



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 07:58 PM BST

PDB ID : 4U50  
Title : Crystal structure of Verrucarin bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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	:	<b>FAILED</b>
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

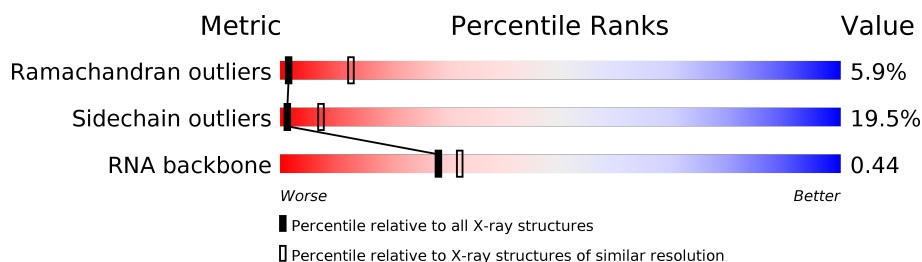
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



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


























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	63% 30% 5% •
1	6	1800	64% 31% 5%
2	S0	251	62% 18% • 18%
2	s0	251	63% 17% • 18%
3	S1	254	59% 24% • 16%
3	s1	254	64% 20% • 15%
4	S2	253	68% 17% • 14%
4	s2	253	63% 22% • 14%









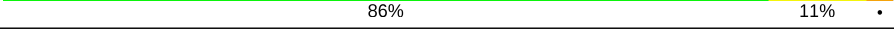


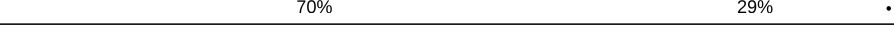

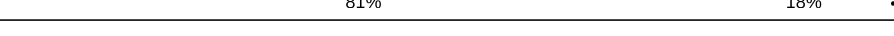


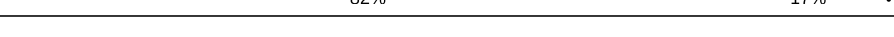

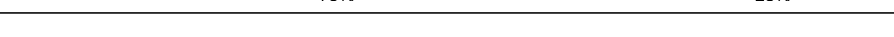
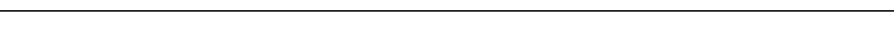

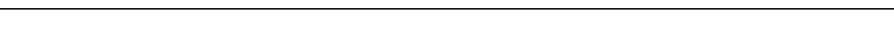
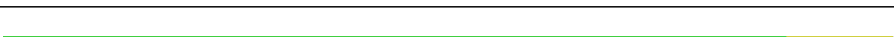


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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3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















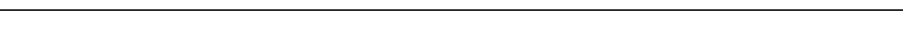




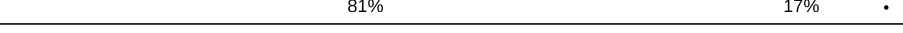





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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107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












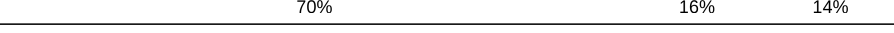



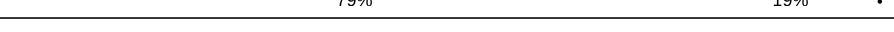



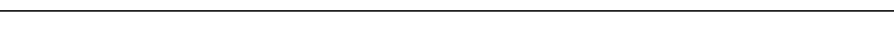
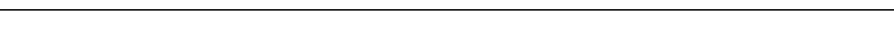

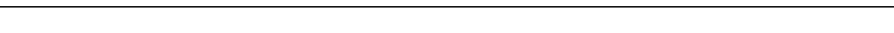
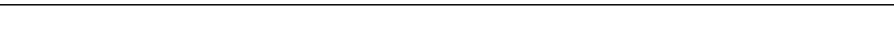

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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6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















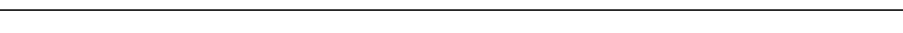




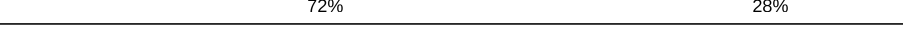





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Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9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

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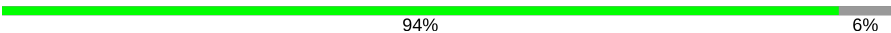


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Mol	Chain	Length	Quality of chain
68	O2	129	 78%19%..
68	o2	129	 79%19%..
69	O3	106	 87%12%.
69	o3	106	 81%18%.
70	O4	120	 77%16%7%.
70	o4	120	 75%16%7%.
71	O5	119	 78%21%.
71	o5	119	 77%22%.
72	O6	99	 76%21%.
72	o6	99	 71%26%.
73	O7	87	 84%14%.
73	o7	87	 86%14%
74	O8	77	 77%23%
74	o8	77	 81%18%.
75	O9	50	 84%16%
75	o9	50	 80%20%
76	Q0	52	 73%25%.
76	q0	52	 75%23%.
77	Q1	25	 72%28%
77	q1	25	 72%28%
78	Q2	105	 75%23%.
78	q2	105	 79%19%.
79	Q3	91	 86%14%
79	q3	91	 79%21%
80	e0	62	 73%26%.

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Mol	Chain	Length	Quality of chain
81	p0	311	 39% 7% 54%
82	m2	160	 94% 6%
83	p1	47	 100%
84	p2	46	 100%

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411230 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
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
E1	77	ALA	GLY	conflict	UNP P05759
e1	77	ALA	GLY	conflict	UNP P05759

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	17	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	18	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	19	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O		0	0	0
			1543	962	315	266				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	m3	194	Total	C	N	O	0	0	0
			1548	965	316	267			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 82 is a protein called UNKNOWN PROTEIN m2.

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

- 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	4	Total	Mg	0	0
			4	4		
85	n8	5	Total	Mg	0	0
			5	5		
85	o1	1	Total	Mg	0	0
			1	1		
85	N5	2	Total	Mg	0	0
			2	2		
85	6	146	Total	Mg	0	0
			146	146		
85	sM	2	Total	Mg	0	0
			2	2		
85	O4	1	Total	Mg	0	0
			1	1		
85	m5	3	Total	Mg	0	0
			3	3		
85	l3	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	C1	1	Total 1	Mg 1	0	0
85	M1	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	122	Total 122	Mg 122	0	0
85	n0	3	Total 3	Mg 3	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	2	Total 2	Mg 2	0	0
85	M5	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	S2	2	Total 2	Mg 2	0	0
85	L8	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
85	SM	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	497	Total 497	Mg 497	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	1	Total 1	Mg 1	0	0

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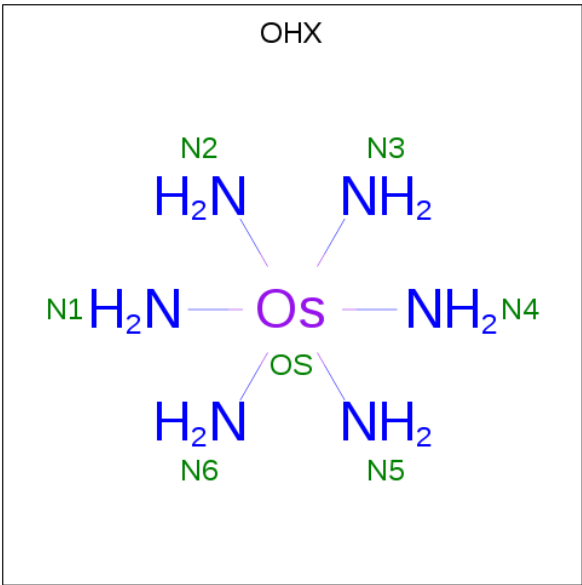
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	s6	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	1	Total 1	Mg 1	0	0
85	1	470	Total 470	Mg 470	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	3	Total 3	Mg 3	0	0
85	O2	1	Total 1	Mg 1	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o3	1	Total 1	Mg 1	0	0
85	d3	3	Total 3	Mg 3	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	25	Total 25	Mg 25	0	0
85	n6	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	2	Total 2	Mg 2	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N8	4	Total 4	Mg 4	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	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	1	Total 1	Mg 1	0	0
85	7	16	Total 16	Mg 16	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	d4	1	Total 1	Mg 1	0	0
85	N6	2	Total 2	Mg 2	0	0
85	8	15	Total 15	Mg 15	0	0
85	l4	2	Total 2	Mg 2	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0
85	3	14	Total 14	Mg 14	0	0

- 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		
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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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			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
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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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86	2	1	Total	N	Os	0	0
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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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86	2	1	Total	N	Os	0	0
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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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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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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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			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
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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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86	2	1	Total	N	Os	0	0
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			7	6	1		
86	2	1	Total	N	Os	0	0
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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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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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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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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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86	2	1	Total	N	Os	0	0
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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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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
86	2	1	Total	N	Os	0	0
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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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86	2	1	Total	N	Os	0	0
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86	S6	1	Total	N	Os	0	0
			7	6	1		
86	S8	1	Total	N	Os	0	0
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86	C3	1	Total	N	Os	0	0
			7	6	1		
86	C5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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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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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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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		

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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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86	1	1	Total	N	Os	0	0
			7	6	1		

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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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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		

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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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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
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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

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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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86	1	1	Total	N	Os	0	0
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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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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N1	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	Q2	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	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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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		

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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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86	6	1	Total	N	Os	0	0
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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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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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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		

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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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86	6	1	Total	N	Os	0	0
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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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			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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

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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	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		
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 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l3	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l4	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l5	1	Total 7	N 6	Os 1	0	0
86	l9	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m0	1	Total 7	N 6	Os 1	0	0
86	m1	1	Total 7	N 6	Os 1	0	0
86	m4	1	Total 7	N 6	Os 1	0	0
86	m5	1	Total 7	N 6	Os 1	0	0
86	m6	1	Total 7	N 6	Os 1	0	0
86	m7	1	Total 7	N 6	Os 1	0	0
86	m8	1	Total 7	N 6	Os 1	0	0
86	n3	1	Total 7	N 6	Os 1	0	0
86	n3	1	Total 7	N 6	Os 1	0	0
86	n6	1	Total 7	N 6	Os 1	0	0
86	n9	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	o2	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	o7	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).

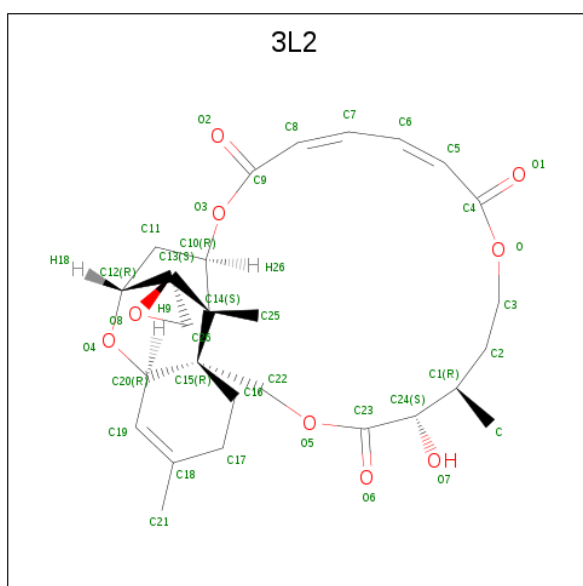
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0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

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

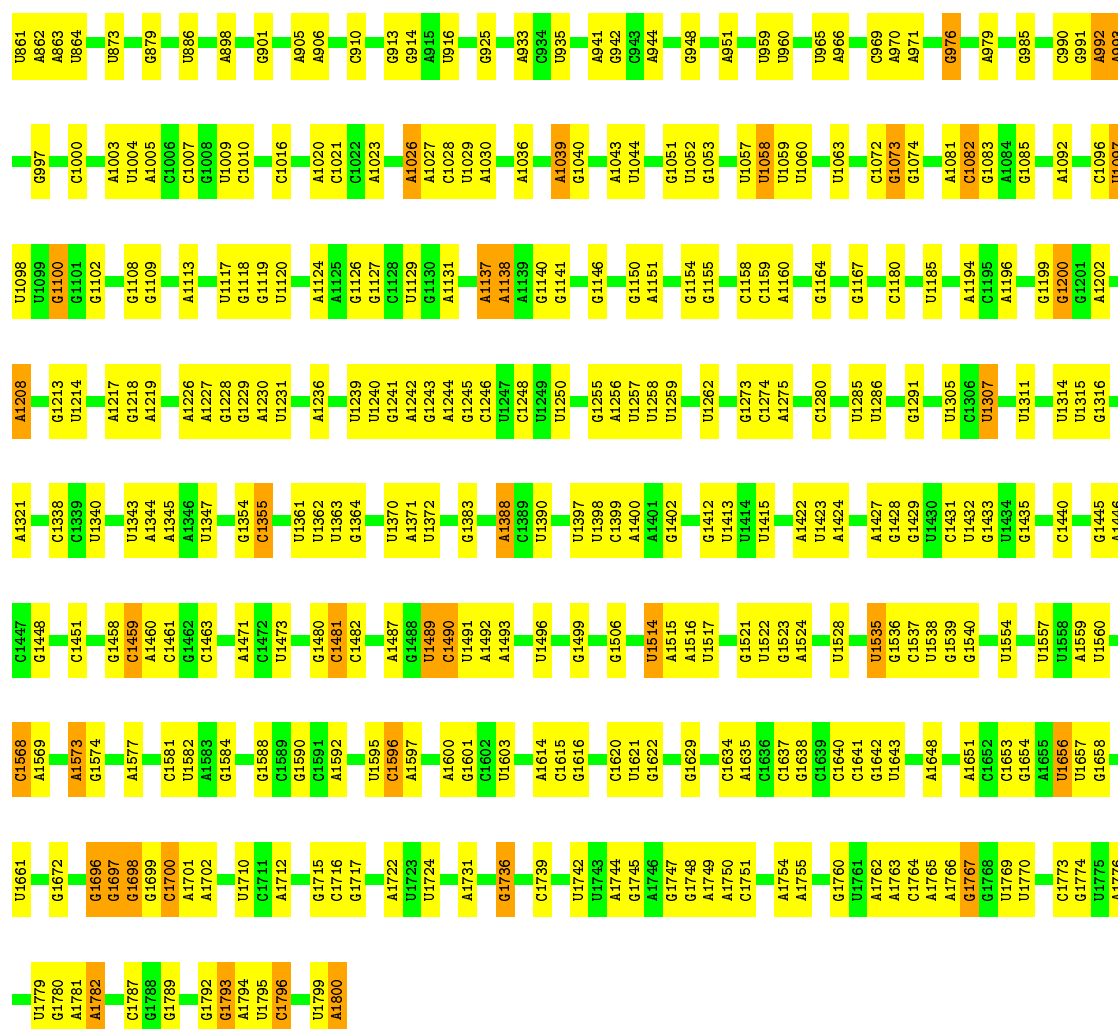
- Molecule 88 is (4S,5R,10E,12Z,16R,16aS,17S,18R,19aR,23aR)-4-hydroxy-5,16a,21-trimethyl-4,5,6,7,16,16a,22,23-octahydro-3H,18H,19aH-spiro[16,18-methano[1,6,12]trioxacyclooctadecino[3,4-d]chromene-17,2'-oxirane]-3,9,14-trione (three-letter code: 3L2) (formula:  $C_{27}H_{34}O_9$ ).



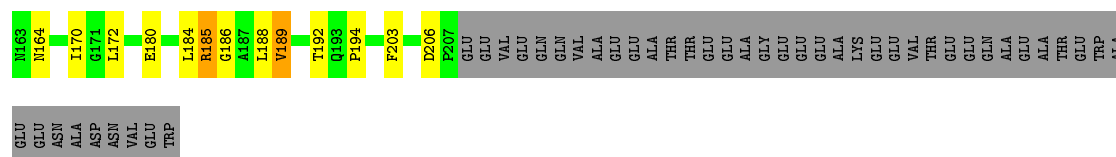
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			36	27	9		
88	5	1	Total	C	O	0	0
			36	27	9		





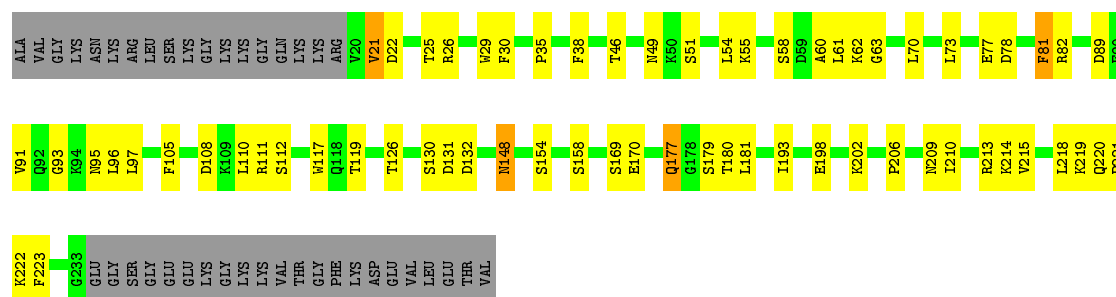






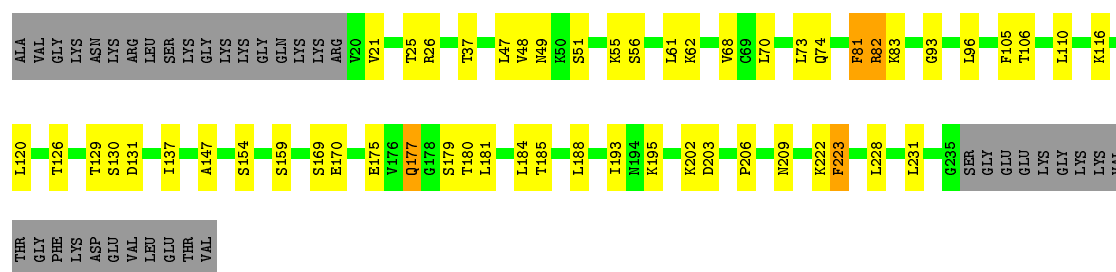
- Molecule 3: 40S ribosomal protein S1-A

Chain S1: 59% 24% 16%



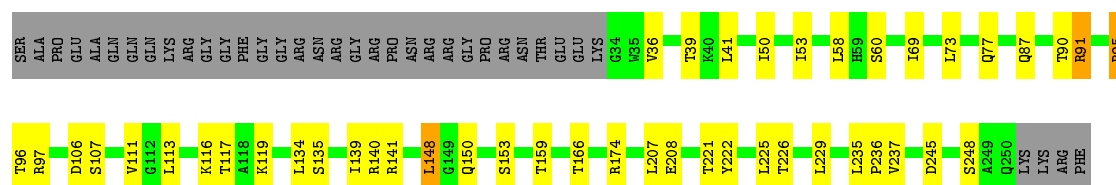
- Molecule 3: 40S ribosomal protein S1-A

