



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 06:32 PM BST

PDB ID : 4U4O  
Title : Crystal structure of Geneticin bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
Resolution : 3.60 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

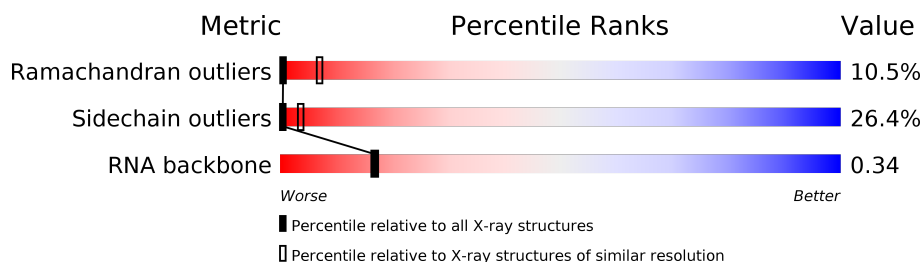
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)


























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	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	


























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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	












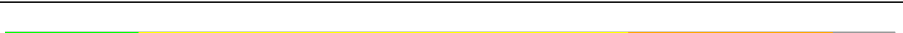


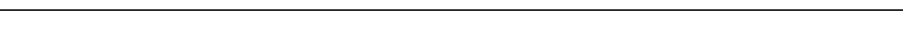
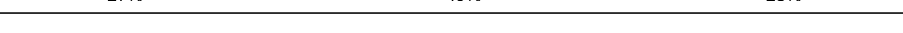
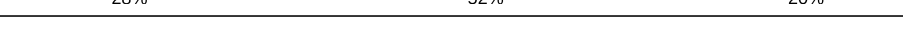


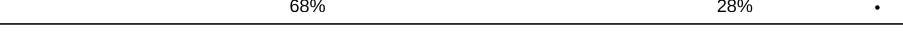





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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107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















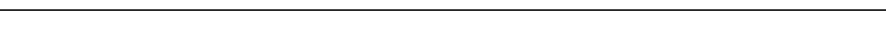




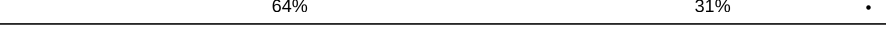





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Mol	Chain	Length	Quality of chain
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	















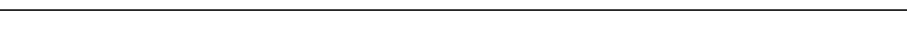




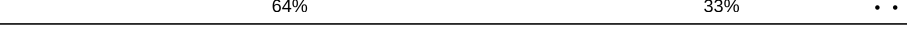





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Mol	Chain	Length	Quality of chain
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	















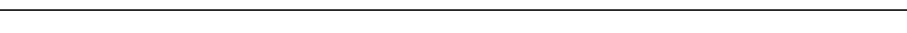




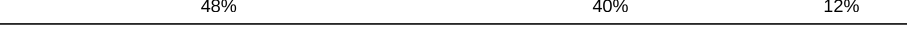





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Mol	Chain	Length	Quality of chain
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	

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Mol	Chain	Length	Quality of chain
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	
81	e1	76	

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Mol	Chain	Length	Quality of chain
82	m2	160	<div><div></div><div>92%</div><div></div><div>6%</div></div>
83	p0	311	<div><div></div><div>36%</div><div>9%</div><div></div><div>54%</div></div>
84	p1	47	<div><div></div><div>100%</div></div>
85	p2	46	<div><div></div><div>100%</div></div>

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411095 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	1791	Total	C	N	O	P	0	0	0
			38149	17055	6738	12565	1791			

- 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			

- 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
			679	402	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	12	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	13	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	14	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	15	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	16	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	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 22 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
O4	113	LYS	-	expression tag	UNP P87262
O4	114	SER	-	expression tag	UNP P87262
O4	115	GLU	-	expression tag	UNP P87262
O4	116	LYS	-	expression tag	UNP P87262
O4	117	LYS	-	expression tag	UNP P87262
O4	118	ALA	-	expression tag	UNP P87262
O4	119	LYS	-	expression tag	UNP P87262
O4	120	LYS	-	expression tag	UNP P87262
o4	110	GLU	-	expression tag	UNP P87262
o4	111	ALA	-	expression tag	UNP P87262
o4	112	ALA	-	expression tag	UNP P87262
o4	113	LYS	-	expression tag	UNP P87262
o4	114	SER	-	expression tag	UNP P87262
o4	115	GLU	-	expression tag	UNP P87262
o4	116	LYS	-	expression tag	UNP P87262
o4	117	LYS	-	expression tag	UNP P87262
o4	118	ALA	-	expression tag	UNP P87262
o4	119	LYS	-	expression tag	UNP P87262
o4	120	LYS	-	expression tag	UNP P87262

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

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

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

- Molecule 84 is a protein called unknown protein chain p1.

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

- Molecule 85 is a protein called unknown protein chain p2.

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

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	2	Total 2	Mg 2	0	0
86	N9	1	Total 1	Mg 1	0	0
86	n8	2	Total 2	Mg 2	0	0
86	o1	1	Total 1	Mg 1	0	0
86	N5	2	Total 2	Mg 2	0	0
86	6	150	Total 150	Mg 150	0	0
86	n4	1	Total 1	Mg 1	0	0
86	m5	2	Total 2	Mg 2	0	0
86	l3	6	Total 6	Mg 6	0	0
86	M1	1	Total 1	Mg 1	0	0
86	d6	1	Total 1	Mg 1	0	0
86	2	124	Total 124	Mg 124	0	0
86	O3	1	Total 1	Mg 1	0	0
86	L4	2	Total 2	Mg 2	0	0
86	l7	2	Total 2	Mg 2	0	0
86	M5	2	Total 2	Mg 2	0	0
86	o0	1	Total 1	Mg 1	0	0
86	S2	2	Total 2	Mg 2	0	0
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	M9	1	Total 1	Mg 1	0	0
86	q0	2	Total 2	Mg 2	0	0
86	SM	1	Total 1	Mg 1	0	0
86	c8	1	Total 1	Mg 1	0	0
86	M0	3	Total 3	Mg 3	0	0
86	5	499	Total 499	Mg 499	0	0
86	L5	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	l4	1	Total 1	Mg 1	0	0
86	n9	2	Total 2	Mg 2	0	0
86	1	468	Total 468	Mg 468	0	0
86	s2	1	Total 1	Mg 1	0	0
86	d3	1	Total 1	Mg 1	0	0
86	S8	1	Total 1	Mg 1	0	0
86	l2	1	Total 1	Mg 1	0	0
86	O2	1	Total 1	Mg 1	0	0
86	q3	2	Total 2	Mg 2	0	0
86	o3	2	Total 2	Mg 2	0	0
86	M3	2	Total 2	Mg 2	0	0
86	N3	2	Total 2	Mg 2	0	0
86	N8	4	Total 4	Mg 4	0	0

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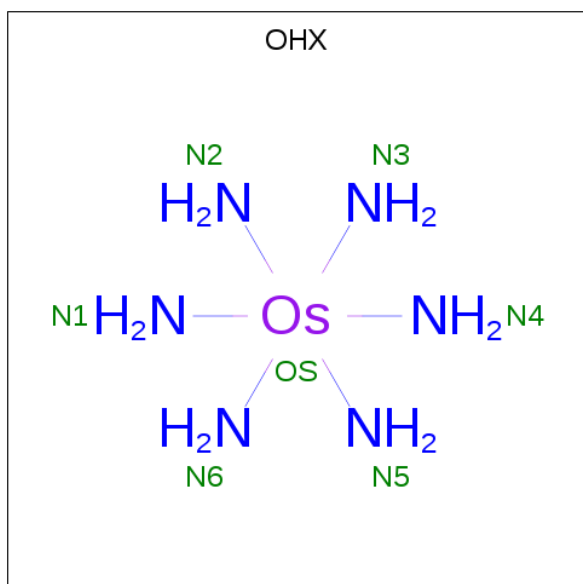
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	4	23	Total 23	Mg 23	0	0
86	D4	1	Total 1	Mg 1	0	0
86	L2	2	Total 2	Mg 2	0	0
86	m1	1	Total 1	Mg 1	0	0
86	l5	3	Total 3	Mg 3	0	0
86	m7	4	Total 4	Mg 4	0	0
86	M7	5	Total 5	Mg 5	0	0
86	m4	1	Total 1	Mg 1	0	0
86	L6	2	Total 2	Mg 2	0	0
86	s1	1	Total 1	Mg 1	0	0
86	l9	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	o2	1	Total 1	Mg 1	0	0
86	c7	1	Total 1	Mg 1	0	0
86	7	15	Total 15	Mg 15	0	0
86	n3	1	Total 1	Mg 1	0	0
86	q1	1	Total 1	Mg 1	0	0
86	L3	2	Total 2	Mg 2	0	0
86	O5	1	Total 1	Mg 1	0	0
86	m6	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	N6	1	Total	Mg	0	0
			1	1		
86	8	17	Total	Mg	0	0
			17	17		
86	m0	1	Total	Mg	0	0
			1	1		
86	M6	1	Total	Mg	0	0
			1	1		
86	N0	1	Total	Mg	0	0
			1	1		
86	3	14	Total	Mg	0	0
			14	14		

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
			7	6	1		
87	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L4	1	Total	N	Os	0	0
			7	6	1		
87	M0	1	Total	N	Os	0	0
			7	6	1		
87	M5	1	Total	N	Os	0	0
			7	6	1		
87	M6	1	Total	N	Os	0	0
			7	6	1		
87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M9	1	Total	N	Os	0	0
			7	6	1		
87	M9	1	Total	N	Os	0	0
			7	6	1		
87	N9	1	Total	N	Os	0	0
			7	6	1		
87	O1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	O2	1	Total	N	Os	0	0
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87	O3	1	Total	N	Os	0	0
			7	6	1		
87	O7	1	Total	N	Os	0	0
			7	6	1		
87	O7	1	Total	N	Os	0	0
			7	6	1		
87	Q2	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	s1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	c3	1	Total 7	N 6	Os 1	0	0
87	c5	1	Total 7	N 6	Os 1	0	0
87	c8	1	Total 7	N 6	Os 1	0	0
87	d4	1	Total 7	N 6	Os 1	0	0
87	d9	1	Total 7	N 6	Os 1	0	0
87	sR	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	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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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		

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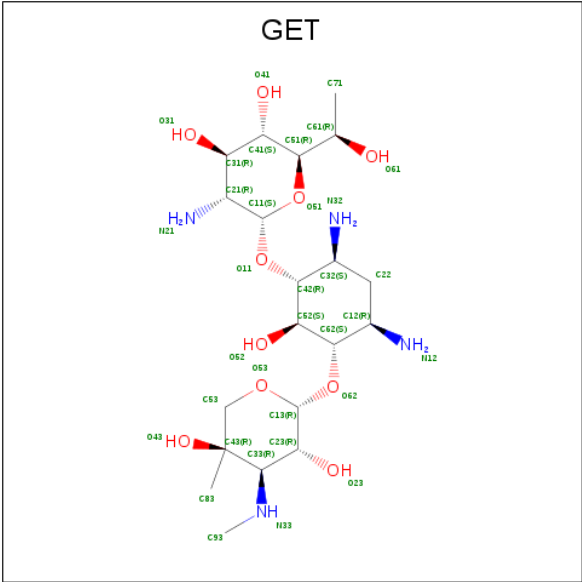
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	19	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m9	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o9	1	Total	N	Os	0	0
			7	6	1		
87	q1	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 88 is GENETICIN (three-letter code: GET) (formula: C<sub>20</sub>H<sub>40</sub>N<sub>4</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	2	1	Total	C	N	O	0	0
			34	20	4	10		

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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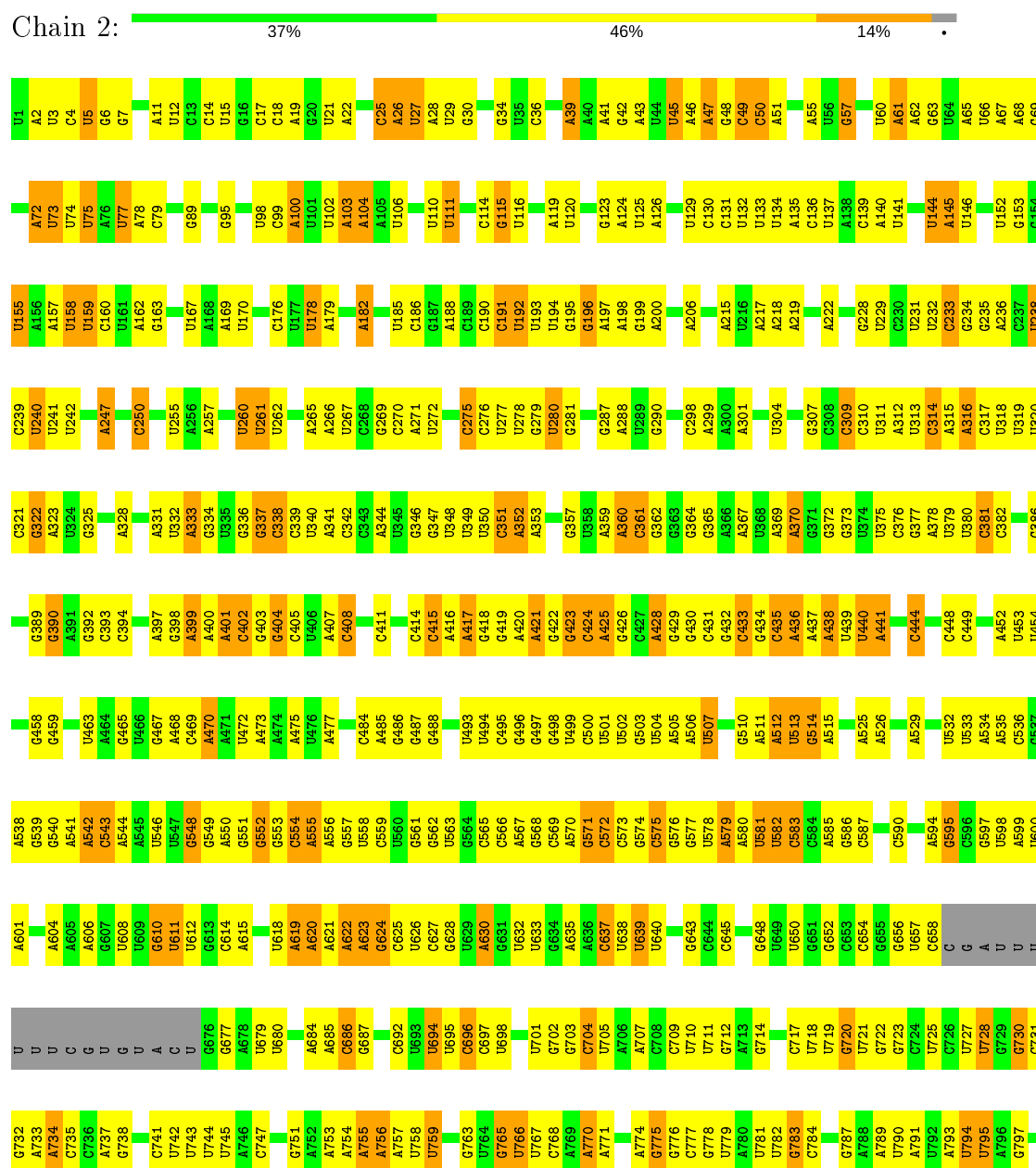
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	D7	1	Total 1	Zn 1	0	0
89	d6	1	Total 1	Zn 1	0	0
89	o7	1	Total 1	Zn 1	0	0
89	O7	1	Total 1	Zn 1	0	0
89	q2	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

#### • Molecule 1: 18S ribosomal RNA



C1751	U1752	A1753	A1754	A1755	A1756	G1757	U1758	C1759	G1760	U1761	A1762	G1763	C1764	A1765	A1766	G1767	G1768	U1769	U1770	U1771	C1772	C1773	G1774	U1775	A1776	G1777	G1778	U1779	C1780	A1781	A1782	C1783	U1784	U1785	G1786	C1787	G1788	C1789	A1790	A1791	G1792	G1793	A1794	U1795	C1796	A1797	U1798	U	A									
C1619	C1620	C1623	C1624	C1625	A1631	C1632	G1633	C1634	A1635	G1636	C1637	C1638	A1639	C1640	C1641	C1642	G1643	G1644	G1645	G1646	U1647	A1648	G1649	U1650	A1651	C1652	C1653	A1654	A1655	U1656	U1657	G1658	A1659	U1660	U1661	G1662	C1663	C1664	U1665	U1666	A1667	G1668	U1669	G1670	A1671	G1672	A1673	C1674	C1675	G1679	G1682	C1683	U1684	G1685	C			
A1475	C1476	U1477	G1478	A1479	G1480	C1481	A1482	A1483	G1484	C1485	G1486	U1489	C1490	A1491	A1492	A1493	U1496	U1497	G1498	G1499	C1500	C1501	G1502	A1503	G1504	A1505	G1506	U1514	A1515	A1516	U1517	U1520	C1521	U1522	G1523	A1524	A1525	A1526	C1530	G1531	U1532	C1533	G1534	U1535	G1536	C1537	U1538	G1539	G1540	A1541	G1542	G1546	A1547					
G1412	U1413	C1414	U1415	G1416	A1417	G1418	U1419	A1420	A1421	A1422	U1423	A1424	A1425	C1426	A1427	G1428	U1430	U1431	U1432	G1433	U1434	G1435	A1436	U1437	G1438	C1439	U1443	A1444	A1445	A1446	C1447	G1448	U1452	G1453	G1454	G1455	C1456	G1457	G1458	C1459	C1461	G1462	C1463	G1464	G1465	U1466	U1467	U1468	C1469	C1470	A1471	C1472	G1474					
A1475	G1476	G1477	G1478	A1479	G1480	C1481	A1482	A1483	G1484	C1485	G1486	U1489	C1490	A1491	A1492	A1493	U1496	U1497	G1498	G1499	C1500	C1501	G1502	A1503	G1504	A1505	G1506	U1514	A1515	A1516	U1517	U1520	C1521	U1522	G1523	A1524	A1525	A1526	C1530	G1531	U1532	C1533	G1534	U1535	G1536	C1537	U1538	G1539	G1540	A1541	G1542	G1546	A1547					
A1550	U1551	U1552	G1553	U1554	A1555	A1556	U1557	U1558	U1559	U1560	U1561	C1565	C1568	C1569	A1570	C1571	G1572	A1573	G1574	U1579	U1582	A1583	G1584	A1587	G1588	C1589	G1590	C1591	G1594	U1595	C1596	A1597	U1598	C1599	A1600	G1601	C1602	G1605	C1606	G1607	U1608	U1609	G1610	A1611	U1613	A1614	C1615	G1616	U1617	G1618	C1618							
C1619	C1620	C1623	C1624	C1625	A1631	C1632	G1633	C1634	A1635	G1636	C1637	C1638	A1639	C1640	C1641	C1642	G1643	G1644	G1645	G1646	U1647	A1648	G1649	U1650	A1651	C1652	C1653	A1654	A1655	U1656	U1657	A1658	A1659	U1660	U1661	G1662	C1663	C1664	U1665	U1666	A1667	G1668	U1669	G1670	A1671	G1672	A1673	C1674	C1675	G1679	G1682	C1683	U1684	G1685	C			
U	U	A	G	A	G	A	A	G	G	G	G	C	A	A	A	C	C	A	U	U	U	C	U	C	A	A	C	G1717	G1720	U1724	G1727	A1728	C1729	A1730	A1731	A1732	C1733	U1734	U1735	G1736	U1737	U1738	C1739	A1740	U1741	U1742	U1743	A1744	G1745	A1746	G1747	G1748	A1749	A1750				
C980	C983	C983	A984	G985	U986	A974	C975	G976	A977	A978	A979	G980	U981	U982	A983	G984	U985	G986	G987	A988	U989	C990	G991	A992	A993	G994	G997	C1000	A1001	G1002	A1003	U1004	A1005	C1006	C1007	U1008	U1009	C1010	G1011	U1015	C1016	A1019	A1020	C949	C1021	C1022	A1023	U1024	A1025	A1026	A1027	C1028	U1029	A1030	U965	U1031	C1032	A967
C1033	C1037	U1038	A1039	G1040	A1043	U1044	C1045	G1046	G1050	G1051	U1052	G1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	A1061	A1062	U1071	C1072	G1073	G1074	C1075	A1076	C1077	C1078	U1079	U1080	A1081	C1082	U1083	A1084	G1085	A1086	A1092	A1093	U1094	U1095	C1096	U1097	U1098	U1099	G1100	G1101	A1102	U1103	U1104	G1108	C1174	U1175	G1109	G1110			
G1111	G1112	A1113	G1114	G1119	U1120	C1121	G1122	A1124	G1125	G1126	G1127	U1128	U1129	A1130	U1131	A1132	A1133	U1134	U1135	U1136	A1137	A1138	A1139	G1140	G1141	A1142	A1143	U1144	U1145	A1146	A1147	C1148	G1149	G1150	A1151	A1152	G1155	C1156	A1157	C1158	A1159	A1160	C1161	G1162	A1163	G1164	G1165	A1166	U1167	U1168	G1172	C1173	C1174	U1175	G1176			
C1177	G1178	C1179	U1181	U1182	A1183	U1184	U1185	U1186	A1189	C1190	U1191	C1192	A1193	A1194	C1195	A1196	C1197	G1198	G1199	U1200	G1201	A1202	A1203	A1204	C1205	U1206	C1207	A1208	C1209	A1211	G1212	U1213	U1214	C1215	G1216	G1217	G1218	C1219	C1220	A1226	A1227	G1228	G1229	C1235	A1236	G1237	U1240	G1241	A1244	G1245	C1246	U1247						
U1250	U1251	C1252	G1255	U1258	U1259	U1260	G1261	G1264	G1265	U1266	G1267	G1268	U1269	G1270	G1271	G1272	U1273	C1274	A1275	U1276	G1277	G1278	C1279	G1280	C1281	U1282	U1283	C1284	U1285	U1286	A1287	G1288	U1289	U1290	G1291	G1295	A1296	G1297	U1298	G1299	A1300	U1301	U1302	U1303	C1306	U1307	U1311	U1314	U1315	G1316								
U1320	A1321	A1322	C1323	G1324	A1329	C1332	A1336	C1337	C1338	C1339	U1340	A1341	C1342	U1343	G1344	A1345	U1346	U1347	G1348	G1354	C1355	U1356	A1357	G1358	C1359	A1360	U1361	U1362	U1363	U1370	A1371	U1372	C1373	C1374	A1375	U1378	G1385	G1386	C1389	U1390	A1391	U1392	C1393	U1398	C1399	A1400	U1407	G1408	G1409									
G1412	U1413	C1414	U1415	G1416	A1417	G1418	U1419	A1420	A1421	A1422	U1423	A1424	A1425	C1426	A1427	G1428	U1430	U1431	U1432	G1433	U1434	G1435	A1436	U1437	G1438	C1439	U1443	A1444	A1445	A1446	C1447	G1448	U1452	G1453	G1454	G1455	C1456	G1457	G1458	C1459	C1461	G1462	C1463	G1464	G1465	U1466	U1467	U1468	C1469	C1470	A1471	C1472	G1474					
A1475	C1476	G1477	G1478	A1479	G1480	C1481	A1482	A1483	G1484	C1485	G1486	U1489	C1490	A1491	A1492	A1493	U1496	U1497	G1498	G1499	C1500	C1501	G1502	A1503	G1504	A1505	G1506	U1514	A1515	A1516	U1517	U1520	C1521	U1522	G1523	A1524	A1525	A1526	C1530	G1531	U1532	C1533	G1534	U1535	G1536	C1537	U1538	G1539	G1540	A1541	G1542	G1546	A1547					
A1550	U1551	U1552	G1553	U1554	A1555	A1556	U1557	U1558	U1559	U1560	U1561	C1565	C1568	C1569	A1570	C1571	G1572	A1573	G1574	U1579	U1582	A1583	G1584	A1587	G1588	C1589	G1590	C1591	G1594	U1595	C1596	A1597	U1598	C1599	A1600	G1601	C1602	G1605	C1606	G1607	U1608	U1609	G1610	A1611	U1613	A1614	C1615	G1616	U1617	G1618	C1618							
C1619	C1620	C1623	C1624	C1625	A1631	C1632	G1633	C1634	A1635	G1636	C1637	C1638	A1639	C1640	C1641	C1642	G1643	G1644	G1645	G1646	U1647	A1648	G1649	U1650	A1651	C1652	C1653	A1654	A1655	U1656	U1657	A1658	A1659	U1660	U1661	G1662	C1663	C1664	U1665	U1666	A1667	G1668	U1669	G1670	A1671	G1672	A1673	C1674	C1675	G1679	G1682	C1683	U1684	G1685	C			
U	U	A	G	A	G	A	A	G	G	G	G	C	A	A	A	C	C	A	U	U	U	C	U	C	A	A	C	G1717	G1720	U1724	G1727	A1728	C1729	A1730	A1731	A1732	C1733	U1734	U1735	G1736	U1737	U1738	C1739	A1740	U1741	U1742	U1743	A1744	G1745	A1746	G1747	G1748	A1749	A1750				
C980	C983	C983	A984	G985	U986	A974	C975	G976	A977	A978	A979	G980	U981	U982	A983	G984	U985	G986	G987	A988	U989	C990	G991	A992	A993	G994	G997	C1000	A1001	G1002	A1003	U1004	A1005	C1006	C1007	U1008	U1009	C1010	G1011	U1015	C1016	A1019	A1020	C949	C1021	C1022	A1023	U1024	A1025	A1026	A1027	C1028	U1029	A1030	U965	U1031	C1032	A967
C1033	C1037	U1038	A1039	G1040	A1043	U1044	C1045	G1046	G1050	G1051	U1052	G1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	A1061	A1062	U1071	C1072	G1073	G1074	C1075	A1076	C1077	C1078	U1079	U1080	A1081	C1082	U1083	A1084	G1085	A1086	A1092	A1093	U1094	U1095	C1096	U1097	U1098	U1099	G1100	G1101	A1102	U1103	U1104	G1108	C1174	U1175	G1109	G1110			
G1111	G1112	A1113	G1114	G1119	U1120	C1121	G1122	A1124	G1125	G1126	G1127	U1128	U1129	A1130	U1131	A1132	A1133	U1134	U1135	U1136	A1137	A1138	A1139	G1140	G1141	A1142	A1143	U1144	U1145	A1146	A1147	C1148	G1149	G1150	A1151	A1152	G1155	C1156	A1157	C1158	A1159	A1160	C1161	G1162	A1163	G1164	G1165	A1166	U1167	U1168	G1172	C1173	C1174	U1175	G1176			
C1177	G1178	C1179	U1181	U1182	A1183	U1184	U1185	U1186	A1189	C1190	U1191	C1192	A1193	A1194	C1195	A1196	C1197	G1198	G1199	U1200	G1201	A1202	A1203	A1204	C1205	U1206	C1207	A1208	C1209	A1211	G1212	U1213	U1214	C1215	G1216	G1217	G1218	C1219	C1220	A1226	A1227	G1228	G1229	C1235	A1236	G1237	U1240	G1241	A1244	G1245	C1246	U1247						
U1250	U1251	C1252	G1255	U1258	U1259	U1260	G1261	G1264	G1265	U1266	G1267	G1268	U1269	G1270	G1271	G1272	U1273	C1274	A1275	U1276	G1277	G1278	C1279	G1280	C1281	U1282	U1283	C1284	U1285	U1286	A1287	G1288	U1289	U1290	G1291	G1295	A1296	G1297	U1298	G1299	A1300	U1301	U1302	U1303	C1306	U1307	U1311	U1314	U1315	G1316								
U1320	A1321	A1322	C1323	G1324	A1329	C1332	A1336	C1337	C1338	C1339	U1340	A1341	C1342	U1343	G1344	A1345	U1346	U1347	G1348	G1354	C1355	U1356	A1357	G1358	C1359	A1360	U1361	U1362	U1363	U1370	A1371	U1372	C1373	C1374	A1375	U1378	G1385	G1386	C1389	U1390	A1391	U1392	C1393	U1398	C1399	A1400	U1407	G1408	G1409									
G1412	U1413	C1414	U1415	G1416	A1417	G14																																																				

● Molecule 1: 18S ribosomal RNA

Chain 6:  26% 52% 22% .





