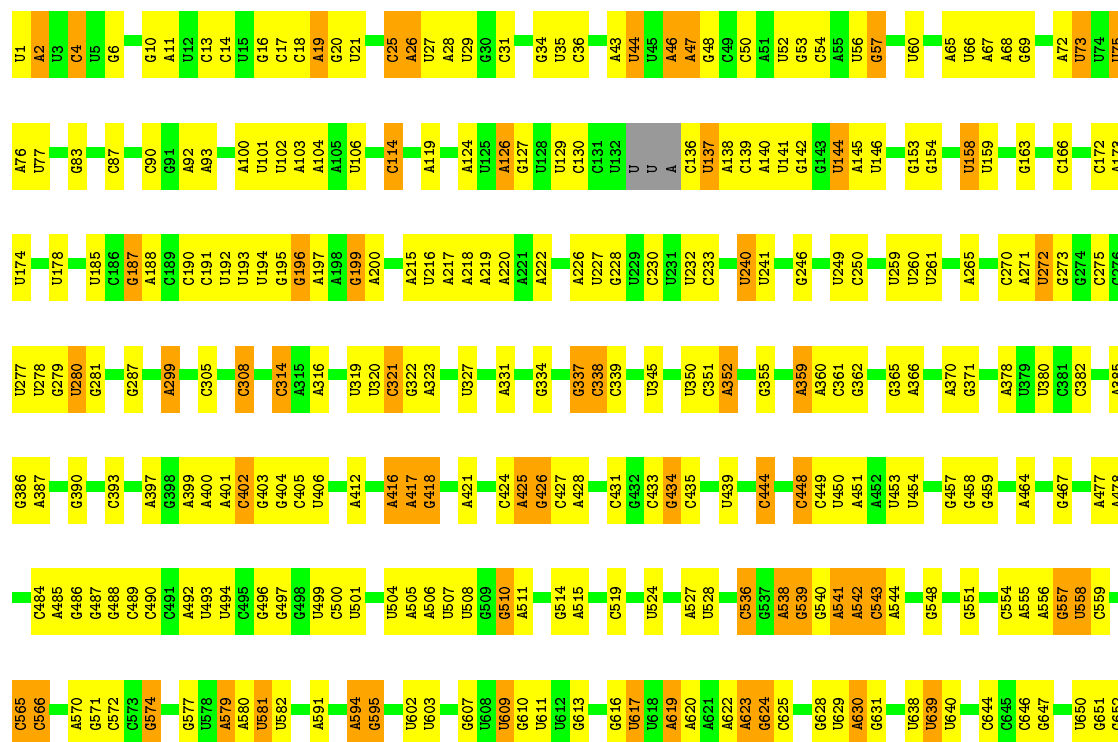
3 Residue-property plots

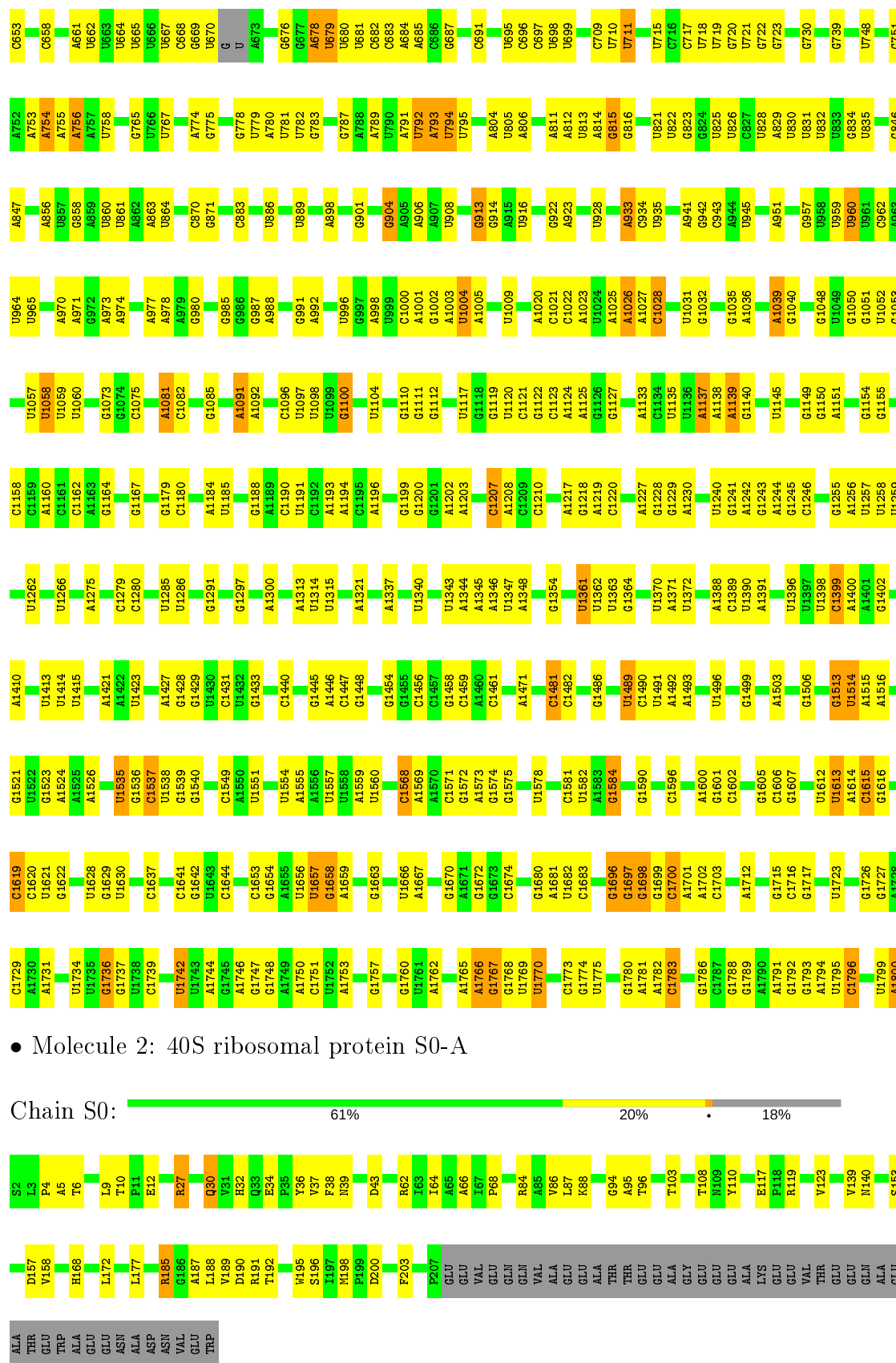
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

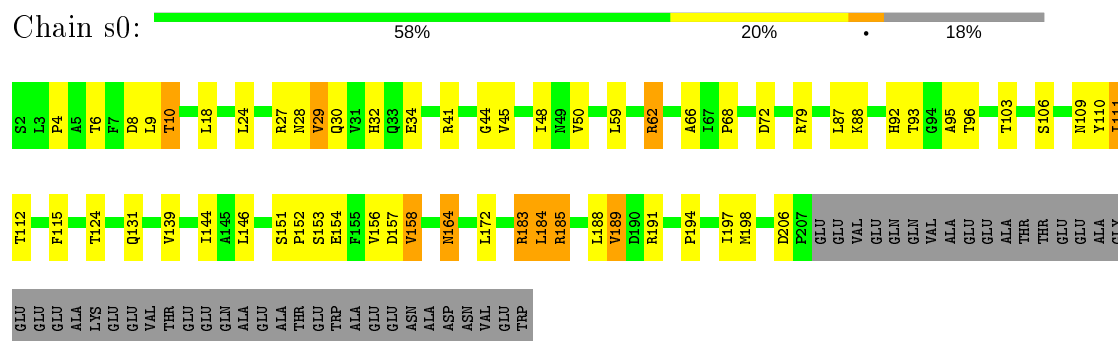
- Molecule 1: 18S ribosomal RNA



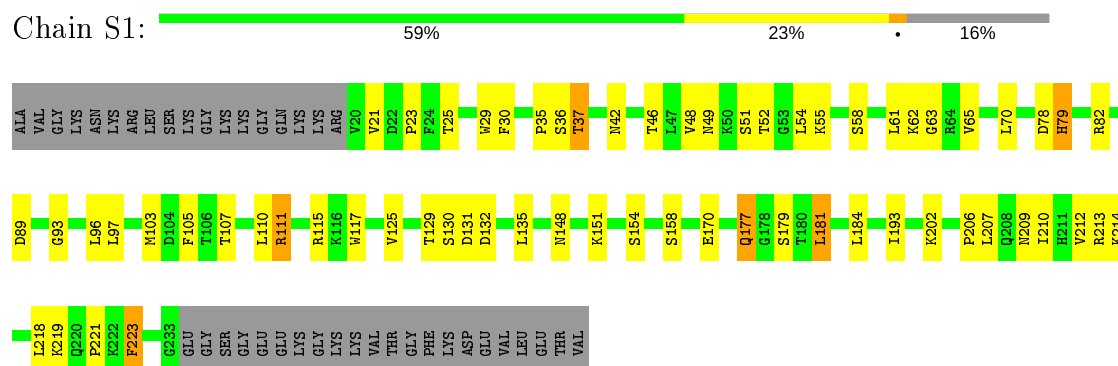




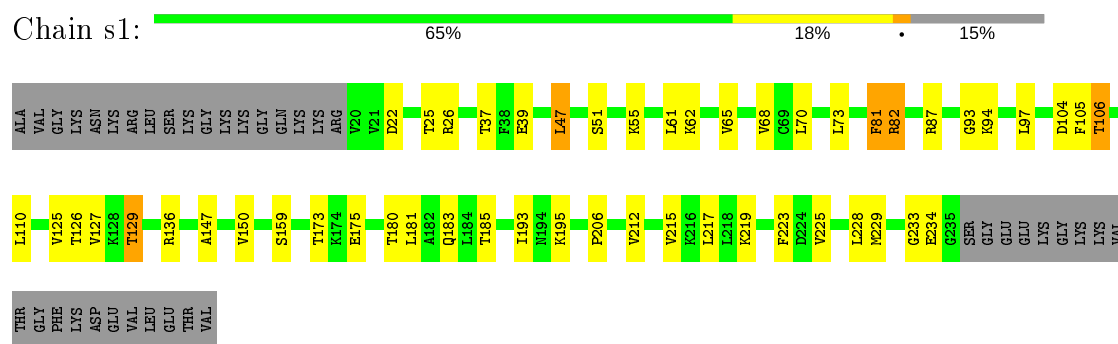
• Molecule 2: 40S ribosomal protein S0-A



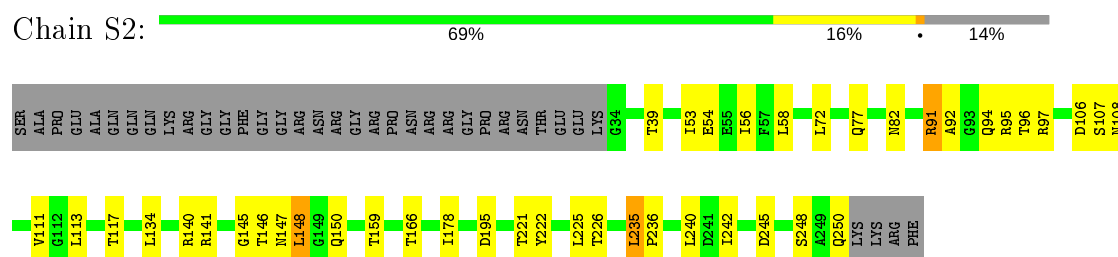
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 3: 40S ribosomal protein S1-A

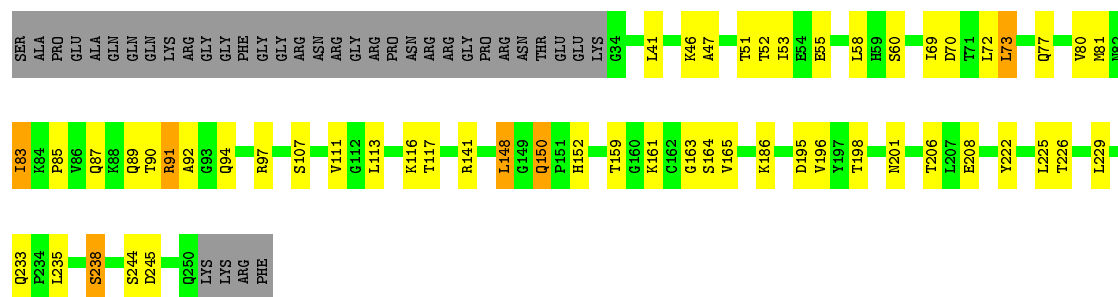


- Molecule 4: 40S ribosomal protein S2



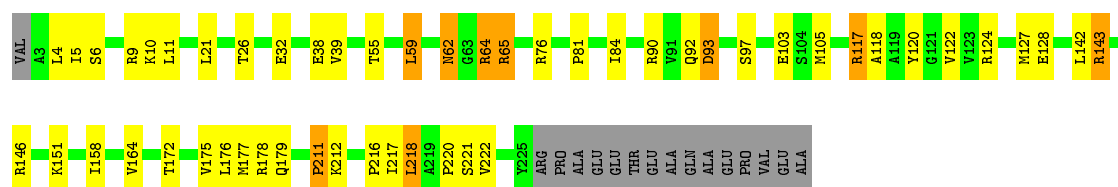
- Molecule 4: 40S ribosomal protein S2





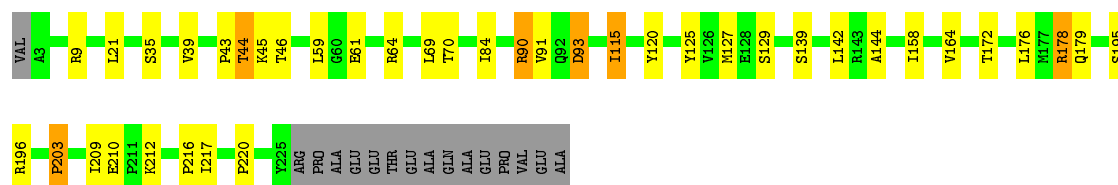
- Molecule 5: 40S ribosomal protein S3

Chain S3: 72% 18% 7%



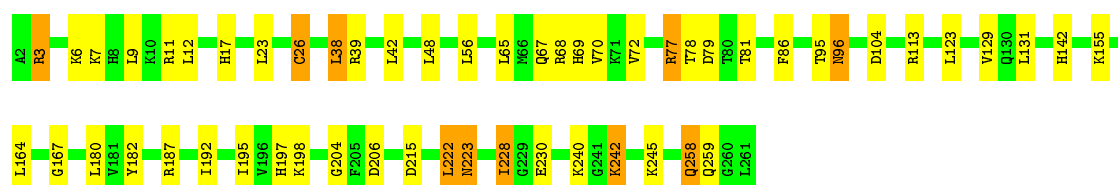
- Molecule 5: 40S ribosomal protein S3

Chain s3: 77% 14% 7%



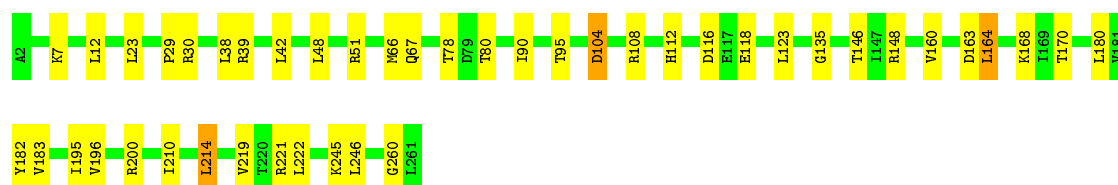
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 79% 17% 4%



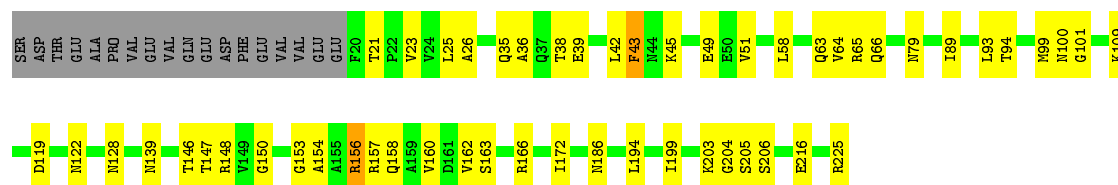
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 83% 16% 1%



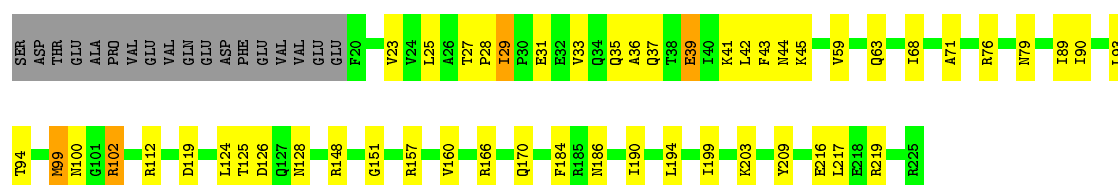
- Molecule 7: 40S ribosomal protein S5

Chain S5: 