Chain s1: 64% 20% 15%



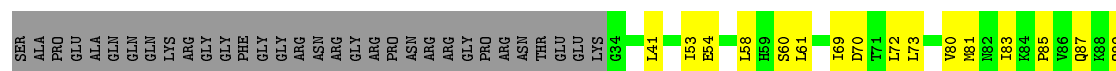
- Molecule 4: 40S ribosomal protein S2

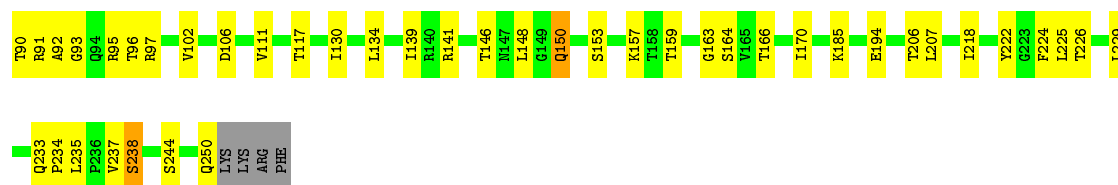
Chain S2: 68% 17% 14%



- Molecule 4: 40S ribosomal protein S2

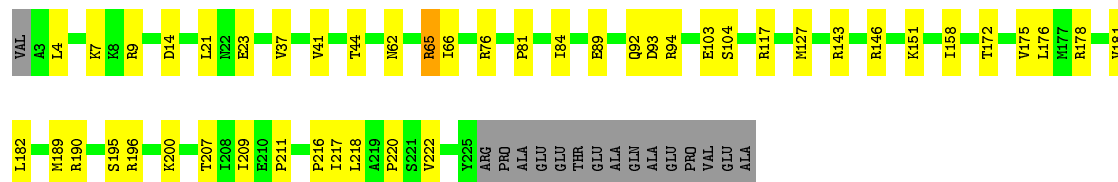
Chain s2: 63% 22% 14%





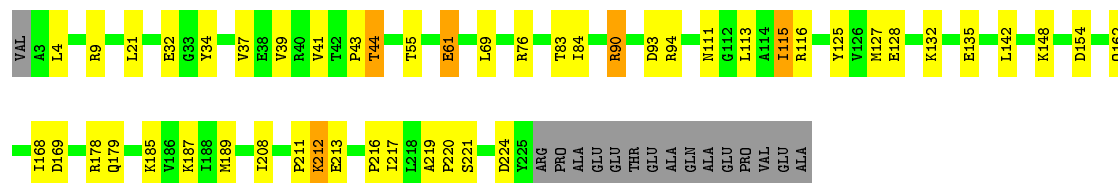
- Molecule 5: 40S ribosomal protein S3

Chain S3: 74% 19% 7%



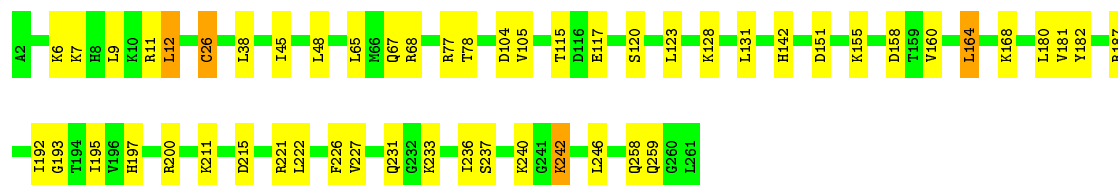
- Molecule 5: 40S ribosomal protein S3

Chain s3: 73% 18% 7%



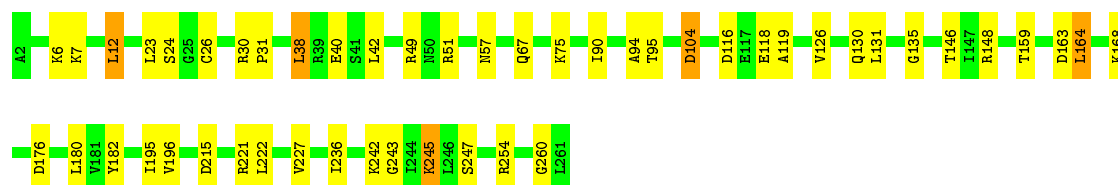
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 80% 19% 1%



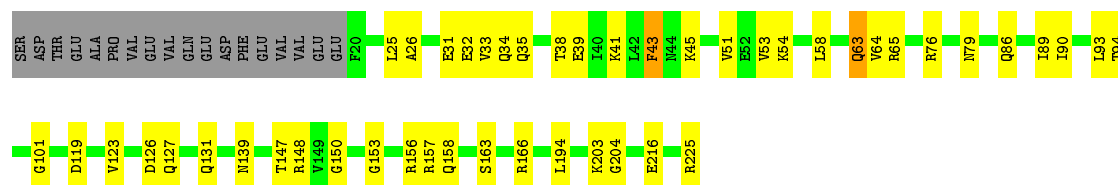
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 81% 17% 2%

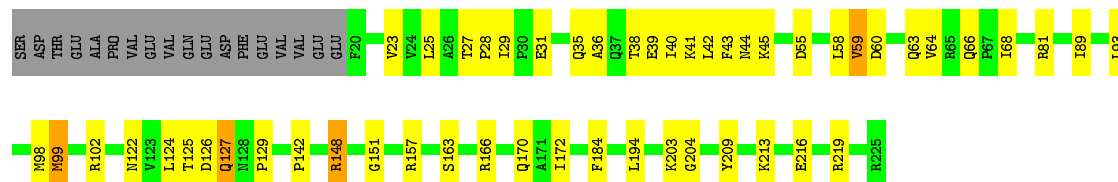


- Molecule 7: 40S ribosomal protein S5

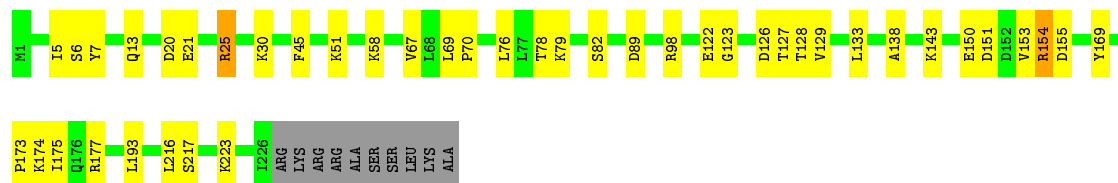
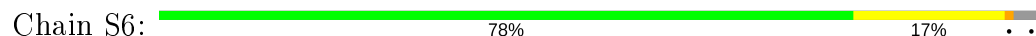
Chain S5: 71% 20% 8%



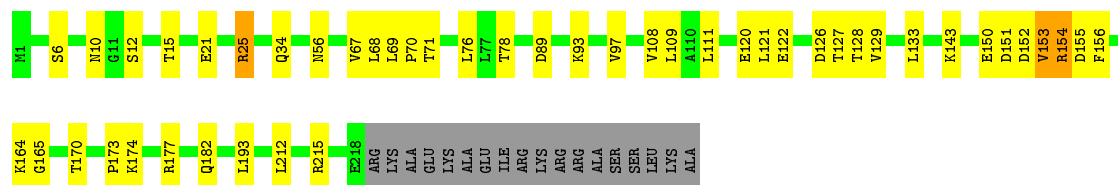
• Molecule 7: 40S ribosomal protein S5



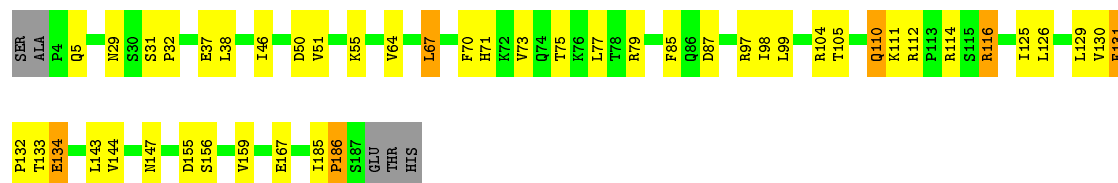
• Molecule 8: 40S ribosomal protein S6-A



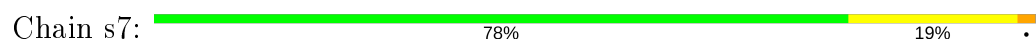
• Molecule 8: 40S ribosomal protein S6-A

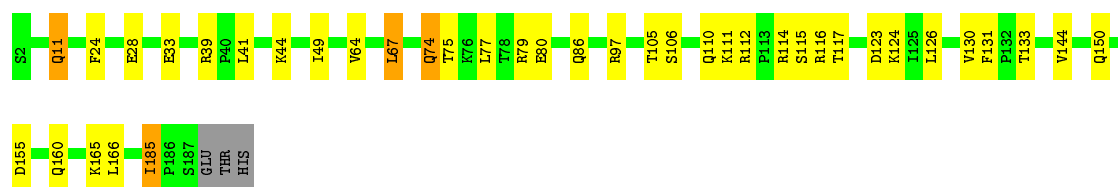


• Molecule 9: 40S ribosomal protein S7-A

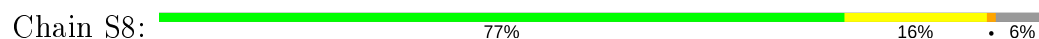


• Molecule 9: 40S ribosomal protein S7-A

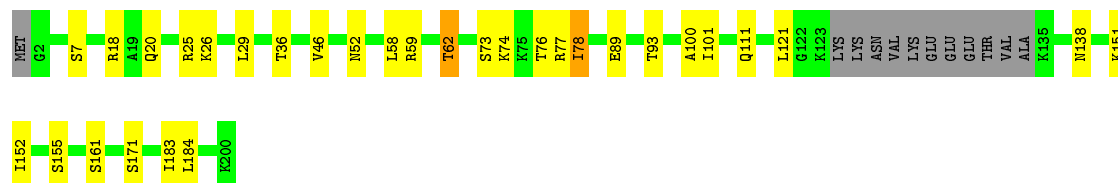




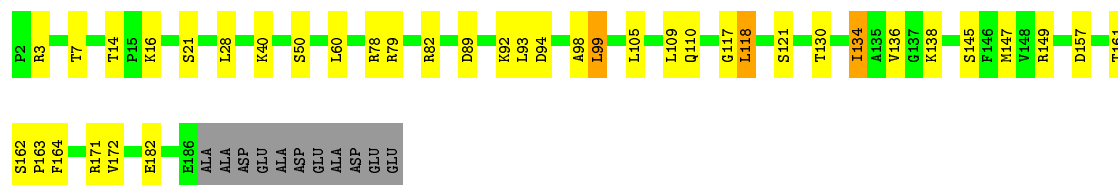
- Molecule 10: 40S ribosomal protein S8-A



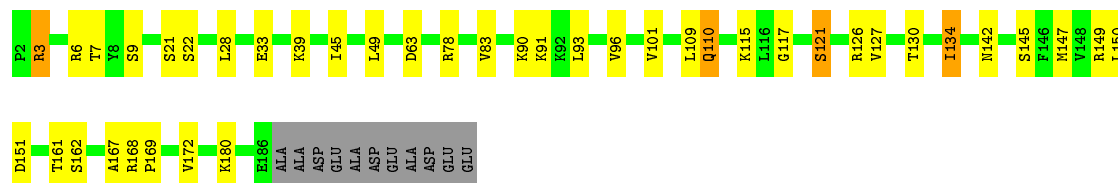
- Molecule 10: 40S ribosomal protein S8-A



- Molecule 11: 40S ribosomal protein S9-A



- Molecule 11: 40S ribosomal protein S9-A



- Molecule 12: 40S ribosomal protein S10-A





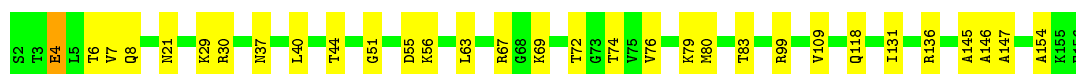
- Molecule 12: 40S ribosomal protein S10-A

Chain c0: 67% 22% 9%



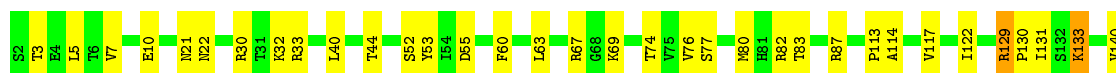
- Molecule 13: 40S ribosomal protein S11-A

Chain C1: 80% 19% 1%



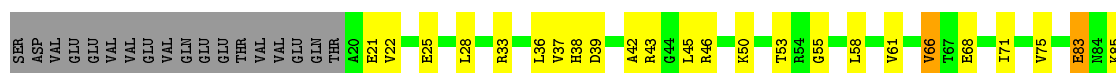
- Molecule 13: 40S ribosomal protein S11-A

Chain c1: 72% 21% 6%



- Molecule 14: 40S ribosomal protein S12

Chain C2: 56% 28% 13%




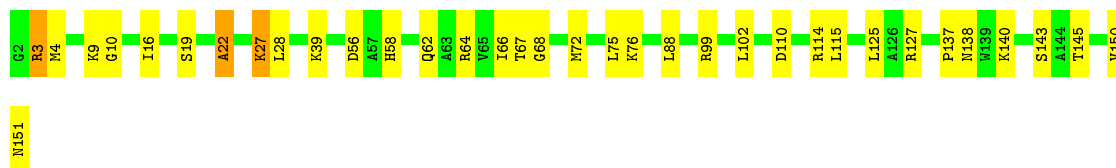
- Molecule 14: 40S ribosomal protein S12

Chain c2: 56% 28% 13%




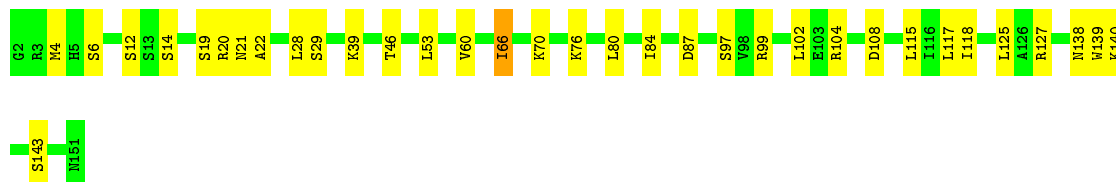
- Molecule 15: 40S ribosomal protein S13

Chain C3:  77% 21% .



- Molecule 15: 40S ribosomal protein S13

Chain c3:  77% 22% .



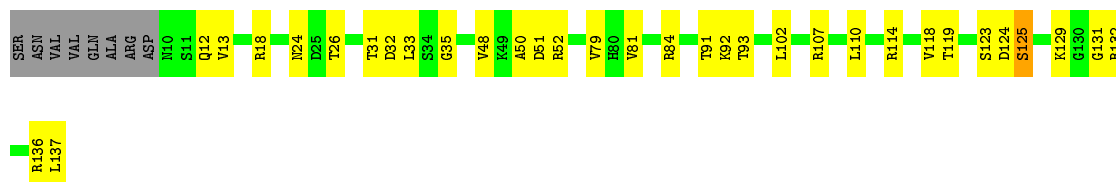
- Molecule 16: 40S ribosomal protein S14-A

Chain C4:  74% 16% 7% .



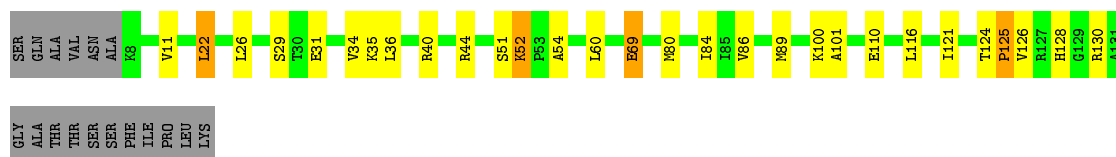
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:  70% 24% 6% .



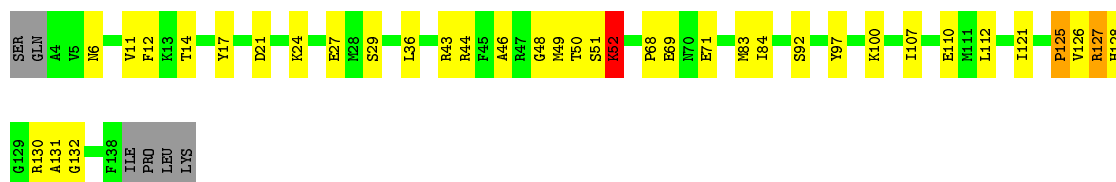
- Molecule 17: 40S ribosomal protein S15

Chain C5:  67% 18% 12% .



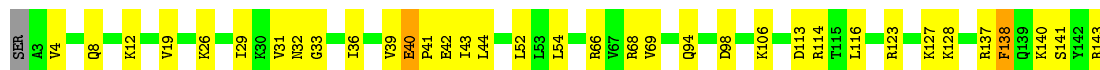
- Molecule 17: 40S ribosomal protein S15

Chain c5:  70% 24% . . .



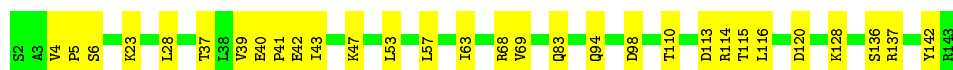
- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 75% 23% ..