- Molecule 2: 40S ribosomal protein S0-A

Frequency	Percentage
Daily	55%
Weekly	25%
Monthly	2%
Never	18%



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

• Molecule 2: 40S ribosomal protein S0-A

Chain s0: 54% 25% 18%

S2 L3 P4 A5 T6 L9 T10 E12 Q15 T22 E23 L24 N28 V29 Q30 Q31 R41 V50 V58 L59 R62 I63 I64 A65 P68 M69 D72 T80 R84 A85 V86 L87 A95 T96 P97 I98 T103 Y110 I111 T112 R113 S114 F115

R119 I122 R127 S128 D129 A130 Q131 I133 V139 H140 I141 L146 P152 S153 E154 F155 V156 D157 V158 N164 R165 G166 K167 L172 L177 A178 R179 E180 V181 L182 R183 L184 R185 G186 A187 L188 V189 P194 W195 S196 Y202 R205 D206 P207 GLU GLU VAL GLU

• Molecule 3: 40S ribosomal protein S1-A

Chain S1: 55% 27% 16%

ALA VAL GLY LYS ASN LYS ARG LEU SER LYS GLY LYS LYS GLY GLN LYS ARG V20 V21 T25 R26 P25 S26 T37 F38 E39 M40 V43 T46 M49 L54 S58 D59 A60 L61 K62 G63 R64 L70 L73 D78 H79 S80 F81 R82 K85 D89

G93 R94 L96 L97 H101 D104 F105 R111 K116 T119 V125 T126 K128 T129 S130 D131 I137 Q149 S154 Y155 S158 S169 T173 V176 Q177 G178 S179 T180 L181 S186 K187 L188 E191 V192 I193 N194 E198 N199 K202

• Molecule 3: 40S ribosomal protein S1-A

Chain s1: 59% 24% 15%

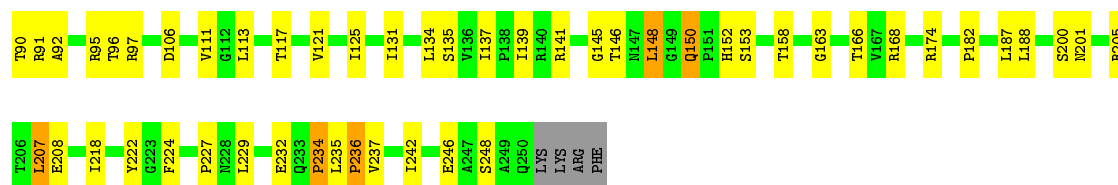
ALA VAL GLY LYS ASN LYS ARG LEU SER LYS GLY LYS LYS GLY GLN LYS ARG V20 V21 D22 R26 S36 T37 R41 T46 L47 K50 K55 D59 A60 L61 K62 V65 V66 L70 L73 S76 E77 D78 H79 S80 F81 R82 D89 E90 G93

T98 N99 F105 T106 T107 D108 R115 T126 T129 S130 D131 I137 A147 S154 S158 S159 H160 I161 T173 T180 L181 T185 L188 E191 V192 I193 N194 A200 T201 K202 F205 P206 L207 Q208 M209 I210 H211 L218 R222 F223 D224

• Molecule 4: 40S ribosomal protein S2

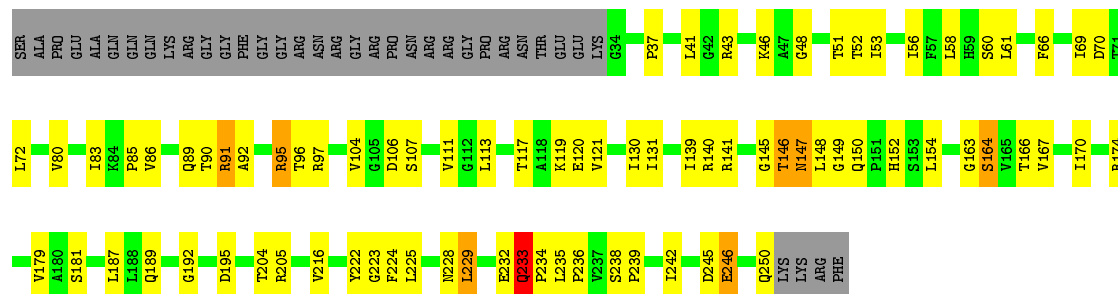
Chain S2: 59% 24% 14%

SER ALA ALA GLU GLU ALA GLN GLN LYS ARG GLY GLY PHE VAL THR GLY ARG ASN ARG ARG GLY ARG PRQ ARG R35 V38 L41 T53 E54 L58 H59 S60 L61 D70 T71 L72 G75 L76 Q77 R85 V86 Q87 R88 Q89



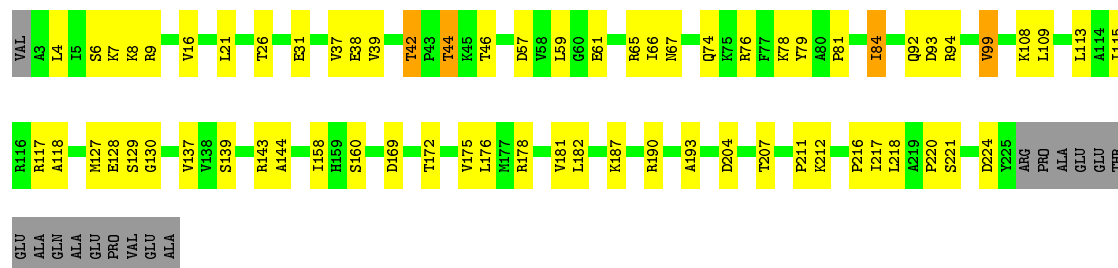
• Molecule 4: 40S ribosomal protein S2

Chain s2: 54% 29% 14%



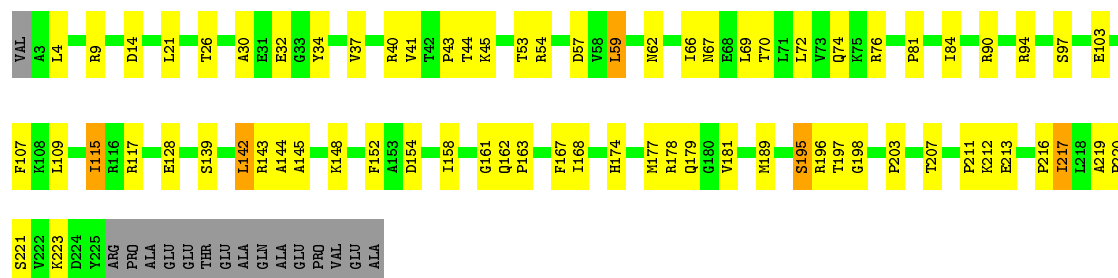
• Molecule 5: 40S ribosomal protein S3

Chain S3: 65% 26% 7%



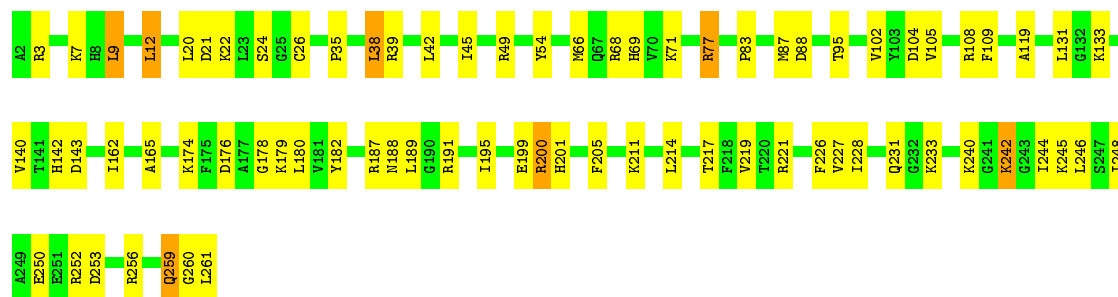
• Molecule 5: 40S ribosomal protein S3

Chain s3: 63% 28% 7%



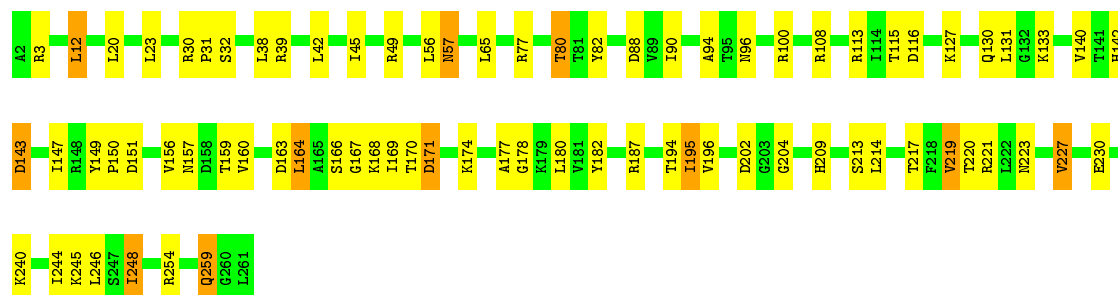
• Molecule 6: 40S ribosomal protein S4-A

Chain S4: 71% 27%



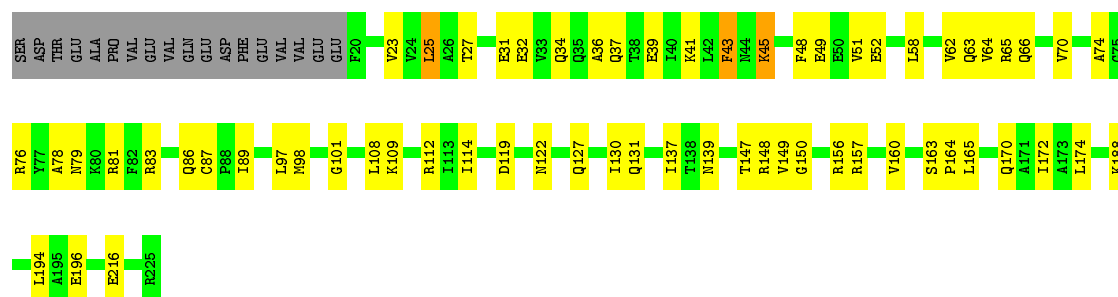
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 70% 26%



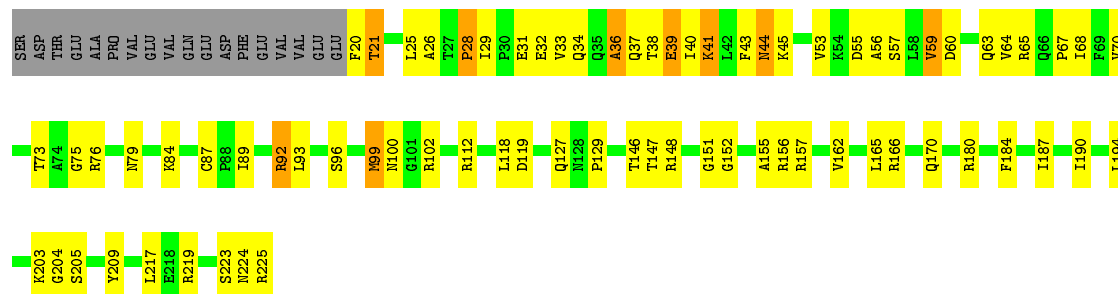
- Molecule 7: 40S ribosomal protein S5

Chain S5: 64% 27% 8%



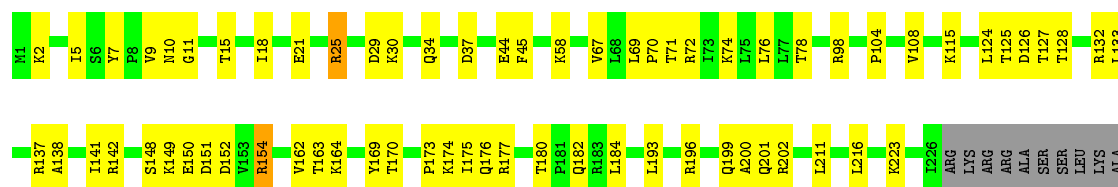
- Molecule 7: 40S ribosomal protein S5

Chain s5: 58% 29% 8%



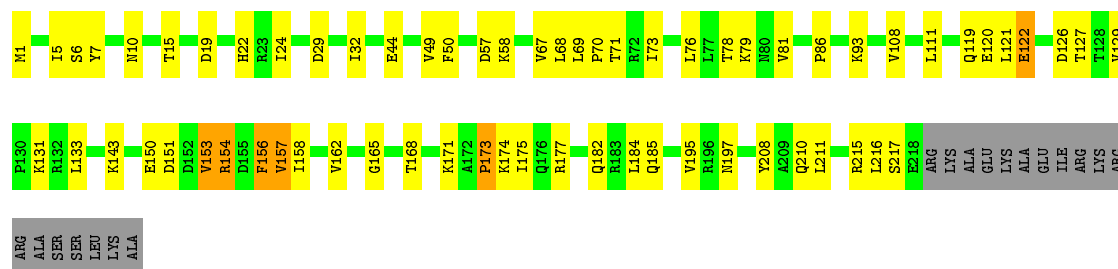
- Molecule 8: 40S ribosomal protein S6-A

Chain S6:  67% 28% . .



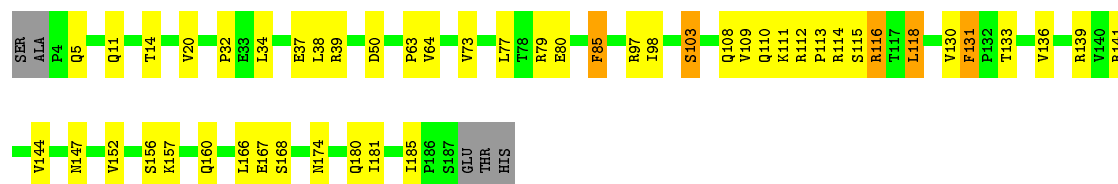
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:  64% 25% . 8%



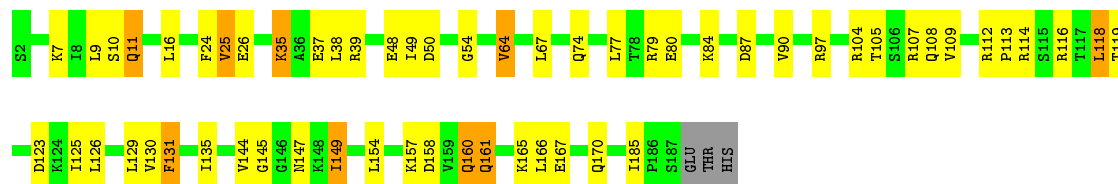
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:  71% 23% . .



• Molecule 9: 40S ribosomal protein S7-A

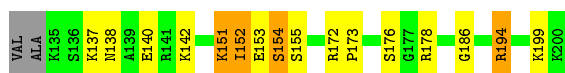
Chain s7:  68% 26% 5% .



• Molecule 10: 40S ribosomal protein S8-A

Chain S8:  72% 19% . 6%





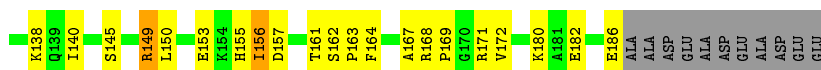
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 67% 26% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 67% 25% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 65% 26% 6%



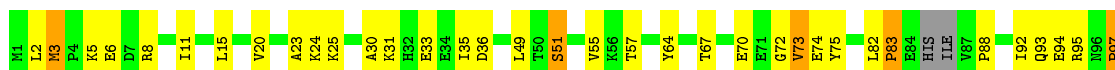
- Molecule 12: 40S ribosomal protein S10-A

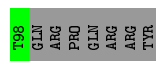
Chain C0: 57% 30% 9%



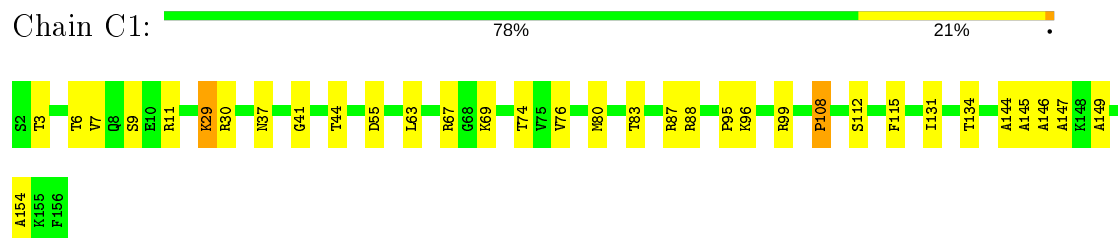
- Molecule 12: 40S ribosomal protein S10-A

Chain c0: 58% 29% 5% 9%

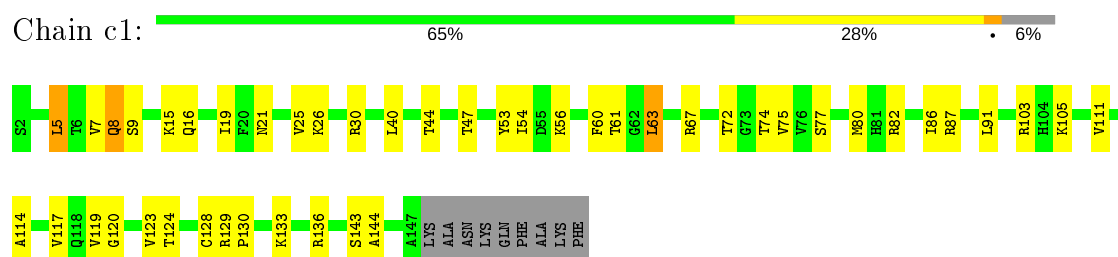




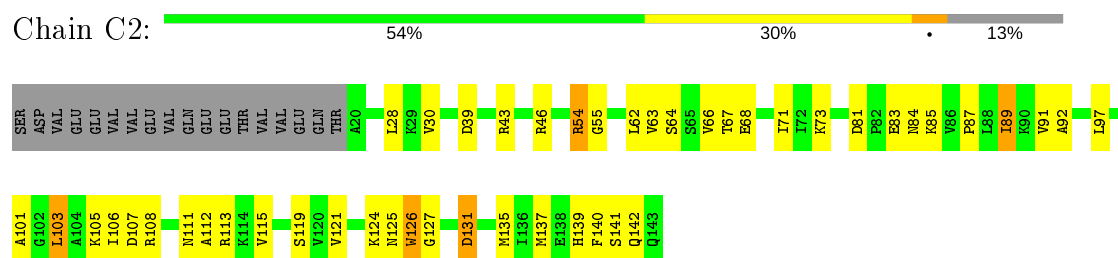
- Molecule 13: 40S ribosomal protein S11-A



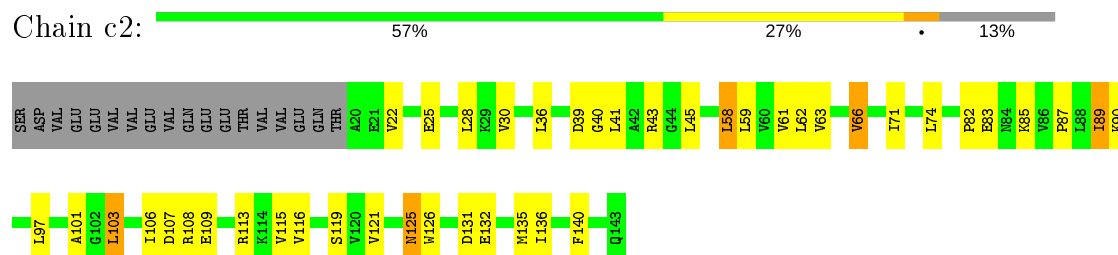
- Molecule 13: 40S ribosomal protein S11-A



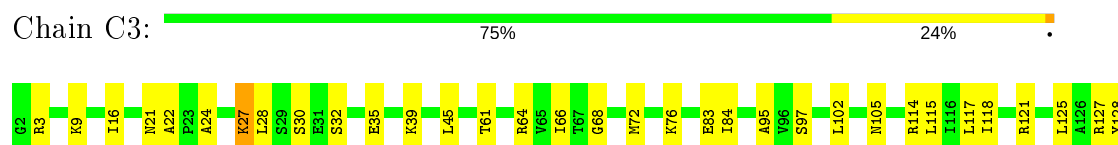
- Molecule 14: 40S ribosomal protein S12



- Molecule 14: 40S ribosomal protein S12



- Molecule 15: 40S ribosomal protein S13

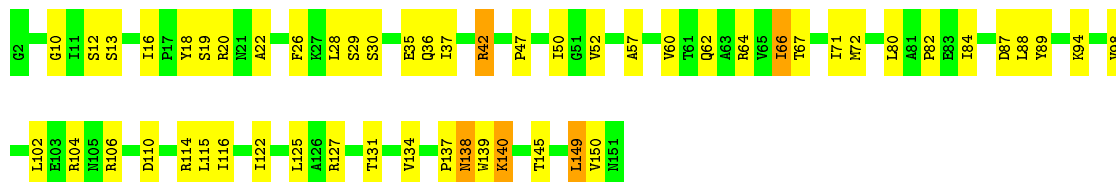






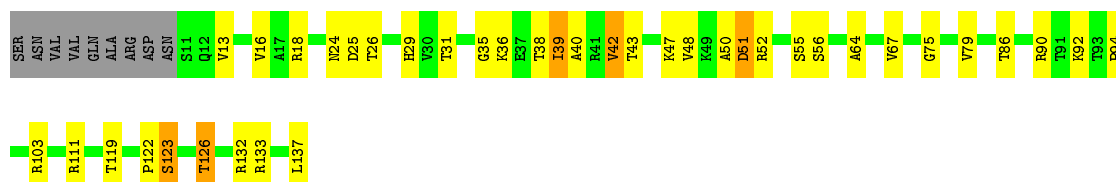
- Molecule 15: 40S ribosomal protein S13

Chain c3: 64% 33%



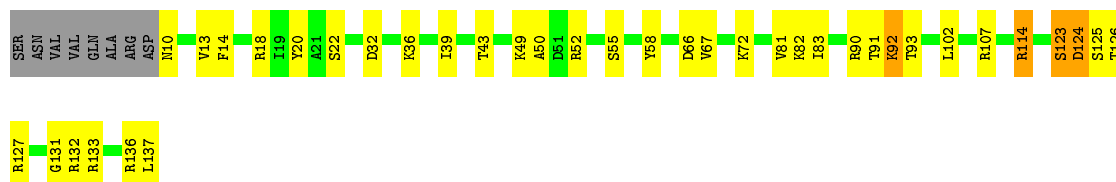
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 65% 25% 7%



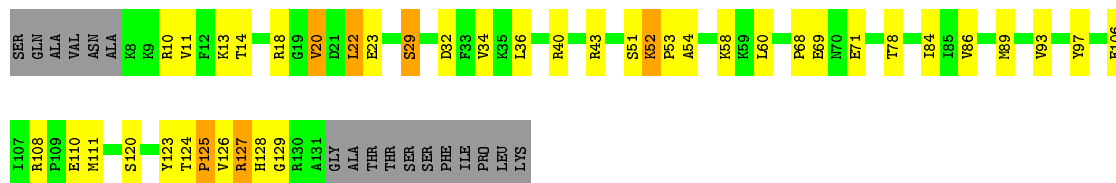
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 66% 25% 6%



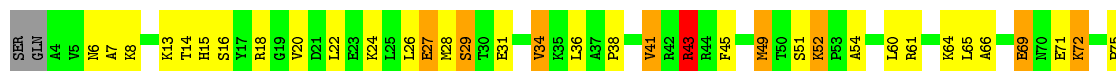
- Molecule 17: 40S ribosomal protein S15

Chain C5: 59% 25% 12%



- Molecule 17: 40S ribosomal protein S15

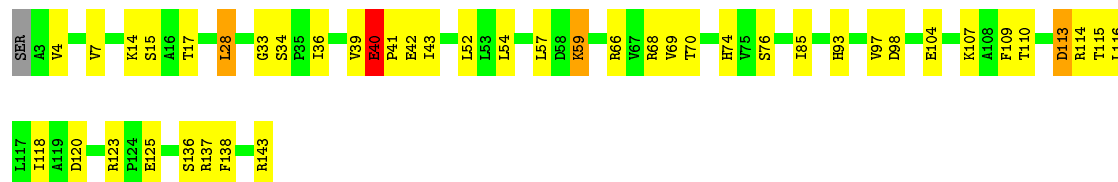
Chain c5: 60% 28% 7%





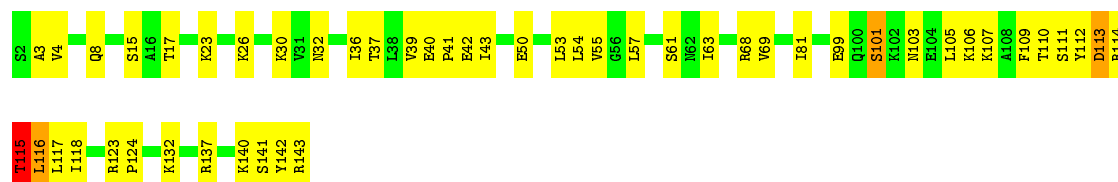
- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 68% 28% ..



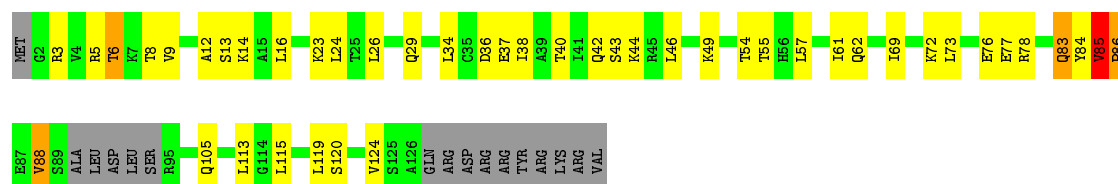
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 65% 32% ..



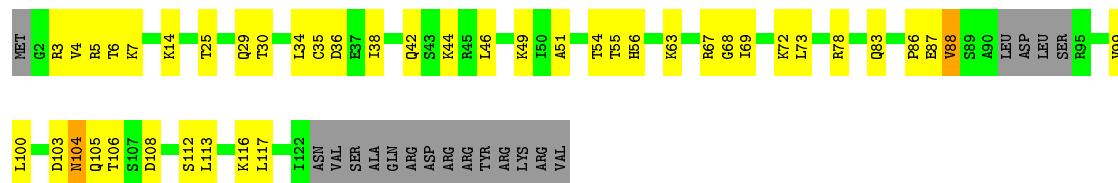
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 55% 29% 12% ..



- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 54% 30% 14% .



- Molecule 20: 40S ribosomal protein S18-A

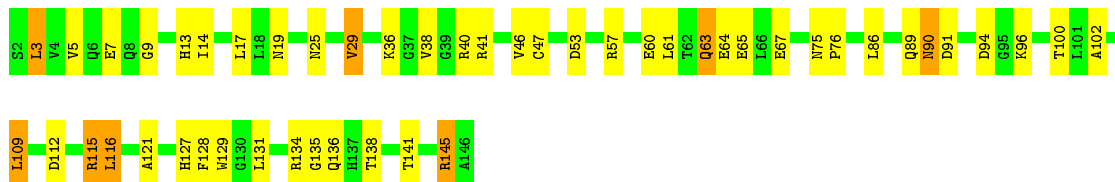
Chain C8: 77% 21% .




R145  
A146

- Molecule 20: 40S ribosomal protein S18-A

Chain c8:  66% 28% 6%




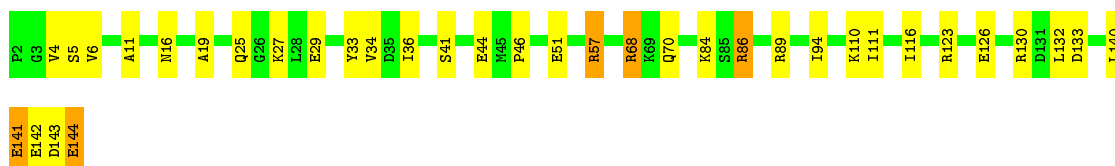
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:  73% 24% .



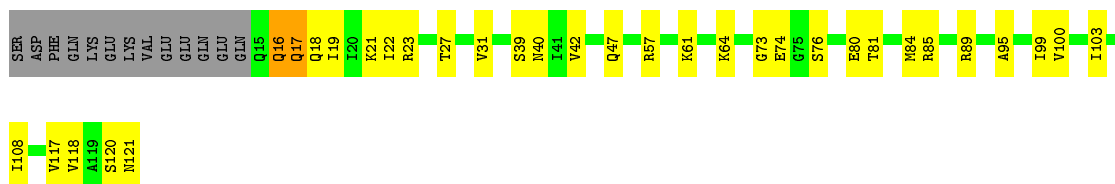
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:  75% 22% .