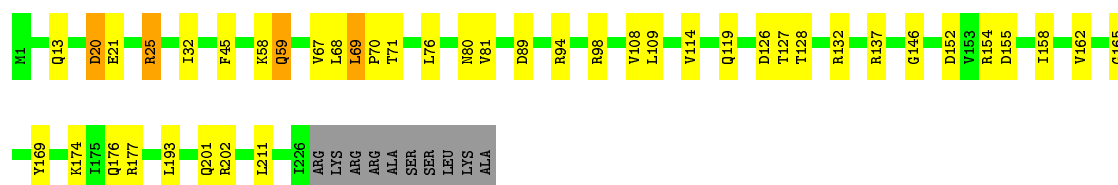
- Molecule 7: 40S ribosomal protein S5

Chain s5: 



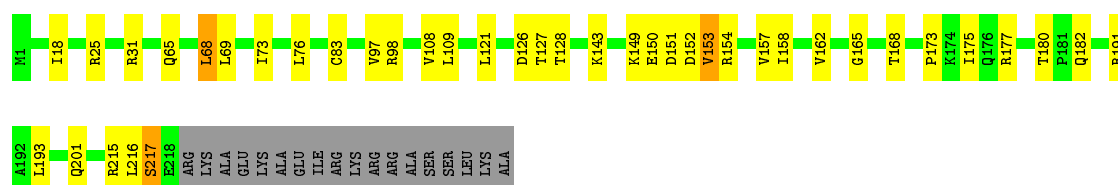
- Molecule 8: 40S ribosomal protein S6-A

Chain S6: 



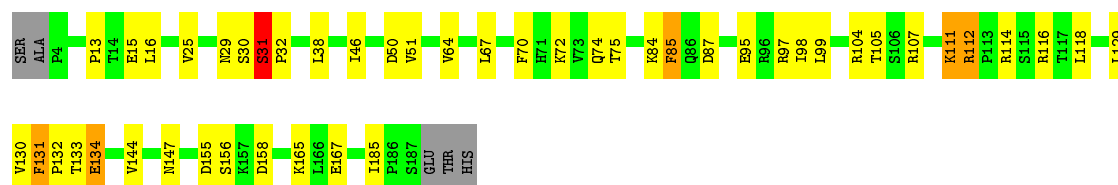
- Molecule 8: 40S ribosomal protein S6-A

Chain s6: 



- Molecule 9: 40S ribosomal protein S7-A

Chain S7: 



- Molecule 12: 40S ribosomal protein S10-A

M1	I11	H12	V20	F27	N28	Q29	A30	K31	H32	I35	T50	S51	K52	Q53	V54	V55	K56	S60	W61	E74	N81	L82	I86	W87	P88	E94	R95	N96	PRO	THR	GIN	ARG	PRO	GIN	ARG	ARG	TRV
----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | L2 | N3 | P4 | K5 | L15 | V20 | A23 | K24 | A30 | K31 | H32 | I35 | D36 | L49 | T50 | S51 | V55 | K56 | T57 | E70 | E71 | L82 | P83 | P84 | HIS | I1E | V87 | P88 | I92 | Q93 | E94 | N95 | N96 | P97 | T98 | GLN | ARG | PRO | ARG | GLN | ARG | ARG | ARG |
|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|------|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|
| F156 | S2 | T3 | E4 | V7 | E10 | I21 | V25 | K29 | R30 | L40 | T44 | D55 | L63 | R67 | G68 | R69 | I70 | L71 | K79 | R80 | T83 | P85 | V96 | R99 | K105 | V109 | P113 | Q118 | V123 | Q127 | C128 | R136 | V140 | A145 | A154 | G155 |
|------|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|

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|------|------|
| F137 | S2 |
| N138 | T3 |
| V139 | E4 |
| V140 | T5 |
| | L6 |
| S143 | V7 |
| A144 | E10 |
| G147 | N21 |
| ALA | N22 |
| ASN | |
| LYS | T27 |
| GLN | T31 |
| PHE | K32 |
| ALA | R33 |
| LYS | K34 |
| PHE | V35 |
| | L40 |
| | T44 |
| | T47 |
| | D55 |
| | F60 |
| | V64 |
| | R67 |
| | E68 |
| | K69 |
| | V76 |
| | S77 |
| | I86 |
| | P95 |
| | K96 |
| | V109 |
| | S112 |
| | R116 |
| | D121 |
| | I122 |
| | V123 |
| | C128 |
| | R129 |
| | K133 |
| | R136 |

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|------|-----|
| L97 | SER |
| L103 | ASP |
| L106 | VAL |
| D107 | GLU |
| R113 | GLU |
| K114 | VAL |
| V115 | GLN |
| V116 | GLU |
| G117 | THR |
| A118 | VAL |
| S119 | VAL |
| N125 | GLU |
| W126 | GLN |
| G127 | THR |
| A128 | E20 |
| E129 | E21 |
| T130 | V22 |
| D131 | E25 |
| E132 | E25 |
| E138 | L28 |
| H139 | R29 |
| F140 | V30 |
| Q143 | R33 |
| | T34 |
| | A35 |
| | L36 |
| | V37 |
| | R43 |
| | R50 |
| | A51 |
| | L52 |
| | T53 |
| | R54 |
| | G55 |
| | V66 |
| | T67 |
| | E68 |
| | I71 |
| | E83 |
| | V86 |
| | P87 |
| | L88 |
| | R89 |
| | K90 |
| | V91 |
| | A92 |
| | D93 |

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|--|-----|--|-----|--|-----|-----|--|-----|-----|--|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|--|------|------|------|
| SER | ASP | VAL | GLU | GLU | VAL | VAL | GLU | GLN | GLU | THR | VAL | VAL | GLU | GLN | THR | A20 | E21 | V22 | | V30 | | L36 | V37 | H38 | D39 | | L45 | | L52 | | L58 | L59 | | L62 | V63 | | I71 | | L74 | | F82 | E83 | N84 | K85 | V86 | F87 | L88 | I89 | K90 | V91 | | L97 | | A101 | G102 | L103 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|--|-----|-----|-----|-----|--|-----|--|-----|--|-----|-----|--|-----|-----|--|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|--|------|------|------|



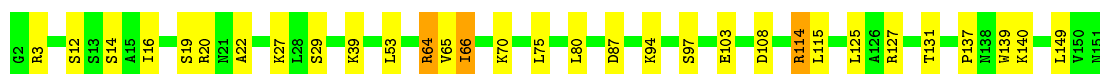
- Molecule 15: 40S ribosomal protein S13

Chain C3: 84% 13%



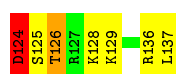
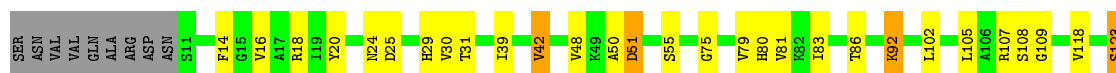
- Molecule 15: 40S ribosomal protein S13

Chain c3: 79% 19%



- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 67% 22% 7%



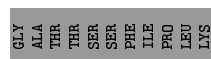
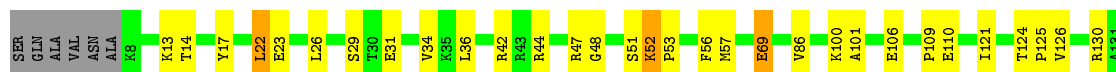
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 68% 24% 6%



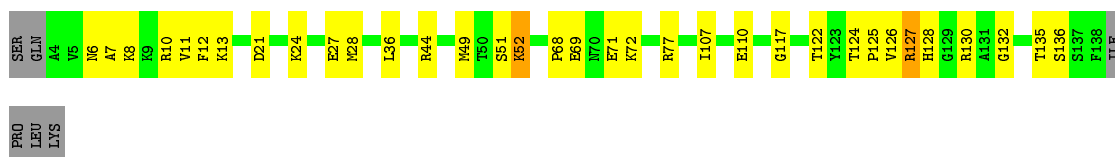
- Molecule 17: 40S ribosomal protein S15

Chain C5: 66% 20% 12%



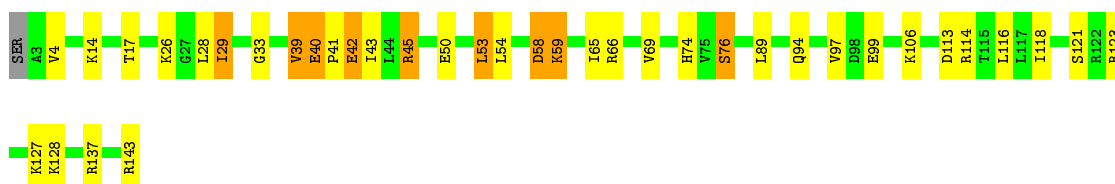
- Molecule 17: 40S ribosomal protein S15

Chain c5: 72% 23%



- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 73% 20% 6%



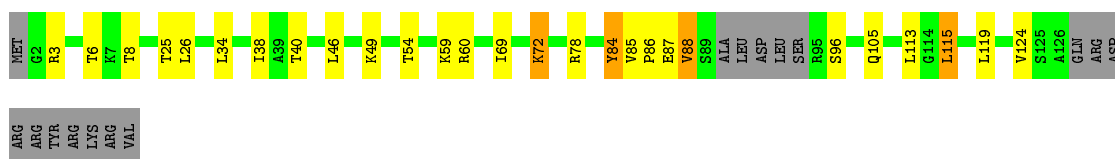
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 75% 25%



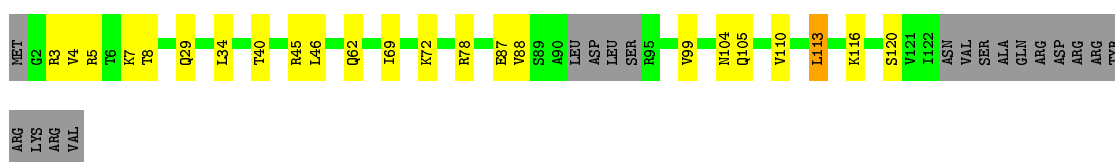
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 68% 17% 12%



- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 69% 16% 14%

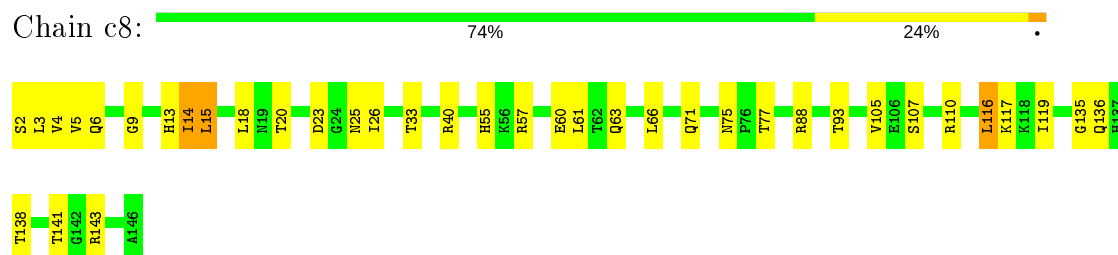


- Molecule 20: 40S ribosomal protein S18-A

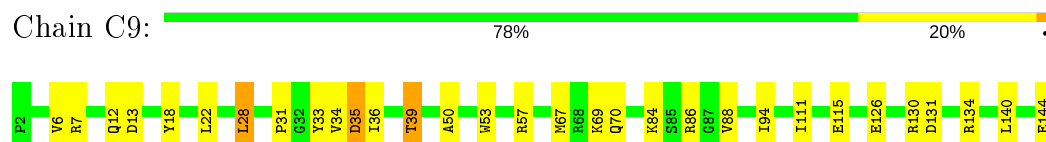
Chain C8: 74% 20% 6%



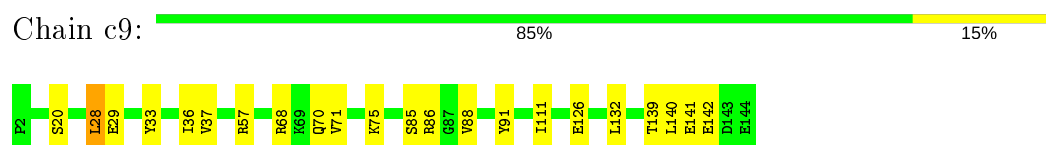
- Molecule 20: 40S ribosomal protein S18-A



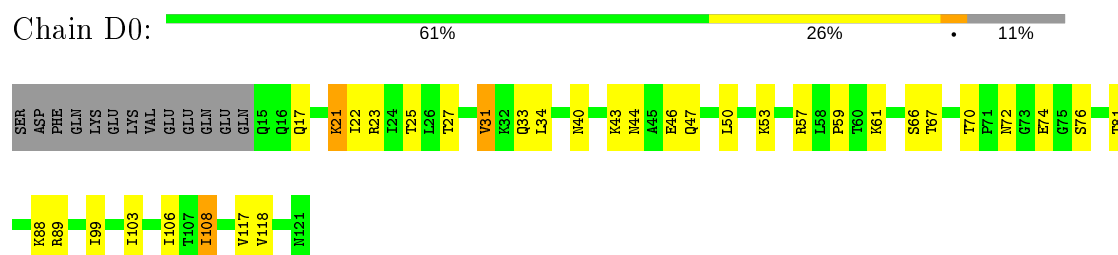
- Molecule 21: 40S ribosomal protein S19-A



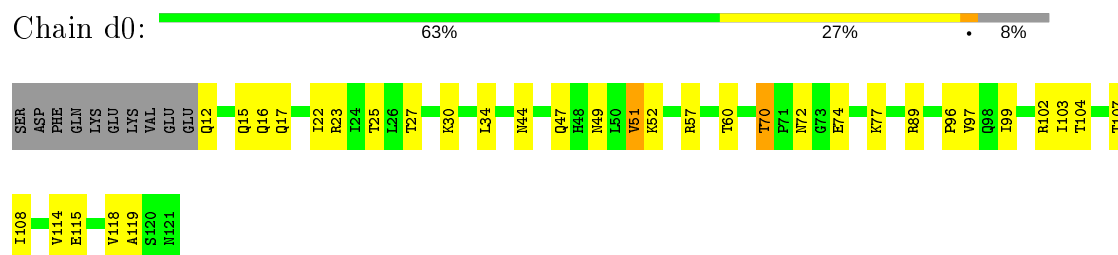
- Molecule 21: 40S ribosomal protein S19-A



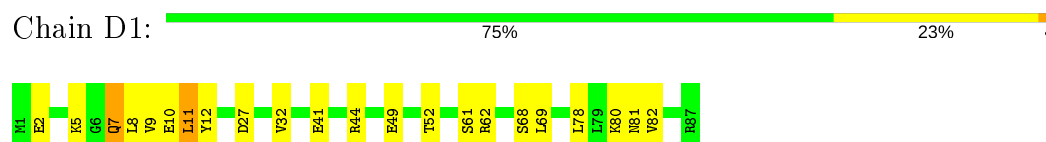
- Molecule 22: 40S ribosomal protein S20



- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A




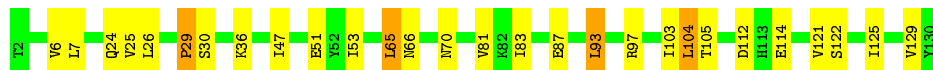
- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  72% 28%



- Molecule 24: 40S ribosomal protein S22-A

Chain D2:  78% 19%




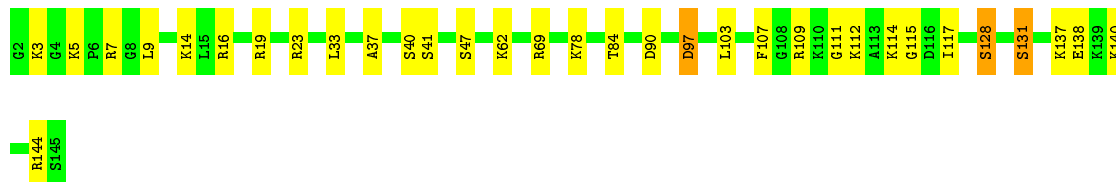
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:  87% 12%




- Molecule 25: 40S ribosomal protein S23-A

Chain D3:  77% 21%




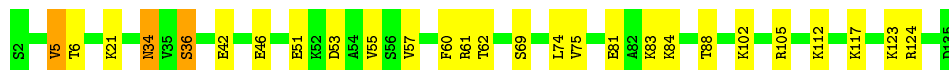
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:  79% 20%



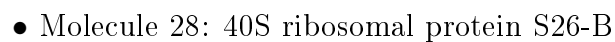
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:  80% 18%



- Molecule 26: 40S ribosomal protein S24-A

Chain d4:  75% 23%





- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 71% 24% 5%



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 80% 12% 5% • 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 75% 20% • •



- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 71% 22% • •



- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 72% 27% •



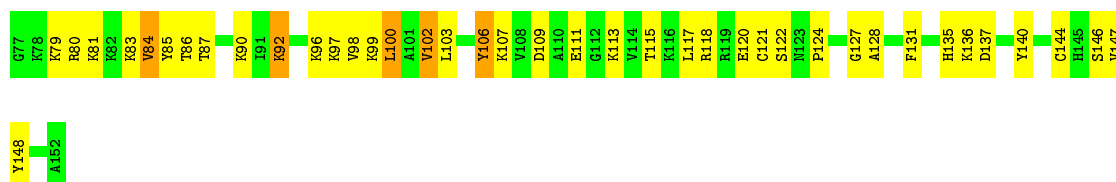
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 50% 33% 11% 7%