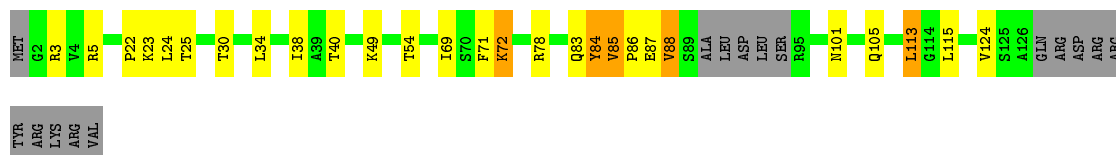
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 79% 21%



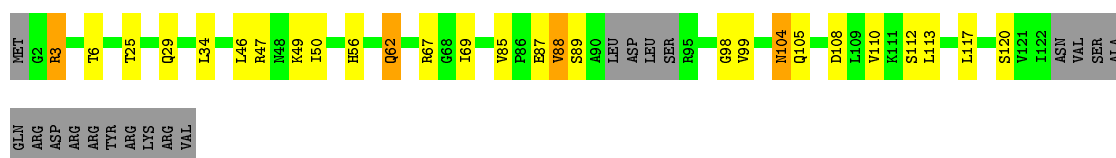
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 68% 16% 12%



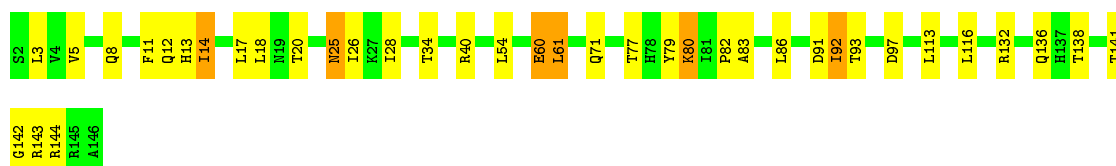
- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 66% 17% 14%

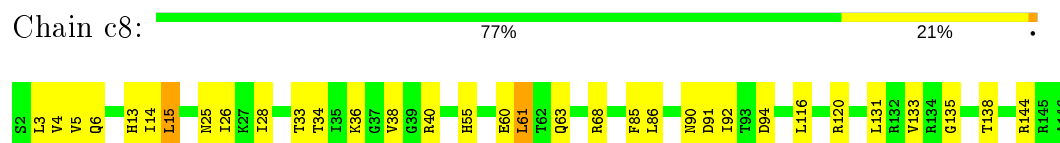


- Molecule 20: 40S ribosomal protein S18-A

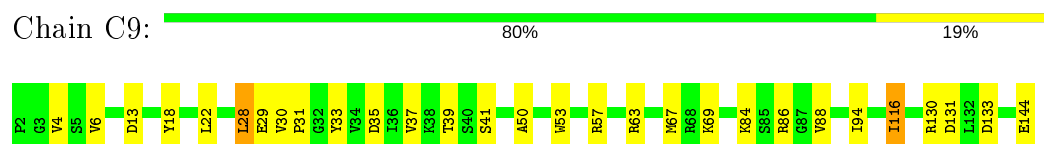
Chain C8: 74% 22%



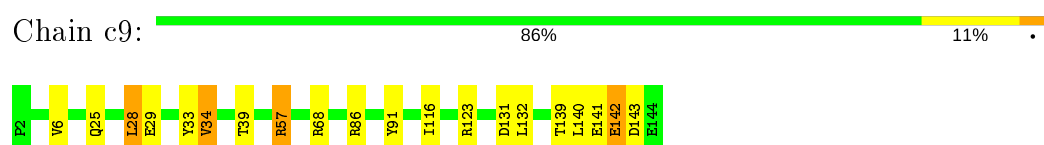
- Molecule 20: 40S ribosomal protein S18-A



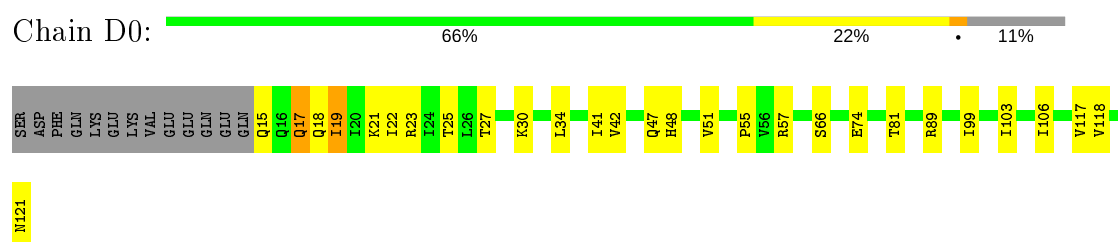
- Molecule 21: 40S ribosomal protein S19-A



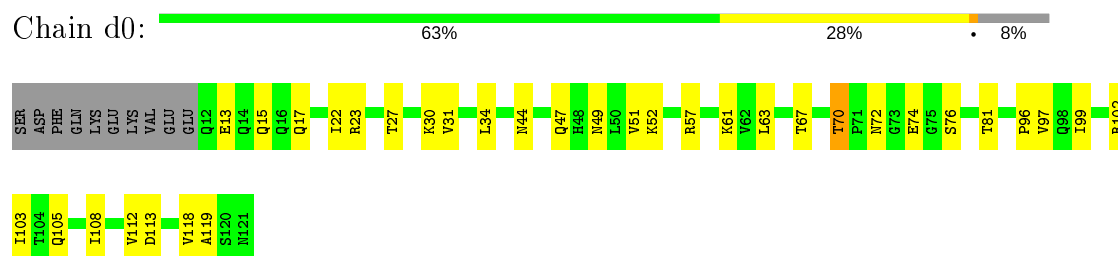
- Molecule 21: 40S ribosomal protein S19-A



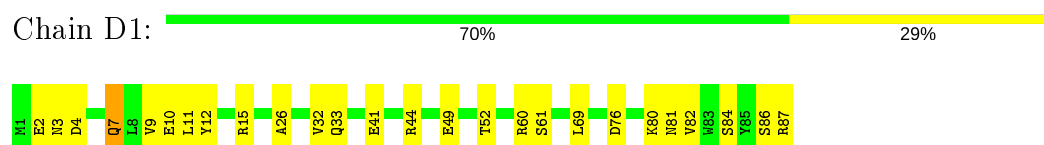
- Molecule 22: 40S ribosomal protein S20



- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A



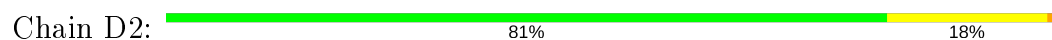
- Molecule 23: 40S ribosomal protein S21-A







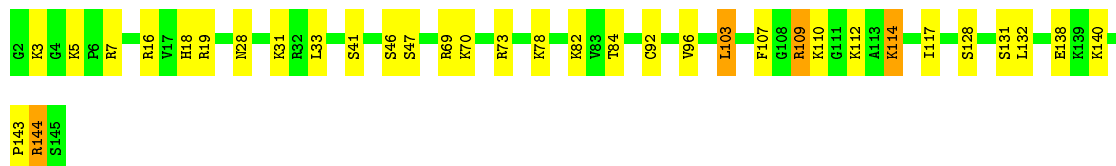
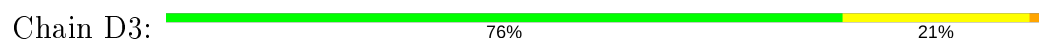
- Molecule 24: 40S ribosomal protein S22-A



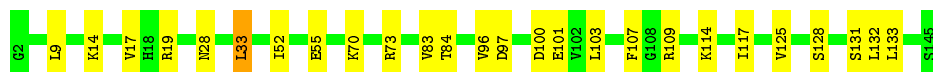
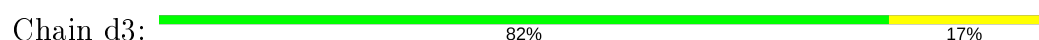
- Molecule 24: 40S ribosomal protein S22-A



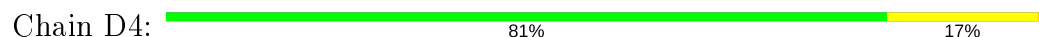
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A

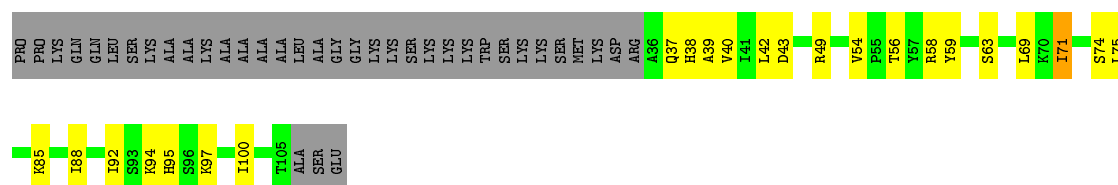


- Molecule 26: 40S ribosomal protein S24-A



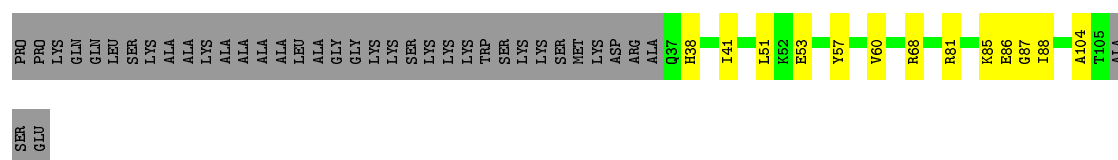
- Molecule 27: 40S ribosomal protein S25-A

Chain D5: 



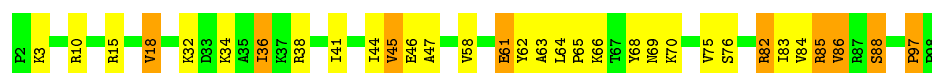
- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 




- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 




- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 




- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 



- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 



- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 



- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 67% 23% 6% 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 69% 24% . .



- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 67% 29% .



- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 83% 15% .



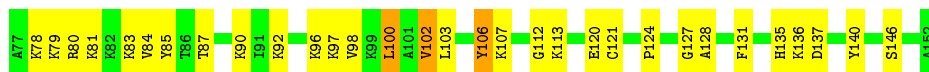
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 50% 42% . 7%



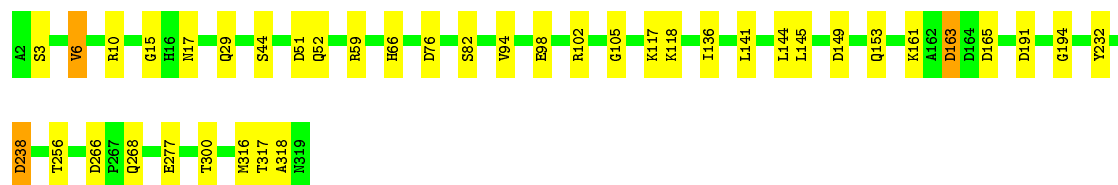
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 59% 37% .



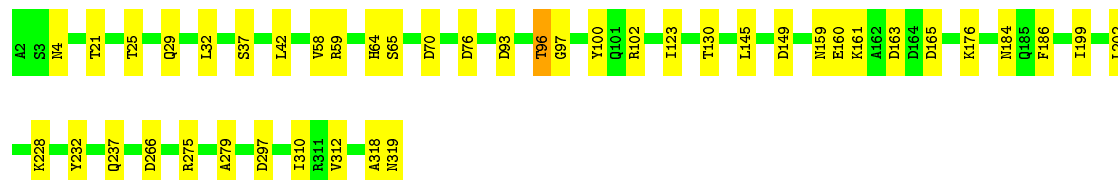
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR: 87% 12% .



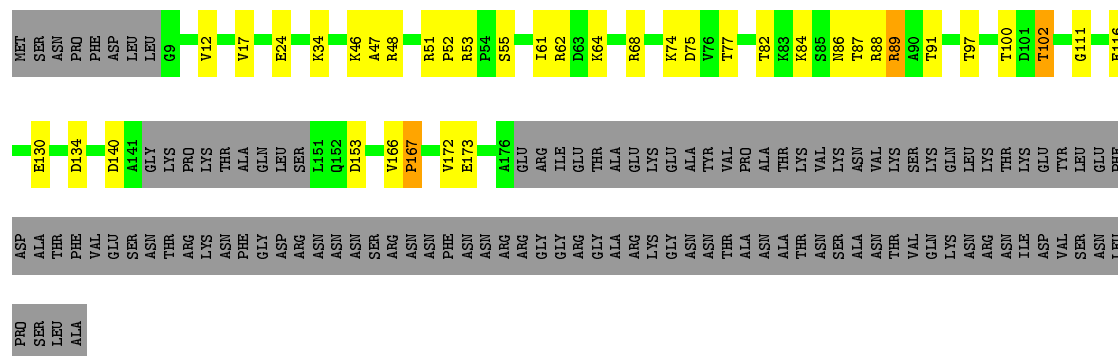
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 86% 13%



