



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 12, 2020 – 07:12 PM BST

PDB ID : 4U3N  
Title : Crystal structure of CCA trinucleotide bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-22  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
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) : 2.14.4.dev1

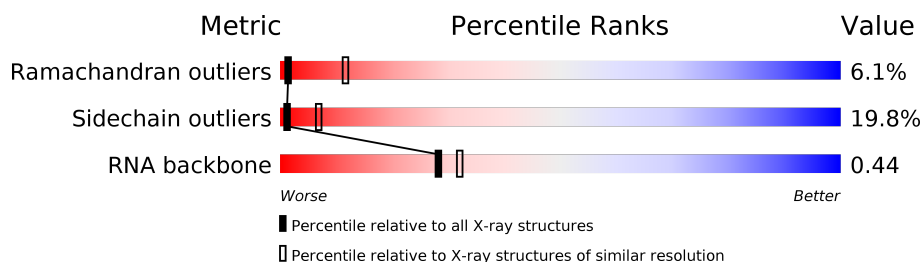
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



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





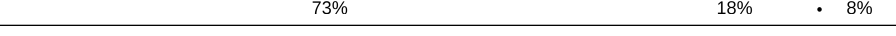
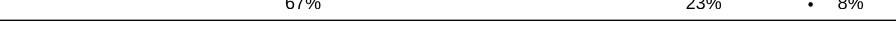
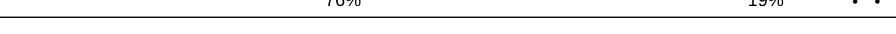
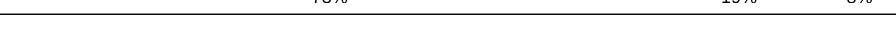
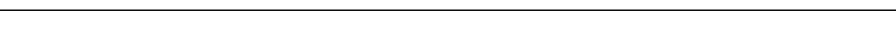

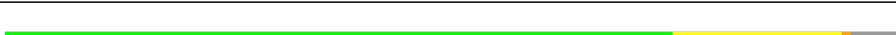














The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	64% 29% . .
1	6	1800	64% 30% 5%
2	S0	251	64% 15% . 18%
2	s0	251	61% 20% . 18%
3	S1	254	57% 24% . 16%
3	s1	254	65% 19% . 15%
4	S2	253	63% 22% . 14%
4	s2	253	64% 20% . 14%

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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
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	
17	c5	141	















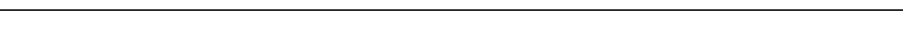




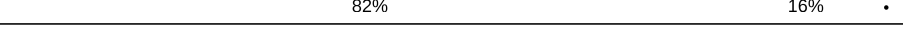





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Mol	Chain	Length	Quality of chain
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	











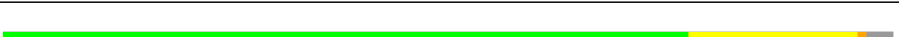


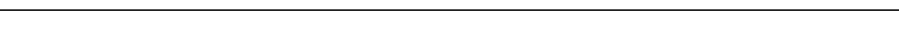











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Mol	Chain	Length	Quality of chain
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	


























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Mol	Chain	Length	Quality of chain
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	
56	N0	172	


























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Mol	Chain	Length	Quality of chain
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	
68	o2	129	

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Mol	Chain	Length	Quality of chain
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	c0	105	
81	e0	62	
82	e1	76	

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Mol	Chain	Length	Quality of chain
83	m2	160	<div><div></div><div>94%</div><div>6%</div></div>
84	p0	311	<div><div></div><div>37%</div><div>8%</div><div>54%</div></div>
85	p1	47	<div><div></div><div>100%</div></div>
86	p2	46	<div><div></div><div>100%</div></div>

## 2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 411288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

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

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

- Molecule 35 is a protein called Suppressor protein STM1.



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	S	0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O	S	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 S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 81 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S31.

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

- Molecule 83 is a protein called UNKNOWN PROTEIN m2.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 86 is a protein called UNKNOWN PROTEIN p2.

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

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	L7	4	Total	Mg	0	0
			4	4		
87	n8	3	Total	Mg	0	0
			3	3		
87	o1	1	Total	Mg	0	0
			1	1		
87	N5	1	Total	Mg	0	0
			1	1		
87	6	144	Total	Mg	0	0
			144	144		
87	sM	1	Total	Mg	0	0
			1	1		
87	O4	1	Total	Mg	0	0
			1	1		
87	m5	5	Total	Mg	0	0
			5	5		
87	l3	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	M1	1	Total 1	Mg 1	0	0
87	d6	1	Total 1	Mg 1	0	0
87	2	124	Total 124	Mg 124	0	0
87	n0	3	Total 3	Mg 3	0	0
87	L4	1	Total 1	Mg 1	0	0
87	l7	1	Total 1	Mg 1	0	0
87	M5	2	Total 2	Mg 2	0	0
87	c9	1	Total 1	Mg 1	0	0
87	L8	1	Total 1	Mg 1	0	0
87	D3	1	Total 1	Mg 1	0	0
87	o4	1	Total 1	Mg 1	0	0
87	M9	1	Total 1	Mg 1	0	0
87	q0	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	c8	1	Total 1	Mg 1	0	0
87	M0	2	Total 2	Mg 2	0	0
87	c1	1	Total 1	Mg 1	0	0
87	5	502	Total 502	Mg 502	0	0
87	L5	1	Total 1	Mg 1	0	0
87	O7	1	Total 1	Mg 1	0	0
87	s6	1	Total 1	Mg 1	0	0

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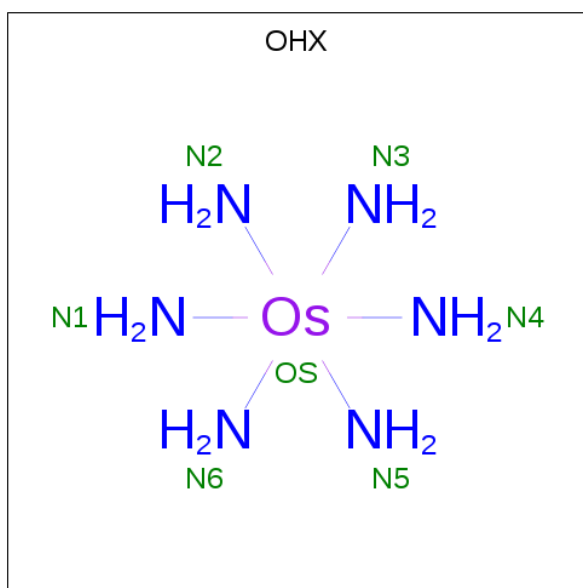
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	l4	2	Total 2	Mg 2	0	0
87	d4	1	Total 1	Mg 1	0	0
87	1	477	Total 477	Mg 477	0	0
87	d3	1	Total 1	Mg 1	0	0
87	S8	1	Total 1	Mg 1	0	0
87	m1	2	Total 2	Mg 2	0	0
87	O2	1	Total 1	Mg 1	0	0
87	q3	2	Total 2	Mg 2	0	0
87	o3	1	Total 1	Mg 1	0	0
87	M3	2	Total 2	Mg 2	0	0
87	N3	3	Total 3	Mg 3	0	0
87	4	19	Total 19	Mg 19	0	0
87	n6	2	Total 2	Mg 2	0	0
87	S4	2	Total 2	Mg 2	0	0
87	L2	1	Total 1	Mg 1	0	0
87	l5	2	Total 2	Mg 2	0	0
87	m7	5	Total 5	Mg 5	0	0
87	M7	4	Total 4	Mg 4	0	0
87	N8	5	Total 5	Mg 5	0	0
87	s1	1	Total 1	Mg 1	0	0
87	m6	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	s8	3	Total 3	Mg 3	0	0
87	c7	2	Total 2	Mg 2	0	0
87	7	15	Total 15	Mg 15	0	0
87	n3	2	Total 2	Mg 2	0	0
87	q1	1	Total 1	Mg 1	0	0
87	L3	3	Total 3	Mg 3	0	0
87	O5	1	Total 1	Mg 1	0	0
87	l2	1	Total 1	Mg 1	0	0
87	8	16	Total 16	Mg 16	0	0
87	M6	1	Total 1	Mg 1	0	0
87	N0	1	Total 1	Mg 1	0	0
87	3	14	Total 14	Mg 14	0	0

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	3	1	Total	N	Os	0	0
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88	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	L3	1	Total	N	Os	0	0
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88	L3	1	Total	N	Os	0	0
			7	6	1		
88	L3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	M5	1	Total	N	Os	0	0
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88	M7	1	Total	N	Os	0	0
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88	M7	1	Total	N	Os	0	0
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88	M8	1	Total	N	Os	0	0
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88	M9	1	Total	N	Os	0	0
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88	N9	1	Total	N	Os	0	0
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88	O3	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	s1	1	Total 7	N 6	Os 1	0	0
88	s1	1	Total 7	N 6	Os 1	0	0
88	s8	1	Total 7	N 6	Os 1	0	0
88	c1	1	Total 7	N 6	Os 1	0	0
88	c3	1	Total 7	N 6	Os 1	0	0
88	c5	1	Total 7	N 6	Os 1	0	0
88	c8	1	Total 7	N 6	Os 1	0	0
88	d4	1	Total 7	N 6	Os 1	0	0
88	d9	1	Total 7	N 6	Os 1	0	0
88	sR	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	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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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		

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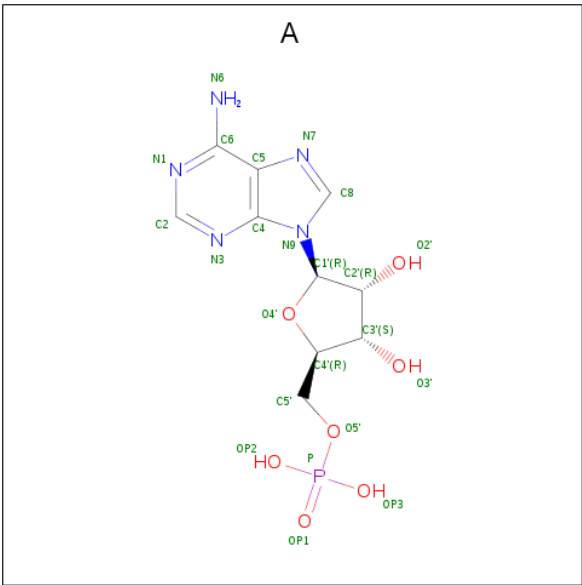
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	l4	1	Total	N	Os	0	0
			7	6	1		
88	l4	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l9	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m1	1	Total	N	Os	0	0
			7	6	1		
88	m4	1	Total	N	Os	0	0
			7	6	1		
88	m5	1	Total	N	Os	0	0
			7	6	1		
88	m6	1	Total	N	Os	0	0
			7	6	1		
88	n3	1	Total	N	Os	0	0
			7	6	1		
88	n3	1	Total	N	Os	0	0
			7	6	1		
88	n9	1	Total	N	Os	0	0
			7	6	1		
88	o3	1	Total	N	Os	0	0
			7	6	1		
88	o7	1	Total	N	Os	0	0
			7	6	1		
88	q2	1	Total	N	Os	0	0
			7	6	1		

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

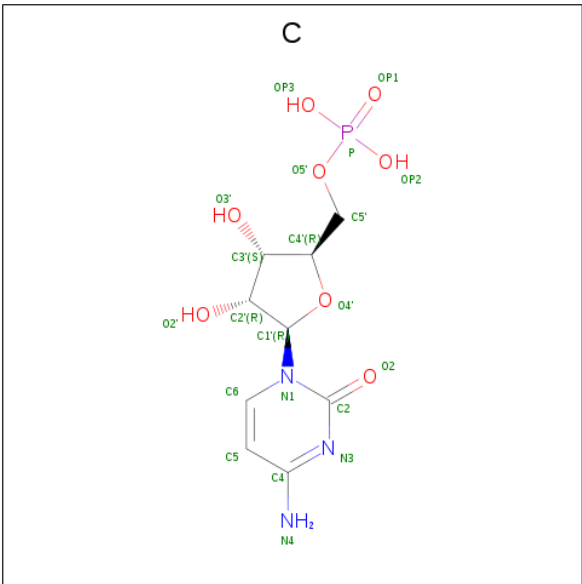
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	q0	1	Total Zn 1 1	0	0
89	D6	1	Total Zn 1 1	0	0
89	Q2	1	Total Zn 1 1	0	0
89	e1	1	Total Zn 1 1	0	0
89	Q3	1	Total Zn 1 1	0	0
89	D9	1	Total Zn 1 1	0	0
89	E1	1	Total Zn 1 1	0	0
89	Q0	1	Total Zn 1 1	0	0
89	d7	1	Total Zn 1 1	0	0
89	q3	1	Total Zn 1 1	0	0
89	d9	1	Total Zn 1 1	0	0
89	D7	1	Total Zn 1 1	0	0
89	d6	1	Total Zn 1 1	0	0
89	o7	1	Total Zn 1 1	0	0
89	O7	1	Total Zn 1 1	0	0
89	q2	1	Total Zn 1 1	0	0

- Molecule 90 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
90	1	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
90	5	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 91 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula:  $C_9H_{14}N_3O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

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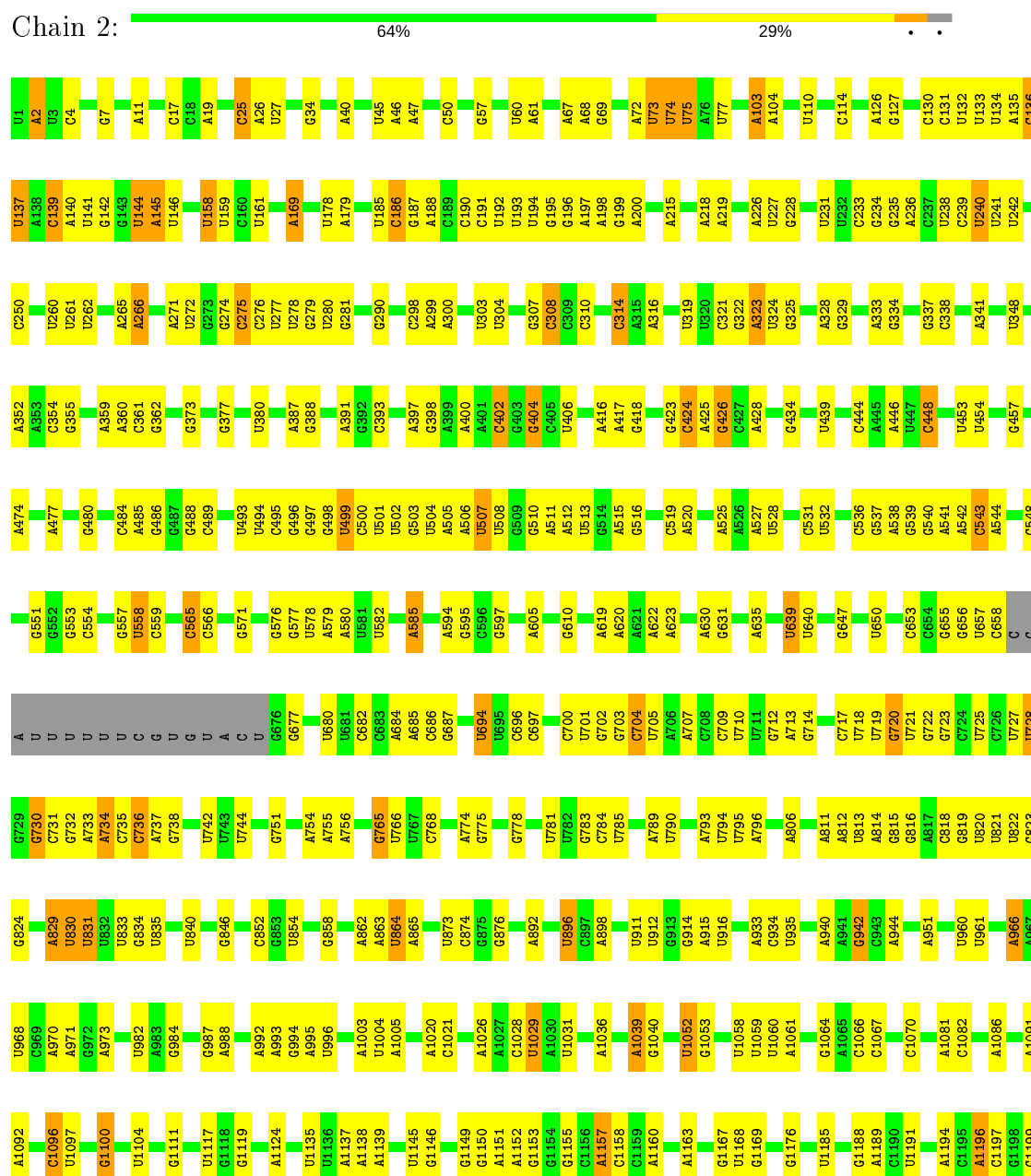
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

### 3 Residue-property plots

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

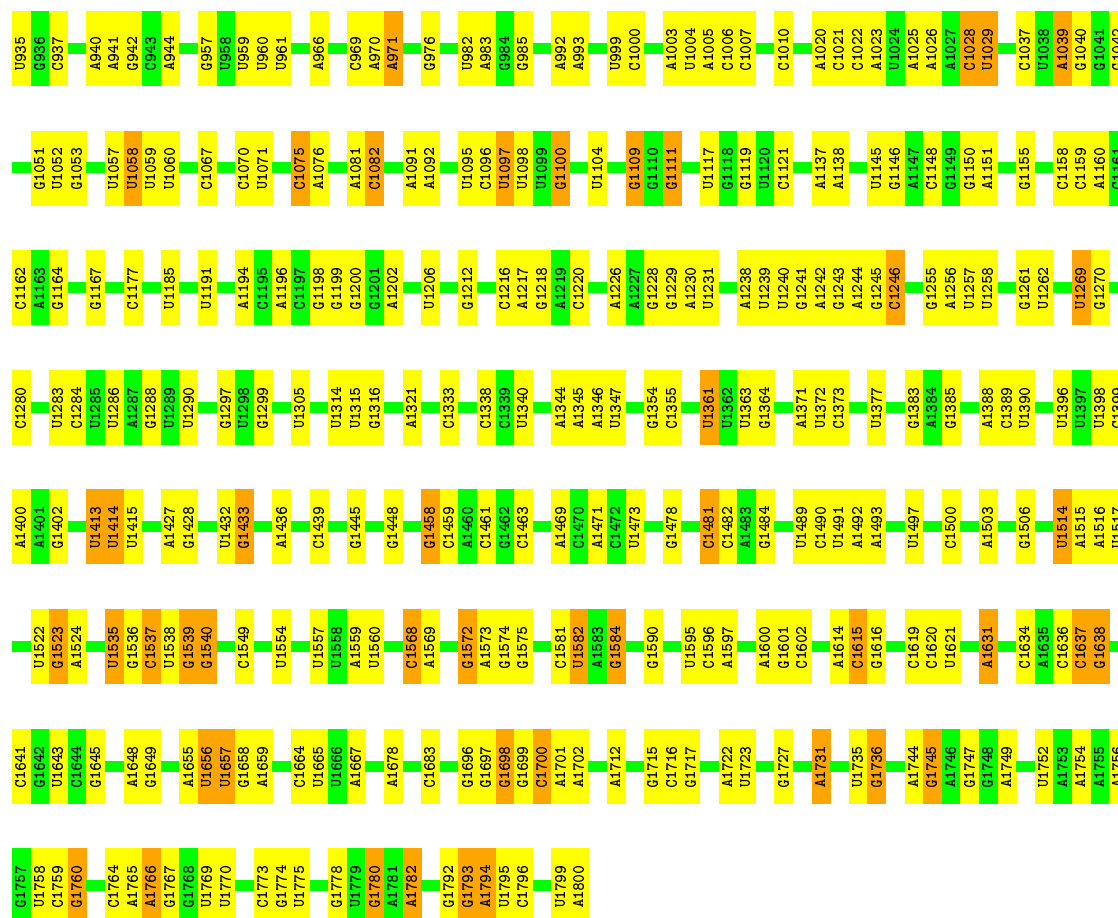
Note EDS failed to run properly.

- Molecule 1: 18S ribosomal RNA



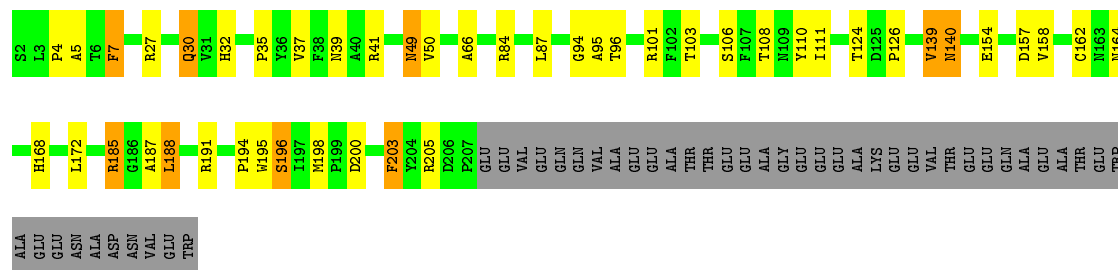






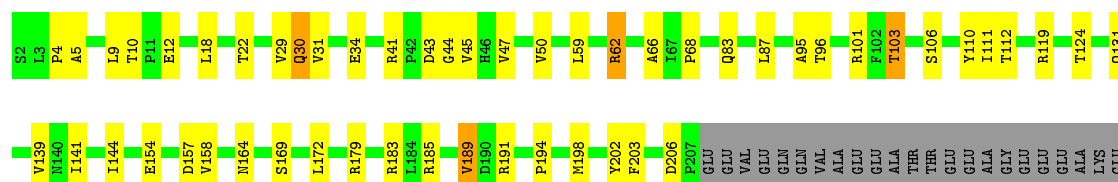
• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 64% 15% 18%

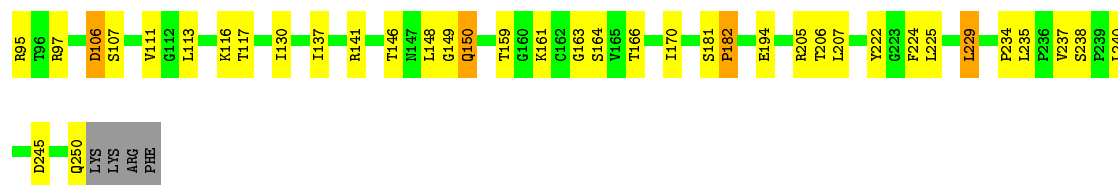


• Molecule 2: 40S ribosomal protein S0-A

Chain s0: 61% 20% 18%

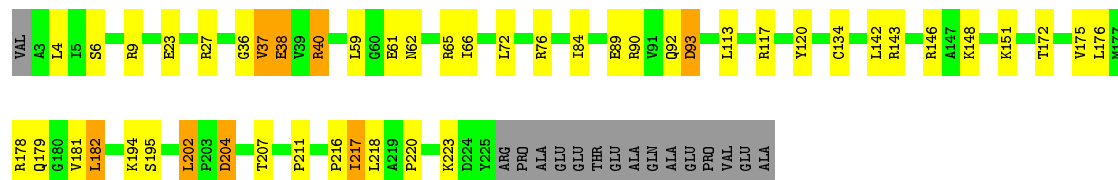






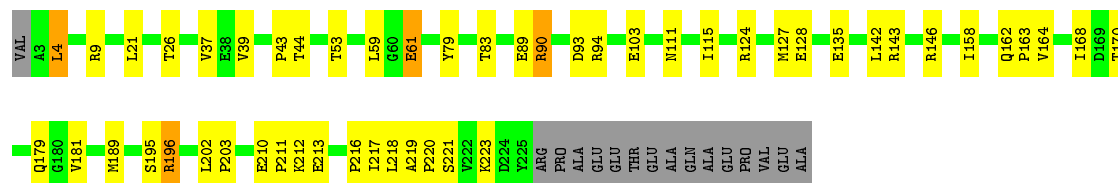
- Molecule 5: 40S ribosomal protein S3

Chain S3:



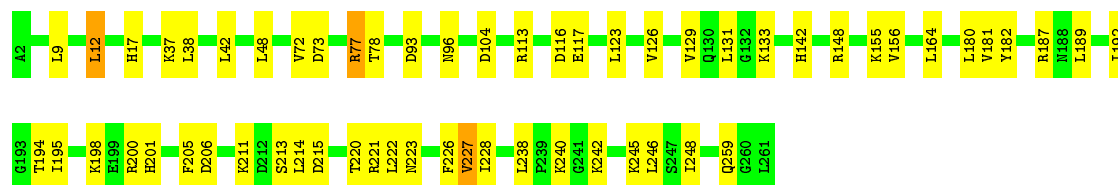
- Molecule 5: 40S ribosomal protein S3

Chain s3:



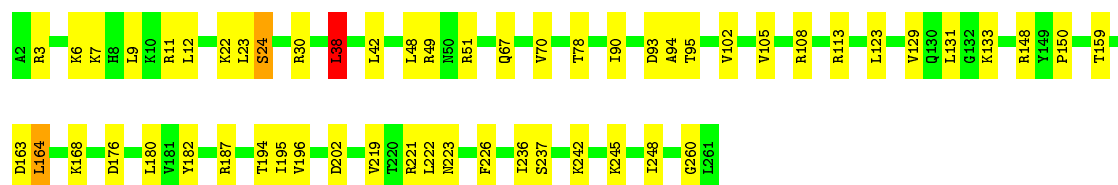
- Molecule 6: 40S ribosomal protein S4-A