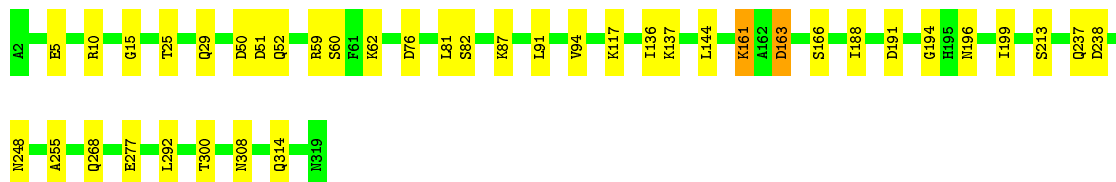
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 47% 46% 7%



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

Chain SR: 87% 12% •



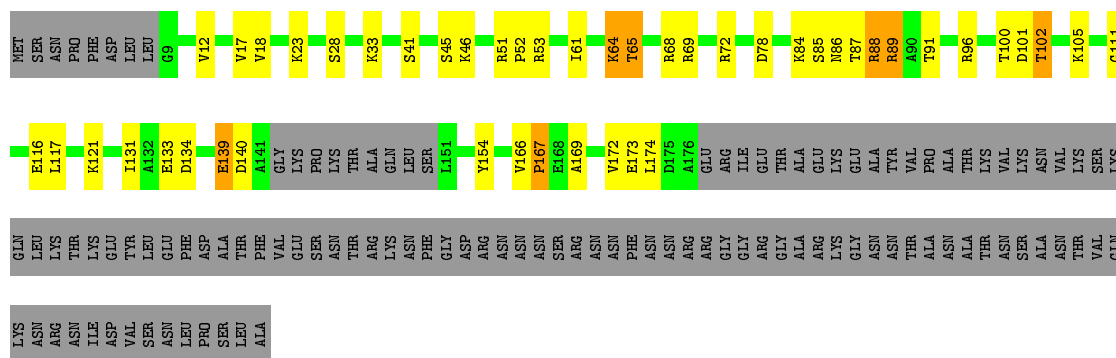
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 87% 13% •



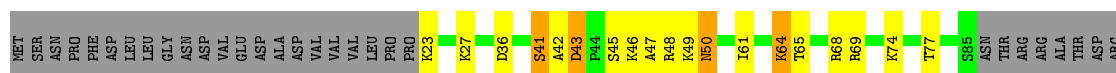
- Molecule 35: Suppressor protein STM1

Chain SM: 41% 15% • 42%



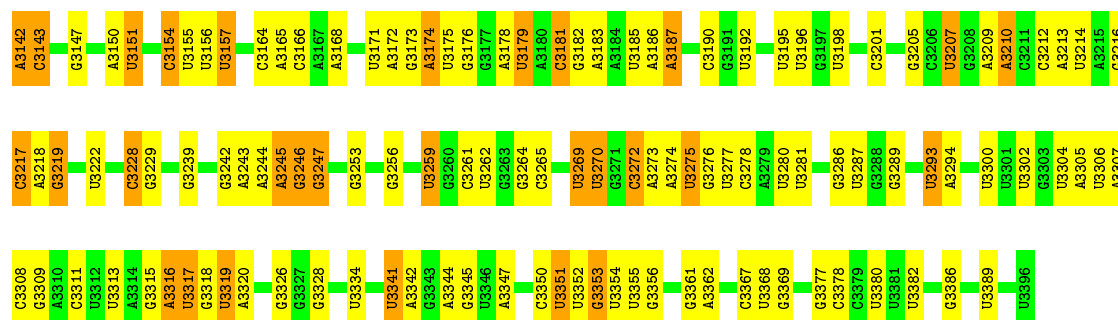
- Molecule 35: Suppressor protein STM1

Chain sM: 30% 7% • 62%

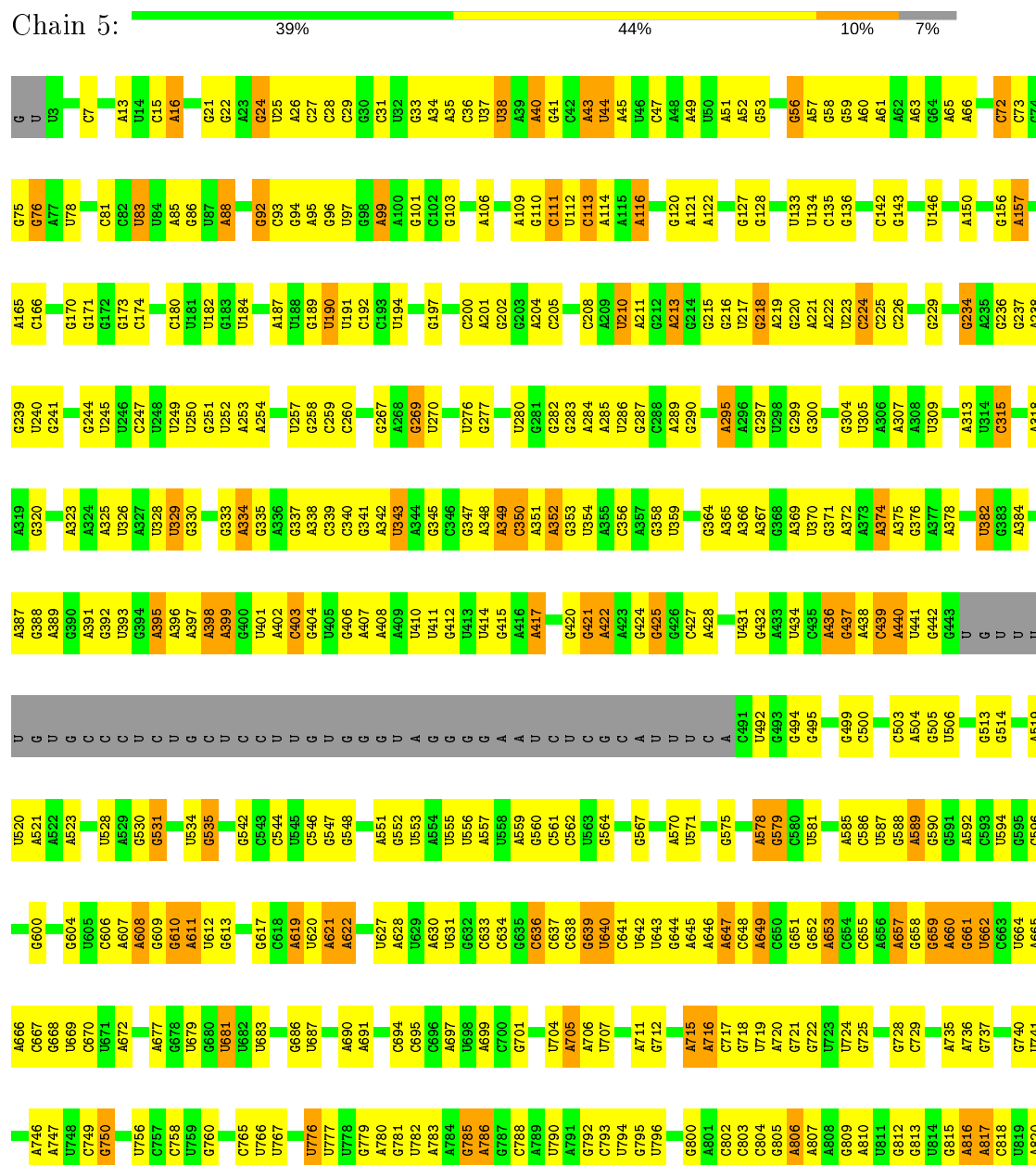


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G	G1919	A1841	A1760	C1548	A1475	U1641	C1339	U1265	A1965	U1122	U1041	U966	A904
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C	U1930	A1850	A1654	A1559	G1488			A1274	A1197	G1131	C975		A915
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U3139	U2973	A2843	U2908	U2759	U2687	U2623	U	U2462	U2398	A2332	A2178	C
G3140	G2974	C2844	U2909	G2777	U2688	G2624	G	U2463	U2399	U2333	C2179	U
U3141	U2975	U2845	U2910	U2778	U2689	U2625	A	U2464	U2400	U2334	U2180	C
C3142	A2976	A2846	U2911	U2779	U2690	A2626	G	U2465	A2401	U2335	G2181	A
U3143	U2976	U2847	U2912	A2780	U2691	G2627	C	U2466	A2402	U2336		
U3144	C2977	G2848	U2913	U2781	U2692	U2628	U	U2467	A2403	C2337		
	U2978	C2849	U2914	U2782	U2693	U2629	U	U2468	A2404	U2338		
	G2979	U2915	U2915	U2783	U2694	U2630	C	U2469		U2339		
	U2979	G2917	U2917	G2787	U2695	C2630	G	U2470		C2340		
		A2851			U2696	C2631		U2471		C2341		
					U2697	C2632		U2472		C2342		
					U2698	G2633		U2473		C2343		
					U2699	G2634		U2474		C2344		
					U2700	G2635		U2475		C2345		
					U2701	G2636		U2476		C2346		
					U2702	G2637		U2477		C2347		
					U2703	G2638		U2478		C2348		
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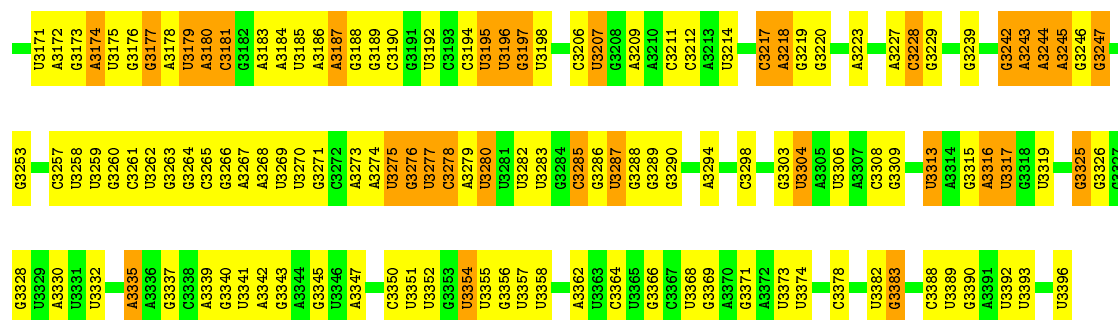


● Molecule 36: 25S ribosomal RNA



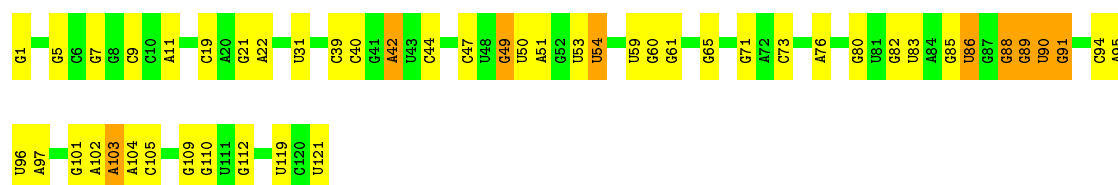


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G3102	A3032	G2960	U2826	G2753	C2685	A2609	U2509	A	A2384	A2313	A2243	G2157	G
G3103	G2962	G2961	U2827	G2754	G2686	G2610	G2510	G	G2385	G2314	A2244	A2158	U
U3104	G3033	U2963	G2828	C2755	A2687	U2611	A2511	G	A2386	G2315	G2245	G2159	C
U3105	G3034	C2963	U2829	G2756	G2688	G2614	C2512	G	A2387	G2316	G2246	G2160	G
A3106	U3038	G2964	G2830	U2757	U2689	G2615	U2513	U	U2388	U2318	G2247	G2161	C
U3107	C3039	G2968	G2831	A2758	A2690	G2616	U2514	U	C2389	G2248	G2249	A2164	U
C3110	A3040	A2969	A2832	U2762	A2691	U2617	A2515	U	G2390	G2249	G2250	G2165	U
C3115	U3041	G2970	A2833	U2763	A2692	G2618	A2523	G	G2391	G2250	G2251	G2169	C
U3119	U3042	A2971	U2835	U2767	C2693	G2619	A2524	A	G2392	A2326	G2252	G2170	U
C3120	C3043	G2972	G2836	U2767	A2694	G2620	G2525	A	G2393	U2327	A2253	G2171	A
U3121	G3044	G2973	A2837	G2770	A2695	G2621	C2526	U	G2394	G2337	G2254	A2172	C
A3122	A3045	U2974	U2838	U2771	A2696	G2622	G2530	A	U2334	A2254	U2255	A2173	A
A3123	U3046	U2975	G2842	U2771	A2697	G2623	C2531	U	A2397	A2256	G2257	G2174	U
A3124	U3047	U2976	U2843	C2772	G2698	G2624	U2542	G	G2398	G2258	C2257	U2175	U
G3125	A3048	G2977	C2844	C2773	G2699	A2626	U2543	G	U2336	U2259	U2258	U2176	A
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C3127	U3050	U2979	U2846	C2775	A2703	U2631	C2549	G	C2338	U2269	U2269	A2183	C
G3128	U3051	C2980	A2847	G2776	A2704	U2632	U2541	G	U2339	A2270	A2271	U2184	C
C3129	G3052	C2983	G2848	G2777	A2705	G2633	U2542	A	A2340	G2271	G2272	U2185	C
U3130	G3053	G2984	U2849	G2778	G2706	U2634	U2543	C	C2405	U2264	U2264	U2186	C
A3131	U3054	C2985	C2850	U2783	C2707	A2635	G2549	U	C2406	U2264	U2264	U2187	C
C3132	U3055	U2986	A2851	U2783	C2708	A2636	U2550	U	U2407	U2264	U2264	G2187	C
C3133	U3056	U2987	C2852	G2787	C2709	A2637	U2551	C	U2408	U2264	U2264	A2188	C
G3134	U3057	C2988	U2853	C2788	C2710	G2638	C2552	G	C2409	U2264	U2264	U2189	C
U3135	A3058	U2989	U2854	C2788	C2711	U2639	U2553	C	U2410	U2264	U2264	U2190	C
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A3141	A3070	U2995	U2860	C2797	C2717	G2644	C2559	U	U2416	U2264	U2264	G2200	C
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C3143	G3075	C2997	U2862	C2799	G2714	C2646	U2570	G	A2418	U2264	U2264	G2202	C
C3144	C3076	A3000	U2863	U2799	U2715	A2647	U2571	A	A2419	U2264	U2264	G2203	C
C3145	A3077	C3001	U2864	U2725	C2726	G2648	C2572	A	C2420	U2264	U2264	G2204	C
G3146	U3078	U3002	U2865	C2726	A2727	A2649	G2573	U	U2421	U2264	U2264	G2205	C
G3147	U3079	G3003	C2870	A2728	G2728	U2650	G2574	U	C2422	U2264	U2264	G2206	C
U3148	G3080	C3004	G2871	G2729	U2729	U2652	G2584	C	G2425	U2264	U2264	G2207	C
C3081	A3086	A3085	A2872	U2806	G2730	C2653	G2585	C	U2426	U2264	U2264	G2208	C
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G3083	A3088	A3087	U2874	A2808	G2732	C2655	U2587	C	A2430	U2264	U2264	G2210	C
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U3157	A3091	C3090	C2877	C2812	U2735	G2660	C2594	C	U2433	U2264	U2264	U2140	C
C3158	U3092	U3091	G2878	A2813	A2736	G2661	A2595	C	G2434	U2264	U2264	U2141	C
C3159	G3093	C3092	C2879	G2814	C2737	G2662	U2596	C	U2435	U2264	U2264	U2142	C
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C3161	C3095	C3094	U2881	G2816	U2739	C2664	U2598	U	G2437	U2264	U2264	U2224	C
C3162	A3096	U3095	U2882	A2817	A2740	U2668	C2600	A	A2438	U2264	U2264	G2231	C
A3163	C3097	G3022	U2883	U2818	U2741	A2673	A2601	U	G2439	U2264	U2264	G2232	C
A3164	C3098	C3097	U2884	U2819	U2742	A2674	G2602	A	U2440	U2264	U2264	A2145	C
A3165	U3099	C3098	U2885	A2820	A2743	A2675	G2603	U	G2441	U2264	U2264	G2233	C
C3166	G3025	U3099	U2886	C2821	U2744	A2676	U2604	C	U2442	U2264	U2264	A2146	C
A3167	C3096	U3098	U2887	A2822	A2747	A2677	G2605	U	A2443	U2264	U2264	G2234	C
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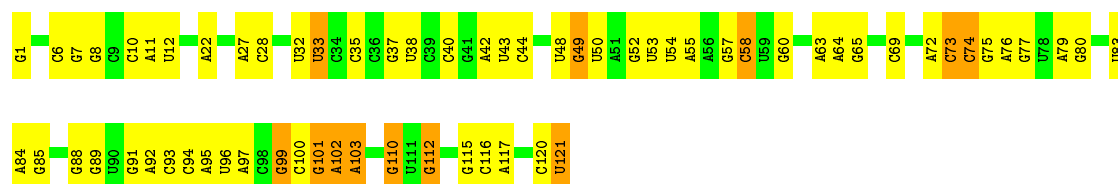
• Molecule 37: 5S ribosomal RNA