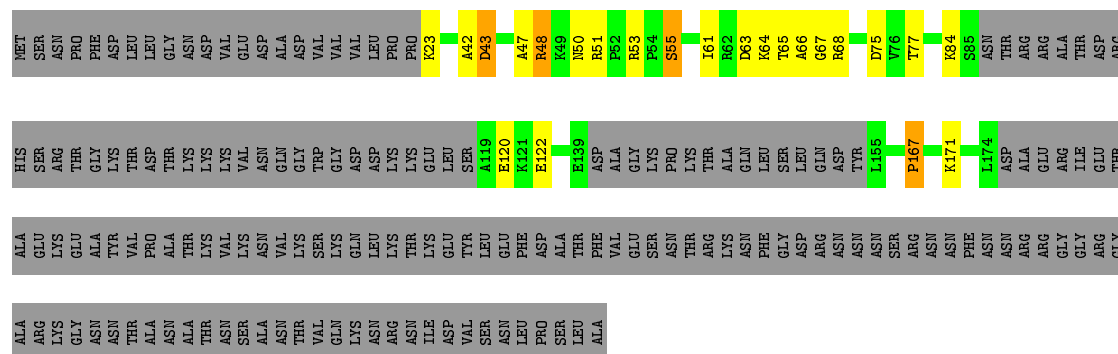
- Molecule 35: Suppressor protein STM1

Chain SM: 44% 13% 42%



- Molecule 35: Suppressor protein STM1

Chain sM: 30% 7% 62%

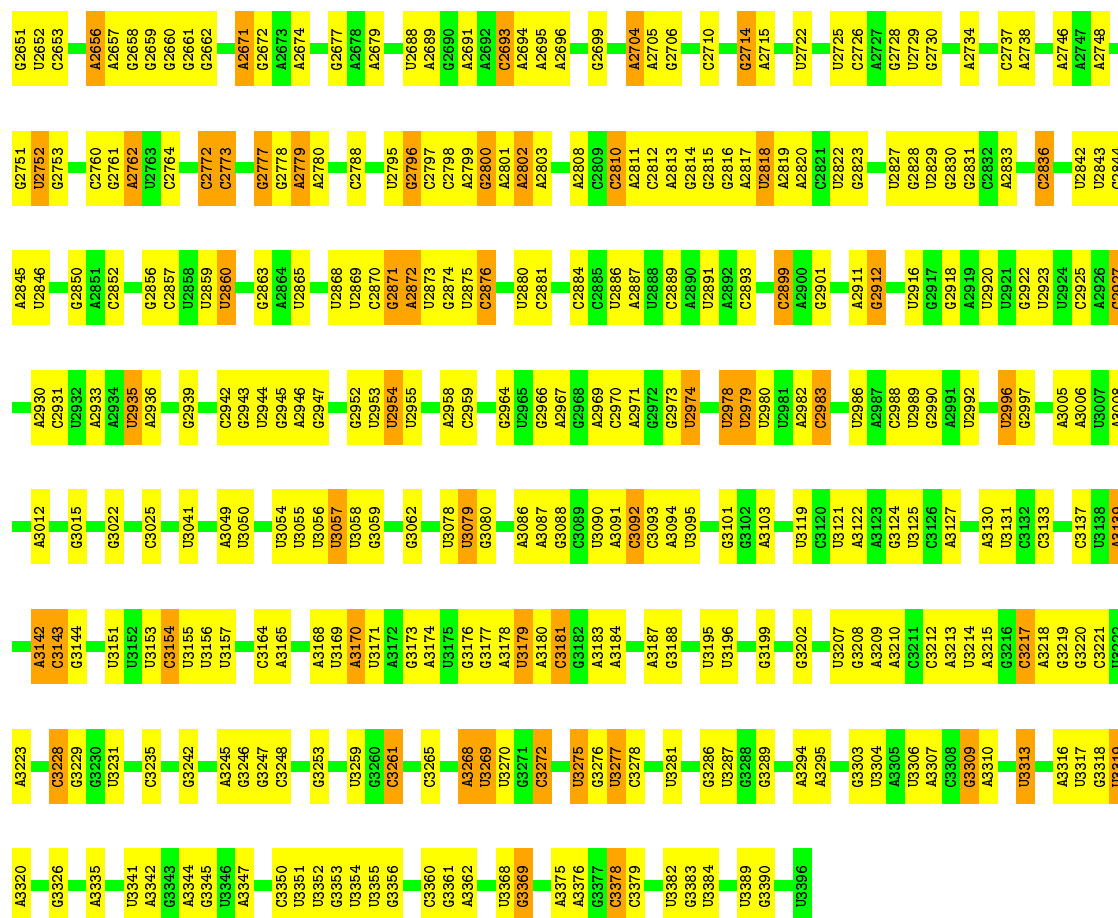


- Molecule 36: 25S ribosomal RNA

Chain 1: 52% 34% 6% 7%

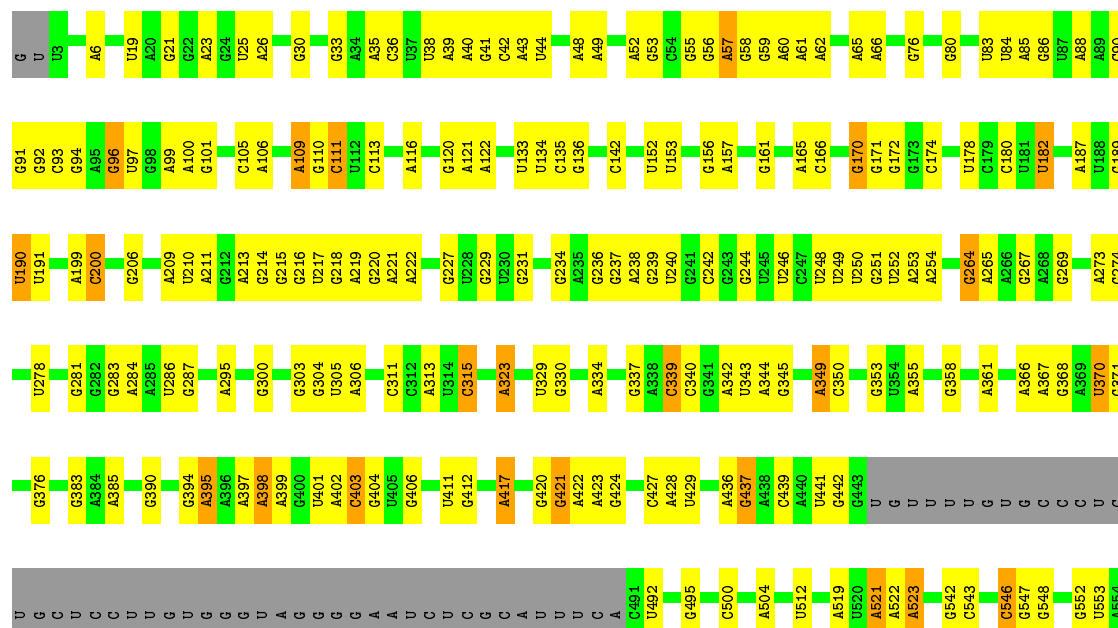
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U1235	A1157	A1094	A917	U822	G723	G652	U556	G	A398	U305	G205	G92	U3
G1236	A1158	U1094	C918	G830	G725	A653	A557	G	A399	G306	G206	G93	G
G1237	C1159	U1095	U919	A831	G726	G654	U558	A	G400	A306	U210	G94	U9
C1238	C1160	U1096	A920	G832	G730	G655	A559	G	U401	C311	A211	G95	A
U1241	G1161	G1097	A921	G833	G731	A656	U560	U	A402	C312	A212	G96	A13
G1242	U1162	A1098	U922	G834	G732	A657	U561	A	C403	U313	U213	G97	U14
G1243	A1163	C923	C923	G835	G733	G658	U562	C	G404	C314	U214	G98	C15
G1244	G1164	G924	G924	G836	G734	G659	U563	U	U405	C315	G218	G99	A99
A1245	A1165	G1101	A925	A843	A744	G660	U564	U	U406	C316	A219	A100	G18
G1246	G1166	A1102	A926	C849	G754	G661	A578	G	A407	G320	G220	G104	G24
U1247	U1167	G1103	C927	U850	A755	C663	G579	C	A408	A323	A221	U25	U25
C1248	U1168	G1104	G928	C851	A756	U664	C580	A	A409	A324	C226	A26	A26
G1249	G1105	G1010	A929	G852	C757	U665	U581	U	G420	U326	G229	C27	C27
G1250	G1106	C1017	U932	G853	C758	G667	G582	U	G421	U327	G230	C28	C28
A1251	C1107	G1018	A933	G854	C759	U668	U583	U	A422	U328	G231	C29	C29
U1258	U1110	G1019	G934	A858	G763	U669	A585	C	A423	U329	G232	G33	G33
G1262	U1111	G1020	U935	G859	U764	G670	A586	G	A424	C332	C233	A116	A116
A1263	A1112	G1021	U936	G860	U765	U671	C586	U	U428	G335	G236	U117	A39
G1264	U1113	G1022	A937	C861	U766	A672	U589	U	U430	G336	A238	A121	A40
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G1266	G1115	A1025	U939	G863	G768	U674	C599	U	C435	C340	U240	A123	C42
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G1268	G1117	G1027	G941	A866	G770	A677	C594	U	C437	C344	C242	G132	U46
U1269	C1118	C1032	U942	G867	G771	U678	U599	U	U438	G347	U245	U133	C47
A1270	C1119	G1033	U943	C868	U776	G679	G604	U	U439	A348	U246	U134	A48
U1271	U1120	A1036	U944	G869	U777	U680	U605	U	U440	C350	C247	C135	A49
C1272	U1121	C1037	C945	G870	U778	U681	G511	U	U	G353	U249	G155	G53
A1273	U1122	U1041	C946	C873	A780	U682	U507	U	U	U359	U250	G156	G54
C1274	U1123	C1043	A951	U874	G781	U683	G509	U	U	G360	U251	A157	G55
U1278	G1126	U1044	A952	G878	G785	A690	U510	U	U	A361	G267	G161	G56
G1279	U1127	C1045	G953	U879	A786	A691	U511	U	U	U362	A268	U182	A57
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G1281	A1130	A1048	C957	C881	C788	C695	U518	U	U	A364	U270	U184	A61
C1282	G1131	C1049	C958	A882	A789	A699	A519	U	U	A365	G277	A65	A62
G1285	C1132	A1052	C959	A883	U790	C700	U520	U	U	G368	G281	A66	A66
A1286	G1133	U1052	U960	A884	C793	G701	U521	U	U	U370	G282	A67	A67
U1287	A1134	A1053	C961	U885	U794	C702	A522	U	U	G371	G283	A71	A71
C1296	C1135	A1054	A962	C893	G795	G703	A523	U	U	A372	A284	C72	C72
C1297	U1138	A1055	A963	G894	U796	U704	A524	U	U	A375	A285	C73	C73
A1301	G1139	A1061	A964	A895	U797	A705	G531	U	U	G376	U296	G76	G76
U1302	G1142	A1064	U965	A896	G800	U706	U534	U	U	A377	A289	C81	C81
A1303	U1143	A1065	G968	U897	A801	G708	G535	U	U	A378	A290	U187	U187
C1304	G1144	C1068	C969	G900	C802	A709	C543	U	U	A379	A291	U188	U188
G1306	U1145	C1069	G971	G901	C803	G712	C544	U	U	A380	A292	U189	U189
U1307	G1148	A1072	A973	U905	A806	U713	C545	U	U	A381	A293	U190	U190
A1308	G1149	G1072	G974	G906	A807	G714	U546	U	U	A382	A294	U191	U191
U1309	U1150	U1081	U979	G907	A808	A715	C547	U	U	A383	A295	U192	U192
G1310	U1151	U1082	A980	G908	U810	A716	G548	U	U	A384	A296	G86	G86
U1313	G1152	G1083	U981	G909	U811	G717	A646	U	U	A385	A297	U87	U87
C1232	A1154	A1155	C982	G910	G815	U718	A647	U	U	A386	A298	A88	A88
				A914	A816	A720	A649	U	U	A387	A299	A89	A89





• Molecule 36: 25S ribosomal RNA

Chain 5: 51% 35% 7% 7%





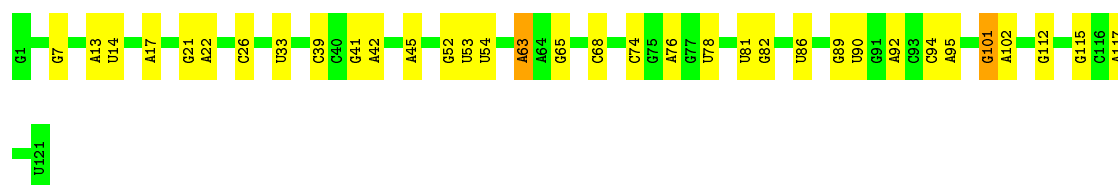


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U3058	A2972	U2752	U2835	A2900	G2555	G2415	U2349	C2279	U2193	U2112	G
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G3065	G2973	G2754	C2839	A2902	C2566	U2417	U2352	A2281	C2195	C2114	C
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C3004	C3004	U2795	U2864	U2930	G2610	G	U2379	U2310	U2226	C2146	G
A3005	A3005	U2796	U2865	C2931	G2611	U	U2380	G2311	C2227	A2147	C
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		U2822	U2891	U2960	U2637	C	U2408	U2338	G2262	U2181	C
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		U2824	U2893	U2962	U2639	C	U2410	U2340	G2264	U2183	C
		U2825	U2894	U2963	U2640	C	U2411	U2341	G2265	U2184	C
		U2826	U2895	U2964	U2641	C	U2412	U2342	G2266	U2185	C
		U2827	U2896	U2965	U2642	C	U2413	U2343	G2267	U2186	C
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		U2832	U2901	U2970	U2647	C	U2418	U2348	G2272	U2191	C
		U2833	U2902	U2971	U2648	C	U2419	U2349	G2273	U2192	C
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		U2835	U2904	U2973	U2650	C	U2421	U2351	G2275	U2194	C
		U2836	U2905	U2974	U2651	C	U2422	U2352	G2276	U2195	C
		U2837	U2906	U2975	U2652	C	U2423	U2353	G2277	U2196	C
		U2838	U2907	U2976	U2653	C	U2424	U2354	G2278	U2197	C
		U2839	U2908	U2977	U2654	C	U2425	U2355	G2279	U2198	C
		U2840	U2909	U2978	U2655	C	U2426	U2356	G2280	U2199	C
		U2841	U2910	U2979	U2656	C	U2427	U2357	G2281	U2200	C
		U2842	U2911	U2980	U2657	C	U2428	U2358	G2282	U2201	C
		U2843	U2912	U2981	U2658	C	U2429	U2359	G2283	U2202	C
		U2844	U2913	U2982	U2659	C	U2430	U2360	G2284	U2203	C
		U2845	U2914	U2983	U2660	C	U2431	U2361	G2285	U2204	C
		U2846	U2915	U2984	U2661	C	U2432	U2362	G2286	U2205	C
		U2847	U2916	U2985	U2662	C	U2433	U2363	G2287	U2206	C
		U2848	U2917	U2986	U2663	C	U2434	U2364	G2288	U2207	C
		U2849	U2918	U2987	U2664	C	U2435	U2365	G2289	U2208	C
		U2850	U2919	U2988	U2665	C	U2436	U2366	G2290	U2209	C
		U2851	U2920	U2989	U2666	C	U2437	U2367	G2291	U2210	C
		U2852	U2921	U2990	U2667	C	U2438	U2368	G2292	U2211	C
		U2853	U2922	U2991	U2668	C	U2439	U2369	G2293	U2212	C
		U2854	U2923	U2992	U2669	C	U2440	U2370	G2294	U2213	C
		U2855	U2924	U2993	U2670	C	U2441	U2371	G2295	U2214	C
		U2856	U2925	U2994	U2671	C	U2442	U2372	G2296	U2215	C
		U2857	U2926	U2995	U2672	C	U2443	U2373	G2297	U2216	C
		U2858	U2927	U2996	U2673	C	U2444	U2374	G2298	U2217	C
		U2859	U2928	U2997	U2674	C	U2445	U2375	G2299	U2218	C
		U2860	U2929	U2998	U2675	C	U2446	U2376	G2300	U2219	C
		U2861	U2930	U2999	U2676	C	U2447	U2377	G2301	U2220	C
		U2862	U2931	U3000	U2677	C	U2448	U2378	G2302	U2221	C
		U2863	U2932	U3001	U2678	C	U2449	U2379	G2303	U2222	C
		U2864	U2933	U3002	U2679	C	U2450	U2380	G2304	U2223	C
		U2865	U2934	U3003	U2680	C	U2451	U2381	G2305	U2224	C
		U2866	U2935	U3004	U2681	C	U2452	U2382	G2306	U2225	C
		U2867	U2936	U3005	U2682	C	U2453	U2383	G2307	U2226	C
		U2868	U2937	U3006	U2683	C	U2454	U2384	G2308	U2227	C
		U2869	U2938	U3007	U2684	C	U2455	U2385	G2309	U2228	C
		U2870	U2939	U3008	U2685	C	U2456	U2386	G2310	U2229	C
		U2871	U2940	U3009	U2686	C	U2457	U2387	G2311	U2230	C
		U2872	U2941	U3010	U2687	C	U2458	U2388	G2312	U2231	C
		U2873	U2942	U3011	U2688	C	U2459	U2389	G2313	U2232	C
		U2874	U2943	U3012	U2689	C	U2460	U2390	G2314	U2233	C
		U2875	U2944	U3013	U2690	C	U2461	U2391	G2315	U2234	C
		U2876	U2945	U3014	U2691	C	U2462	U2392	G2316	U2235	C
		U2877	U2946	U3015	U2692	C	U2463	U2393	G2317	U2236	C
		U2878	U2947	U3016	U2693	C	U2464	U2394	G2318	U2237	C
		U2879	U2948	U3017	U2694	C	U2465	U2395	G2319	U2238	C
		U2880	U2949	U3018	U2695	C	U2466	U2396	G2320	U2239	C
		U2881	U2950	U3019	U2696	C	U2467	U2397	G2321	U2240	C
		U2882	U2951	U3020	U2697	C	U2468	U2398	G2322	U2241	C
		U2883									



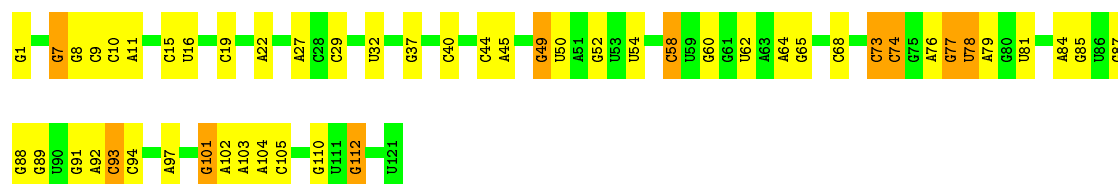
• Molecule 37: 5S ribosomal RNA

Chain 3: 72% 26% .



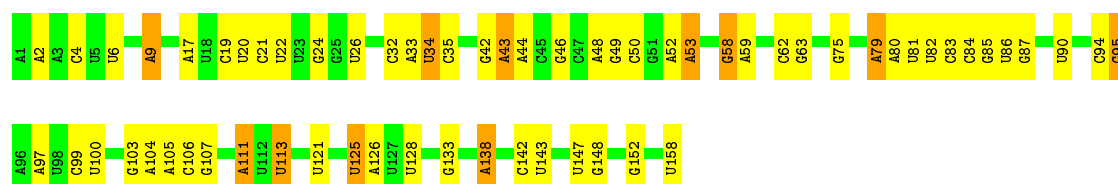
• Molecule 37: 5S ribosomal RNA

Chain 7: 58% 34% 8%



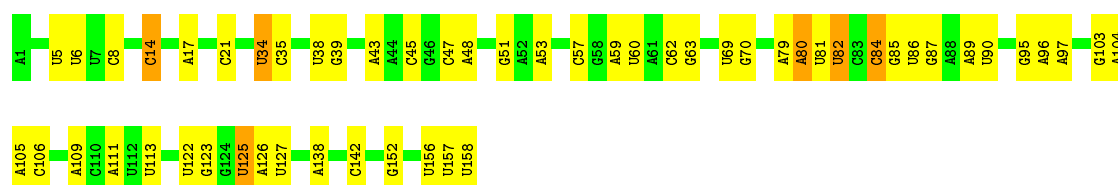
• Molecule 38: 5.8S ribosomal RNA

Chain 4: 60% 33% 7%

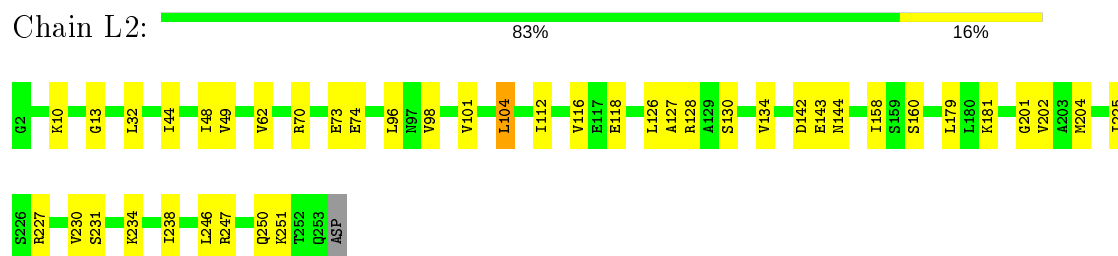


• Molecule 38: 5.8S ribosomal RNA

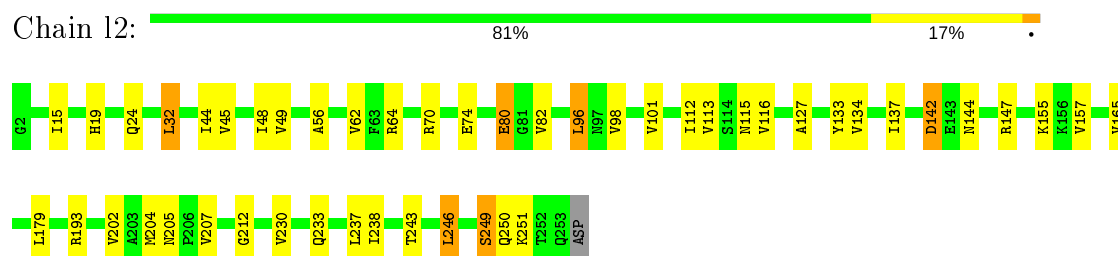
Chain 8: 66% 30% .



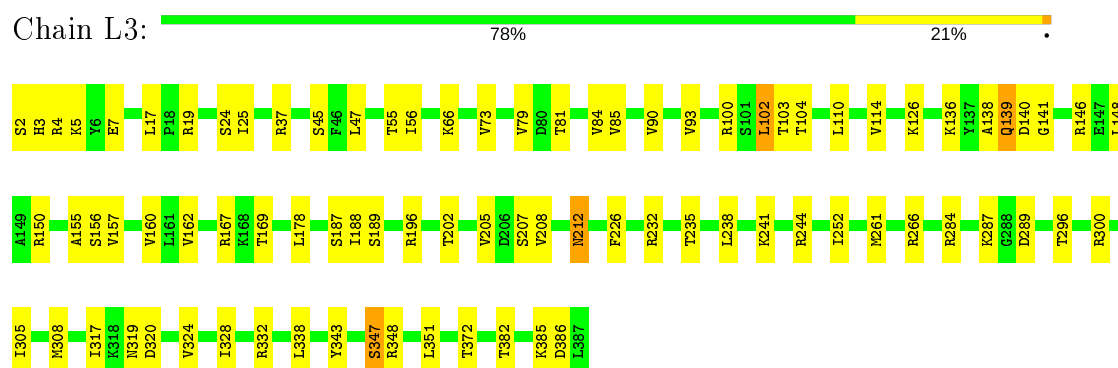
- Molecule 39: 60S ribosomal protein L2-A



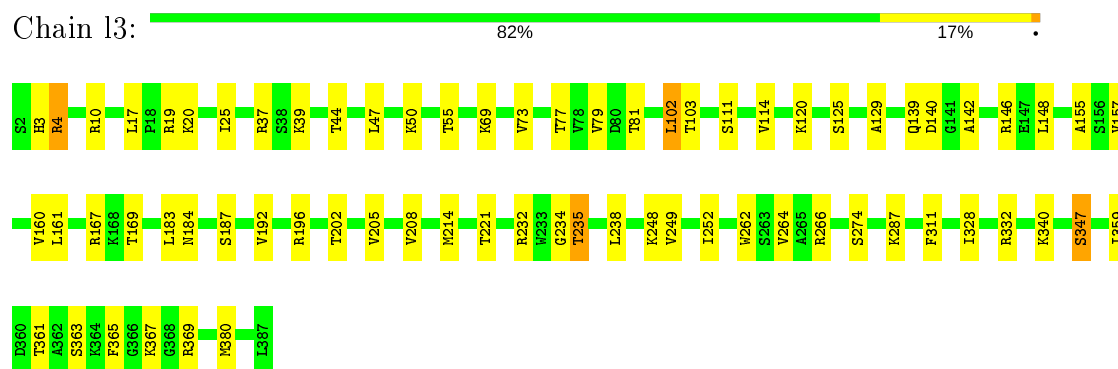
- Molecule 39: 60S ribosomal protein L2-A