- Molecule 22: 40S ribosomal protein S20

Chain D0:  62% 26% . 11%



- Molecule 22: 40S ribosomal protein S20

Chain d0:  49% 38% 5% 8%





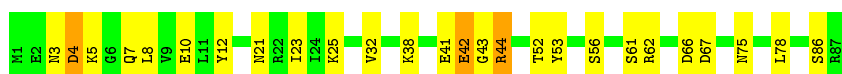
- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 68% 28% 5%



- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 70% 26% 4%



- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 72% 26% 2%



- Molecule 24: 40S ribosomal protein S22-A

Chain d2: 78% 20% 2%



- Molecule 25: 40S ribosomal protein S23-A

Chain D3: 58% 36% 6%



- Molecule 25: 40S ribosomal protein S23-A

Chain d3: 71% 27% 2%





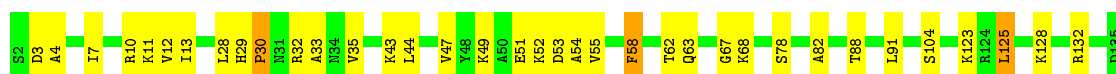
- Molecule 26: 40S ribosomal protein S24-A

Chain D4: 78% 18%



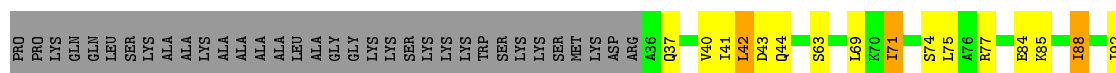
- Molecule 26: 40S ribosomal protein S24-A

Chain d4: 73% 25%



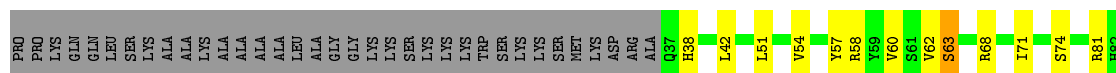
- Molecule 27: 40S ribosomal protein S25-A

Chain D5: 46% 17% 35%



- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 45% 18% 36%



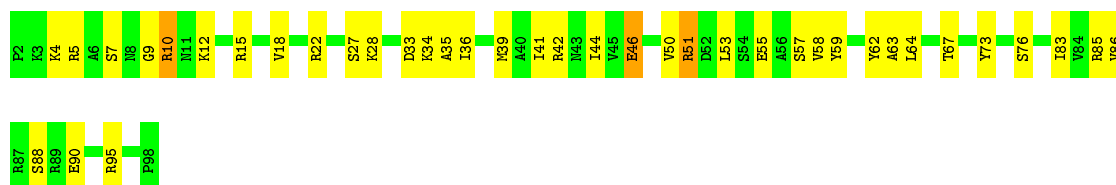
- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 60% 31% 9%



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 60% 37%



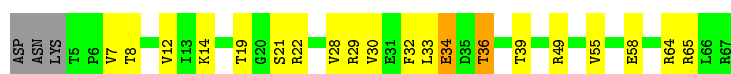
- Molecule 29: 40S ribosomal protein S27-A



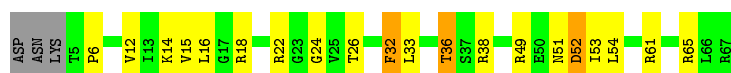
- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A

A2	K3	G6	K13	V14	K15	S16	K20	V21	E22	K23	T24	E25	K26	P27	R33	L38	L39	R42	V47	T48	L49	V50	N51	G52	K53	R54	R55	M56	S61
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- Chain E1:  53% 37% 7%

[illegible]

- Chain SR:  80% 19%

[illegible]

- Chain sR:  80% 19%

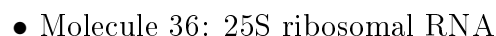
[illegible]

- Chain SM:  40% 16% . 42%

SER	LYS	A90
ALA	ASN	T91
ASN	VAL	D92
THR	LYS	
VAL	SER	T100
GLN	LYS	D101
LYS	GLN	T102
ASN	LEU	
ARG	LYS	V106
ASN	THR	
ILE	LYS	D112
ASP	GLU	D113
VAL	TYR	K114
SER	LEU	K115
ASN	GLU	E116
LEU	PHE	
PRO	ASP	E120
SER	ALA	
LEU	THR	E133
ALA	PHE	D134
	VAL	
	GLU	E139
	SER	D140
	ASN	A141
	THR	GLY
	ARG	LVS
	LYS	PRO
	ASN	LVS
	PHE	THR
	GLY	ALA
	ASP	GLN
	ARG	LEU
	ASN	SER
	ASN	L151
	ASN	Q152
	SER	D153
	ARG	
	ASN	V166
	ASN	P167
	PHE	
	ASN	E173
	ASN	
	ARG	A176
	PRO	GLU
	GLY	ARG
	GLY	I1E
	ARG	GLU
	GLY	THR
	ALA	ALA
	LYS	LVS
	GLY	GLU
	ASN	ALA
	ASN	TYR
	THR	VAL
	ALA	PRO
	ASN	ALA
	ALA	THR
	THR	LVS
	ASN	R89

- Molecule 35: Suppressor protein STM1

Response	Percentage
Yes	27%
No	9%
Don't know	62%



Response	Percentage
Yes, U.S. should take action to reduce greenhouse gas emissions	16%
No, U.S. should not take action to reduce greenhouse gas emissions	54%
U.S. should take action to reduce greenhouse gas emissions, but not as fast as the European Union	22%
U.S. should not take action to reduce greenhouse gas emissions	7%





G1586	A1587	A1588	A1589	G1592	A1593	A1594	A1595	A1596	G1599	U1580	U1601	U1602	G1603	G1604	A1605	A1606	A1607	A1608	A1609	A1610	A1613	G1614	G1617	G1618	A1619	U1620	A1621	U1622	A1623	G1624	U1627	G1628	U1629	U1630	G1631	A1632	G1633	G1634	G1635	U1636	G1639	G1640	A1641	A1642	A1643	A1644	U1645	G1646	G1650	U1651	A1656																																																																																						
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G951	U952	C953	U954	U955	U956	C957	C958	U959	U960	G961	A962	G963	G964	A965	U966	U967	G968	C969	A970	G971	U972	A973	G974	C975	U976	C977	A978	C979	U980	A981	U982	C983	A984	U985	A986	U987	U988	A989	U990	C991	U992	A993	G994	U995	U996	A997	A998	G999	U1000	G1001	A1002	U1003	U1004	G1005	A1006	U1007	G1008	U1009	G1010	A1011																																																																													
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G765	U766	U767	C768	G769	G770	A771	U772	U773	G774	A775	U776	U777	U778	G779	U780	G781	U782	A783	A784	G785	A786	G787	C788	A789	U790	G791	G792	C793	U794	U795	U796	U797	G798	A801	C802	C803	C804	G805	U871	U872	C873	A808	U874	G875	A876	C877	C878	U879	U880	C881	A882	A883	A884	U885	A886	U887	A888	U889	C890																																																																														
G700	G701	G702	G703	U704	A705	U706	U707	G708	A709	U710	A711	G712	U713	G714	A715	A716	C717	U718	U719	A720	G721	G722	G723	G724	G725	G726	G727	C728	G729	C730	U731	C732	G733	C734	A735	A736	G737	G740	U741	G742	C743	U881	U882	U883	G884	G885	U887	G888	U889	A890	A891	A892	A893	C894	C895	C896	U897	U898	U899	U900																																																																													
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A2482	U2483	U2484	G2485	U2486	U2487	A2488	A2489	A2490	A2491	A2492	A2493	A2494	A2495	A2496	A2497	A2498	A2499	A2500	A2501	A2502	A2503	A2504	A2505	A2506	A2507	A2508	A2509	A2510	A2511	A2512	A2513	A2514	A2515	A2516	A2517	A2518	A2519	A2520	A2521	A2522	A2523	A2524	A2525	A2526	A2527	A2528	A2529	A2530	A2531	A2532	A2533	A2534	A2535	A2536	A2537	A2538	A2539	A2540	A2541	A2542	A2543	A2544	A2545	A2546	A2547	A2548	A2549	A2550	A2551	A2552	A2553	A2554	A2555	A2556	A2557	A2558	U2559	U2560	A2561	U2562		
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G2311	A2312	U2313	U2314	U2315	U2316	U2317	U2318	U2319	U2320	U2321	U2322	U2323	U2324	U2325	U2326	U2327	U2328	U2329	U2330	U2331	U2332	U2333	U2334	U2335	U2336	U2337	U2338	U2339	U2340	U2341	U2342	U2343	U2344	U2345	U2346	U2347	U2348	U2349	U2350	U2351	U2352	U2353	U2354	U2355	U2356	U2357	U2358	U2359	U2360	U2361	U2362	U2363	U2364	U2365	U2366	U2367	U2368	U2369	U2370	U2371	U2372																					
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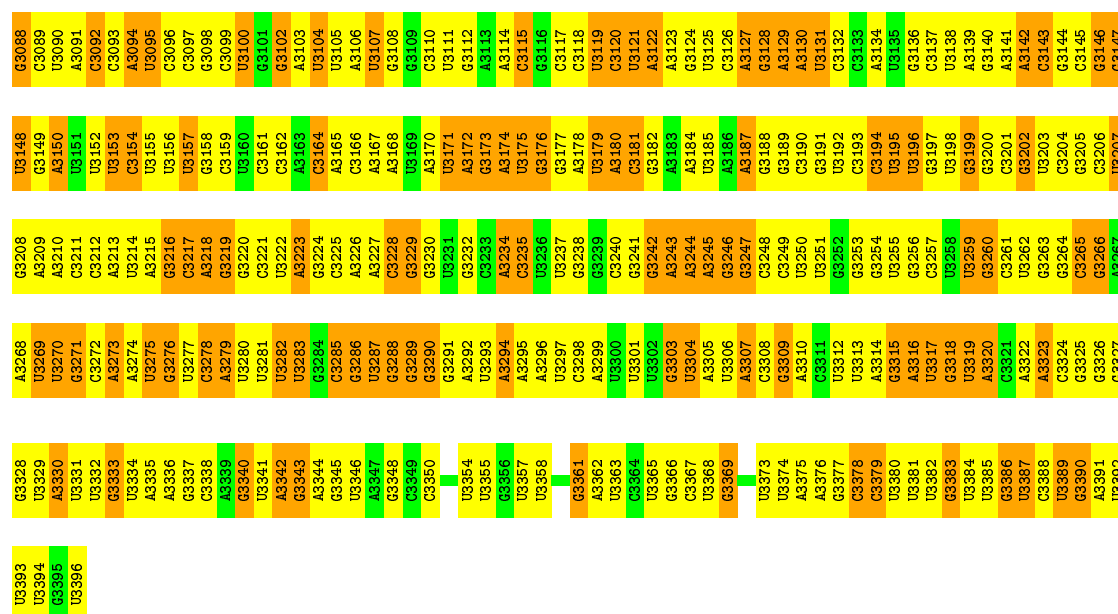
- Molecule 36: 25S ribosomal RNA

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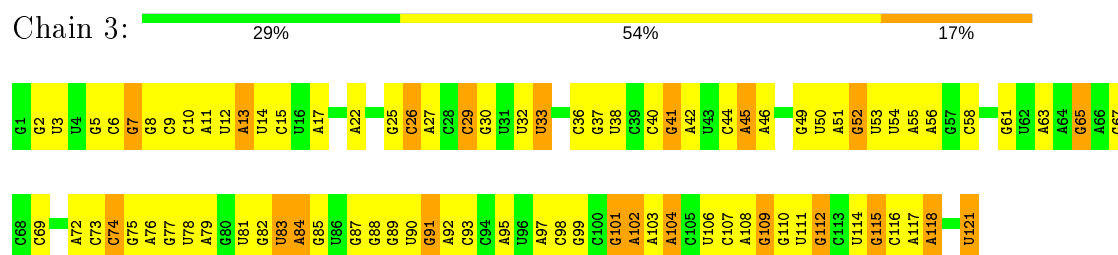
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G1010	G950	C890	G768	C769	A705	A645	C577	G514	G391	G330	A265	C200	C132	A70
A1011	A951	C891	A830	G769	A706	A646	A578	C515	G392	G331	A266	A201	U133	C69
G1012	A952	U892	G831	G770	U707	A647	C579	G517	U393	G332	G267	G202	U134	A71
G1013	G953	C893	G832	A771	G708	C648	C580	G518	G394	G333	A268	G206	C135	C72
U1014	U954	C894	G833	U772	A709	A649	U581	G519	A395	A334	G269	G136	G137	G73
U1015	U955	A895	U834	G773	A710	C650	G582	A519	A396	G335	U270	G138	G74	G75
C1016	U956	A896	G835	G774	A711	G651	G583	U520	A397	G336	C208	G139	G76	A77
C1017	C957	U897	A836	A775	G712	G652	G584	A521	A398	C338	G272	A209	G78	A78
G1018	C958	U898	A837	U776	U713	A653	A522	A523	A399	C339	A273	U210	G79	A79
U1019	U959	U899	U777	G714	G715	C655	G586	U524	G401	C340	G274	A211	G142	U79
G1020	U960	U900	U778	A715	A716	A656	G588	C525	U401	A342	U275	G212	G143	U79
G1021	C961	G901	A841	G779	A716	A657	G589	C526	A402	G403	U276	A213	A144	G80
U1022	A962	G902	G842	A780	C717	G658	G590	U527	G404	U343	G277	G214	G145	C81
C1023	G963	U903	A843	G781	G718	A659	G591	A528	U405	A344	U278	G216	U146	C82
G1024	G964	A904	G844	U782	U719	C660	G592	U529	G406	G345	U279	G217	U147	
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U1026	U966	A906	A846	A784	G721	G661	C593	G530	G408	G347	G281	G218	G86	G86
A1027	A967	G907	A847	U785	G722	U682	U594	G531	A348	A348	G282	A219	A151	U87
G968	G968	G908	A848	A786	U723	G683	G595	A532	A349	A349	G283	G220	U152	A88
C969	C969	G909	C849	G787	U724	U664	C596	A533	C350	A350	A284	A221	U153	A89
A970	A970	G910	U850	C788	G725	A665	U534	U534	A351	A351	A285	A222	U154	C90
G971	G971	C911	C851	A789	G726	A666	U601	G535	A352	A352	U286	U223	G155	G91
U1033	A972	G912	U852	U790	G727	C687	U536	U536	G414	G414	G287	G219	G156	G92
U1034	A973	A913	G853	A791	G728	G688	G604	A537	A416	U854	G288	G226	A157	C93
G974	G974	A914	G854	G792	C729	U689	U605	G538	A417	A355	A289	G94	G158	C94
C975	C975	A915	U855	C793	C670	C606	G606	U539	A418	C356	G290	U228	U159	A95
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A1040	C977	A917	G857	G795	C732	A672	A608	U542	G420	G358	U292	U230	G162	U97
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C1063	C1000	G940	G880	C757	C695	G695	G635	G567	U381	A374	A255	A255	U190	A121
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G1066	A1003	U943	A883	U821	U698	U698	C638	A570	U384	A384	A323	G258	C193	
	U1004	C944	A884	G822	A699	A699	G639	U571	U	A385	A324	C259	U194	U126
	G1005	C945	U885	C823	C700	U640	A572	A572	U	A386	A325	C260	U195	G127
	A1006	U946	C886	G764	G701	C641	C573	G510	U	A387	A326	G196	G128	A129
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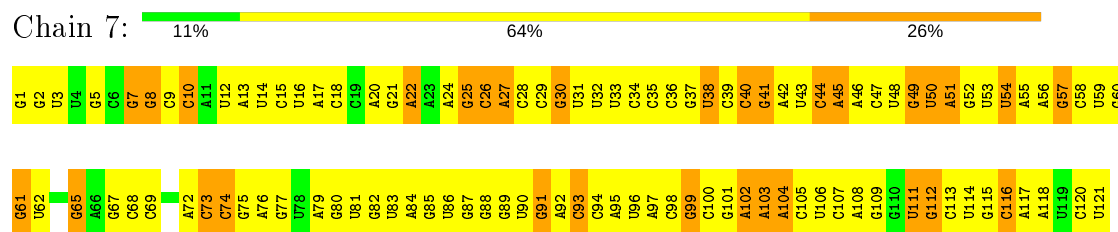
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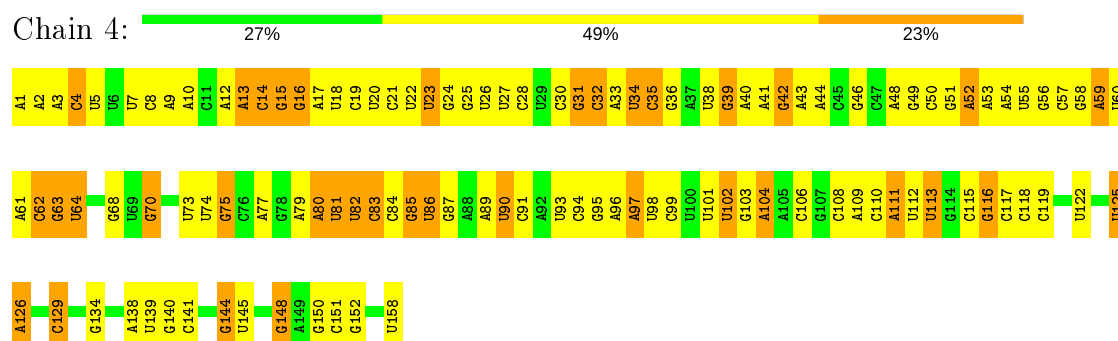
• Molecule 37: 5S ribosomal RNA



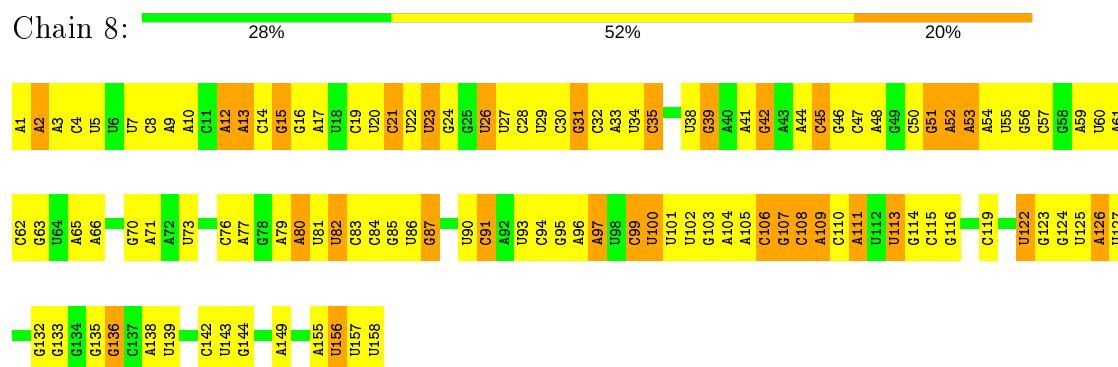
• Molecule 37: 5S ribosomal RNA



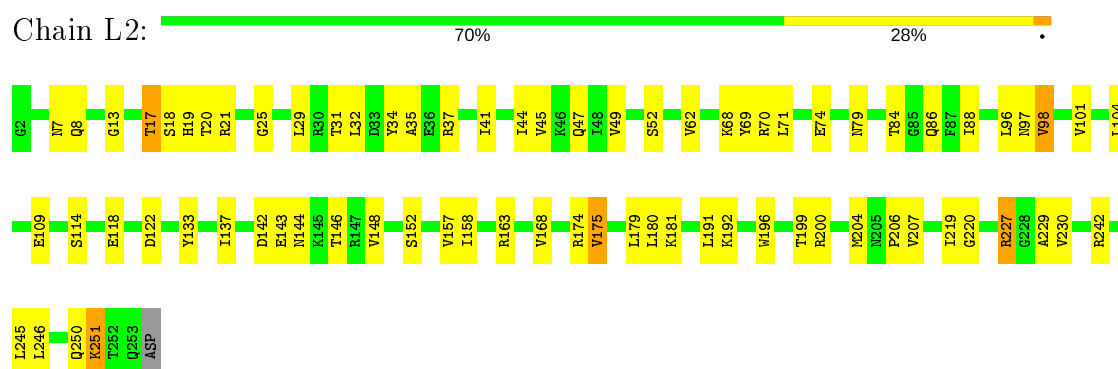
• Molecule 38: 5.8S ribosomal RNA



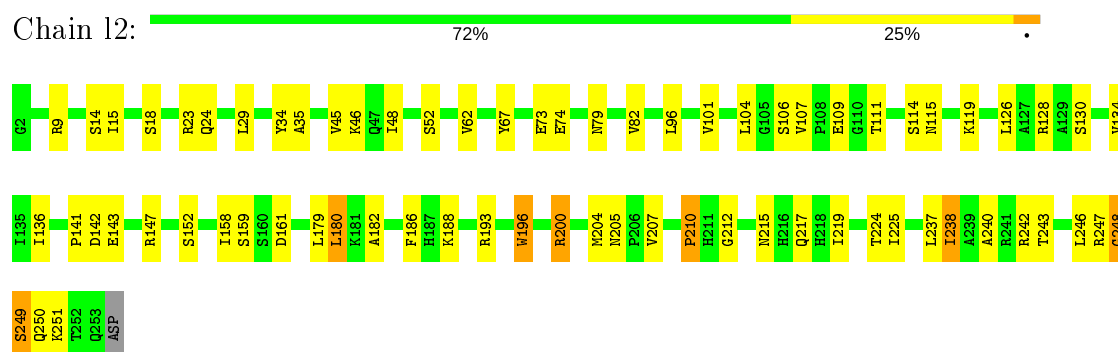
- Molecule 38: 5.8S ribosomal RNA



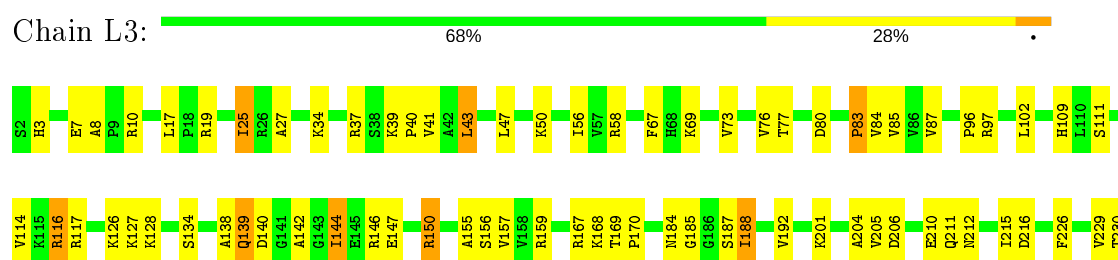
- Molecule 39: 60S ribosomal protein L2-A



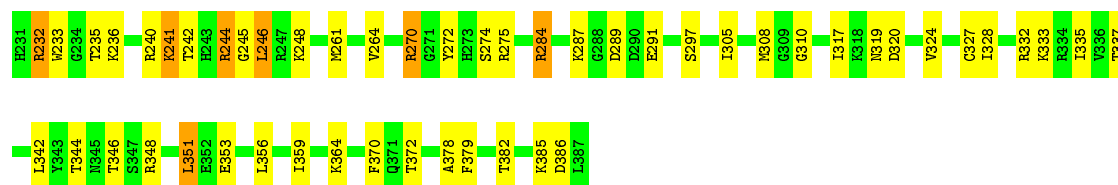
- Molecule 39: 60S ribosomal protein L2-A



- Molecule 40: 60S ribosomal protein L3

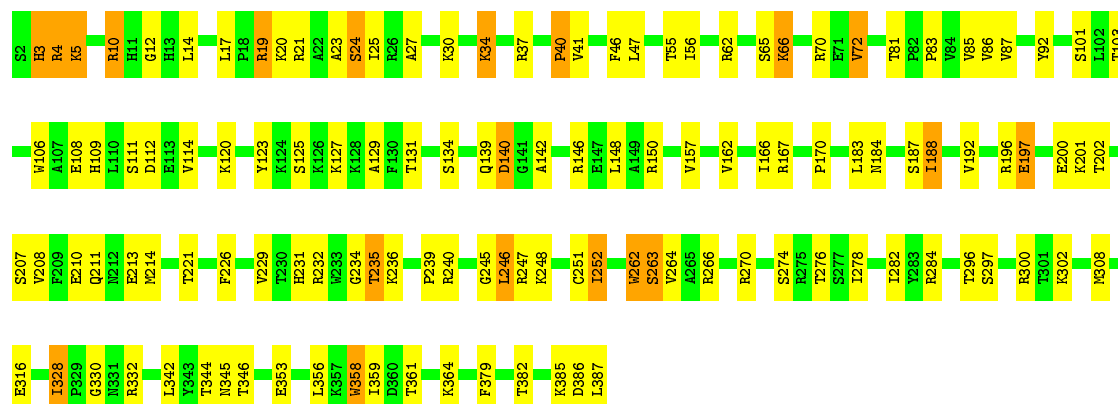






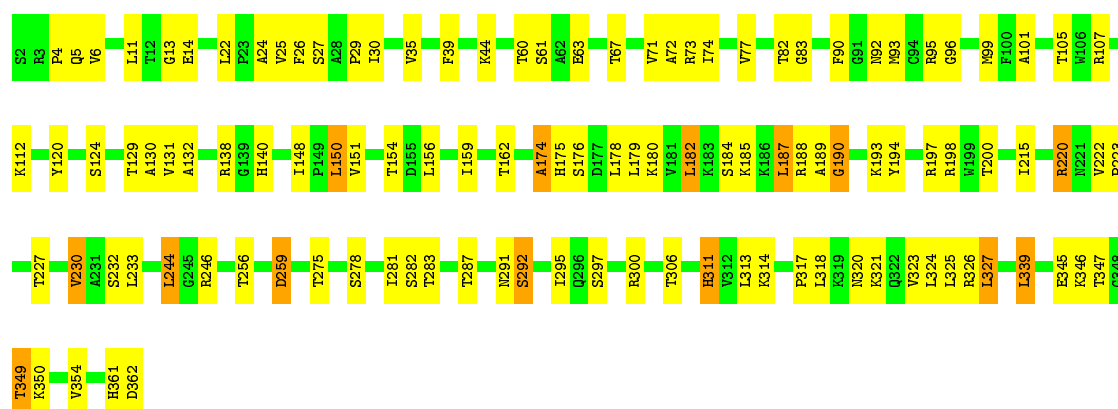
• Molecule 40: 60S ribosomal protein L3

Chain 13: 67% 27% 5%



• Molecule 41: 60S ribosomal protein L4-A

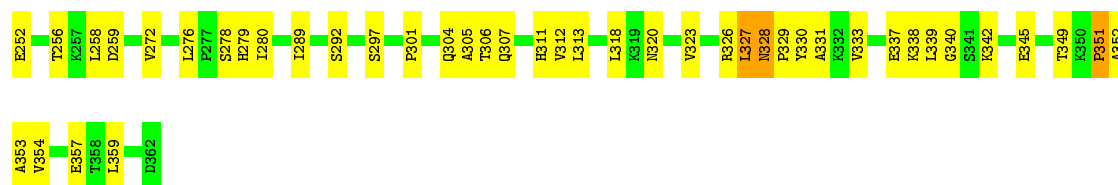
Chain L4: 68% 28% 4%



• Molecule 41: 60S ribosomal protein L4-A

Chain 14: 68% 29% 3%

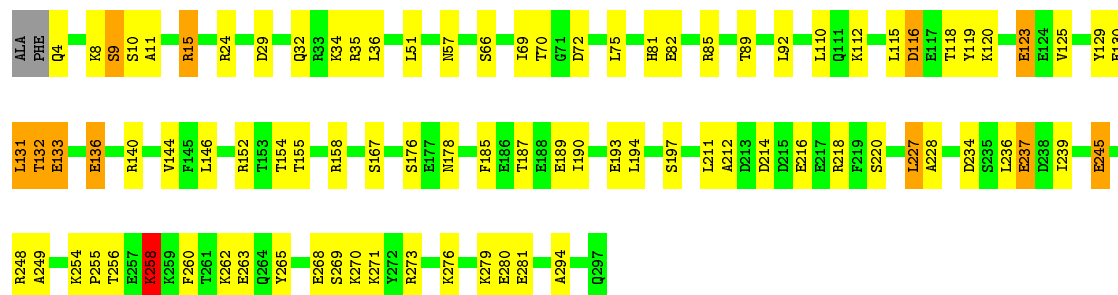




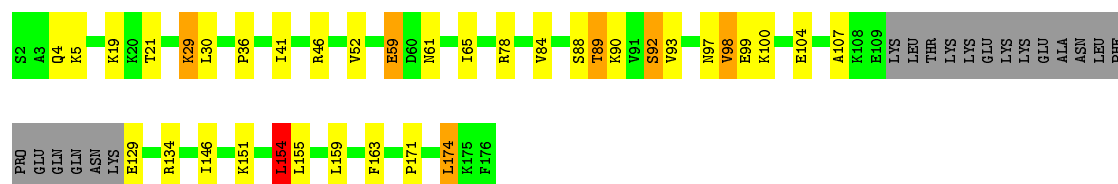
• Molecule 42: 60S ribosomal protein L5



• Molecule 42: 60S ribosomal protein L5

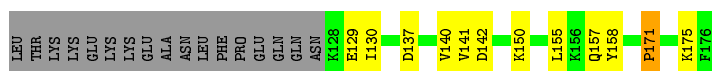


• Molecule 43: 60S ribosomal protein L6-A



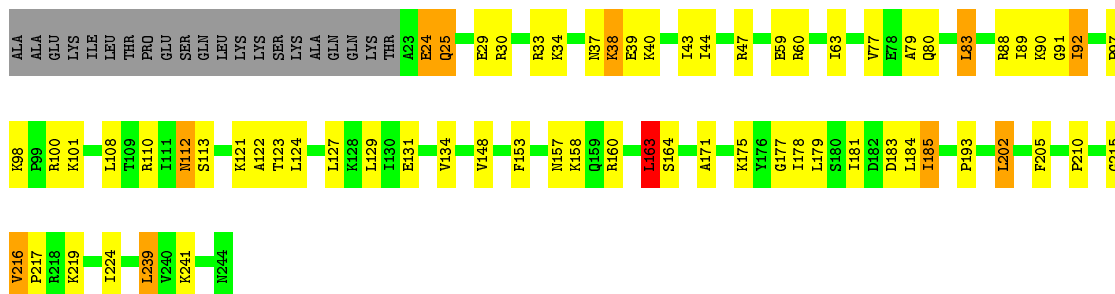
• Molecule 43: 60S ribosomal protein L6-A





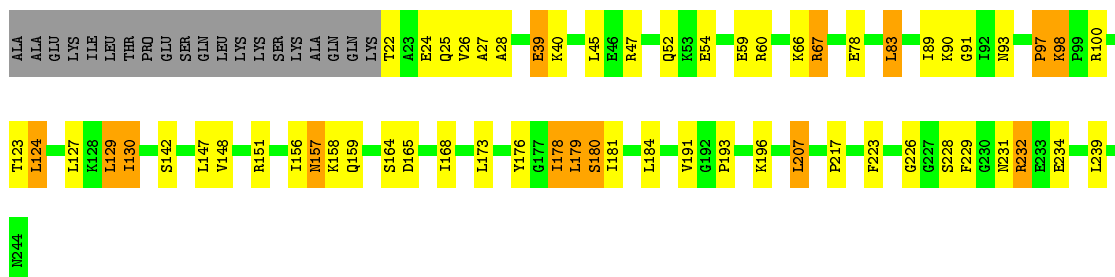
- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 63% 23% 9%



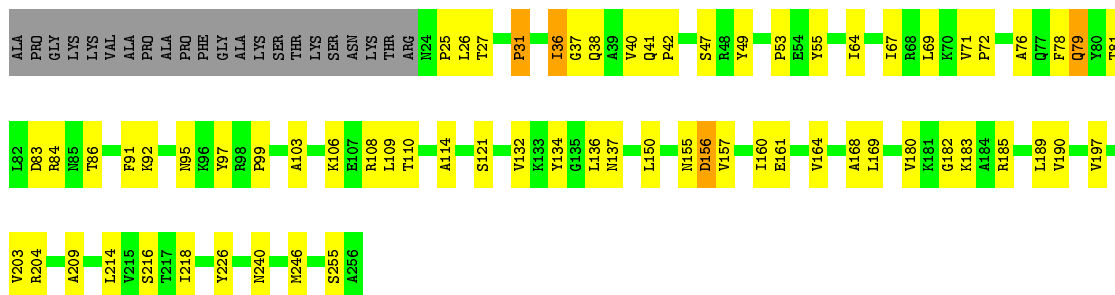
- Molecule 44: 60S ribosomal protein L7-A

Chain 17: 67% 19% 6% 8%



- Molecule 45: 60S ribosomal protein L8-A

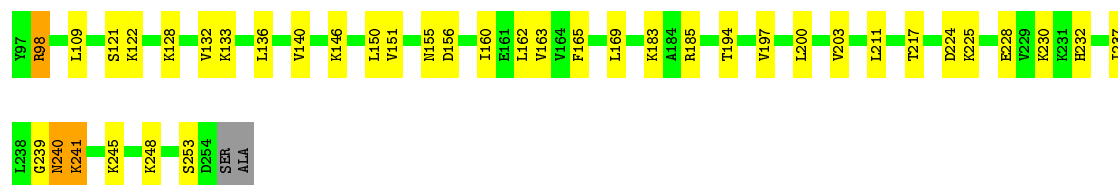
Chain L8: 65% 25% 9%



- Molecule 45: 60S ribosomal protein L8-A

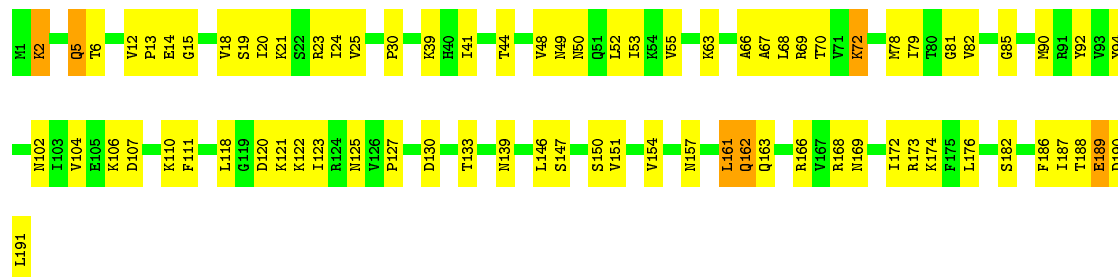
Chain 18: 67% 21% 9%





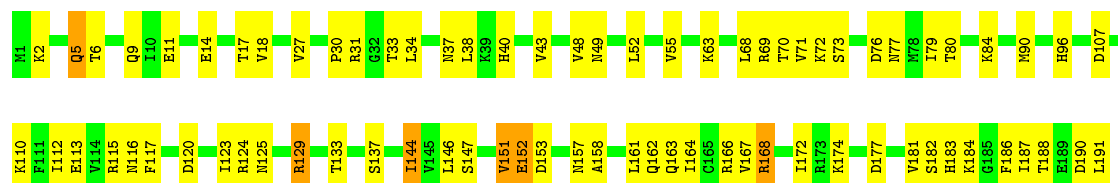
- Molecule 46: 60S ribosomal protein L9-A

Chain L9: 59% 38%



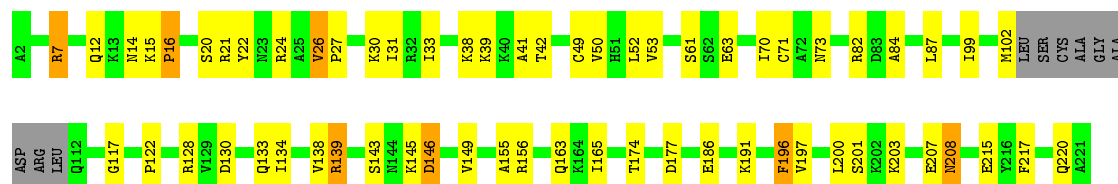
- Molecule 46: 60S ribosomal protein L9-A

Chain l9: 60% 37%



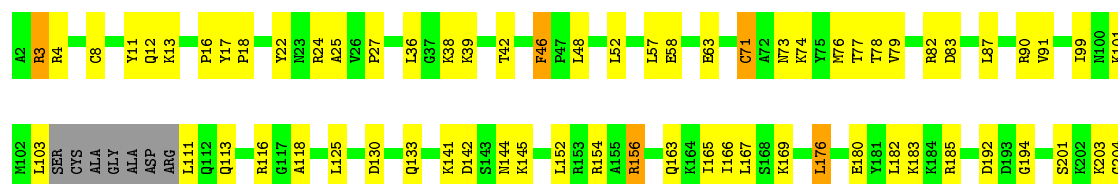
- Molecule 47: 60S ribosomal protein L10

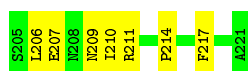
Chain M0: 68% 25%



- Molecule 47: 60S ribosomal protein L10

Chain m0: 63% 31%





- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 66% 27% . . .