Chain S4:



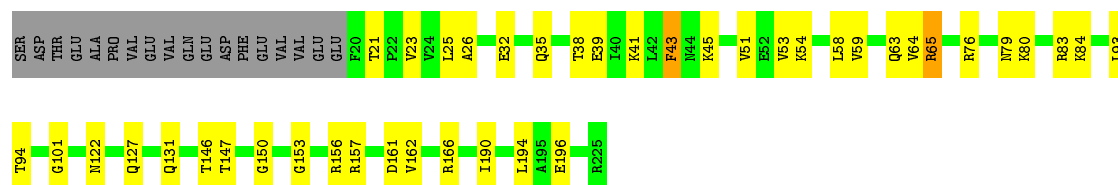
- Molecule 6: 40S ribosomal protein S4-A

Chain s4:



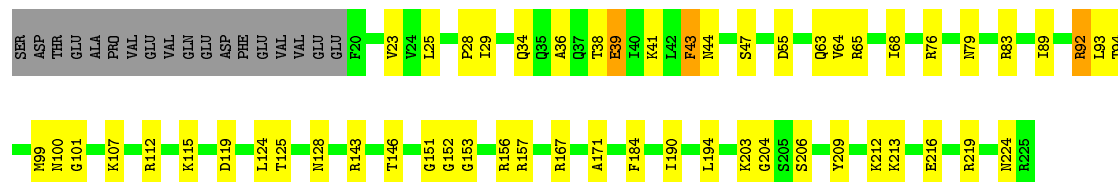
- Molecule 7: 40S ribosomal protein S5

Chain S5:



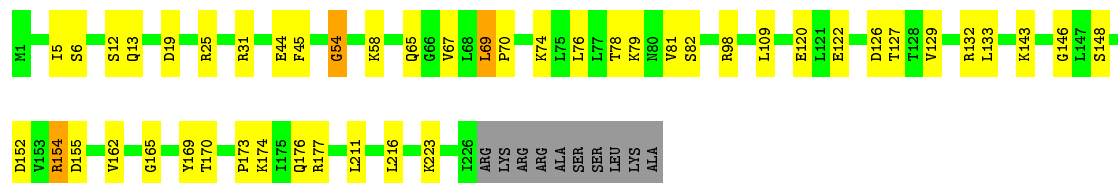
• Molecule 7: 40S ribosomal protein S5

Chain s5: 67% 23% 8%



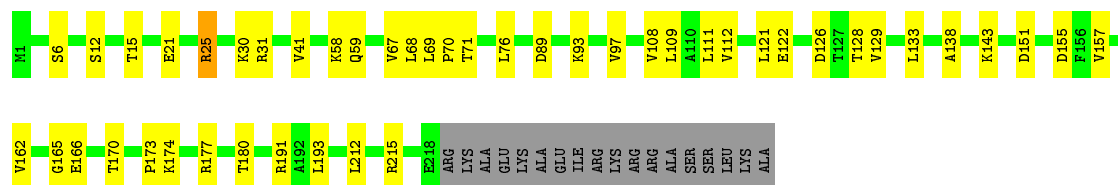
• Molecule 8: 40S ribosomal protein S6-A

Chain S6: 76% 19% 8%



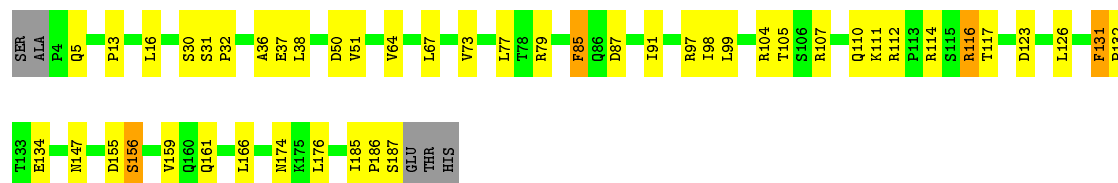
• Molecule 8: 40S ribosomal protein S6-A

Chain s6: 73% 19% 8%



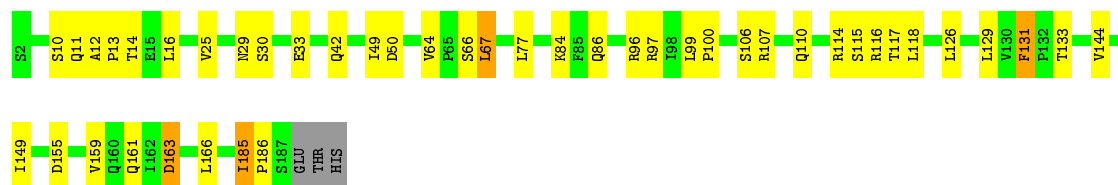
• Molecule 9: 40S ribosomal protein S7-A

Chain S7: 72% 23% 8%



• Molecule 9: 40S ribosomal protein S7-A

Chain s7: 75% 21% 8%



- Molecule 10: 40S ribosomal protein S8-A

- Molecule 10: 40S ribosomal protein S8-A

- Molecule 11: 40S ribosomal protein S9-A

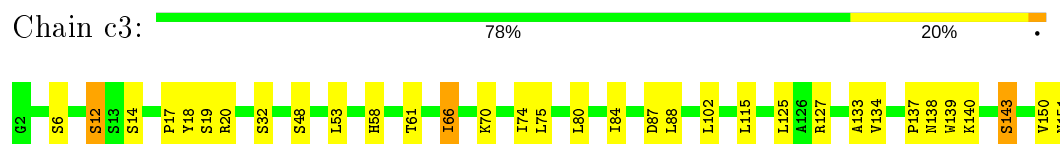
- Molecule 11: 40S ribosomal protein S9-A

- Molecule 12: 40S ribosomal protein S10-A

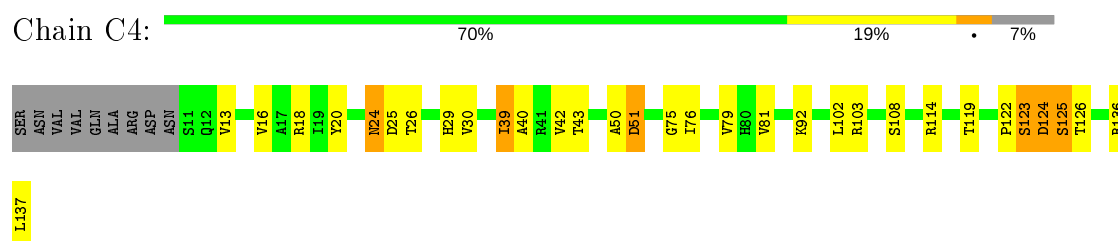




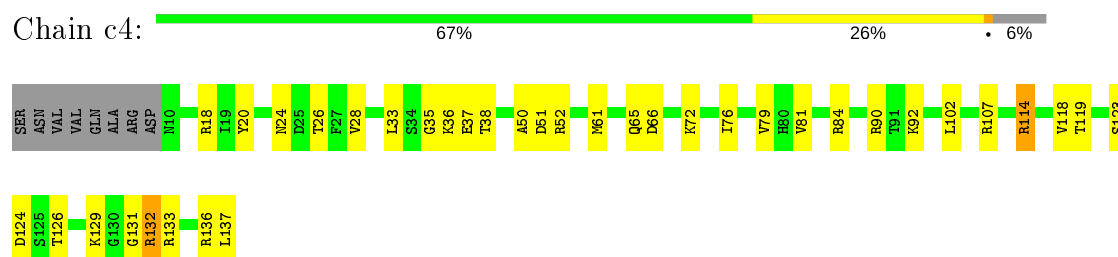
## • Molecule 15: 40S ribosomal protein S13



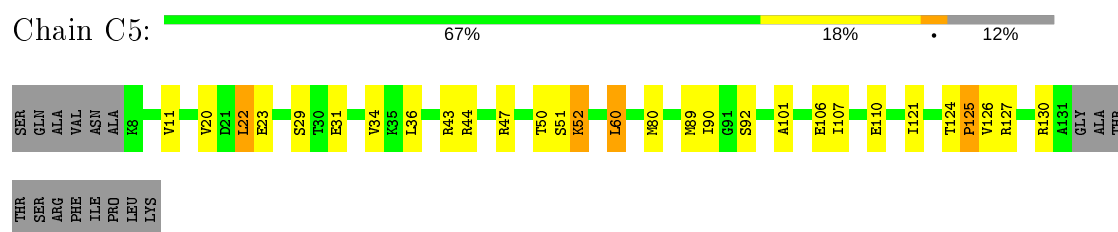
## • Molecule 16: 40S ribosomal protein S14-A



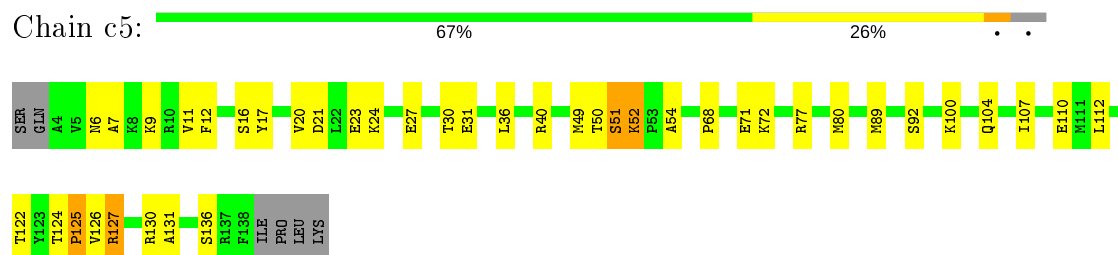
## • Molecule 16: 40S ribosomal protein S14-A



## • Molecule 17: 40S ribosomal protein S15



## • Molecule 17: 40S ribosomal protein S15



## • Molecule 18: 40S ribosomal protein S16-A





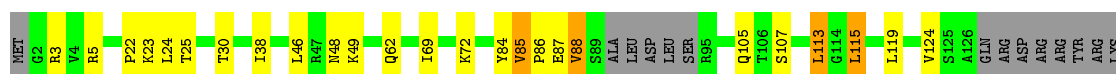
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 78% 20%



- Molecule 19: 40S ribosomal protein S17-A

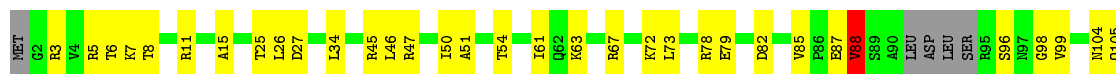
Chain C7: 70% 15% 12%



ARG  
VAL

- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 60% 25% 14%



L113  
K116  
S120  
V121  
I122  
ASN  
VAL  
SER  
ALA  
GLN  
ARG  
ASP  
ARG  
TYR  
LYS  
ARG  
VAL

- Molecule 20: 40S ribosomal protein S18-A

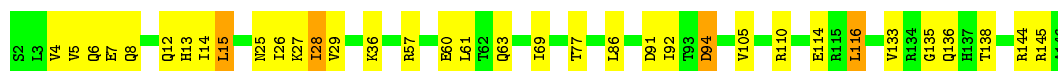
Chain C8: 74% 20% 6%



R143  
R144  
R145  
A146

- Molecule 20: 40S ribosomal protein S18-A

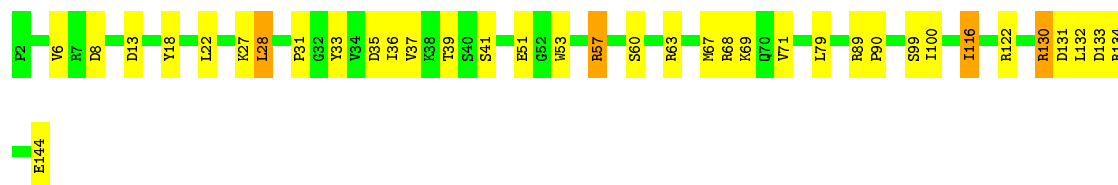
Chain c8: 76% 21%



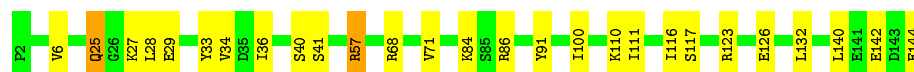
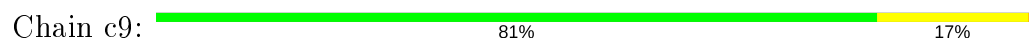
- Molecule 21: 40S ribosomal protein S19-A

Chain C9: 75% 22%





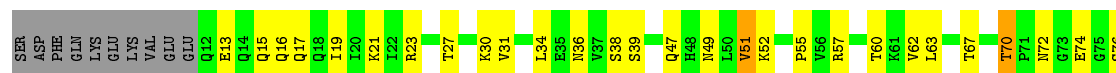
- Molecule 21: 40S ribosomal protein S19-A



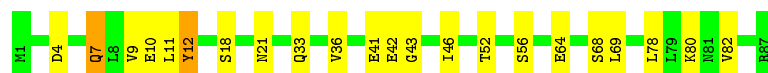
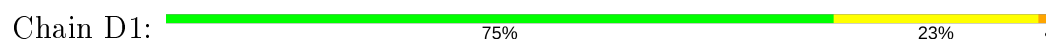
- Molecule 22: 40S ribosomal protein S20



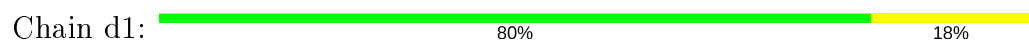
- Molecule 22: 40S ribosomal protein S20



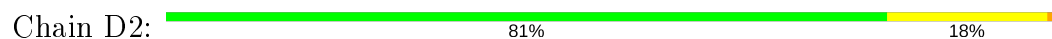
- Molecule 23: 40S ribosomal protein S21-A

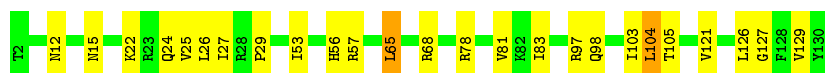


- Molecule 23: 40S ribosomal protein S21-A



- Molecule 24: 40S ribosomal protein S22-A





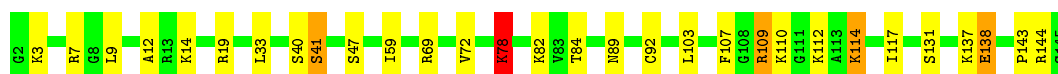
- Molecule 24: 40S ribosomal protein S22-A

Chain d2: 86% 13%



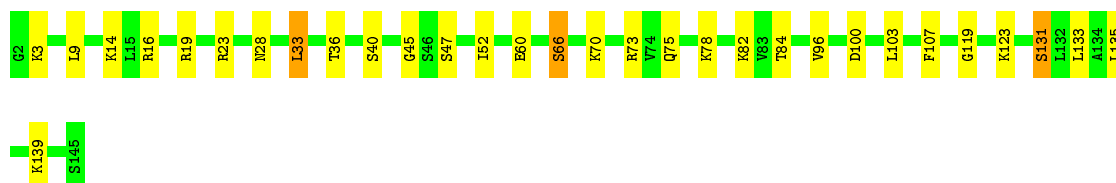
- Molecule 25: 40S ribosomal protein S23-A

Chain D3: 79% 17%



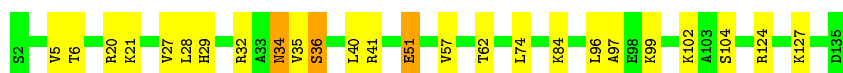
- Molecule 25: 40S ribosomal protein S23-A

Chain d3: 78% 19%



- Molecule 26: 40S ribosomal protein S24-A

Chain D4: 81% 16%



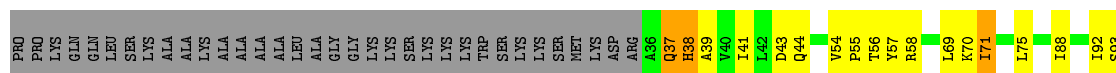
- Molecule 26: 40S ribosomal protein S24-A

Chain d4: 78% 21%



- Molecule 27: 40S ribosomal protein S25-A

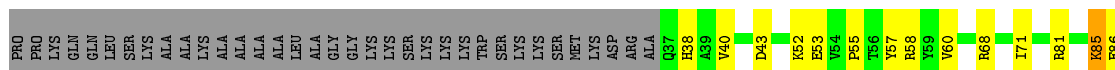
Chain D5: 43% 18% 5% 35%





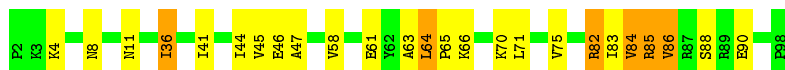
- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 47% 17% 36%



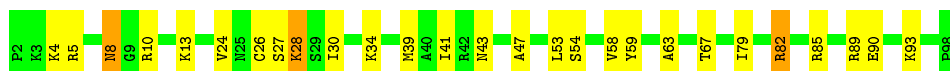
- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 74% 20% 6%



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 72% 25% 3%



- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 77% 20% 3%



- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 80% 17% 3%



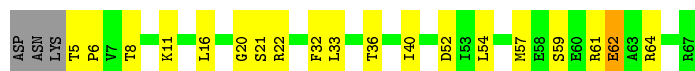
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 67% 24% 5% 5%




- Molecule 30: 40S ribosomal protein S28-A

Chain d8:  67% 27% • 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:  82% 13% • •




- Molecule 31: 40S ribosomal protein S29-A

Chain d9:  67% 29% •



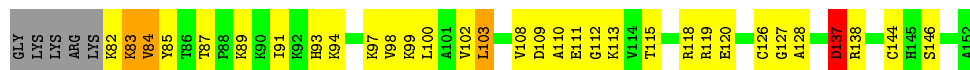
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:  85% 13% •




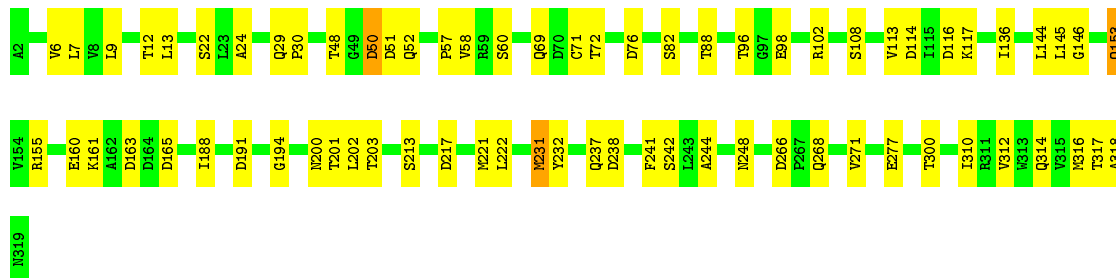
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:  51% 37% • • 7%




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

Chain SR:  78% 21% •



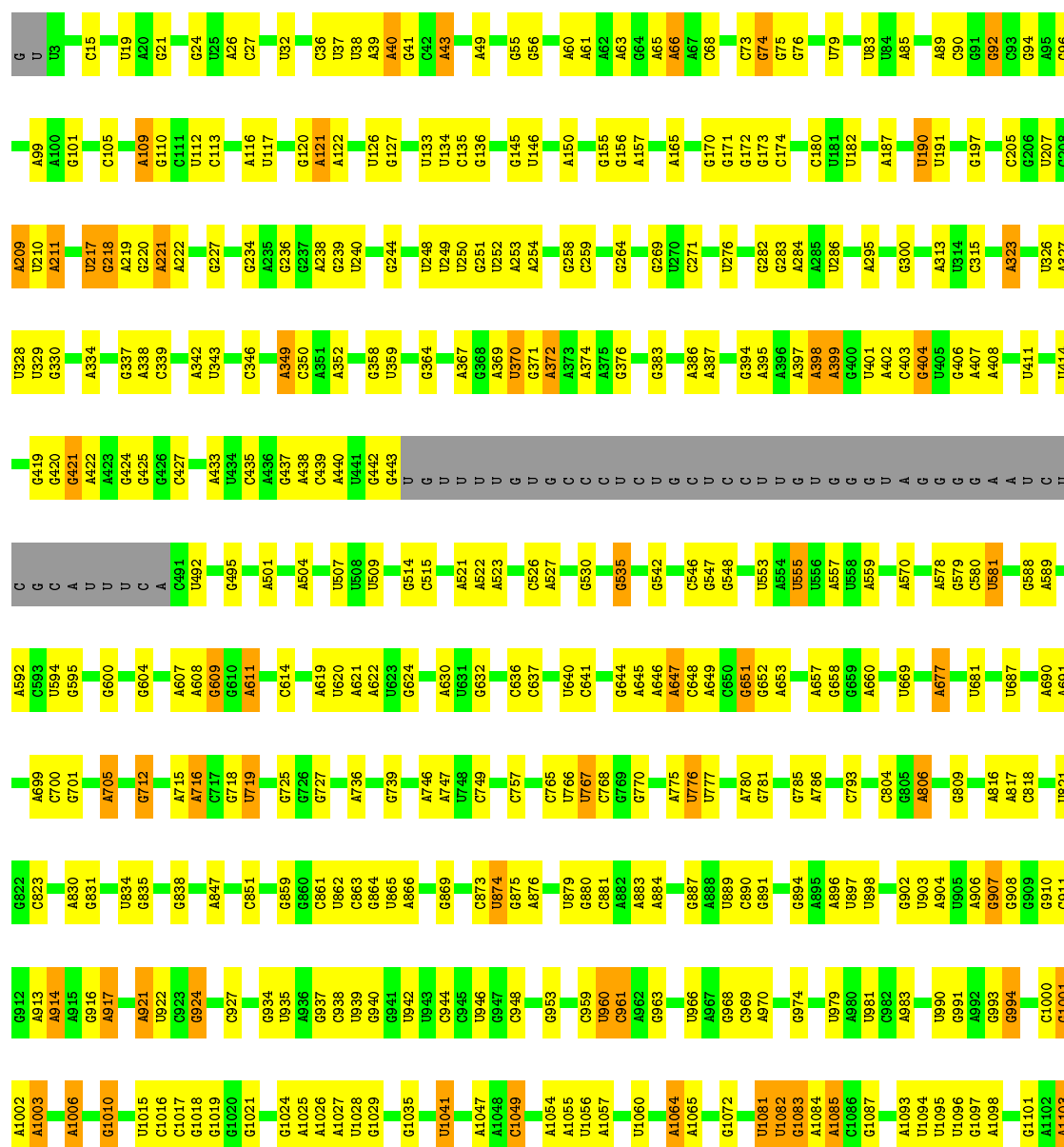
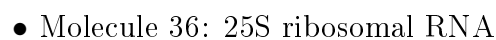
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:  89% 10% •



