



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 07:42 PM BST

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

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

We welcome your comments at [validation@mail.wwpdb.org](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**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

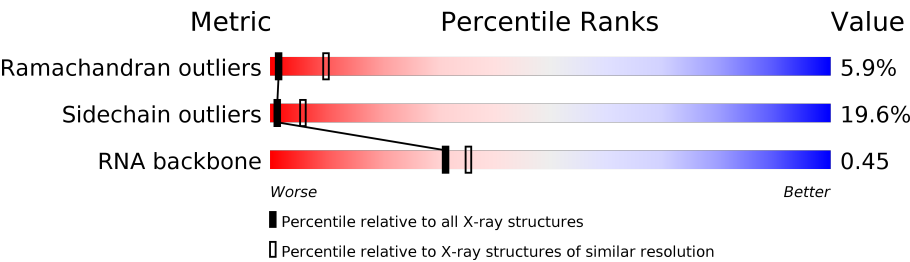
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)















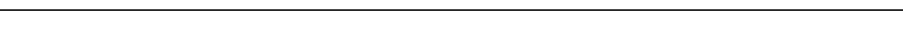




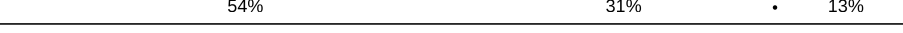





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	<div><div>64%</div><div>30%</div><div>.</div><div>.</div></div>
1	6	1800	<div><div>65%</div><div>30%</div><div>5%</div></div>
2	S0	251	<div><div>64%</div><div>16%</div><div>.</div><div>18%</div></div>
2	s0	251	<div><div>61%</div><div>20%</div><div>.</div><div>18%</div></div>
3	S1	254	<div><div>58%</div><div>22%</div><div>.</div><div>16%</div></div>
3	s1	254	<div><div>65%</div><div>18%</div><div>.</div><div>15%</div></div>
4	S2	253	<div><div>67%</div><div>17%</div><div>.</div><div>14%</div></div>
4	s2	253	<div><div>64%</div><div>20%</div><div>.</div><div>14%</div></div>




















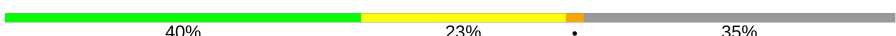





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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3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














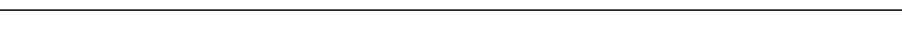











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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107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


























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















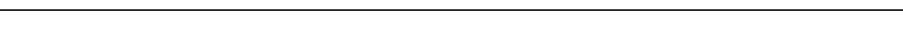




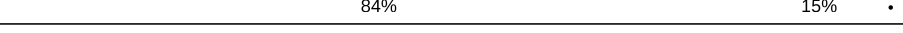





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Mol	Chain	Length	Quality of chain
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6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















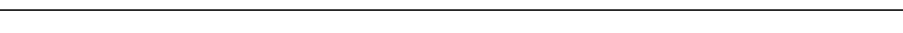




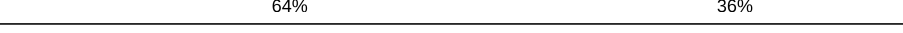





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Mol	Chain	Length	Quality of chain
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9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

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Mol	Chain	Length	Quality of chain
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	

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

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C5	137	SER	ARG	conflict	UNP Q01855
c5	137	SER	ARG	conflict	UNP Q01855

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			679	402	140	137				

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	13	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	14	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	16	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 22 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called Unknown protein m2.

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

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

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

- Molecule 83 is a protein called Unknown protein p1.

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

- Molecule 84 is a protein called Unknown protein p2.

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	m6	2	Total 2	Mg 2	0	0
85	n8	5	Total 5	Mg 5	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	145	Total 145	Mg 145	0	0
85	sM	2	Total 2	Mg 2	0	0
85	O4	1	Total 1	Mg 1	0	0
85	m5	3	Total 3	Mg 3	0	0
85	l3	3	Total 3	Mg 3	0	0
85	M1	2	Total 2	Mg 2	0	0
85	n0	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	121	Total 121	Mg 121	0	0
85	O3	1	Total 1	Mg 1	0	0
85	S6	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0
85	l7	3	Total 3	Mg 3	0	0
85	M5	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	S2	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L8	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0
85	M9	2	Total 2	Mg 2	0	0
85	q0	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	3	Total 3	Mg 3	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	497	Total 497	Mg 497	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	1	471	Total 471	Mg 471	0	0
85	s2	1	Total 1	Mg 1	0	0
85	D0	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	l2	2	Total 2	Mg 2	0	0
85	d3	2	Total 2	Mg 2	0	0
85	o7	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	M3	3	Total 3	Mg 3	0	0

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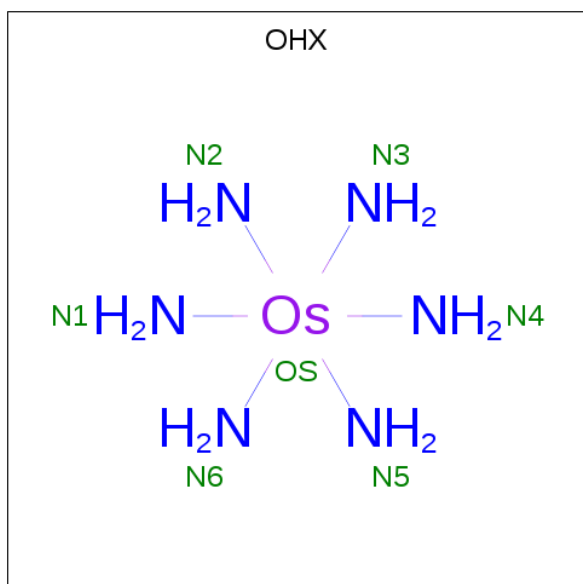
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N3	3	Total 3	Mg 3	0	0
85	4	23	Total 23	Mg 23	0	0
85	n6	1	Total 1	Mg 1	0	0
85	S4	1	Total 1	Mg 1	0	0
85	L2	2	Total 2	Mg 2	0	0
85	m1	1	Total 1	Mg 1	0	0
85	l5	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	4	Total 4	Mg 4	0	0
85	m4	1	Total 1	Mg 1	0	0
85	N8	3	Total 3	Mg 3	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	l8	1	Total 1	Mg 1	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	16	Total 16	Mg 16	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	3	Total 3	Mg 3	0	0
85	s4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N6	1	Total	Mg	0	0
			1	1		
85	8	15	Total	Mg	0	0
			15	15		
85	14	1	Total	Mg	0	0
			1	1		
85	M6	1	Total	Mg	0	0
			1	1		
85	N0	1	Total	Mg	0	0
			1	1		
85	3	13	Total	Mg	0	0
			13	13		