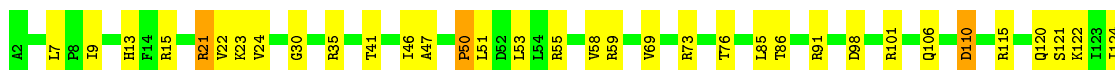
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 57% 32% 8% .



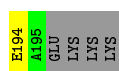
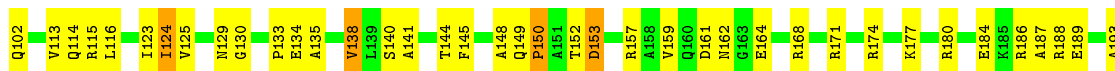
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 71% 24% . .



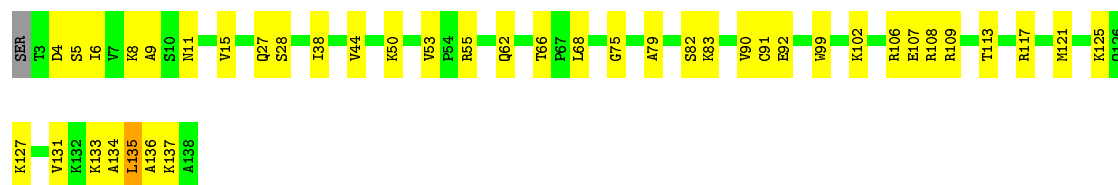
- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 59% 37% . .

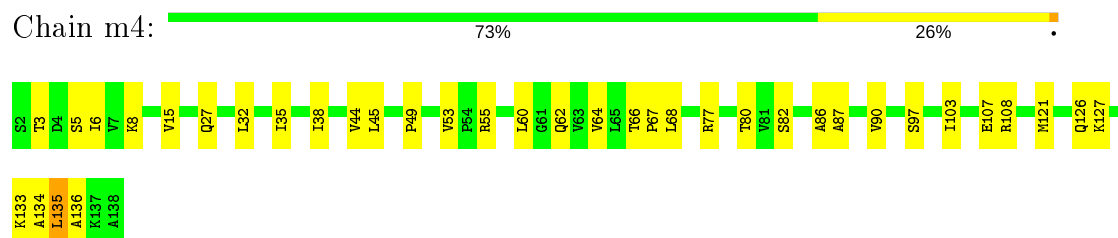


- Molecule 50: 60S ribosomal protein L14-A

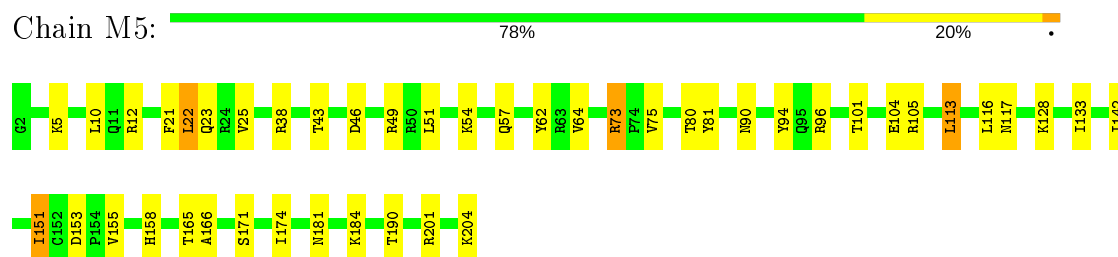
Chain M4: 69% 29% . .



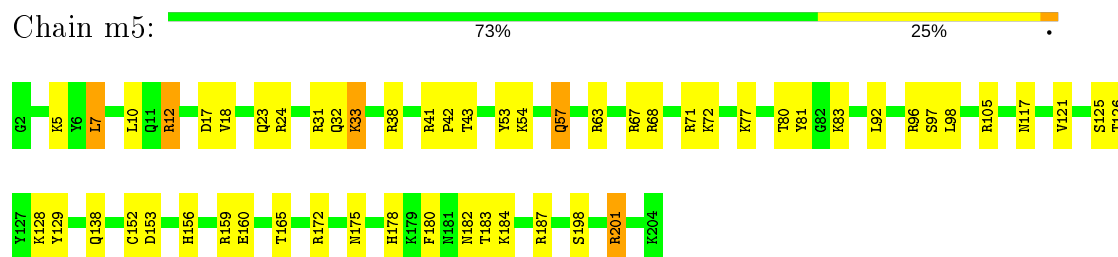
- Molecule 50: 60S ribosomal protein L14-A



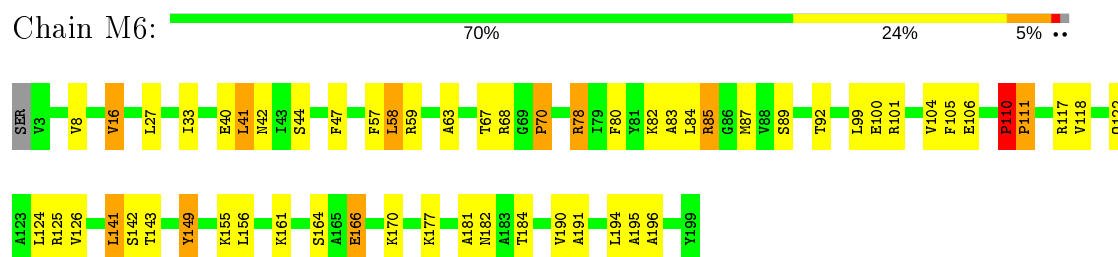
- Molecule 51: 60S ribosomal protein L15-A



- Molecule 51: 60S ribosomal protein L15-A

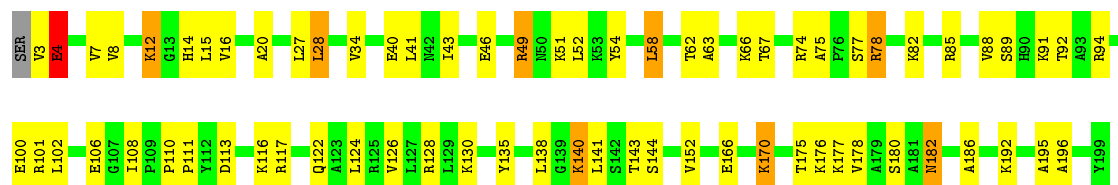


- Molecule 52: 60S ribosomal protein L16-A



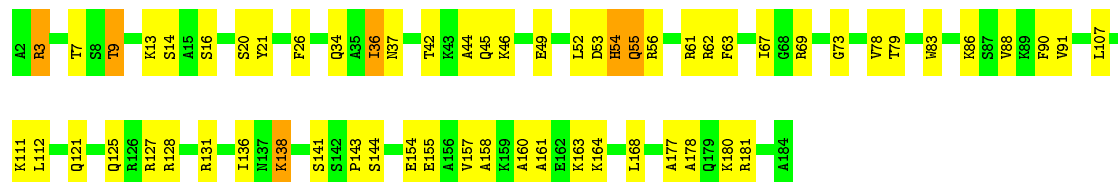
- Molecule 52: 60S ribosomal protein L16-A





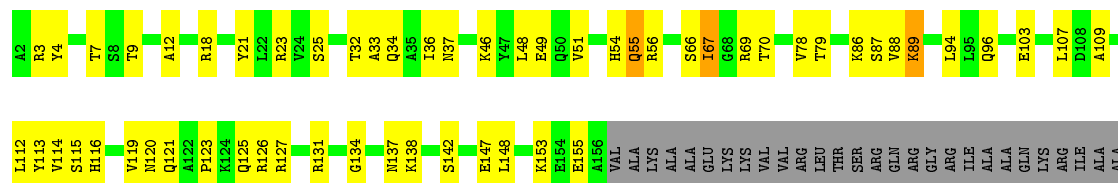
• Molecule 53: 60S ribosomal protein L17-A

Chain M7: 67% 30%



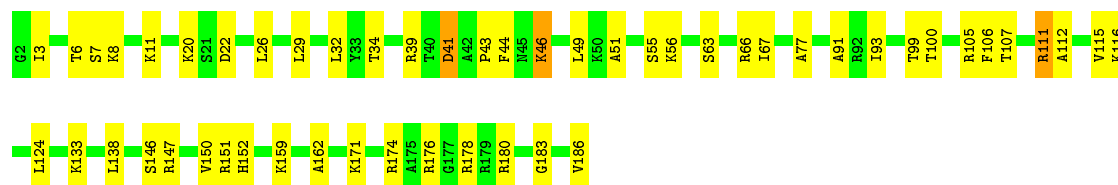
• Molecule 53: 60S ribosomal protein L17-A

Chain m7: 54% 30% 15%



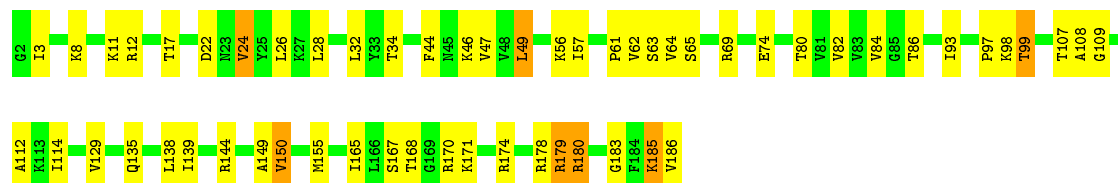
• Molecule 54: 60S ribosomal protein L18-A

Chain M8: 72% 26%



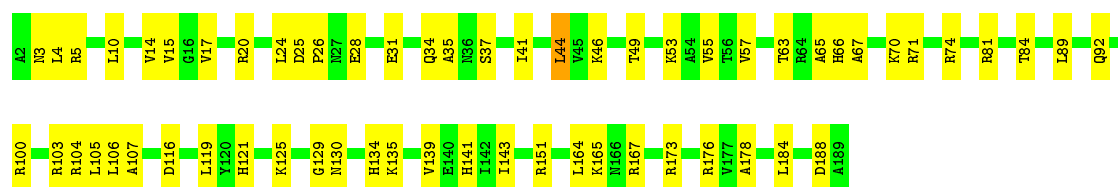
• Molecule 54: 60S ribosomal protein L18-A

Chain m8: 69% 27%

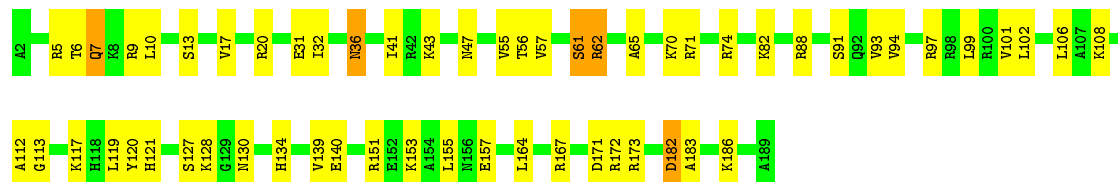


• Molecule 55: 60S ribosomal protein L19-A

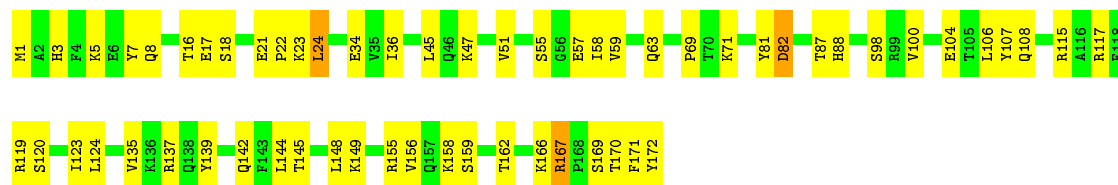
Chain M9: 68% 31%



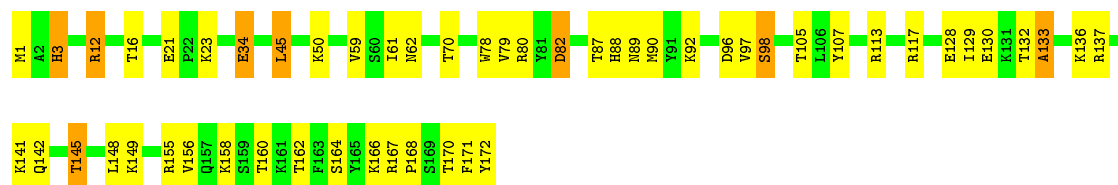
• Molecule 55: 60S ribosomal protein L19-A



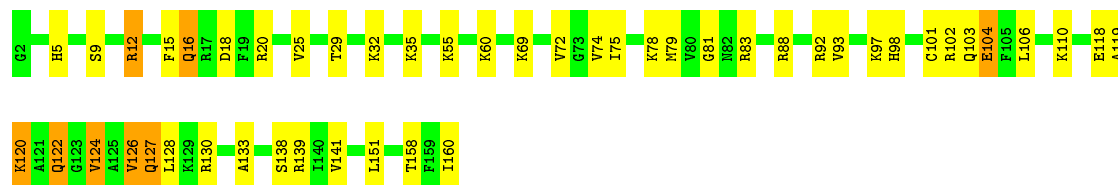
• Molecule 56: 60S ribosomal protein L20-A



• Molecule 56: 60S ribosomal protein L20-A



• Molecule 57: 60S ribosomal protein L21-A



• Molecule 57: 60S ribosomal protein L21-A

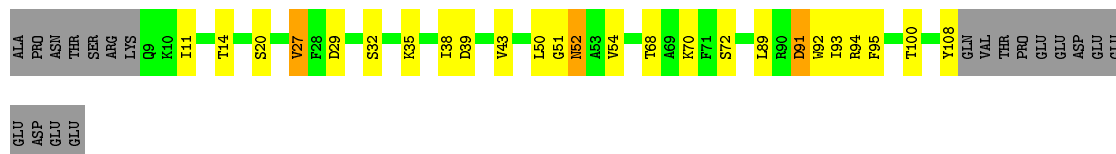






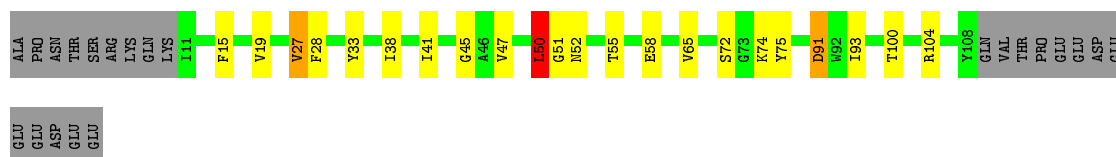
- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 63% 18% 17%



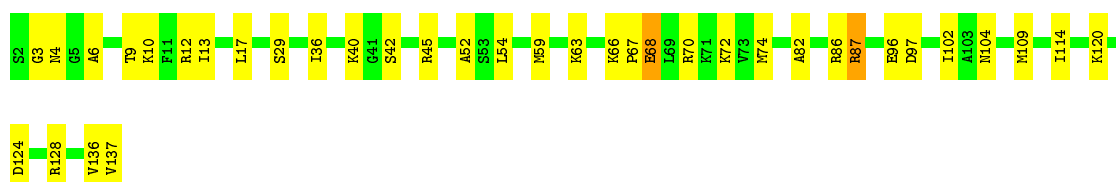
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 63% 16% 18%



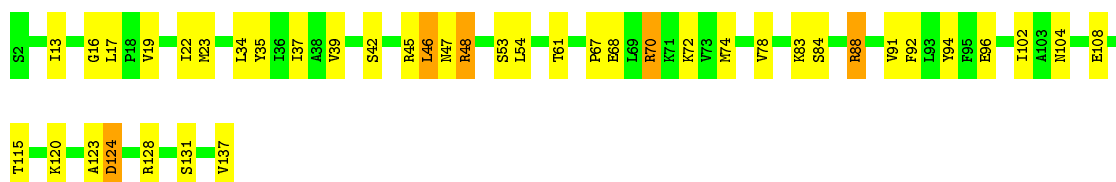
- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 73% 26%



- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 70% 26%

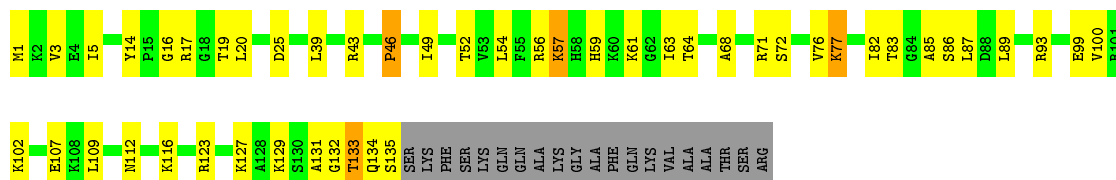


- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 46% 15% 37%

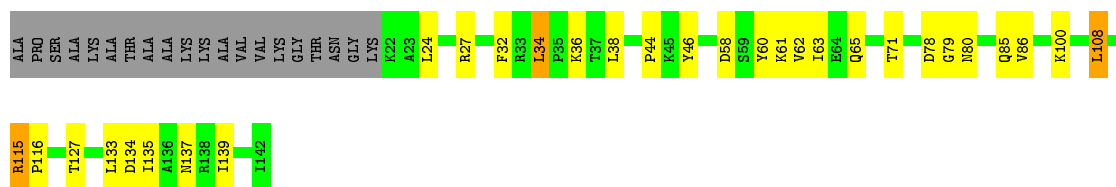
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:  56% 28% • 13%



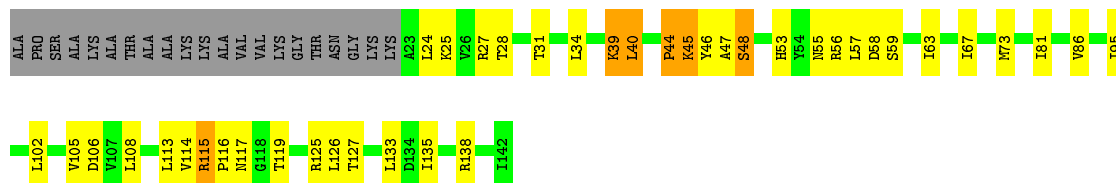
- Molecule 61: 60S ribosomal protein L25

Chain N5:  65% 19% • 14%



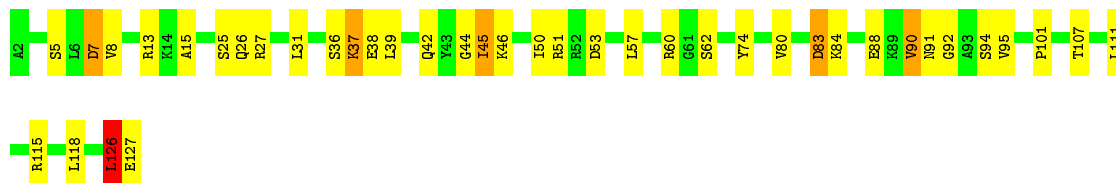
- Molecule 61: 60S ribosomal protein L25

Chain n5:  56% 25% • 15%



- Molecule 62: 60S ribosomal protein L26-A

Chain N6:  68% 27% 5%



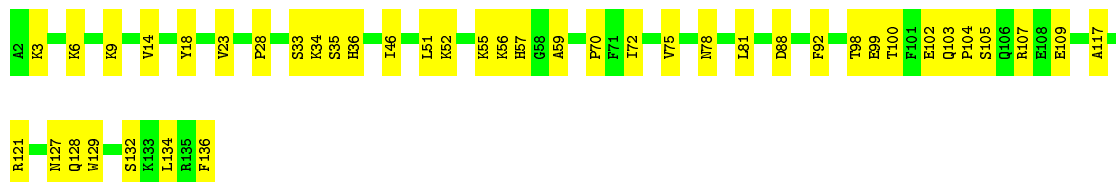
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:  62% 33% 5%



- Molecule 63: 60S ribosomal protein L27-A

Chain N7:   69% 31%



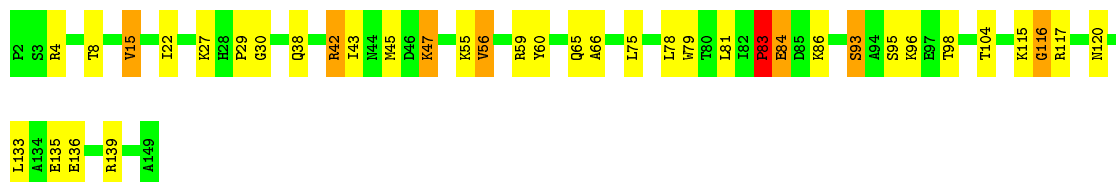
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:   76% 23%



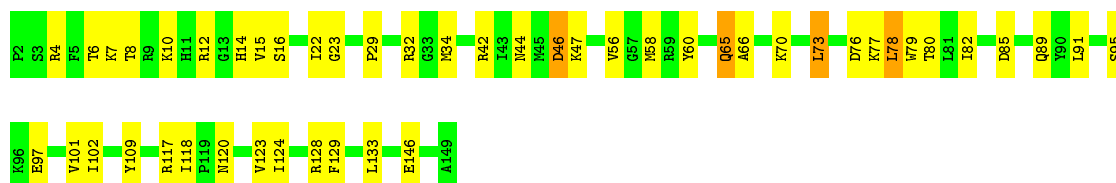
- Molecule 64: 60S ribosomal protein L28

Chain N8:    74% 20% 5%



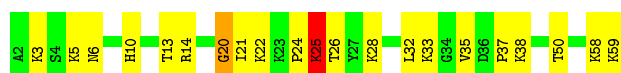
- Molecule 64: 60S ribosomal protein L28

Chain n8:    68% 30%



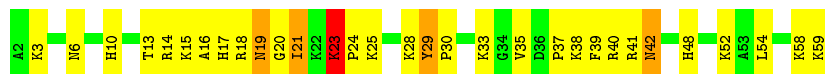
- Molecule 65: 60S ribosomal protein L29

Chain N9:    64% 33%



- Molecule 65: 60S ribosomal protein L29

Chain n9:  47% 45% 7% •



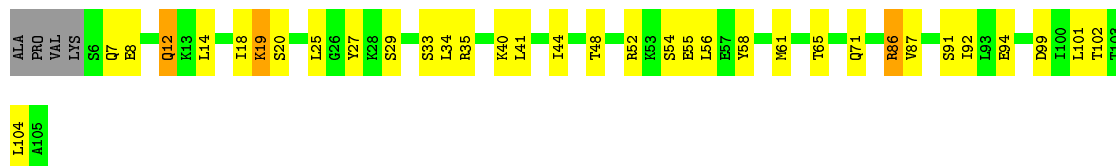
- Molecule 66: 60S ribosomal protein L30

Chain O0:  73% 19% • 7%



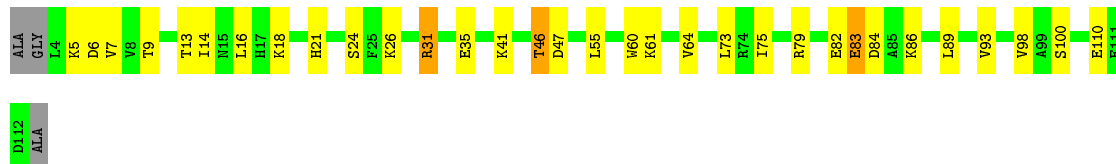
- Molecule 66: 60S ribosomal protein L30

Chain o0:  63% 30% • •



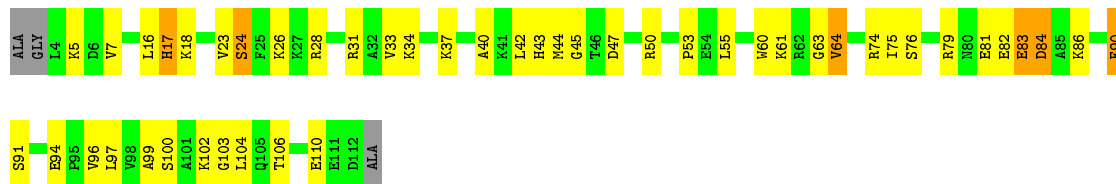
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  69% 26% • •



- Molecule 67: 60S ribosomal protein L31-A

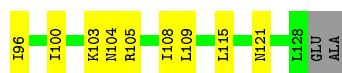
Chain o1:  55% 37% 5% •



- Molecule 68: 60S ribosomal protein L32

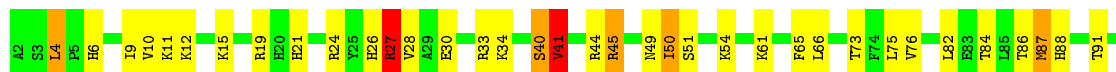
Chain O2:  63% 33% • • •





- Molecule 68: 60S ribosomal protein L32

Chain o2: 67% 25% 5% ..



- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 74% 23% ..



- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 65% 30% 5% ..



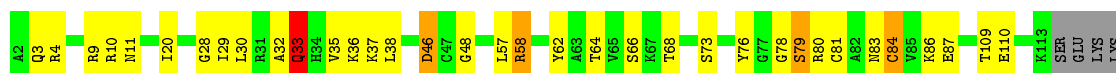
- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 61% 27% 6% 6% ..

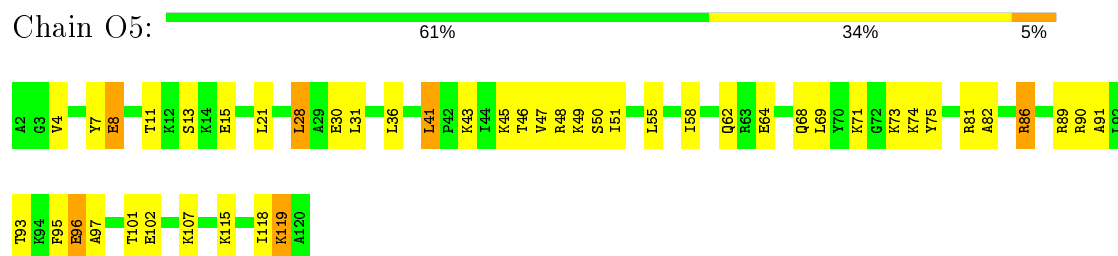


- Molecule 70: 60S ribosomal protein L34-A

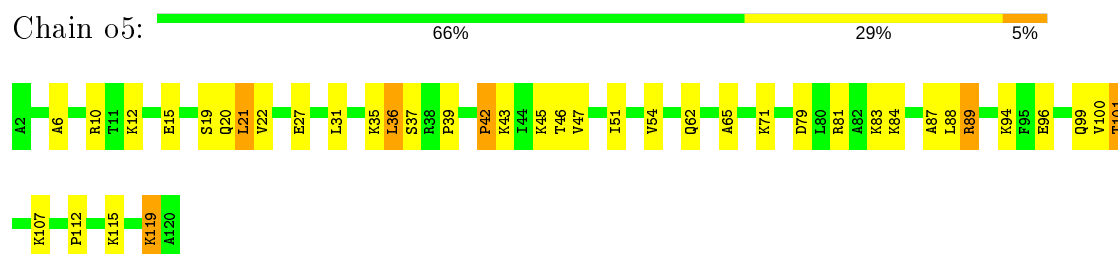
Chain o4: 65% 25% .. 6%



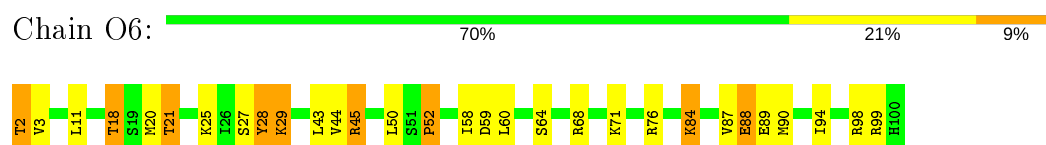
- Molecule 71: 60S ribosomal protein L35-A



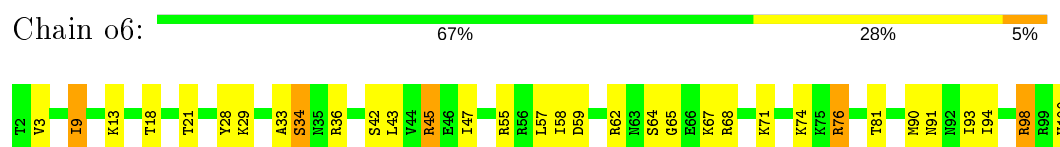
- Molecule 71: 60S ribosomal protein L35-A



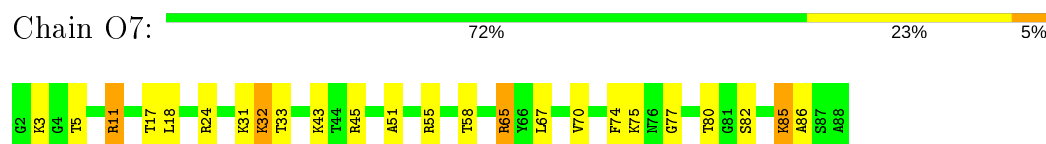
- Molecule 72: 60S ribosomal protein L36-A



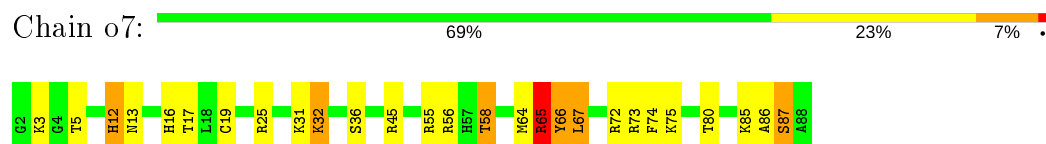
- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A

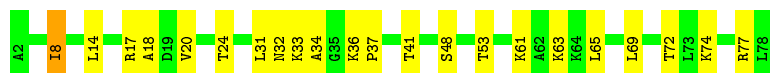


- Molecule 73: 60S ribosomal protein L37-A




- Molecule 74: 60S ribosomal protein L38

Chain O8:  71% 27%



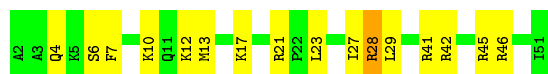
- Molecule 74: 60S ribosomal protein L38

Chain o8:  77% 22%



- Molecule 75: 60S ribosomal protein L39

Chain O9:  68% 30%



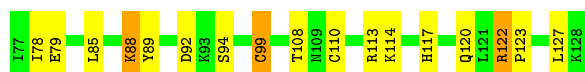
- Molecule 75: 60S ribosomal protein L39

Chain o9:  70% 30%



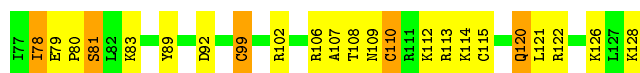
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  67% 27% 6%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  56% 35% 10%



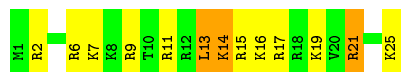
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  52% 48%



- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  48% 40% 12%



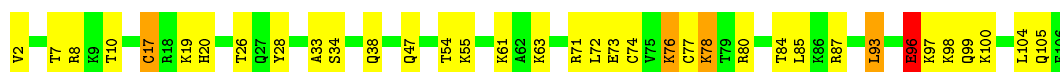
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  69% 29% .