A1715	C1581	C1385	C1224	C1352	U1042	C957	A884	U766	G658	C576	G	U401
U1716	C1582	A1386	C1227	A1153	C1045	C958	U885	U767	G659	C577	G	A402
U1717	U1583	G1389	G1314	G1142	A1046	C959	C886	G770	A660	A578	A	C403
U1724	C1585	A1390	C1316	A1143	A1047	U960	C887		G661	G579	G	G406
C1725	G1586	G1391	C1317	U1144	A1048	C961	U889	U776	U662	C580	G	
G1736	A1587	A1393	A1318	U1144	C1049	G964	C890	U777	U663	U581	G	A409
A1741	U1495	A1394	G1319	G1148	U1058	A965	C893	A780	C667	G582	A	A412
U1742	C1496	G1395	C1320	A1150	A1061	U966	C894	G781	U668	A585	A	
G1743	C1497	C1396	U1321	U1151	A1062	A967	A895	U782	U669	C586	U	G415
A1749	A1503	U1398	C1322	G1152	A1063	G968	A896	A783	C670	U587	U	G416
G1750	C1504	A1399	C1327	G1153	G1063	C969	U897	A784	U671	G588	C	A417
A1751	C1505	G1400	C1328	A1154	A1064	A970	U898	G785	A672	A589	C	
G1752	A1506	A1401	U1329	C1155	A1065	G971	U899		U673	G590	G	A418
U1605	C1507	C1402	A1330	C1156	U1065	A972	G900	C788	G674	G591	C	G419
A1757	A1508	U1405	U1331	G1157	C1068	G972	G901		U675	A592	A	G420
U1607	G1510	A1406	A1158	A1158	U1068	U976		A791	A677	C593	U	A422
C1761	C1516	A1407	A1159	A1159	U1071	U979	A906	G792		U594	U	
C1762	G1520	G1408	C1161	C1160	G1072	U980	G907	C793	U681	G604	C	G426
U1765	C1521	U1410	A1162	A1163	A1079	U981	G908		U682		A	U429
G1766	G1521	C1342	A1163	A1163	A1080	C982	G909	U797	U683	A608	C	
C1767	U1526	G1343	G1164	A1164	U1081	A983	G910			G609	U	
U1768	G1527	G1344	A1165	A1165	U1082	G984	A914	G800	A691	G610	U	G432
G1769	C1528	G1345	G1166	G1166	G1083	G988	A915	C802	C686	A611	G	A433
U1770	G1528	U1346	U1167	U1167	U1087	U988	G916	C803		U612	G	U434
G1775	A1534	U1347	G1171	G1171	A1093	G991	A917	C804	A699	G613	A	C435
C1779	A1535	U1348	A1179	A1179	U1094	A992	U919	G805	C700	A619	U	A438
G1780	G1536	A1350	U1269	U1269	U1095	G993	G920	A806	G701	U620	U	C439
C1639	U1537	U1351	A1180	A1180	U1096	G994	A921	A807	C702	A621	U	A440
U1643	C1548	C1353	A1181	A1181	G1097	A997	U922	A808	G703	G517	G	
C1644	U1549	G1354	C1182	C1182	U1098	A997	C923	G809	U704	G518	U	
G1646	U1553	A1355	C1183	C1183	A1099	G1000	G924	A810	A705	A519	C	
C1657	C1556	U1356	G1187	G1187	U1099	G1001	A926	A816	A706	U623	U	
G1658	U1556	G1357	U1191	U1191	A1102	A1002	C931	A817	G708	U626	U	
U1659	C1556	C1360	C1192	C1192	A1103	A1006	G934	C818	G712	U627	U	
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A1809	C1562	C1364	A1200	A1200	U1111	G1013	A937	C717	C717	C637	U	G
A1810	C1563	G1365	C1201	C1201	A1112	U1017	C938	G718	U719	C638	U	
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U1821	U1571	A1373	A1304	A1304	U1121	G1029	U946	C861	U748	A647	U	
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A1835	U1577	G1379	A1217	A1217	U1124	A1037	C949		C752	C650	U	
A1836	C1578	G1380	U1218	U1218	A1129	C1037	G950	G878	G763	G651	U	
U1837	U1579	A1381	U1222	U1222	A1130	A1040	G953	U879	U764	A652	G	
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U3055	G2946	G2761	C2675	C2594	C		C2343	C2257	A2158	A	G	G1951	U1840
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U3079	G2977	G2874	A2692	G2610	U2513	U	G2365	U2282	G2188	C	C	C	A1859
G3080	U2978	A2780	C2693	U2611	U2514	G	C2366	G2283	U2193	A	A	U	G1860
C3081	U2979	G2786	A2694	U2612	A2515	U	C2366	C2284	G2194	C	C	U	C1866
A3086	U2980	G2787	A2695	U2613	A	G	G2369	U2285	C2195	A	U	G	A1867
A3087	A2981	G2791	A2697	G2614	U2520	G	G2370	A2196	C2196	A	C	U	G1868
C3088	A2982	G2795	G2698	U2617	U2521	G	G2371	A2197	C2197	U	U	C	U1871
C3092	U2983	U2796	G2699	G2618	G2522	U	A2372	U2289	A2198	A	U	A	A1879
A3103	G2979	G2797	G2700	G2619	A2523	U	C2373	U2290	U2200	C	G	A	U1880
U3107	U2986	C2797	U2701	G2620	U2532	U	C2374	G2201	G2201	C	C	C	A1881
U3111	A2987	G2798	A2702	G2621	G2533	A	C2376	U2205	U2205	C	G	C	U1882
A3113	C2988	A2703	G2703	C2622	U2534	G	C2383	A2208	A2208	C	C	C	A1883
U3129	U2989	A2704	G2704	G2623	G2534	U	A2384	U2209	G2210	C	A	A	A1884
G3112	G2990	A2705	A2705	G2624	U2538	A	G2385	C2304	G2211	C	C	C	U1885
A3114	A2801	A2802	G2714	C2625	C2539	A	U2388	G2305	U2211	C	U	U	A1886
U3119	C2898	A2803			A2540	U	C2391	C2212	G2212	C	G	G	A1891
G3120	C2899	C2810	U2718	U2629	U2541	G	G2392	U2109	G2110	C	U	U	G1892
U3121	A2911	G2816	U2719	U2630	U2542	U	C2393	G2111	G2111	C	G	G	A1893
A3122	C2912	G2817	G2720	U2631	U2543	G	G2394	G2112	U2112	C	U	U	G1894
A3123	G2913	A2817	U2721	G2632	U2547	U	G2395	G2113	A2113	C	U	C	A1895
A3130	U2914	U2818	U2722	U2633	A2548	G	C2397	G2114	G2114	C	U	U	A1896
U3131	U2915	U2819	U2723	U2634	C2549	A	A2401	A2117	A2117	C	A	G	A1901
G3132	U2916	A2819	U2725	A2635	C2549	G	A2402	C2118	C2118	C	A	C	G1902
A3140	G2917	G2823	U2726	A2636	U2550	C	G2403	G2121	G2121	C	U	U	U1903
A3141	A2918	G2827	C2727	A2637	U2551	U	A2404	G2122	G2122	C	U	G	G1904
A3142	G2919	U2728	U2728	G2638	U2552	U	G2405	G2123	G2123	C	G	U	G1905
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U3148	U2923	G2730	U2730	A2640	U2554	G	G2407	G2130	G2130	C	G	G	A1909
U3153	C2924	G2731	U2731	U2641	G2555	U	A2408	G2131	A2131	C	U	A	A1910
C3154	G2925	A2831	G2732	A2642	A2561	C	A2409	G2132	G2132	C	U	C	U1912
U3155	A2926	G2733	G2733	G2643	C2560	C	G2409	G2133	G2133	C	U	C	A1913
U3156	C2927	G2734	U2734	C2644	C2561	A	U2408	G2134	G2134	C	U	C	U1920
U3157	C2928	C2737	G2745	A2647	C2568	G	U2409	U2327	U2327	C	U	C	G1928
	G3028	G2746	A2746	U2652	A2569	U	G2410	A2242	A2242	C	U	U	G1929
	A3029	A2747	A2747	C2653	U2570	U	U2411	U2140	U2140	C	U	G	
	G3030	G2748	A2748	U2571	U2571	G	G2412	A2243	A2243	C	U	G	
	C3034	G2749	A2656	G2572	G2573	A	A2413	A2244	A2244	C	U	G	
	U3037	U2750	G2657	G2573	A	A	U2417	C2245	C2245	C	U	G	
	A2845	G2753	G2658	G2585	U	U	G2418	G2249	G2249	C	U	G	
	U2846	G2754	G2662	G2586	A	A	U2336	U2153	U2153	C	U	G	
	A2847	C2755	G2663	U2587	C	C	A2419			C	U	G	





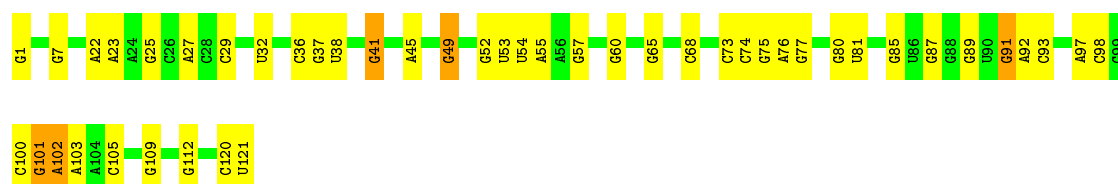
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G2394	A2320	C2237	C2144	C1843	A1588	G1500	U1405	G1314	U1111	A1112
G2395	G2323	A2243	C2147	C1846	A1589	G1500	U1405	U1315	G1199	G1113
G2396	A2324	A2244	U2148	A1847	G1592	A1503	G1416	C1316	A1200	U1114
A2397	G2325	C2245	U2148	G1848	A1593	A1504	G1417	C1316	C1201	G1115
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G2400	U2327	C2248	C2156	G1851	U1595	G1507	C1420	U1329	A1204	
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A2402	A2332	G2250	A2158	U1941	G1598	C1508	G1422	U1331	G1206	U1124
G2403	C2333	G2251	C2163	A1858	A1750		G1422	A1332	U1207	U1125
A2404	U2334	G2252	C2163	G1863	G1751	U1511	A1428		G1208	
G2405	G2335	G2253	A2164	A1864	C1755	U1512	G1429	U1336	U1128	
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C2407	C2337	U2254	A2166	G1868	C1756	G1514	G1431	G1340	A1130	
U2408	C2338	A2255	A2167	C1869	C1762	C1516	C1432	A1343	G1131	
		A2256	C2168	C1869	U1763	C1517	A1433		A1217	
U2411	A2341	U2260	G2169	A1874	U1764	U1518	G1434	G1346	U1219	C1141
G2412	C2342	C2267	U2175	G1878	U1765	U1519	A1435	U1347	G1222	G1142
U2416	U2343	C2267	U2176	A1879	G1766	U1628	C1437	U1348		U1144
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A2419	C2350	G2272	C2179	G1882	G1770	G1635	G1441	U1351	C1232	G1148
C2420	U2351	G2273	C2185	A1882	G1780	G1639	G1442	A1352	G1149	
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C2422	C2353	A2279	C2186	A1884	G1781	G1641	G1444	G1354	G1237	U1150
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	G2355	A2281	C2192	A1886	C1788	A1643	A1446	U1356	G1239	G1152
U2426		U2282	C2195	A1891	G1789	C1548		G1357	A1240	A1153
U2427	A2358	G2283	C2196	A1892	G1789	U1549	G1449	U1357	U1241	A1154
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A2430		G2289	C2200	A1895	U1795	G1555	A1452		A1244	A1158
U2434	A2363	C2290	G2201	A1896	G1795	G1556	A1452	U1367	A1245	
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A2438	A2372	U2294	U2205	G1899	A1798	C1562	A1462	G1371	U1258	G1161
G2440	A2373	A2295	U2206	G1899	A1799	C1563	A1462	C1372		
A2441	C2374	U2296	A2207	A1900	C1803	U1564	A1465	A1373	G1262	U1167
G2442	G2375	U2299	A2208	A1901	C1803	U1565	A1466	G1374	A1263	U1168
A2443	G2376	C2299	U2209	G1902	A1810	G1566	A1467	G1375	G1264	A1169
	C2377	A2303	U2210	U1903	A1810	U1567	A1468	C1376	U1265	G1170
A	U2378	G2304	G2211	G1906	A1814		G1473		G1266	G1171
U	U2379	G2304	G2212	U1906	U1815	U1570		A1381		
A	A2380	G2305	G2123	A1909	A1816	A1571	G1480	U1384	G1284	G1178
G	G2381	C2306	G2123	C1917	G1817	U1572	A1481	C1385	G1285	A1179
A	G2382	C2307	A2131	C1917	U1818	G1573	A1482	A1386		A1180
G	C2383	C2308	C2132	U1920	U1818	C1574	A1483	A1387	C1292	U1181
G	A2384	A2309	G2133	U1921	U1821	A1575	U1484	G1389	A1302	C1183
U	G2385	U2310	C2134	A1922	C1822	G1576	A1489	A1390	A1304	
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A	A2390	A2233	A2138	G1927	G1713	C1581	G1493		A1308	U1191

- Molecule 37: 5S ribosomal RNA

Satisfaction Level	Percentage
Satisfied	79%
Not Satisfied	21%

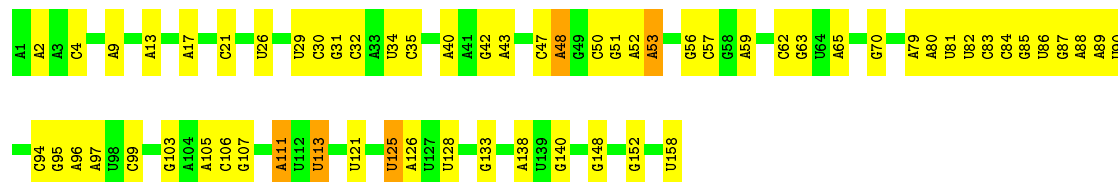
- Molecule 37: 5S ribosomal RNA

Response	Percentage
U.S. should take more action to reduce global warming	62%
U.S. should take less action to reduce global warming	34%
Other/Unsure	4%



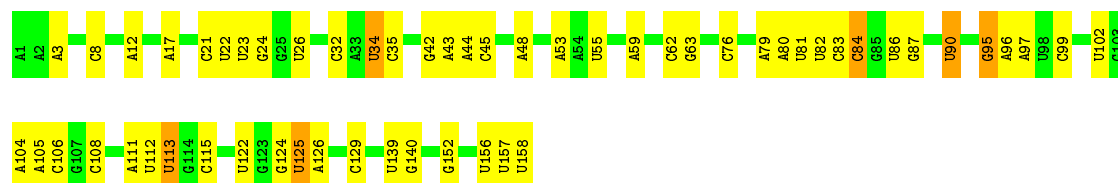
- Molecule 38: 5.8S ribosomal RNA

Chain 4: 61% 36% .



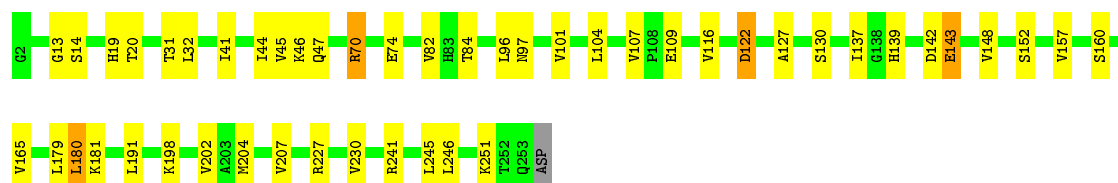
- Molecule 38: 5.8S ribosomal RNA

Chain 8: 65% 32% .



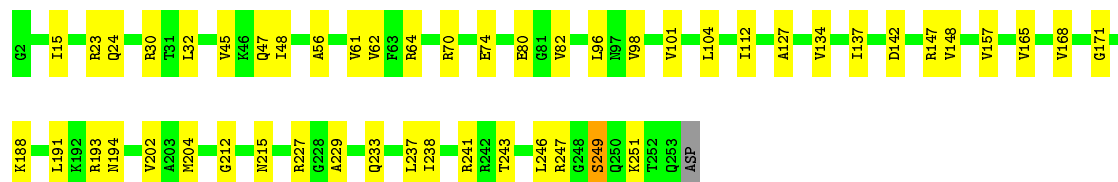
- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 81% 17% .



- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 80% 19% .



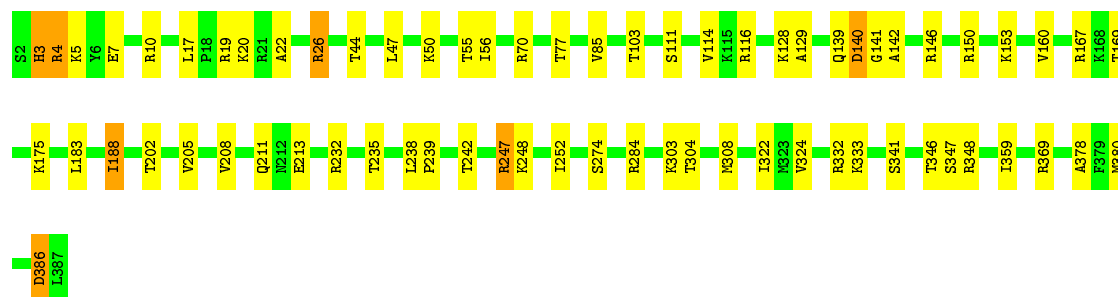
- Molecule 40: 60S ribosomal protein L3

Chain L3: 81% 18% .



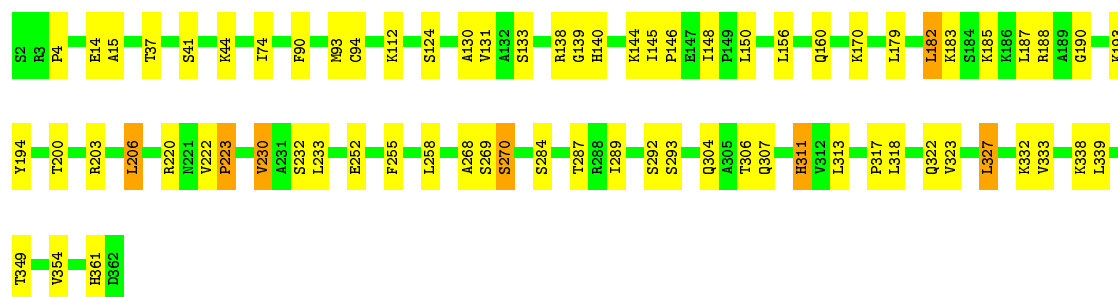
- Molecule 40: 60S ribosomal protein L3

Chain 13: 82% 16%



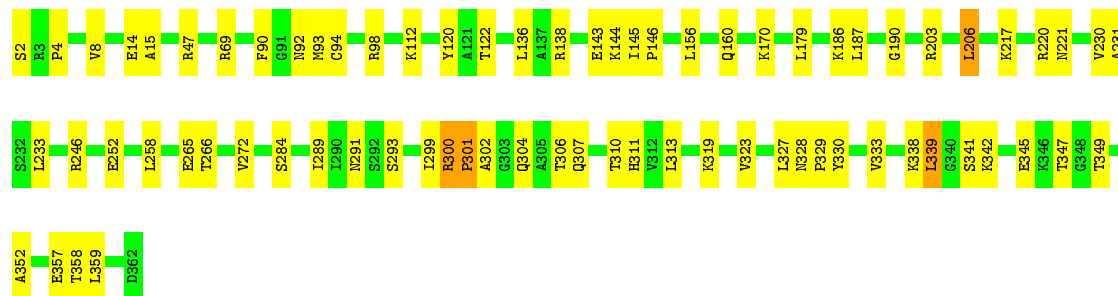
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 80% 18%




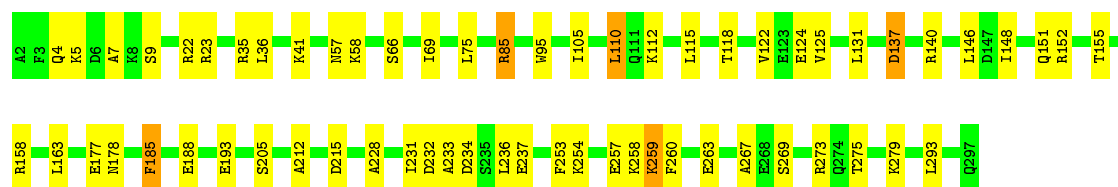
- Molecule 41: 60S ribosomal protein L4-A

Chain 14: 80% 19%




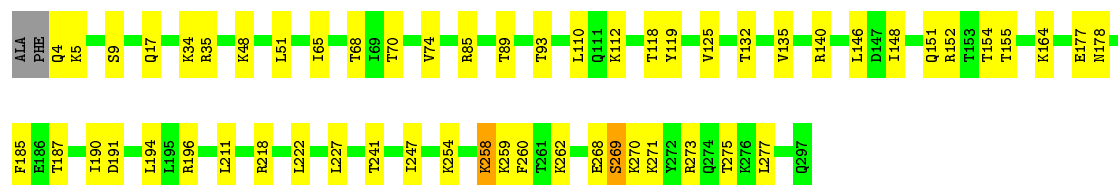
- Molecule 42: 60S ribosomal protein L5

Chain L5:  79% 19%



- Molecule 42: 60S ribosomal protein L5

Chain l5:  80% 18%



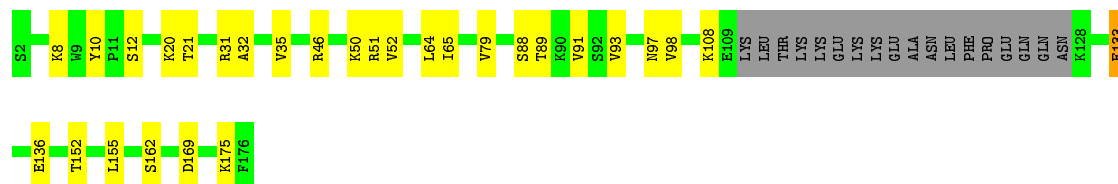
- Molecule 43: 60S ribosomal protein L6-A

Chain L6:  74% 15% 11%




- Molecule 43: 60S ribosomal protein L6-A

Chain l6:  73% 16% 10%




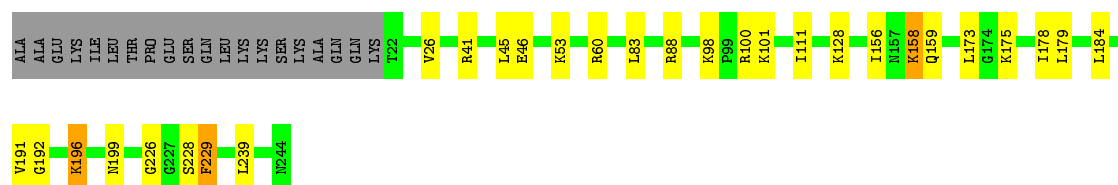
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:  79% 11% 9%



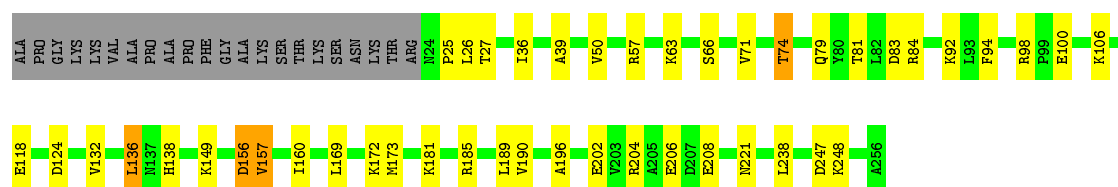
- Molecule 44: 60S ribosomal protein L7-A

Chain 17:  80% 11% • 8%



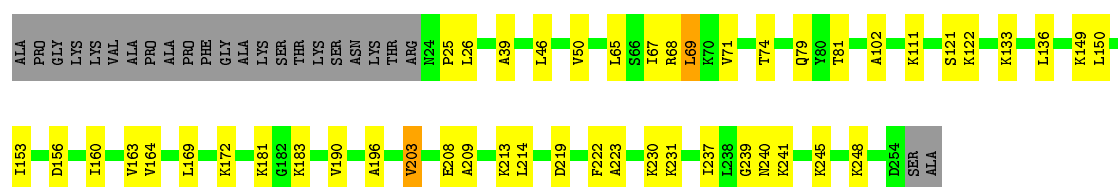
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:  74% 16% • 9%




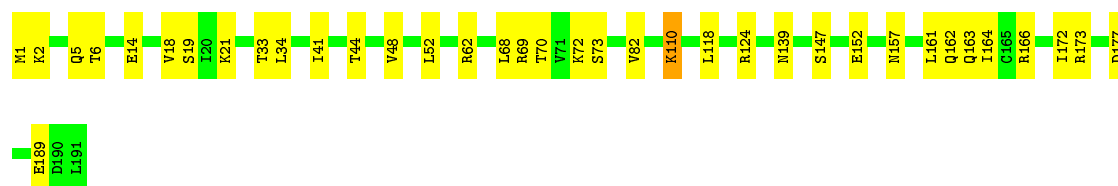
- Molecule 45: 60S ribosomal protein L8-A

Chain l8:  72% 18% • 9%




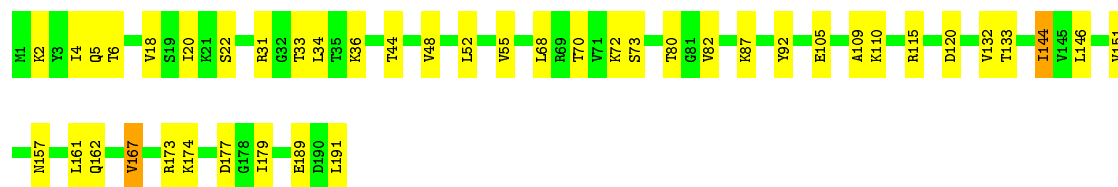
- Molecule 46: 60S ribosomal protein L9-A

Chain L9:  81% 19% •




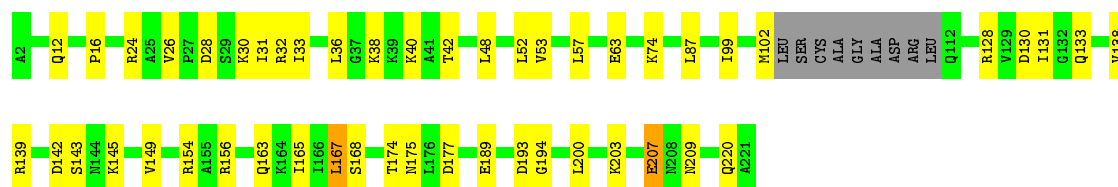
- Molecule 46: 60S ribosomal protein L9-A

Chain l9:  77% 21% •




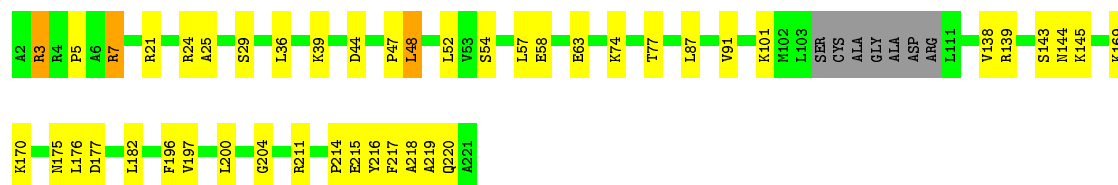
- Molecule 47: 60S ribosomal protein L10

Chain M0:  74% 21% ..



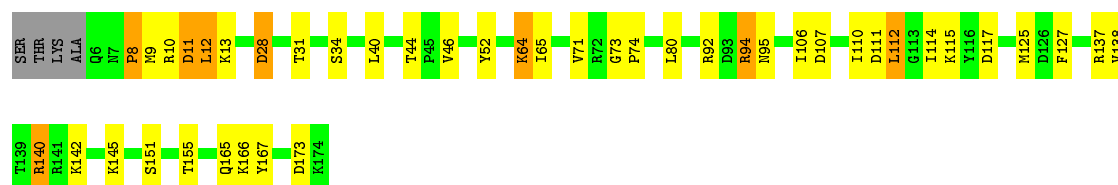
- Molecule 47: 60S ribosomal protein L10

Chain m0:  76% 19% ..



- Molecule 48: 60S ribosomal protein L11-B

Chain M1:  73% 20% 5% .