Chain 3: 60% 33% 7%



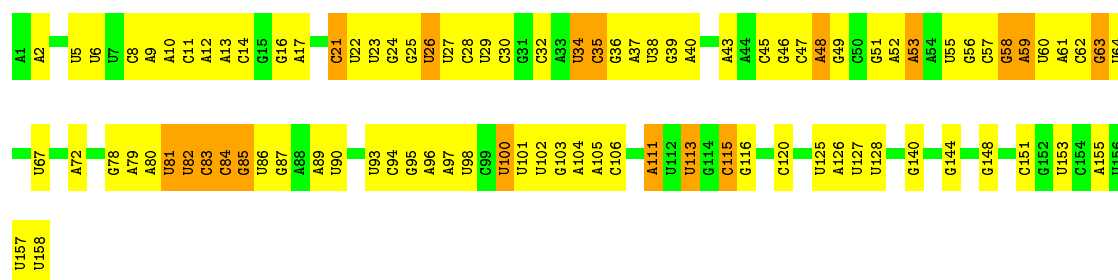
• Molecule 37: 5S ribosomal RNA

Chain 7: 46% 44% 10%



• Molecule 38: 5.8S ribosomal RNA

Chain 4: 41% 47% 11%



• Molecule 38: 5.8S ribosomal RNA

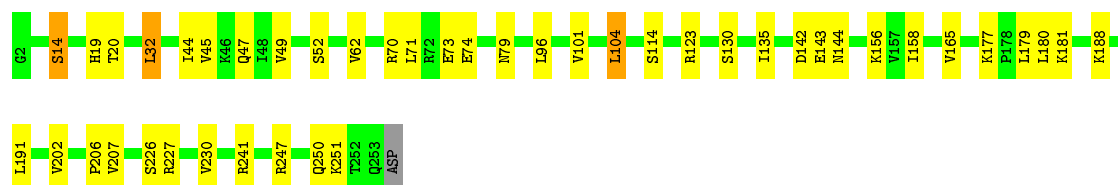
Chain 8: 55% 35% 10%





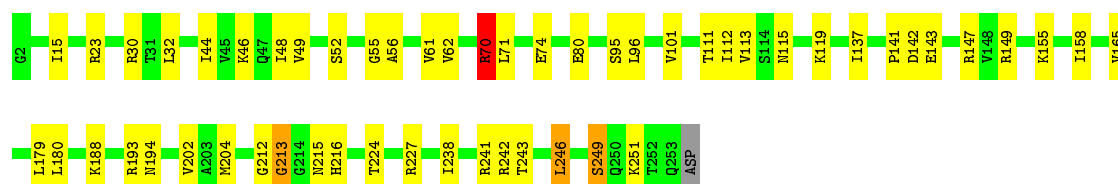
- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 82% 16%



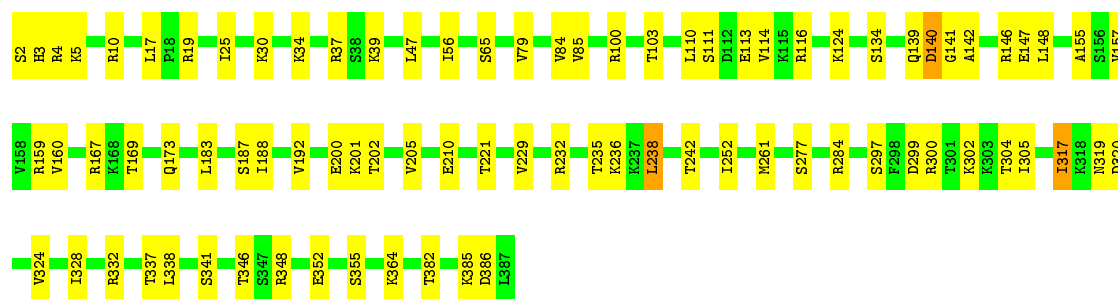
- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 78% 20%



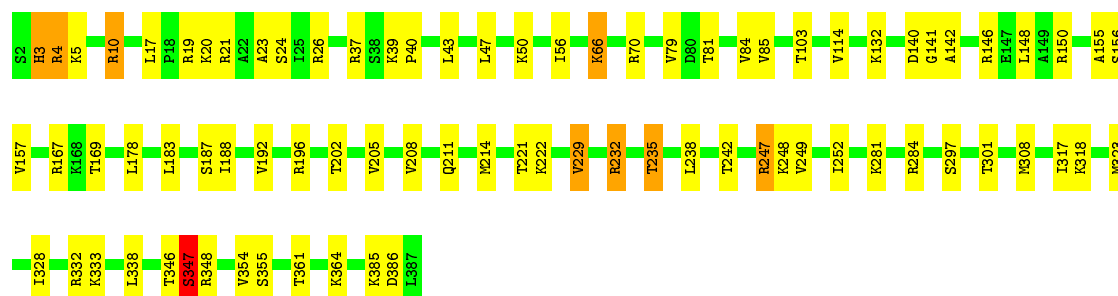
- Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 21%

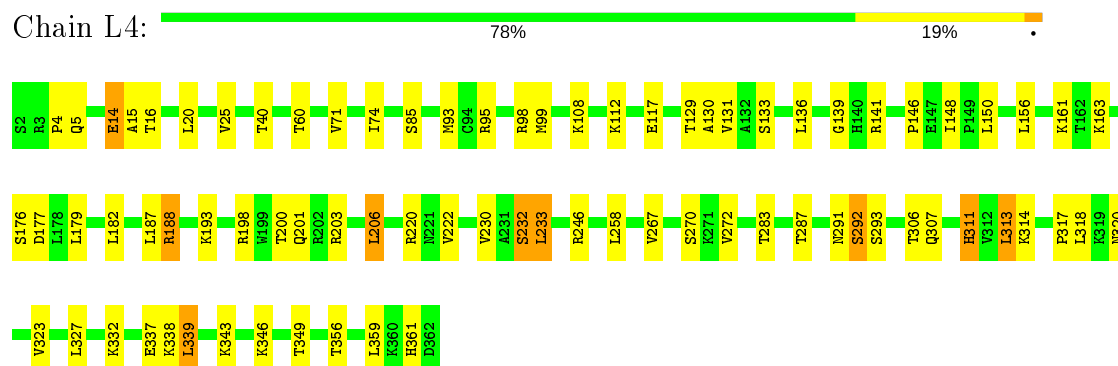


- Molecule 40: 60S ribosomal protein L3

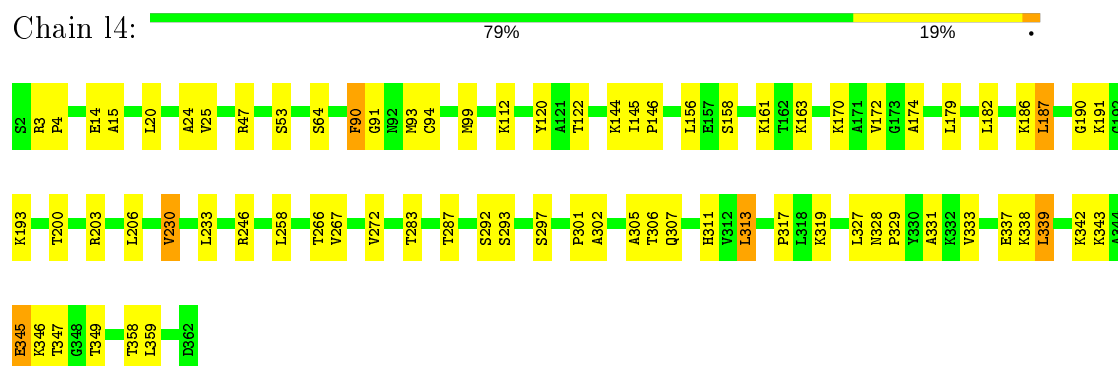
Chain L3: 79% 19%



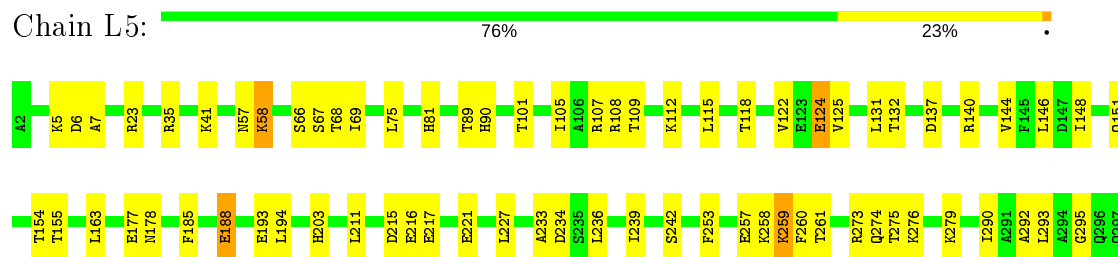
• Molecule 41: 60S ribosomal protein L4-A



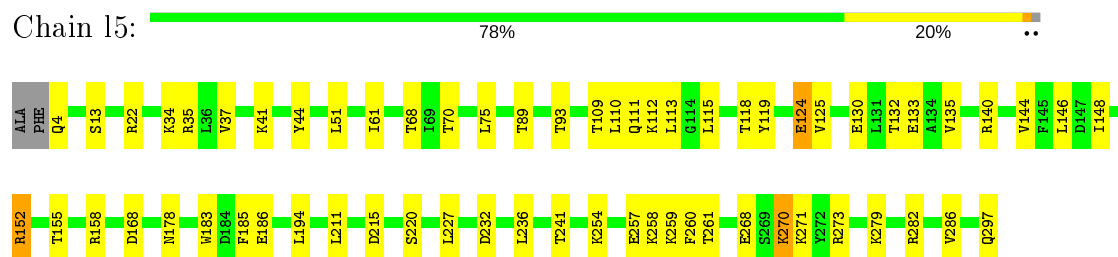
• Molecule 41: 60S ribosomal protein L4-A



• Molecule 42: 60S ribosomal protein L5



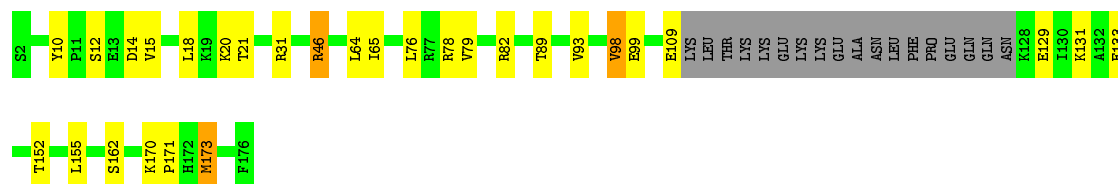
• Molecule 42: 60S ribosomal protein L5



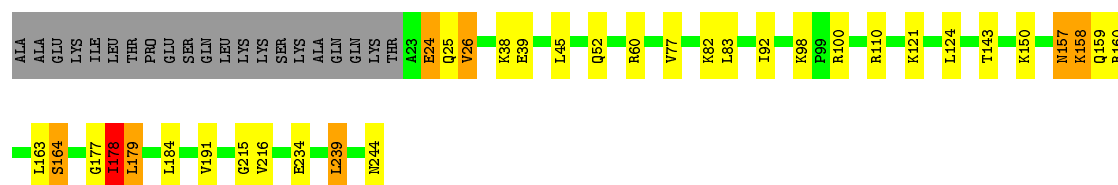
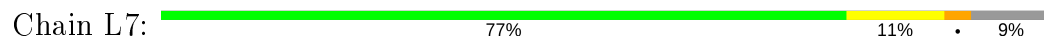
• Molecule 43: 60S ribosomal protein L6-A



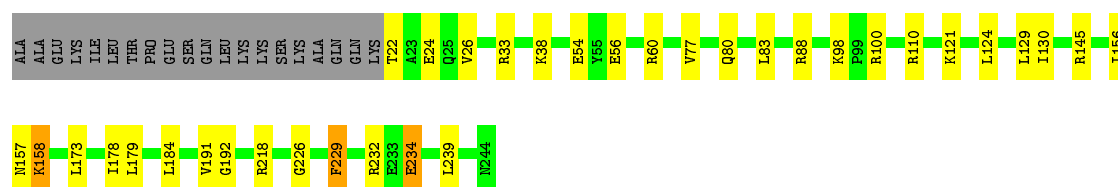
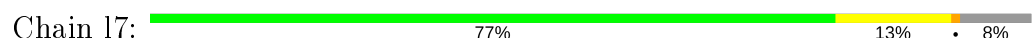
- Molecule 43: 60S ribosomal protein L6-A



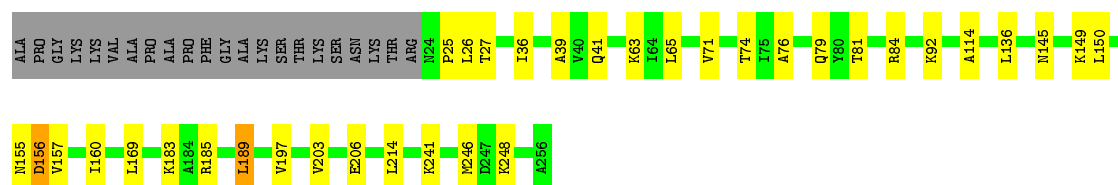
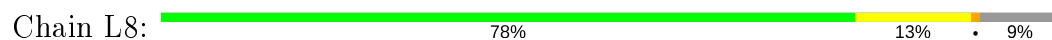
- Molecule 44: 60S ribosomal protein L7-A



- Molecule 44: 60S ribosomal protein L7-A

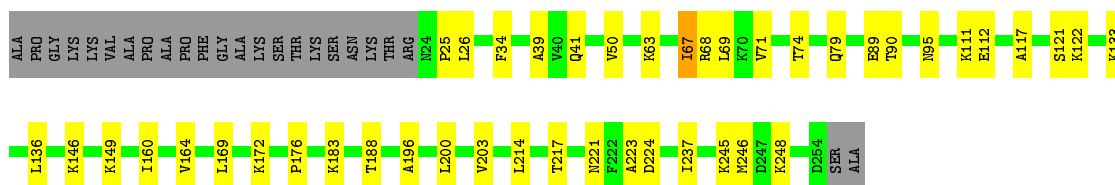


- Molecule 45: 60S ribosomal protein L8-A



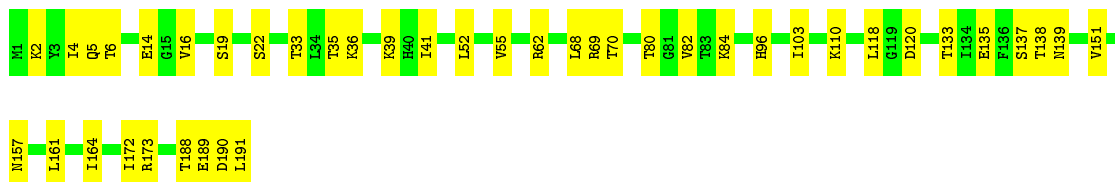
- Molecule 45: 60S ribosomal protein L8-A





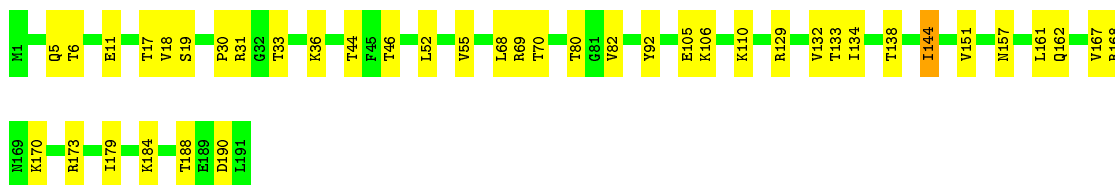
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 78% 22%



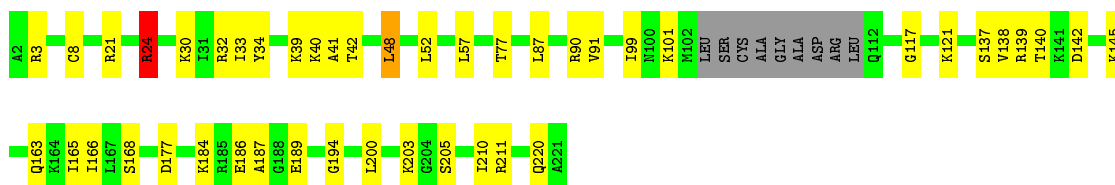
- Molecule 46: 60S ribosomal protein L9-A

Chain l9: 79% 21%



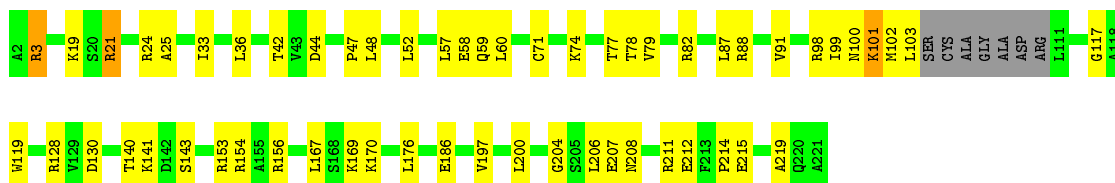
- Molecule 47: 60S ribosomal protein L10

Chain M0: 75% 20%



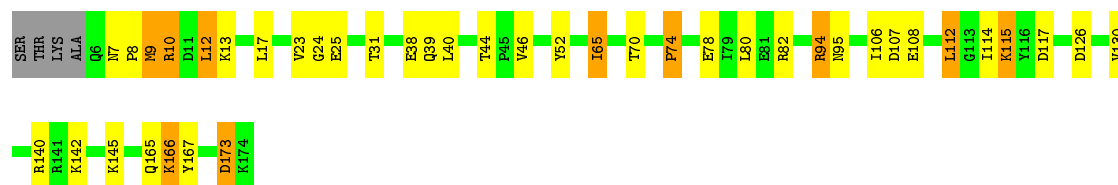
- Molecule 47: 60S ribosomal protein L10

Chain m0: 71% 25%



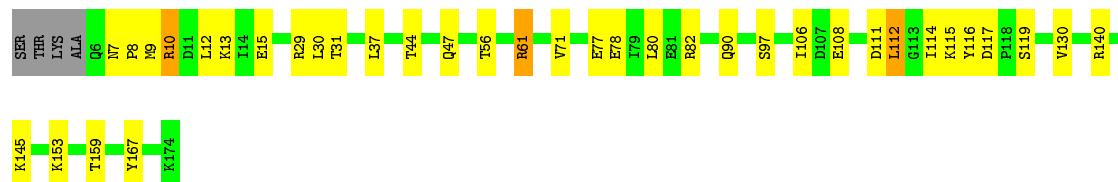
- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 74% 18% 6%



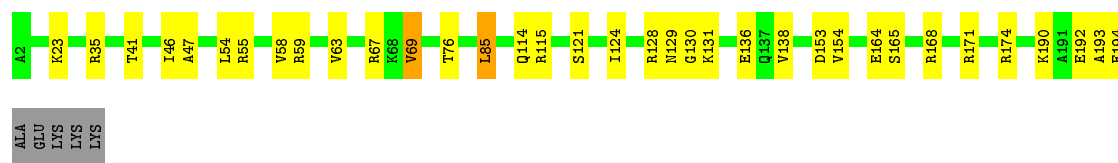
• Molecule 48: 60S ribosomal protein L11-B

Chain m1: 76% 20% ..