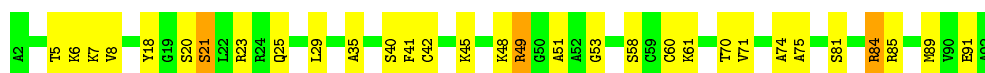
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  66% 30% . .



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  66% 31% .



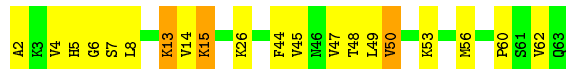
- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  70% 24% 5%



- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  68% 27% 5%



- Molecule 81: Ubiquitin-40S ribosomal protein S31

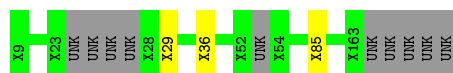
Chain e1:  46% 47% 7%




- Molecule 82: unknown protein chain m2

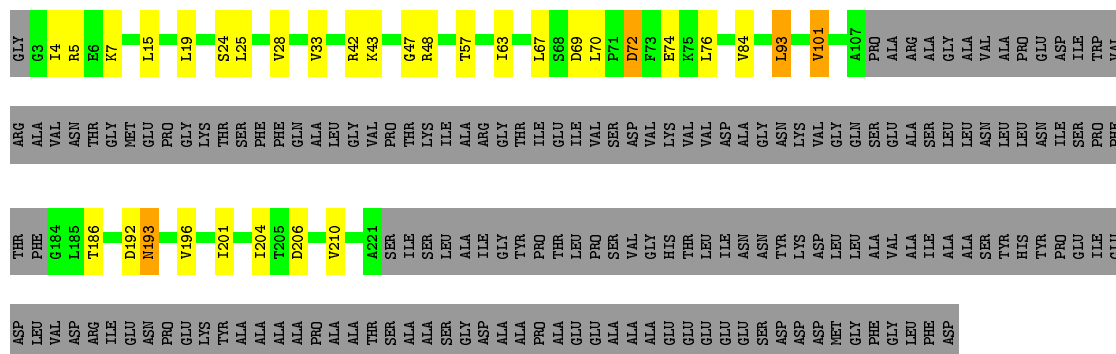


Chain m2:  92% 6%



- Molecule 83: 60S acidic ribosomal protein P0

Chain p0:  36% 9% 54%



- Molecule 84: unknown protein chain p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 85: unknown protein chain 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, $\alpha$ , $\beta$ , $\gamma$	437.00Å 286.75Å 305.18Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	135.58 – 3.60	Depositor
% Data completeness (in resolution range)	100.0 (135.58-3.60)	Depositor
$R_{merge}$	0.52	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.190 , 0.267	Depositor
Wilson B-factor (Å <sup>2</sup> )	115.6	Xtriage
Anisotropy	0.083	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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, GET

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	1.08	91/41698 (0.2%)	1.83	1528/64972 (2.4%)
1	6	1.44	367/42663 (0.9%)	2.19	2982/66472 (4.5%)
2	S0	0.60	0/1617	0.83	0/2215
2	s0	0.75	0/1623	0.92	1/2222 (0.0%)
3	S1	0.46	0/1735	0.74	0/2335
3	s1	0.67	0/1748	0.87	3/2352 (0.1%)
4	S2	0.74	2/1665 (0.1%)	0.90	2/2263 (0.1%)
4	s2	0.87	1/1665 (0.1%)	1.01	4/2263 (0.2%)
5	S3	0.72	0/1759	0.86	1/2368 (0.0%)
5	s3	0.72	0/1759	0.89	1/2368 (0.0%)
6	S4	0.65	0/2109	0.86	2/2839 (0.1%)
6	s4	0.77	0/2109	0.90	1/2839 (0.0%)
7	S5	0.54	0/1629	0.76	0/2202
7	s5	0.89	1/1629 (0.1%)	1.02	4/2202 (0.2%)
8	S6	0.64	0/1823	0.79	0/2439
8	s6	0.88	0/1779	0.99	2/2379 (0.1%)
9	S7	0.54	0/1506	0.75	0/2028
9	s7	0.68	0/1516	0.91	2/2043 (0.1%)
10	S8	0.79	0/1514	0.92	1/2021 (0.0%)
10	s8	0.86	0/1514	0.94	1/2021 (0.0%)
11	S9	0.65	0/1519	0.84	1/2035 (0.0%)
11	s9	0.79	0/1519	0.91	2/2035 (0.1%)
12	C0	0.66	0/790	0.86	2/1069 (0.2%)
12	c0	0.56	0/777	0.87	2/1049 (0.2%)
13	C1	0.82	0/1240	0.88	0/1675
13	c1	0.91	0/1194	1.00	2/1610 (0.1%)
14	C2	0.51	0/900	0.80	1/1224 (0.1%)
14	c2	0.46	0/900	0.69	1/1224 (0.1%)
15	C3	0.59	0/1215	0.76	0/1638
15	c3	0.80	0/1215	0.96	2/1638 (0.1%)
16	C4	0.50	0/901	0.79	0/1217
16	c4	0.76	0/960	0.91	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.69	0/998	0.81	0/1341
17	c5	0.89	0/1060	1.05	3/1426 (0.2%)
18	C6	0.60	0/1125	0.89	3/1510 (0.2%)
18	c6	0.93	0/1131	1.06	2/1518 (0.1%)
19	C7	0.59	0/935	0.87	3/1254 (0.2%)
19	c7	0.80	0/914	0.91	1/1224 (0.1%)
20	C8	0.61	0/1211	0.82	0/1628
20	c8	0.92	2/1211 (0.2%)	1.08	5/1628 (0.3%)
21	C9	0.61	0/1130	0.83	0/1517
21	c9	0.94	1/1130 (0.1%)	1.01	2/1517 (0.1%)
22	D0	0.65	0/865	0.83	0/1169
22	d0	0.79	0/892	0.97	1/1205 (0.1%)
23	D1	0.65	0/693	0.88	2/935 (0.2%)
23	d1	0.79	0/693	0.92	0/935
24	D2	0.63	0/1038	0.89	1/1395 (0.1%)
24	d2	0.88	0/1038	0.98	1/1395 (0.1%)
25	D3	0.90	1/1139 (0.1%)	1.04	1/1518 (0.1%)
25	d3	1.17	5/1139 (0.4%)	1.14	4/1518 (0.3%)
26	D4	0.66	0/1087	0.80	0/1449
26	d4	0.77	0/1087	0.92	0/1449
27	D5	0.61	0/571	0.84	0/768
27	d5	0.81	0/566	0.96	0/761
28	D6	0.66	0/782	0.84	0/1047
28	d6	0.81	0/782	0.92	1/1047 (0.1%)
29	D7	0.53	0/620	0.81	1/838 (0.1%)
29	d7	0.67	0/620	0.93	2/838 (0.2%)
30	D8	0.49	0/499	0.74	0/670
30	d8	0.76	0/499	0.97	1/670 (0.1%)
31	D9	0.75	0/452	0.86	0/600
31	d9	0.97	0/452	0.97	0/600
32	E0	0.69	0/483	0.87	0/643
33	E1	0.65	0/577	0.90	0/770
34	SR	0.54	0/2494	0.72	0/3393
34	sR	0.69	0/2495	0.85	2/3395 (0.1%)
35	SM	0.72	0/1113	0.91	2/1502 (0.1%)
35	sM	0.77	0/682	0.98	1/921 (0.1%)
36	1	1.76	1434/75394 (1.9%)	2.53	7929/117545 (6.7%)
36	5	1.87	1867/75414 (2.5%)	2.61	8463/117575 (7.2%)
37	3	1.50	28/2883 (1.0%)	2.28	214/4491 (4.8%)
37	7	2.04	91/2883 (3.2%)	2.85	410/4491 (9.1%)
38	4	1.54	29/3746 (0.8%)	2.42	331/5832 (5.7%)
38	8	1.43	34/3746 (0.9%)	2.16	250/5832 (4.3%)
39	L2	0.98	1/1948 (0.1%)	1.08	2/2617 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	l2	0.96	1/1946 (0.1%)	1.03	4/2614 (0.2%)
40	L3	1.12	3/3146 (0.1%)	1.12	11/4228 (0.3%)
40	l3	1.32	9/3146 (0.3%)	1.24	17/4228 (0.4%)
41	L4	1.03	0/2800	1.15	13/3790 (0.3%)
41	l4	1.02	1/2800 (0.0%)	1.11	5/3790 (0.1%)
42	L5	0.84	1/2425 (0.0%)	0.97	2/3271 (0.1%)
42	l5	1.16	2/2408 (0.1%)	1.08	3/3248 (0.1%)
43	L6	1.15	2/1260 (0.2%)	1.17	4/1694 (0.2%)
43	l6	1.18	2/1269 (0.2%)	1.15	3/1705 (0.2%)
44	L7	1.09	0/1821	1.13	9/2451 (0.4%)
44	l7	1.26	3/1828 (0.2%)	1.17	7/2461 (0.3%)
45	L8	0.74	0/1836	0.91	0/2481
45	l8	0.72	0/1795	0.86	1/2429 (0.0%)
46	L9	0.97	0/1539	1.07	1/2073 (0.0%)
46	l9	1.33	4/1539 (0.3%)	1.23	8/2073 (0.4%)
47	M0	1.02	4/1741 (0.2%)	1.04	1/2335 (0.0%)
47	m0	1.23	5/1758 (0.3%)	1.20	7/2358 (0.3%)
48	M1	0.80	1/1374 (0.1%)	0.93	3/1842 (0.2%)
48	m1	1.09	3/1374 (0.2%)	1.09	5/1842 (0.3%)
49	M3	0.96	2/1568 (0.1%)	1.09	4/2106 (0.2%)
49	m3	0.87	0/1573	1.02	0/2113
50	M4	1.10	0/1068	1.13	1/1438 (0.1%)
50	m4	1.30	1/1074 (0.1%)	1.15	3/1446 (0.2%)
51	M5	0.97	0/1757	1.04	5/2354 (0.2%)
51	m5	0.84	0/1757	0.93	2/2354 (0.1%)
52	M6	1.25	6/1585 (0.4%)	1.28	12/2128 (0.6%)
52	m6	1.54	9/1585 (0.6%)	1.38	14/2128 (0.7%)
53	M7	1.21	3/1443 (0.2%)	1.09	3/1944 (0.2%)
53	m7	1.18	1/1250 (0.1%)	1.19	2/1683 (0.1%)
54	M8	1.03	0/1465	1.12	5/1965 (0.3%)
54	m8	0.98	1/1465 (0.1%)	1.06	3/1965 (0.2%)
55	M9	0.84	0/1538	0.92	3/2050 (0.1%)
55	m9	0.88	1/1538 (0.1%)	0.92	2/2050 (0.1%)
56	N0	1.05	0/1481	1.10	5/1990 (0.3%)
56	n0	1.46	7/1481 (0.5%)	1.21	5/1990 (0.3%)
57	N1	1.09	1/1300 (0.1%)	1.10	4/1743 (0.2%)
57	n1	1.28	6/1300 (0.5%)	1.17	5/1743 (0.3%)
58	N2	0.73	1/812 (0.1%)	0.89	1/1099 (0.1%)
58	n2	0.73	0/794	0.84	1/1076 (0.1%)
59	N3	1.09	2/1018 (0.2%)	1.07	3/1369 (0.2%)
59	n3	1.35	7/1018 (0.7%)	1.28	7/1369 (0.5%)
60	N4	0.90	0/712	0.98	1/958 (0.1%)
60	n4	1.04	0/1052	1.04	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	N5	0.86	1/979 (0.1%)	1.00	4/1321 (0.3%)
61	n5	0.85	0/974	1.03	2/1314 (0.2%)
62	N6	0.92	0/1004	1.11	6/1341 (0.4%)
62	n6	0.89	0/1004	1.02	5/1341 (0.4%)
63	N7	0.68	0/1118	0.89	1/1497 (0.1%)
63	n7	0.67	0/1118	0.83	0/1497
64	N8	1.05	0/1204	1.10	5/1612 (0.3%)
64	n8	0.98	1/1204 (0.1%)	1.08	2/1612 (0.1%)
65	N9	0.98	0/473	1.07	1/629 (0.2%)
65	n9	1.12	1/473 (0.2%)	1.33	3/629 (0.5%)
66	O0	0.71	0/751	0.87	0/1008
66	o0	0.69	0/775	0.88	2/1040 (0.2%)
67	O1	0.90	0/890	1.00	1/1196 (0.1%)
67	o1	1.13	2/897 (0.2%)	1.20	3/1205 (0.2%)
68	O2	1.21	2/1041 (0.2%)	1.20	4/1394 (0.3%)
68	o2	1.15	2/1041 (0.2%)	1.13	5/1394 (0.4%)
69	O3	1.32	2/868 (0.2%)	1.23	3/1168 (0.3%)
69	o3	1.38	3/868 (0.3%)	1.19	2/1168 (0.2%)
70	O4	0.84	0/890	1.00	4/1189 (0.3%)
70	o4	0.83	1/890 (0.1%)	0.99	2/1189 (0.2%)
71	O5	0.98	2/978 (0.2%)	1.09	2/1301 (0.2%)
71	o5	0.82	0/974	0.89	1/1297 (0.1%)
72	O6	0.84	0/778	0.98	1/1034 (0.1%)
72	o6	0.79	0/777	0.98	1/1033 (0.1%)
73	O7	1.08	0/696	1.20	4/923 (0.4%)
73	o7	0.99	0/696	1.07	3/923 (0.3%)
74	O8	0.72	0/618	0.84	0/826
74	o8	0.66	0/614	0.90	0/822
75	O9	1.05	0/443	1.19	3/588 (0.5%)
75	o9	0.82	0/443	0.99	0/588
76	Q0	1.04	2/423 (0.5%)	1.14	1/562 (0.2%)
76	q0	1.58	3/423 (0.7%)	1.44	5/562 (0.9%)
77	Q1	0.76	0/234	1.11	2/300 (0.7%)
77	q1	1.03	0/234	1.30	3/300 (1.0%)
78	Q2	1.12	1/860 (0.1%)	1.07	2/1136 (0.2%)
78	q2	1.13	2/860 (0.2%)	1.09	2/1136 (0.2%)
79	Q3	1.04	0/701	1.10	3/934 (0.3%)
79	q3	1.07	1/701 (0.1%)	1.05	0/934
80	e0	0.81	0/499	0.95	0/665
81	e1	0.51	0/619	0.87	0/822
83	p0	0.75	0/1091	0.85	0/1472
All	All	1.39	4070/429970 (0.9%)	1.97	22469/631198 (3.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S0	0	2
2	s0	0	2
3	s1	0	3
5	S3	0	2
5	s3	0	2
6	s4	0	2
7	s5	0	3
9	s7	0	1
11	S9	0	2
11	s9	0	1
12	C0	0	2
15	c3	0	1
16	C4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	3
19	C7	0	1
19	c7	0	2
20	c8	0	1
21	c9	0	1
22	d0	0	1
23	D1	0	1
24	D2	0	1
24	d2	0	2
25	D3	0	2
26	D4	0	1
26	d4	0	2
27	D5	0	1
27	d5	0	1
28	D6	0	1
28	d6	0	1
33	E1	0	2
35	SM	0	1
39	l2	0	2
40	L3	0	3
40	l3	0	5
41	L4	0	5
41	l4	0	2
42	L5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	l5	0	3
43	L6	0	2
43	l6	0	1
44	L7	0	2
44	l7	0	3
45	l8	0	1
47	M0	0	2
47	m0	0	1
48	m1	0	1
49	m3	0	2
52	M6	0	2
52	m6	0	2
53	M7	0	1
53	m7	0	2
54	m8	0	1
56	n0	0	2
57	N1	0	1
57	n1	0	1
60	n4	0	1
61	n5	0	1
63	N7	0	2
64	N8	0	4
64	n8	0	2
65	N9	0	2
65	n9	0	1
67	o1	0	1
68	o2	0	2
69	O3	0	2
70	O4	0	2
70	o4	0	2
72	O6	0	1
76	q0	0	1
80	e0	0	2
81	e1	0	1
82	m2	0	3
83	p0	0	1
All	All	0	130

The worst 5 of 4070 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	15.17	2.08	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	806	A	N9-C4	-14.79	1.28	1.37
37	7	89	G	C6-O6	14.62	1.37	1.24
36	5	2397	A	N9-C4	-14.38	1.29	1.37
36	5	2875	U	N1-C2	13.97	1.51	1.38

The worst 5 of 22469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-25.15	110.91	126.00
37	7	44	C	C6-N1-C2	24.27	130.01	120.30
36	5	648	C	N3-C4-C5	-23.62	112.45	121.90
36	5	884	A	N1-C6-N6	23.07	132.44	118.60
38	4	94	C	C6-N1-C2	22.99	129.50	120.30

There are no chirality outliers.

5 of 130 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S0	29	VAL	Peptide
2	S0	6	THR	Peptide
5	S3	144	ALA	Peptide
5	S3	42	THR	Peptide
11	S9	15	PRO	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%)	137 (67%)	42 (21%)	25 (12%)	0	5
2	s0	204/251 (81%)	139 (68%)	31 (15%)	34 (17%)	0	3
3	S1	212/254 (84%)	142 (67%)	42 (20%)	28 (13%)	0	4
3	s1	214/254 (84%)	155 (72%)	39 (18%)	20 (9%)	0	9
4	S2	215/253 (85%)	148 (69%)	47 (22%)	20 (9%)	0	9
4	s2	215/253 (85%)	156 (73%)	30 (14%)	29 (14%)	0	4
5	S3	221/239 (92%)	154 (70%)	48 (22%)	19 (9%)	1	10
5	s3	221/239 (92%)	147 (66%)	51 (23%)	23 (10%)	0	7
6	S4	258/260 (99%)	184 (71%)	44 (17%)	30 (12%)	0	6
6	s4	258/260 (99%)	175 (68%)	53 (20%)	30 (12%)	0	6
7	S5	204/224 (91%)	129 (63%)	46 (22%)	29 (14%)	0	4
7	s5	204/224 (91%)	124 (61%)	51 (25%)	29 (14%)	0	4
8	S6	224/236 (95%)	166 (74%)	37 (16%)	21 (9%)	0	8
8	s6	216/236 (92%)	165 (76%)	36 (17%)	15 (7%)	1	14
9	S7	182/189 (96%)	131 (72%)	35 (19%)	16 (9%)	1	9
9	s7	184/189 (97%)	126 (68%)	37 (20%)	21 (11%)	0	6
10	S8	184/200 (92%)	132 (72%)	32 (17%)	20 (11%)	0	6
10	s8	184/200 (92%)	144 (78%)	26 (14%)	14 (8%)	1	12
11	S9	183/196 (93%)	128 (70%)	36 (20%)	19 (10%)	0	7
11	s9	183/196 (93%)	122 (67%)	42 (23%)	19 (10%)	0	7
12	C0	94/105 (90%)	54 (57%)	21 (22%)	19 (20%)	0	1
12	c0	92/105 (88%)	56 (61%)	17 (18%)	19 (21%)	0	1
13	C1	153/155 (99%)	113 (74%)	22 (14%)	18 (12%)	0	5
13	c1	144/155 (93%)	108 (75%)	20 (14%)	16 (11%)	0	6
14	C2	122/142 (86%)	71 (58%)	22 (18%)	29 (24%)	0	0
14	c2	122/142 (86%)	65 (53%)	36 (30%)	21 (17%)	0	2
15	C3	148/150 (99%)	107 (72%)	29 (20%)	12 (8%)	1	11
15	c3	148/150 (99%)	95 (64%)	28 (19%)	25 (17%)	0	2
16	C4	125/136 (92%)	80 (64%)	25 (20%)	20 (16%)	0	3
16	c4	126/136 (93%)	90 (71%)	24 (19%)	12 (10%)	0	8
17	C5	122/141 (86%)	78 (64%)	26 (21%)	18 (15%)	0	3
17	c5	133/141 (94%)	75 (56%)	29 (22%)	29 (22%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	105 (76%)	22 (16%)	12 (9%)	1	10
18	c6	140/142 (99%)	97 (69%)	24 (17%)	19 (14%)	0	4
19	C7	116/136 (85%)	76 (66%)	22 (19%)	18 (16%)	0	3
19	c7	113/136 (83%)	73 (65%)	29 (26%)	11 (10%)	0	8
20	C8	143/145 (99%)	107 (75%)	27 (19%)	9 (6%)	1	17
20	c8	143/145 (99%)	98 (68%)	27 (19%)	18 (13%)	0	5
21	C9	141/143 (99%)	99 (70%)	31 (22%)	11 (8%)	1	11
21	c9	141/143 (99%)	98 (70%)	36 (26%)	7 (5%)	2	21
22	D0	105/120 (88%)	74 (70%)	22 (21%)	9 (9%)	1	10
22	d0	108/120 (90%)	75 (69%)	15 (14%)	18 (17%)	0	3
23	D1	85/87 (98%)	53 (62%)	18 (21%)	14 (16%)	0	3
23	d1	85/87 (98%)	64 (75%)	14 (16%)	7 (8%)	1	10
24	D2	127/129 (98%)	91 (72%)	28 (22%)	8 (6%)	1	17
24	d2	127/129 (98%)	105 (83%)	17 (13%)	5 (4%)	3	27
25	D3	142/144 (99%)	87 (61%)	29 (20%)	26 (18%)	0	2
25	d3	142/144 (99%)	119 (84%)	16 (11%)	7 (5%)	2	21
26	D4	132/134 (98%)	98 (74%)	25 (19%)	9 (7%)	1	15
26	d4	132/134 (98%)	101 (76%)	17 (13%)	14 (11%)	0	7
27	D5	68/107 (64%)	43 (63%)	16 (24%)	9 (13%)	0	4
27	d5	67/107 (63%)	45 (67%)	14 (21%)	8 (12%)	0	5
28	D6	95/97 (98%)	53 (56%)	18 (19%)	24 (25%)	0	0
28	d6	95/97 (98%)	71 (75%)	16 (17%)	8 (8%)	1	10
29	D7	79/81 (98%)	58 (73%)	14 (18%)	7 (9%)	1	9
29	d7	79/81 (98%)	61 (77%)	11 (14%)	7 (9%)	1	9
30	D8	61/66 (92%)	45 (74%)	11 (18%)	5 (8%)	1	10
30	d8	61/66 (92%)	39 (64%)	14 (23%)	8 (13%)	0	4
31	D9	51/55 (93%)	32 (63%)	11 (22%)	8 (16%)	0	3
31	d9	51/55 (93%)	35 (69%)	8 (16%)	8 (16%)	0	3
32	E0	58/60 (97%)	34 (59%)	16 (28%)	8 (14%)	0	4
33	E1	69/76 (91%)	39 (56%)	13 (19%)	17 (25%)	0	0
34	SR	316/318 (99%)	237 (75%)	56 (18%)	23 (7%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	sR	316/318 (99%)	251 (79%)	46 (15%)	19 (6%)	1	17
35	SM	155/273 (57%)	90 (58%)	40 (26%)	25 (16%)	0	3
35	sM	98/273 (36%)	59 (60%)	20 (20%)	19 (19%)	0	2
39	L2	250/253 (99%)	197 (79%)	31 (12%)	22 (9%)	1	9
39	l2	250/253 (99%)	192 (77%)	42 (17%)	16 (6%)	1	17
40	L3	384/386 (100%)	290 (76%)	63 (16%)	31 (8%)	1	11
40	l3	384/386 (100%)	299 (78%)	53 (14%)	32 (8%)	1	10
41	L4	359/361 (99%)	260 (72%)	62 (17%)	37 (10%)	0	7
41	l4	359/361 (99%)	251 (70%)	68 (19%)	40 (11%)	0	6
42	L5	294/296 (99%)	200 (68%)	58 (20%)	36 (12%)	0	5
42	l5	292/296 (99%)	221 (76%)	44 (15%)	27 (9%)	1	9
43	L6	152/175 (87%)	123 (81%)	17 (11%)	12 (8%)	1	11
43	l6	153/175 (87%)	107 (70%)	27 (18%)	19 (12%)	0	5
44	L7	220/243 (90%)	154 (70%)	45 (20%)	21 (10%)	0	8
44	l7	221/243 (91%)	165 (75%)	34 (15%)	22 (10%)	0	8
45	L8	231/255 (91%)	137 (59%)	65 (28%)	29 (13%)	0	5
45	l8	229/255 (90%)	155 (68%)	52 (23%)	22 (10%)	0	8
46	L9	189/191 (99%)	137 (72%)	30 (16%)	22 (12%)	0	6
46	l9	189/191 (99%)	142 (75%)	27 (14%)	20 (11%)	0	7
47	M0	207/220 (94%)	148 (72%)	38 (18%)	21 (10%)	0	7
47	m0	209/220 (95%)	149 (71%)	41 (20%)	19 (9%)	1	9
48	M1	167/173 (96%)	116 (70%)	27 (16%)	24 (14%)	0	4
48	m1	167/173 (96%)	120 (72%)	27 (16%)	20 (12%)	0	5
49	M3	191/198 (96%)	134 (70%)	46 (24%)	11 (6%)	1	18
49	m3	192/198 (97%)	126 (66%)	37 (19%)	29 (15%)	0	3
50	M4	134/137 (98%)	97 (72%)	25 (19%)	12 (9%)	1	9
50	m4	135/137 (98%)	92 (68%)	35 (26%)	8 (6%)	1	18
51	M5	201/203 (99%)	151 (75%)	38 (19%)	12 (6%)	1	17
51	m5	201/203 (99%)	151 (75%)	35 (17%)	15 (8%)	1	12
52	M6	195/198 (98%)	146 (75%)	36 (18%)	13 (7%)	1	15
52	m6	195/198 (98%)	151 (77%)	26 (13%)	18 (9%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	M7	181/183 (99%)	128 (71%)	34 (19%)	19 (10%)	0	7
53	m7	153/183 (84%)	111 (72%)	29 (19%)	13 (8%)	1	10
54	M8	183/185 (99%)	132 (72%)	36 (20%)	15 (8%)	1	10
54	m8	183/185 (99%)	134 (73%)	36 (20%)	13 (7%)	1	14
55	M9	186/188 (99%)	136 (73%)	33 (18%)	17 (9%)	1	9
55	m9	186/188 (99%)	125 (67%)	40 (22%)	21 (11%)	0	6
56	N0	170/172 (99%)	139 (82%)	21 (12%)	10 (6%)	1	18
56	n0	170/172 (99%)	145 (85%)	16 (9%)	9 (5%)	2	19
57	N1	157/159 (99%)	115 (73%)	28 (18%)	14 (9%)	1	9
57	n1	157/159 (99%)	121 (77%)	27 (17%)	9 (6%)	1	18
58	N2	98/120 (82%)	65 (66%)	26 (26%)	7 (7%)	1	14
58	n2	96/120 (80%)	64 (67%)	24 (25%)	8 (8%)	1	10
59	N3	134/136 (98%)	109 (81%)	16 (12%)	9 (7%)	1	15
59	n3	134/136 (98%)	113 (84%)	12 (9%)	9 (7%)	1	15
60	N4	96/155 (62%)	63 (66%)	16 (17%)	17 (18%)	0	2
60	n4	133/155 (86%)	88 (66%)	25 (19%)	20 (15%)	0	3
61	N5	119/141 (84%)	81 (68%)	30 (25%)	8 (7%)	1	15
61	n5	118/141 (84%)	91 (77%)	17 (14%)	10 (8%)	1	10
62	N6	124/126 (98%)	94 (76%)	18 (14%)	12 (10%)	0	8
62	n6	124/126 (98%)	92 (74%)	17 (14%)	15 (12%)	0	5
63	N7	133/135 (98%)	98 (74%)	19 (14%)	16 (12%)	0	5
63	n7	133/135 (98%)	94 (71%)	26 (20%)	13 (10%)	0	8
64	N8	146/148 (99%)	100 (68%)	30 (20%)	16 (11%)	0	6
64	n8	146/148 (99%)	104 (71%)	28 (19%)	14 (10%)	0	8
65	N9	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	9
65	n9	56/58 (97%)	33 (59%)	14 (25%)	9 (16%)	0	3
66	O0	95/104 (91%)	82 (86%)	10 (10%)	3 (3%)	4	31
66	o0	98/104 (94%)	75 (76%)	18 (18%)	5 (5%)	2	20
67	O1	107/112 (96%)	86 (80%)	12 (11%)	9 (8%)	1	10
67	o1	107/112 (96%)	73 (68%)	14 (13%)	20 (19%)	0	2
68	O2	125/129 (97%)	95 (76%)	20 (16%)	10 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	o2	125/129 (97%)	89 (71%)	23 (18%)	13 (10%)	0	7
69	O3	104/106 (98%)	90 (86%)	7 (7%)	7 (7%)	1	15
69	o3	104/106 (98%)	82 (79%)	13 (12%)	9 (9%)	1	9
70	O4	110/119 (92%)	80 (73%)	19 (17%)	11 (10%)	0	8
70	o4	110/119 (92%)	75 (68%)	24 (22%)	11 (10%)	0	8
71	O5	117/119 (98%)	75 (64%)	28 (24%)	14 (12%)	0	5
71	o5	117/119 (98%)	80 (68%)	18 (15%)	19 (16%)	0	3
72	O6	97/99 (98%)	69 (71%)	16 (16%)	12 (12%)	0	5
72	o6	97/99 (98%)	67 (69%)	18 (19%)	12 (12%)	0	5
73	O7	85/87 (98%)	63 (74%)	16 (19%)	6 (7%)	1	14
73	o7	85/87 (98%)	60 (71%)	14 (16%)	11 (13%)	0	5
74	O8	75/77 (97%)	55 (73%)	12 (16%)	8 (11%)	0	7
74	o8	75/77 (97%)	53 (71%)	18 (24%)	4 (5%)	2	19
75	O9	48/50 (96%)	34 (71%)	10 (21%)	4 (8%)	1	10
75	o9	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	10
76	Q0	50/52 (96%)	32 (64%)	12 (24%)	6 (12%)	0	5
76	q0	50/52 (96%)	39 (78%)	6 (12%)	5 (10%)	0	8
77	Q1	23/25 (92%)	18 (78%)	3 (13%)	2 (9%)	1	9
77	q1	23/25 (92%)	16 (70%)	3 (13%)	4 (17%)	0	2
78	Q2	103/105 (98%)	75 (73%)	20 (19%)	8 (8%)	1	11
78	q2	103/105 (98%)	83 (81%)	14 (14%)	6 (6%)	1	18
79	Q3	89/91 (98%)	59 (66%)	16 (18%)	14 (16%)	0	3
79	q3	89/91 (98%)	71 (80%)	9 (10%)	9 (10%)	0	7
80	e0	60/62 (97%)	37 (62%)	14 (23%)	9 (15%)	0	3
81	e1	74/76 (97%)	28 (38%)	26 (35%)	20 (27%)	0	0
83	p0	139/311 (45%)	103 (74%)	27 (19%)	9 (6%)	1	16
All	All	22333/24141 (92%)	15914 (71%)	4073 (18%)	2346 (10%)	0	7