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



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
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86	1	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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			7	6	1		
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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			7	6	1		
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	O1	1	Total	N	Os	0	0
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86	O2	1	Total	N	Os	0	0
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86	O3	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	s1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	s4	1	Total	N	Os	0	0
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86	s8	1	Total	N	Os	0	0
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86	c8	1	Total	N	Os	0	0
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86	d4	1	Total	N	Os	0	0
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86	d9	1	Total	N	Os	0	0
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86	sR	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	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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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q1	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

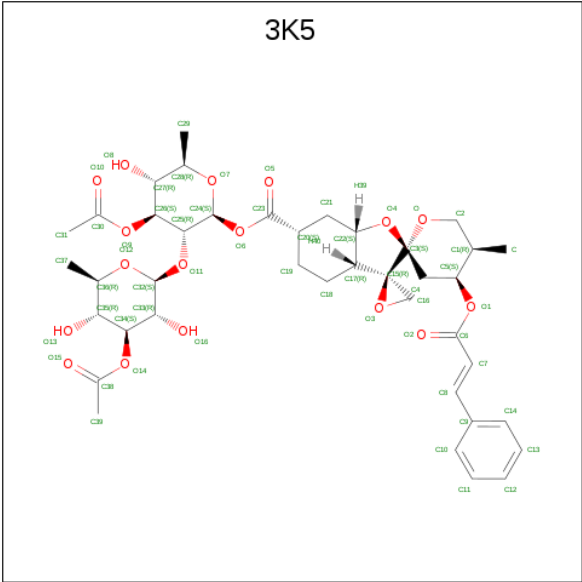
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		

- Molecule 88 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-  
 {[ (2R,2'S,3a'R,4'S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahy-  
 drodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose  
 (three-letter code: 3K5) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>17</sub>).



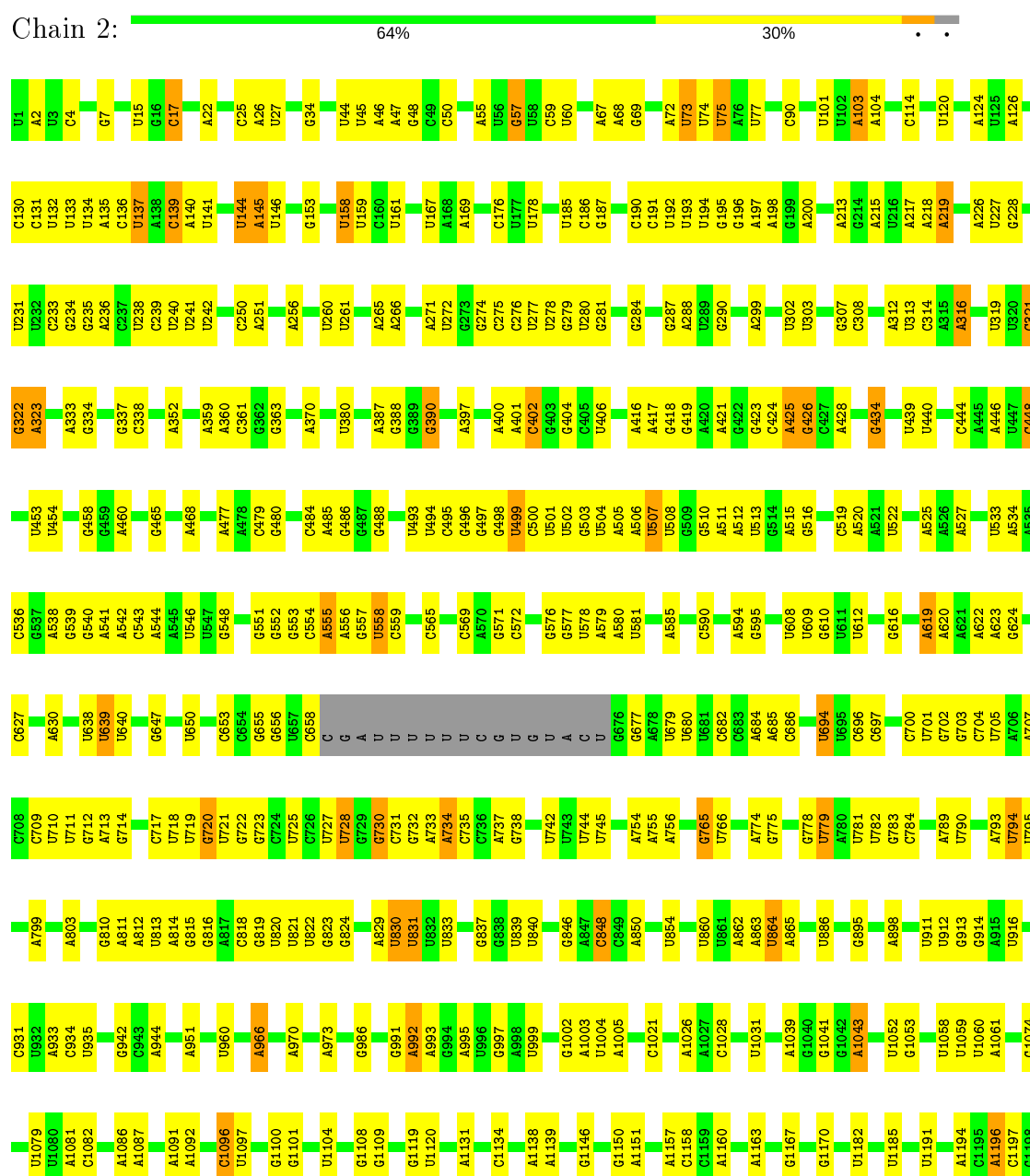
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	1	1	Total	C	O	0	0
			57	40	17		
88	5	1	Total	C	O	0	0
			57	40	17		