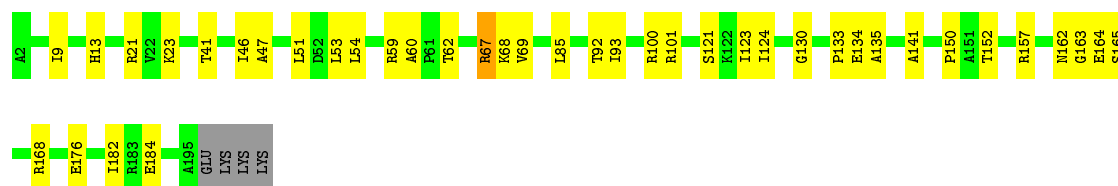
• Molecule 49: 60S ribosomal protein L13-A

Chain M3: 80% 17% ..



• Molecule 49: 60S ribosomal protein L13-A

Chain m3: 78% 20% ..



• Molecule 50: 60S ribosomal protein L14-A

Chain M4: 80% 18% ...

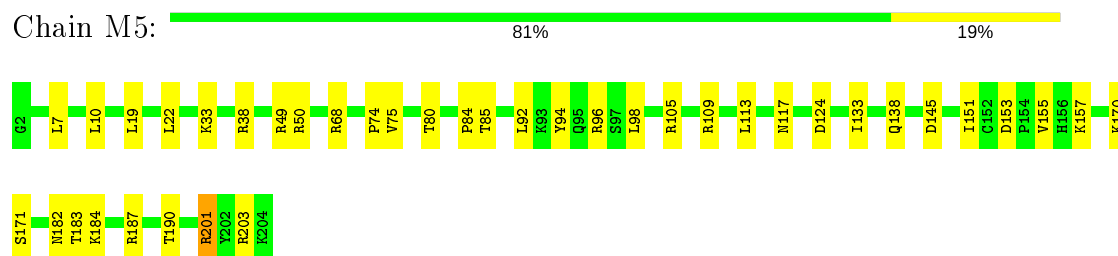


• Molecule 50: 60S ribosomal protein L14-A

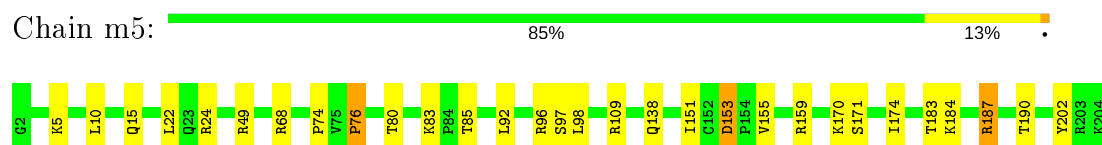
Chain m4: 85% 14% .



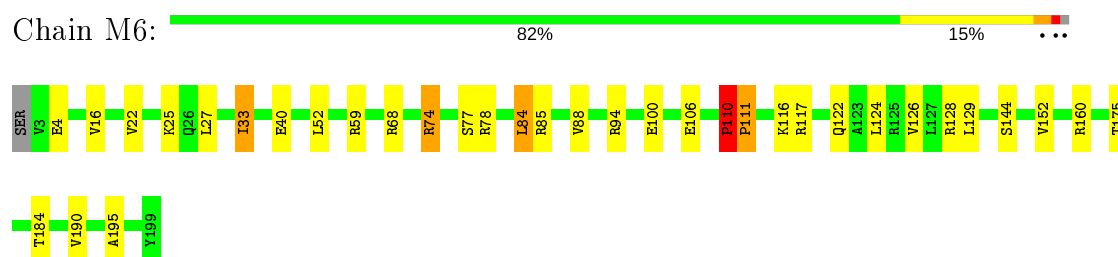
- Molecule 51: 60S ribosomal protein L15-A



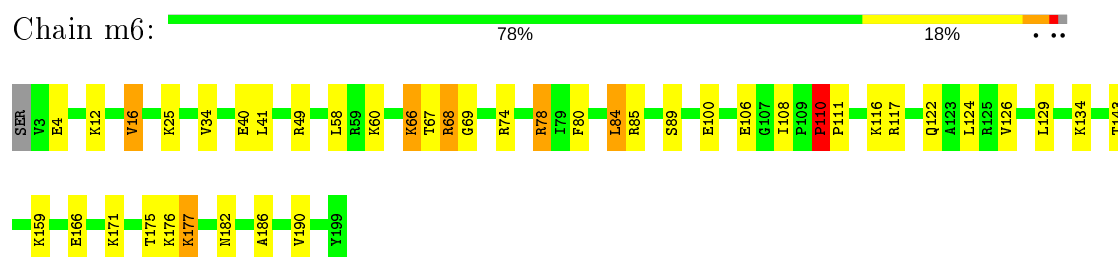
- Molecule 51: 60S ribosomal protein L15-A



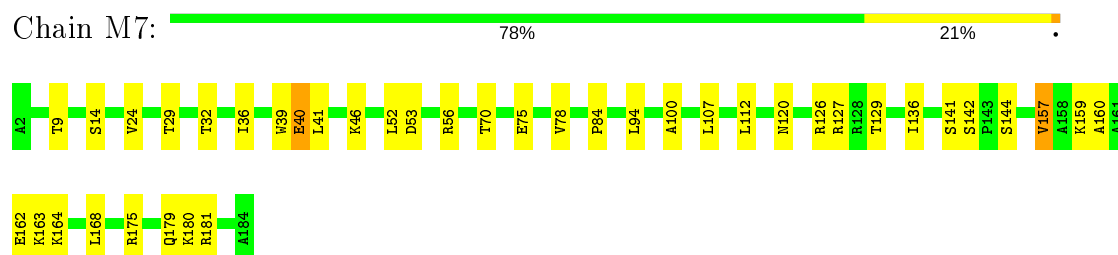
- Molecule 52: 60S ribosomal protein L16-A



- Molecule 52: 60S ribosomal protein L16-A

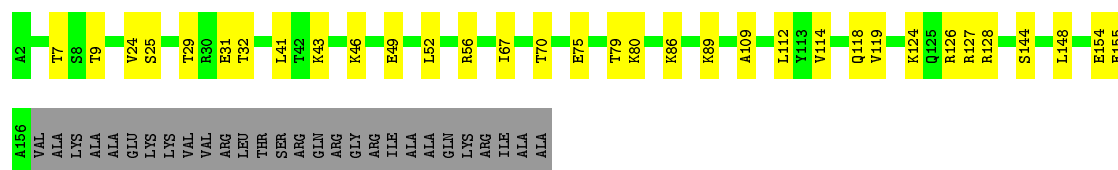


- Molecule 53: 60S ribosomal protein L17-A




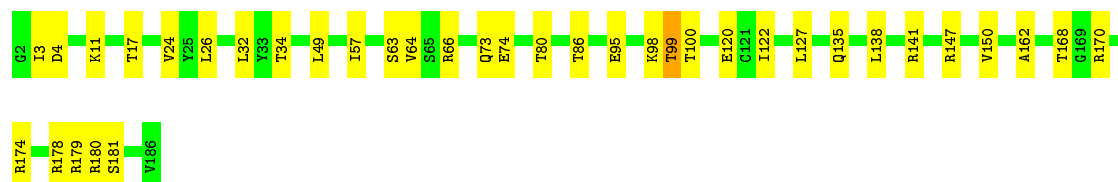
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:  67% 18% 15%




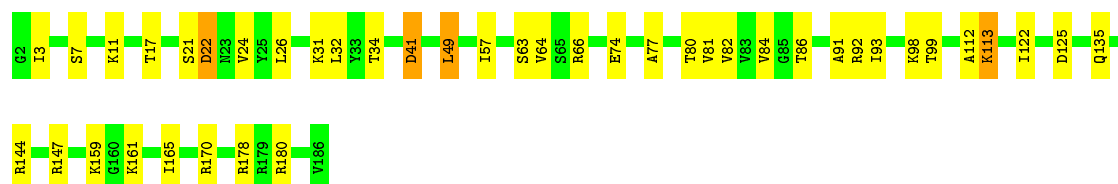
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:  80% 19% .




- Molecule 54: 60S ribosomal protein L18-A

Chain m8:  77% 21% .




- Molecule 55: 60S ribosomal protein L19-A

Chain M9:  84% 15% .




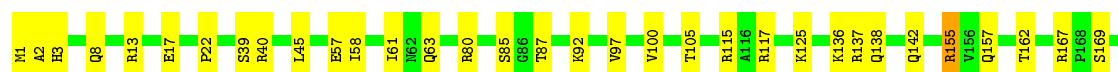
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:  84% 16% .




- Molecule 56: 60S ribosomal protein L20-A

Chain N0:  80% 19% .

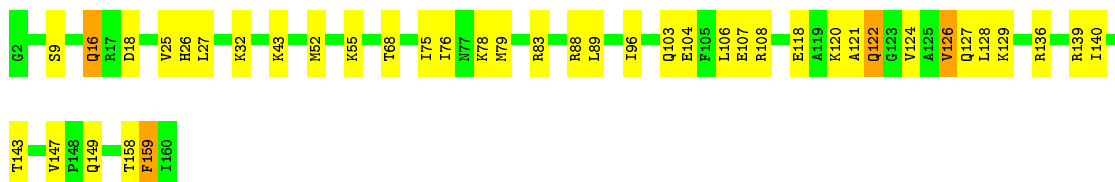


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- Molecule 56: 60S ribosomal protein L20-A

Chain n0:  81% 19%


- Molecule 57: 60S ribosomal protein L21-A

Chain N1:  74% 23%


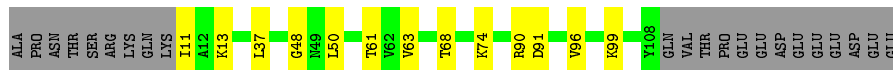
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:  79% 18%


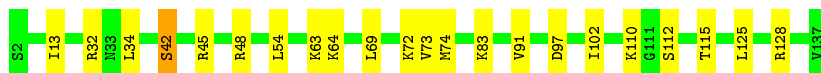

- Molecule 58: 60S ribosomal protein L22-A

Chain N2:  71% 13% 17%



- Molecule 58: 60S ribosomal protein L22-A

Chain n2:  71% 11% 18%


- Molecule 59: 60S ribosomal protein L23-A

Chain N3:  84% 15%


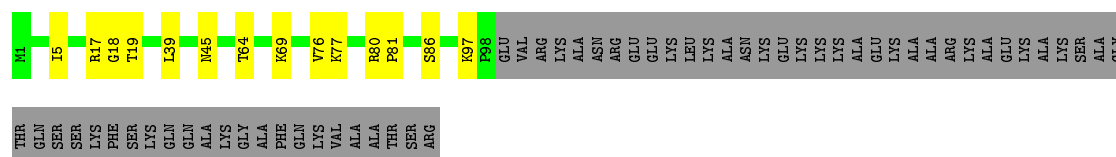
- Molecule 59: 60S ribosomal protein L23-A

Chain n3:  88% 11%



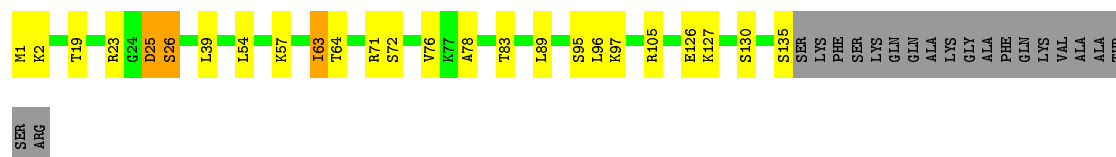
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:  54% 9% 37%



- Molecule 60: 60S ribosomal protein L24-A

Chain n4:  71% 14% 13%



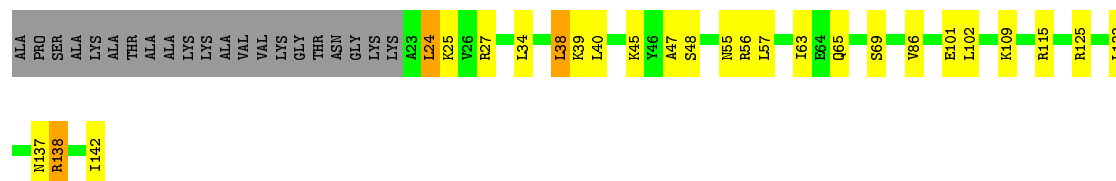
- Molecule 61: 60S ribosomal protein L25

Chain N5:  67% 18% 14%




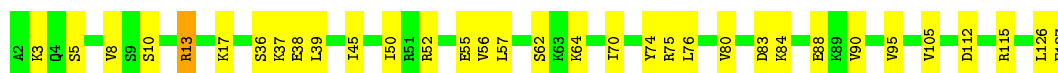
- Molecule 61: 60S ribosomal protein L25

Chain n5:  67% 16% 15%



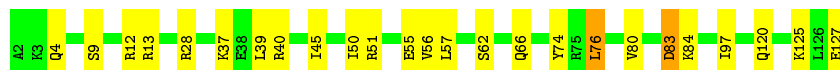
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  74% 25%



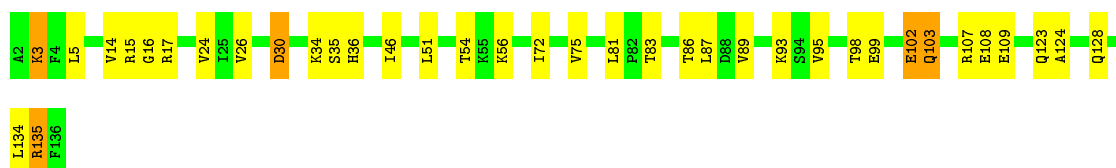
- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 80% 18%



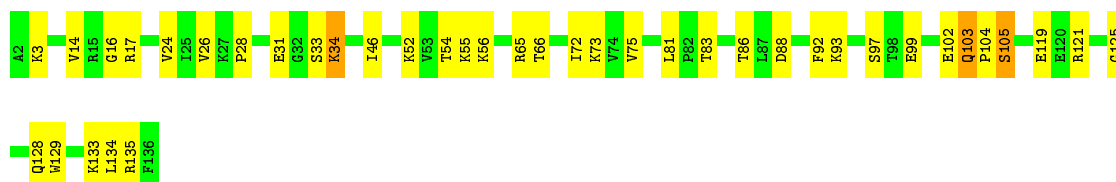
- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 73% 24%



- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 70% 27%



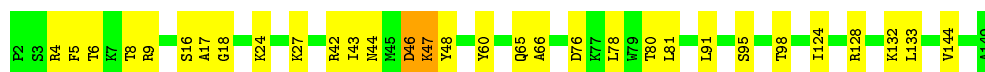
- Molecule 64: 60S ribosomal protein L28

Chain N8: 81% 16%



- Molecule 64: 60S ribosomal protein L28

Chain n8: 79% 20%

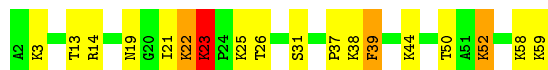


- Molecule 65: 60S ribosomal protein L29

Chain N9: 79% 17%



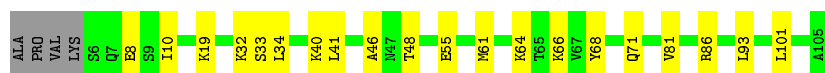
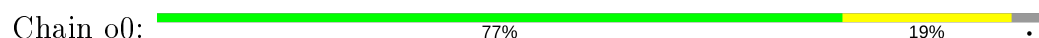
- Molecule 65: 60S ribosomal protein L29