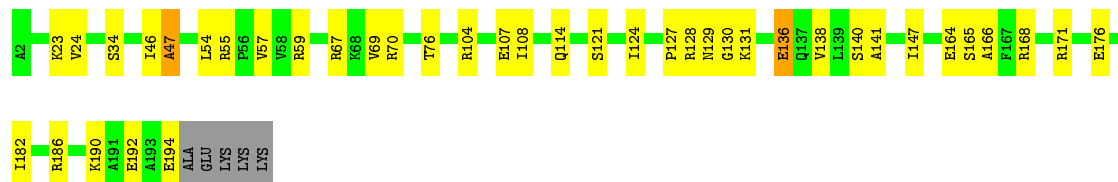
- Molecule 48: 60S ribosomal protein L11-B

Chain m1:  73% 22% ..

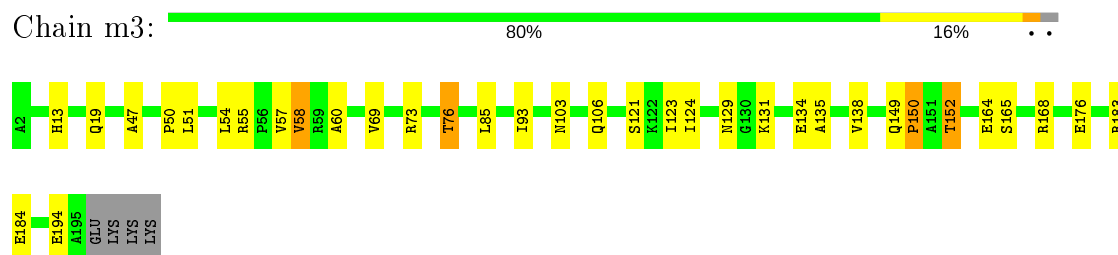


- Molecule 49: 60S ribosomal protein L13-A

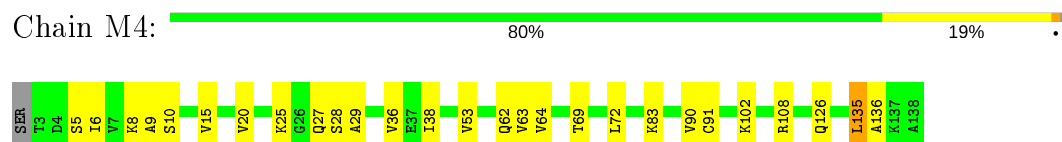
Chain M3:  77% 19% ..



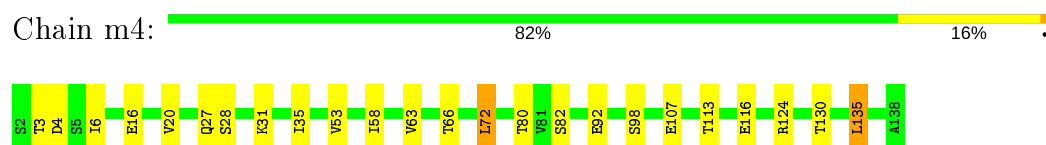
- Molecule 49: 60S ribosomal protein L13-A



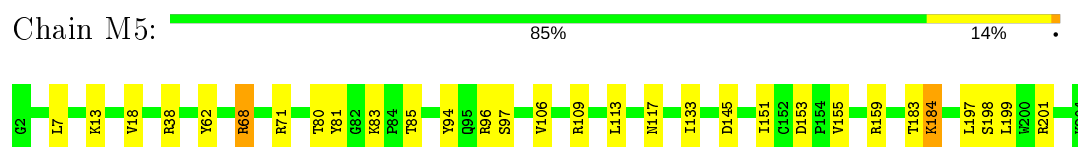
- Molecule 50: 60S ribosomal protein L14-A



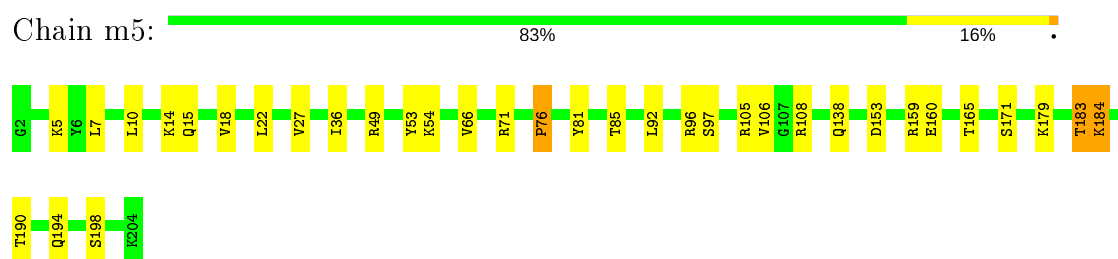
- Molecule 50: 60S ribosomal protein L14-A



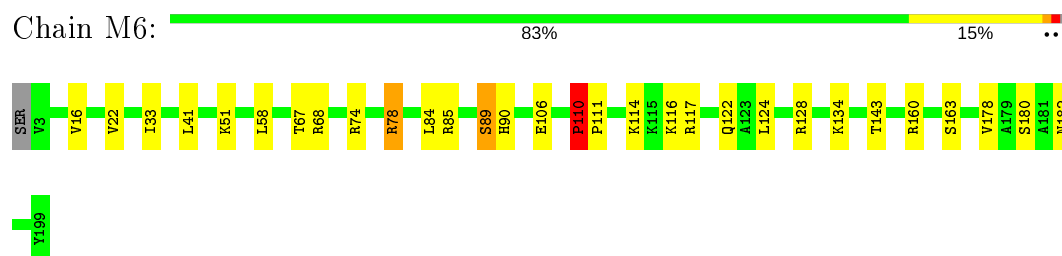
- Molecule 51: 60S ribosomal protein L15-A



- Molecule 51: 60S ribosomal protein L15-A

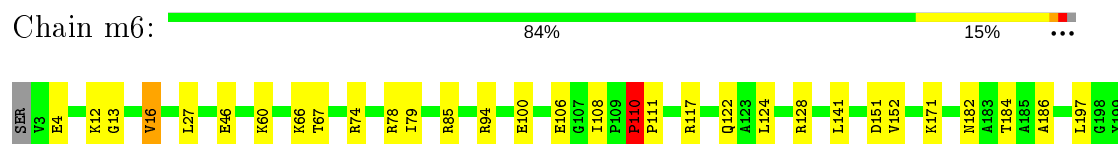


- Molecule 52: 60S ribosomal protein L16-A

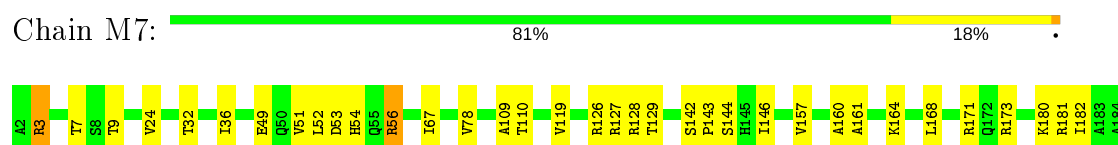




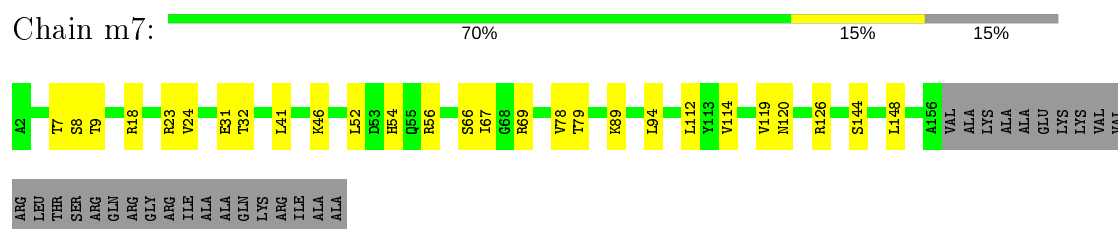
- Molecule 52: 60S ribosomal protein L16-A



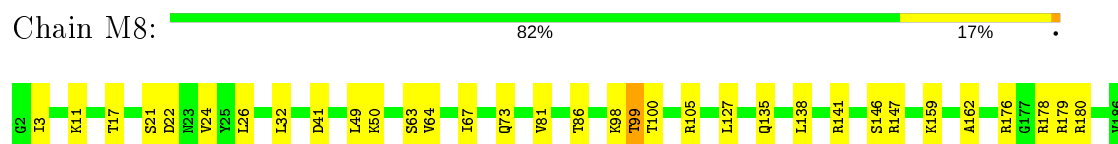
- Molecule 53: 60S ribosomal protein L17-A



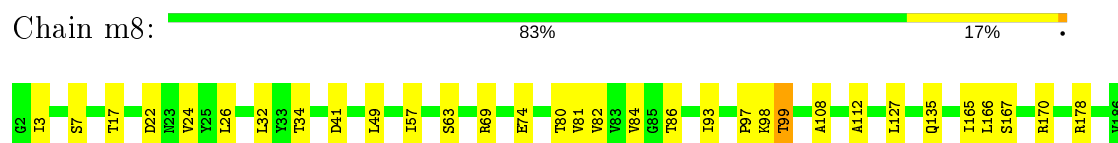
- Molecule 53: 60S ribosomal protein L17-A



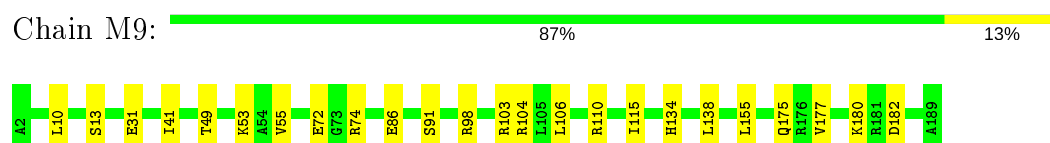
- Molecule 54: 60S ribosomal protein L18-A



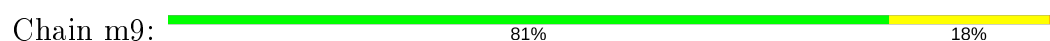
- Molecule 54: 60S ribosomal protein L18-A

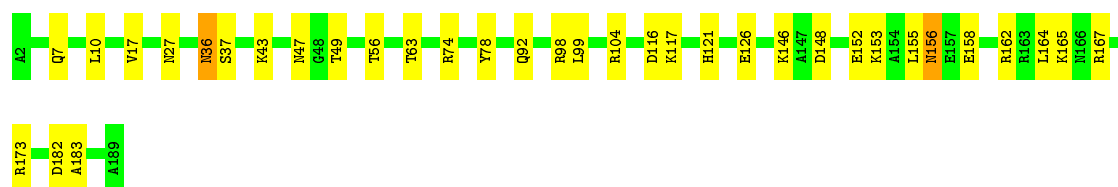


- Molecule 55: 60S ribosomal protein L19-A

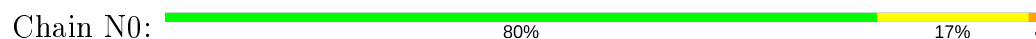


- Molecule 55: 60S ribosomal protein L19-A

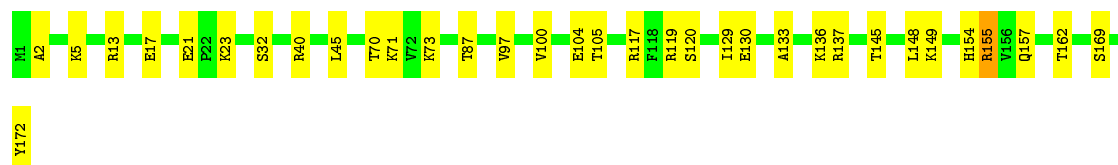
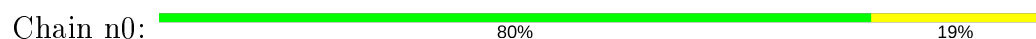




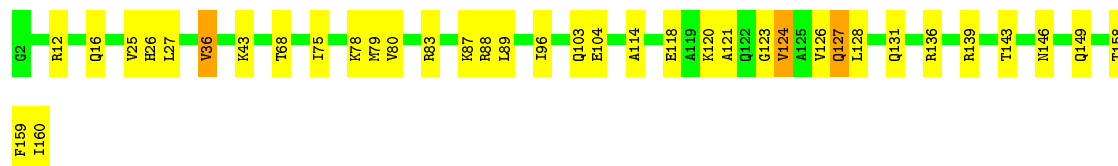
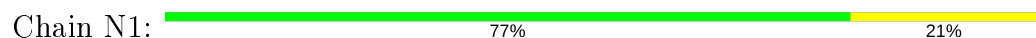
- Molecule 56: 60S ribosomal protein L20-A



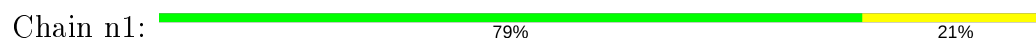
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 57: 60S ribosomal protein L21-A



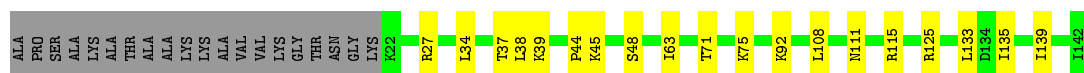
- Molecule 57: 60S ribosomal protein L21-A



- Molecule 58: 60S ribosomal protein L22-A



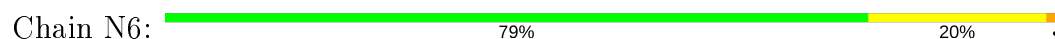




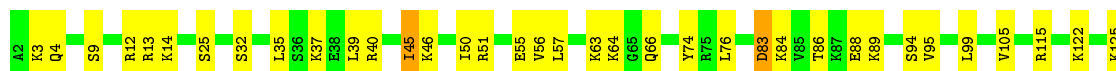
- Molecule 61: 60S ribosomal protein L25



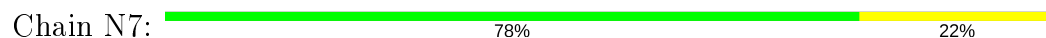
- Molecule 62: 60S ribosomal protein L26-A



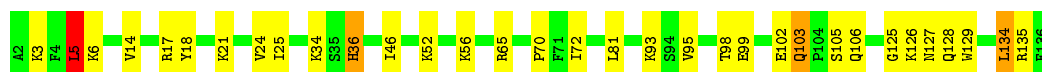
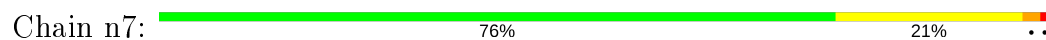
- Molecule 62: 60S ribosomal protein L26-A



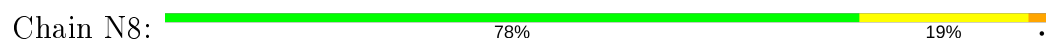
- Molecule 63: 60S ribosomal protein L27-A



- Molecule 63: 60S ribosomal protein L27-A



- Molecule 64: 60S ribosomal protein L28





- Molecule 64: 60S ribosomal protein L28

Chain n8: 81% 18%



- Molecule 65: 60S ribosomal protein L29

Chain N9: 78% 22%



- Molecule 65: 60S ribosomal protein L29

Chain n9: 78% 19%



- Molecule 66: 60S ribosomal protein L30

Chain O0: 72% 20% 7%



- Molecule 66: 60S ribosomal protein L30

Chain o0: 80% 16%



- Molecule 67: 60S ribosomal protein L31-A

Chain O1: 77% 19%

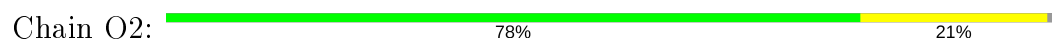


- Molecule 67: 60S ribosomal protein L31-A

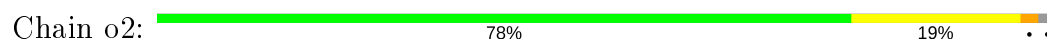
Chain o1: 69% 29%



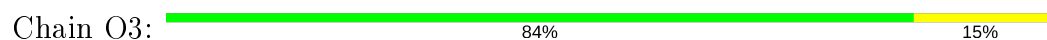
- Molecule 68: 60S ribosomal protein L32



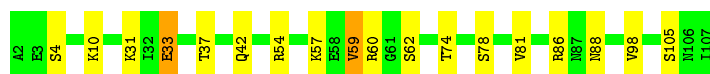
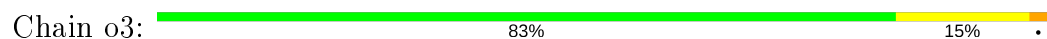
- Molecule 68: 60S ribosomal protein L32



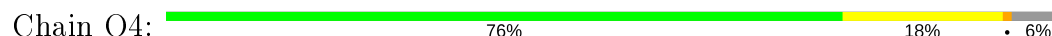
- Molecule 69: 60S ribosomal protein L33-A



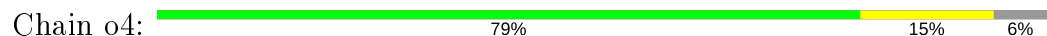
- Molecule 69: 60S ribosomal protein L33-A



- Molecule 70: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L34-A



- Molecule 71: 60S ribosomal protein L35-A





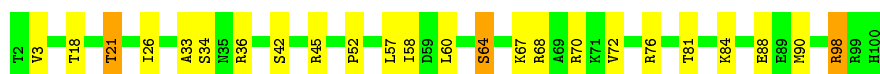
- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 79% 20%



- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 76% 21%



- Molecule 72: 60S ribosomal protein L36-A

Chain o6: 74% 23%



- Molecule 73: 60S ribosomal protein L37-A

Chain O7: 79% 20%



- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 77% 21%



- Molecule 74: 60S ribosomal protein L38

Chain O8: 71% 29%

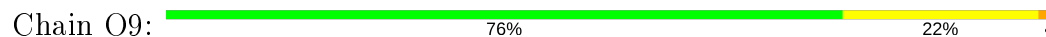


- Molecule 74: 60S ribosomal protein L38

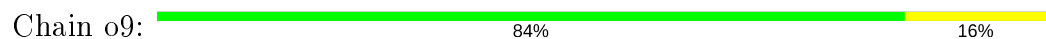
Chain o8: 81% 19%



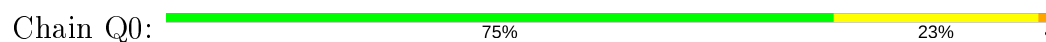
- Molecule 75: 60S ribosomal protein L39



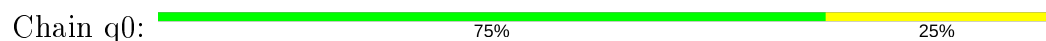
- Molecule 75: 60S ribosomal protein L39



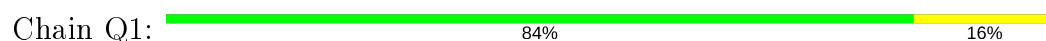
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



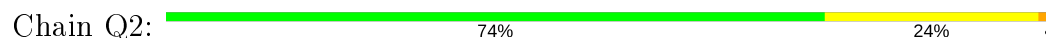
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A



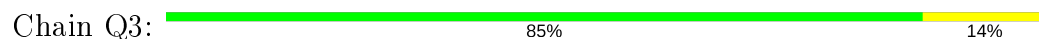




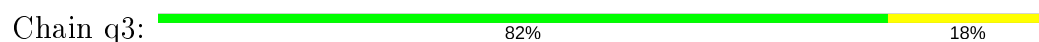
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



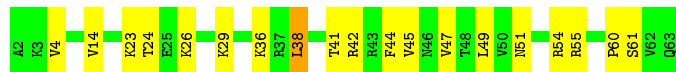
- Molecule 79: 60S ribosomal protein L43-A



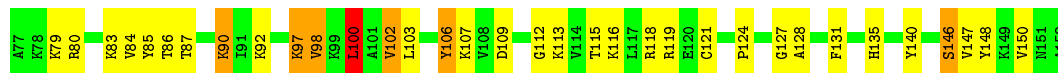
- Molecule 80: 40S ribosomal protein S10-A



- Molecule 81: 40S ribosomal protein S30-A

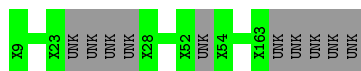


- Molecule 82: Ubiquitin-40S ribosomal protein S31

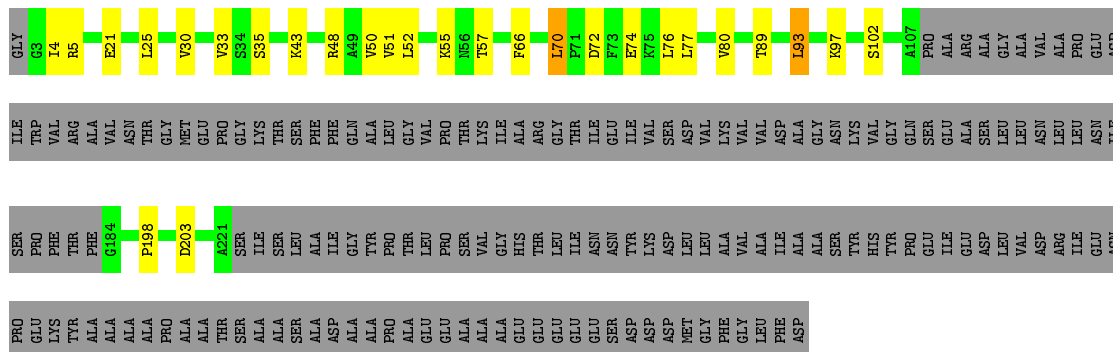
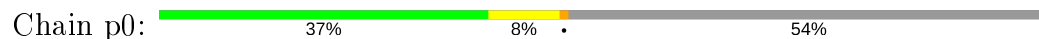


- Molecule 83: UNKNOWN PROTEIN m2





- Molecule 84: 60S acidic ribosomal protein P0



- Molecule 85: UNKNOWN PROTEIN p1



There are no outlier residues recorded for this chain.

- Molecule 86: UNKNOWN PROTEIN p2



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, $\alpha$ , $\beta$ , $\gamma$	436.02Å 287.59Å 304.52Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	49.82 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (49.82-3.20)	Depositor
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.181 , 0.237	Depositor
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtriage
Anisotropy	0.157	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	2	0.68	1/41698 (0.0%)	1.28	292/64972 (0.4%)
1	6	0.81	13/42765 (0.0%)	1.38	456/66634 (0.7%)
2	S0	0.43	0/1617	0.67	0/2215
2	s0	0.49	0/1623	0.72	0/2222
3	S1	0.37	0/1735	0.69	2/2335 (0.1%)
3	s1	0.51	0/1748	0.70	1/2352 (0.0%)
4	S2	0.45	0/1665	0.65	0/2263
4	s2	0.54	0/1665	0.72	1/2263 (0.0%)
5	S3	0.45	0/1759	0.68	2/2368 (0.1%)
5	s3	0.45	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.71	0/2839
6	s4	0.52	0/2109	0.75	2/2839 (0.1%)
7	S5	0.38	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.71	1/2202 (0.0%)
8	S6	0.45	0/1823	0.63	1/2439 (0.0%)
8	s6	0.51	0/1779	0.68	0/2379
9	S7	0.42	0/1506	0.63	0/2028
9	s7	0.44	0/1516	0.70	1/2043 (0.0%)
10	S8	0.51	0/1514	0.76	1/2021 (0.0%)
10	s8	0.59	0/1514	0.77	1/2021 (0.0%)
11	S9	0.43	0/1519	0.65	0/2035
11	s9	0.53	0/1519	0.75	1/2035 (0.0%)
12	C0	0.43	0/790	0.66	1/1069 (0.1%)
13	C1	0.55	0/1240	0.69	0/1675
13	c1	0.60	0/1194	0.80	2/1610 (0.1%)
14	C2	0.35	0/900	0.65	1/1224 (0.1%)
14	c2	0.32	0/900	0.60	1/1224 (0.1%)
15	C3	0.47	0/1215	0.69	3/1638 (0.2%)
15	c3	0.54	0/1215	0.75	1/1638 (0.1%)
16	C4	0.37	0/901	0.64	0/1217
16	c4	0.52	0/960	0.73	0/1290
17	C5	0.44	0/998	0.66	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	c5	0.47	0/1060	0.66	0/1426
18	C6	0.43	0/1125	0.69	2/1510 (0.1%)
18	c6	0.48	0/1131	0.71	1/1518 (0.1%)
19	C7	0.40	0/935	0.66	0/1254
19	c7	0.48	0/914	0.72	0/1224
20	C8	0.43	0/1211	0.66	1/1628 (0.1%)
20	c8	0.50	0/1211	0.70	2/1628 (0.1%)
21	C9	0.44	0/1130	0.67	1/1517 (0.1%)
21	c9	0.49	0/1130	0.72	2/1517 (0.1%)
22	D0	0.45	0/865	0.66	0/1169
22	d0	0.49	0/892	0.70	0/1205
23	D1	0.39	0/693	0.59	0/935
23	d1	0.49	0/693	0.70	0/935
24	D2	0.46	0/1038	0.75	2/1395 (0.1%)
24	d2	0.64	0/1038	0.78	1/1395 (0.1%)
25	D3	0.58	0/1139	0.74	0/1518
25	d3	0.64	0/1139	0.82	2/1518 (0.1%)
26	D4	0.41	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.69	0/1449
27	D5	0.39	0/571	0.77	2/768 (0.3%)
27	d5	0.42	0/566	0.69	0/761
28	D6	0.40	0/782	0.60	0/1047
28	d6	0.53	0/782	0.69	0/1047
29	D7	0.42	0/620	0.68	0/838
29	d7	0.44	0/620	0.68	0/838
30	D8	0.34	0/499	0.62	0/670
30	d8	0.38	0/499	0.64	0/670
31	D9	0.50	0/452	0.74	1/600 (0.2%)
31	d9	0.56	0/452	0.71	0/600
32	E0	0.40	0/483	0.64	0/643
33	E1	0.41	0/577	0.78	0/770
34	SR	0.39	0/2494	0.63	0/3393
34	sR	0.39	0/2495	0.60	0/3395
35	SM	0.45	0/1113	0.68	2/1502 (0.1%)
35	sM	0.41	0/683	0.63	1/923 (0.1%)
36	1	1.01	59/75394 (0.1%)	1.57	1453/117545 (1.2%)
36	5	1.05	74/75414 (0.1%)	1.58	1442/117575 (1.2%)
37	3	0.87	0/2883	1.32	14/4491 (0.3%)
37	7	1.02	1/2883 (0.0%)	1.60	54/4491 (1.2%)
38	4	0.95	1/3746 (0.0%)	1.51	47/5832 (0.8%)
38	8	0.89	0/3746	1.43	43/5832 (0.7%)
39	L2	0.65	0/1948	0.81	2/2617 (0.1%)
39	l2	0.64	0/1946	0.83	0/2614