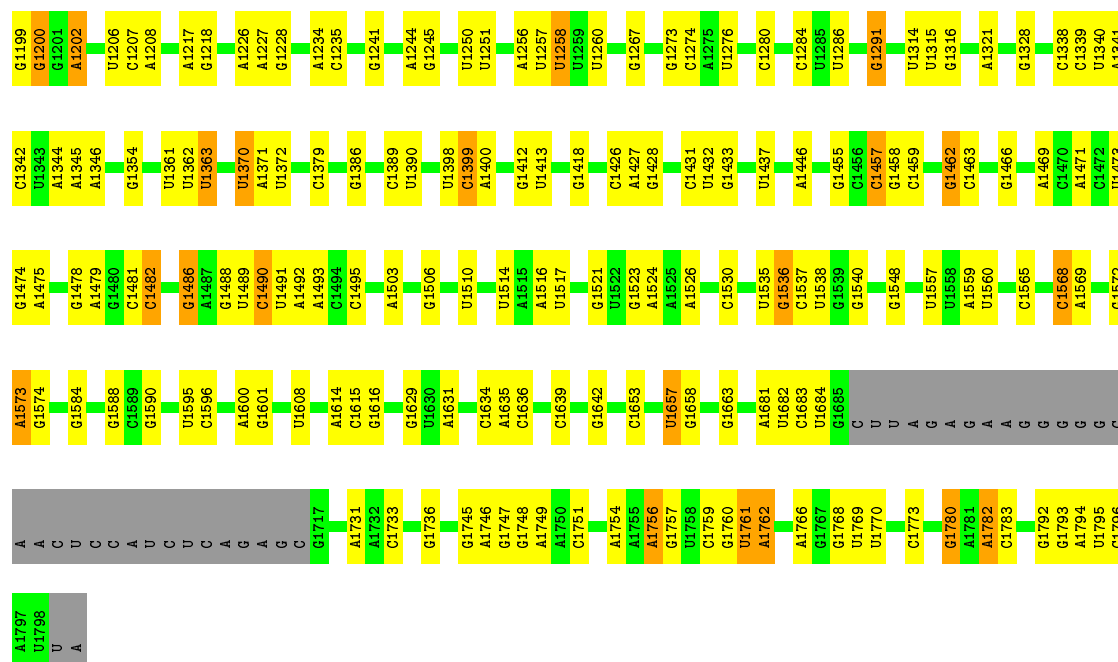
### 3 Residue-property plots

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.