5 of 2346 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN

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Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	95	ALA
2	S0	132	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	117 (71%)	47 (29%)	0	3
2	s0	165/209 (79%)	123 (74%)	42 (26%)	0	4
3	S1	191/223 (86%)	139 (73%)	52 (27%)	0	3
3	s1	192/223 (86%)	147 (77%)	45 (23%)	1	5
4	S2	176/204 (86%)	126 (72%)	50 (28%)	0	3
4	s2	176/204 (86%)	119 (68%)	57 (32%)	0	2
5	S3	182/194 (94%)	133 (73%)	49 (27%)	0	3
5	s3	182/194 (94%)	131 (72%)	51 (28%)	0	3
6	S4	221/221 (100%)	170 (77%)	51 (23%)	1	5
6	s4	221/221 (100%)	165 (75%)	56 (25%)	0	4
7	S5	173/190 (91%)	136 (79%)	37 (21%)	1	7
7	s5	173/190 (91%)	125 (72%)	48 (28%)	0	3
8	S6	188/201 (94%)	139 (74%)	49 (26%)	0	4
8	s6	187/201 (93%)	132 (71%)	55 (29%)	0	2
9	S7	165/169 (98%)	127 (77%)	38 (23%)	1	5
9	s7	165/169 (98%)	122 (74%)	43 (26%)	0	4
10	S8	150/161 (93%)	118 (79%)	32 (21%)	1	7
10	s8	150/161 (93%)	106 (71%)	44 (29%)	0	2
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	5
11	s9	158/165 (96%)	116 (73%)	42 (27%)	0	3
12	C0	77/98 (79%)	58 (75%)	19 (25%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c0	73/98 (74%)	54 (74%)	19 (26%)	0	4
13	C1	129/136 (95%)	111 (86%)	18 (14%)	3	21
13	c1	129/136 (95%)	98 (76%)	31 (24%)	0	4
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0	4
14	c2	88/118 (75%)	62 (70%)	26 (30%)	0	2
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	7
15	c3	127/127 (100%)	96 (76%)	31 (24%)	0	4
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	3
16	c4	97/104 (93%)	67 (69%)	30 (31%)	0	2
17	C5	101/117 (86%)	72 (71%)	29 (29%)	0	3
17	c5	103/117 (88%)	73 (71%)	30 (29%)	0	2
18	C6	117/118 (99%)	83 (71%)	34 (29%)	0	2
18	c6	118/118 (100%)	87 (74%)	31 (26%)	0	4
19	C7	94/124 (76%)	65 (69%)	29 (31%)	0	2
19	c7	92/124 (74%)	61 (66%)	31 (34%)	0	1
20	C8	128/128 (100%)	101 (79%)	27 (21%)	1	7
20	c8	128/128 (100%)	96 (75%)	32 (25%)	0	4
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0	3
21	c9	115/115 (100%)	85 (74%)	30 (26%)	0	4
22	D0	100/113 (88%)	74 (74%)	26 (26%)	0	4
22	d0	103/113 (91%)	67 (65%)	36 (35%)	0	1
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	8
23	d1	74/74 (100%)	52 (70%)	22 (30%)	0	2
24	D2	110/110 (100%)	81 (74%)	29 (26%)	0	4
24	d2	110/110 (100%)	88 (80%)	22 (20%)	1	8
25	D3	119/119 (100%)	79 (66%)	40 (34%)	0	1
25	d3	119/119 (100%)	89 (75%)	30 (25%)	0	4
26	D4	112/112 (100%)	88 (79%)	24 (21%)	1	7
26	d4	112/112 (100%)	89 (80%)	23 (20%)	1	7
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	5
27	d5	61/88 (69%)	47 (77%)	14 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0	3
28	d6	83/83 (100%)	51 (61%)	32 (39%)	0	0
29	D7	70/70 (100%)	57 (81%)	13 (19%)	1	10
29	d7	70/70 (100%)	54 (77%)	16 (23%)	1	5
30	D8	56/59 (95%)	39 (70%)	17 (30%)	0	2
30	d8	56/59 (95%)	42 (75%)	14 (25%)	0	4
31	D9	47/48 (98%)	34 (72%)	13 (28%)	0	3
31	d9	47/48 (98%)	32 (68%)	15 (32%)	0	2
32	E0	51/51 (100%)	35 (69%)	16 (31%)	0	2
33	E1	62/66 (94%)	47 (76%)	15 (24%)	0	4
34	SR	260/261 (100%)	216 (83%)	44 (17%)	2	14
34	sR	260/261 (100%)	213 (82%)	47 (18%)	1	11
35	SM	97/228 (42%)	68 (70%)	29 (30%)	0	2
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	3
39	L2	193/195 (99%)	138 (72%)	55 (28%)	0	3
39	l2	192/195 (98%)	137 (71%)	55 (29%)	0	3
40	L3	321/322 (100%)	229 (71%)	92 (29%)	0	3
40	l3	321/322 (100%)	235 (73%)	86 (27%)	0	3
41	L4	288/288 (100%)	212 (74%)	76 (26%)	0	4
41	l4	288/288 (100%)	208 (72%)	80 (28%)	0	3
42	L5	244/244 (100%)	195 (80%)	49 (20%)	1	8
42	l5	243/244 (100%)	176 (72%)	67 (28%)	0	3
43	L6	134/152 (88%)	110 (82%)	24 (18%)	2	11
43	l6	135/152 (89%)	105 (78%)	30 (22%)	1	6
44	L7	186/204 (91%)	138 (74%)	48 (26%)	0	4
44	l7	187/204 (92%)	146 (78%)	41 (22%)	1	6
45	L8	187/207 (90%)	144 (77%)	43 (23%)	1	5
45	l8	177/207 (86%)	134 (76%)	43 (24%)	0	4
46	L9	171/171 (100%)	110 (64%)	61 (36%)	0	1
46	l9	171/171 (100%)	119 (70%)	52 (30%)	0	2
47	M0	177/186 (95%)	135 (76%)	42 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	m0	179/186 (96%)	131 (73%)	48 (27%)	0	3
48	M1	147/150 (98%)	111 (76%)	36 (24%)	0	4
48	m1	147/150 (98%)	91 (62%)	56 (38%)	0	0
49	M3	154/158 (98%)	114 (74%)	40 (26%)	0	4
49	m3	154/158 (98%)	102 (66%)	52 (34%)	0	1
50	M4	107/108 (99%)	78 (73%)	29 (27%)	0	3
50	m4	108/108 (100%)	81 (75%)	27 (25%)	0	4
51	M5	175/175 (100%)	143 (82%)	32 (18%)	1	10
51	m5	175/175 (100%)	132 (75%)	43 (25%)	0	4
52	M6	160/161 (99%)	120 (75%)	40 (25%)	0	4
52	m6	160/161 (99%)	119 (74%)	41 (26%)	0	4
53	M7	140/145 (97%)	98 (70%)	42 (30%)	0	2
53	m7	125/145 (86%)	83 (66%)	42 (34%)	0	1
54	M8	150/150 (100%)	115 (77%)	35 (23%)	1	5
54	m8	150/150 (100%)	104 (69%)	46 (31%)	0	2
55	M9	153/153 (100%)	112 (73%)	41 (27%)	0	3
55	m9	153/153 (100%)	113 (74%)	40 (26%)	0	4
56	N0	156/156 (100%)	108 (69%)	48 (31%)	0	2
56	n0	156/156 (100%)	114 (73%)	42 (27%)	0	3
57	N1	136/136 (100%)	100 (74%)	36 (26%)	0	3
57	n1	136/136 (100%)	100 (74%)	36 (26%)	0	3
58	N2	87/106 (82%)	68 (78%)	19 (22%)	1	6
58	n2	85/106 (80%)	68 (80%)	17 (20%)	1	8
59	N3	104/104 (100%)	79 (76%)	25 (24%)	0	4
59	n3	104/104 (100%)	78 (75%)	26 (25%)	0	4
60	N4	57/129 (44%)	45 (79%)	12 (21%)	1	7
60	n4	100/129 (78%)	69 (69%)	31 (31%)	0	2
61	N5	104/117 (89%)	83 (80%)	21 (20%)	1	8
61	n5	104/117 (89%)	70 (67%)	34 (33%)	0	2
62	N6	109/109 (100%)	80 (73%)	29 (27%)	0	3
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1	8
63	n7	115/115 (100%)	93 (81%)	22 (19%)	1	9
64	N8	118/118 (100%)	95 (80%)	23 (20%)	1	9
64	n8	118/118 (100%)	85 (72%)	33 (28%)	0	3
65	N9	46/46 (100%)	30 (65%)	16 (35%)	0	1
65	n9	46/46 (100%)	23 (50%)	23 (50%)	0	0
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1	5
66	o0	84/87 (97%)	54 (64%)	30 (36%)	0	1
67	O1	92/96 (96%)	67 (73%)	25 (27%)	0	3
67	o1	94/96 (98%)	67 (71%)	27 (29%)	0	3
68	O2	109/110 (99%)	73 (67%)	36 (33%)	0	2
68	o2	109/110 (99%)	78 (72%)	31 (28%)	0	3
69	O3	90/90 (100%)	71 (79%)	19 (21%)	1	7
69	o3	90/90 (100%)	62 (69%)	28 (31%)	0	2
70	O4	95/101 (94%)	66 (70%)	29 (30%)	0	2
70	o4	95/101 (94%)	70 (74%)	25 (26%)	0	4
71	O5	104/104 (100%)	69 (66%)	35 (34%)	0	1
71	o5	103/104 (99%)	77 (75%)	26 (25%)	0	4
72	O6	81/81 (100%)	56 (69%)	25 (31%)	0	2
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	2
73	O7	70/70 (100%)	51 (73%)	19 (27%)	0	3
73	o7	70/70 (100%)	48 (69%)	22 (31%)	0	2
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	6
74	o8	67/68 (98%)	52 (78%)	15 (22%)	1	6
75	O9	45/45 (100%)	35 (78%)	10 (22%)	1	6
75	o9	45/45 (100%)	34 (76%)	11 (24%)	0	4
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	5
76	q0	47/47 (100%)	33 (70%)	14 (30%)	0	2
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	65 (72%)	25 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	q2	90/90 (100%)	58 (64%)	32 (36%)	0	1
79	Q3	71/71 (100%)	54 (76%)	17 (24%)	0	4
79	q3	71/71 (100%)	49 (69%)	22 (31%)	0	2
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	6
81	e1	66/66 (100%)	41 (62%)	25 (38%)	0	1
83	p0	105/253 (42%)	79 (75%)	26 (25%)	0	4
All	All	18730/20239 (92%)	13794 (74%)	4936 (26%)	0	4

5 of 4936 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	O6	59	ASP
10	s8	56	ARG
64	n8	102	ILE
76	Q0	127	LEU
5	s3	66	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
5	s3	74	GLN
13	c1	37	ASN
64	n8	25	HIS
5	s3	179	GLN
6	s4	224	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	613 (35%)	71 (4%)
1	6	1787/1800 (99%)	650 (36%)	64 (3%)
36	1	3145/3396 (92%)	1010 (32%)	106 (3%)
36	5	3145/3396 (92%)	1037 (32%)	115 (3%)
37	3	120/121 (99%)	34 (28%)	2 (1%)
37	7	120/121 (99%)	30 (25%)	3 (2%)
38	4	157/158 (99%)	51 (32%)	7 (4%)
38	8	157/158 (99%)	57 (36%)	3 (1%)
All	All	10378/10950 (94%)	3482 (33%)	371 (3%)

5 of 3482 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	5	U
1	2	25	C
1	2	26	A

5 of 371 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3228	C
1	6	664	U
36	5	3011	A
36	1	3318	G
1	6	103	A