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	L3	0.62	0/3146	0.77	0/4228
40	l3	0.76	0/3146	0.84	3/4228 (0.1%)
41	L4	0.70	1/2800 (0.0%)	0.88	3/3790 (0.1%)
41	l4	0.68	1/2800 (0.0%)	0.85	3/3790 (0.1%)
42	L5	0.51	0/2425	0.67	0/3271
42	l5	0.65	0/2408	0.76	0/3248
43	L6	0.65	0/1260	0.79	0/1694
43	l6	0.66	0/1269	0.76	1/1705 (0.1%)
44	L7	0.68	0/1821	0.85	2/2451 (0.1%)
44	l7	0.74	0/1828	0.80	2/2461 (0.1%)
45	L8	0.51	0/1836	0.69	0/2481
45	l8	0.52	0/1795	0.67	0/2429
46	L9	0.60	0/1539	0.71	0/2073
46	l9	0.70	0/1539	0.80	0/2073
47	M0	0.64	0/1741	0.76	2/2335 (0.1%)
47	m0	0.67	0/1758	0.80	3/2358 (0.1%)
48	M1	0.49	0/1374	0.71	1/1842 (0.1%)
48	m1	0.59	0/1374	0.81	2/1842 (0.1%)
49	M3	0.68	0/1568	0.80	1/2106 (0.0%)
49	m3	0.61	0/1573	0.78	0/2113
50	M4	0.61	0/1068	0.74	0/1438
50	m4	0.68	0/1074	0.80	1/1446 (0.1%)
51	M5	0.65	0/1757	0.79	1/2354 (0.0%)
51	m5	0.64	0/1757	0.77	0/2354
52	M6	0.70	0/1585	0.86	3/2128 (0.1%)
52	m6	0.84	0/1585	0.92	3/2128 (0.1%)
53	M7	0.67	0/1443	0.80	1/1944 (0.1%)
53	m7	0.78	0/1250	0.81	0/1683
54	M8	0.67	0/1465	0.85	2/1965 (0.1%)
54	m8	0.66	0/1465	0.86	2/1965 (0.1%)
55	M9	0.51	0/1538	0.66	0/2050
55	m9	0.57	0/1538	0.65	0/2050
56	N0	0.64	0/1481	0.82	3/1990 (0.2%)
56	n0	0.73	0/1481	0.83	2/1990 (0.1%)
57	N1	0.68	0/1300	0.79	0/1743
57	n1	0.74	0/1300	0.79	0/1743
58	N2	0.44	0/812	0.63	0/1099
58	n2	0.46	0/794	0.62	0/1076
59	N3	0.62	0/1018	0.78	1/1369 (0.1%)
59	n3	0.69	0/1018	0.83	1/1369 (0.1%)
60	N4	0.50	0/712	0.64	0/958
60	n4	0.61	0/1052	0.70	0/1398
61	N5	0.53	0/979	0.74	1/1321 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	n5	0.58	0/974	0.74	1/1314 (0.1%)
62	N6	0.63	0/1004	0.82	1/1341 (0.1%)
62	n6	0.57	0/1004	0.78	1/1341 (0.1%)
63	N7	0.49	0/1118	0.66	0/1497
63	n7	0.47	0/1118	0.67	0/1497
64	N8	0.72	0/1204	0.86	1/1612 (0.1%)
64	n8	0.69	0/1204	0.82	0/1612
65	N9	0.60	0/473	0.78	0/629
65	n9	0.63	0/473	0.89	1/629 (0.2%)
66	O0	0.47	0/751	0.64	0/1008
66	o0	0.49	0/775	0.69	0/1040
67	O1	0.60	0/890	0.74	0/1196
67	o1	0.66	0/897	0.81	0/1205
68	O2	0.79	0/1041	0.87	0/1394
68	o2	0.74	0/1041	0.87	2/1394 (0.1%)
69	O3	0.79	0/868	0.85	0/1168
69	o3	0.79	0/868	0.83	0/1168
70	O4	0.59	0/890	0.79	2/1189 (0.2%)
70	o4	0.57	0/890	0.81	0/1189
71	O5	0.62	0/978	0.77	0/1301
71	o5	0.53	0/974	0.67	0/1297
72	O6	0.57	0/778	0.74	0/1034
72	o6	0.55	0/777	0.70	0/1033
73	O7	0.67	0/696	0.94	4/923 (0.4%)
73	o7	0.64	0/696	0.81	1/923 (0.1%)
74	O8	0.48	0/618	0.64	1/826 (0.1%)
74	o8	0.45	0/614	0.64	0/822
75	O9	0.64	0/443	0.83	0/588
75	o9	0.63	0/443	0.76	0/588
76	Q0	0.64	0/423	0.73	0/562
76	q0	0.81	1/423 (0.2%)	0.85	0/562
77	Q1	0.66	0/234	0.84	0/300
77	q1	0.65	0/234	0.98	2/300 (0.7%)
78	Q2	0.74	1/860 (0.1%)	0.83	0/1136
78	q2	0.69	0/860	0.79	1/1136 (0.1%)
79	Q3	0.67	0/701	0.77	0/934
79	q3	0.65	0/701	0.80	0/934
80	c0	0.40	0/777	0.66	3/1049 (0.3%)
81	e0	0.49	0/499	0.72	0/665
82	e1	0.38	0/619	0.74	1/822 (0.1%)
84	p0	0.44	0/1092	0.63	1/1474 (0.1%)
All	All	0.80	153/430074 (0.0%)	1.26	3913/631364 (0.6%)

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
3	s1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	s8	0	1
13	C1	0	1
15	c3	0	1
16	C4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	3
22	d0	0	1
25	D3	0	1
26	d4	0	2
27	D5	0	3
27	d5	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	2
42	l5	0	2
43	l6	0	1
44	l7	0	2
45	L8	0	2
48	M1	0	2
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	2
56	n0	0	1
57	N1	0	1
60	n4	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
82	e1	0	1
All	All	0	52



The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.64	1.28	1.38
36	5	3008	A	N9-C4	-8.98	1.32	1.37
36	5	2358	A	N9-C4	-8.04	1.33	1.37
36	1	1114	U	C2-N3	-7.72	1.32	1.37
36	1	2714	G	N9-C4	-7.69	1.31	1.38

The worst 5 of 3913 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-21.84	112.90	126.00
36	5	1152	G	N3-C4-C5	21.63	139.41	128.60
36	5	1152	G	C2-N3-C4	-18.18	102.81	111.90
36	1	2714	G	N3-C4-C5	17.75	137.47	128.60
36	1	1308	A	O5'-P-OP2	-16.96	90.35	110.70

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	127	GLN	Peptide
16	C4	124	ASP	Peptide
18	C6	40	GLU	Peptide
19	C7	22	PRO	Peptide
9	S7	131	PHE	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	143 (70%)	34 (17%)	27 (13%)	0	1
2	s0	204/251 (81%)	152 (74%)	33 (16%)	19 (9%)	0	3
3	S1	212/254 (84%)	141 (66%)	38 (18%)	33 (16%)	0	1
3	s1	214/254 (84%)	171 (80%)	30 (14%)	13 (6%)	1	12
4	S2	215/253 (85%)	173 (80%)	27 (13%)	15 (7%)	1	8
4	s2	215/253 (85%)	184 (86%)	21 (10%)	10 (5%)	2	17
5	S3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	1	9
5	s3	221/239 (92%)	174 (79%)	31 (14%)	16 (7%)	1	7
6	S4	258/260 (99%)	206 (80%)	34 (13%)	18 (7%)	1	8
6	s4	258/260 (99%)	210 (81%)	28 (11%)	20 (8%)	1	6
7	S5	204/224 (91%)	154 (76%)	34 (17%)	16 (8%)	1	6
7	s5	204/224 (91%)	154 (76%)	35 (17%)	15 (7%)	1	7
8	S6	224/236 (95%)	197 (88%)	15 (7%)	12 (5%)	2	14
8	s6	216/236 (92%)	184 (85%)	22 (10%)	10 (5%)	2	18
9	S7	182/189 (96%)	136 (75%)	25 (14%)	21 (12%)	0	2
9	s7	184/189 (97%)	141 (77%)	28 (15%)	15 (8%)	1	5
10	S8	184/200 (92%)	148 (80%)	23 (12%)	13 (7%)	1	8
10	s8	184/200 (92%)	155 (84%)	16 (9%)	13 (7%)	1	8
11	S9	183/196 (93%)	147 (80%)	26 (14%)	10 (6%)	2	14
11	s9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	3	22
12	C0	94/105 (90%)	68 (72%)	17 (18%)	9 (10%)	0	3
13	C1	153/155 (99%)	114 (74%)	24 (16%)	15 (10%)	0	3
13	c1	144/155 (93%)	122 (85%)	16 (11%)	6 (4%)	3	20
14	C2	122/142 (86%)	67 (55%)	34 (28%)	21 (17%)	0	0
14	c2	122/142 (86%)	67 (55%)	32 (26%)	23 (19%)	0	0
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	3	21
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	1	9
16	C4	125/136 (92%)	90 (72%)	19 (15%)	16 (13%)	0	1
16	c4	126/136 (93%)	96 (76%)	19 (15%)	11 (9%)	1	4
17	C5	122/141 (86%)	88 (72%)	22 (18%)	12 (10%)	0	3
17	c5	133/141 (94%)	94 (71%)	20 (15%)	19 (14%)	0	1
18	C6	139/142 (98%)	117 (84%)	11 (8%)	11 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	1	14
19	C7	116/136 (85%)	87 (75%)	21 (18%)	8 (7%)	1	8
19	c7	113/136 (83%)	84 (74%)	19 (17%)	10 (9%)	1	4
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	5
20	c8	143/145 (99%)	115 (80%)	18 (13%)	10 (7%)	1	8
21	C9	141/143 (99%)	120 (85%)	14 (10%)	7 (5%)	2	16
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	2	20
22	D0	105/120 (88%)	82 (78%)	19 (18%)	4 (4%)	3	22
22	d0	108/120 (90%)	87 (81%)	10 (9%)	11 (10%)	0	3
23	D1	85/87 (98%)	64 (75%)	12 (14%)	9 (11%)	0	2
23	d1	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	3	24
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	6	34
24	d2	127/129 (98%)	112 (88%)	14 (11%)	1 (1%)	19	58
25	D3	142/144 (99%)	109 (77%)	19 (13%)	14 (10%)	0	3
25	d3	142/144 (99%)	119 (84%)	18 (13%)	5 (4%)	3	24
26	D4	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	1	12
26	d4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	1	7
27	D5	68/107 (64%)	44 (65%)	11 (16%)	13 (19%)	0	0
27	d5	67/107 (63%)	49 (73%)	11 (16%)	7 (10%)	0	3
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0	1
28	d6	95/97 (98%)	67 (70%)	18 (19%)	10 (10%)	0	3
29	D7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1	4
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1	4
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	0	3
30	d8	61/66 (92%)	43 (70%)	13 (21%)	5 (8%)	1	5
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	22
31	d9	51/55 (93%)	36 (71%)	9 (18%)	6 (12%)	0	2
32	E0	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	9	42
33	E1	69/76 (91%)	38 (55%)	12 (17%)	19 (28%)	0	0
34	SR	316/318 (99%)	244 (77%)	45 (14%)	27 (8%)	1	4
34	sR	316/318 (99%)	261 (83%)	42 (13%)	13 (4%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	SM	155/273 (57%)	111 (72%)	27 (17%)	17 (11%)	0	2
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0	1
39	L2	250/253 (99%)	224 (90%)	17 (7%)	9 (4%)	3	23
39	l2	250/253 (99%)	214 (86%)	23 (9%)	13 (5%)	2	15
40	L3	384/386 (100%)	322 (84%)	45 (12%)	17 (4%)	2	19
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	3	24
41	L4	359/361 (99%)	297 (83%)	34 (10%)	28 (8%)	1	6
41	l4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	1	12
42	L5	294/296 (99%)	237 (81%)	35 (12%)	22 (8%)	1	7
42	l5	292/296 (99%)	253 (87%)	32 (11%)	7 (2%)	6	34
43	L6	152/175 (87%)	134 (88%)	12 (8%)	6 (4%)	3	22
43	l6	153/175 (87%)	130 (85%)	17 (11%)	6 (4%)	3	22
44	L7	220/243 (90%)	184 (84%)	26 (12%)	10 (4%)	2	18
44	l7	221/243 (91%)	189 (86%)	27 (12%)	5 (2%)	6	34
45	L8	231/255 (91%)	189 (82%)	31 (13%)	11 (5%)	2	17
45	l8	229/255 (90%)	188 (82%)	23 (10%)	18 (8%)	1	6
46	L9	189/191 (99%)	166 (88%)	21 (11%)	2 (1%)	14	51
46	l9	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	4	26
47	M0	207/220 (94%)	171 (83%)	28 (14%)	8 (4%)	3	22
47	m0	209/220 (95%)	172 (82%)	23 (11%)	14 (7%)	1	9
48	M1	167/173 (96%)	122 (73%)	29 (17%)	16 (10%)	0	3
48	m1	167/173 (96%)	141 (84%)	15 (9%)	11 (7%)	1	9
49	M3	191/198 (96%)	154 (81%)	26 (14%)	11 (6%)	1	13
49	m3	192/198 (97%)	150 (78%)	28 (15%)	14 (7%)	1	7
50	M4	134/137 (98%)	113 (84%)	12 (9%)	9 (7%)	1	9
50	m4	135/137 (98%)	118 (87%)	16 (12%)	1 (1%)	22	61
51	M5	201/203 (99%)	183 (91%)	14 (7%)	4 (2%)	7	38
51	m5	201/203 (99%)	181 (90%)	16 (8%)	4 (2%)	7	38
52	M6	195/198 (98%)	176 (90%)	12 (6%)	7 (4%)	3	23
52	m6	195/198 (98%)	179 (92%)	10 (5%)	6 (3%)	4	26
53	M7	181/183 (99%)	144 (80%)	27 (15%)	10 (6%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	m7	153/183 (84%)	132 (86%)	18 (12%)	3 (2%)	7	38
54	M8	183/185 (99%)	154 (84%)	24 (13%)	5 (3%)	5	30
54	m8	183/185 (99%)	151 (82%)	26 (14%)	6 (3%)	4	25
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	67
55	m9	186/188 (99%)	167 (90%)	14 (8%)	5 (3%)	5	30
56	N0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	8	41
56	n0	170/172 (99%)	160 (94%)	7 (4%)	3 (2%)	8	41
57	N1	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	2	18
57	n1	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	4	26
58	N2	98/120 (82%)	72 (74%)	15 (15%)	11 (11%)	0	2
58	n2	96/120 (80%)	78 (81%)	15 (16%)	3 (3%)	4	26
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	10	44
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
60	N4	96/155 (62%)	78 (81%)	13 (14%)	5 (5%)	2	15
60	n4	133/155 (86%)	109 (82%)	15 (11%)	9 (7%)	1	9
61	N5	119/141 (84%)	106 (89%)	11 (9%)	2 (2%)	9	42
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	7
62	N6	124/126 (98%)	104 (84%)	14 (11%)	6 (5%)	2	17
62	n6	124/126 (98%)	112 (90%)	8 (6%)	4 (3%)	4	26
63	N7	133/135 (98%)	111 (84%)	11 (8%)	11 (8%)	1	5
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	1	5
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	2	17
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	3	24
65	N9	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	2	14
65	n9	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	4
66	O0	95/104 (91%)	76 (80%)	15 (16%)	4 (4%)	3	20
66	o0	98/104 (94%)	85 (87%)	13 (13%)	0	100	100
67	O1	107/112 (96%)	91 (85%)	8 (8%)	8 (8%)	1	7
67	o1	107/112 (96%)	85 (79%)	13 (12%)	9 (8%)	1	5
68	O2	125/129 (97%)	108 (86%)	17 (14%)	0	100	100
68	o2	125/129 (97%)	109 (87%)	9 (7%)	7 (6%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	O3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	4	28
69	o3	104/106 (98%)	96 (92%)	4 (4%)	4 (4%)	3	22
70	O4	110/119 (92%)	94 (86%)	14 (13%)	2 (2%)	8	41
70	o4	110/119 (92%)	100 (91%)	9 (8%)	1 (1%)	17	56
71	O5	117/119 (98%)	99 (85%)	10 (8%)	8 (7%)	1	9
71	o5	117/119 (98%)	95 (81%)	17 (14%)	5 (4%)	2	20
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	11
72	o6	97/99 (98%)	76 (78%)	15 (16%)	6 (6%)	1	11
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	3	24
73	o7	85/87 (98%)	70 (82%)	11 (13%)	4 (5%)	2	17
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	3	21
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	3	21
75	O9	48/50 (96%)	40 (83%)	6 (12%)	2 (4%)	3	20
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
76	Q0	50/52 (96%)	39 (78%)	9 (18%)	2 (4%)	3	21
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	7	38
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	20
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	1	13
78	q2	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	8	39
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	3	24
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	14	51
80	c0	92/105 (88%)	59 (64%)	16 (17%)	17 (18%)	0	0
81	e0	60/62 (97%)	43 (72%)	10 (17%)	7 (12%)	0	2
82	e1	74/76 (97%)	34 (46%)	21 (28%)	19 (26%)	0	0
84	p0	139/311 (45%)	116 (84%)	16 (12%)	7 (5%)	2	16
All	All	22333/24141 (92%)	18253 (82%)	2722 (12%)	1358 (6%)	1	12

5 of 1358 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	66	ALA
2	S0	111	ILE

### 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%)	136 (83%)	28 (17%)	2	10
2	s0	165/209 (79%)	127 (77%)	38 (23%)	1	3
3	S1	191/223 (86%)	151 (79%)	40 (21%)	1	6
3	s1	192/223 (86%)	153 (80%)	39 (20%)	1	6
4	S2	176/204 (86%)	130 (74%)	46 (26%)	0	2
4	s2	176/204 (86%)	129 (73%)	47 (27%)	0	2
5	S3	182/194 (94%)	143 (79%)	39 (21%)	1	5
5	s3	182/194 (94%)	143 (79%)	39 (21%)	1	5
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	7
6	s4	221/221 (100%)	184 (83%)	37 (17%)	2	10
7	S5	173/190 (91%)	145 (84%)	28 (16%)	2	11
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1	3
8	S6	188/201 (94%)	151 (80%)	37 (20%)	1	7
8	s6	187/201 (93%)	150 (80%)	37 (20%)	1	7
9	S7	165/169 (98%)	136 (82%)	29 (18%)	2	9
9	s7	165/169 (98%)	134 (81%)	31 (19%)	1	8
10	S8	150/161 (93%)	122 (81%)	28 (19%)	1	8
10	s8	150/161 (93%)	124 (83%)	26 (17%)	2	10
11	S9	158/165 (96%)	124 (78%)	34 (22%)	1	5
11	s9	158/165 (96%)	126 (80%)	32 (20%)	1	6
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	10
13	c1	129/136 (95%)	109 (84%)	20 (16%)	2	12
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0	2
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	1
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	5
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	8
16	C4	81/104 (78%)	60 (74%)	21 (26%)	0	2
16	c4	97/104 (93%)	69 (71%)	28 (29%)	0	1
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	6
17	c5	103/117 (88%)	78 (76%)	25 (24%)	0	2
18	C6	117/118 (99%)	89 (76%)	28 (24%)	0	3
18	c6	118/118 (100%)	95 (80%)	23 (20%)	1	7
19	C7	94/124 (76%)	75 (80%)	19 (20%)	1	6
19	c7	92/124 (74%)	66 (72%)	26 (28%)	0	1
20	C8	128/128 (100%)	96 (75%)	32 (25%)	0	2
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	6
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0	1
21	c9	115/115 (100%)	93 (81%)	22 (19%)	1	8
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2	10
22	d0	103/113 (91%)	71 (69%)	32 (31%)	0	0
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	6
23	d1	74/74 (100%)	59 (80%)	15 (20%)	1	6
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	6
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2	12
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	9
25	d3	119/119 (100%)	92 (77%)	27 (23%)	1	4
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2	9
26	d4	112/112 (100%)	91 (81%)	21 (19%)	1	8
27	D5	61/88 (69%)	50 (82%)	11 (18%)	1	9
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1	7
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	d6	83/83 (100%)	63 (76%)	20 (24%)	0	3
29	D7	70/70 (100%)	55 (79%)	15 (21%)	1	5
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2	12
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0	1
30	d8	56/59 (95%)	41 (73%)	15 (27%)	0	2
31	D9	47/48 (98%)	41 (87%)	6 (13%)	4	20
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	5
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2	9
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1
34	SR	260/261 (100%)	214 (82%)	46 (18%)	2	9
34	sR	260/261 (100%)	237 (91%)	23 (9%)	10	36
35	SM	97/228 (42%)	79 (81%)	18 (19%)	1	8
35	sM	54/228 (24%)	40 (74%)	14 (26%)	0	2
39	L2	193/195 (99%)	153 (79%)	40 (21%)	1	6
39	l2	192/195 (98%)	156 (81%)	36 (19%)	1	8
40	L3	320/322 (99%)	260 (81%)	60 (19%)	1	8
40	l3	319/322 (99%)	259 (81%)	60 (19%)	1	8
41	L4	288/288 (100%)	241 (84%)	47 (16%)	2	11
41	l4	288/288 (100%)	236 (82%)	52 (18%)	1	8
42	L5	244/244 (100%)	199 (82%)	45 (18%)	1	8
42	l5	243/244 (100%)	194 (80%)	49 (20%)	1	6
43	L6	134/152 (88%)	113 (84%)	21 (16%)	2	12
43	l6	135/152 (89%)	113 (84%)	22 (16%)	2	11
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	19
44	l7	187/204 (92%)	163 (87%)	24 (13%)	4	20
45	L8	187/207 (90%)	151 (81%)	36 (19%)	1	8
45	l8	177/207 (86%)	145 (82%)	32 (18%)	1	8
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	6
46	l9	171/171 (100%)	132 (77%)	39 (23%)	1	4
47	M0	177/186 (95%)	136 (77%)	41 (23%)	1	3
47	m0	179/186 (96%)	148 (83%)	31 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	5
48	m1	147/150 (98%)	112 (76%)	35 (24%)	0	3
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1	7
49	m3	154/158 (98%)	129 (84%)	25 (16%)	2	11
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	9
50	m4	108/108 (100%)	84 (78%)	24 (22%)	1	4
51	M5	175/175 (100%)	148 (85%)	27 (15%)	2	13
51	m5	175/175 (100%)	142 (81%)	33 (19%)	1	8
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2	11
52	m6	160/161 (99%)	136 (85%)	24 (15%)	3	14
53	M7	140/145 (97%)	114 (81%)	26 (19%)	1	8
53	m7	125/145 (86%)	101 (81%)	24 (19%)	1	8
54	M8	150/150 (100%)	123 (82%)	27 (18%)	1	9
54	m8	150/150 (100%)	125 (83%)	25 (17%)	2	10
55	M9	153/153 (100%)	130 (85%)	23 (15%)	3	14
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1	6
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	6
56	n0	156/156 (100%)	127 (81%)	29 (19%)	1	8
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	3
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	5
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2	10
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1	5
59	N3	104/104 (100%)	85 (82%)	19 (18%)	1	8
59	n3	104/104 (100%)	95 (91%)	9 (9%)	10	37
60	N4	57/129 (44%)	47 (82%)	10 (18%)	2	9
60	n4	100/129 (78%)	84 (84%)	16 (16%)	2	11
61	N5	104/117 (89%)	88 (85%)	16 (15%)	2	13
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	6
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1	6
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0	0
63	N7	115/115 (100%)	96 (84%)	19 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	n7	115/115 (100%)	89 (77%)	26 (23%)	1	4
64	N8	118/118 (100%)	90 (76%)	28 (24%)	1	3
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1	8
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	7
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	10
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1	3
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1	6
67	O1	92/96 (96%)	75 (82%)	17 (18%)	1	8
67	o1	94/96 (98%)	71 (76%)	23 (24%)	0	2
68	O2	109/110 (99%)	82 (75%)	27 (25%)	0	2
68	o2	109/110 (99%)	89 (82%)	20 (18%)	1	8
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2	10
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	9
70	O4	95/101 (94%)	76 (80%)	19 (20%)	1	6
70	o4	95/101 (94%)	78 (82%)	17 (18%)	2	9
71	O5	104/104 (100%)	79 (76%)	25 (24%)	0	3
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	6
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	2
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0	1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	1	8
73	o7	70/70 (100%)	53 (76%)	17 (24%)	0	2
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	2
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	9
75	O9	45/45 (100%)	34 (76%)	11 (24%)	0	2
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	9
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0	2
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	3
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	10
77	q1	23/23 (100%)	18 (78%)	5 (22%)	1	5
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	0	2
78	q2	90/90 (100%)	65 (72%)	25 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	10
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	6
80	c0	73/98 (74%)	65 (89%)	8 (11%)	6	26
81	e0	53/53 (100%)	40 (76%)	13 (24%)	0	2
82	e1	66/66 (100%)	45 (68%)	21 (32%)	0	0
84	p0	105/253 (42%)	84 (80%)	21 (20%)	1	6
All	All	18727/20239 (92%)	15017 (80%)	3710 (20%)	1	7