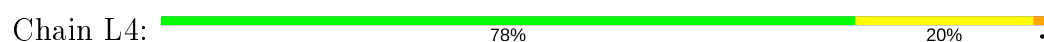
- Molecule 40: 60S ribosomal protein L3

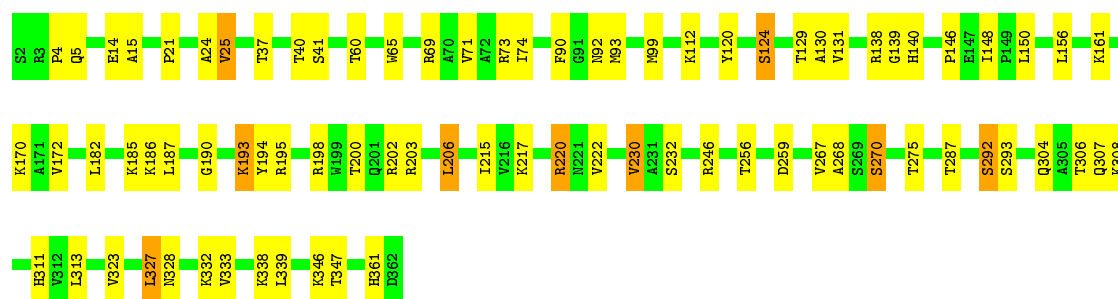


- Molecule 40: 60S ribosomal protein L3

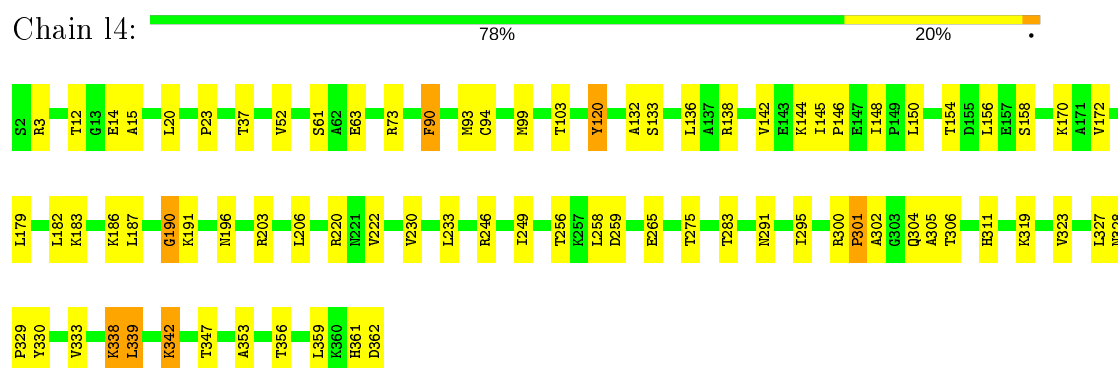


- Molecule 41: 60S ribosomal protein L4-A

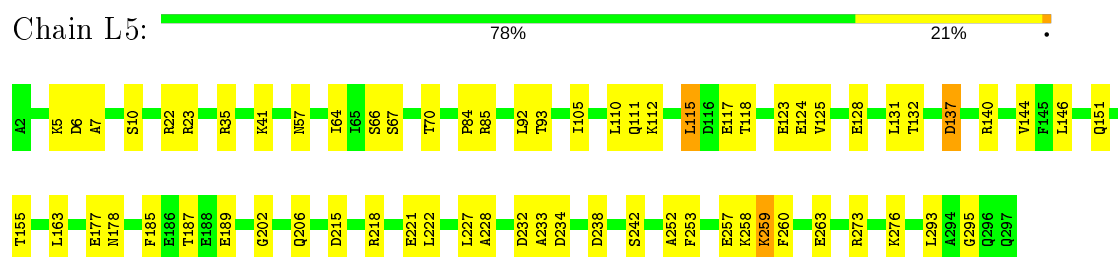




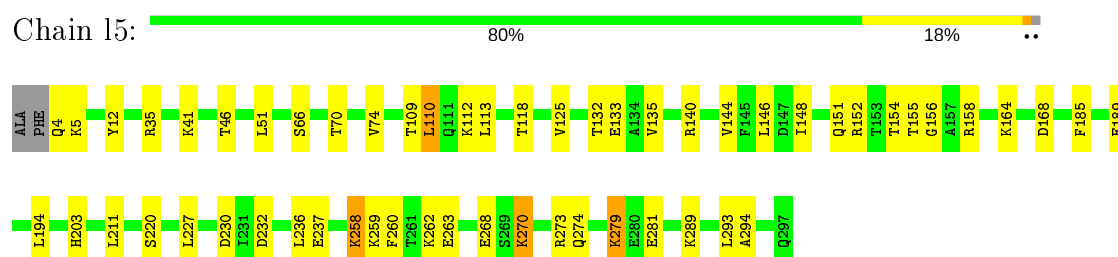
- Molecule 41: 60S ribosomal protein L4-A



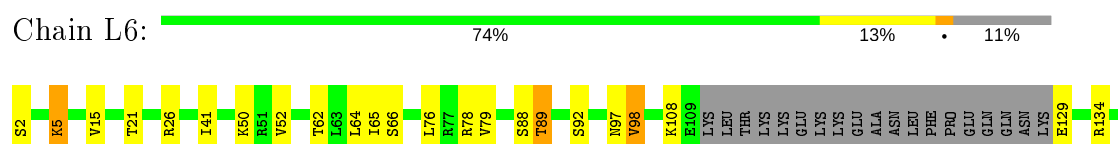
- Molecule 42: 60S ribosomal protein L5



- Molecule 42: 60S ribosomal protein L5



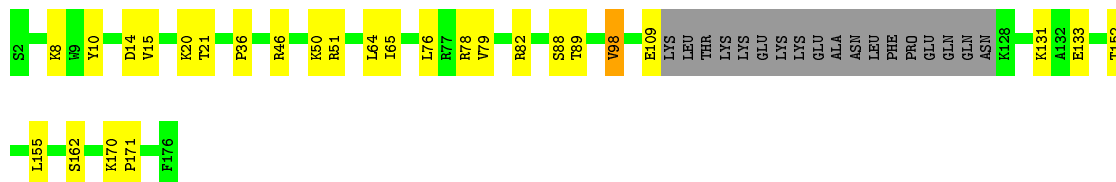
- Molecule 43: 60S ribosomal protein L6-A





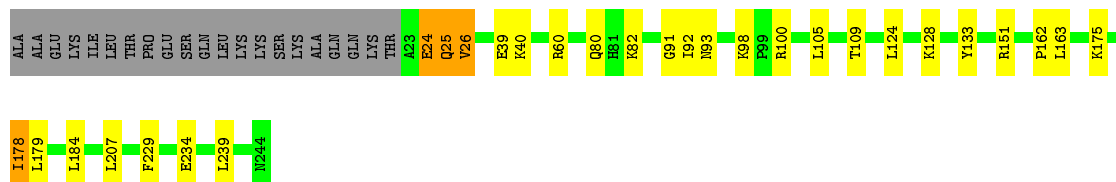
- Molecule 43: 60S ribosomal protein L6-A

Chain l6: 74% 15% 10%



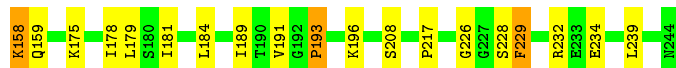
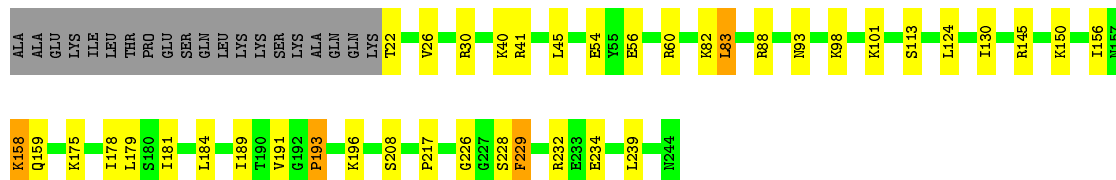
- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 79% 10% 9%



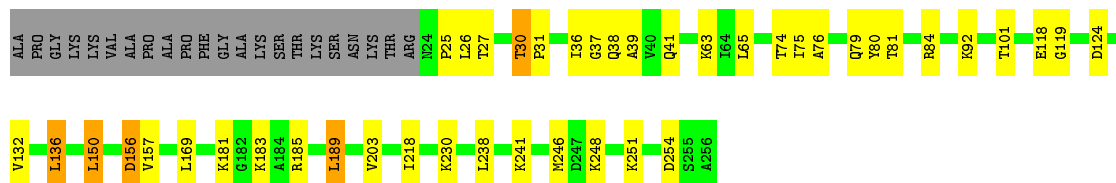
- Molecule 44: 60S ribosomal protein L7-A

Chain l7: 75% 15% 8%



- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 75% 15% 9%



- Molecule 45: 60S ribosomal protein L8-A

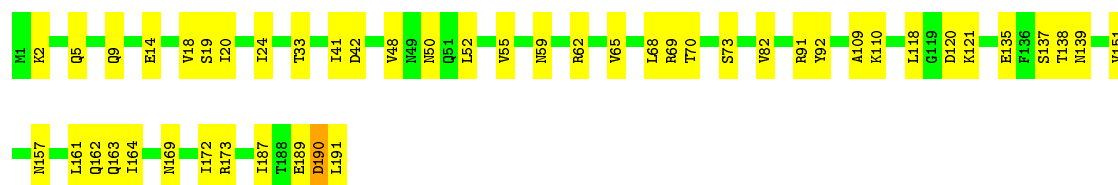
Chain l8: 73% 17% 9%





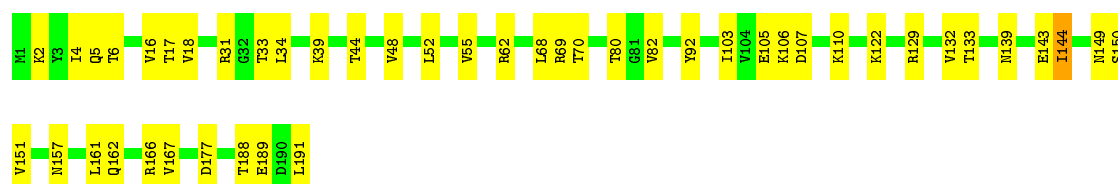
- Molecule 46: 60S ribosomal protein L9-A

Chain L9:  75%  24%



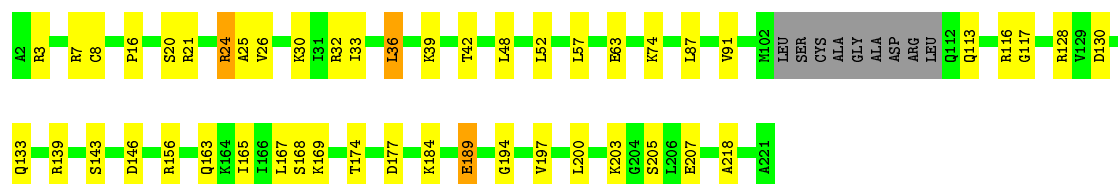
- Molecule 46: 60S ribosomal protein L9-A

Chain l9:  76%  24%



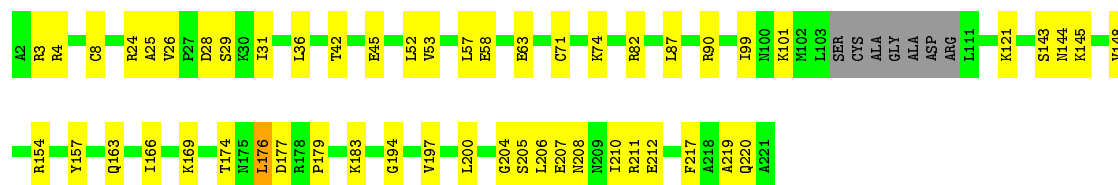
- Molecule 47: 60S ribosomal protein L10

Chain M0:  74%  20%



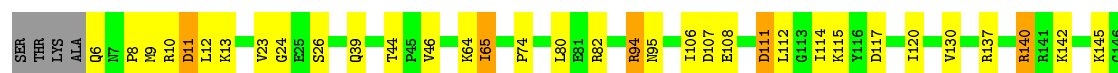
- Molecule 47: 60S ribosomal protein L10

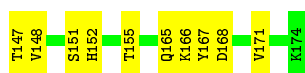
Chain m0:  73%  24%



- Molecule 48: 60S ribosomal protein L11-B

Chain M1:  72%  23%





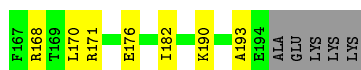
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 76% 19%



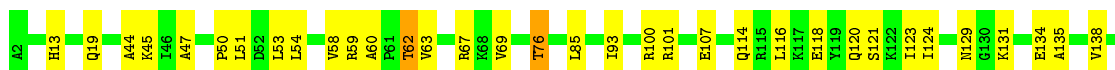
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 76% 20%



- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 75% 21%



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 82% 15%




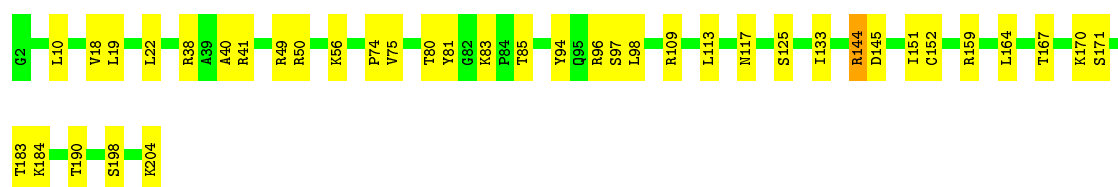
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 85% 15%




- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  81% 19%



- Molecule 51: 60S ribosomal protein L15-A

Chain m5:  86% 13%




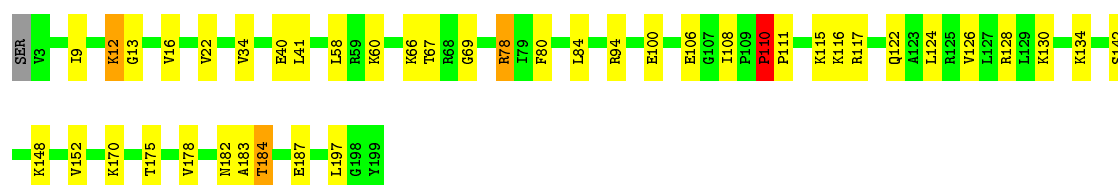
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:  88% 10%




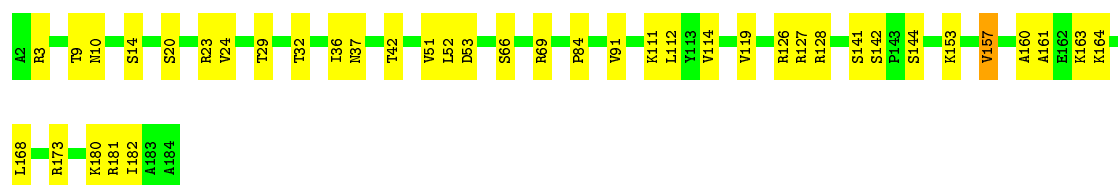
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:  78% 19%



- Molecule 53: 60S ribosomal protein L17-A

Chain M7:  78% 21%



- Molecule 53: 60S ribosomal protein L17-A


Chain m7:  67% 17% 15%






VAL  
ALA  
LYS  
ALA  
ALA  
GLU  
LYS  
LYS  
VAL  
VAL  
ARG  
LEU  
TER  
SER  
ARG  
GLN  
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ALA  
GLN  
LYS  
ARG  
TLE  
ALA  
ALA

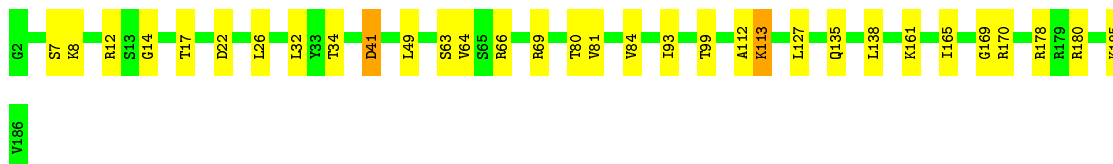
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:  84% 15% .



- Molecule 54: 60S ribosomal protein L18-A

Chain m8:  83% 16% .




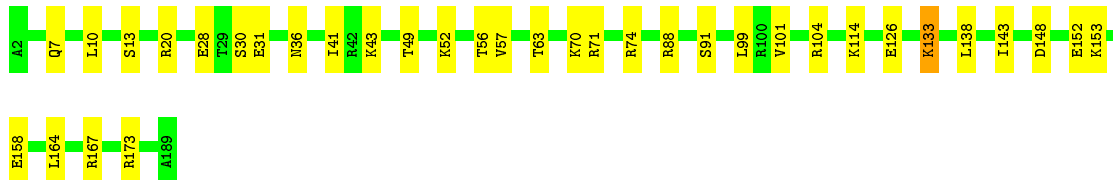
- Molecule 55: 60S ribosomal protein L19-A

Chain M9:  88% 12% .



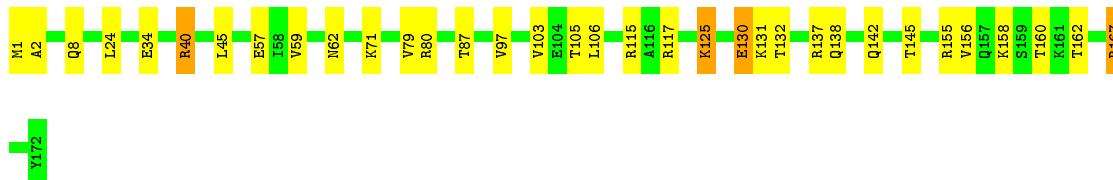
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:  81% 18% .




- Molecule 56: 60S ribosomal protein L20-A

Chain N0:  80% 17% .

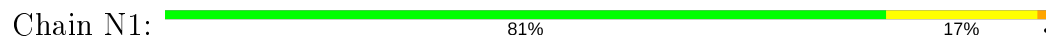


- Molecule 56: 60S ribosomal protein L20-A

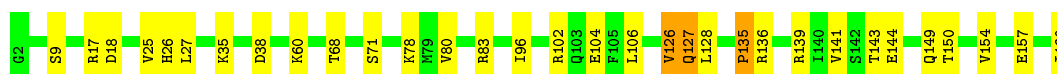
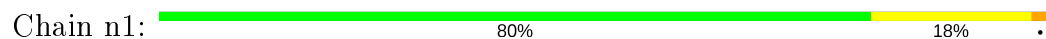
Chain n0:  83% 17% .