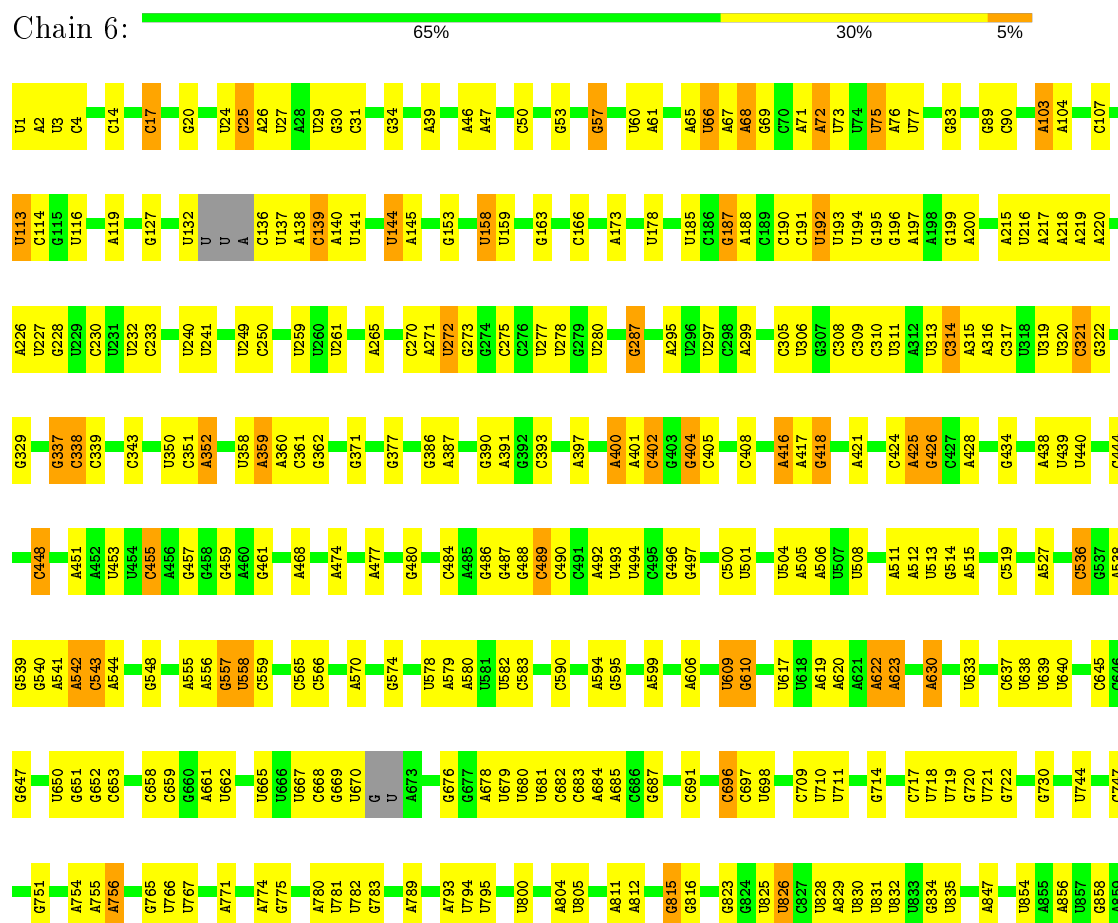
- Molecule 1: 18S ribosomal RNA



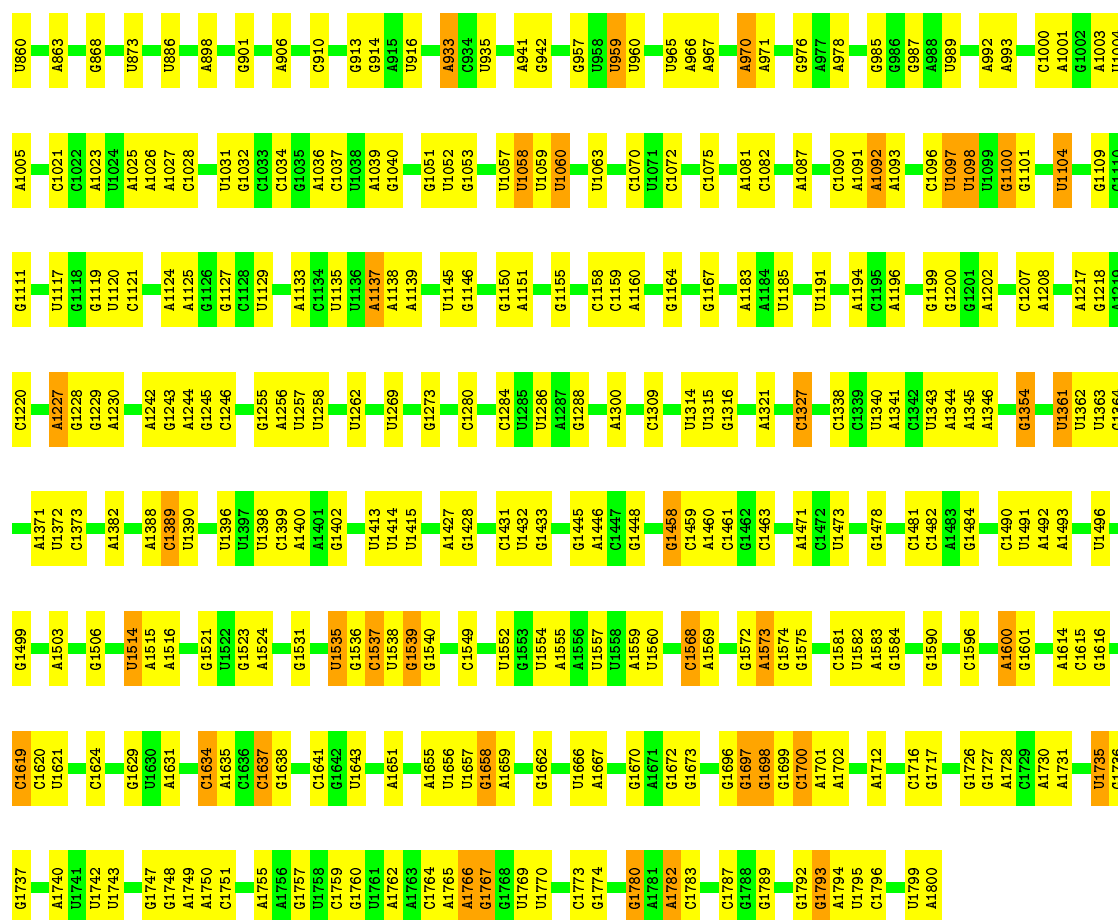


• Molecule 1: 18S ribosomal RNA

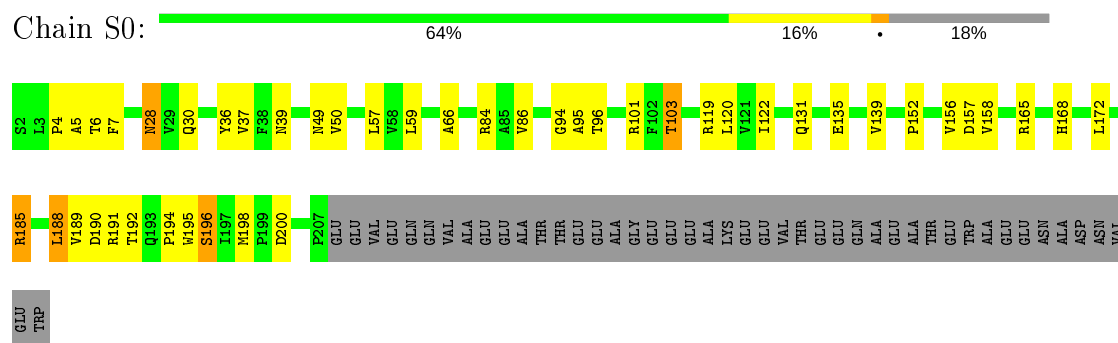
Chain 6:



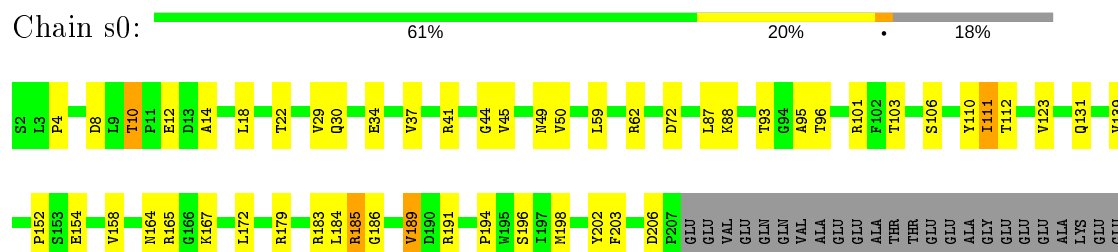




- Molecule 2: 40S ribosomal protein S0-A



- Molecule 2: 40S ribosomal protein S0-A



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

• Molecule 3: 40S ribosomal protein S1-A

Chain S1: 58% 22% 16%

ALA  
VAL  
GLY  
LYS  
ASN  
LYS  
LYS  
ARG  
LEU  
SER  
LYS  
GLY  
LYS  
LYS  
GLY  
GLN  
LYS  
LYS  
LYS  
ARG  
V20  
V21  
T25  
V29  
F30  
P35  
M42  
T46  
L47  
V48  
M49  
K50  
S51  
L54  
K55  
S58  
D59  
A60  
L61  
K62  
G63  
R64  
V65  
L70  
E77  
D78  
F81  
R82  
K85  
D89  
G93  
L97  
D104  
F105  
D108  
R111  
W117  
V125  
T126  
D131  
D132  
I137  
R144  
K145  
Q146  
A147  
M148  
S154  
S158  
S169  
V176  
Q177  
G178  
S179  
T180  
L181  
A182  
I193  
T201  
K202  
D203  
R204  
F205  
P206  
N209  
I210  
R213  
K214  
L217  
L218  
K219  
Q220  
P221  
F223  
D224  
V225  
G226  
G233  
GLU  
GLY  
SER  
GLY  
GLY  
GLU  
GLU  
GLN  
LYS  
LYS  
LYS  
LYS  
VAL  
THR  
PHE  
GLY  
PHE  
LYS  
ASP  
GLU  
VAL  
LEU  
GLU  
THR  
VAL

• Molecule 3: 40S ribosomal protein S1-A

Chain s1: 65% 18% 15%

ALA  
VAL  
GLY  
LYS  
ASN  
LYS  
LYS  
ARG  
LEU  
SER  
LYS  
GLY  
LYS  
LYS  
GLY  
GLN  
LYS  
LYS  
LYS  
ARG  
V20  
V21  
D22  
T25  
T37  
L47  
D59  
K62  
L70  
L73  
Q74  
D78  
F81  
R82  
K83  
D89  
E90  
G93  
K94  
L97  
F105  
D108  
V114  
L120  
T129  
S130  
D131  
T137  
Q146  
R152  
S159  
S169  
T173  
Q177  
L181  
A182  
Q183  
L184  
I193  
N194  
K195  
E196  
I197  
R202  
P206  
L207  
N209  
V212  
R213  
K214  
L218  
R219  
K222  
P223  
L228  
L231  
H232  
G235  
SER  
GLY  
GLU  
GLU  
LYS  
GLY  
LYS  
VAL  
THR  
GLY  
PHE  
LYS  
ASP  
VAL  
LEU  
THR  
VAL

• Molecule 4: 40S ribosomal protein S2

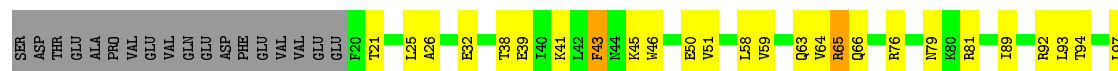
Chain S2: 67% 17% 14%

SER  
ALA  
PRO  
GLU  
ALA  
GLN  
GLN  
GLN  
LYS  
ARG  
GLY  
GLY  
PHE  
GLY  
GLY  
ARG  
ASN  
ARG  
GLY  
ARG  
PRO  
ASN  
THR  
GLU  
GLU  
LYS  
G34  
V35  
V36  
L41  
I53  
E54  
I69  
D70  
L76  
Q77  
I83  
Q87  
K88  
Q89  
R91  
Q94  
R95  
R96  
R97  
S107  
V111  
L113  
T117  
A118  
I119  
I130  
L134  
T137  
P138  
I139  
R140  
R141  
G145  
T146  
M147  
L148  
G149  
Q150  
S153  
L154  
T166  
P162  
L187  
N201  
L207  
E208  
Y222  
L225  
T226  
L235  
P236  
I245  
E246  
Q250  
LYS  
LYS  
ARG  
PHE

• Molecule 4: 40S ribosomal protein S2

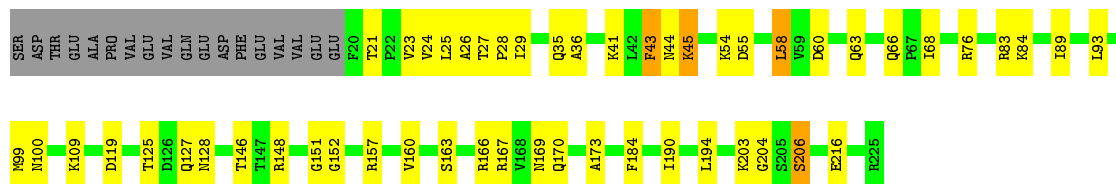
Chain s2: 64% 20% 14%

SER  
ALA  
PRO  
GLU  
ALA  
GLN  
GLN  
GLN  
LYS  
ARG  
GLY  
GLY  
PHE  
GLY  
GLY  
ARG  
ASN  
ARG  
GLY  
ARG  
PRO  
ASN  
THR  
GLU  
GLU  
LYS  
G34  
L41  
K46  
T51  
T52  
I53  
L58  
H59  
S60  
L61  
I69  
L73  
Q77  
D78  
E79  
V80  
V81  
N82  
R83  
K84  
P85  
V86  
Q87  
R88  
Q89  
T90  
R91  
A92  
G93  
R95  
T96  
D106  
S107  
V111  
G112  
L113  
T117  
A118  
K119  
E120  
V121  
R141  
T146  
M147  
L148  
G149  
Q150  
T159  
G163  
S164  
V165  
T166  
I170  
V179  
K185  
K186  
Q199  
T206  
L207  
Y222  
L225  
L229  
P234  
L235