5 of 3710 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	8	ARG
8	s6	12	SER
63	n7	135	ARG
72	O6	45	ARG
3	s1	77	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
47	M0	162	GLN
3	s1	149	GLN
53	m7	34	GLN
54	M8	152	HIS
59	N3	33	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	488 (27%)	56 (3%)
1	6	1792/1800 (99%)	474 (26%)	57 (3%)
36	1	3145/3396 (92%)	688 (21%)	83 (2%)
36	5	3145/3396 (92%)	687 (21%)	76 (2%)
37	3	120/121 (99%)	14 (11%)	0
37	7	120/121 (99%)	24 (20%)	1 (0%)
38	4	157/158 (99%)	38 (24%)	2 (1%)
38	8	157/158 (99%)	37 (23%)	2 (1%)
All	All	10383/10950 (94%)	2450 (23%)	277 (2%)

5 of 2450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 277 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3169	U
1	6	417	A
36	5	2896	A
36	1	3228	C
38	4	125	U

## 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 2563 ligands modelled in this entry, 1424 are monoatomic - leaving 1139 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	$\# Z  > 2$
88	OHX	5	4019	-	0,6,6	0.00	-	-		
88	OHX	5	4150	-	0,6,6	0.00	-	-		
88	OHX	5	4064	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3934	-	0,6,6	0.00	-	-		
88	OHX	6	2119	-	0,6,6	0.00	-	-		
88	OHX	2	2122	-	0,6,6	0.00	-	-		
88	OHX	1	3992	-	0,6,6	0.00	-	-		
88	OHX	5	4224	-	0,6,6	0.00	-	-		
88	OHX	5	4191	-	0,6,6	0.00	-	-		
88	OHX	2	2058	-	0,6,6	0.00	-	-		
88	OHX	1	4088	-	0,6,6	0.00	-	-		
88	OHX	1	4036	-	0,6,6	0.00	-	-		
88	OHX	6	2086	-	0,6,6	0.00	-	-		
88	OHX	5	4049	-	0,6,6	0.00	-	-		
88	OHX	1	4064	-	0,6,6	0.00	-	-		
88	OHX	2	2031	-	0,6,6	0.00	-	-		
88	OHX	7	225	-	0,6,6	0.00	-	-		
88	OHX	1	4055	-	0,6,6	0.00	-	-		
88	OHX	5	4065	-	0,6,6	0.00	-	-		
88	OHX	1	3928	-	0,6,6	0.00	-	-		
88	OHX	2	2100	-	0,6,6	0.00	-	-		
88	OHX	6	2095	-	0,6,6	0.00	-	-		
88	OHX	1	4125	-	0,6,6	0.00	-	-		
88	OHX	2	2041	-	0,6,6	0.00	-	-		
88	OHX	1	3978	-	0,6,6	0.00	-	-		
88	OHX	1	4075	-	0,6,6	0.00	-	-		
88	OHX	1	3976	-	0,6,6	0.00	-	-		
88	OHX	5	4137	-	0,6,6	0.00	-	-		
88	OHX	6	2167	-	0,6,6	0.00	-	-		
88	OHX	1	4139	-	0,6,6	0.00	-	-		
88	OHX	1	4223	-	0,6,6	0.00	-	-		
88	OHX	2	2065	-	0,6,6	0.00	-	-		
88	OHX	5	3941	-	0,6,6	0.00	-	-		
88	OHX	2	2035	-	0,6,6	0.00	-	-		
88	OHX	1	3892	-	0,6,6	0.00	-	-		
88	OHX	5	4100	-	0,6,6	0.00	-	-		
88	OHX	1	4077	-	0,6,6	0.00	-	-		
88	OHX	1	4057	-	0,6,6	0.00	-	-		
88	OHX	1	4058	-	0,6,6	0.00	-	-		
88	OHX	1	4107	-	0,6,6	0.00	-	-		
88	OHX	5	4084	-	0,6,6	0.00	-	-		
88	OHX	2	2070	-	0,6,6	0.00	-	-		
88	OHX	1	3913	-	0,6,6	0.00	-	-		
88	OHX	3	222	-	0,6,6	0.00	-	-		
88	OHX	5	3917	-	0,6,6	0.00	-	-		
88	OHX	1	3908	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	4	229	-	0,6,6	0.00	-	-		
88	OHX	5	4005	-	0,6,6	0.00	-	-		
88	OHX	1	4144	-	0,6,6	0.00	-	-		
88	OHX	6	2134	-	0,6,6	0.00	-	-		
88	OHX	1	3955	-	0,6,6	0.00	-	-		
88	OHX	2	2110	-	0,6,6	0.00	-	-		
88	OHX	6	2135	-	0,6,6	0.00	-	-		
88	OHX	6	2183	-	0,6,6	0.00	-	-		
88	OHX	15	305	-	0,6,6	0.00	-	-		
88	OHX	2	2057	-	0,6,6	0.00	-	-		
88	OHX	5	4037	-	0,6,6	0.00	-	-		
88	OHX	1	3990	-	0,6,6	0.00	-	-		
88	OHX	1	4123	-	0,6,6	0.00	-	-		
88	OHX	5	3995	-	0,6,6	0.00	-	-		
88	OHX	1	4033	-	0,6,6	0.00	-	-		
88	OHX	5	3904	-	0,6,6	0.00	-	-		
88	OHX	6	2145	-	0,6,6	0.00	-	-		
88	OHX	5	4042	-	0,6,6	0.00	-	-		
88	OHX	5	4004	-	0,6,6	0.00	-	-		
88	OHX	6	2126	-	0,6,6	0.00	-	-		
88	OHX	2	2107	-	0,6,6	0.00	-	-		
88	OHX	5	3928	-	0,6,6	0.00	-	-		
88	OHX	1	3963	-	0,6,6	0.00	-	-		
88	OHX	5	3903	-	0,6,6	0.00	-	-		
88	OHX	5	4240	-	0,6,6	0.00	-	-		
88	OHX	5	4104	-	0,6,6	0.00	-	-		
88	OHX	5	4182	-	0,6,6	0.00	-	-		
88	OHX	5	3932	-	0,6,6	0.00	-	-		
88	OHX	5	4235	-	0,6,6	0.00	-	-		
88	OHX	2	2105	-	0,6,6	0.00	-	-		
88	OHX	2	2104	-	0,6,6	0.00	-	-		
88	OHX	5	4222	-	0,6,6	0.00	-	-		
88	OHX	5	4148	-	0,6,6	0.00	-	-		
88	OHX	5	4105	-	0,6,6	0.00	-	-		
88	OHX	1	3895	-	0,6,6	0.00	-	-		
88	OHX	1	4042	-	0,6,6	0.00	-	-		
88	OHX	7	224	-	0,6,6	0.00	-	-		
88	OHX	5	4013	-	0,6,6	0.00	-	-		
88	OHX	5	4029	-	0,6,6	0.00	-	-		
88	OHX	5	3930	-	0,6,6	0.00	-	-		
88	OHX	5	4068	-	0,6,6	0.00	-	-		
88	OHX	2	2166	-	0,6,6	0.00	-	-		
88	OHX	1	4186	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	4195	-	0,6,6	0.00	-	-		
88	OHX	m4	201	-	0,6,6	0.00	-	-		
88	OHX	5	3957	-	0,6,6	0.00	-	-		
88	OHX	1	4052	-	0,6,6	0.00	-	-		
88	OHX	1	4156	-	0,6,6	0.00	-	-		
88	OHX	1	4153	-	0,6,6	0.00	-	-		
88	OHX	5	4129	-	0,6,6	0.00	-	-		
88	OHX	1	4004	-	0,6,6	0.00	-	-		
88	OHX	2	2121	-	0,6,6	0.00	-	-		
88	OHX	5	4051	-	0,6,6	0.00	-	-		
88	OHX	5	4135	-	0,6,6	0.00	-	-		
88	OHX	1	4218	-	0,6,6	0.00	-	-		
88	OHX	6	2064	-	0,6,6	0.00	-	-		
88	OHX	5	4190	-	0,6,6	0.00	-	-		
88	OHX	5	4034	-	0,6,6	0.00	-	-		
88	OHX	5	3939	-	0,6,6	0.00	-	-		
88	OHX	1	4120	-	0,6,6	0.00	-	-		
88	OHX	6	2153	-	0,6,6	0.00	-	-		
88	OHX	2	2044	-	0,6,6	0.00	-	-		
88	OHX	5	4071	-	0,6,6	0.00	-	-		
88	OHX	1	4040	-	0,6,6	0.00	-	-		
88	OHX	6	2049	-	0,6,6	0.00	-	-		
88	OHX	5	4091	-	0,6,6	0.00	-	-		
88	OHX	O3	201	-	0,6,6	0.00	-	-		
88	OHX	5	4086	-	0,6,6	0.00	-	-		
88	OHX	6	2152	-	0,6,6	0.00	-	-		
88	OHX	1	4065	-	0,6,6	0.00	-	-		
88	OHX	1	4104	-	0,6,6	0.00	-	-		
88	OHX	2	2073	-	0,6,6	0.00	-	-		
88	OHX	5	4059	-	0,6,6	0.00	-	-		
88	OHX	5	4053	-	0,6,6	0.00	-	-		
88	OHX	O7	104	-	0,6,6	0.00	-	-		
88	OHX	2	2056	-	0,6,6	0.00	-	-		
88	OHX	5	4142	-	0,6,6	0.00	-	-		
88	OHX	1	4145	-	0,6,6	0.00	-	-		
88	OHX	2	2043	-	0,6,6	0.00	-	-		
88	OHX	1	4067	-	0,6,6	0.00	-	-		
88	OHX	6	2070	-	0,6,6	0.00	-	-		
88	OHX	5	4007	-	0,6,6	0.00	-	-		
88	OHX	1	4022	-	0,6,6	0.00	-	-		
88	OHX	1	4116	-	0,6,6	0.00	-	-		
88	OHX	8	218	-	0,6,6	0.00	-	-		
88	OHX	n3	204	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	4179	-	0,6,6	0.00	-	-		
88	OHX	5	4196	-	0,6,6	0.00	-	-		
88	OHX	8	227	-	0,6,6	0.00	-	-		
88	OHX	1	3903	-	0,6,6	0.00	-	-		
88	OHX	6	2155	-	0,6,6	0.00	-	-		
88	OHX	6	2077	-	0,6,6	0.00	-	-		
88	OHX	6	2117	-	0,6,6	0.00	-	-		
88	OHX	o3	202	-	0,6,6	0.00	-	-		
88	OHX	1	3897	-	0,6,6	0.00	-	-		
88	OHX	5	4256	-	0,6,6	0.00	-	-		
88	OHX	5	3960	-	0,6,6	0.00	-	-		
88	OHX	5	4127	-	0,6,6	0.00	-	-		
88	OHX	1	3982	-	0,6,6	0.00	-	-		
88	OHX	1	4085	-	0,6,6	0.00	-	-		
88	OHX	2	2178	-	0,6,6	0.00	-	-		
88	OHX	1	3905	-	0,6,6	0.00	-	-		
88	OHX	5	4201	-	0,6,6	0.00	-	-		
88	OHX	2	2153	-	0,6,6	0.00	-	-		
88	OHX	5	4095	-	0,6,6	0.00	-	-		
88	OHX	1	4012	-	0,6,6	0.00	-	-		
88	OHX	c8	202	-	0,6,6	0.00	-	-		
88	OHX	1	3882	-	0,6,6	0.00	-	-		
88	OHX	2	2146	-	0,6,6	0.00	-	-		
88	OHX	2	2080	-	0,6,6	0.00	-	-		
88	OHX	5	4066	-	0,6,6	0.00	-	-		
88	OHX	2	2118	-	0,6,6	0.00	-	-		
88	OHX	1	3898	-	0,6,6	0.00	-	-		
88	OHX	m6	203	-	0,6,6	0.00	-	-		
88	OHX	5	4209	-	0,6,6	0.00	-	-		
88	OHX	1	4118	-	0,6,6	0.00	-	-		
88	OHX	1	4079	-	0,6,6	0.00	-	-		
88	OHX	6	2163	-	0,6,6	0.00	-	-		
88	OHX	2	2029	-	0,6,6	0.00	-	-		
88	OHX	5	3915	-	0,6,6	0.00	-	-		
88	OHX	6	2097	-	0,6,6	0.00	-	-		
88	OHX	6	2146	-	0,6,6	0.00	-	-		
88	OHX	1	4132	-	0,6,6	0.00	-	-		
88	OHX	1	4152	-	0,6,6	0.00	-	-		
88	OHX	1	4014	-	0,6,6	0.00	-	-		
88	OHX	8	226	-	0,6,6	0.00	-	-		
88	OHX	5	4236	-	0,6,6	0.00	-	-		
88	OHX	5	4039	-	0,6,6	0.00	-	-		
88	OHX	1	4208	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2086	-	0,6,6	0.00	-	-		
88	OHX	5	4056	-	0,6,6	0.00	-	-		
88	OHX	5	4157	-	0,6,6	0.00	-	-		
88	OHX	3	224	-	0,6,6	0.00	-	-		
88	OHX	6	2164	-	0,6,6	0.00	-	-		
88	OHX	2	2141	-	0,6,6	0.00	-	-		
88	OHX	1	3944	-	0,6,6	0.00	-	-		
88	OHX	5	4184	-	0,6,6	0.00	-	-		
88	OHX	1	4109	-	0,6,6	0.00	-	-		
88	OHX	1	4043	-	0,6,6	0.00	-	-		
88	OHX	5	4158	-	0,6,6	0.00	-	-		
88	OHX	M8	201	-	0,6,6	0.00	-	-		
88	OHX	5	4173	-	0,6,6	0.00	-	-		
88	OHX	1	3937	-	0,6,6	0.00	-	-		
88	OHX	5	3989	-	0,6,6	0.00	-	-		
88	OHX	2	2113	-	0,6,6	0.00	-	-		
88	OHX	1	3918	-	0,6,6	0.00	-	-		
88	OHX	m5	306	-	0,6,6	0.00	-	-		
88	OHX	6	2149	-	0,6,6	0.00	-	-		
88	OHX	6	2091	-	0,6,6	0.00	-	-		
88	OHX	5	4242	-	0,6,6	0.00	-	-		
88	OHX	6	2112	-	0,6,6	0.00	-	-		
88	OHX	5	3948	-	0,6,6	0.00	-	-		
88	OHX	5	3901	-	0,6,6	0.00	-	-		
88	OHX	l3	405	-	0,6,6	0.00	-	-		
88	OHX	2	2115	-	0,6,6	0.00	-	-		
88	OHX	5	3952	-	0,6,6	0.00	-	-		
88	OHX	2	2164	-	0,6,6	0.00	-	-		
88	OHX	2	2064	-	0,6,6	0.00	-	-		
88	OHX	1	4194	-	0,6,6	0.00	-	-		
88	OHX	5	3946	-	0,6,6	0.00	-	-		
88	OHX	6	2138	-	0,6,6	0.00	-	-		
88	OHX	6	2052	-	0,6,6	0.00	-	-		
88	OHX	1	4076	-	0,6,6	0.00	-	-		
88	OHX	1	4114	-	0,6,6	0.00	-	-		
88	OHX	d4	202	-	0,6,6	0.00	-	-		
88	OHX	5	4141	-	0,6,6	0.00	-	-		
88	OHX	2	2149	-	0,6,6	0.00	-	-		
88	OHX	1	4016	-	0,6,6	0.00	-	-		
88	OHX	5	4063	-	0,6,6	0.00	-	-		
88	OHX	5	4062	-	0,6,6	0.00	-	-		
88	OHX	5	4111	-	0,6,6	0.00	-	-		
88	OHX	1	3890	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2148	-	0,6,6	0.00	-	-		
88	OHX	5	4228	-	0,6,6	0.00	-	-		
88	OHX	1	4197	-	0,6,6	0.00	-	-		
88	OHX	2	2152	-	0,6,6	0.00	-	-		
88	OHX	1	4192	-	0,6,6	0.00	-	-		
88	OHX	1	4176	-	0,6,6	0.00	-	-		
88	OHX	2	2097	-	0,6,6	0.00	-	-		
88	OHX	5	3958	-	0,6,6	0.00	-	-		
88	OHX	2	2085	-	0,6,6	0.00	-	-		
88	OHX	6	2099	-	0,6,6	0.00	-	-		
88	OHX	5	4125	-	0,6,6	0.00	-	-		
88	OHX	1	4027	-	0,6,6	0.00	-	-		
88	OHX	S8	302	-	0,6,6	0.00	-	-		
88	OHX	5	4024	-	0,6,6	0.00	-	-		
88	OHX	2	2127	-	0,6,6	0.00	-	-		
88	OHX	1	4196	-	0,6,6	0.00	-	-		
88	OHX	5	4221	-	0,6,6	0.00	-	-		
88	OHX	1	4013	-	0,6,6	0.00	-	-		
88	OHX	1	3998	-	0,6,6	0.00	-	-		
88	OHX	2	2054	-	0,6,6	0.00	-	-		
88	OHX	5	4092	-	0,6,6	0.00	-	-		
88	OHX	5	4215	-	0,6,6	0.00	-	-		
88	OHX	1	4200	-	0,6,6	0.00	-	-		
88	OHX	5	4210	-	0,6,6	0.00	-	-		
88	OHX	1	4205	-	0,6,6	0.00	-	-		
88	OHX	1	3902	-	0,6,6	0.00	-	-		
88	OHX	5	4082	-	0,6,6	0.00	-	-		
88	OHX	5	4154	-	0,6,6	0.00	-	-		
88	OHX	1	3979	-	0,6,6	0.00	-	-		
88	OHX	8	230	-	0,6,6	0.00	-	-		
88	OHX	1	3974	-	0,6,6	0.00	-	-		
88	OHX	1	4054	-	0,6,6	0.00	-	-		
88	OHX	6	2142	-	0,6,6	0.00	-	-		
88	OHX	6	2180	-	0,6,6	0.00	-	-		
88	OHX	1	4174	-	0,6,6	0.00	-	-		
88	OHX	2	2091	-	0,6,6	0.00	-	-		
88	OHX	1	3980	-	0,6,6	0.00	-	-		
88	OHX	5	4241	-	0,6,6	0.00	-	-		
88	OHX	1	4024	-	0,6,6	0.00	-	-		
88	OHX	c1	202	-	0,6,6	0.00	-	-		
88	OHX	5	4134	-	0,6,6	0.00	-	-		
88	OHX	1	4021	-	0,6,6	0.00	-	-		
88	OHX	5	4200	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2079	-	0,6,6	0.00	-	-		
88	OHX	5	4234	-	0,6,6	0.00	-	-		
88	OHX	5	4217	-	0,6,6	0.00	-	-		
88	OHX	o7	502	-	0,6,6	0.00	-	-		
88	OHX	1	4129	-	0,6,6	0.00	-	-		
88	OHX	5	3945	-	0,6,6	0.00	-	-		
88	OHX	1	4202	-	0,6,6	0.00	-	-		
88	OHX	1	4099	-	0,6,6	0.00	-	-		
88	OHX	5	4156	-	0,6,6	0.00	-	-		
88	OHX	6	2191	-	0,6,6	0.00	-	-		
88	OHX	5	4232	-	0,6,6	0.00	-	-		
88	OHX	6	2175	-	0,6,6	0.00	-	-		
88	OHX	1	4204	-	0,6,6	0.00	-	-		
88	OHX	1	4148	-	0,6,6	0.00	-	-		
88	OHX	5	3922	-	0,6,6	0.00	-	-		
88	OHX	1	4119	-	0,6,6	0.00	-	-		
88	OHX	6	2075	-	0,6,6	0.00	-	-		
88	OHX	1	4003	-	0,6,6	0.00	-	-		
88	OHX	M0	303	-	0,6,6	0.00	-	-		
88	OHX	1	4135	-	0,6,6	0.00	-	-		
88	OHX	5	4251	-	0,6,6	0.00	-	-		
88	OHX	2	2136	-	0,6,6	0.00	-	-		
88	OHX	3	221	-	0,6,6	0.00	-	-		
88	OHX	5	4047	-	0,6,6	0.00	-	-		
88	OHX	5	3942	-	0,6,6	0.00	-	-		
88	OHX	6	2195	-	0,6,6	0.00	-	-		
88	OHX	5	3925	-	0,6,6	0.00	-	-		
88	OHX	1	4147	-	0,6,6	0.00	-	-		
88	OHX	1	4213	-	0,6,6	0.00	-	-		
88	OHX	6	2154	-	0,6,6	0.00	-	-		
88	OHX	2	2134	-	0,6,6	0.00	-	-		
88	OHX	6	2092	-	0,6,6	0.00	-	-		
88	OHX	5	4044	-	0,6,6	0.00	-	-		
88	OHX	5	4036	-	0,6,6	0.00	-	-		
88	OHX	5	4204	-	0,6,6	0.00	-	-		
88	OHX	5	4130	-	0,6,6	0.00	-	-		
88	OHX	5	4205	-	0,6,6	0.00	-	-		
88	OHX	6	2106	-	0,6,6	0.00	-	-		
88	OHX	5	4002	-	0,6,6	0.00	-	-		
88	OHX	1	4087	-	0,6,6	0.00	-	-		
88	OHX	5	4143	-	0,6,6	0.00	-	-		
88	OHX	5	3974	-	0,6,6	0.00	-	-		
88	OHX	2	2169	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3977	-	0,6,6	0.00	-	-		
88	OHX	1	4006	-	0,6,6	0.00	-	-		
88	OHX	5	4072	-	0,6,6	0.00	-	-		
88	OHX	5	4160	-	0,6,6	0.00	-	-		
88	OHX	5	4117	-	0,6,6	0.00	-	-		
88	OHX	5	3991	-	0,6,6	0.00	-	-		
88	OHX	1	4029	-	0,6,6	0.00	-	-		
88	OHX	5	4172	-	0,6,6	0.00	-	-		
88	OHX	1	4018	-	0,6,6	0.00	-	-		
88	OHX	5	4054	-	0,6,6	0.00	-	-		
88	OHX	5	3951	-	0,6,6	0.00	-	-		
88	OHX	2	2120	-	0,6,6	0.00	-	-		
88	OHX	6	2168	-	0,6,6	0.00	-	-		
88	OHX	6	2096	-	0,6,6	0.00	-	-		
88	OHX	6	2104	-	0,6,6	0.00	-	-		
88	OHX	7	216	-	0,6,6	0.00	-	-		
88	OHX	6	2176	-	0,6,6	0.00	-	-		
88	OHX	5	3992	-	0,6,6	0.00	-	-		
88	OHX	2	2171	-	0,6,6	0.00	-	-		
88	OHX	6	2137	-	0,6,6	0.00	-	-		
88	OHX	2	2075	-	0,6,6	0.00	-	-		
88	OHX	5	4152	-	0,6,6	0.00	-	-		
88	OHX	5	4144	-	0,6,6	0.00	-	-		
88	OHX	1	4032	-	0,6,6	0.00	-	-		
88	OHX	5	3924	-	0,6,6	0.00	-	-		
88	OHX	5	3993	-	0,6,6	0.00	-	-		
88	OHX	2	2032	-	0,6,6	0.00	-	-		
88	OHX	2	2048	-	0,6,6	0.00	-	-		
88	OHX	1	4035	-	0,6,6	0.00	-	-		
88	OHX	d9	102	-	0,6,6	0.00	-	-		
88	OHX	2	2155	-	0,6,6	0.00	-	-		
88	OHX	5	4079	-	0,6,6	0.00	-	-		
88	OHX	1	3954	-	0,6,6	0.00	-	-		
88	OHX	5	4114	-	0,6,6	0.00	-	-		
88	OHX	2	2131	-	0,6,6	0.00	-	-		
88	OHX	1	3943	-	0,6,6	0.00	-	-		
88	OHX	5	4239	-	0,6,6	0.00	-	-		
88	OHX	5	3944	-	0,6,6	0.00	-	-		
88	OHX	5	3905	-	0,6,6	0.00	-	-		
88	OHX	5	4080	-	0,6,6	0.00	-	-		
88	OHX	2	2159	-	0,6,6	0.00	-	-		
88	OHX	2	2092	-	0,6,6	0.00	-	-		
88	OHX	2	2109	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2028	-	0,6,6	0.00	-	-		
88	OHX	1	4164	-	0,6,6	0.00	-	-		
88	OHX	4	230	-	0,6,6	0.00	-	-		
88	OHX	6	2074	-	0,6,6	0.00	-	-		
88	OHX	5	4162	-	0,6,6	0.00	-	-		
88	OHX	1	4133	-	0,6,6	0.00	-	-		
88	OHX	2	2072	-	0,6,6	0.00	-	-		
88	OHX	1	4191	-	0,6,6	0.00	-	-		
88	OHX	2	2101	-	0,6,6	0.00	-	-		
88	OHX	4	231	-	0,6,6	0.00	-	-		
88	OHX	5	4131	-	0,6,6	0.00	-	-		
88	OHX	5	4223	-	0,6,6	0.00	-	-		