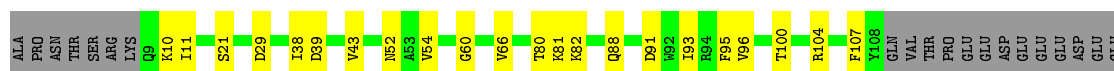
- Molecule 57: 60S ribosomal protein L21-A



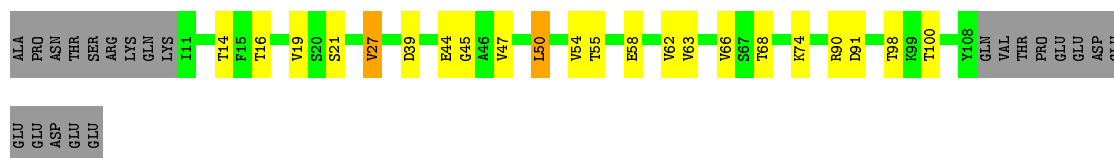
- Molecule 57: 60S ribosomal protein L21-A



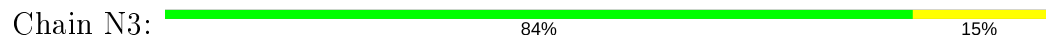
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A



- Molecule 59: 60S ribosomal protein L23-A

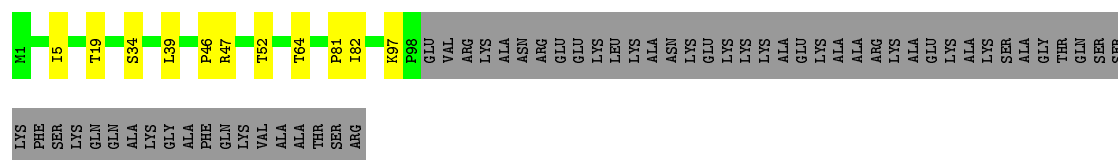


- Molecule 59: 60S ribosomal protein L23-A



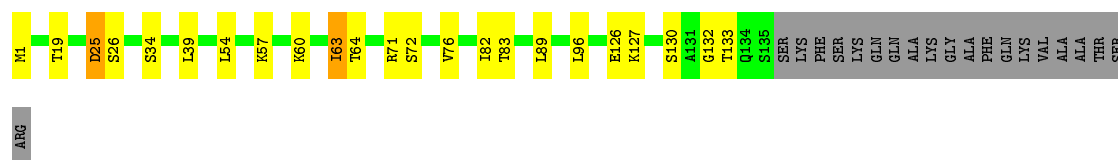
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:  56% 7% 37%



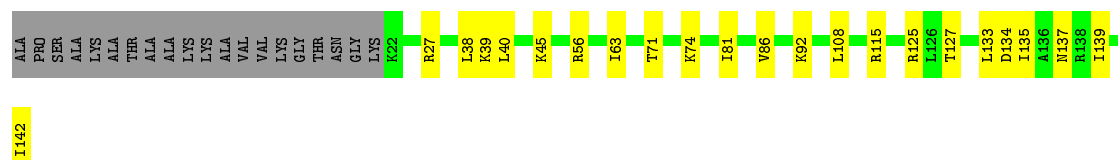
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:  72% 14% 13%



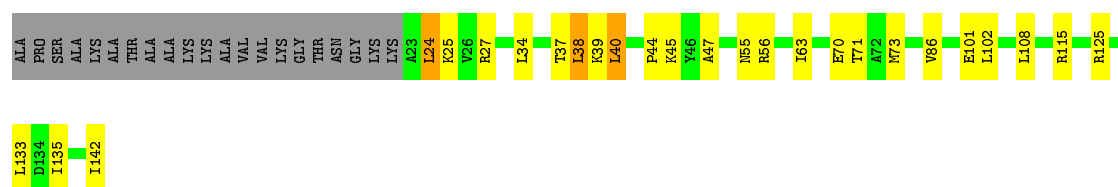
- Molecule 61: 60S ribosomal protein L25

Chain N5:  70% 16% 14%




- Molecule 61: 60S ribosomal protein L25

Chain n5:  67% 16% 15%




- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  82% 15% 3%




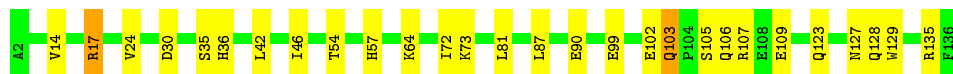
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:  75% 22% 3%




- Molecule 63: 60S ribosomal protein L27-A

Chain N7:  79% 19%




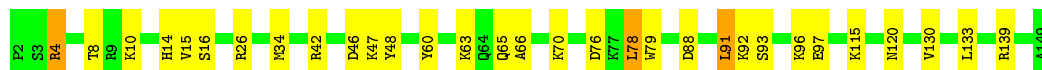
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:  78% 20%




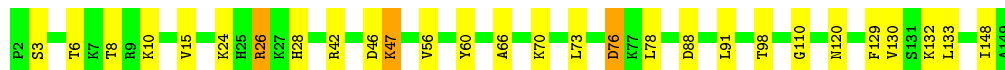
- Molecule 64: 60S ribosomal protein L28

Chain N8:  79% 19%




- Molecule 64: 60S ribosomal protein L28

Chain n8:  81% 17%




- Molecule 65: 60S ribosomal protein L29

Chain N9:  81% 19%




- Molecule 65: 60S ribosomal protein L29

Chain n9:  76% 22%




- Molecule 66: 60S ribosomal protein L30

Chain O0:  76% 17% 7%




- Molecule 66: 60S ribosomal protein L30

Chain o0:  78% 17% . .




- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  76% 20% . .




- Molecule 67: 60S ribosomal protein L31-A

Chain o1:  77% 21% .




- Molecule 68: 60S ribosomal protein L32

Chain O2:  78% 19% . .




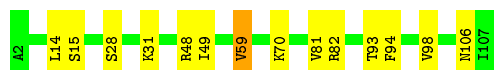
- Molecule 68: 60S ribosomal protein L32

Chain o2:  79% 19% . .




- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  87% 12% .




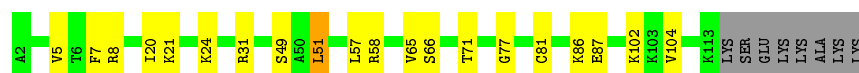
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:  81% 18% .



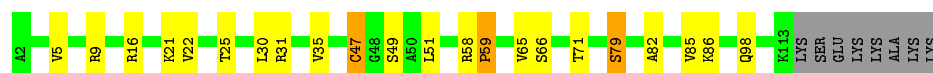
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  77% 16% 7%




- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  75% 16% 7%



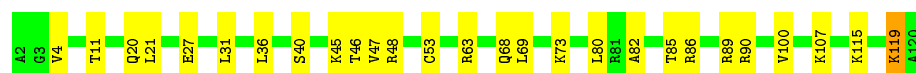
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  78% 21% 1%




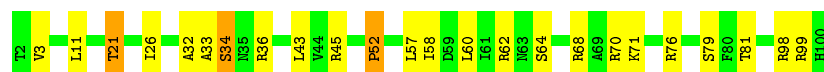
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  77% 22% 1%



- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  76% 21% 3%




- Molecule 72: 60S ribosomal protein L36-A

Chain o6:  71% 26% 3%




- Molecule 73: 60S ribosomal protein L37-A

Chain O7:  84% 14% 2%




- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  86% 14%




- Molecule 74: 60S ribosomal protein L38

Chain O8:  77% 23%




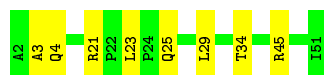
- Molecule 74: 60S ribosomal protein L38

Chain o8:  81% 18%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  84% 16%




- Molecule 75: 60S ribosomal protein L39

Chain o9:  80% 20%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  73% 25%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  75% 23%



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  72% 28%




- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  72% 28%




- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  75% 23%




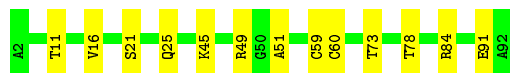
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  79% 19%




- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  86% 14%



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  79% 21%



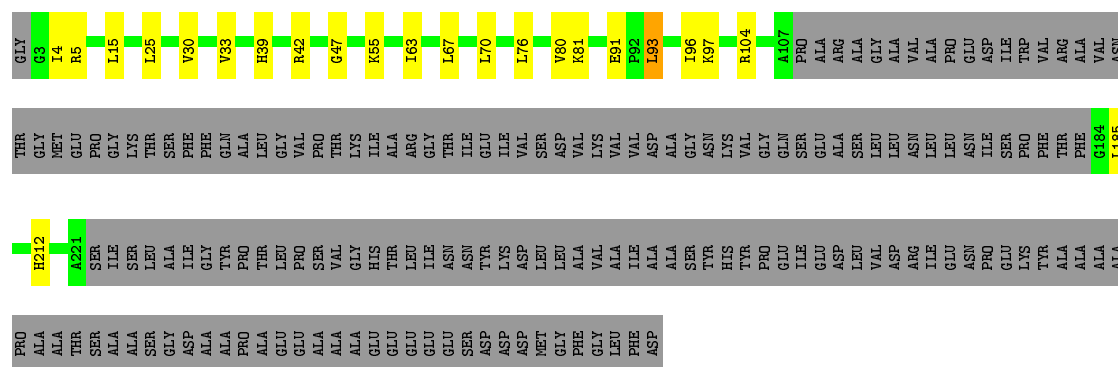
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  73% 26%



- Molecule 81: 60S acidic ribosomal protein P0





- Molecule 82: UNKNOWN PROTEIN\_m2



- Molecule 83: UNKNOWN PROTEIN p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 84: UNKNOWN PROTEIN p2

Chain p2:  100%

There are no outlier residues recorded for this chain.

## 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, $\alpha$ , $\beta$ , $\gamma$	434.39Å 285.58Å 303.06Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	49.88 – 3.20	Depositor
% Data completeness (in resolution range)	99.9 (49.88-3.20)	Depositor
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.212 , 0.262	Depositor
Wilson B-factor (Å <sup>2</sup> )	72.4	Xtriage
Anisotropy	0.130	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, OHX, MG, 3L2

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	0.70	1/41698 (0.0%)	1.28	289/64972 (0.4%)
1	6	0.80	10/42765 (0.0%)	1.35	400/66634 (0.6%)
2	S0	0.45	0/1617	0.66	0/2215
2	s0	0.45	0/1623	0.68	0/2222
3	S1	0.38	0/1735	0.63	0/2335
3	s1	0.49	0/1748	0.69	0/2352
4	S2	0.48	0/1665	0.66	0/2263
4	s2	0.56	0/1665	0.74	0/2263
5	S3	0.47	0/1759	0.64	0/2368
5	s3	0.39	0/1759	0.59	0/2368
6	S4	0.46	0/2109	0.69	1/2839 (0.0%)
6	s4	0.49	0/2109	0.74	1/2839 (0.0%)
7	S5	0.37	0/1629	0.58	0/2202
7	s5	0.42	0/1629	0.66	1/2202 (0.0%)
8	S6	0.45	0/1823	0.65	0/2439
8	s6	0.49	0/1779	0.68	0/2379
9	S7	0.42	0/1506	0.65	0/2028
9	s7	0.43	0/1516	0.62	0/2043
10	S8	0.52	0/1514	0.67	0/2021
10	s8	0.58	0/1514	0.73	0/2021
11	S9	0.46	0/1519	0.65	0/2035
11	s9	0.52	0/1519	0.75	1/2035 (0.0%)
12	C0	0.43	0/790	0.70	1/1069 (0.1%)
12	c0	0.36	0/777	0.64	3/1049 (0.3%)
13	C1	0.55	0/1240	0.67	0/1675
13	c1	0.58	0/1194	0.71	0/1610
14	C2	0.35	0/900	0.63	0/1224
14	c2	0.30	0/900	0.60	1/1224 (0.1%)
15	C3	0.47	0/1215	0.69	2/1638 (0.1%)
15	c3	0.53	0/1215	0.69	0/1638
16	C4	0.40	0/901	0.70	0/1217
16	c4	0.49	0/960	0.74	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.43	0/998	0.64	0/1341
17	c5	0.44	0/1060	0.67	0/1426
18	C6	0.42	0/1125	0.69	2/1510 (0.1%)
18	c6	0.43	0/1131	0.67	0/1518
19	C7	0.43	0/935	0.64	0/1254
19	c7	0.43	0/914	0.67	0/1224
20	C8	0.41	0/1211	0.64	0/1628
20	c8	0.44	0/1211	0.68	1/1628 (0.1%)
21	C9	0.42	0/1130	0.65	0/1517
21	c9	0.44	0/1130	0.68	2/1517 (0.1%)
22	D0	0.42	0/865	0.64	0/1169
22	d0	0.43	0/892	0.64	0/1205
23	D1	0.44	0/693	0.63	0/935
23	d1	0.49	0/693	0.65	0/935
24	D2	0.50	0/1038	0.73	2/1395 (0.1%)
24	d2	0.56	0/1038	0.74	1/1395 (0.1%)
25	D3	0.59	0/1139	0.75	1/1518 (0.1%)
25	d3	0.66	0/1139	0.82	2/1518 (0.1%)
26	D4	0.43	0/1087	0.63	0/1449
26	d4	0.48	0/1087	0.69	0/1449
27	D5	0.38	0/571	0.69	0/768
27	d5	0.38	0/566	0.63	0/761
28	D6	0.48	0/782	0.73	0/1047
28	d6	0.59	0/782	0.73	0/1047
29	D7	0.42	0/620	0.65	0/838
29	d7	0.45	0/620	0.69	0/838
30	D8	0.35	0/499	0.59	0/670
30	d8	0.43	0/499	0.69	0/670
31	D9	0.52	0/452	0.71	1/600 (0.2%)
31	d9	0.45	0/452	0.67	0/600
32	E0	0.45	0/483	0.57	0/643
33	E1	0.42	0/577	0.76	0/770
33	e1	0.38	0/619	0.72	0/822
34	SR	0.36	0/2494	0.56	0/3393
34	sR	0.36	0/2495	0.58	0/3395
35	SM	0.51	0/1113	0.69	2/1502 (0.1%)
35	sM	0.47	0/683	0.67	1/923 (0.1%)
36	1	1.08	76/75394 (0.1%)	1.62	1625/117545 (1.4%)
36	5	1.10	110/75414 (0.1%)	1.64	1765/117575 (1.5%)
37	3	0.90	3/2883 (0.1%)	1.38	19/4491 (0.4%)
37	7	1.03	1/2883 (0.0%)	1.66	70/4491 (1.6%)
38	4	1.00	0/3746	1.57	67/5832 (1.1%)
38	8	0.90	2/3746 (0.1%)	1.41	29/5832 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.67	0/1948	0.81	1/2617 (0.0%)
39	l2	0.65	0/1946	0.82	1/2614 (0.0%)
40	L3	0.70	0/3146	0.81	1/4228 (0.0%)
40	l3	0.77	0/3146	0.85	3/4228 (0.1%)
41	L4	0.77	0/2800	0.91	5/3790 (0.1%)
41	l4	0.72	1/2800 (0.0%)	0.87	2/3790 (0.1%)
42	L5	0.52	0/2425	0.69	0/3271
42	l5	0.67	0/2408	0.77	1/3248 (0.0%)
43	L6	0.71	0/1260	0.82	1/1694 (0.1%)
43	l6	0.71	0/1269	0.78	0/1705
44	L7	0.73	0/1821	0.84	0/2451
44	l7	0.82	0/1828	0.86	2/2461 (0.1%)
45	L8	0.53	0/1836	0.68	1/2481 (0.0%)
45	l8	0.49	0/1795	0.66	0/2429
46	L9	0.64	0/1539	0.75	0/2073
46	l9	0.73	0/1539	0.81	0/2073
47	M0	0.69	1/1741 (0.1%)	0.81	5/2335 (0.2%)
47	m0	0.70	1/1758 (0.1%)	0.85	1/2358 (0.0%)
48	M1	0.51	0/1374	0.69	1/1842 (0.1%)
48	m1	0.64	0/1374	0.78	2/1842 (0.1%)
49	M3	0.71	0/1568	0.83	2/2106 (0.1%)
49	m3	0.62	0/1573	0.80	0/2113
50	M4	0.70	0/1068	0.79	0/1438
50	m4	0.76	0/1074	0.80	1/1446 (0.1%)
51	M5	0.72	1/1757 (0.1%)	0.84	2/2354 (0.1%)
51	m5	0.63	0/1757	0.83	3/2354 (0.1%)
52	M6	0.81	0/1585	0.84	2/2128 (0.1%)
52	m6	0.96	2/1585 (0.1%)	0.95	4/2128 (0.2%)
53	M7	0.73	0/1443	0.80	1/1944 (0.1%)
53	m7	0.86	0/1250	0.84	0/1683
54	M8	0.75	0/1465	0.88	0/1965
54	m8	0.67	0/1465	0.85	0/1965
55	M9	0.53	0/1538	0.66	0/2050
55	m9	0.54	0/1538	0.65	0/2050
56	N0	0.73	0/1481	0.79	1/1990 (0.1%)
56	n0	0.82	0/1481	0.86	0/1990
57	N1	0.71	0/1300	0.80	1/1743 (0.1%)
57	n1	0.80	1/1300 (0.1%)	0.83	2/1743 (0.1%)
58	N2	0.40	0/812	0.60	0/1099
58	n2	0.46	0/794	0.67	0/1076
59	N3	0.70	0/1018	0.87	2/1369 (0.1%)
59	n3	0.79	0/1018	0.84	0/1369
60	N4	0.52	0/712	0.67	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	n4	0.58	0/1052	0.72	0/1398
61	N5	0.62	0/979	0.77	0/1321
61	n5	0.58	0/974	0.77	0/1314
62	N6	0.68	0/1004	0.85	2/1341 (0.1%)
62	n6	0.66	0/1004	0.82	1/1341 (0.1%)
63	N7	0.48	0/1118	0.67	0/1497
63	n7	0.47	0/1118	0.66	1/1497 (0.1%)
64	N8	0.73	0/1204	0.90	1/1612 (0.1%)
64	n8	0.72	0/1204	0.83	0/1612
65	N9	0.66	0/473	0.76	0/629
65	n9	0.71	0/473	0.94	1/629 (0.2%)
66	O0	0.49	0/751	0.63	0/1008
66	o0	0.46	0/775	0.63	0/1040
67	O1	0.61	0/890	0.73	0/1196
67	o1	0.72	0/897	0.80	0/1205
68	O2	0.76	0/1041	0.86	1/1394 (0.1%)
68	o2	0.79	0/1041	0.87	0/1394
69	O3	0.90	0/868	0.95	2/1168 (0.2%)
69	o3	0.87	0/868	0.90	0/1168
70	O4	0.56	0/890	0.75	1/1189 (0.1%)
70	o4	0.51	0/890	0.73	0/1189
71	O5	0.66	0/978	0.80	1/1301 (0.1%)
71	o5	0.53	0/974	0.68	0/1297
72	O6	0.62	0/778	0.78	0/1034
72	o6	0.54	0/777	0.72	0/1033
73	O7	0.73	0/696	1.03	4/923 (0.4%)
73	o7	0.61	0/696	0.80	0/923
74	O8	0.52	0/618	0.61	0/826
74	o8	0.45	0/614	0.59	0/822
75	O9	0.71	0/443	0.83	0/588
75	o9	0.67	0/443	0.81	0/588
76	Q0	0.65	0/423	0.80	0/562
76	q0	0.84	0/423	0.91	1/562 (0.2%)
77	Q1	0.63	0/234	0.93	0/300
77	q1	0.68	0/234	0.91	0/300
78	Q2	0.82	1/860 (0.1%)	0.80	0/1136
78	q2	0.76	1/860 (0.1%)	0.82	1/1136 (0.1%)
79	Q3	0.71	0/701	0.82	0/934
79	q3	0.66	0/701	0.76	2/934 (0.2%)
80	e0	0.56	0/499	0.72	0/665
81	p0	4.55	1/1091 (0.1%)	1.38	2/1472 (0.1%)
All	All	0.87	213/430073 (0.0%)	1.28	4359/631362 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	2
9	S7	0	1
9	s7	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	1
22	d0	0	1
27	D5	0	1
28	D6	0	1
33	E1	0	1
39	l2	0	1
40	l3	0	1
41	L4	0	1
42	l5	0	1
43	L6	0	1
43	l6	0	1
44	l7	0	1
45	L8	0	1
49	M3	0	1
52	M6	0	1
52	m6	0	1
54	m8	0	2
56	n0	0	2
57	N1	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
72	o6	0	1
81	p0	1	0
All	All	1	35