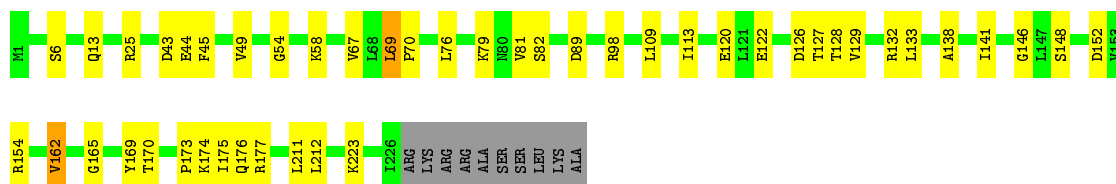
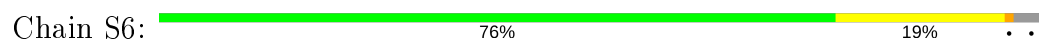




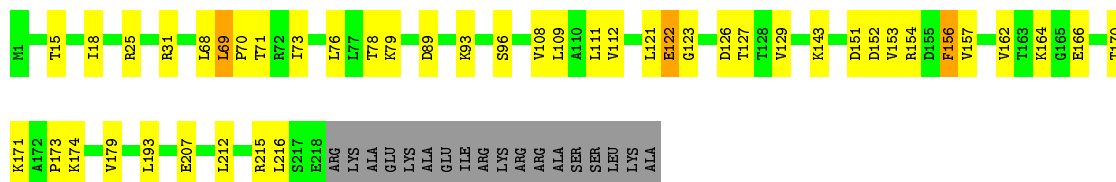
• Molecule 7: 40S ribosomal protein S5



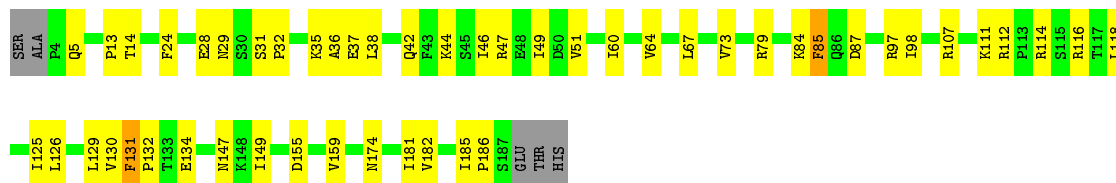
• Molecule 8: 40S ribosomal protein S6-A



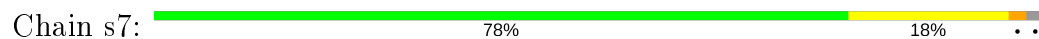
• Molecule 8: 40S ribosomal protein S6-A



• Molecule 9: 40S ribosomal protein S7-A



• Molecule 9: 40S ribosomal protein S7-A





- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 78% 15% 6%



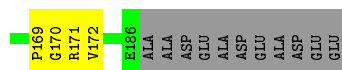
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 74% 20% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 74% 19% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 73% 20% 6%

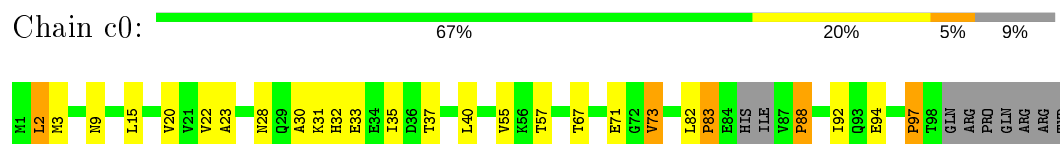


- Molecule 12: 40S ribosomal protein S10-A

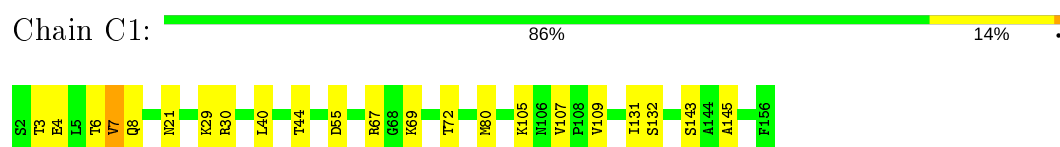
Chain C0: 74% 14% 9%



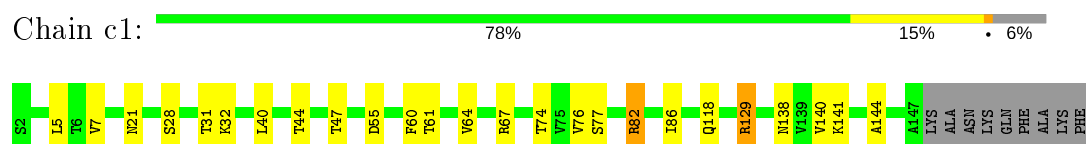
- Molecule 12: 40S ribosomal protein S10-A