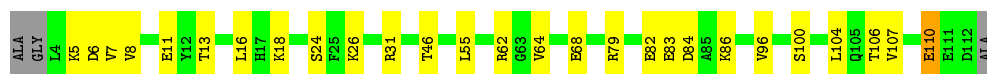
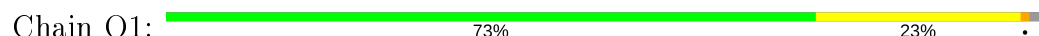
- Molecule 66: 60S ribosomal protein L30



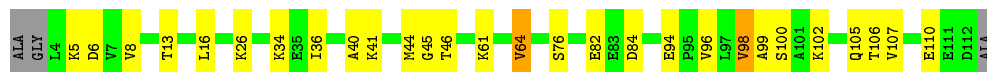
- Molecule 66: 60S ribosomal protein L30



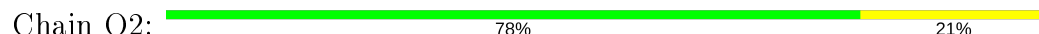
- Molecule 67: 60S ribosomal protein L31-A



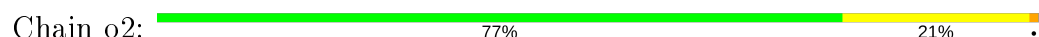
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32



- Molecule 68: 60S ribosomal protein L32





- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 86% 13%



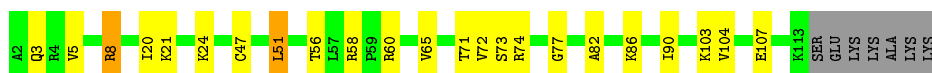
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 83% 17%



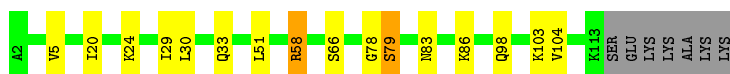
- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 75% 18% 6%



- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 81% 12% 6%



- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 70% 29%



- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 78% 22%



- Molecule 72: 60S ribosomal protein L36-A

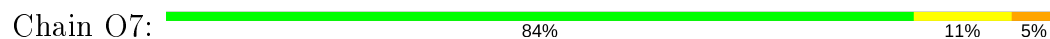
Chain O6: 72% 26%



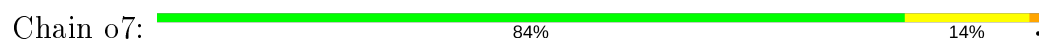
- Molecule 72: 60S ribosomal protein L36-A



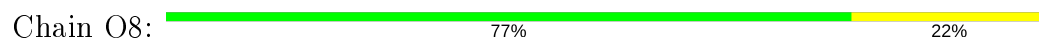
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 73: 60S ribosomal protein L37-A



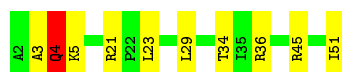
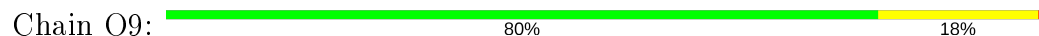
- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38

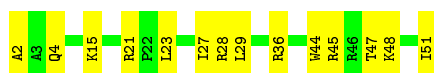


- Molecule 75: 60S ribosomal protein L39

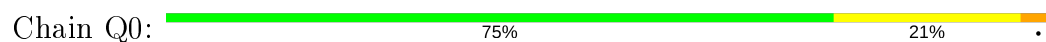


- Molecule 75: 60S ribosomal protein L39

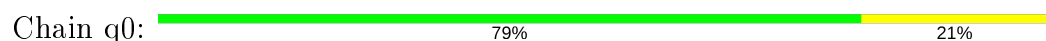




- Molecule 76: Ubiquitin-60S ribosomal protein L40



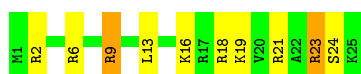
- Molecule 76: Ubiquitin-60S ribosomal protein L40



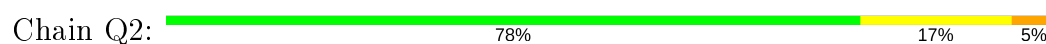
- Molecule 77: 60S ribosomal protein L41-A



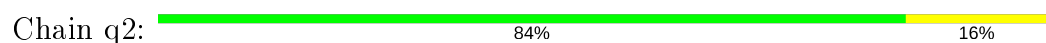
- Molecule 77: 60S ribosomal protein L41-A



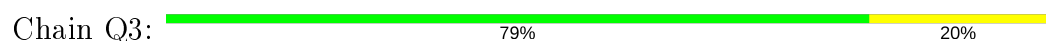
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.39Å 286.22Å 303.33Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	299.62 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (299.62-3.00)	Depositor
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.207 , 0.258	Depositor
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.193	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411206	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3J2, ZN, 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	0.87	13/41698 (0.0%)	1.42	462/64972 (0.7%)
1	6	0.97	33/42765 (0.1%)	1.48	645/66634 (1.0%)
2	S0	0.49	0/1617	0.69	0/2215
2	s0	0.52	0/1623	0.73	1/2222 (0.0%)
3	S1	0.42	0/1735	0.68	2/2335 (0.1%)
3	s1	0.54	0/1748	0.74	1/2352 (0.0%)
4	S2	0.54	0/1665	0.72	0/2263
4	s2	0.62	0/1665	0.81	2/2263 (0.1%)
5	S3	0.54	0/1759	0.72	1/2368 (0.0%)
5	s3	0.46	0/1759	0.65	0/2368
6	S4	0.56	0/2109	0.79	2/2839 (0.1%)
6	s4	0.56	0/2109	0.80	0/2839
7	S5	0.43	0/1629	0.63	0/2202
7	s5	0.47	0/1629	0.67	0/2202
8	S6	0.54	0/1823	0.72	0/2439
8	s6	0.64	1/1779 (0.1%)	0.74	0/2379
9	S7	0.48	0/1506	0.70	1/2028 (0.0%)
9	s7	0.52	0/1516	0.73	0/2043
10	S8	0.65	0/1514	0.82	1/2021 (0.0%)
10	s8	0.65	0/1514	0.79	1/2021 (0.0%)
11	S9	0.54	0/1519	0.74	1/2035 (0.0%)
11	s9	0.59	0/1519	0.80	4/2035 (0.2%)
12	C0	0.44	0/790	0.68	1/1069 (0.1%)
12	c0	0.39	0/777	0.66	3/1049 (0.3%)
13	C1	0.68	1/1239 (0.1%)	0.74	0/1673
13	c1	0.66	0/1194	0.82	1/1610 (0.1%)
14	C2	0.42	0/900	0.65	0/1224
14	c2	0.32	0/900	0.58	0/1224
15	C3	0.60	0/1215	0.73	2/1638 (0.1%)
15	c3	0.62	0/1215	0.82	2/1638 (0.1%)
16	C4	0.42	0/901	0.69	0/1217
16	c4	0.58	0/960	0.84	3/1290 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.54	0/998	0.78	1/1341 (0.1%)
17	c5	0.51	0/1060	0.69	0/1426
18	C6	0.50	0/1125	0.75	2/1510 (0.1%)
18	c6	0.52	0/1131	0.71	0/1518
19	C7	0.49	0/935	0.69	0/1254
19	c7	0.52	0/914	0.70	0/1224
20	C8	0.48	0/1211	0.72	1/1628 (0.1%)
20	c8	0.51	0/1211	0.73	2/1628 (0.1%)
21	C9	0.48	0/1130	0.69	0/1517
21	c9	0.52	0/1130	0.68	1/1517 (0.1%)
22	D0	0.51	0/865	0.70	0/1169
22	d0	0.53	0/892	0.69	0/1205
23	D1	0.55	0/693	0.70	0/935
23	d1	0.59	0/693	0.79	0/935
24	D2	0.58	0/1038	0.80	3/1395 (0.2%)
24	d2	0.66	0/1038	0.80	1/1395 (0.1%)
25	D3	0.73	0/1139	0.85	1/1518 (0.1%)
25	d3	0.74	0/1139	0.83	1/1518 (0.1%)
26	D4	0.53	0/1087	0.66	0/1449
26	d4	0.57	0/1087	0.78	0/1449
27	D5	0.43	0/571	0.75	0/768
27	d5	0.46	0/566	0.69	0/761
28	D6	0.48	0/782	0.72	0/1047
28	d6	0.60	0/782	0.75	0/1047
29	D7	0.50	0/620	0.70	0/838
29	d7	0.53	0/620	0.73	0/838
30	D8	0.43	0/499	0.62	0/670
30	d8	0.45	0/499	0.69	0/670
31	D9	0.63	0/452	0.85	1/600 (0.2%)
31	d9	0.57	0/452	0.75	1/600 (0.2%)
32	E0	0.54	0/483	0.68	0/643
33	E1	0.53	0/577	0.86	0/770
33	e1	0.42	0/619	0.72	0/822
34	SR	0.42	0/2494	0.63	1/3393 (0.0%)
34	sR	0.42	0/2495	0.59	0/3395
35	SM	0.58	0/1113	0.78	2/1502 (0.1%)
35	sM	0.55	0/683	0.78	2/923 (0.2%)
36	1	1.38	411/75394 (0.5%)	1.86	2927/117545 (2.5%)
36	5	1.40	457/75414 (0.6%)	1.87	2915/117575 (2.5%)
37	3	1.08	4/2883 (0.1%)	1.61	59/4491 (1.3%)
37	7	1.39	14/2883 (0.5%)	1.82	95/4491 (2.1%)
38	4	1.32	12/3746 (0.3%)	1.84	130/5832 (2.2%)
38	8	1.20	10/3746 (0.3%)	1.71	88/5832 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.86	0/1948	0.93	2/2617 (0.1%)
39	l2	0.84	1/1946 (0.1%)	0.95	5/2614 (0.2%)
40	L3	0.87	1/3146 (0.0%)	0.93	2/4228 (0.0%)
40	l3	0.98	2/3146 (0.1%)	0.96	6/4228 (0.1%)
41	L4	0.93	0/2800	1.03	10/3790 (0.3%)
41	l4	0.90	1/2800 (0.0%)	0.95	5/3790 (0.1%)
42	L5	0.66	0/2425	0.75	0/3271
42	l5	0.87	2/2408 (0.1%)	0.89	2/3248 (0.1%)
43	L6	0.93	0/1260	0.91	1/1694 (0.1%)
43	l6	0.95	0/1269	0.97	4/1705 (0.2%)
44	L7	0.92	1/1821 (0.1%)	0.98	7/2451 (0.3%)
44	l7	1.01	4/1828 (0.2%)	0.98	3/2461 (0.1%)
45	L8	0.68	0/1836	0.76	1/2481 (0.0%)
45	l8	0.59	0/1795	0.71	0/2429
46	L9	0.77	0/1539	0.85	0/2073
46	l9	0.88	1/1539 (0.1%)	0.87	0/2073
47	M0	0.81	1/1741 (0.1%)	0.90	4/2335 (0.2%)
47	m0	0.88	1/1758 (0.1%)	0.98	6/2358 (0.3%)
48	M1	0.59	0/1374	0.80	1/1842 (0.1%)
48	m1	0.75	0/1374	0.85	2/1842 (0.1%)
49	M3	0.88	0/1568	0.93	1/2106 (0.0%)
49	m3	0.82	1/1573 (0.1%)	0.92	2/2113 (0.1%)
50	M4	0.88	0/1068	0.87	1/1438 (0.1%)
50	m4	0.96	0/1074	0.92	1/1446 (0.1%)
51	M5	0.90	0/1757	0.99	4/2354 (0.2%)
51	m5	0.78	1/1757 (0.1%)	0.91	2/2354 (0.1%)
52	M6	1.08	5/1585 (0.3%)	1.04	9/2128 (0.4%)
52	m6	1.18	4/1585 (0.3%)	1.08	6/2128 (0.3%)
53	M7	0.91	1/1443 (0.1%)	0.91	0/1944
53	m7	1.00	0/1250	0.97	0/1683
54	M8	0.90	0/1465	0.96	4/1965 (0.2%)
54	m8	0.90	0/1465	1.01	3/1965 (0.2%)
55	M9	0.69	0/1538	0.74	0/2050
55	m9	0.70	0/1538	0.77	0/2050
56	N0	0.89	0/1481	0.93	4/1990 (0.2%)
56	n0	1.01	0/1481	0.97	4/1990 (0.2%)
57	N1	0.87	0/1300	0.88	0/1743
57	n1	1.00	2/1300 (0.2%)	0.96	2/1743 (0.1%)
58	N2	0.49	0/812	0.66	0/1099
58	n2	0.54	0/794	0.72	0/1076
59	N3	0.87	0/1018	0.93	0/1369
59	n3	0.97	1/1018 (0.1%)	1.04	4/1369 (0.3%)
60	N4	0.70	0/712	0.77	1/958 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.75	0/1052	0.80	1/1398 (0.1%)
61	N5	0.80	0/979	0.91	1/1321 (0.1%)
61	n5	0.73	0/974	0.91	1/1314 (0.1%)
62	N6	0.83	0/1004	0.99	2/1341 (0.1%)
62	n6	0.87	1/1004 (0.1%)	0.98	2/1341 (0.1%)
63	N7	0.64	0/1118	0.78	1/1497 (0.1%)
63	n7	0.55	0/1118	0.71	0/1497
64	N8	0.93	0/1204	1.01	2/1612 (0.1%)
64	n8	0.90	1/1204 (0.1%)	0.95	2/1612 (0.1%)
65	N9	0.79	0/473	0.91	1/629 (0.2%)
65	n9	0.96	0/473	1.05	2/629 (0.3%)
66	O0	0.57	0/751	0.74	1/1008 (0.1%)
66	o0	0.55	0/775	0.69	0/1040
67	O1	0.75	0/890	0.80	1/1196 (0.1%)
67	o1	0.90	0/897	0.89	0/1205
68	O2	0.98	0/1041	1.04	4/1394 (0.3%)
68	o2	1.03	1/1041 (0.1%)	1.03	1/1394 (0.1%)
69	O3	1.14	3/868 (0.3%)	0.98	0/1168
69	o3	1.06	0/868	0.96	0/1168
70	O4	0.74	0/890	0.94	5/1189 (0.4%)
70	o4	0.69	0/890	0.82	1/1189 (0.1%)
71	O5	0.88	1/978 (0.1%)	0.91	2/1301 (0.2%)
71	o5	0.68	0/974	0.80	0/1297
72	O6	0.75	0/778	0.88	0/1034
72	o6	0.64	0/777	0.75	0/1033
73	O7	0.96	0/696	1.05	3/923 (0.3%)
73	o7	0.85	0/696	0.96	1/923 (0.1%)
74	O8	0.61	0/618	0.73	0/826
74	o8	0.53	0/614	0.76	1/822 (0.1%)
75	O9	0.91	0/443	0.93	0/588
75	o9	0.82	0/443	0.96	0/588
76	Q0	0.89	1/423 (0.2%)	0.95	1/562 (0.2%)
76	q0	1.00	0/423	1.01	0/562
77	Q1	0.75	0/234	0.96	1/300 (0.3%)
77	q1	0.92	0/234	1.15	3/300 (1.0%)
78	Q2	1.02	1/860 (0.1%)	0.94	1/1136 (0.1%)
78	q2	0.88	0/860	0.91	1/1136 (0.1%)
79	Q3	0.90	0/701	0.94	1/934 (0.1%)
79	q3	0.84	0/701	0.90	0/934
80	e0	0.60	0/499	0.78	0/665
82	p0	0.48	0/1092	0.61	0/1474
All	All	1.06	995/430073 (0.2%)	1.45	7522/631362 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
3	s1	0	1
5	s3	0	1
6	S4	0	1
7	S5	0	1
7	s5	0	2
9	S7	0	2
9	s7	0	1
16	C4	0	1
16	c4	0	1
18	c6	0	2
19	c7	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	2
28	D6	0	2
33	E1	0	1
33	e1	0	1
39	L2	0	1
39	l2	0	3
41	L4	0	1
41	l4	0	1
42	L5	0	2
42	l5	0	1
43	L6	0	1
44	L7	0	1
44	l7	0	1
45	l8	0	1
48	M1	0	1
49	M3	0	1
51	M5	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
56	N0	0	1
56	n0	0	1
57	N1	0	1
59	n3	0	1
60	n4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	N7	0	1
64	N8	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	2
67	O1	0	2
67	o1	0	1
71	o5	0	1
72	O6	0	2
75	O9	0	1
75	o9	0	1
76	Q0	0	1
78	Q2	0	2
All	All	0	65

The worst 5 of 995 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	16.46	2.10	1.82
36	5	1152	G	N9-C4	-12.28	1.28	1.38
36	5	2872	A	N9-C4	-12.03	1.30	1.37
57	n1	104	GLU	CB-CG	10.19	1.71	1.52
36	1	3181	C	N3-C4	-9.73	1.27	1.33

The worst 5 of 7522 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	27.54	142.37	128.60
36	5	1152	G	N3-C4-N9	-26.81	109.91	126.00
36	1	2945	G	O5'-P-OP2	-22.04	84.25	110.70
36	5	1152	G	C2-N3-C4	-21.23	101.28	111.90
36	5	922	U	N3-C2-O2	-21.19	107.37	122.20

There are no chirality outliers.