The worst 5 of 213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	p0	212	HIS	CA-CB	149.59	4.83	1.53
78	Q2	17	CYS	CB-SG	13.09	2.04	1.82
36	5	1152	G	N9-C4	-11.55	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	9.39	1.98	1.82
36	1	656	A	N3-C4	-7.83	1.30	1.34

The worst 5 of 4359 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	p0	212	HIS	N-CA-CB	-47.24	25.57	110.60
36	5	1152	G	N3-C4-C5	23.22	140.21	128.60
36	5	1152	G	N3-C4-N9	-22.85	112.29	126.00
36	5	1152	G	C2-N3-C4	-18.92	102.44	111.90
36	5	780	A	O5'-P-OP1	-14.51	92.64	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
81	p0	212	HIS	CA

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
9	S7	131	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	150 (74%)	31 (15%)	23 (11%)	0	2
2	s0	204/251 (81%)	156 (76%)	28 (14%)	20 (10%)	0	3
3	S1	212/254 (84%)	148 (70%)	40 (19%)	24 (11%)	0	2
3	s1	214/254 (84%)	171 (80%)	31 (14%)	12 (6%)	2	14
4	S2	215/253 (85%)	180 (84%)	24 (11%)	11 (5%)	2	15
4	s2	215/253 (85%)	177 (82%)	28 (13%)	10 (5%)	2	17
5	S3	221/239 (92%)	183 (83%)	27 (12%)	11 (5%)	2	16
5	s3	221/239 (92%)	170 (77%)	35 (16%)	16 (7%)	1	7
6	S4	258/260 (99%)	205 (80%)	43 (17%)	10 (4%)	3	22
6	s4	258/260 (99%)	209 (81%)	28 (11%)	21 (8%)	1	5
7	S5	204/224 (91%)	156 (76%)	30 (15%)	18 (9%)	1	4
7	s5	204/224 (91%)	158 (78%)	27 (13%)	19 (9%)	0	3
8	S6	224/236 (95%)	192 (86%)	21 (9%)	11 (5%)	2	17
8	s6	216/236 (92%)	186 (86%)	18 (8%)	12 (6%)	2	14
9	S7	182/189 (96%)	132 (72%)	29 (16%)	21 (12%)	0	2
9	s7	184/189 (97%)	148 (80%)	24 (13%)	12 (6%)	1	10
10	S8	184/200 (92%)	153 (83%)	19 (10%)	12 (6%)	1	10
10	s8	184/200 (92%)	163 (89%)	16 (9%)	5 (3%)	5	30
11	S9	183/196 (93%)	147 (80%)	25 (14%)	11 (6%)	1	12
11	s9	183/196 (93%)	149 (81%)	24 (13%)	10 (6%)	2	14
12	C0	94/105 (90%)	72 (77%)	12 (13%)	10 (11%)	0	2
12	c0	92/105 (88%)	67 (73%)	11 (12%)	14 (15%)	0	1
13	C1	153/155 (99%)	119 (78%)	22 (14%)	12 (8%)	1	6
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	1	10
14	C2	122/142 (86%)	68 (56%)	29 (24%)	25 (20%)	0	0
14	c2	122/142 (86%)	64 (52%)	36 (30%)	22 (18%)	0	0
15	C3	148/150 (99%)	122 (82%)	17 (12%)	9 (6%)	1	12
15	c3	148/150 (99%)	111 (75%)	28 (19%)	9 (6%)	1	12
16	C4	125/136 (92%)	88 (70%)	25 (20%)	12 (10%)	0	3
16	c4	126/136 (93%)	97 (77%)	19 (15%)	10 (8%)	1	6
17	C5	122/141 (86%)	86 (70%)	24 (20%)	12 (10%)	0	3
17	c5	133/141 (94%)	90 (68%)	27 (20%)	16 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	119 (86%)	11 (8%)	9 (6%)	1	10
18	c6	140/142 (99%)	113 (81%)	17 (12%)	10 (7%)	1	8
19	C7	116/136 (85%)	90 (78%)	15 (13%)	11 (10%)	0	3
19	c7	113/136 (83%)	85 (75%)	17 (15%)	11 (10%)	0	3
20	C8	143/145 (99%)	112 (78%)	19 (13%)	12 (8%)	1	5
20	c8	143/145 (99%)	112 (78%)	23 (16%)	8 (6%)	2	14
21	C9	141/143 (99%)	122 (86%)	11 (8%)	8 (6%)	1	14
21	c9	141/143 (99%)	118 (84%)	18 (13%)	5 (4%)	3	24
22	D0	105/120 (88%)	81 (77%)	17 (16%)	7 (7%)	1	9
22	d0	108/120 (90%)	85 (79%)	12 (11%)	11 (10%)	0	3
23	D1	85/87 (98%)	59 (69%)	15 (18%)	11 (13%)	0	1
23	d1	85/87 (98%)	69 (81%)	11 (13%)	5 (6%)	1	12
24	D2	127/129 (98%)	108 (85%)	16 (13%)	3 (2%)	6	34
24	d2	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	19	58
25	D3	142/144 (99%)	109 (77%)	18 (13%)	15 (11%)	0	2
25	d3	142/144 (99%)	123 (87%)	15 (11%)	4 (3%)	5	29
26	D4	132/134 (98%)	107 (81%)	17 (13%)	8 (6%)	1	12
26	d4	132/134 (98%)	102 (77%)	17 (13%)	13 (10%)	0	3
27	D5	68/107 (64%)	45 (66%)	14 (21%)	9 (13%)	0	1
27	d5	67/107 (63%)	53 (79%)	10 (15%)	4 (6%)	1	12
28	D6	95/97 (98%)	59 (62%)	16 (17%)	20 (21%)	0	0
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	5
29	D7	79/81 (98%)	63 (80%)	12 (15%)	4 (5%)	2	15
29	d7	79/81 (98%)	61 (77%)	13 (16%)	5 (6%)	1	10
30	D8	61/66 (92%)	50 (82%)	9 (15%)	2 (3%)	4	25
30	d8	61/66 (92%)	40 (66%)	15 (25%)	6 (10%)	0	3
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1	12
31	d9	51/55 (93%)	43 (84%)	4 (8%)	4 (8%)	1	6
32	E0	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	2	15
33	E1	69/76 (91%)	38 (55%)	13 (19%)	18 (26%)	0	0
33	e1	74/76 (97%)	35 (47%)	19 (26%)	20 (27%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	277 (88%)	28 (9%)	11 (4%)	3	24
34	sR	316/318 (99%)	274 (87%)	31 (10%)	11 (4%)	3	24
35	SM	155/273 (57%)	106 (68%)	30 (19%)	19 (12%)	0	2
35	sM	98/273 (36%)	63 (64%)	18 (18%)	17 (17%)	0	0
39	L2	250/253 (99%)	220 (88%)	20 (8%)	10 (4%)	3	21
39	l2	250/253 (99%)	207 (83%)	31 (12%)	12 (5%)	2	17
40	L3	384/386 (100%)	326 (85%)	42 (11%)	16 (4%)	3	20
40	l3	384/386 (100%)	344 (90%)	31 (8%)	9 (2%)	6	34
41	L4	359/361 (99%)	286 (80%)	46 (13%)	27 (8%)	1	7
41	l4	359/361 (99%)	297 (83%)	36 (10%)	26 (7%)	1	7
42	L5	294/296 (99%)	245 (83%)	27 (9%)	22 (8%)	1	7
42	l5	292/296 (99%)	243 (83%)	39 (13%)	10 (3%)	3	24
43	L6	152/175 (87%)	133 (88%)	15 (10%)	4 (3%)	5	31
43	l6	153/175 (87%)	131 (86%)	17 (11%)	5 (3%)	4	25
44	L7	220/243 (90%)	189 (86%)	24 (11%)	7 (3%)	4	26
44	l7	221/243 (91%)	194 (88%)	18 (8%)	9 (4%)	3	21
45	L8	231/255 (91%)	181 (78%)	35 (15%)	15 (6%)	1	10
45	l8	229/255 (90%)	166 (72%)	45 (20%)	18 (8%)	1	6
46	L9	189/191 (99%)	156 (82%)	25 (13%)	8 (4%)	3	20
46	l9	189/191 (99%)	163 (86%)	19 (10%)	7 (4%)	3	22
47	M0	207/220 (94%)	166 (80%)	33 (16%)	8 (4%)	3	22
47	m0	209/220 (95%)	163 (78%)	32 (15%)	14 (7%)	1	9
48	M1	167/173 (96%)	127 (76%)	19 (11%)	21 (13%)	0	1
48	m1	167/173 (96%)	138 (83%)	20 (12%)	9 (5%)	2	14
49	M3	191/198 (96%)	155 (81%)	23 (12%)	13 (7%)	1	9
49	m3	192/198 (97%)	151 (79%)	22 (12%)	19 (10%)	0	3
50	M4	134/137 (98%)	115 (86%)	12 (9%)	7 (5%)	2	15
50	m4	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	6	35
51	M5	201/203 (99%)	181 (90%)	12 (6%)	8 (4%)	3	21
51	m5	201/203 (99%)	175 (87%)	21 (10%)	5 (2%)	5	32
52	M6	195/198 (98%)	181 (93%)	11 (6%)	3 (2%)	10	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m6	195/198 (98%)	171 (88%)	17 (9%)	7 (4%)	3	23
53	M7	181/183 (99%)	151 (83%)	21 (12%)	9 (5%)	2	16
53	m7	153/183 (84%)	137 (90%)	14 (9%)	2 (1%)	12	47
54	M8	183/185 (99%)	156 (85%)	21 (12%)	6 (3%)	4	25
54	m8	183/185 (99%)	155 (85%)	23 (13%)	5 (3%)	5	30
55	M9	186/188 (99%)	163 (88%)	21 (11%)	2 (1%)	14	51
55	m9	186/188 (99%)	158 (85%)	26 (14%)	2 (1%)	14	51
56	N0	170/172 (99%)	157 (92%)	8 (5%)	5 (3%)	4	28
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	25	64
57	N1	157/159 (99%)	136 (87%)	16 (10%)	5 (3%)	4	26
57	n1	157/159 (99%)	134 (85%)	18 (12%)	5 (3%)	4	26
58	N2	98/120 (82%)	72 (74%)	22 (22%)	4 (4%)	3	21
58	n2	96/120 (80%)	79 (82%)	12 (12%)	5 (5%)	2	15
59	N3	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	6	35
59	n3	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	44
60	N4	96/155 (62%)	70 (73%)	21 (22%)	5 (5%)	2	15
60	n4	133/155 (86%)	109 (82%)	14 (10%)	10 (8%)	1	7
61	N5	119/141 (84%)	107 (90%)	12 (10%)	0	100	100
61	n5	118/141 (84%)	97 (82%)	9 (8%)	12 (10%)	0	3
62	N6	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	6	34
62	n6	124/126 (98%)	102 (82%)	17 (14%)	5 (4%)	3	21
63	N7	133/135 (98%)	113 (85%)	12 (9%)	8 (6%)	1	12
63	n7	133/135 (98%)	111 (84%)	11 (8%)	11 (8%)	1	5
64	N8	146/148 (99%)	117 (80%)	19 (13%)	10 (7%)	1	9
64	n8	146/148 (99%)	113 (77%)	23 (16%)	10 (7%)	1	9
65	N9	56/58 (97%)	49 (88%)	6 (11%)	1 (2%)	8	41
65	n9	56/58 (97%)	43 (77%)	8 (14%)	5 (9%)	1	4
66	O0	95/104 (91%)	88 (93%)	6 (6%)	1 (1%)	14	51
66	o0	98/104 (94%)	85 (87%)	8 (8%)	5 (5%)	2	15
67	O1	107/112 (96%)	88 (82%)	11 (10%)	8 (8%)	1	7
67	o1	107/112 (96%)	89 (83%)	12 (11%)	6 (6%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O2	125/129 (97%)	111 (89%)	12 (10%)	2 (2%)	9	43
68	o2	125/129 (97%)	105 (84%)	16 (13%)	4 (3%)	4	26
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	4	28
69	o3	104/106 (98%)	93 (89%)	7 (7%)	4 (4%)	3	22
70	O4	110/120 (92%)	96 (87%)	13 (12%)	1 (1%)	17	56
70	o4	110/120 (92%)	92 (84%)	14 (13%)	4 (4%)	3	23
71	O5	117/119 (98%)	104 (89%)	9 (8%)	4 (3%)	3	24
71	o5	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	5	31
72	O6	97/99 (98%)	73 (75%)	17 (18%)	7 (7%)	1	7
72	o6	97/99 (98%)	80 (82%)	11 (11%)	6 (6%)	1	11
73	O7	85/87 (98%)	73 (86%)	12 (14%)	0	100	100
73	o7	85/87 (98%)	71 (84%)	12 (14%)	2 (2%)	6	34
74	O8	75/77 (97%)	63 (84%)	11 (15%)	1 (1%)	12	47
74	o8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	1	9
75	O9	48/50 (96%)	38 (79%)	9 (19%)	1 (2%)	7	37
75	o9	48/50 (96%)	43 (90%)	3 (6%)	2 (4%)	3	20
76	Q0	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	1	12
76	q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3	21
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	17 (74%)	6 (26%)	0	100	100
78	Q2	103/105 (98%)	79 (77%)	15 (15%)	9 (9%)	1	4
78	q2	103/105 (98%)	90 (87%)	10 (10%)	3 (3%)	4	28
79	Q3	89/91 (98%)	77 (86%)	11 (12%)	1 (1%)	14	51
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	14	51
80	e0	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	9
81	p0	139/311 (45%)	120 (86%)	16 (12%)	3 (2%)	6	35
All	All	22333/24143 (92%)	18254 (82%)	2761 (12%)	1318 (6%)	1	12

5 of 1318 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
2	S0	66	ALA
2	S0	95	ALA
2	S0	139	VAL