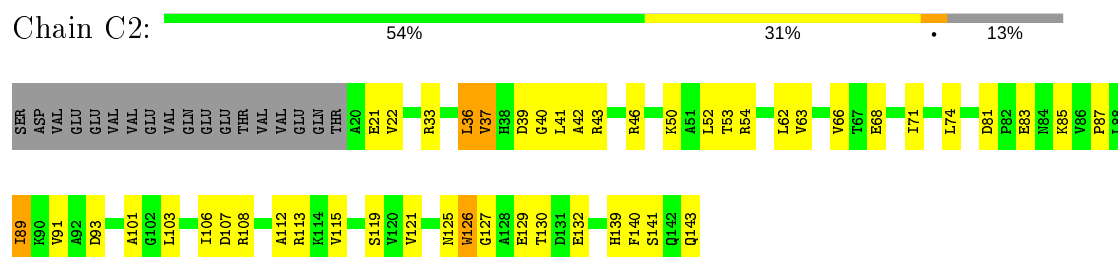
- Molecule 13: 40S ribosomal protein S11-A



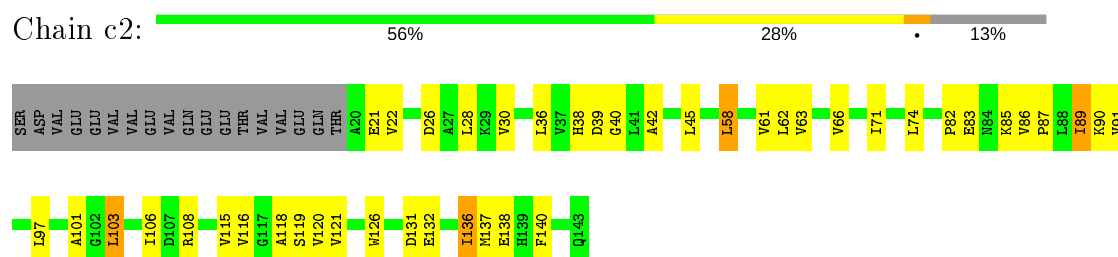
- Molecule 13: 40S ribosomal protein S11-A



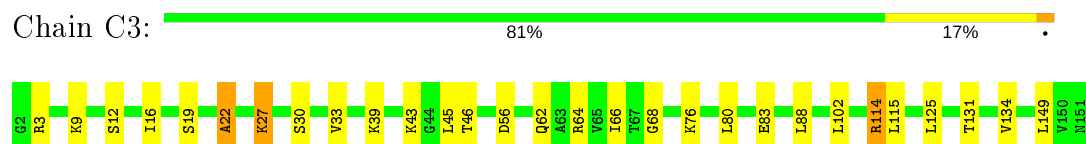
- Molecule 14: 40S ribosomal protein S12




- Molecule 14: 40S ribosomal protein S12



- Molecule 15: 40S ribosomal protein S13



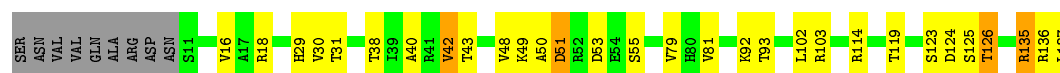
- Molecule 15: 40S ribosomal protein S13

Chain c3:  79% 19%



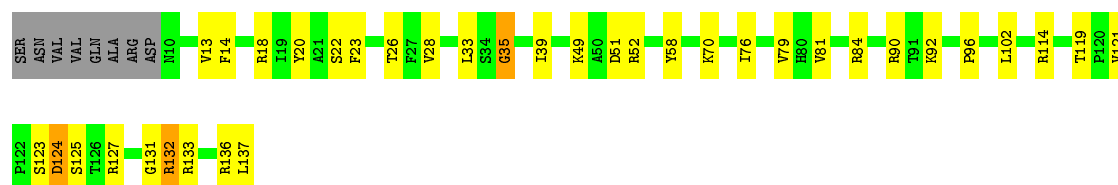
- Molecule 16: 40S ribosomal protein S14-A

Chain C4:  71% 19% 7%



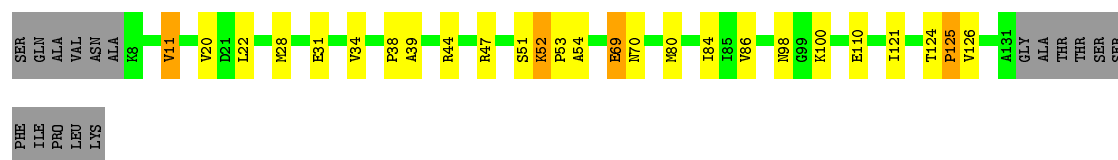
- Molecule 16: 40S ribosomal protein S14-A

Chain c4:  68% 24% 6%



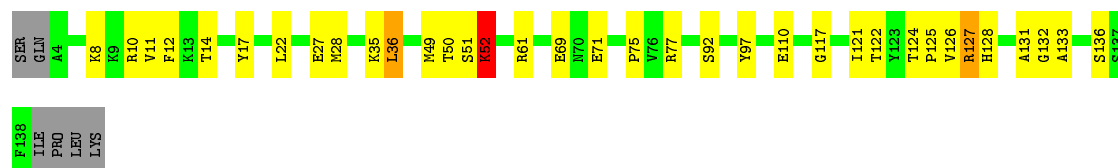
- Molecule 17: 40S ribosomal protein S15

Chain C5:  70% 16% 12%




- Molecule 17: 40S ribosomal protein S15

Chain c5:  71% 23%



- Molecule 18: 40S ribosomal protein S16-A

Chain C6:  77% 21%



- Molecule 18: 40S ribosomal protein S16-A

S2  
A3  
V4  
K23  
L28  
T37  
L38  
V39  
E40  
P41  
E42  
I43  
V48  
L53  
L54  
V55  
G56  
L57  
R68  
V69  
T70  
I81  
R82  
Q83  
Q94  
V97  
K106  
T110  
D113  
R114  
T115  
L116  
L117  
I118  
R137  
R143