5 of 65 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	S1	177	GLN	Peptide
6	S4	167	GLY	Peptide
7	S5	49	GLU	Peptide
9	S7	131	PHE	Peptide

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Mol	Chain	Res	Type	Group
9	S7	31	SER	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%)	145 (71%)	36 (18%)	23 (11%)	0	2
2	s0	204/251 (81%)	151 (74%)	28 (14%)	25 (12%)	0	1
3	S1	212/254 (84%)	144 (68%)	40 (19%)	28 (13%)	0	1
3	s1	214/254 (84%)	169 (79%)	31 (14%)	14 (6%)	1	7
4	S2	215/253 (85%)	180 (84%)	23 (11%)	12 (6%)	2	10
4	s2	215/253 (85%)	183 (85%)	20 (9%)	12 (6%)	2	10
5	S3	221/239 (92%)	175 (79%)	32 (14%)	14 (6%)	1	7
5	s3	221/239 (92%)	182 (82%)	22 (10%)	17 (8%)	1	5
6	S4	258/260 (99%)	202 (78%)	36 (14%)	20 (8%)	1	4
6	s4	258/260 (99%)	211 (82%)	31 (12%)	16 (6%)	1	8
7	S5	204/224 (91%)	158 (78%)	25 (12%)	21 (10%)	0	2
7	s5	204/224 (91%)	152 (74%)	37 (18%)	15 (7%)	1	5
8	S6	224/236 (95%)	187 (84%)	28 (12%)	9 (4%)	3	17
8	s6	216/236 (92%)	180 (83%)	26 (12%)	10 (5%)	2	14
9	S7	182/189 (96%)	136 (75%)	28 (15%)	18 (10%)	0	2
9	s7	184/189 (97%)	133 (72%)	37 (20%)	14 (8%)	1	5
10	S8	184/200 (92%)	160 (87%)	16 (9%)	8 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	s8	184/200 (92%)	157 (85%)	18 (10%)	9 (5%)	2	13
11	S9	183/196 (93%)	150 (82%)	25 (14%)	8 (4%)	2	15
11	s9	183/196 (93%)	143 (78%)	28 (15%)	12 (7%)	1	6
12	C0	94/105 (90%)	69 (73%)	16 (17%)	9 (10%)	0	3
12	c0	92/105 (88%)	67 (73%)	9 (10%)	16 (17%)	0	0
13	C1	153/155 (99%)	123 (80%)	19 (12%)	11 (7%)	1	5
13	c1	144/155 (93%)	121 (84%)	13 (9%)	10 (7%)	1	6
14	C2	122/142 (86%)	70 (57%)	28 (23%)	24 (20%)	0	0
14	c2	122/142 (86%)	73 (60%)	32 (26%)	17 (14%)	0	1
15	C3	148/150 (99%)	120 (81%)	22 (15%)	6 (4%)	3	16
15	c3	148/150 (99%)	117 (79%)	20 (14%)	11 (7%)	1	5
16	C4	125/136 (92%)	81 (65%)	28 (22%)	16 (13%)	0	1
16	c4	126/136 (93%)	99 (79%)	14 (11%)	13 (10%)	0	2
17	C5	122/141 (86%)	91 (75%)	18 (15%)	13 (11%)	0	2
17	c5	133/141 (94%)	95 (71%)	20 (15%)	18 (14%)	0	1
18	C6	139/142 (98%)	111 (80%)	14 (10%)	14 (10%)	0	2
18	c6	140/142 (99%)	115 (82%)	17 (12%)	8 (6%)	1	10
19	C7	116/136 (85%)	86 (74%)	18 (16%)	12 (10%)	0	2
19	c7	113/136 (83%)	86 (76%)	20 (18%)	7 (6%)	1	8
20	C8	143/145 (99%)	110 (77%)	20 (14%)	13 (9%)	1	3
20	c8	143/145 (99%)	112 (78%)	22 (15%)	9 (6%)	1	7
21	C9	141/143 (99%)	116 (82%)	17 (12%)	8 (6%)	1	10
21	c9	141/143 (99%)	120 (85%)	18 (13%)	3 (2%)	7	33
22	D0	105/120 (88%)	81 (77%)	16 (15%)	8 (8%)	1	5
22	d0	108/120 (90%)	80 (74%)	19 (18%)	9 (8%)	1	4
23	D1	85/87 (98%)	62 (73%)	15 (18%)	8 (9%)	0	3
23	d1	85/87 (98%)	68 (80%)	9 (11%)	8 (9%)	0	3
24	D2	127/129 (98%)	100 (79%)	23 (18%)	4 (3%)	4	23
24	d2	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	9	40
25	D3	142/144 (99%)	112 (79%)	17 (12%)	13 (9%)	1	3
25	d3	142/144 (99%)	121 (85%)	16 (11%)	5 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	D4	132/134 (98%)	108 (82%)	17 (13%)	7 (5%)	2	11
26	d4	132/134 (98%)	104 (79%)	16 (12%)	12 (9%)	1	3
27	D5	68/107 (64%)	46 (68%)	13 (19%)	9 (13%)	0	1
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	2	14
28	D6	95/97 (98%)	55 (58%)	24 (25%)	16 (17%)	0	0
28	d6	95/97 (98%)	73 (77%)	12 (13%)	10 (10%)	0	2
29	D7	79/81 (98%)	60 (76%)	14 (18%)	5 (6%)	1	7
29	d7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1	3
30	D8	61/66 (92%)	47 (77%)	12 (20%)	2 (3%)	4	21
30	d8	61/66 (92%)	44 (72%)	13 (21%)	4 (7%)	1	6
31	D9	51/55 (93%)	43 (84%)	5 (10%)	3 (6%)	1	9
31	d9	51/55 (93%)	37 (72%)	9 (18%)	5 (10%)	0	2
32	E0	58/60 (97%)	44 (76%)	11 (19%)	3 (5%)	2	12
33	E1	69/76 (91%)	30 (44%)	19 (28%)	20 (29%)	0	0
33	e1	74/76 (97%)	37 (50%)	16 (22%)	21 (28%)	0	0
34	SR	316/318 (99%)	263 (83%)	45 (14%)	8 (2%)	5	28
34	sR	316/318 (99%)	256 (81%)	48 (15%)	12 (4%)	3	18
35	SM	155/273 (57%)	103 (66%)	29 (19%)	23 (15%)	0	1
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0	1
39	L2	250/253 (99%)	222 (89%)	19 (8%)	9 (4%)	3	19
39	l2	250/253 (99%)	211 (84%)	29 (12%)	10 (4%)	3	17
40	L3	384/386 (100%)	339 (88%)	29 (8%)	16 (4%)	3	16
40	l3	384/386 (100%)	342 (89%)	29 (8%)	13 (3%)	3	20
41	L4	359/361 (99%)	301 (84%)	39 (11%)	19 (5%)	2	11
41	l4	359/361 (99%)	303 (84%)	36 (10%)	20 (6%)	2	10
42	L5	294/296 (99%)	235 (80%)	37 (13%)	22 (8%)	1	5
42	l5	292/296 (99%)	247 (85%)	34 (12%)	11 (4%)	3	18
43	L6	152/175 (87%)	137 (90%)	12 (8%)	3 (2%)	7	34
43	l6	153/175 (87%)	129 (84%)	20 (13%)	4 (3%)	5	27
44	L7	220/243 (90%)	192 (87%)	20 (9%)	8 (4%)	3	19
44	l7	221/243 (91%)	201 (91%)	14 (6%)	6 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	L8	231/255 (91%)	188 (81%)	36 (16%)	7 (3%)	4	24
45	l8	229/255 (90%)	180 (79%)	33 (14%)	16 (7%)	1	6
46	L9	189/191 (99%)	164 (87%)	21 (11%)	4 (2%)	7	33
46	l9	189/191 (99%)	169 (89%)	16 (8%)	4 (2%)	7	33
47	M0	207/220 (94%)	174 (84%)	25 (12%)	8 (4%)	3	17
47	m0	209/220 (95%)	167 (80%)	26 (12%)	16 (8%)	1	5
48	M1	167/173 (96%)	130 (78%)	21 (13%)	16 (10%)	0	3
48	m1	167/173 (96%)	139 (83%)	17 (10%)	11 (7%)	1	6
49	M3	191/198 (96%)	165 (86%)	17 (9%)	9 (5%)	2	14
49	m3	192/198 (97%)	152 (79%)	26 (14%)	14 (7%)	1	5
50	M4	134/137 (98%)	114 (85%)	10 (8%)	10 (8%)	1	5
50	m4	135/137 (98%)	122 (90%)	11 (8%)	2 (2%)	10	42
51	M5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	5	28
51	m5	201/203 (99%)	180 (90%)	16 (8%)	5 (2%)	5	28
52	M6	195/198 (98%)	182 (93%)	10 (5%)	3 (2%)	10	42
52	m6	195/198 (98%)	172 (88%)	15 (8%)	8 (4%)	3	16
53	M7	181/183 (99%)	149 (82%)	21 (12%)	11 (6%)	1	8
53	m7	153/183 (84%)	133 (87%)	17 (11%)	3 (2%)	7	34
54	M8	183/185 (99%)	161 (88%)	16 (9%)	6 (3%)	4	21
54	m8	183/185 (99%)	148 (81%)	24 (13%)	11 (6%)	1	9
55	M9	186/188 (99%)	162 (87%)	21 (11%)	3 (2%)	9	40
55	m9	186/188 (99%)	156 (84%)	25 (13%)	5 (3%)	5	26
56	N0	170/172 (99%)	154 (91%)	14 (8%)	2 (1%)	13	48
56	n0	170/172 (99%)	153 (90%)	15 (9%)	2 (1%)	13	48
57	N1	157/159 (99%)	135 (86%)	13 (8%)	9 (6%)	1	10
57	n1	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	3	18
58	N2	98/120 (82%)	75 (76%)	18 (18%)	5 (5%)	2	12
58	n2	96/120 (80%)	77 (80%)	16 (17%)	3 (3%)	4	23
59	N3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10	42
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
60	N4	96/155 (62%)	72 (75%)	16 (17%)	8 (8%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	n4	133/155 (86%)	101 (76%)	21 (16%)	11 (8%)	1	4
61	N5	119/141 (84%)	100 (84%)	17 (14%)	2 (2%)	9	39
61	n5	118/141 (84%)	103 (87%)	7 (6%)	8 (7%)	1	6
62	N6	124/126 (98%)	114 (92%)	8 (6%)	2 (2%)	9	40
62	n6	124/126 (98%)	109 (88%)	12 (10%)	3 (2%)	6	29
63	N7	133/135 (98%)	102 (77%)	21 (16%)	10 (8%)	1	5
63	n7	133/135 (98%)	101 (76%)	20 (15%)	12 (9%)	1	3
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	2	13
64	n8	146/148 (99%)	128 (88%)	14 (10%)	4 (3%)	5	26
65	N9	56/58 (97%)	43 (77%)	12 (21%)	1 (2%)	8	37
65	n9	56/58 (97%)	40 (71%)	9 (16%)	7 (12%)	0	1
66	O0	95/104 (91%)	88 (93%)	5 (5%)	2 (2%)	7	33
66	o0	98/104 (94%)	88 (90%)	8 (8%)	2 (2%)	7	34
67	O1	107/112 (96%)	95 (89%)	8 (8%)	4 (4%)	3	19
67	o1	107/112 (96%)	86 (80%)	14 (13%)	7 (6%)	1	7
68	O2	125/129 (97%)	113 (90%)	11 (9%)	1 (1%)	19	57
68	o2	125/129 (97%)	108 (86%)	12 (10%)	5 (4%)	3	17
69	O3	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	15	53
69	o3	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	8	36
70	O4	110/119 (92%)	100 (91%)	6 (6%)	4 (4%)	3	19
70	o4	110/119 (92%)	99 (90%)	7 (6%)	4 (4%)	3	19
71	O5	117/119 (98%)	108 (92%)	7 (6%)	2 (2%)	9	39
71	o5	117/119 (98%)	104 (89%)	7 (6%)	6 (5%)	2	12
72	O6	97/99 (98%)	79 (81%)	13 (13%)	5 (5%)	2	12
72	o6	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	7	33
73	O7	85/87 (98%)	71 (84%)	11 (13%)	3 (4%)	3	20
73	o7	85/87 (98%)	73 (86%)	10 (12%)	2 (2%)	6	29
74	O8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	11
74	o8	75/77 (97%)	57 (76%)	15 (20%)	3 (4%)	3	17
75	O9	48/50 (96%)	42 (88%)	4 (8%)	2 (4%)	3	16
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	Q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3	17
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7	34
77	Q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	15
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	84 (82%)	12 (12%)	7 (7%)	1	6
78	q2	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
79	Q3	89/91 (98%)	74 (83%)	11 (12%)	4 (4%)	2	14
79	q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	6	31
80	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	2
82	p0	139/311 (45%)	113 (81%)	22 (16%)	4 (3%)	4	24
All	All	22333/24141 (92%)	18316 (82%)	2723 (12%)	1294 (6%)	1	10

5 of 1294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	5	ALA
2	S0	30	GLN
2	S0	39	ASN
2	S0	66	ALA