88	OHX	1	4131	-	0,6,6	0.00	-	-		
88	OHX	1	4155	-	0,6,6	0.00	-	-		
88	OHX	5	3971	-	0,6,6	0.00	-	-		
88	OHX	1	4193	-	0,6,6	0.00	-	-		
88	OHX	1	4100	-	0,6,6	0.00	-	-		
88	OHX	5	4069	-	0,6,6	0.00	-	-		
88	OHX	5	4103	-	0,6,6	0.00	-	-		
88	OHX	5	3978	-	0,6,6	0.00	-	-		
88	OHX	1	3950	-	0,6,6	0.00	-	-		
88	OHX	1	3893	-	0,6,6	0.00	-	-		
88	OHX	5	4192	-	0,6,6	0.00	-	-		
88	OHX	6	2101	-	0,6,6	0.00	-	-		
88	OHX	6	2063	-	0,6,6	0.00	-	-		
88	OHX	6	2200	-	0,6,6	0.00	-	-		
88	OHX	6	2066	-	0,6,6	0.00	-	-		
88	OHX	1	4140	-	0,6,6	0.00	-	-		
88	OHX	5	4246	-	0,6,6	0.00	-	-		
88	OHX	1	4201	-	0,6,6	0.00	-	-		
88	OHX	1	4217	-	0,6,6	0.00	-	-		
88	OHX	1	3934	-	0,6,6	0.00	-	-		
88	OHX	6	2056	-	0,6,6	0.00	-	-		
88	OHX	2	2114	-	0,6,6	0.00	-	-		
88	OHX	5	3937	-	0,6,6	0.00	-	-		
88	OHX	5	3919	-	0,6,6	0.00	-	-		
88	OHX	5	4094	-	0,6,6	0.00	-	-		
88	OHX	1	4138	-	0,6,6	0.00	-	-		
88	OHX	2	2154	-	0,6,6	0.00	-	-		
88	OHX	2	2087	-	0,6,6	0.00	-	-		
88	OHX	5	3947	-	0,6,6	0.00	-	-		
88	OHX	1	4103	-	0,6,6	0.00	-	-		
88	OHX	s1	302	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	4106	-	0,6,6	0.00	-	-		
88	OHX	6	2065	-	0,6,6	0.00	-	-		
88	OHX	1	3899	-	0,6,6	0.00	-	-		
88	OHX	2	2112	-	0,6,6	0.00	-	-		
88	OHX	2	2140	-	0,6,6	0.00	-	-		
88	OHX	5	4248	-	0,6,6	0.00	-	-		
88	OHX	1	4001	-	0,6,6	0.00	-	-		
88	OHX	7	215	-	0,6,6	0.00	-	-		
88	OHX	1	3914	-	0,6,6	0.00	-	-		
88	OHX	6	2186	-	0,6,6	0.00	-	-		
88	OHX	1	4215	-	0,6,6	0.00	-	-		
88	OHX	7	226	-	0,6,6	0.00	-	-		
88	OHX	6	2083	-	0,6,6	0.00	-	-		
88	OHX	m1	203	-	0,6,6	0.00	-	-		
88	OHX	l3	406	-	0,6,6	0.00	-	-		
88	OHX	2	2180	-	0,6,6	0.00	-	-		
88	OHX	5	4188	-	0,6,6	0.00	-	-		
88	OHX	1	4066	-	0,6,6	0.00	-	-		
88	OHX	2	2137	-	0,6,6	0.00	-	-		
88	OHX	3	216	-	0,6,6	0.00	-	-		
88	OHX	8	217	-	0,6,6	0.00	-	-		
88	OHX	5	3983	-	0,6,6	0.00	-	-		
88	OHX	1	3920	-	0,6,6	0.00	-	-		
88	OHX	6	2093	-	0,6,6	0.00	-	-		
88	OHX	1	3984	-	0,6,6	0.00	-	-		
88	OHX	1	4009	-	0,6,6	0.00	-	-		
88	OHX	3	223	-	0,6,6	0.00	-	-		
88	OHX	1	4061	-	0,6,6	0.00	-	-		
88	OHX	6	2177	-	0,6,6	0.00	-	-		
88	OHX	1	4044	-	0,6,6	0.00	-	-		
88	OHX	5	3943	-	0,6,6	0.00	-	-		
88	OHX	5	4108	-	0,6,6	0.00	-	-		
88	OHX	1	4159	-	0,6,6	0.00	-	-		
88	OHX	2	2117	-	0,6,6	0.00	-	-		
88	OHX	1	3938	-	0,6,6	0.00	-	-		
88	OHX	L3	404	-	0,6,6	0.00	-	-		
88	OHX	1	3901	-	0,6,6	0.00	-	-		
88	OHX	5	4008	-	0,6,6	0.00	-	-		
88	OHX	6	2190	-	0,6,6	0.00	-	-		
88	OHX	2	2167	-	0,6,6	0.00	-	-		
88	OHX	1	3874	-	0,6,6	0.00	-	-		
88	OHX	5	4140	-	0,6,6	0.00	-	-		
88	OHX	5	3920	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2174	-	0,6,6	0.00	-	-		
88	OHX	6	2141	-	0,6,6	0.00	-	-		
88	OHX	1	4173	-	0,6,6	0.00	-	-		
88	OHX	1	4034	-	0,6,6	0.00	-	-		
88	OHX	2	2103	-	0,6,6	0.00	-	-		
88	OHX	1	4183	-	0,6,6	0.00	-	-		
88	OHX	6	2058	-	0,6,6	0.00	-	-		
88	OHX	2	2126	-	0,6,6	0.00	-	-		
88	OHX	6	2067	-	0,6,6	0.00	-	-		
88	OHX	5	4107	-	0,6,6	0.00	-	-		
88	OHX	5	3931	-	0,6,6	0.00	-	-		
88	OHX	8	219	-	0,6,6	0.00	-	-		
88	OHX	6	2166	-	0,6,6	0.00	-	-		
88	OHX	1	3924	-	0,6,6	0.00	-	-		
88	OHX	6	2156	-	0,6,6	0.00	-	-		
88	OHX	6	2078	-	0,6,6	0.00	-	-		
88	OHX	6	2158	-	0,6,6	0.00	-	-		
88	OHX	5	4016	-	0,6,6	0.00	-	-		
88	OHX	6	2131	-	0,6,6	0.00	-	-		
88	OHX	1	4094	-	0,6,6	0.00	-	-		
88	OHX	5	4099	-	0,6,6	0.00	-	-		
88	OHX	6	2151	-	0,6,6	0.00	-	-		
88	OHX	1	3886	-	0,6,6	0.00	-	-		
88	OHX	5	3913	-	0,6,6	0.00	-	-		
88	OHX	6	2068	-	0,6,6	0.00	-	-		
88	OHX	5	4237	-	0,6,6	0.00	-	-		
88	OHX	6	2184	-	0,6,6	0.00	-	-		
88	OHX	2	2083	-	0,6,6	0.00	-	-		
88	OHX	6	2189	-	0,6,6	0.00	-	-		
88	OHX	2	2038	-	0,6,6	0.00	-	-		
88	OHX	5	4118	-	0,6,6	0.00	-	-		
88	OHX	m0	301	-	0,6,6	0.00	-	-		
88	OHX	2	2098	-	0,6,6	0.00	-	-		
88	OHX	1	4184	-	0,6,6	0.00	-	-		
88	OHX	5	4123	-	0,6,6	0.00	-	-		
88	OHX	7	218	-	0,6,6	0.00	-	-		
88	OHX	L4	402	-	0,6,6	0.00	-	-		
88	OHX	5	4159	-	0,6,6	0.00	-	-		
88	OHX	5	3984	-	0,6,6	0.00	-	-		
88	OHX	1	4041	-	0,6,6	0.00	-	-		
88	OHX	1	4166	-	0,6,6	0.00	-	-		
88	OHX	2	2053	-	0,6,6	0.00	-	-		
88	OHX	5	4197	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3969	-	0,6,6	0.00	-	-		
88	OHX	1	4097	-	0,6,6	0.00	-	-		
88	OHX	2	2145	-	0,6,6	0.00	-	-		
88	OHX	6	2173	-	0,6,6	0.00	-	-		
88	OHX	2	2173	-	0,6,6	0.00	-	-		
88	OHX	6	2114	-	0,6,6	0.00	-	-		
88	OHX	5	4023	-	0,6,6	0.00	-	-		
88	OHX	5	3926	-	0,6,6	0.00	-	-		
88	OHX	1	4142	-	0,6,6	0.00	-	-		
88	OHX	6	2053	-	0,6,6	0.00	-	-		
88	OHX	6	2169	-	0,6,6	0.00	-	-		
88	OHX	2	2179	-	0,6,6	0.00	-	-		
88	OHX	2	2108	-	0,6,6	0.00	-	-		
88	OHX	1	4111	-	0,6,6	0.00	-	-		
88	OHX	1	3968	-	0,6,6	0.00	-	-		
88	OHX	2	2062	-	0,6,6	0.00	-	-		
88	OHX	6	2136	-	0,6,6	0.00	-	-		
88	OHX	5	3906	-	0,6,6	0.00	-	-		
88	OHX	5	4003	-	0,6,6	0.00	-	-		
88	OHX	1	3957	-	0,6,6	0.00	-	-		
88	OHX	1	3891	-	0,6,6	0.00	-	-		
88	OHX	6	2160	-	0,6,6	0.00	-	-		
88	OHX	1	3997	-	0,6,6	0.00	-	-		
88	OHX	5	4216	-	0,6,6	0.00	-	-		
88	OHX	1	3995	-	0,6,6	0.00	-	-		
88	OHX	5	4167	-	0,6,6	0.00	-	-		
88	OHX	2	2165	-	0,6,6	0.00	-	-		
88	OHX	1	3948	-	0,6,6	0.00	-	-		
88	OHX	5	4219	-	0,6,6	0.00	-	-		
88	OHX	1	4207	-	0,6,6	0.00	-	-		
88	OHX	5	3997	-	0,6,6	0.00	-	-		
88	OHX	1	4098	-	0,6,6	0.00	-	-		
88	OHX	6	2140	-	0,6,6	0.00	-	-		
88	OHX	5	4025	-	0,6,6	0.00	-	-		
88	OHX	13	404	-	0,6,6	0.00	-	-		
88	OHX	5	4258	-	0,6,6	0.00	-	-		
88	OHX	1	4053	-	0,6,6	0.00	-	-		
88	OHX	1	4056	-	0,6,6	0.00	-	-		
88	OHX	2	2160	-	0,6,6	0.00	-	-		
88	OHX	6	2170	-	0,6,6	0.00	-	-		
88	OHX	2	2133	-	0,6,6	0.00	-	-		
88	OHX	2	2156	-	0,6,6	0.00	-	-		
88	OHX	2	2158	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2090	-	0,6,6	0.00	-	-		
88	OHX	6	2107	-	0,6,6	0.00	-	-		
88	OHX	6	2162	-	0,6,6	0.00	-	-		
88	OHX	1	3981	-	0,6,6	0.00	-	-		
88	OHX	L3	406	-	0,6,6	0.00	-	-		
88	OHX	n9	101	-	0,6,6	0.00	-	-		
88	OHX	2	2088	-	0,6,6	0.00	-	-		
88	OHX	1	3935	-	0,6,6	0.00	-	-		
88	OHX	c5	201	-	0,6,6	0.00	-	-		
88	OHX	5	4139	-	0,6,6	0.00	-	-		
88	OHX	6	2147	-	0,6,6	0.00	-	-		
88	OHX	6	2124	-	0,6,6	0.00	-	-		
88	OHX	1	3879	-	0,6,6	0.00	-	-		
88	OHX	6	2085	-	0,6,6	0.00	-	-		
88	OHX	1	4051	-	0,6,6	0.00	-	-		
88	OHX	1	3945	-	0,6,6	0.00	-	-		
88	OHX	5	4145	-	0,6,6	0.00	-	-		
88	OHX	6	2125	-	0,6,6	0.00	-	-		
88	OHX	1	4046	-	0,6,6	0.00	-	-		
88	OHX	1	4209	-	0,6,6	0.00	-	-		
88	OHX	5	4077	-	0,6,6	0.00	-	-		
88	OHX	5	4050	-	0,6,6	0.00	-	-		
88	OHX	6	2122	-	0,6,6	0.00	-	-		
88	OHX	1	3877	-	0,6,6	0.00	-	-		
88	OHX	2	2147	-	0,6,6	0.00	-	-		
88	OHX	N9	101	-	0,6,6	0.00	-	-		
88	OHX	6	2082	-	0,6,6	0.00	-	-		
88	OHX	5	3923	-	0,6,6	0.00	-	-		
88	OHX	1	4063	-	0,6,6	0.00	-	-		
88	OHX	1	4095	-	0,6,6	0.00	-	-		
88	OHX	1	4017	-	0,6,6	0.00	-	-		
88	OHX	2	2061	-	0,6,6	0.00	-	-		
88	OHX	1	3941	-	0,6,6	0.00	-	-		
88	OHX	6	2198	-	0,6,6	0.00	-	-		
88	OHX	1	3989	-	0,6,6	0.00	-	-		
88	OHX	6	2196	-	0,6,6	0.00	-	-		
88	OHX	1	3970	-	0,6,6	0.00	-	-		
88	OHX	1	4167	-	0,6,6	0.00	-	-		
88	OHX	1	4007	-	0,6,6	0.00	-	-		
88	OHX	5	4225	-	0,6,6	0.00	-	-		
88	OHX	1	3993	-	0,6,6	0.00	-	-		
88	OHX	5	4163	-	0,6,6	0.00	-	-		
88	OHX	1	4210	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	4045	-	0,6,6	0.00	-	-		
88	OHX	5	4238	-	0,6,6	0.00	-	-		
88	OHX	1	4211	-	0,6,6	0.00	-	-		
88	OHX	5	4126	-	0,6,6	0.00	-	-		
88	OHX	1	4072	-	0,6,6	0.00	-	-		
88	OHX	6	2181	-	0,6,6	0.00	-	-		
88	OHX	1	3931	-	0,6,6	0.00	-	-		
88	OHX	5	3956	-	0,6,6	0.00	-	-		
88	OHX	6	2094	-	0,6,6	0.00	-	-		
88	OHX	5	3967	-	0,6,6	0.00	-	-		
88	OHX	1	4084	-	0,6,6	0.00	-	-		
88	OHX	2	2060	-	0,6,6	0.00	-	-		
88	OHX	1	3922	-	0,6,6	0.00	-	-		
88	OHX	5	3979	-	0,6,6	0.00	-	-		
88	OHX	6	2187	-	0,6,6	0.00	-	-		
88	OHX	2	2096	-	0,6,6	0.00	-	-		
88	OHX	5	4128	-	0,6,6	0.00	-	-		
88	OHX	1	3880	-	0,6,6	0.00	-	-		
88	OHX	1	4026	-	0,6,6	0.00	-	-		
88	OHX	5	3994	-	0,6,6	0.00	-	-		
88	OHX	14	403	-	0,6,6	0.00	-	-		
88	OHX	6	2185	-	0,6,6	0.00	-	-		
88	OHX	1	4212	-	0,6,6	0.00	-	-		
88	OHX	5	4194	-	0,6,6	0.00	-	-		
88	OHX	5	4116	-	0,6,6	0.00	-	-		
88	OHX	2	2094	-	0,6,6	0.00	-	-		
88	OHX	6	2193	-	0,6,6	0.00	-	-		
88	OHX	5	3950	-	0,6,6	0.00	-	-		
88	OHX	6	2045	-	0,6,6	0.00	-	-		
88	OHX	1	4069	-	0,6,6	0.00	-	-		
88	OHX	5	3977	-	0,6,6	0.00	-	-		
88	OHX	1	4126	-	0,6,6	0.00	-	-		
88	OHX	1	3912	-	0,6,6	0.00	-	-		
88	OHX	1	4170	-	0,6,6	0.00	-	-		
88	OHX	1	3986	-	0,6,6	0.00	-	-		
88	OHX	5	4052	-	0,6,6	0.00	-	-		
88	OHX	1	3983	-	0,6,6	0.00	-	-		
88	OHX	D9	102	-	0,6,6	0.00	-	-		
88	OHX	1	4039	-	0,6,6	0.00	-	-		
88	OHX	1	4049	-	0,6,6	0.00	-	-		
88	OHX	5	3907	-	0,6,6	0.00	-	-		
88	OHX	1	4117	-	0,6,6	0.00	-	-		
88	OHX	2	2033	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	D3	202	-	0,6,6	0.00	-	-		
88	OHX	1	3875	-	0,6,6	0.00	-	-		
88	OHX	5	4124	-	0,6,6	0.00	-	-		
88	OHX	c3	201	-	0,6,6	0.00	-	-		
88	OHX	1	4222	-	0,6,6	0.00	-	-		
88	OHX	1	4162	-	0,6,6	0.00	-	-		
88	OHX	1	4025	-	0,6,6	0.00	-	-		
88	OHX	6	2116	-	0,6,6	0.00	-	-		
88	OHX	5	3962	-	0,6,6	0.00	-	-		
88	OHX	5	4250	-	0,6,6	0.00	-	-		
88	OHX	1	3889	-	0,6,6	0.00	-	-		
88	OHX	2	2026	-	0,6,6	0.00	-	-		
88	OHX	5	4233	-	0,6,6	0.00	-	-		
88	OHX	1	3925	-	0,6,6	0.00	-	-		
88	OHX	5	4249	-	0,6,6	0.00	-	-		
88	OHX	6	2199	-	0,6,6	0.00	-	-		
88	OHX	5	4088	-	0,6,6	0.00	-	-		
88	OHX	1	4062	-	0,6,6	0.00	-	-		
88	OHX	6	2172	-	0,6,6	0.00	-	-		
88	OHX	1	4038	-	0,6,6	0.00	-	-		
88	OHX	2	2144	-	0,6,6	0.00	-	-		
88	OHX	6	2120	-	0,6,6	0.00	-	-		
88	OHX	1	3927	-	0,6,6	0.00	-	-		
88	OHX	1	3926	-	0,6,6	0.00	-	-		
88	OHX	5	4010	-	0,6,6	0.00	-	-		
88	OHX	6	2133	-	0,6,6	0.00	-	-		
88	OHX	5	4212	-	0,6,6	0.00	-	-		
88	OHX	1	3930	-	0,6,6	0.00	-	-		
88	OHX	2	2175	-	0,6,6	0.00	-	-		
88	OHX	6	2194	-	0,6,6	0.00	-	-		
88	OHX	5	3914	-	0,6,6	0.00	-	-		
88	OHX	2	2142	-	0,6,6	0.00	-	-		
88	OHX	1	3996	-	0,6,6	0.00	-	-		
88	OHX	5	4006	-	0,6,6	0.00	-	-		
88	OHX	1	4080	-	0,6,6	0.00	-	-		
88	OHX	5	4041	-	0,6,6	0.00	-	-		
88	OHX	1	4060	-	0,6,6	0.00	-	-		
88	OHX	2	2037	-	0,6,6	0.00	-	-		
88	OHX	6	2060	-	0,6,6	0.00	-	-		
88	OHX	5	4102	-	0,6,6	0.00	-	-		
88	OHX	5	4093	-	0,6,6	0.00	-	-		
88	OHX	2	2047	-	0,6,6	0.00	-	-		
88	OHX	5	4096	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3975	-	0,6,6	0.00	-	-		
88	OHX	2	2042	-	0,6,6	0.00	-	-		
88	OHX	5	3910	-	0,6,6	0.00	-	-		
88	OHX	1	3959	-	0,6,6	0.00	-	-		
88	OHX	1	4000	-	0,6,6	0.00	-	-		
88	OHX	6	2148	-	0,6,6	0.00	-	-		
88	OHX	1	4136	-	0,6,6	0.00	-	-		
88	OHX	6	2081	-	0,6,6	0.00	-	-		
88	OHX	O7	103	-	0,6,6	0.00	-	-		
88	OHX	5	3936	-	0,6,6	0.00	-	-		
88	OHX	3	219	-	0,6,6	0.00	-	-		
88	OHX	C8	201	-	0,6,6	0.00	-	-		
88	OHX	2	2157	-	0,6,6	0.00	-	-		
88	OHX	5	3949	-	0,6,6	0.00	-	-		
88	OHX	5	4213	-	0,6,6	0.00	-	-		
88	OHX	5	4174	-	0,6,6	0.00	-	-		
88	OHX	5	4106	-	0,6,6	0.00	-	-		
88	OHX	5	4012	-	0,6,6	0.00	-	-		
88	OHX	1	3969	-	0,6,6	0.00	-	-		
88	OHX	1	4154	-	0,6,6	0.00	-	-		
88	OHX	5	4001	-	0,6,6	0.00	-	-		
88	OHX	1	4185	-	0,6,6	0.00	-	-		
88	OHX	5	4243	-	0,6,6	0.00	-	-		
88	OHX	2	2045	-	0,6,6	0.00	-	-		
88	OHX	1	4168	-	0,6,6	0.00	-	-		
88	OHX	5	4155	-	0,6,6	0.00	-	-		
88	OHX	1	3951	-	0,6,6	0.00	-	-		
88	OHX	5	4085	-	0,6,6	0.00	-	-		
88	OHX	5	4033	-	0,6,6	0.00	-	-		
88	OHX	5	3985	-	0,6,6	0.00	-	-		
88	OHX	2	2024	-	0,6,6	0.00	-	-		
88	OHX	4	220	-	0,6,6	0.00	-	-		
88	OHX	5	4189	-	0,6,6	0.00	-	-		
88	OHX	2	2055	-	0,6,6	0.00	-	-		
88	OHX	2	2093	-	0,6,6	0.00	-	-		
88	OHX	6	2108	-	0,6,6	0.00	-	-		
88	OHX	5	4178	-	0,6,6	0.00	-	-		
88	OHX	5	4244	-	0,6,6	0.00	-	-		
88	OHX	15	306	-	0,6,6	0.00	-	-		
88	OHX	7	217	-	0,6,6	0.00	-	-		
88	OHX	1	4068	-	0,6,6	0.00	-	-		
88	OHX	6	2115	-	0,6,6	0.00	-	-		
88	OHX	1	4110	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3896	-	0,6,6	0.00	-	-		
88	OHX	6	2143	-	0,6,6	0.00	-	-		
88	OHX	5	3965	-	0,6,6	0.00	-	-		
88	OHX	1	4010	-	0,6,6	0.00	-	-		
88	OHX	2	2163	-	0,6,6	0.00	-	-		
88	OHX	1	3900	-	0,6,6	0.00	-	-		
88	OHX	M9	202	-	0,6,6	0.00	-	-		
88	OHX	6	2051	-	0,6,6	0.00	-	-		
88	OHX	5	4075	-	0,6,6	0.00	-	-		
88	OHX	1	4019	-	0,6,6	0.00	-	-		
88	OHX	6	2165	-	0,6,6	0.00	-	-		
88	OHX	1	3946	-	0,6,6	0.00	-	-		
88	OHX	1	4105	-	0,6,6	0.00	-	-		
88	OHX	2	2063	-	0,6,6	0.00	-	-		
88	OHX	1	3947	-	0,6,6	0.00	-	-		
88	OHX	1	4206	-	0,6,6	0.00	-	-		
88	OHX	7	222	-	0,6,6	0.00	-	-		
88	OHX	4	233	-	0,6,6	0.00	-	-		
88	OHX	6	2057	-	0,6,6	0.00	-	-		
88	OHX	1	4130	-	0,6,6	0.00	-	-		
88	OHX	6	2059	-	0,6,6	0.00	-	-		
88	OHX	1	4115	-	0,6,6	0.00	-	-		
88	OHX	1	3884	-	0,6,6	0.00	-	-		
88	OHX	1	4101	-	0,6,6	0.00	-	-		
88	OHX	3	220	-	0,6,6	0.00	-	-		
88	OHX	1	4128	-	0,6,6	0.00	-	-		
88	OHX	2	2111	-	0,6,6	0.00	-	-		
88	OHX	8	223	-	0,6,6	0.00	-	-		
88	OHX	5	4253	-	0,6,6	0.00	-	-		
88	OHX	1	3988	-	0,6,6	0.00	-	-		
88	OHX	1	4177	-	0,6,6	0.00	-	-		
88	OHX	5	4097	-	0,6,6	0.00	-	-		
88	OHX	5	4098	-	0,6,6	0.00	-	-		
88	OHX	M7	205	-	0,6,6	0.00	-	-		
88	OHX	6	2088	-	0,6,6	0.00	-	-		
88	OHX	1	4146	-	0,6,6	0.00	-	-		
88	OHX	1	4108	-	0,6,6	0.00	-	-		
88	OHX	1	3953	-	0,6,6	0.00	-	-		
88	OHX	1	4078	-	0,6,6	0.00	-	-		
88	OHX	1	4165	-	0,6,6	0.00	-	-		
88	OHX	5	4057	-	0,6,6	0.00	-	-		
88	OHX	2	2071	-	0,6,6	0.00	-	-		
88	OHX	15	303	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3909	-	0,6,6	0.00	-	-		
88	OHX	1	3883	-	0,6,6	0.00	-	-		
88	OHX	5	4119	-	0,6,6	0.00	-	-		
88	OHX	6	2076	-	0,6,6	0.00	-	-		
88	OHX	6	2174	-	0,6,6	0.00	-	-		
88	OHX	s8	304	-	0,6,6	0.00	-	-		
88	OHX	2	2177	-	0,6,6	0.00	-	-		
88	OHX	2	2084	-	0,6,6	0.00	-	-		
88	OHX	7	223	-	0,6,6	0.00	-	-		
88	OHX	4	224	-	0,6,6	0.00	-	-		
88	OHX	5	4132	-	0,6,6	0.00	-	-		
88	OHX	1	3964	-	0,6,6	0.00	-	-		
88	OHX	5	3908	-	0,6,6	0.00	-	-		