### 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%)	133 (81%)	31 (19%)	1	8
2	s0	165/209 (79%)	132 (80%)	33 (20%)	1	6
3	S1	191/223 (86%)	146 (76%)	45 (24%)	1	3
3	s1	192/223 (86%)	146 (76%)	46 (24%)	0	3
4	S2	176/204 (86%)	138 (78%)	38 (22%)	1	5
4	s2	176/204 (86%)	126 (72%)	50 (28%)	0	1
5	S3	182/194 (94%)	146 (80%)	36 (20%)	1	7
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1	6
6	S4	221/221 (100%)	175 (79%)	46 (21%)	1	6
6	s4	221/221 (100%)	189 (86%)	32 (14%)	3	15
7	S5	173/190 (91%)	142 (82%)	31 (18%)	2	9
7	s5	173/190 (91%)	139 (80%)	34 (20%)	1	7
8	S6	188/201 (94%)	154 (82%)	34 (18%)	1	8
8	s6	187/201 (93%)	149 (80%)	38 (20%)	1	6
9	S7	165/169 (98%)	134 (81%)	31 (19%)	1	8
9	s7	165/169 (98%)	135 (82%)	30 (18%)	1	8
10	S8	150/161 (93%)	126 (84%)	24 (16%)	2	11
10	s8	150/161 (93%)	122 (81%)	28 (19%)	1	8
11	S9	158/165 (96%)	127 (80%)	31 (20%)	1	7
11	s9	158/165 (96%)	124 (78%)	34 (22%)	1	5
12	C0	77/98 (79%)	63 (82%)	14 (18%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c0	73/98 (74%)	61 (84%)	12 (16%)	2	11
13	C1	129/136 (95%)	109 (84%)	20 (16%)	2	12
13	c1	129/136 (95%)	101 (78%)	28 (22%)	1	5
14	C2	88/118 (75%)	63 (72%)	25 (28%)	0	1
14	c2	88/118 (75%)	60 (68%)	28 (32%)	0	0
15	C3	127/127 (100%)	99 (78%)	28 (22%)	1	5
15	c3	127/127 (100%)	101 (80%)	26 (20%)	1	6
16	C4	81/104 (78%)	62 (76%)	19 (24%)	1	3
16	c4	97/104 (93%)	73 (75%)	24 (25%)	0	2
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	6
17	c5	103/117 (88%)	79 (77%)	24 (23%)	1	3
18	C6	117/118 (99%)	90 (77%)	27 (23%)	1	3
18	c6	118/118 (100%)	99 (84%)	19 (16%)	2	11
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	6
19	c7	92/124 (74%)	73 (79%)	19 (21%)	1	6
20	C8	128/128 (100%)	96 (75%)	32 (25%)	0	2
20	c8	128/128 (100%)	102 (80%)	26 (20%)	1	6
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	6
21	c9	115/115 (100%)	97 (84%)	18 (16%)	2	12
22	D0	100/113 (88%)	77 (77%)	23 (23%)	1	3
22	d0	103/113 (91%)	80 (78%)	23 (22%)	1	4
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	5
23	d1	74/74 (100%)	61 (82%)	13 (18%)	2	9
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	6
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4	20
25	D3	119/119 (100%)	97 (82%)	22 (18%)	1	8
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2	9
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	10
26	d4	112/112 (100%)	90 (80%)	22 (20%)	1	7
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	3
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	3
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2	12
29	D7	70/70 (100%)	64 (91%)	6 (9%)	10	38
29	d7	70/70 (100%)	55 (79%)	15 (21%)	1	5
30	D8	56/59 (95%)	42 (75%)	14 (25%)	0	2
30	d8	56/59 (95%)	39 (70%)	17 (30%)	0	0
31	D9	47/48 (98%)	34 (72%)	13 (28%)	0	1
31	d9	47/48 (98%)	35 (74%)	12 (26%)	0	2
32	E0	51/51 (100%)	43 (84%)	8 (16%)	2	12
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0	2
33	e1	66/66 (100%)	52 (79%)	14 (21%)	1	5
34	SR	260/261 (100%)	228 (88%)	32 (12%)	4	21
34	sR	260/261 (100%)	227 (87%)	33 (13%)	4	20
35	SM	97/228 (42%)	77 (79%)	20 (21%)	1	6
35	sM	54/228 (24%)	45 (83%)	9 (17%)	2	10
39	L2	193/195 (99%)	161 (83%)	32 (17%)	2	10
39	l2	192/195 (98%)	152 (79%)	40 (21%)	1	6
40	L3	321/322 (100%)	249 (78%)	72 (22%)	1	4
40	l3	318/322 (99%)	256 (80%)	62 (20%)	1	7
41	L4	288/288 (100%)	231 (80%)	57 (20%)	1	7
41	l4	288/288 (100%)	231 (80%)	57 (20%)	1	7
42	L5	244/244 (100%)	197 (81%)	47 (19%)	1	8
42	l5	243/244 (100%)	195 (80%)	48 (20%)	1	7
43	L6	134/152 (88%)	111 (83%)	23 (17%)	2	10
43	l6	135/152 (89%)	113 (84%)	22 (16%)	2	11
44	L7	186/204 (91%)	160 (86%)	26 (14%)	3	16
44	l7	187/204 (92%)	155 (83%)	32 (17%)	2	10
45	L8	187/207 (90%)	156 (83%)	31 (17%)	2	10
45	l8	177/207 (86%)	146 (82%)	31 (18%)	2	9
46	L9	171/171 (100%)	131 (77%)	40 (23%)	1	3
46	l9	171/171 (100%)	131 (77%)	40 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	M0	177/186 (95%)	140 (79%)	37 (21%)	1	6
47	m0	179/186 (96%)	141 (79%)	38 (21%)	1	5
48	M1	147/150 (98%)	120 (82%)	27 (18%)	1	8
48	m1	147/150 (98%)	115 (78%)	32 (22%)	1	5
49	M3	154/158 (98%)	125 (81%)	29 (19%)	1	8
49	m3	154/158 (98%)	125 (81%)	29 (19%)	1	8
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	10
50	m4	108/108 (100%)	89 (82%)	19 (18%)	2	9
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%)	140 (88%)	20 (12%)	4	21
52	m6	160/161 (99%)	126 (79%)	34 (21%)	1	5
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	4
53	m7	125/145 (86%)	94 (75%)	31 (25%)	0	2
54	M8	150/150 (100%)	125 (83%)	25 (17%)	2	10
54	m8	150/150 (100%)	123 (82%)	27 (18%)	1	9
55	M9	153/153 (100%)	132 (86%)	21 (14%)	3	17
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	4
56	N0	156/156 (100%)	124 (80%)	32 (20%)	1	6
56	n0	156/156 (100%)	130 (83%)	26 (17%)	2	10
57	N1	136/136 (100%)	110 (81%)	26 (19%)	1	8
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	6
58	N2	87/106 (82%)	69 (79%)	18 (21%)	1	6
58	n2	85/106 (80%)	66 (78%)	19 (22%)	1	4
59	N3	104/104 (100%)	85 (82%)	19 (18%)	1	8
59	n3	104/104 (100%)	93 (89%)	11 (11%)	6	27
60	N4	57/129 (44%)	51 (90%)	6 (10%)	7	28
60	n4	100/129 (78%)	85 (85%)	15 (15%)	3	14
61	N5	104/117 (89%)	82 (79%)	22 (21%)	1	5
61	n5	104/117 (89%)	87 (84%)	17 (16%)	2	11
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	n6	109/109 (100%)	81 (74%)	28 (26%)	0	2
63	N7	115/115 (100%)	93 (81%)	22 (19%)	1	8
63	n7	115/115 (100%)	94 (82%)	21 (18%)	1	8
64	N8	118/118 (100%)	95 (80%)	23 (20%)	1	7
64	n8	118/118 (100%)	99 (84%)	19 (16%)	2	11
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	7
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	10
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1	6
66	o0	84/87 (97%)	69 (82%)	15 (18%)	2	9
67	O1	92/96 (96%)	74 (80%)	18 (20%)	1	7
67	o1	94/96 (98%)	77 (82%)	17 (18%)	1	8
68	O2	109/110 (99%)	85 (78%)	24 (22%)	1	5
68	o2	109/110 (99%)	87 (80%)	22 (20%)	1	6
69	O3	90/90 (100%)	79 (88%)	11 (12%)	5	22
69	o3	90/90 (100%)	73 (81%)	17 (19%)	1	8
70	O4	95/102 (93%)	76 (80%)	19 (20%)	1	6
70	o4	95/102 (93%)	74 (78%)	21 (22%)	1	4
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	5
71	o5	103/104 (99%)	78 (76%)	25 (24%)	0	2
72	O6	81/81 (100%)	61 (75%)	20 (25%)	0	2
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	0
73	O7	70/70 (100%)	57 (81%)	13 (19%)	1	8
73	o7	70/70 (100%)	60 (86%)	10 (14%)	3	15
74	O8	68/68 (100%)	51 (75%)	17 (25%)	0	2
74	o8	67/68 (98%)	56 (84%)	11 (16%)	2	11
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	12
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	9
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0	2
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	3
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	0
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	Q2	90/90 (100%)	72 (80%)	18 (20%)	1	6
78	q2	90/90 (100%)	70 (78%)	20 (22%)	1	4
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	10
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	4
80	e0	53/53 (100%)	39 (74%)	14 (26%)	0	2
81	p0	105/253 (42%)	85 (81%)	20 (19%)	1	8
All	All	18727/20241 (92%)	15073 (80%)	3654 (20%)	1	7

5 of 3654 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	O3	98	VAL
8	s6	78	THR
63	n7	121	ARG
72	O6	45	ARG
3	s1	116	LYS

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

Mol	Chain	Res	Type
55	M9	130	ASN
5	s3	74	GLN
52	m6	90	HIS
57	N1	49	GLN
65	N9	45	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	495 (28%)	62 (3%)
1	6	1793/1800 (99%)	481 (26%)	53 (2%)
36	1	3145/3396 (92%)	712 (22%)	87 (2%)
36	5	3145/3396 (92%)	700 (22%)	82 (2%)
37	3	120/121 (99%)	21 (17%)	2 (1%)
37	7	120/121 (99%)	22 (18%)	2 (1%)
38	4	157/158 (99%)	40 (25%)	5 (3%)
38	8	157/158 (99%)	40 (25%)	2 (1%)
All	All	10384/10950 (94%)	2511 (24%)	295 (2%)

5 of 2511 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U

5 of 295 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	2818	U
1	6	187	G
36	5	2801	A
36	1	3121	U
37	3	13	A

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2560 ligands modelled in this entry, 1426 are monoatomic - leaving 1134 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	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	3978	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	m1	203	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	5	3894	-	0,6,6	0.00	-	-		
86	OHX	n3	203	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	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	3900	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	O3	201	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	o3	202	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	7	228	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	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	2138	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	M7	205	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	5	3900	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	6	2187	1	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	5	3897	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	1	3864	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	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	2086	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	L4	403	-	0,6,6	0.00	-	-		
86	OHX	2	2022	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	m5	304	-	0,6,6	0.00	-	-		
86	OHX	1	4211	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	n3	204	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	c8	202	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	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	4153	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
88	3L2	5	4246	-	40,40,40	1.23	5 (12%)	59,62,62	1.67	9 (15%)
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	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	2073	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	1	3871	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	1	3870	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	M7	204	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	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	4149	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	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	2028	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	4	240	-	0,6,6	0.00	-	-		
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	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	2050	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	S6	301	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	5	3893	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	5	3895	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	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	4131	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	m7	206	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	l9	600	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	6	2045	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	n9	102	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	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	4142	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	4	241	-	0,6,6	0.00	-	-		
86	OHX	8	231	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	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	4214	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	l5	302	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
88	3L2	1	4212	-	40,40,40	0.68	1 (2%)	59,62,62	1.41	8 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	m8	201	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	m4	201	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	8	230	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	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	2106	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	3	225	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		
86	OHX	7	217	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	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	4016	-	0,6,6	0.00	-	-		
86	OHX	6	2095	1	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	6	2046	-	0,6,6	0.00	-	-		
86	OHX	s4	301	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	M5	302	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	s9	201	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	Q2	503	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	3	226	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	4	239	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	14	404	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	m0	301	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	5	3896	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	5	3898	-	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	4081	-	0,6,6	0.00	-	-		
86	OHX	5	3892	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	o7	502	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	O7	103	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	1	3866	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	M9	202	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	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	2035	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	5	3899	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	3869	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	1	3865	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	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	4122	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	1	3867	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	M0	303	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	d4	202	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	l3	406	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	1	3863	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	o2	201	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	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	3999	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	13	405	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	m6	202	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	n6	202	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4200	-	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	3967	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	2	2023	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	N1	201	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	1	3868	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	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	4047	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	o7	503	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	L3	403	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	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	3947	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	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	3L2	5	4246	-	-	3/31/89/89	0/4/5/5
88	3L2	1	4212	-	-	4/31/89/89	0/4/5/5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4246	3L2	O8-C13	-2.76	1.39	1.44
88	5	4246	3L2	C25-C14	-2.64	1.47	1.53
88	1	4212	3L2	O8-C13	2.63	1.49	1.44
88	5	4246	3L2	C22-C15	2.46	1.57	1.53
88	5	4246	3L2	O3-C9	-2.40	1.29	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	4246	3L2	O7-C24-C1	-5.73	98.81	110.40
88	5	4246	3L2	C16-C15-C20	5.61	111.97	107.90
88	1	4212	3L2	C7-C8-C9	4.25	133.81	123.36
88	1	4212	3L2	C15-C14-C10	4.01	112.53	108.19
88	5	4246	3L2	C11-C10-C14	3.90	108.30	106.07

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	1	4212	3L2	C16-C15-C22-O5
88	1	4212	3L2	C5-C6-C7-C8
88	1	4212	3L2	C5-C4-O-C3
88	5	4246	3L2	C6-C7-C8-C9
88	1	4212	3L2	O1-C4-O-C3

There are no ring outliers.

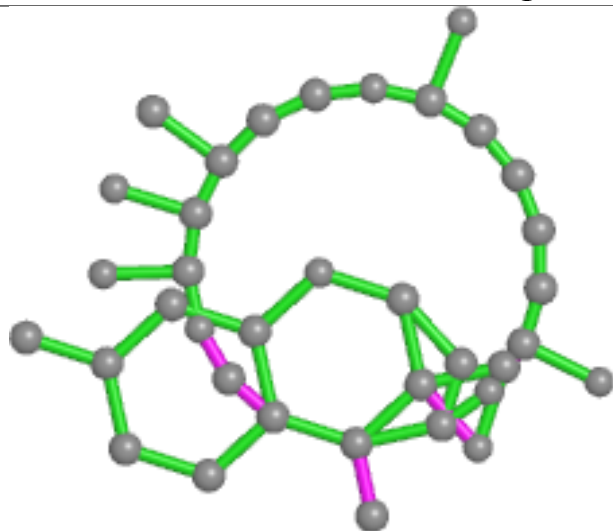
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	S6	301	OHX	0	1

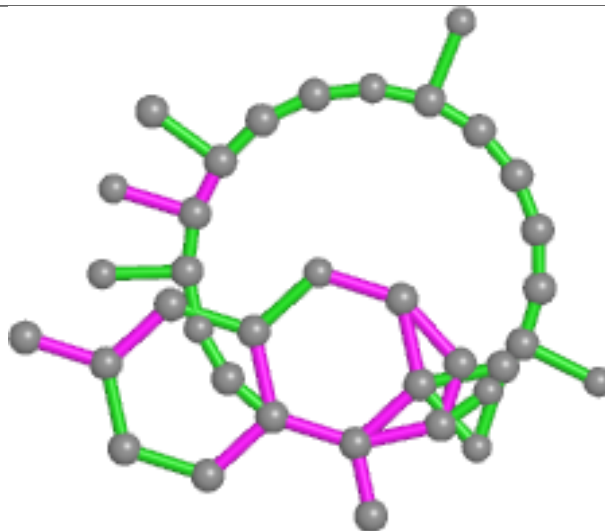
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



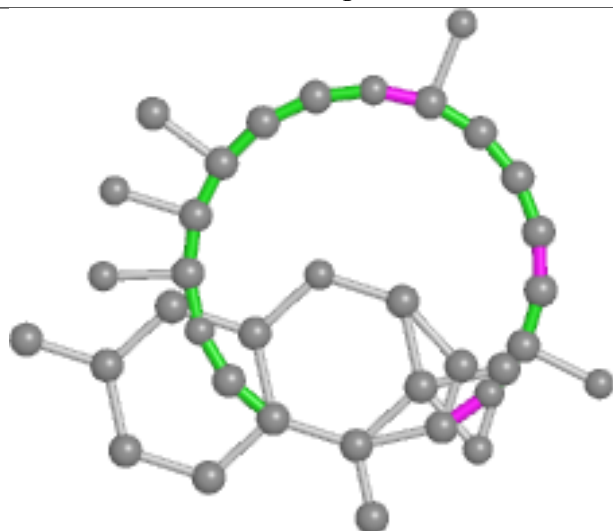
## Ligand 3L2 5 4246



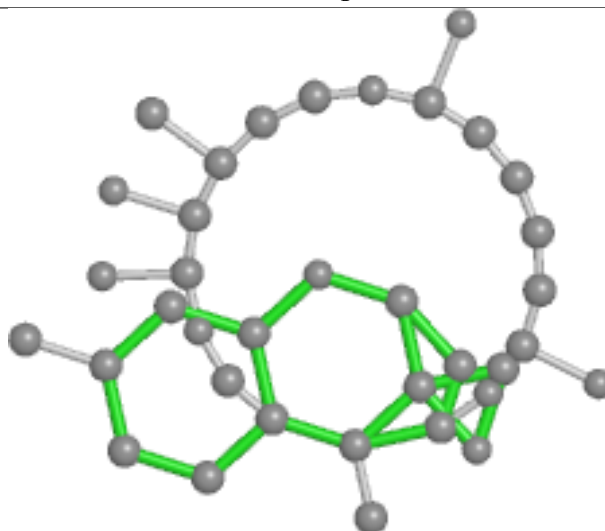
Bond lengths



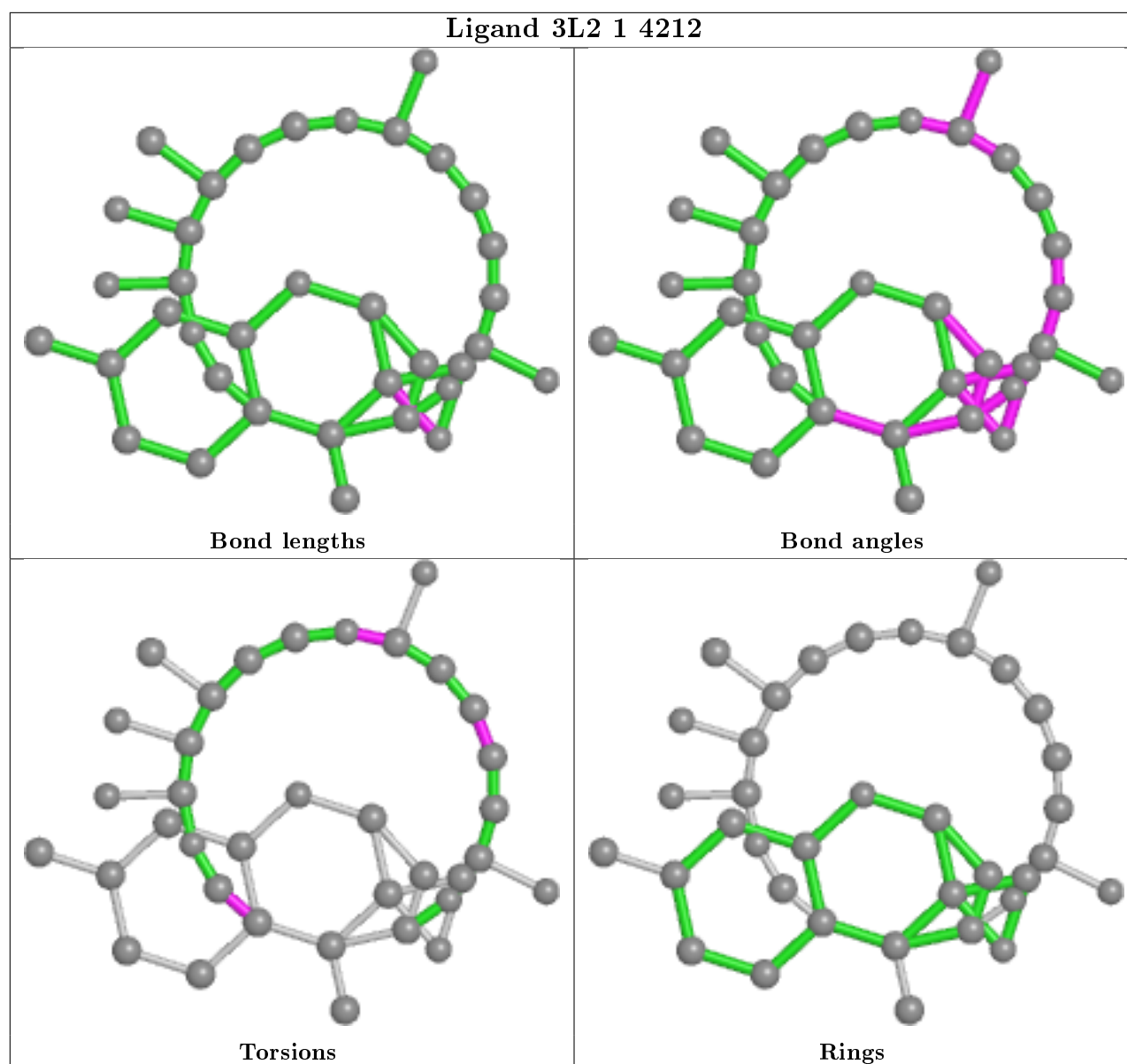
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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