5.3.2 Protein sidechains ⓘ

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%)	132 (80%)	32 (20%)	1	7
2	s0	165/209 (79%)	120 (73%)	45 (27%)	0	2
3	S1	191/223 (86%)	152 (80%)	39 (20%)	1	6
3	s1	192/223 (86%)	152 (79%)	40 (21%)	1	5
4	S2	176/204 (86%)	142 (81%)	34 (19%)	1	8
4	s2	176/204 (86%)	129 (73%)	47 (27%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S3	182/194 (94%)	136 (75%)	46 (25%)	0	3
5	s3	182/194 (94%)	154 (85%)	28 (15%)	2	13
6	S4	221/221 (100%)	179 (81%)	42 (19%)	1	8
6	s4	221/221 (100%)	190 (86%)	31 (14%)	3	16
7	S5	173/190 (91%)	140 (81%)	33 (19%)	1	8
7	s5	173/190 (91%)	135 (78%)	38 (22%)	1	4
8	S6	188/201 (94%)	150 (80%)	38 (20%)	1	6
8	s6	187/201 (93%)	155 (83%)	32 (17%)	2	10
9	S7	165/169 (98%)	132 (80%)	33 (20%)	1	7
9	s7	165/169 (98%)	136 (82%)	29 (18%)	2	10
10	S8	150/161 (93%)	132 (88%)	18 (12%)	5	22
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	15
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	4
11	s9	158/165 (96%)	130 (82%)	28 (18%)	2	9
12	C0	77/98 (79%)	63 (82%)	14 (18%)	1	9
12	c0	73/98 (74%)	62 (85%)	11 (15%)	3	14
13	C1	129/136 (95%)	106 (82%)	23 (18%)	2	9
13	c1	129/136 (95%)	101 (78%)	28 (22%)	1	5
14	C2	88/118 (75%)	64 (73%)	24 (27%)	0	2
14	c2	88/118 (75%)	64 (73%)	24 (27%)	0	2
15	C3	127/127 (100%)	106 (84%)	21 (16%)	2	11
15	c3	127/127 (100%)	106 (84%)	21 (16%)	2	11
16	C4	81/104 (78%)	55 (68%)	26 (32%)	0	1
16	c4	97/104 (93%)	74 (76%)	23 (24%)	1	3
17	C5	101/117 (86%)	81 (80%)	20 (20%)	1	7
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	10
18	C6	117/118 (99%)	86 (74%)	31 (26%)	0	2
18	c6	118/118 (100%)	93 (79%)	25 (21%)	1	5
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	6
19	c7	92/124 (74%)	76 (83%)	16 (17%)	2	10
20	C8	128/128 (100%)	97 (76%)	31 (24%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	4
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1	4
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	11
22	D0	100/113 (88%)	71 (71%)	29 (29%)	0	2
22	d0	103/113 (91%)	77 (75%)	26 (25%)	0	3
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	5
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	5
24	D2	110/110 (100%)	85 (77%)	25 (23%)	1	4
24	d2	110/110 (100%)	95 (86%)	15 (14%)	3	17
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	8
25	d3	119/119 (100%)	94 (79%)	25 (21%)	1	5
26	D4	112/112 (100%)	89 (80%)	23 (20%)	1	6
26	d4	112/112 (100%)	90 (80%)	22 (20%)	1	7
27	D5	61/88 (69%)	44 (72%)	17 (28%)	0	2
27	d5	61/88 (69%)	54 (88%)	7 (12%)	5	24
28	D6	83/83 (100%)	65 (78%)	18 (22%)	1	5
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2	13
29	D7	70/70 (100%)	60 (86%)	10 (14%)	3	15
29	d7	70/70 (100%)	54 (77%)	16 (23%)	1	4
30	D8	56/59 (95%)	42 (75%)	14 (25%)	0	3
30	d8	56/59 (95%)	48 (86%)	8 (14%)	3	15
31	D9	47/48 (98%)	38 (81%)	9 (19%)	1	8
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	5
32	E0	51/51 (100%)	36 (71%)	15 (29%)	0	1
33	E1	62/66 (94%)	42 (68%)	20 (32%)	0	1
33	e1	66/66 (100%)	43 (65%)	23 (35%)	0	1
34	SR	260/261 (100%)	227 (87%)	33 (13%)	4	19
34	sR	260/261 (100%)	230 (88%)	30 (12%)	5	24
35	SM	97/228 (42%)	68 (70%)	29 (30%)	0	1
35	sM	54/228 (24%)	42 (78%)	12 (22%)	1	4
39	L2	193/195 (99%)	158 (82%)	35 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	l2	192/195 (98%)	152 (79%)	40 (21%)	1	5
40	L3	320/322 (99%)	252 (79%)	68 (21%)	1	5
40	l3	320/322 (99%)	249 (78%)	71 (22%)	1	4
41	L4	288/288 (100%)	229 (80%)	59 (20%)	1	6
41	l4	288/288 (100%)	234 (81%)	54 (19%)	1	8
42	L5	244/244 (100%)	193 (79%)	51 (21%)	1	5
42	l5	243/244 (100%)	193 (79%)	50 (21%)	1	6
43	L6	134/152 (88%)	108 (81%)	26 (19%)	1	7
43	l6	135/152 (89%)	110 (82%)	25 (18%)	1	8
44	L7	186/204 (91%)	159 (86%)	27 (14%)	3	15
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3	15
45	L8	187/207 (90%)	158 (84%)	29 (16%)	2	13
45	l8	177/207 (86%)	149 (84%)	28 (16%)	2	12
46	L9	171/171 (100%)	133 (78%)	38 (22%)	1	4
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	5
47	M0	177/186 (95%)	140 (79%)	37 (21%)	1	5
47	m0	179/186 (96%)	141 (79%)	38 (21%)	1	5
48	M1	147/150 (98%)	114 (78%)	33 (22%)	1	4
48	m1	147/150 (98%)	120 (82%)	27 (18%)	1	9
49	M3	154/158 (98%)	128 (83%)	26 (17%)	2	11
49	m3	154/158 (98%)	130 (84%)	24 (16%)	2	13
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	9
50	m4	108/108 (100%)	90 (83%)	18 (17%)	2	11
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	10
51	m5	175/175 (100%)	150 (86%)	25 (14%)	3	15
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2	11
52	m6	160/161 (99%)	127 (79%)	33 (21%)	1	6
53	M7	140/145 (97%)	111 (79%)	29 (21%)	1	6
53	m7	125/145 (86%)	95 (76%)	30 (24%)	0	3
54	M8	150/150 (100%)	122 (81%)	28 (19%)	1	8
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	M9	153/153 (100%)	124 (81%)	29 (19%)	1	8
55	m9	153/153 (100%)	126 (82%)	27 (18%)	2	10
56	N0	156/156 (100%)	126 (81%)	30 (19%)	1	8
56	n0	156/156 (100%)	129 (83%)	27 (17%)	2	10
57	N1	136/136 (100%)	101 (74%)	35 (26%)	0	3
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	6
58	N2	87/106 (82%)	77 (88%)	10 (12%)	5	24
58	n2	85/106 (80%)	75 (88%)	10 (12%)	5	22
59	N3	104/104 (100%)	83 (80%)	21 (20%)	1	6
59	n3	104/104 (100%)	92 (88%)	12 (12%)	5	24
60	N4	57/129 (44%)	52 (91%)	5 (9%)	10	36
60	n4	100/129 (78%)	85 (85%)	15 (15%)	3	14
61	N5	104/117 (89%)	80 (77%)	24 (23%)	1	4
61	n5	104/117 (89%)	84 (81%)	20 (19%)	1	8
62	N6	109/109 (100%)	79 (72%)	30 (28%)	0	2
62	n6	109/109 (100%)	88 (81%)	21 (19%)	1	8
63	N7	115/115 (100%)	85 (74%)	30 (26%)	0	2
63	n7	115/115 (100%)	84 (73%)	31 (27%)	0	2
64	N8	118/118 (100%)	95 (80%)	23 (20%)	1	7
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	6
65	N9	46/46 (100%)	35 (76%)	11 (24%)	0	3
65	n9	46/46 (100%)	34 (74%)	12 (26%)	0	2
66	O0	81/87 (93%)	67 (83%)	14 (17%)	2	10
66	o0	84/87 (97%)	66 (79%)	18 (21%)	1	5
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	4
67	o1	94/96 (98%)	72 (77%)	22 (23%)	1	4
68	O2	109/110 (99%)	86 (79%)	23 (21%)	1	5
68	o2	109/110 (99%)	87 (80%)	22 (20%)	1	6
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	17
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	9
70	O4	95/101 (94%)	77 (81%)	18 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	o4	95/101 (94%)	82 (86%)	13 (14%)	3	17
71	O5	104/104 (100%)	72 (69%)	32 (31%)	0	1
71	o5	103/104 (99%)	84 (82%)	19 (18%)	1	9
72	O6	81/81 (100%)	58 (72%)	23 (28%)	0	2
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	10
73	o7	70/70 (100%)	57 (81%)	13 (19%)	1	8
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	4
74	o8	67/68 (98%)	49 (73%)	18 (27%)	0	2
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	7
75	o9	45/45 (100%)	33 (73%)	12 (27%)	0	2
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	5
76	q0	47/47 (100%)	37 (79%)	10 (21%)	1	5
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
77	q1	23/23 (100%)	13 (56%)	10 (44%)	0	0
78	Q2	90/90 (100%)	73 (81%)	17 (19%)	1	8
78	q2	90/90 (100%)	74 (82%)	16 (18%)	2	9
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	5
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1	7
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	5
82	p0	105/253 (42%)	81 (77%)	24 (23%)	1	4
All	All	18728/20239 (92%)	14998 (80%)	3730 (20%)	1	7

5 of 3730 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	O0	87	VAL
6	s4	200	ARG
64	n8	27	LYS
69	O3	33	GLU
79	Q3	32	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
74	O8	32	ASN
9	s7	122	HIS
57	n1	131	GLN
2	s0	140	ASN
7	s5	186	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	512 (29%)	56 (3%)
1	6	1792/1800 (99%)	463 (25%)	53 (2%)
36	1	3145/3396 (92%)	702 (22%)	92 (2%)
36	5	3145/3396 (92%)	717 (22%)	94 (2%)
37	3	120/121 (99%)	24 (20%)	2 (1%)
37	7	120/121 (99%)	23 (19%)	1 (0%)
38	4	157/158 (99%)	40 (25%)	4 (2%)
38	8	157/158 (99%)	40 (25%)	4 (2%)
All	All	10383/10950 (94%)	2521 (24%)	306 (2%)

5 of 2521 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 306 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3228	C
1	6	542	A
36	5	2971	A
36	1	3315	G
1	6	66	U

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

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 2562 ligands modelled in this entry, 1429 are monoatomic - leaving 1133 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	6	2085	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	S9	201	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	6	2206	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	L3	403	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
88	3J2	1	4209	-	28,30,30	1.57	5 (17%)	32,52,52	2.00	6 (18%)
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	c8	203	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4249	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	o7	502	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	n6	202	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	O7	105	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	m0	303	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	1	3866	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	m6	202	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	5	4234	86	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	6	2205	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	O2	201	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	3J2	5	4254	-	28,30,30	1.56	7 (25%)	32,52,52	1.75	8 (25%)
86	OHX	1	3869	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3915	-	0,6,6	0.00	-	-	-	-
86	OHX	d4	201	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3952	-	0,6,6	0.00	-	-	-	-
86	OHX	8	218	-	0,6,6	0.00	-	-	-	-
86	OHX	8	216	-	0,6,6	0.00	-	-	-	-
86	OHX	M6	202	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2102	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2126	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4020	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4087	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4211	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4124	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3942	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4170	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4252	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4175	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3870	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3898	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4180	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4052	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3929	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3997	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4004	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4248	-	0,6,6	0.00	-	-	-	-
86	OHX	m7	206	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3972	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4241	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2177	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4236	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4084	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4186	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2054	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4092	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4150	-	0,6,6	0.00	-	-	-	-
86	OHX	1	4200	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4089	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2191	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4154	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2134	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4178	-	0,6,6	0.00	-	-	-	-
86	OHX	5	4073	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	4	223	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	13	404	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	q1	101	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	m8	201	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	13	403	-	0,6,6	0.00	-	-		
86	OHX	5	3900	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	2	2147	86	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	5	4253	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	l5	302	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	7	229	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	2	2180	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	M7	205	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	L4	403	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	Q2	502	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	O9	101	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	M8	202	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	1	4000	86	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	m1	203	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	m9	201	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	5	3944	86	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	C1	201	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	M7	204	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	O3	202	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	o3	202	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	5	4251	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	2	2032	86	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	M9	202	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	8	230	-	0,6,6	0.00	-	-		
86	OHX	1	3865	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	1	3864	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	6	2208	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	6	2207	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	M5	304	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	N9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	1	3863	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	n3	202	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	m5	305	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	7	228	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4250	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	8	231	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	M0	303	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	19	202	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	n9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	1	4168	86	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	15	304	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		

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	3J2	5	4254	-	-	0/2/65/65	0/5/5/5
88	3J2	1	4209	-	-	0/2/65/65	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4209	3J2	C4-C13	4.52	1.47	1.40
88	1	4209	3J2	C3-C1	4.40	1.57	1.51
88	5	4254	3J2	C4-C3	-4.14	1.34	1.39
88	5	4254	3J2	C4-C13	3.57	1.46	1.40
88	5	4254	3J2	C14-C13	-3.05	1.34	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4209	3J2	O6-C5-C6	-5.77	97.42	109.61
88	1	4209	3J2	O2-C11-C12	5.14	123.51	117.72
88	5	4254	3J2	C18-C8-C9	-4.85	99.90	108.96
88	1	4209	3J2	O1-C3-C1	-4.21	107.25	112.52
88	5	4254	3J2	O6-C5-C6	-4.13	100.89	109.61

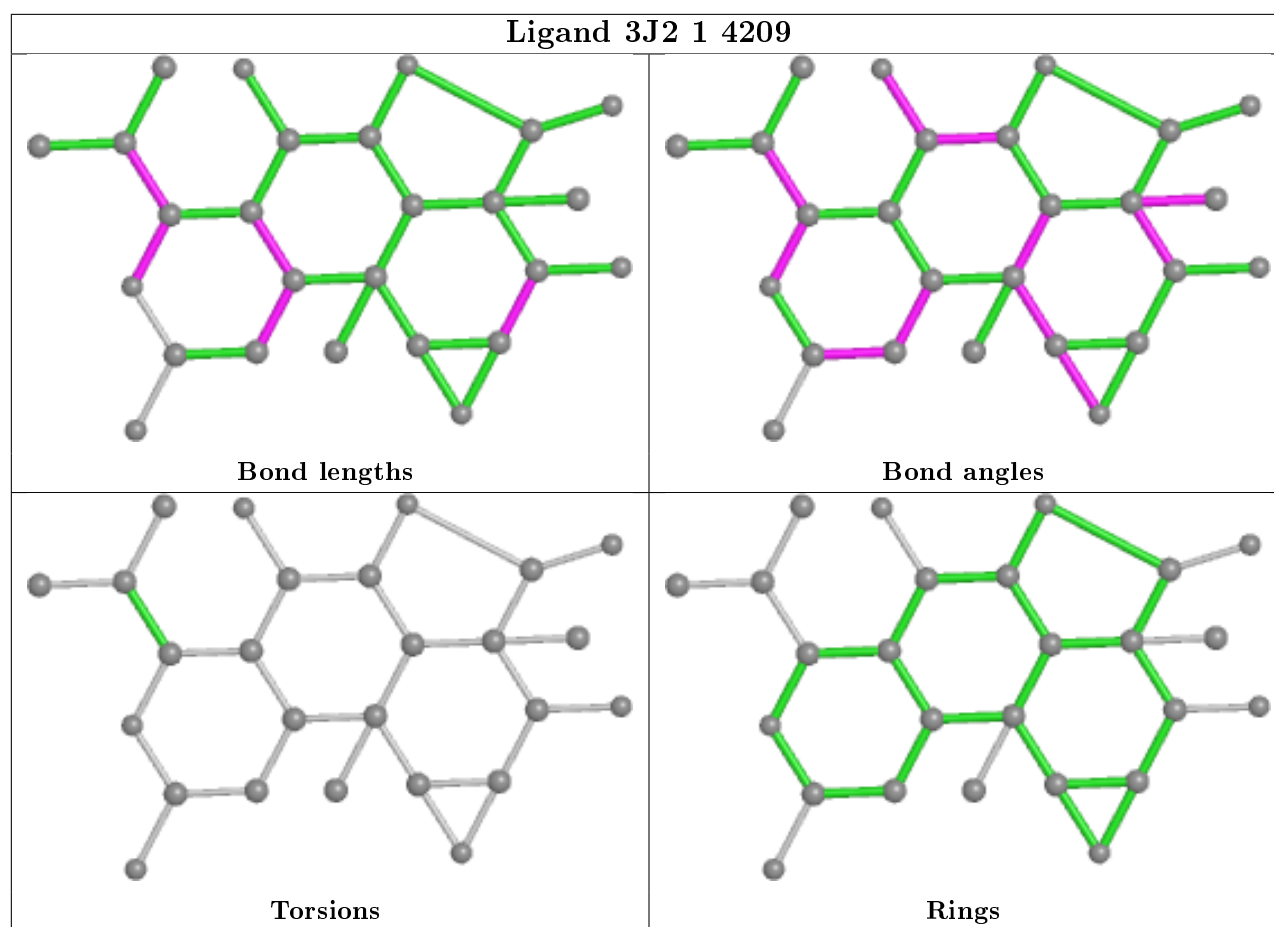
There are no chirality outliers.

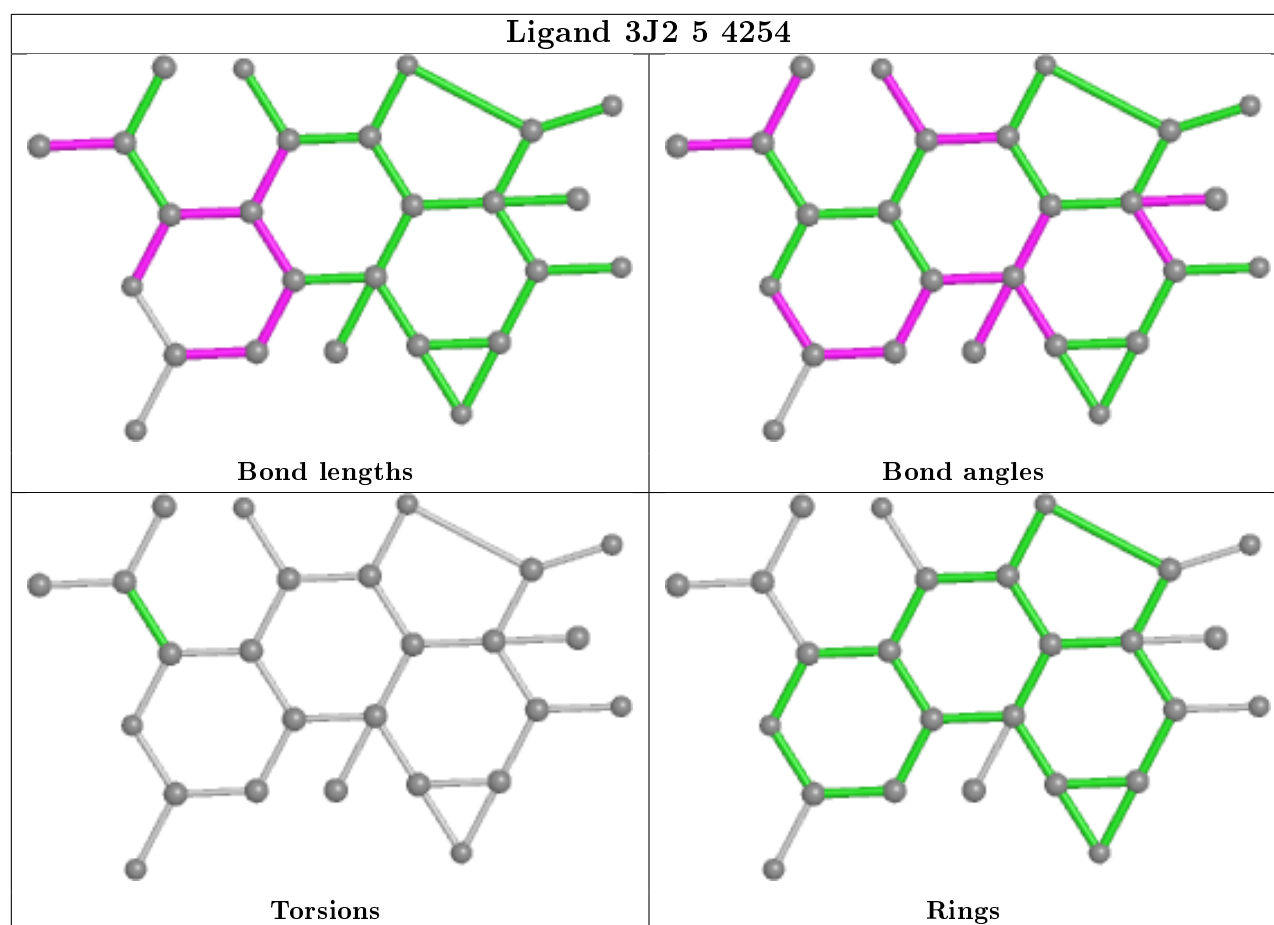
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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