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2558 ligands modelled in this entry, 1426 are monoatomic - leaving 1132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
87	OHX	1	4019	-	0,6,6	0.00	-	-		
87	OHX	1	4150	-	0,6,6	0.00	-	-		
87	OHX	6	2061	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2025	-	0,6,6	0.00	-	-		
87	OHX	1	3934	-	0,6,6	0.00	-	-		
87	OHX	5	4125	-	0,6,6	0.00	-	-		
87	OHX	5	4244	-	0,6,6	0.00	-	-		
87	OHX	6	2182	-	0,6,6	0.00	-	-		
87	OHX	2	2078	-	0,6,6	0.00	-	-		
87	OHX	8	225	-	0,6,6	0.00	-	-		
87	OHX	5	3992	-	0,6,6	0.00	-	-		
87	OHX	2	2135	-	0,6,6	0.00	-	-		
87	OHX	1	4191	-	0,6,6	0.00	-	-		
87	OHX	5	4033	-	0,6,6	0.00	-	-		
87	OHX	1	4004	-	0,6,6	0.00	-	-		
87	OHX	5	4036	-	0,6,6	0.00	-	-		
87	OHX	1	4064	-	0,6,6	0.00	-	-		
87	OHX	1	4069	-	0,6,6	0.00	-	-		
87	OHX	1	4049	-	0,6,6	0.00	-	-		
87	OHX	5	4064	-	0,6,6	0.00	-	-		
87	OHX	3	225	-	0,6,6	0.00	-	-		
87	OHX	5	4055	-	0,6,6	0.00	-	-		
87	OHX	5	4108	-	0,6,6	0.00	-	-		
87	OHX	1	3978	-	0,6,6	0.00	-	-		
87	OHX	5	4240	-	0,6,6	0.00	-	-		
87	OHX	6	2060	-	0,6,6	0.00	-	-		
87	OHX	5	3928	-	0,6,6	0.00	-	-		
87	OHX	6	2178	-	0,6,6	0.00	-	-		
87	OHX	5	4001	-	0,6,6	0.00	-	-		
87	OHX	5	3978	-	0,6,6	0.00	-	-		
87	OHX	6	2096	-	0,6,6	0.00	-	-		
87	OHX	5	3976	-	0,6,6	0.00	-	-		
87	OHX	4	228	-	0,6,6	0.00	-	-		
87	OHX	5	4139	-	0,6,6	0.00	-	-		
87	OHX	5	4223	-	0,6,6	0.00	-	-		
87	OHX	1	3941	-	0,6,6	0.00	-	-		
87	OHX	2	2034	-	0,6,6	0.00	-	-		
87	OHX	m0	303	-	0,6,6	0.00	-	-		
87	OHX	6	2076	-	0,6,6	0.00	-	-		
87	OHX	1	4100	-	0,6,6	0.00	-	-		
87	OHX	6	2198	-	0,6,6	0.00	-	-		
87	OHX	8	233	-	0,6,6	0.00	-	-		
87	OHX	5	4057	-	0,6,6	0.00	-	-		
87	OHX	5	4058	-	0,6,6	0.00	-	-		
87	OHX	5	4107	-	0,6,6	0.00	-	-		
87	OHX	1	4072	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2045	-	0,6,6	0.00	-	-		
87	OHX	1	4084	-	0,6,6	0.00	-	-		
87	OHX	5	3913	-	0,6,6	0.00	-	-		
87	OHX	sR	401	-	0,6,6	0.00	-	-		
87	OHX	2	2174	-	0,6,6	0.00	-	-		
87	OHX	5	3908	-	0,6,6	0.00	-	-		
87	OHX	5	4144	-	0,6,6	0.00	-	-		
87	OHX	5	3955	-	0,6,6	0.00	-	-		
87	OHX	19	202	-	0,6,6	0.00	-	-		
87	OHX	5	4191	-	0,6,6	0.00	-	-		
87	OHX	1	4158	-	0,6,6	0.00	-	-		
87	OHX	1	4037	-	0,6,6	0.00	-	-		
87	OHX	5	4123	-	0,6,6	0.00	-	-		
87	OHX	N9	102	-	0,6,6	0.00	-	-		
87	OHX	1	3995	-	0,6,6	0.00	-	-		
87	OHX	1	3904	-	0,6,6	0.00	-	-		
87	OHX	2	2116	-	0,6,6	0.00	-	-		
87	OHX	1	3887	-	0,6,6	0.00	-	-		
87	OHX	1	4209	-	0,6,6	0.00	-	-		
87	OHX	6	2200	-	0,6,6	0.00	-	-		
87	OHX	1	4042	-	0,6,6	0.00	-	-		
87	OHX	5	4088	-	0,6,6	0.00	-	-		
87	OHX	1	3928	-	0,6,6	0.00	-	-		
87	OHX	5	3963	-	0,6,6	0.00	-	-		
87	OHX	1	3903	-	0,6,6	0.00	-	-		
87	OHX	2	2151	-	0,6,6	0.00	-	-		
87	OHX	1	4104	-	0,6,6	0.00	-	-		
87	OHX	1	4182	-	0,6,6	0.00	-	-		
87	OHX	1	3932	-	0,6,6	0.00	-	-		
87	OHX	6	2053	-	0,6,6	0.00	-	-		
87	OHX	6	2144	-	0,6,6	0.00	-	-		
87	OHX	2	2120	-	0,6,6	0.00	-	-		
87	OHX	2	2133	-	0,6,6	0.00	-	-		
87	OHX	1	4148	-	0,6,6	0.00	-	-		
87	OHX	1	4105	-	0,6,6	0.00	-	-		
87	OHX	5	3895	-	0,6,6	0.00	-	-		
87	OHX	5	4042	-	0,6,6	0.00	-	-		
87	OHX	3	224	-	0,6,6	0.00	-	-		
87	OHX	6	2175	-	0,6,6	0.00	-	-		
87	OHX	1	4029	-	0,6,6	0.00	-	-		
87	OHX	6	2199	-	0,6,6	0.00	-	-		
87	OHX	1	3930	-	0,6,6	0.00	-	-		
87	OHX	6	2203	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2060	-	0,6,6	0.00	-	-		
87	OHX	1	4068	-	0,6,6	0.00	-	-		
87	OHX	6	2114	-	0,6,6	0.00	-	-		
87	OHX	6	2055	-	0,6,6	0.00	-	-		
87	OHX	5	4186	-	0,6,6	0.00	-	-		
87	OHX	6	2195	-	0,6,6	0.00	-	-		
87	OHX	4	239	-	0,6,6	0.00	-	-		
87	OHX	5	4195	-	0,6,6	0.00	-	-		
87	OHX	1	3957	-	0,6,6	0.00	-	-		
87	OHX	5	4052	-	0,6,6	0.00	-	-		
87	OHX	5	4156	-	0,6,6	0.00	-	-		
87	OHX	L3	404	-	0,6,6	0.00	-	-		
87	OHX	5	4153	-	0,6,6	0.00	-	-		
87	OHX	1	4129	-	0,6,6	0.00	-	-		
87	OHX	6	2185	-	0,6,6	0.00	-	-		
87	OHX	7	221	-	0,6,6	0.00	-	-		
87	OHX	5	4018	-	0,6,6	0.00	-	-		
87	OHX	1	4051	-	0,6,6	0.00	-	-		
87	OHX	1	4135	-	0,6,6	0.00	-	-		
87	OHX	5	4193	-	0,6,6	0.00	-	-		
87	OHX	2	2081	-	0,6,6	0.00	-	-		
87	OHX	1	3910	-	0,6,6	0.00	-	-		
87	OHX	1	4190	-	0,6,6	0.00	-	-		
87	OHX	1	4034	-	0,6,6	0.00	-	-		
87	OHX	1	3939	-	0,6,6	0.00	-	-		
87	OHX	6	2194	-	0,6,6	0.00	-	-		
87	OHX	5	4120	-	0,6,6	0.00	-	-		
87	OHX	1	4178	-	0,6,6	0.00	-	-		
87	OHX	2	2112	-	0,6,6	0.00	-	-		
87	OHX	1	3884	-	0,6,6	0.00	-	-		
87	OHX	q2	502	-	0,6,6	0.00	-	-		
87	OHX	C5	201	-	0,6,6	0.00	-	-		
87	OHX	1	3948	-	0,6,6	0.00	-	-		
87	OHX	1	4091	-	0,6,6	0.00	-	-		
87	OHX	1	4086	-	0,6,6	0.00	-	-		
87	OHX	1	3909	-	0,6,6	0.00	-	-		
87	OHX	5	4065	-	0,6,6	0.00	-	-		
87	OHX	5	4104	-	0,6,6	0.00	-	-		
87	OHX	5	4137	-	0,6,6	0.00	-	-		
87	OHX	5	4090	-	0,6,6	0.00	-	-		
87	OHX	1	4059	-	0,6,6	0.00	-	-		
87	OHX	1	4053	-	0,6,6	0.00	-	-		
87	OHX	2	2094	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4142	-	0,6,6	0.00	-	-		
87	OHX	6	2067	-	0,6,6	0.00	-	-		
87	OHX	5	4145	-	0,6,6	0.00	-	-		
87	OHX	5	4067	-	0,6,6	0.00	-	-		
87	OHX	5	4116	-	0,6,6	0.00	-	-		
87	OHX	5	4213	-	0,6,6	0.00	-	-		
87	OHX	5	4179	-	0,6,6	0.00	-	-		
87	OHX	2	2108	-	0,6,6	0.00	-	-		
87	OHX	1	4065	-	0,6,6	0.00	-	-		
87	OHX	5	4089	-	0,6,6	0.00	-	-		
87	OHX	5	3903	-	0,6,6	0.00	-	-		
87	OHX	5	4182	-	0,6,6	0.00	-	-		
87	OHX	5	4124	-	0,6,6	0.00	-	-		
87	OHX	5	3897	-	0,6,6	0.00	-	-		
87	OHX	2	2143	-	0,6,6	0.00	-	-		
87	OHX	1	3960	-	0,6,6	0.00	-	-		
87	OHX	6	2100	-	0,6,6	0.00	-	-		
87	OHX	1	4127	-	0,6,6	0.00	-	-		
87	OHX	5	3982	-	0,6,6	0.00	-	-		
87	OHX	1	4009	-	0,6,6	0.00	-	-		
87	OHX	O3	202	-	0,6,6	0.00	-	-		
87	OHX	5	4241	-	0,6,6	0.00	-	-		
87	OHX	5	3905	-	0,6,6	0.00	-	-		
87	OHX	1	4201	-	0,6,6	0.00	-	-		
87	OHX	1	4095	-	0,6,6	0.00	-	-		
87	OHX	5	4012	-	0,6,6	0.00	-	-		
87	OHX	2	2165	-	0,6,6	0.00	-	-		
87	OHX	1	4171	-	0,6,6	0.00	-	-		
87	OHX	1	4061	-	0,6,6	0.00	-	-		
87	OHX	15	306	-	0,6,6	0.00	-	-		
87	OHX	6	2063	-	0,6,6	0.00	-	-		
87	OHX	5	3936	-	0,6,6	0.00	-	-		
87	OHX	5	3898	-	0,6,6	0.00	-	-		
87	OHX	1	4207	-	0,6,6	0.00	-	-		
87	OHX	2	2059	-	0,6,6	0.00	-	-		
87	OHX	5	4118	-	0,6,6	0.00	-	-		
87	OHX	5	4079	-	0,6,6	0.00	-	-		
87	OHX	1	3891	-	0,6,6	0.00	-	-		
87	OHX	8	227	-	0,6,6	0.00	-	-		
87	OHX	6	2111	-	0,6,6	0.00	-	-		
87	OHX	8	231	-	0,6,6	0.00	-	-		
87	OHX	2	2097	-	0,6,6	0.00	-	-		
87	OHX	5	4132	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4152	-	0,6,6	0.00	-	-		
87	OHX	5	4014	-	0,6,6	0.00	-	-		
87	OHX	2	2088	-	0,6,6	0.00	-	-		
87	OHX	1	4039	-	0,6,6	0.00	-	-		
87	OHX	5	4208	-	0,6,6	0.00	-	-		
87	OHX	1	4076	-	0,6,6	0.00	-	-		
88	GET	2	2181	-	33,36,36	0.49	0	43,55,55	1.87	12 (27%)
87	OHX	1	4177	-	0,6,6	0.00	-	-		
87	OHX	1	4056	-	0,6,6	0.00	-	-		
87	OHX	2	2037	-	0,6,6	0.00	-	-		
87	OHX	6	2071	-	0,6,6	0.00	-	-		
87	OHX	7	224	-	0,6,6	0.00	-	-		
87	OHX	5	3944	-	0,6,6	0.00	-	-		
87	OHX	2	2076	-	0,6,6	0.00	-	-		
87	OHX	1	4184	-	0,6,6	0.00	-	-		
87	OHX	5	4109	-	0,6,6	0.00	-	-		
87	OHX	5	4043	-	0,6,6	0.00	-	-		
87	OHX	6	2177	-	0,6,6	0.00	-	-		
87	OHX	6	2084	-	0,6,6	0.00	-	-		
87	OHX	1	4173	-	0,6,6	0.00	-	-		
87	OHX	5	3937	-	0,6,6	0.00	-	-		
87	OHX	1	3989	-	0,6,6	0.00	-	-		
87	OHX	5	3918	-	0,6,6	0.00	-	-		
87	OHX	5	4077	-	0,6,6	0.00	-	-		
87	OHX	6	2095	-	0,6,6	0.00	-	-		
87	OHX	2	2153	-	0,6,6	0.00	-	-		
87	OHX	4	230	-	0,6,6	0.00	-	-		
87	OHX	1	3890	-	0,6,6	0.00	-	-		
87	OHX	5	4040	-	0,6,6	0.00	-	-		
87	OHX	6	2050	-	0,6,6	0.00	-	-		
87	OHX	1	3901	-	0,6,6	0.00	-	-		
87	OHX	o7	502	-	0,6,6	0.00	-	-		
87	OHX	6	2204	-	0,6,6	0.00	-	-		
87	OHX	2	2026	-	0,6,6	0.00	-	-		
87	OHX	6	2197	-	0,6,6	0.00	-	-		
87	OHX	5	4049	-	0,6,6	0.00	-	-		
87	OHX	2	2080	-	0,6,6	0.00	-	-		
87	OHX	1	3946	-	0,6,6	0.00	-	-		
87	OHX	6	2187	-	0,6,6	0.00	-	-		
87	OHX	5	4076	-	0,6,6	0.00	-	-		
87	OHX	5	4114	-	0,6,6	0.00	-	-		
87	OHX	1	4141	-	0,6,6	0.00	-	-		
87	OHX	1	4063	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2047	-	0,6,6	0.00	-	-		
87	OHX	6	2066	-	0,6,6	0.00	-	-		
87	OHX	1	4062	-	0,6,6	0.00	-	-		
87	OHX	1	4111	-	0,6,6	0.00	-	-		
87	OHX	6	2148	-	0,6,6	0.00	-	-		
87	OHX	2	2139	-	0,6,6	0.00	-	-		
87	OHX	2	2083	-	0,6,6	0.00	-	-		
87	OHX	5	4219	-	0,6,6	0.00	-	-		
87	OHX	5	4176	-	0,6,6	0.00	-	-		
87	OHX	1	3875	-	0,6,6	0.00	-	-		
87	OHX	1	3958	-	0,6,6	0.00	-	-		
87	OHX	5	3907	-	0,6,6	0.00	-	-		
87	OHX	o3	203	-	0,6,6	0.00	-	-		
87	OHX	5	4027	-	0,6,6	0.00	-	-		
87	OHX	1	4024	-	0,6,6	0.00	-	-		
87	OHX	2	2130	-	0,6,6	0.00	-	-		
87	OHX	5	4013	-	0,6,6	0.00	-	-		
87	OHX	5	3998	-	0,6,6	0.00	-	-		
87	OHX	1	4092	-	0,6,6	0.00	-	-		
87	OHX	n3	202	-	0,6,6	0.00	-	-		
87	OHX	6	2059	-	0,6,6	0.00	-	-		
87	OHX	5	4200	-	0,6,6	0.00	-	-		
87	OHX	2	2105	-	0,6,6	0.00	-	-		
87	OHX	5	4205	-	0,6,6	0.00	-	-		
87	OHX	5	3902	-	0,6,6	0.00	-	-		
87	OHX	1	3869	-	0,6,6	0.00	-	-		
87	OHX	L3	405	-	0,6,6	0.00	-	-		
87	OHX	6	2072	-	0,6,6	0.00	-	-		
87	OHX	1	3888	-	0,6,6	0.00	-	-		
87	OHX	5	3979	-	0,6,6	0.00	-	-		
87	OHX	1	3886	-	0,6,6	0.00	-	-		
87	OHX	5	3974	-	0,6,6	0.00	-	-		
87	OHX	5	4054	-	0,6,6	0.00	-	-		
87	OHX	1	3919	-	0,6,6	0.00	-	-		
87	OHX	5	4192	-	0,6,6	0.00	-	-		
87	OHX	5	4174	-	0,6,6	0.00	-	-		
87	OHX	1	3873	-	0,6,6	0.00	-	-		
87	OHX	5	3980	-	0,6,6	0.00	-	-		
87	OHX	2	2150	-	0,6,6	0.00	-	-		
87	OHX	5	4024	-	0,6,6	0.00	-	-		
87	OHX	1	4134	-	0,6,6	0.00	-	-		
87	OHX	5	4021	-	0,6,6	0.00	-	-		
87	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
87	OHX	6	2116	-	0,6,6	0.00	-	-		
87	OHX	s8	303	-	0,6,6	0.00	-	-		
87	OHX	2	2024	-	0,6,6	0.00	-	-		
87	OHX	1	3880	-	0,6,6	0.00	-	-		
87	OHX	2	2121	-	0,6,6	0.00	-	-		
87	OHX	2	2102	-	0,6,6	0.00	-	-		
87	OHX	5	4129	-	0,6,6	0.00	-	-		
87	OHX	1	3945	-	0,6,6	0.00	-	-		
87	OHX	5	4202	-	0,6,6	0.00	-	-		
87	OHX	5	4099	-	0,6,6	0.00	-	-		
87	OHX	6	2070	-	0,6,6	0.00	-	-		
87	OHX	1	3927	-	0,6,6	0.00	-	-		
87	OHX	2	2127	-	0,6,6	0.00	-	-		
87	OHX	5	4060	-	0,6,6	0.00	-	-		
87	OHX	5	4204	-	0,6,6	0.00	-	-		
87	OHX	M0	304	-	0,6,6	0.00	-	-		
87	OHX	1	3922	-	0,6,6	0.00	-	-		
87	OHX	6	2129	-	0,6,6	0.00	-	-		
87	OHX	4	229	-	0,6,6	0.00	-	-		
87	OHX	5	4135	-	0,6,6	0.00	-	-		
87	OHX	2	2144	-	0,6,6	0.00	-	-		
87	OHX	d9	102	-	0,6,6	0.00	-	-		
87	OHX	1	4047	-	0,6,6	0.00	-	-		
87	OHX	1	3942	-	0,6,6	0.00	-	-		
87	OHX	1	4125	-	0,6,6	0.00	-	-		
87	OHX	1	3925	-	0,6,6	0.00	-	-		
87	OHX	5	4147	-	0,6,6	0.00	-	-		
87	OHX	2	2027	-	0,6,6	0.00	-	-		
87	OHX	1	3900	-	0,6,6	0.00	-	-		
87	OHX	6	2209	-	0,6,6	0.00	-	-		
87	OHX	5	3920	-	0,6,6	0.00	-	-		
87	OHX	1	4044	-	0,6,6	0.00	-	-		
87	OHX	1	4036	-	0,6,6	0.00	-	-		
87	OHX	1	4204	-	0,6,6	0.00	-	-		
87	OHX	2	2072	-	0,6,6	0.00	-	-		
87	OHX	1	4130	-	0,6,6	0.00	-	-		
87	OHX	1	4205	-	0,6,6	0.00	-	-		
87	OHX	6	2135	-	0,6,6	0.00	-	-		
87	OHX	6	2168	-	0,6,6	0.00	-	-		
87	OHX	5	4228	-	0,6,6	0.00	-	-		
87	OHX	1	4164	-	0,6,6	0.00	-	-		
87	OHX	1	4143	-	0,6,6	0.00	-	-		
87	OHX	1	3974	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3977	-	0,6,6	0.00	-	-		
87	OHX	5	4006	-	0,6,6	0.00	-	-		
87	OHX	6	2154	-	0,6,6	0.00	-	-		
87	OHX	1	4117	-	0,6,6	0.00	-	-		
87	OHX	1	3879	-	0,6,6	0.00	-	-		
87	OHX	1	3991	-	0,6,6	0.00	-	-		
87	OHX	5	4029	-	0,6,6	0.00	-	-		
87	OHX	1	4172	-	0,6,6	0.00	-	-		
87	OHX	1	4054	-	0,6,6	0.00	-	-		
87	OHX	1	3951	-	0,6,6	0.00	-	-		
87	OHX	1	4187	-	0,6,6	0.00	-	-		
87	OHX	D9	102	-	0,6,6	0.00	-	-		
87	OHX	5	4242	-	0,6,6	0.00	-	-		
87	OHX	3	216	-	0,6,6	0.00	-	-		
87	OHX	2	2044	-	0,6,6	0.00	-	-		
87	OHX	1	3992	-	0,6,6	0.00	-	-		
87	OHX	5	4187	-	0,6,6	0.00	-	-		
87	OHX	5	3991	-	0,6,6	0.00	-	-		
87	OHX	5	4096	-	0,6,6	0.00	-	-		
87	OHX	1	4152	-	0,6,6	0.00	-	-		
87	OHX	2	2100	-	0,6,6	0.00	-	-		
87	OHX	o9	101	-	0,6,6	0.00	-	-		
87	OHX	1	4144	-	0,6,6	0.00	-	-		
87	OHX	1	3924	-	0,6,6	0.00	-	-		
87	OHX	2	2031	-	0,6,6	0.00	-	-		
87	OHX	1	3993	-	0,6,6	0.00	-	-		
87	OHX	5	4035	-	0,6,6	0.00	-	-		
87	OHX	1	4170	-	0,6,6	0.00	-	-		
87	OHX	1	4210	-	0,6,6	0.00	-	-		
87	OHX	1	4114	-	0,6,6	0.00	-	-		
87	OHX	6	2206	-	0,6,6	0.00	-	-		
87	OHX	5	3943	-	0,6,6	0.00	-	-		
87	OHX	2	2087	-	0,6,6	0.00	-	-		
87	OHX	1	3944	-	0,6,6	0.00	-	-		
87	OHX	1	4212	-	0,6,6	0.00	-	-		
87	OHX	1	3905	-	0,6,6	0.00	-	-		
87	OHX	5	4163	-	0,6,6	0.00	-	-		
87	OHX	1	3981	-	0,6,6	0.00	-	-		
87	OHX	1	3870	-	0,6,6	0.00	-	-		
87	OHX	6	2051	-	0,6,6	0.00	-	-		
87	OHX	L4	403	-	0,6,6	0.00	-	-		
87	OHX	5	3940	-	0,6,6	0.00	-	-		
87	OHX	5	4164	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	8	220	-	0,6,6	0.00	-	-		
87	OHX	1	4160	-	0,6,6	0.00	-	-		
87	OHX	6	2077	-	0,6,6	0.00	-	-		
87	OHX	5	4133	-	0,6,6	0.00	-	-		
87	OHX	5	4236	-	0,6,6	0.00	-	-		
87	OHX	1	4154	-	0,6,6	0.00	-	-		
87	OHX	5	4084	-	0,6,6	0.00	-	-		
87	OHX	2	2111	-	0,6,6	0.00	-	-		
87	OHX	1	4131	-	0,6,6	0.00	-	-		
87	OHX	2	2132	-	0,6,6	0.00	-	-		
87	OHX	5	4131	-	0,6,6	0.00	-	-		
87	OHX	6	2052	-	0,6,6	0.00	-	-		
87	OHX	5	4155	-	0,6,6	0.00	-	-		
87	OHX	6	2138	-	0,6,6	0.00	-	-		
87	OHX	1	3971	-	0,6,6	0.00	-	-		
87	OHX	2	2090	-	0,6,6	0.00	-	-		
87	OHX	5	4100	-	0,6,6	0.00	-	-		
87	OHX	6	2143	-	0,6,6	0.00	-	-		
87	OHX	1	4103	-	0,6,6	0.00	-	-		
87	OHX	L3	403	-	0,6,6	0.00	-	-		
87	OHX	5	3950	-	0,6,6	0.00	-	-		
87	OHX	1	4192	-	0,6,6	0.00	-	-		
87	OHX	O2	202	-	0,6,6	0.00	-	-		
87	OHX	1	3917	-	0,6,6	0.00	-	-		
87	OHX	1	3912	-	0,6,6	0.00	-	-		
87	OHX	5	4140	-	0,6,6	0.00	-	-		
87	OHX	2	2157	-	0,6,6	0.00	-	-		
87	OHX	5	4201	-	0,6,6	0.00	-	-		
87	OHX	5	4217	-	0,6,6	0.00	-	-		
87	OHX	5	3934	-	0,6,6	0.00	-	-		
87	OHX	6	2174	-	0,6,6	0.00	-	-		
87	OHX	1	3937	-	0,6,6	0.00	-	-		
87	OHX	2	2142	-	0,6,6	0.00	-	-		
87	OHX	1	4094	-	0,6,6	0.00	-	-		
87	OHX	2	2084	-	0,6,6	0.00	-	-		
87	OHX	5	4138	-	0,6,6	0.00	-	-		
87	OHX	1	3947	-	0,6,6	0.00	-	-		
87	OHX	5	4103	-	0,6,6	0.00	-	-		
87	OHX	1	3889	-	0,6,6	0.00	-	-		
87	OHX	5	4106	-	0,6,6	0.00	-	-		
87	OHX	5	3899	-	0,6,6	0.00	-	-		
87	OHX	1	4206	-	0,6,6	0.00	-	-		
87	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
87	OHX	2	2061	-	0,6,6	0.00	-	-		
87	OHX	5	4243	-	0,6,6	0.00	-	-		
87	OHX	2	2159	-	0,6,6	0.00	-	-		
87	OHX	1	3866	-	0,6,6	0.00	-	-		
87	OHX	2	2073	-	0,6,6	0.00	-	-		
87	OHX	5	4168	-	0,6,6	0.00	-	-		
87	OHX	3	215	-	0,6,6	0.00	-	-		
87	OHX	5	3914	-	0,6,6	0.00	-	-		
87	OHX	5	4194	-	0,6,6	0.00	-	-		
87	OHX	5	4215	-	0,6,6	0.00	-	-		
87	OHX	13	408	-	0,6,6	0.00	-	-		
87	OHX	6	2207	-	0,6,6	0.00	-	-		
87	OHX	1	4082	-	0,6,6	0.00	-	-		
87	OHX	2	2030	-	0,6,6	0.00	-	-		
87	OHX	2	2071	-	0,6,6	0.00	-	-		
87	OHX	5	4066	-	0,6,6	0.00	-	-		
87	OHX	6	2189	-	0,6,6	0.00	-	-		
87	OHX	6	2132	-	0,6,6	0.00	-	-		
87	OHX	1	3983	-	0,6,6	0.00	-	-		
87	OHX	6	2102	-	0,6,6	0.00	-	-		
87	OHX	6	2147	-	0,6,6	0.00	-	-		
87	OHX	5	3984	-	0,6,6	0.00	-	-		
87	OHX	7	223	-	0,6,6	0.00	-	-		
87	OHX	5	4061	-	0,6,6	0.00	-	-		
87	OHX	5	4044	-	0,6,6	0.00	-	-		
87	OHX	1	3943	-	0,6,6	0.00	-	-		
87	OHX	1	4108	-	0,6,6	0.00	-	-		
87	OHX	M6	202	-	0,6,6	0.00	-	-		
87	OHX	5	4159	-	0,6,6	0.00	-	-		
87	OHX	SR	401	-	0,6,6	0.00	-	-		
87	OHX	5	3901	-	0,6,6	0.00	-	-		
87	OHX	1	4167	-	0,6,6	0.00	-	-		
87	OHX	5	4150	-	0,6,6	0.00	-	-		
87	OHX	1	4140	-	0,6,6	0.00	-	-		
87	OHX	1	3920	-	0,6,6	0.00	-	-		
87	OHX	1	4208	-	0,6,6	0.00	-	-		
87	OHX	2	2065	-	0,6,6	0.00	-	-		
87	OHX	5	4173	-	0,6,6	0.00	-	-		
87	OHX	5	4034	-	0,6,6	0.00	-	-		
87	OHX	6	2107	-	0,6,6	0.00	-	-		
87	OHX	5	4183	-	0,6,6	0.00	-	-		
87	OHX	4	238	-	0,6,6	0.00	-	-		
87	OHX	1	4107	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3931	-	0,6,6	0.00	-	-		
87	OHX	6	2106	-	0,6,6	0.00	-	-		
87	OHX	5	4227	-	0,6,6	0.00	-	-		
87	OHX	6	2079	-	0,6,6	0.00	-	-		
87	OHX	5	3997	-	0,6,6	0.00	-	-		
87	OHX	5	4094	-	0,6,6	0.00	-	-		
87	OHX	1	4099	-	0,6,6	0.00	-	-		
87	OHX	2	2161	-	0,6,6	0.00	-	-		
87	OHX	6	2191	-	0,6,6	0.00	-	-		
87	OHX	1	3913	-	0,6,6	0.00	-	-		
87	OHX	5	4170	-	0,6,6	0.00	-	-		
87	OHX	2	2122	-	0,6,6	0.00	-	-		
87	OHX	6	2183	-	0,6,6	0.00	-	-		
87	OHX	6	2083	-	0,6,6	0.00	-	-		
87	OHX	5	4196	-	0,6,6	0.00	-	-		
87	OHX	1	3921	-	0,6,6	0.00	-	-		
87	OHX	4	231	-	0,6,6	0.00	-	-		
87	OHX	5	4210	-	0,6,6	0.00	-	-		
87	OHX	2	2172	-	0,6,6	0.00	-	-		
87	OHX	1	4118	-	0,6,6	0.00	-	-		
87	OHX	5	4184	-	0,6,6	0.00	-	-		
87	OHX	1	4123	-	0,6,6	0.00	-	-		
87	OHX	1	3896	-	0,6,6	0.00	-	-		
87	OHX	2	2110	-	0,6,6	0.00	-	-		
87	OHX	1	3882	-	0,6,6	0.00	-	-		
87	OHX	4	227	-	0,6,6	0.00	-	-		
87	OHX	6	2176	-	0,6,6	0.00	-	-		
87	OHX	1	3916	-	0,6,6	0.00	-	-		
87	OHX	1	3984	-	0,6,6	0.00	-	-		
87	OHX	8	222	-	0,6,6	0.00	-	-		
87	OHX	5	4229	-	0,6,6	0.00	-	-		
87	OHX	5	4041	-	0,6,6	0.00	-	-		
87	OHX	2	2113	-	0,6,6	0.00	-	-		
87	OHX	5	4235	-	0,6,6	0.00	-	-		
87	OHX	5	4009	-	0,6,6	0.00	-	-		
87	OHX	C8	201	-	0,6,6	0.00	-	-		
87	OHX	5	3924	-	0,6,6	0.00	-	-		
87	OHX	1	3969	-	0,6,6	0.00	-	-		
87	OHX	2	2098	-	0,6,6	0.00	-	-		
87	OHX	6	2173	-	0,6,6	0.00	-	-		
87	OHX	5	4008	-	0,6,6	0.00	-	-		
87	OHX	5	4128	-	0,6,6	0.00	-	-		
87	OHX	2	2171	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2038	-	0,6,6	0.00	-	-		
87	OHX	5	4142	-	0,6,6	0.00	-	-		
87	OHX	5	4239	-	0,6,6	0.00	-	-		
87	OHX	6	2093	-	0,6,6	0.00	-	-		
87	OHX	D3	202	-	0,6,6	0.00	-	-		
87	OHX	6	2179	-	0,6,6	0.00	-	-		
87	OHX	5	4111	-	0,6,6	0.00	-	-		
87	OHX	5	3968	-	0,6,6	0.00	-	-		
87	OHX	5	3926	-	0,6,6	0.00	-	-		
87	OHX	5	3990	-	0,6,6	0.00	-	-		
87	OHX	1	3906	-	0,6,6	0.00	-	-		
87	OHX	5	4086	-	0,6,6	0.00	-	-		
87	OHX	5	3957	-	0,6,6	0.00	-	-		
87	OHX	14	403	-	0,6,6	0.00	-	-		
87	OHX	2	2103	-	0,6,6	0.00	-	-		
87	OHX	1	4018	-	0,6,6	0.00	-	-		
87	OHX	5	3948	-	0,6,6	0.00	-	-		
87	OHX	1	3952	-	0,6,6	0.00	-	-		
87	OHX	5	4207	-	0,6,6	0.00	-	-		
87	OHX	1	4011	-	0,6,6	0.00	-	-		
87	OHX	5	4098	-	0,6,6	0.00	-	-		
87	OHX	1	4157	-	0,6,6	0.00	-	-		
87	OHX	1	4025	-	0,6,6	0.00	-	-		
87	OHX	6	2205	-	0,6,6	0.00	-	-		
87	OHX	2	2062	-	0,6,6	0.00	-	-		
87	OHX	5	4053	-	0,6,6	0.00	-	-		
87	OHX	Q2	502	-	0,6,6	0.00	-	-		
87	OHX	6	2120	-	0,6,6	0.00	-	-		
87	OHX	5	4056	-	0,6,6	0.00	-	-		
87	OHX	6	2081	-	0,6,6	0.00	-	-		
87	OHX	6	2125	-	0,6,6	0.00	-	-		
87	OHX	2	2175	-	0,6,6	0.00	-	-		
87	OHX	1	3872	-	0,6,6	0.00	-	-		
87	OHX	2	2050	-	0,6,6	0.00	-	-		
87	OHX	S8	302	-	0,6,6	0.00	-	-		
87	OHX	1	4013	-	0,6,6	0.00	-	-		
87	OHX	5	3981	-	0,6,6	0.00	-	-		
87	OHX	c8	202	-	0,6,6	0.00	-	-		
87	OHX	8	221	-	0,6,6	0.00	-	-		
87	OHX	1	3999	-	0,6,6	0.00	-	-		
87	OHX	2	2148	-	0,6,6	0.00	-	-		
87	OHX	5	3935	-	0,6,6	0.00	-	-		
87	OHX	5	4148	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4139	-	0,6,6	0.00	-	-		
87	OHX	6	2117	-	0,6,6	0.00	-	-		
87	OHX	2	2068	-	0,6,6	0.00	-	-		
87	OHX	2	2104	-	0,6,6	0.00	-	-		
87	OHX	2	2125	-	0,6,6	0.00	-	-		
87	OHX	5	4051	-	0,6,6	0.00	-	-		
87	OHX	5	3945	-	0,6,6	0.00	-	-		
87	OHX	1	4145	-	0,6,6	0.00	-	-		
87	OHX	6	2082	-	0,6,6	0.00	-	-		
87	OHX	5	4046	-	0,6,6	0.00	-	-		
87	OHX	6	2089	-	0,6,6	0.00	-	-		
87	OHX	1	4077	-	0,6,6	0.00	-	-		
87	OHX	6	2139	-	0,6,6	0.00	-	-		
87	OHX	1	4050	-	0,6,6	0.00	-	-		
87	OHX	2	2089	-	0,6,6	0.00	-	-		
87	OHX	5	4082	-	0,6,6	0.00	-	-		
87	OHX	6	2099	-	0,6,6	0.00	-	-		
87	OHX	2	2033	-	0,6,6	0.00	-	-		
87	OHX	7	216	-	0,6,6	0.00	-	-		
87	OHX	1	4016	-	0,6,6	0.00	-	-		
87	OHX	6	2124	-	0,6,6	0.00	-	-		
87	OHX	6	2128	-	0,6,6	0.00	-	-		
87	OHX	1	4181	-	0,6,6	0.00	-	-		
87	OHX	5	4063	-	0,6,6	0.00	-	-		
87	OHX	3	219	-	0,6,6	0.00	-	-		
87	OHX	5	4095	-	0,6,6	0.00	-	-		
87	OHX	6	2196	-	0,6,6	0.00	-	-		
87	OHX	5	4017	-	0,6,6	0.00	-	-		
87	OHX	5	3941	-	0,6,6	0.00	-	-		
87	OHX	1	4128	-	0,6,6	0.00	-	-		
87	OHX	2	2119	-	0,6,6	0.00	-	-		
87	OHX	5	3989	-	0,6,6	0.00	-	-		
87	OHX	2	2032	-	0,6,6	0.00	-	-		
87	OHX	5	3970	-	0,6,6	0.00	-	-		
87	OHX	5	4167	-	0,6,6	0.00	-	-		
87	OHX	5	4007	-	0,6,6	0.00	-	-		
87	OHX	2	2134	-	0,6,6	0.00	-	-		
87	OHX	5	3993	-	0,6,6	0.00	-	-		
87	OHX	5	4081	-	0,6,6	0.00	-	-		
87	OHX	6	2058	-	0,6,6	0.00	-	-		
87	OHX	5	4080	-	0,6,6	0.00	-	-		
87	OHX	1	4045	-	0,6,6	0.00	-	-		
87	OHX	2	2086	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4218	-	0,6,6	0.00	-	-		
87	OHX	c3	201	-	0,6,6	0.00	-	-		
87	OHX	2	2029	-	0,6,6	0.00	-	-		
87	OHX	1	3956	-	0,6,6	0.00	-	-		
87	OHX	6	2075	-	0,6,6	0.00	-	-		
87	OHX	1	3967	-	0,6,6	0.00	-	-		
87	OHX	5	4022	-	0,6,6	0.00	-	-		
87	OHX	1	3892	-	0,6,6	0.00	-	-		
87	OHX	5	3922	-	0,6,6	0.00	-	-		
87	OHX	2	2095	-	0,6,6	0.00	-	-		
87	OHX	2	2051	-	0,6,6	0.00	-	-		
87	OHX	1	3979	-	0,6,6	0.00	-	-		
87	OHX	1	3874	-	0,6,6	0.00	-	-		
87	OHX	2	2167	-	0,6,6	0.00	-	-		
87	OHX	6	2123	-	0,6,6	0.00	-	-		
87	OHX	4	225	-	0,6,6	0.00	-	-		
87	OHX	5	4026	-	0,6,6	0.00	-	-		
87	OHX	1	3994	-	0,6,6	0.00	-	-		
87	OHX	1	4060	-	0,6,6	0.00	-	-		
87	OHX	6	2098	-	0,6,6	0.00	-	-		
87	OHX	6	2184	-	0,6,6	0.00	-	-		
87	OHX	1	3895	-	0,6,6	0.00	-	-		
87	OHX	1	3883	-	0,6,6	0.00	-	-		
87	OHX	5	4197	-	0,6,6	0.00	-	-		
87	OHX	5	4212	-	0,6,6	0.00	-	-		
87	OHX	1	4194	-	0,6,6	0.00	-	-		
87	OHX	5	4074	-	0,6,6	0.00	-	-		
87	OHX	1	4116	-	0,6,6	0.00	-	-		
87	OHX	5	4169	-	0,6,6	0.00	-	-		
87	OHX	1	3876	-	0,6,6	0.00	-	-		
87	OHX	1	4113	-	0,6,6	0.00	-	-		
87	OHX	1	3950	-	0,6,6	0.00	-	-		
87	OHX	5	4069	-	0,6,6	0.00	-	-		
87	OHX	1	3977	-	0,6,6	0.00	-	-		
87	OHX	5	3912	-	0,6,6	0.00	-	-		
87	OHX	1	4070	-	0,6,6	0.00	-	-		
87	OHX	5	3986	-	0,6,6	0.00	-	-		
87	OHX	1	4052	-	0,6,6	0.00	-	-		
87	OHX	5	3983	-	0,6,6	0.00	-	-		
87	OHX	2	2096	-	0,6,6	0.00	-	-		
87	OHX	3	218	-	0,6,6	0.00	-	-		
87	OHX	1	3907	-	0,6,6	0.00	-	-		
87	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
87	OHX	5	4117	-	0,6,6	0.00	-	-		
87	OHX	1	3881	-	0,6,6	0.00	-	-		
87	OHX	6	2057	-	0,6,6	0.00	-	-		
87	OHX	1	4124	-	0,6,6	0.00	-	-		
87	OHX	5	4071	-	0,6,6	0.00	-	-		
87	OHX	5	4222	-	0,6,6	0.00	-	-		
87	OHX	5	4162	-	0,6,6	0.00	-	-		
87	OHX	5	4025	-	0,6,6	0.00	-	-		
87	OHX	1	3962	-	0,6,6	0.00	-	-		
87	OHX	2	2145	-	0,6,6	0.00	-	-		
87	OHX	m1	202	-	0,6,6	0.00	-	-		
87	OHX	5	4246	-	0,6,6	0.00	-	-		
87	OHX	2	2126	-	0,6,6	0.00	-	-		
87	OHX	5	3925	-	0,6,6	0.00	-	-		
87	OHX	6	2186	-	0,6,6	0.00	-	-		
87	OHX	n9	103	-	0,6,6	0.00	-	-		
87	OHX	2	2158	-	0,6,6	0.00	-	-		
87	OHX	5	4004	-	0,6,6	0.00	-	-		
87	OHX	5	4062	-	0,6,6	0.00	-	-		
87	OHX	6	2190	-	0,6,6	0.00	-	-		
87	OHX	4	224	-	0,6,6	0.00	-	-		
87	OHX	5	4038	-	0,6,6	0.00	-	-		
87	OHX	m9	201	-	0,6,6	0.00	-	-		
87	OHX	6	2105	-	0,6,6	0.00	-	-		
87	OHX	6	2104	-	0,6,6	0.00	-	-		
87	OHX	1	4010	-	0,6,6	0.00	-	-		
87	OHX	5	3995	-	0,6,6	0.00	-	-		
87	OHX	5	3930	-	0,6,6	0.00	-	-		
87	OHX	q1	102	-	0,6,6	0.00	-	-		
87	OHX	6	2192	-	0,6,6	0.00	-	-		
87	OHX	5	4237	-	0,6,6	0.00	-	-		
87	OHX	1	3914	-	0,6,6	0.00	-	-		
87	OHX	2	2054	-	0,6,6	0.00	-	-		
87	OHX	1	4169	-	0,6,6	0.00	-	-		
87	OHX	4	234	-	0,6,6	0.00	-	-		
87	OHX	6	2166	-	0,6,6	0.00	-	-		
87	OHX	1	4041	-	0,6,6	0.00	-	-		
87	OHX	1	4007	-	0,6,6	0.00	-	-		
87	OHX	1	4102	-	0,6,6	0.00	-	-		
87	OHX	5	3927	-	0,6,6	0.00	-	-		
87	OHX	1	4093	-	0,6,6	0.00	-	-		
87	OHX	1	4096	-	0,6,6	0.00	-	-		
87	OHX	1	3975	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2035	-	0,6,6	0.00	-	-		
87	OHX	8	226	-	0,6,6	0.00	-	-		
87	OHX	6	2121	-	0,6,6	0.00	-	-		
87	OHX	5	3959	-	0,6,6	0.00	-	-		
87	OHX	7	225	-	0,6,6	0.00	-	-		
87	OHX	5	4000	-	0,6,6	0.00	-	-		
87	OHX	5	4136	-	0,6,6	0.00	-	-		
87	OHX	2	2064	-	0,6,6	0.00	-	-		
87	OHX	6	2171	-	0,6,6	0.00	-	-		
87	OHX	1	4163	-	0,6,6	0.00	-	-		
87	OHX	7	219	-	0,6,6	0.00	-	-		
87	OHX	2	2055	-	0,6,6	0.00	-	-		
87	OHX	4	237	-	0,6,6	0.00	-	-		
87	OHX	1	3899	-	0,6,6	0.00	-	-		
87	OHX	1	4198	-	0,6,6	0.00	-	-		
87	OHX	1	4174	-	0,6,6	0.00	-	-		
87	OHX	1	3936	-	0,6,6	0.00	-	-		
87	OHX	2	2049	-	0,6,6	0.00	-	-		
87	OHX	5	3969	-	0,6,6	0.00	-	-		
87	OHX	5	4154	-	0,6,6	0.00	-	-		
87	OHX	1	4001	-	0,6,6	0.00	-	-		
87	OHX	5	4185	-	0,6,6	0.00	-	-		
87	OHX	2	2042	-	0,6,6	0.00	-	-		
87	OHX	8	228	-	0,6,6	0.00	-	-		
87	OHX	2	2152	-	0,6,6	0.00	-	-		
87	OHX	1	4132	-	0,6,6	0.00	-	-		
87	OHX	1	4161	-	0,6,6	0.00	-	-		
87	OHX	6	2073	-	0,6,6	0.00	-	-		
87	OHX	5	3951	-	0,6,6	0.00	-	-		
87	OHX	5	4166	-	0,6,6	0.00	-	-		
87	OHX	1	4033	-	0,6,6	0.00	-	-		
87	OHX	1	4002	-	0,6,6	0.00	-	-		
87	OHX	6	2056	-	0,6,6	0.00	-	-		
87	OHX	2	2070	-	0,6,6	0.00	-	-		
87	OHX	1	4008	-	0,6,6	0.00	-	-		
87	OHX	1	3871	-	0,6,6	0.00	-	-		
87	OHX	1	4071	-	0,6,6	0.00	-	-		
87	OHX	2	2109	-	0,6,6	0.00	-	-		
87	OHX	2	2155	-	0,6,6	0.00	-	-		
87	OHX	3	217	-	0,6,6	0.00	-	-		
87	OHX	5	4068	-	0,6,6	0.00	-	-		
87	OHX	5	4083	-	0,6,6	0.00	-	-		
87	OHX	2	2117	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2118	-	0,6,6	0.00	-	-		
87	OHX	5	4110	-	0,6,6	0.00	-	-		
87	OHX	5	3896	-	0,6,6	0.00	-	-		
87	OHX	1	3918	-	0,6,6	0.00	-	-		
87	OHX	m7	205	-	0,6,6	0.00	-	-		
87	OHX	1	4081	-	0,6,6	0.00	-	-		
87	OHX	5	3900	-	0,6,6	0.00	-	-		
87	OHX	1	4003	-	0,6,6	0.00	-	-		
87	OHX	4	232	-	0,6,6	0.00	-	-		
87	OHX	6	2145	-	0,6,6	0.00	-	-		
87	OHX	1	4075	-	0,6,6	0.00	-	-		
87	OHX	1	4106	-	0,6,6	0.00	-	-		
87	OHX	5	4019	-	0,6,6	0.00	-	-		
87	OHX	1	4080	-	0,6,6	0.00	-	-		
87	OHX	5	4221	-	0,6,6	0.00	-	-		
87	OHX	5	3946	-	0,6,6	0.00	-	-		
87	OHX	2	2043	-	0,6,6	0.00	-	-		
87	OHX	5	4105	-	0,6,6	0.00	-	-		
87	OHX	6	2146	-	0,6,6	0.00	-	-		
87	OHX	6	2080	-	0,6,6	0.00	-	-		
87	OHX	5	3947	-	0,6,6	0.00	-	-		
87	OHX	2	2173	-	0,6,6	0.00	-	-		
87	OHX	5	4206	-	0,6,6	0.00	-	-		
87	OHX	6	2118	-	0,6,6	0.00	-	-		
87	OHX	5	4130	-	0,6,6	0.00	-	-		
87	OHX	6	2133	-	0,6,6	0.00	-	-		
87	OHX	1	3878	-	0,6,6	0.00	-	-		
87	OHX	5	4115	-	0,6,6	0.00	-	-		
87	OHX	2	2163	-	0,6,6	0.00	-	-		
87	OHX	5	4101	-	0,6,6	0.00	-	-		
87	OHX	1	4089	-	0,6,6	0.00	-	-		
87	OHX	5	3910	-	0,6,6	0.00	-	-		
87	OHX	2	2146	-	0,6,6	0.00	-	-		
87	OHX	5	3988	-	0,6,6	0.00	-	-		
87	OHX	2	2178	-	0,6,6	0.00	-	-		
87	OHX	6	2078	-	0,6,6	0.00	-	-		
87	OHX	1	4097	-	0,6,6	0.00	-	-		
87	OHX	1	4023	-	0,6,6	0.00	-	-		
87	OHX	5	4146	-	0,6,6	0.00	-	-		
87	OHX	1	3926	-	0,6,6	0.00	-	-		
87	OHX	5	3953	-	0,6,6	0.00	-	-		
87	OHX	6	2086	-	0,6,6	0.00	-	-		
87	OHX	5	4165	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4057	-	0,6,6	0.00	-	-		
87	OHX	8	219	-	0,6,6	0.00	-	-		
87	OHX	5	4092	-	0,6,6	0.00	-	-		
87	OHX	5	4234	-	0,6,6	0.00	-	-		
87	OHX	6	2141	-	0,6,6	0.00	-	-		
87	OHX	1	4119	-	0,6,6	0.00	-	-		
87	OHX	1	4203	-	0,6,6	0.00	-	-		
87	OHX	3	223	-	0,6,6	0.00	-	-		
87	OHX	6	2113	-	0,6,6	0.00	-	-		
87	OHX	2	2091	-	0,6,6	0.00	-	-		
87	OHX	5	3964	-	0,6,6	0.00	-	-		
87	OHX	1	3908	-	0,6,6	0.00	-	-		
87	OHX	1	4156	-	0,6,6	0.00	-	-		
87	OHX	5	4199	-	0,6,6	0.00	-	-		
87	OHX	5	4102	-	0,6,6	0.00	-	-		
87	OHX	5	4230	-	0,6,6	0.00	-	-		
87	OHX	6	2115	-	0,6,6	0.00	-	-		
87	OHX	1	3935	-	0,6,6	0.00	-	-		
87	OHX	1	4155	-	0,6,6	0.00	-	-		
87	OHX	6	2164	-	0,6,6	0.00	-	-		
87	OHX	5	4180	-	0,6,6	0.00	-	-		
87	OHX	2	2041	-	0,6,6	0.00	-	-		
87	OHX	6	2064	-	0,6,6	0.00	-	-		
87	OHX	5	4047	-	0,6,6	0.00	-	-		
87	OHX	2	2138	-	0,6,6	0.00	-	-		
87	OHX	1	3929	-	0,6,6	0.00	-	-		
87	OHX	5	4037	-	0,6,6	0.00	-	-		
87	OHX	1	4202	-	0,6,6	0.00	-	-		
87	OHX	1	3877	-	0,6,6	0.00	-	-		
87	OHX	O1	202	-	0,6,6	0.00	-	-		
87	OHX	6	2119	-	0,6,6	0.00	-	-		
87	OHX	1	4133	-	0,6,6	0.00	-	-		
87	OHX	5	4188	-	0,6,6	0.00	-	-		
87	OHX	5	4161	-	0,6,6	0.00	-	-		
87	OHX	1	4074	-	0,6,6	0.00	-	-		
87	OHX	2	2180	-	0,6,6	0.00	-	-		
87	OHX	8	230	-	0,6,6	0.00	-	-		
87	OHX	1	4085	-	0,6,6	0.00	-	-		
87	OHX	5	4050	-	0,6,6	0.00	-	-		
87	OHX	1	4147	-	0,6,6	0.00	-	-		
87	OHX	6	2085	-	0,6,6	0.00	-	-		
87	OHX	2	2099	-	0,6,6	0.00	-	-		
87	OHX	6	2062	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2094	-	0,6,6	0.00	-	-		
87	OHX	6	2127	-	0,6,6	0.00	-	-		
87	OHX	5	3996	-	0,6,6	0.00	-	-		
87	OHX	6	2170	-	0,6,6	0.00	-	-		
87	OHX	6	2054	-	0,6,6	0.00	-	-		
87	OHX	5	4157	-	0,6,6	0.00	-	-		
87	OHX	5	4032	-	0,6,6	0.00	-	-		
87	OHX	1	4166	-	0,6,6	0.00	-	-		
87	OHX	6	2149	-	0,6,6	0.00	-	-		
87	OHX	1	4122	-	0,6,6	0.00	-	-		
87	OHX	5	4127	-	0,6,6	0.00	-	-		
87	OHX	5	4091	-	0,6,6	0.00	-	-		
87	OHX	5	4011	-	0,6,6	0.00	-	-		
87	OHX	2	2028	-	0,6,6	0.00	-	-		
87	OHX	M9	203	-	0,6,6	0.00	-	-		
87	OHX	5	3967	-	0,6,6	0.00	-	-		
87	OHX	6	2091	-	0,6,6	0.00	-	-		
87	OHX	6	2161	-	0,6,6	0.00	-	-		
87	OHX	5	4203	-	0,6,6	0.00	-	-		
87	OHX	5	3938	-	0,6,6	0.00	-	-		
87	OHX	1	4138	-	0,6,6	0.00	-	-		
87	OHX	1	4195	-	0,6,6	0.00	-	-		
87	OHX	2	2179	-	0,6,6	0.00	-	-		
87	OHX	1	4035	-	0,6,6	0.00	-	-		
87	OHX	4	233	-	0,6,6	0.00	-	-		
87	OHX	2	2115	-	0,6,6	0.00	-	-		
87	OHX	O7	103	-	0,6,6	0.00	-	-		
87	OHX	5	4085	-	0,6,6	0.00	-	-		
87	OHX	5	4216	-	0,6,6	0.00	-	-		
87	OHX	1	4015	-	0,6,6	0.00	-	-		
87	OHX	5	4093	-	0,6,6	0.00	-	-		
87	OHX	5	3960	-	0,6,6	0.00	-	-		
87	OHX	2	2164	-	0,6,6	0.00	-	-		
87	OHX	6	2152	-	0,6,6	0.00	-	-		
87	OHX	1	4110	-	0,6,6	0.00	-	-		
87	OHX	l3	407	-	0,6,6	0.00	-	-		
87	OHX	1	4185	-	0,6,6	0.00	-	-		
87	OHX	1	4032	-	0,6,6	0.00	-	-		
87	OHX	l5	304	-	0,6,6	0.00	-	-		
87	OHX	5	4072	-	0,6,6	0.00	-	-		
87	OHX	2	2075	-	0,6,6	0.00	-	-		
87	OHX	1	3988	-	0,6,6	0.00	-	-		
87	OHX	6	2211	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3911	-	0,6,6	0.00	-	-		
87	OHX	1	4088	-	0,6,6	0.00	-	-		
87	OHX	6	2136	-	0,6,6	0.00	-	-		
87	OHX	8	229	-	0,6,6	0.00	-	-		
87	OHX	1	4126	-	0,6,6	0.00	-	-		
87	OHX	8	234	-	0,6,6	0.00	-	-		
87	OHX	1	3949	-	0,6,6	0.00	-	-		
87	OHX	1	4196	-	0,6,6	0.00	-	-		
87	OHX	2	2154	-	0,6,6	0.00	-	-		
87	OHX	1	3954	-	0,6,6	0.00	-	-		
87	OHX	6	2134	-	0,6,6	0.00	-	-		
87	OHX	2	2092	-	0,6,6	0.00	-	-		
87	OHX	5	4238	-	0,6,6	0.00	-	-		
87	OHX	1	4146	-	0,6,6	0.00	-	-		
87	OHX	5	3949	-	0,6,6	0.00	-	-		
87	OHX	5	3971	-	0,6,6	0.00	-	-		
87	OHX	1	4005	-	0,6,6	0.00	-	-		
87	OHX	1	3893	-	0,6,6	0.00	-	-		
87	OHX	5	3956	-	0,6,6	0.00	-	-		
87	OHX	1	4159	-	0,6,6	0.00	-	-		
87	OHX	2	2106	-	0,6,6	0.00	-	-		
87	OHX	1	4193	-	0,6,6	0.00	-	-		
87	OHX	5	3954	-	0,6,6	0.00	-	-		
87	OHX	1	4040	-	0,6,6	0.00	-	-		
87	OHX	1	3985	-	0,6,6	0.00	-	-		
87	OHX	1	3997	-	0,6,6	0.00	-	-		
87	OHX	1	4149	-	0,6,6	0.00	-	-		
87	OHX	6	2169	-	0,6,6	0.00	-	-		
87	OHX	1	3996	36	0,6,6	0.00	-	-		
87	OHX	6	2172	-	0,6,6	0.00	-	-		
87	OHX	1	4020	-	0,6,6	0.00	-	-		
87	OHX	1	3986	-	0,6,6	0.00	-	-		
87	OHX	5	4078	-	0,6,6	0.00	-	-		
87	OHX	5	4226	-	0,6,6	0.00	-	-		
87	OHX	1	3938	-	0,6,6	0.00	-	-		
87	OHX	5	4126	-	0,6,6	0.00	-	-		
87	OHX	5	4141	-	0,6,6	0.00	-	-		
87	OHX	2	2077	-	0,6,6	0.00	-	-		
87	OHX	5	3952	-	0,6,6	0.00	-	-		
87	OHX	5	4059	-	0,6,6	0.00	-	-		
87	OHX	2	2168	-	0,6,6	0.00	-	-		
87	OHX	1	4211	-	0,6,6	0.00	-	-		
87	OHX	5	4198	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2176	-	0,6,6	0.00	-	-		
87	OHX	5	4225	-	0,6,6	0.00	-	-		
87	OHX	1	4017	-	0,6,6	0.00	-	-		
87	OHX	1	3972	-	0,6,6	0.00	-	-		
87	OHX	2	2137	-	0,6,6	0.00	-	-		
87	OHX	1	4153	-	0,6,6	0.00	-	-		
87	OHX	5	4097	-	0,6,6	0.00	-	-		
87	OHX	5	3972	-	0,6,6	0.00	-	-		
87	OHX	5	4214	-	0,6,6	0.00	-	-		
87	OHX	1	4000	-	0,6,6	0.00	-	-		
87	OHX	5	3987	-	0,6,6	0.00	-	-		
87	OHX	6	2181	-	0,6,6	0.00	-	-		
87	OHX	6	2210	-	0,6,6	0.00	-	-		
87	OHX	5	4160	-	0,6,6	0.00	-	-		
87	OHX	5	4190	-	0,6,6	0.00	-	-		
87	OHX	1	3970	-	0,6,6	0.00	-	-		
87	OHX	1	4083	-	0,6,6	0.00	-	-		
87	OHX	6	2155	-	0,6,6	0.00	-	-		
87	OHX	m5	303	-	0,6,6	0.00	-	-		
87	OHX	5	4232	-	0,6,6	0.00	-	-		
87	OHX	6	2131	-	0,6,6	0.00	-	-		
87	OHX	M9	202	-	0,6,6	0.00	-	-		
87	OHX	5	3985	-	0,6,6	0.00	-	-		
87	OHX	5	4028	-	0,6,6	0.00	-	-		
87	OHX	1	3998	-	0,6,6	0.00	-	-		
87	OHX	1	3968	-	0,6,6	0.00	-	-		
87	OHX	5	4045	-	0,6,6	0.00	-	-		
87	OHX	M7	206	-	0,6,6	0.00	-	-		
87	OHX	1	4176	-	0,6,6	0.00	-	-		
87	OHX	5	4016	-	0,6,6	0.00	-	-		
87	OHX	5	4178	-	0,6,6	0.00	-	-		
87	OHX	6	2109	-	0,6,6	0.00	-	-		
87	OHX	1	4180	-	0,6,6	0.00	-	-		
87	OHX	5	4143	-	0,6,6	0.00	-	-		
87	OHX	1	4073	-	0,6,6	0.00	-	-		
87	OHX	1	4026	-	0,6,6	0.00	-	-		
87	OHX	1	3965	-	0,6,6	0.00	-	-		
87	OHX	5	4002	-	0,6,6	0.00	-	-		
87	OHX	1	3940	-	0,6,6	0.00	-	-		
87	OHX	2	2074	-	0,6,6	0.00	-	-		
87	OHX	1	4197	-	0,6,6	0.00	-	-		
87	OHX	1	4006	-	0,6,6	0.00	-	-		
87	OHX	1	4079	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3868	-	0,6,6	0.00	-	-		
87	OHX	6	2163	-	0,6,6	0.00	-	-		
87	OHX	5	4233	-	0,6,6	0.00	-	-		
87	OHX	M5	303	-	0,6,6	0.00	-	-		
87	OHX	1	4028	-	0,6,6	0.00	-	-		
87	OHX	6	2101	-	0,6,6	0.00	-	-		
87	OHX	1	4179	-	0,6,6	0.00	-	-		
87	OHX	2	2066	-	0,6,6	0.00	-	-		
87	OHX	5	3994	-	0,6,6	0.00	-	-		
87	OHX	5	4039	-	0,6,6	0.00	-	-		
87	OHX	1	4090	-	0,6,6	0.00	-	-		
87	OHX	6	2065	-	0,6,6	0.00	-	-		
87	OHX	5	4113	-	0,6,6	0.00	-	-		
87	OHX	1	4043	-	0,6,6	0.00	-	-		
87	OHX	5	3904	-	0,6,6	0.00	-	-		
87	OHX	5	4073	-	0,6,6	0.00	-	-		
87	OHX	1	4058	-	0,6,6	0.00	-	-		
87	OHX	5	3973	-	0,6,6	0.00	-	-		
87	OHX	6	2092	-	0,6,6	0.00	-	-		
87	OHX	2	2101	-	0,6,6	0.00	-	-		
87	OHX	2	2063	-	0,6,6	0.00	-	-		
87	OHX	1	3961	-	0,6,6	0.00	-	-		
87	OHX	2	2149	-	0,6,6	0.00	-	-		
87	OHX	1	4046	-	0,6,6	0.00	-	-		
87	OHX	1	4199	-	0,6,6	0.00	-	-		
87	OHX	3	220	-	0,6,6	0.00	-	-		
87	OHX	2	2056	-	0,6,6	0.00	-	-		
87	OHX	5	4224	-	0,6,6	0.00	-	-		
87	OHX	m4	202	-	0,6,6	0.00	-	-		
87	OHX	5	4158	-	0,6,6	0.00	-	-		
87	OHX	1	4031	-	0,6,6	0.00	-	-		
87	OHX	5	4151	-	0,6,6	0.00	-	-		
87	OHX	1	3955	-	0,6,6	0.00	-	-		
87	OHX	6	2153	-	0,6,6	0.00	-	-		
87	OHX	2	2048	-	0,6,6	0.00	-	-		
87	OHX	6	2087	-	0,6,6	0.00	-	-		
87	OHX	7	218	-	0,6,6	0.00	-	-		
87	OHX	2	2162	-	0,6,6	0.00	-	-		
87	OHX	1	4175	-	0,6,6	0.00	-	-		
87	OHX	1	3885	-	0,6,6	0.00	-	-		
87	OHX	6	2112	-	0,6,6	0.00	-	-		
87	OHX	5	3966	-	0,6,6	0.00	-	-		
87	OHX	1	3915	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3909	-	0,6,6	0.00	-	-		
87	OHX	6	2140	-	0,6,6	0.00	-	-		
87	OHX	1	4162	-	0,6,6	0.00	-	-		
87	OHX	8	223	-	0,6,6	0.00	-	-		
87	OHX	5	3933	-	0,6,6	0.00	-	-		
87	OHX	5	4070	-	0,6,6	0.00	-	-		
87	OHX	5	4030	-	0,6,6	0.00	-	-		
87	OHX	6	2142	-	0,6,6	0.00	-	-		
87	OHX	5	3932	-	0,6,6	0.00	-	-		
87	OHX	2	2128	-	0,6,6	0.00	-	-		
87	OHX	4	240	-	0,6,6	0.00	-	-		
87	OHX	5	3929	-	0,6,6	0.00	-	-		
87	OHX	2	2040	-	0,6,6	0.00	-	-		
87	OHX	6	2180	-	0,6,6	0.00	-	-		
87	OHX	5	3961	-	0,6,6	0.00	-	-		
87	OHX	1	4087	-	0,6,6	0.00	-	-		
87	OHX	1	3976	-	0,6,6	0.00	-	-		
87	OHX	6	2137	-	0,6,6	0.00	-	-		
87	OHX	2	2039	-	0,6,6	0.00	-	-		
87	OHX	5	4119	-	0,6,6	0.00	-	-		
87	OHX	1	4055	-	0,6,6	0.00	-	-		
87	OHX	6	2159	-	0,6,6	0.00	-	-		
87	OHX	1	3953	-	0,6,6	0.00	-	-		
87	OHX	2	2093	-	0,6,6	0.00	-	-		
87	OHX	5	4087	-	0,6,6	0.00	-	-		
87	OHX	8	224	-	0,6,6	0.00	-	-		
87	OHX	6	2069	-	0,6,6	0.00	-	-		
87	OHX	5	3975	-	0,6,6	0.00	-	-		
87	OHX	2	2177	-	0,6,6	0.00	-	-		
87	OHX	8	235	-	0,6,6	0.00	-	-		
87	OHX	1	4109	-	0,6,6	0.00	-	-		
87	OHX	1	4066	-	0,6,6	0.00	-	-		
87	OHX	1	4048	-	0,6,6	0.00	-	-		
87	OHX	5	4010	-	0,6,6	0.00	-	-		
87	OHX	5	3965	-	0,6,6	0.00	-	-		
87	OHX	6	2167	-	0,6,6	0.00	-	-		
87	OHX	1	4012	-	0,6,6	0.00	-	-		
87	OHX	2	2170	-	0,6,6	0.00	-	-		
87	OHX	1	4021	-	0,6,6	0.00	-	-		
87	OHX	1	3911	-	0,6,6	0.00	-	-		
87	OHX	2	2141	-	0,6,6	0.00	-	-		
87	OHX	1	3980	-	0,6,6	0.00	-	-		
87	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
87	OHX	6	2162	-	0,6,6	0.00	-	-		
87	OHX	6	2103	-	0,6,6	0.00	-	-		
87	OHX	6	2157	-	0,6,6	0.00	-	-		
87	OHX	5	4189	-	0,6,6	0.00	-	-		
87	OHX	1	4120	-	0,6,6	0.00	-	-		
87	OHX	2	2058	-	0,6,6	0.00	-	-		
87	OHX	6	2126	-	0,6,6	0.00	-	-		
87	OHX	1	4137	-	0,6,6	0.00	-	-		
87	OHX	2	2085	-	0,6,6	0.00	-	-		
87	OHX	6	2193	-	0,6,6	0.00	-	-		
87	OHX	2	2082	-	0,6,6	0.00	-	-		
87	OHX	2	2166	-	0,6,6	0.00	-	-		
87	OHX	1	3894	-	0,6,6	0.00	-	-		
87	OHX	5	4175	-	0,6,6	0.00	-	-		
87	OHX	4	235	-	0,6,6	0.00	-	-		
87	OHX	2	2057	-	0,6,6	0.00	-	-		
87	OHX	2	2156	-	0,6,6	0.00	-	-		
87	OHX	C3	201	-	0,6,6	0.00	-	-		
87	OHX	1	3990	-	0,6,6	0.00	-	-		
87	OHX	6	2160	-	0,6,6	0.00	-	-		
87	OHX	2	2131	-	0,6,6	0.00	-	-		
87	OHX	1	4151	-	0,6,6	0.00	-	-		
87	OHX	5	4015	-	0,6,6	0.00	-	-		
87	OHX	1	4027	-	0,6,6	0.00	-	-		
87	OHX	14	402	-	0,6,6	0.00	-	-		
87	OHX	1	3933	-	0,6,6	0.00	-	-		
87	OHX	2	2067	-	0,6,6	0.00	-	-		
87	OHX	2	2147	-	0,6,6	0.00	-	-		
87	OHX	5	4020	-	0,6,6	0.00	-	-		
87	OHX	1	4038	-	0,6,6	0.00	-	-		
87	OHX	1	3898	-	0,6,6	0.00	-	-		
87	OHX	15	305	-	0,6,6	0.00	-	-		
87	OHX	1	3897	-	0,6,6	0.00	-	-		
87	OHX	5	3894	-	0,6,6	0.00	-	-		
87	OHX	5	4211	-	0,6,6	0.00	-	-		
87	OHX	5	3916	-	0,6,6	0.00	-	-		
87	OHX	1	4112	-	0,6,6	0.00	-	-		
87	OHX	5	4172	-	0,6,6	0.00	-	-		
87	OHX	1	3964	-	0,6,6	0.00	-	-		
87	OHX	5	3931	-	0,6,6	0.00	-	-		
87	OHX	6	2074	-	0,6,6	0.00	-	-		
87	OHX	6	2122	-	0,6,6	0.00	-	-		
87	OHX	5	3919	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3966	-	0,6,6	0.00	-	-		
87	OHX	m0	302	-	0,6,6	0.00	-	-		
87	OHX	1	4136	-	0,6,6	0.00	-	-		
87	OHX	6	2151	-	0,6,6	0.00	-	-		
87	OHX	1	4186	-	0,6,6	0.00	-	-		
87	OHX	1	4168	-	0,6,6	0.00	-	-		
87	OHX	1	3902	-	0,6,6	0.00	-	-		
87	OHX	1	3867	-	0,6,6	0.00	-	-		
87	OHX	1	4115	-	0,6,6	0.00	-	-		
87	OHX	2	2036	-	0,6,6	0.00	-	-		
87	OHX	4	236	-	0,6,6	0.00	-	-		
87	OHX	6	2201	-	0,6,6	0.00	-	-		
87	OHX	5	4031	-	0,6,6	0.00	-	-		
87	OHX	6	2202	-	0,6,6	0.00	-	-		
87	OHX	5	4134	-	0,6,6	0.00	-	-		
87	OHX	5	3906	-	0,6,6	0.00	-	-		
87	OHX	5	4181	-	0,6,6	0.00	-	-		
87	OHX	7	220	-	0,6,6	0.00	-	-		
87	OHX	1	4183	-	0,6,6	0.00	-	-		
87	OHX	1	4030	-	0,6,6	0.00	-	-		
87	OHX	1	4101	-	0,6,6	0.00	-	-		
87	OHX	2	2114	-	0,6,6	0.00	-	-		
87	OHX	5	4121	-	0,6,6	0.00	-	-		
87	OHX	6	2188	-	0,6,6	0.00	-	-		
87	OHX	1	3963	-	0,6,6	0.00	-	-		
87	OHX	2	2053	-	0,6,6	0.00	-	-		
87	OHX	2	2169	-	0,6,6	0.00	-	-		
87	OHX	6	2108	-	0,6,6	0.00	-	-		
87	OHX	d4	201	-	0,6,6	0.00	-	-		
87	OHX	s1	302	-	0,6,6	0.00	-	-		
87	OHX	7	217	-	0,6,6	0.00	-	-		
87	OHX	1	4067	-	0,6,6	0.00	-	-		
87	OHX	1	4022	-	0,6,6	0.00	-	-		
87	OHX	2	2136	-	0,6,6	0.00	-	-		
87	OHX	5	3921	-	0,6,6	0.00	-	-		
87	OHX	2	2160	-	0,6,6	0.00	-	-		
87	OHX	5	4171	-	0,6,6	0.00	-	-		
87	OHX	6	2130	-	0,6,6	0.00	-	-		
87	OHX	7	222	-	0,6,6	0.00	-	-		
87	OHX	3	222	-	0,6,6	0.00	-	-		
87	OHX	6	2165	-	0,6,6	0.00	-	-		
87	OHX	5	3942	-	0,6,6	0.00	-	-		
87	OHX	1	4189	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3923	-	0,6,6	0.00	-	-		
87	OHX	5	3999	-	0,6,6	0.00	-	-		
87	OHX	2	2069	-	0,6,6	0.00	-	-		
87	OHX	5	4220	-	0,6,6	0.00	-	-		
87	OHX	1	4014	-	0,6,6	0.00	-	-		
87	OHX	1	4188	-	0,6,6	0.00	-	-		
87	OHX	2	2140	-	0,6,6	0.00	-	-		
87	OHX	5	4231	-	0,6,6	0.00	-	-		
87	OHX	6	2097	-	0,6,6	0.00	-	-		
87	OHX	6	2208	-	0,6,6	0.00	-	-		
87	OHX	c5	201	-	0,6,6	0.00	-	-		
87	OHX	l5	307	-	0,6,6	0.00	-	-		
87	OHX	1	4165	-	0,6,6	0.00	-	-		
87	OHX	2	2079	-	0,6,6	0.00	-	-		
87	OHX	5	4048	-	0,6,6	0.00	-	-		
87	OHX	5	4177	-	0,6,6	0.00	-	-		
87	OHX	5	3915	-	0,6,6	0.00	-	-		
87	OHX	6	2156	-	0,6,6	0.00	-	-		
87	OHX	6	2158	-	0,6,6	0.00	-	-		
87	OHX	6	2090	-	0,6,6	0.00	-	-		
87	OHX	5	3962	-	0,6,6	0.00	-	-		
87	OHX	2	2107	-	0,6,6	0.00	-	-		
87	OHX	8	232	-	0,6,6	0.00	-	-		
87	OHX	2	2052	-	0,6,6	0.00	-	-		
87	OHX	1	3973	-	0,6,6	0.00	-	-		
87	OHX	7	226	-	0,6,6	0.00	-	-		
87	OHX	O7	104	-	0,6,6	0.00	-	-		
87	OHX	6	2088	-	0,6,6	0.00	-	-		
87	OHX	3	221	-	0,6,6	0.00	-	-		
87	OHX	1	3923	-	0,6,6	0.00	-	-		
87	OHX	5	4075	-	0,6,6	0.00	-	-		
87	OHX	5	3939	-	0,6,6	0.00	-	-		
87	OHX	1	4098	-	0,6,6	0.00	-	-		
87	OHX	2	2124	-	0,6,6	0.00	-	-		
87	OHX	1	4078	-	0,6,6	0.00	-	-		
87	OHX	5	4005	-	0,6,6	0.00	-	-		
87	OHX	1	3959	-	0,6,6	0.00	-	-		
87	OHX	8	218	-	0,6,6	0.00	-	-		
87	OHX	5	4122	-	0,6,6	0.00	-	-		
87	OHX	2	2123	-	0,6,6	0.00	-	-		
87	OHX	5	4023	-	0,6,6	0.00	-	-		
87	OHX	5	4112	-	0,6,6	0.00	-	-		
87	OHX	5	3958	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3917	-	0,6,6	0.00	-	-		
87	OHX	6	2150	-	0,6,6	0.00	-	-		
87	OHX	5	4245	-	0,6,6	0.00	-	-		
87	OHX	6	2068	-	0,6,6	0.00	-	-		
87	OHX	4	226	-	0,6,6	0.00	-	-		
87	OHX	2	2129	-	0,6,6	0.00	-	-		
87	OHX	5	4149	-	0,6,6	0.00	-	-		
87	OHX	5	4209	-	0,6,6	0.00	-	-		
87	OHX	1	3982	-	0,6,6	0.00	-	-		
87	OHX	5	4003	-	0,6,6	0.00	-	-		
87	OHX	1	3987	-	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	GET	2	2181	-	-	1/13/74/74	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	2	2181	GET	C23-C33-N33	-6.00	94.93	110.84
88	2	2181	GET	O11-C42-C32	-5.70	95.57	109.18
88	2	2181	GET	O62-C62-C12	-3.45	100.96	109.18
88	2	2181	GET	O11-C11-C21	-3.34	102.47	108.22
88	2	2181	GET	C32-C22-C12	2.58	116.47	111.18