88	OHX	15	304	-	0,6,6	0.00	-	-		
88	OHX	1	4102	-	0,6,6	0.00	-	-		
88	OHX	2	2050	-	0,6,6	0.00	-	-		
88	OHX	5	3935	-	0,6,6	0.00	-	-		
88	OHX	1	4090	-	0,6,6	0.00	-	-		
88	OHX	1	4082	-	0,6,6	0.00	-	-		
88	OHX	1	4180	-	0,6,6	0.00	-	-		
88	OHX	5	4061	-	0,6,6	0.00	-	-		
88	OHX	6	2080	-	0,6,6	0.00	-	-		
88	OHX	1	4008	-	0,6,6	0.00	-	-		
88	OHX	1	4047	-	0,6,6	0.00	-	-		
88	OHX	5	4229	-	0,6,6	0.00	-	-		
88	OHX	1	4169	-	0,6,6	0.00	-	-		
88	OHX	5	3929	-	0,6,6	0.00	-	-		
88	OHX	1	4037	-	0,6,6	0.00	-	-		
88	OHX	6	2202	-	0,6,6	0.00	-	-		
88	OHX	5	4202	-	0,6,6	0.00	-	-		
88	OHX	2	2095	-	0,6,6	0.00	-	-		
88	OHX	1	4221	-	0,6,6	0.00	-	-		
88	OHX	2	2027	-	0,6,6	0.00	-	-		
88	OHX	6	2047	-	0,6,6	0.00	-	-		
88	OHX	2	2066	-	0,6,6	0.00	-	-		
88	OHX	2	2067	-	0,6,6	0.00	-	-		
88	OHX	5	4133	-	0,6,6	0.00	-	-		
88	OHX	6	2171	-	0,6,6	0.00	-	-		
88	OHX	1	4188	-	0,6,6	0.00	-	-		
88	OHX	6	2139	-	0,6,6	0.00	-	-		
88	OHX	1	4161	-	0,6,6	0.00	-	-		
88	OHX	5	4074	-	0,6,6	0.00	-	-		
88	OHX	2	2030	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	3	217	-	0,6,6	0.00	-	-		
88	OHX	1	4074	-	0,6,6	0.00	-	-		
88	OHX	1	4050	-	0,6,6	0.00	-	-		
88	OHX	5	4147	-	0,6,6	0.00	-	-		
88	OHX	5	4067	-	0,6,6	0.00	-	-		
88	OHX	2	2161	-	0,6,6	0.00	-	-		
88	OHX	6	2130	-	0,6,6	0.00	-	-		
88	OHX	1	4157	-	0,6,6	0.00	-	-		
88	OHX	6	2100	-	0,6,6	0.00	-	-		
88	OHX	2	2059	-	0,6,6	0.00	-	-		
88	OHX	6	2128	-	0,6,6	0.00	-	-		
88	OHX	5	4011	-	0,6,6	0.00	-	-		
88	OHX	1	4127	-	0,6,6	0.00	-	-		
88	OHX	2	2046	-	0,6,6	0.00	-	-		
88	OHX	1	4091	-	0,6,6	0.00	-	-		
88	OHX	1	3907	-	0,6,6	0.00	-	-		
88	OHX	5	4087	-	0,6,6	0.00	-	-		
88	OHX	5	4257	-	0,6,6	0.00	-	-		
88	OHX	1	3967	-	0,6,6	0.00	-	-		
88	OHX	3	215	-	0,6,6	0.00	-	-		
88	OHX	8	229	-	0,6,6	0.00	-	-		
88	OHX	6	2150	-	0,6,6	0.00	-	-		
88	OHX	1	4203	-	0,6,6	0.00	-	-		
88	OHX	6	2050	-	0,6,6	0.00	-	-		
88	OHX	2	2116	-	0,6,6	0.00	-	-		
88	OHX	5	4138	-	0,6,6	0.00	-	-		
88	OHX	6	2179	-	0,6,6	0.00	-	-		
88	OHX	5	4035	-	0,6,6	0.00	-	-		
88	OHX	6	2121	-	0,6,6	0.00	-	-		
88	OHX	6	2102	-	0,6,6	0.00	-	-		
88	OHX	6	2192	-	0,6,6	0.00	-	-		
88	OHX	M7	206	-	0,6,6	0.00	-	-		
88	OHX	1	4216	-	0,6,6	0.00	-	-		
88	OHX	5	4015	-	0,6,6	0.00	-	-		
88	OHX	1	4093	-	0,6,6	0.00	-	-		
88	OHX	1	3960	-	0,6,6	0.00	-	-		
88	OHX	M5	303	-	0,6,6	0.00	-	-		
88	OHX	1	4182	-	0,6,6	0.00	-	-		
88	OHX	5	4110	-	0,6,6	0.00	-	-		
88	OHX	6	2127	-	0,6,6	0.00	-	-		
88	OHX	5	4185	-	0,6,6	0.00	-	-		
88	OHX	5	4032	-	0,6,6	0.00	-	-		
88	OHX	2	2082	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3988	-	0,6,6	0.00	-	-		
88	OHX	1	3911	-	0,6,6	0.00	-	-		
88	OHX	1	4198	-	0,6,6	0.00	-	-		
88	OHX	6	2144	-	0,6,6	0.00	-	-		
88	OHX	1	4083	-	0,6,6	0.00	-	-		
88	OHX	2	2078	-	0,6,6	0.00	-	-		
88	OHX	1	4070	-	0,6,6	0.00	-	-		
88	OHX	4	227	-	0,6,6	0.00	-	-		
88	OHX	5	3972	-	0,6,6	0.00	-	-		
88	OHX	6	2113	-	0,6,6	0.00	-	-		
88	OHX	5	4245	-	0,6,6	0.00	-	-		
88	OHX	1	3991	-	0,6,6	0.00	-	-		
88	OHX	5	3954	-	0,6,6	0.00	-	-		
88	OHX	2	2172	-	0,6,6	0.00	-	-		
88	OHX	5	4040	-	0,6,6	0.00	-	-		
88	OHX	1	4092	-	0,6,6	0.00	-	-		
88	OHX	1	4096	-	0,6,6	0.00	-	-		
88	OHX	6	2105	1	0,6,6	0.00	-	-		
88	OHX	6	2054	-	0,6,6	0.00	-	-		
88	OHX	1	3949	-	0,6,6	0.00	-	-		
88	OHX	1	3971	-	0,6,6	0.00	-	-		
88	OHX	1	4089	-	0,6,6	0.00	-	-		
88	OHX	6	2072	-	0,6,6	0.00	-	-		
88	OHX	1	3956	-	0,6,6	0.00	-	-		
88	OHX	6	2055	-	0,6,6	0.00	-	-		
88	OHX	5	4198	-	0,6,6	0.00	-	-		
88	OHX	5	4218	-	0,6,6	0.00	-	-		
88	OHX	2	2135	-	0,6,6	0.00	-	-		
88	OHX	2	2168	-	0,6,6	0.00	-	-		
88	OHX	2	2025	-	0,6,6	0.00	-	-		
88	OHX	5	4149	-	0,6,6	0.00	-	-		
88	OHX	8	221	-	0,6,6	0.00	-	-		
88	OHX	5	3996	-	0,6,6	0.00	-	-		
88	OHX	1	3873	-	0,6,6	0.00	-	-		
88	OHX	5	4020	-	0,6,6	0.00	-	-		
88	OHX	5	3986	-	0,6,6	0.00	-	-		
88	OHX	1	4171	-	0,6,6	0.00	-	-		
88	OHX	1	4226	-	0,6,6	0.00	-	-		
88	OHX	5	3938	-	0,6,6	0.00	-	-		
88	OHX	5	3912	-	0,6,6	0.00	-	-		
88	OHX	1	4141	-	0,6,6	0.00	-	-		
88	OHX	1	3952	-	0,6,6	0.00	-	-		
88	OHX	1	4059	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	4000	-	0,6,6	0.00	-	-		
88	OHX	5	4211	-	0,6,6	0.00	-	-		
88	OHX	5	4195	-	0,6,6	0.00	-	-		
88	OHX	6	2044	-	0,6,6	0.00	-	-		
88	OHX	5	4186	-	0,6,6	0.00	-	-		
88	OHX	4	221	-	0,6,6	0.00	-	-		
88	OHX	1	4225	-	0,6,6	0.00	-	-		
88	OHX	5	4017	-	0,6,6	0.00	-	-		
88	OHX	5	3916	-	0,6,6	0.00	-	-		
88	OHX	5	4226	-	0,6,6	0.00	-	-		
88	OHX	5	4153	-	0,6,6	0.00	-	-		
88	OHX	2	2074	-	0,6,6	0.00	-	-		
88	OHX	1	4124	-	0,6,6	0.00	-	-		
88	OHX	4	228	-	0,6,6	0.00	-	-		
88	OHX	n3	203	-	0,6,6	0.00	-	-		
88	OHX	4	222	-	0,6,6	0.00	-	-		
88	OHX	L3	405	-	0,6,6	0.00	-	-		
88	OHX	8	222	-	0,6,6	0.00	-	-		
88	OHX	1	3987	-	0,6,6	0.00	-	-		
88	OHX	1	4224	-	0,6,6	0.00	-	-		
88	OHX	5	4083	-	0,6,6	0.00	-	-		
88	OHX	1	4190	-	0,6,6	0.00	-	-		
88	OHX	5	3970	-	0,6,6	0.00	-	-		
88	OHX	1	4160	-	0,6,6	0.00	-	-		
88	OHX	5	4073	-	0,6,6	0.00	-	-		
88	OHX	q2	504	-	0,6,6	0.00	-	-		
88	OHX	1	3878	-	0,6,6	0.00	-	-		
88	OHX	5	4169	-	0,6,6	0.00	-	-		
88	OHX	6	2182	-	0,6,6	0.00	-	-		
88	OHX	5	3918	-	0,6,6	0.00	-	-		
88	OHX	6	2087	-	0,6,6	0.00	-	-		
88	OHX	1	3985	-	0,6,6	0.00	-	-		
88	OHX	4	225	-	0,6,6	0.00	-	-		
88	OHX	1	4028	-	0,6,6	0.00	-	-		
88	OHX	2	2119	-	0,6,6	0.00	-	-		
88	OHX	5	3998	-	0,6,6	0.00	-	-		
88	OHX	5	3968	-	0,6,6	0.00	-	-		
88	OHX	1	4045	-	0,6,6	0.00	-	-		
88	OHX	5	4176	-	0,6,6	0.00	-	-		
88	OHX	8	228	-	0,6,6	0.00	-	-		
88	OHX	1	4071	-	0,6,6	0.00	-	-		
88	OHX	2	2051	-	0,6,6	0.00	-	-		
88	OHX	6	2197	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	6	2079	-	0,6,6	0.00	-	-		
88	OHX	1	4143	-	0,6,6	0.00	-	-		
88	OHX	5	4026	-	0,6,6	0.00	-	-		
88	OHX	sR	401	-	0,6,6	0.00	-	-		
88	OHX	1	4002	-	0,6,6	0.00	-	-		
88	OHX	5	3940	-	0,6,6	0.00	-	-		
88	OHX	5	4089	-	0,6,6	0.00	-	-		
88	OHX	5	3964	-	0,6,6	0.00	-	-		
88	OHX	5	4122	-	0,6,6	0.00	-	-		
88	OHX	5	4170	-	0,6,6	0.00	-	-		
88	OHX	1	4181	-	0,6,6	0.00	-	-		
88	OHX	5	4009	-	0,6,6	0.00	-	-		
88	OHX	1	3915	-	0,6,6	0.00	-	-		
88	OHX	5	4028	-	0,6,6	0.00	-	-		
88	OHX	1	3923	-	0,6,6	0.00	-	-		
88	OHX	5	4070	-	0,6,6	0.00	-	-		
88	OHX	6	2111	-	0,6,6	0.00	-	-		
88	OHX	1	3994	-	0,6,6	0.00	-	-		
88	OHX	2	2052	-	0,6,6	0.00	-	-		
88	OHX	5	4090	-	0,6,6	0.00	-	-		
88	OHX	1	4187	-	0,6,6	0.00	-	-		
88	OHX	1	4113	-	0,6,6	0.00	-	-		
88	OHX	2	2049	-	0,6,6	0.00	-	-		
88	OHX	5	4043	-	0,6,6	0.00	-	-		
88	OHX	6	2090	-	0,6,6	0.00	-	-		
88	OHX	1	3904	-	0,6,6	0.00	-	-		
88	OHX	2	2143	-	0,6,6	0.00	-	-		
88	OHX	2	2040	-	0,6,6	0.00	-	-		
88	OHX	5	4058	-	0,6,6	0.00	-	-		
88	OHX	1	3973	-	0,6,6	0.00	-	-		
88	OHX	SR	401	-	0,6,6	0.00	-	-		
88	OHX	5	4214	-	0,6,6	0.00	-	-		
88	OHX	1	3906	-	0,6,6	0.00	-	-		
88	OHX	5	3961	-	0,6,6	0.00	-	-		
88	OHX	5	4046	-	0,6,6	0.00	-	-		
88	OHX	6	2157	-	0,6,6	0.00	-	-		
88	OHX	5	4199	-	0,6,6	0.00	-	-		
88	OHX	7	220	-	0,6,6	0.00	-	-		
88	OHX	5	4206	-	0,6,6	0.00	-	-		
88	OHX	8	220	-	0,6,6	0.00	-	-		
88	OHX	1	4011	-	0,6,6	0.00	-	-		
88	OHX	5	4031	-	0,6,6	0.00	-	-		
88	OHX	1	4151	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	3955	-	0,6,6	0.00	-	-		
88	OHX	6	2084	-	0,6,6	0.00	-	-		
88	OHX	1	4137	-	0,6,6	0.00	-	-		
88	OHX	3	218	-	0,6,6	0.00	-	-		
88	OHX	5	4175	-	0,6,6	0.00	-	-		
88	OHX	4	232	-	0,6,6	0.00	-	-		
88	OHX	1	4163	-	0,6,6	0.00	-	-		
88	OHX	1	3966	-	0,6,6	0.00	-	-		
88	OHX	6	2046	-	0,6,6	0.00	-	-		
88	OHX	6	2061	-	0,6,6	0.00	-	-		
88	OHX	1	3909	-	0,6,6	0.00	-	-		
88	OHX	5	3902	-	0,6,6	0.00	-	-		
88	OHX	2	2076	-	0,6,6	0.00	-	-		
88	OHX	6	2073	-	0,6,6	0.00	-	-		
88	OHX	1	3933	-	0,6,6	0.00	-	-		
88	OHX	5	4161	-	0,6,6	0.00	-	-		
88	OHX	m0	302	-	0,6,6	0.00	-	-		
88	OHX	2	2036	-	0,6,6	0.00	-	-		
88	OHX	1	4030	-	0,6,6	0.00	-	-		
88	OHX	1	3932	-	0,6,6	0.00	-	-		
88	OHX	1	3929	-	0,6,6	0.00	-	-		
88	OHX	5	4014	-	0,6,6	0.00	-	-		
88	OHX	1	3961	-	0,6,6	0.00	-	-		
88	OHX	6	2071	-	0,6,6	0.00	-	-		
88	OHX	5	3976	-	0,6,6	0.00	-	-		
88	OHX	5	3999	-	0,6,6	0.00	-	-		
88	OHX	5	3927	-	0,6,6	0.00	-	-		
88	OHX	2	2132	-	0,6,6	0.00	-	-		
88	OHX	5	4055	-	0,6,6	0.00	-	-		
88	OHX	1	3888	-	0,6,6	0.00	-	-		
88	OHX	5	3953	-	0,6,6	0.00	-	-		
88	OHX	2	2102	-	0,6,6	0.00	-	-		
88	OHX	5	4164	-	0,6,6	0.00	-	-		
88	OHX	2	2069	-	0,6,6	0.00	-	-		
88	OHX	1	3975	-	0,6,6	0.00	-	-		
88	OHX	1	4150	-	0,6,6	0.00	-	-		
88	OHX	5	4187	-	0,6,6	0.00	-	-		
88	OHX	1	4178	-	0,6,6	0.00	-	-		
88	OHX	1	4219	-	0,6,6	0.00	-	-		
88	OHX	6	2118	-	0,6,6	0.00	-	-		
88	OHX	5	4109	-	0,6,6	0.00	-	-		
88	OHX	5	3981	-	0,6,6	0.00	-	-		
88	OHX	1	3940	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	5	4081	-	0,6,6	0.00	-	-		
88	OHX	2	2162	-	0,6,6	0.00	-	-		
88	OHX	1	3965	-	0,6,6	0.00	-	-		
88	OHX	1	4081	-	0,6,6	0.00	-	-		
88	OHX	1	4214	-	0,6,6	0.00	-	-		
88	OHX	5	4060	-	0,6,6	0.00	-	-		
88	OHX	6	2178	-	0,6,6	0.00	-	-		
88	OHX	1	3972	-	0,6,6	0.00	-	-		
88	OHX	5	3911	-	0,6,6	0.00	-	-		
88	OHX	5	4254	-	0,6,6	0.00	-	-		
88	OHX	5	3980	-	0,6,6	0.00	-	-		
88	OHX	2	2099	-	0,6,6	0.00	-	-		
88	OHX	5	4121	-	0,6,6	0.00	-	-		
88	OHX	5	4171	-	0,6,6	0.00	-	-		
88	OHX	1	3921	-	0,6,6	0.00	-	-		
88	OHX	1	4189	-	0,6,6	0.00	-	-		
88	OHX	5	4120	-	0,6,6	0.00	-	-		
88	OHX	5	4208	-	0,6,6	0.00	-	-		
88	OHX	2	2077	-	0,6,6	0.00	-	-		
88	OHX	1	3936	-	0,6,6	0.00	-	-		
88	OHX	1	3881	-	0,6,6	0.00	-	-		
88	OHX	s1	303	-	0,6,6	0.00	-	-		
88	OHX	5	4207	-	0,6,6	0.00	-	-		
88	OHX	2	2106	-	0,6,6	0.00	-	-		
88	OHX	5	4247	-	0,6,6	0.00	-	-		
88	OHX	5	4181	-	0,6,6	0.00	-	-		
88	OHX	2	2123	-	0,6,6	0.00	-	-		
88	OHX	2	2170	-	0,6,6	0.00	-	-		
88	OHX	5	4220	-	0,6,6	0.00	-	-		
88	OHX	5	4018	-	0,6,6	0.00	-	-		
88	OHX	1	4015	-	0,6,6	0.00	-	-		
88	OHX	5	4027	-	0,6,6	0.00	-	-		
88	OHX	4	226	-	0,6,6	0.00	-	-		
88	OHX	6	2161	-	0,6,6	0.00	-	-		
88	OHX	5	3933	-	0,6,6	0.00	-	-		
88	OHX	4	223	-	0,6,6	0.00	-	-		
88	OHX	5	4252	-	0,6,6	0.00	-	-		
88	OHX	1	4020	-	0,6,6	0.00	-	-		
88	OHX	5	4038	-	0,6,6	0.00	-	-		
88	OHX	6	2089	-	0,6,6	0.00	-	-		
88	OHX	5	4193	-	0,6,6	0.00	-	-		
88	OHX	2	2128	-	0,6,6	0.00	-	-		
88	OHX	7	219	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2034	-	0,6,6	0.00	-	-		
88	OHX	1	3894	-	0,6,6	0.00	-	-		
88	OHX	2	2039	-	0,6,6	0.00	-	-		
88	OHX	6	2188	-	0,6,6	0.00	-	-		
88	OHX	1	3916	-	0,6,6	0.00	-	-		
88	OHX	5	4112	-	0,6,6	0.00	-	-		
88	OHX	1	4172	-	0,6,6	0.00	-	-		
88	OHX	19	600	-	0,6,6	0.00	-	-		
88	OHX	1	4175	-	0,6,6	0.00	-	-		
88	OHX	6	2110	-	0,6,6	0.00	-	-		
88	OHX	1	3919	-	0,6,6	0.00	-	-		
88	OHX	5	3966	-	0,6,6	0.00	-	-		
88	OHX	5	3921	-	0,6,6	0.00	-	-		
88	OHX	5	4136	-	0,6,6	0.00	-	-		
88	OHX	2	2176	-	0,6,6	0.00	-	-		
88	OHX	1	3876	-	0,6,6	0.00	-	-		
88	OHX	5	4168	-	0,6,6	0.00	-	-		
88	OHX	3	225	-	0,6,6	0.00	-	-		
88	OHX	5	4115	-	0,6,6	0.00	-	-		
88	OHX	C5	201	-	0,6,6	0.00	-	-		
88	OHX	1	4199	-	0,6,6	0.00	-	-		
88	OHX	1	4112	-	0,6,6	0.00	-	-		
88	OHX	1	4031	-	0,6,6	0.00	-	-		
88	OHX	5	3990	-	0,6,6	0.00	-	-		
88	OHX	6	2109	-	0,6,6	0.00	-	-		
88	OHX	1	4134	-	0,6,6	0.00	-	-		
88	OHX	6	2098	-	0,6,6	0.00	-	-		
88	OHX	C3	201	-	0,6,6	0.00	-	-		
88	OHX	1	4005	-	0,6,6	0.00	-	-		
88	OHX	5	4183	-	0,6,6	0.00	-	-		
88	OHX	5	4030	-	0,6,6	0.00	-	-		
88	OHX	5	4101	-	0,6,6	0.00	-	-		
88	OHX	1	4121	-	0,6,6	0.00	-	-		
88	OHX	5	3963	-	0,6,6	0.00	-	-		
88	OHX	5	4203	-	0,6,6	0.00	-	-		
88	OHX	5	4048	-	0,6,6	0.00	-	-		
88	OHX	8	224	-	0,6,6	0.00	-	-		
88	OHX	2	2150	-	0,6,6	0.00	-	-		
88	OHX	14	404	-	0,6,6	0.00	-	-		
88	OHX	5	4022	-	0,6,6	0.00	-	-		
88	OHX	5	4227	-	0,6,6	0.00	-	-		
88	OHX	1	3887	-	0,6,6	0.00	-	-		
88	OHX	6	2103	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	1	3910	-	0,6,6	0.00	-	-		
88	OHX	1	3942	-	0,6,6	0.00	-	-		
88	OHX	5	4146	-	0,6,6	0.00	-	-		
88	OHX	1	3999	-	0,6,6	0.00	-	-		
88	OHX	6	2069	-	0,6,6	0.00	-	-		
88	OHX	1	4220	-	0,6,6	0.00	-	-		
88	OHX	2	2068	-	0,6,6	0.00	-	-		
88	OHX	6	2159	-	0,6,6	0.00	-	-		
88	OHX	5	4255	-	0,6,6	0.00	-	-		
88	OHX	6	2062	-	0,6,6	0.00	-	-		
88	OHX	2	2129	-	0,6,6	0.00	-	-		
88	OHX	5	4166	-	0,6,6	0.00	-	-		
88	OHX	2	2081	-	0,6,6	0.00	-	-		
88	OHX	2	2125	-	0,6,6	0.00	-	-		
88	OHX	1	4086	-	0,6,6	0.00	-	-		
88	OHX	5	4180	-	0,6,6	0.00	-	-		
88	OHX	1	4048	-	0,6,6	0.00	-	-		
88	OHX	5	4165	-	0,6,6	0.00	-	-		
88	OHX	5	4179	-	0,6,6	0.00	-	-		
88	OHX	5	4177	-	0,6,6	0.00	-	-		
88	OHX	1	4073	-	0,6,6	0.00	-	-		
88	OHX	1	3962	-	0,6,6	0.00	-	-		
88	OHX	6	2129	-	0,6,6	0.00	-	-		
88	OHX	1	4158	-	0,6,6	0.00	-	-		
88	OHX	6	2048	-	0,6,6	0.00	-	-		
88	OHX	1	3885	-	0,6,6	0.00	-	-		
88	OHX	5	3973	-	0,6,6	0.00	-	-		
88	OHX	5	4151	-	0,6,6	0.00	-	-		
88	OHX	6	2132	-	0,6,6	0.00	-	-		
88	OHX	7	221	-	0,6,6	0.00	-	-		
88	OHX	6	2201	-	0,6,6	0.00	-	-		
88	OHX	1	3939	-	0,6,6	0.00	-	-		
88	OHX	5	4021	-	0,6,6	0.00	-	-		
88	OHX	5	4231	-	0,6,6	0.00	-	-		
88	OHX	5	4078	-	0,6,6	0.00	-	-		
88	OHX	5	3959	-	0,6,6	0.00	-	-		
88	OHX	2	2023	-	0,6,6	0.00	-	-		
88	OHX	5	4230	-	0,6,6	0.00	-	-		
88	OHX	1	4122	-	0,6,6	0.00	-	-		
88	OHX	2	2089	-	0,6,6	0.00	-	-		
88	OHX	6	2123	-	0,6,6	0.00	-	-		
88	OHX	2	2151	-	0,6,6	0.00	-	-		
88	OHX	1	4023	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	2	2139	-	0,6,6	0.00	-	-		
88	OHX	1	3958	-	0,6,6	0.00	-	-		
88	OHX	1	3917	-	0,6,6	0.00	-	-		
88	OHX	5	4076	-	0,6,6	0.00	-	-		
88	OHX	2	2130	-	0,6,6	0.00	-	-		
88	OHX	5	4113	-	0,6,6	0.00	-	-		
88	OHX	2	2138	-	0,6,6	0.00	-	-		
88	OHX	2	2124	-	0,6,6	0.00	-	-		
88	OHX	1	4149	-	0,6,6	0.00	-	-		
88	OHX	8	225	-	0,6,6	0.00	-	-		
88	OHX	5	3982	-	0,6,6	0.00	-	-		
88	OHX	5	3987	-	0,6,6	0.00	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.