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	2	2181	GET	C52-C62-O62-C13

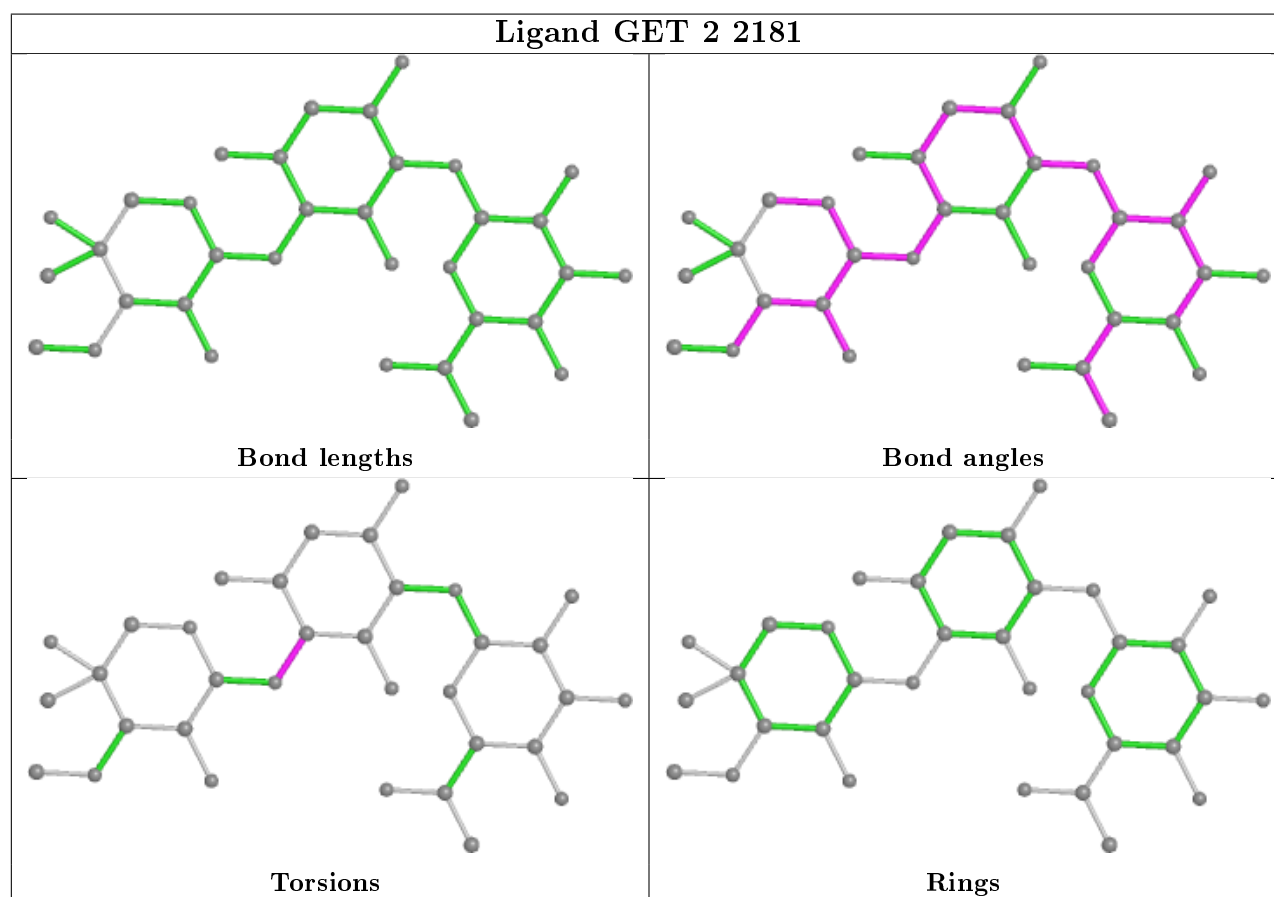
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	4023	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.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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