- |      |     |      |
|------|-----|------|
| S125 | G2  | Met  |
| A126 | GLN | R3   |
|      | ARG | R4   |
|      | ASP | R5   |
|      | ARG | T6   |
|      | ARG | K10  |
|      | TYR | P22  |
|      | ARG | K23  |
|      | LYS | L24  |
|      | ARG | T25  |
|      | VAL | T30  |
|      |     | L34  |
|      |     | T40  |
|      |     | R45  |
|      |     | M58  |
|      |     | Q62  |
|      |     | R67  |
|      |     | G68  |
|      |     | I69  |
|      |     | K72  |
|      |     | R78  |
|      |     | M85  |
|      |     | P86  |
|      |     | E87  |
|      |     | V88  |
|      |     | S89  |
|      |     | ALA  |
|      |     | LEU  |
|      |     | ASP  |
|      |     | LEU  |
|      |     | SER  |
|      |     | R95  |
|      |     | Q105 |
|      |     | V110 |
|      |     | K111 |
|      |     | S112 |
|      |     | L113 |
|      |     | G114 |
|      |     | L115 |
|      |     | P118 |
|      |     | L119 |
|      |     | N123 |
|      |     | I124 |

- | ARG | MET  |
|-----|------|
| ASP | G2   |
| ARG | R3   |
| ARG | V4   |
| TYR | B5   |
| ARG | T6   |
| LYS | K7   |
| ARG | T8   |
| VAL | T25  |
|     | L34  |
|     | I38  |
|     | L46  |
|     | R47  |
|     | R48  |
|     | R49  |
|     | Q62  |
|     | K63  |
|     | T69  |
|     | Q74  |
|     | Q83  |
|     | R84  |
|     | V85  |
|     | R86  |
|     | B87  |
|     | V88  |
|     | S89  |
|     | A90  |
|     | LEU  |
| ASP | ASP  |
| LEU | LEU  |
| SER | SER  |
|     | R95  |
|     | V99  |
|     | T106 |
|     | S107 |
|     | V110 |
|     | L113 |
|     | L117 |
|     | S120 |
|     | V121 |
|     | I122 |
| ASN | ASN  |
| VAL | VAL  |
| SER | SER  |
| ALA | ALA  |
| GLN | GLN  |


- S2  
L3  
V4  
V5  
Q6  
E7  
Q8  
H13  
I14  
I15  
R16  
L17  
T20  
N25  
I28  
R40  
E60  
L61  
E65  
I72  
M73  
Q74  
K80  
I81  
P82  
A83  
D91  
I92  
T93  
Q93  
D97  
K108  
I125  
R132  
Q136  
H137  
T138  
R143  
I144  
L145

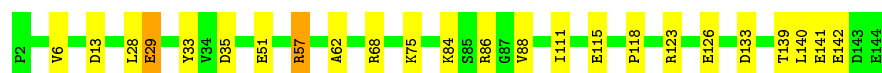
- |      |      |
|------|------|
| R144 | S2   |
| R145 | L3   |
| A146 | V4   |
|      | V5   |
|      | Q6   |
|      | E7   |
|      | Q8   |
|      | H13  |
|      | I14  |
|      | L15  |
|      | L18  |
|      | M19  |
|      | T20  |
|      | T25  |
|      | T26  |
|      | T27  |
|      | T28  |
|      | T33  |
|      | K36  |
|      | G37  |
|      | V38  |
|      | G39  |
|      | R40  |
|      | H55  |
|      | F56  |
|      | R57  |
|      | E60  |
|      | L61  |
|      | T62  |
|      | Q63  |
|      | K30  |
|      | F85  |
|      | N90  |
|      | D91  |
|      | I92  |
|      | V105 |
|      | E106 |
|      | R110 |
|      | L116 |
|      | T119 |
|      | Q136 |
|      | H137 |
|      | T138 |
|      | K139 |

- |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |
|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|
| P2 | V6 | L22 | K27 | L28 | E29 | V30 | P31 | D35 | T36 | V37 | K38 | T39 | A50 | W53 | B57 | S60 | M67 | V71 | R86 | I94 | K103 | I116 | R122 | R130 | D131 | L132 | D133 | R134 | D143 | R144 |
|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|

- 

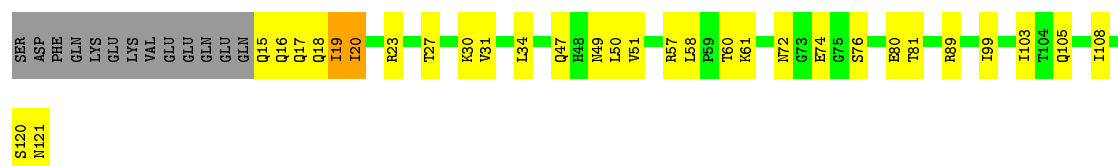


Chain c9:  83% 15% •



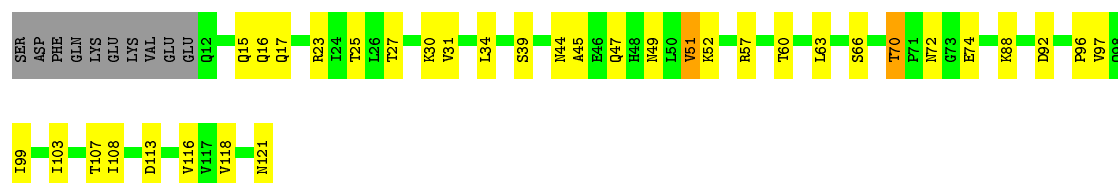
- Molecule 22: 40S ribosomal protein S20

Chain D0:  63% 24% • 11%




- Molecule 22: 40S ribosomal protein S20

Chain d0:  63% 28% • 8%



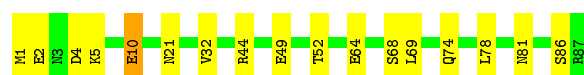
- Molecule 23: 40S ribosomal protein S21-A

Chain D1:  80% 17% •




- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  80% 18% •



- Molecule 24: 40S ribosomal protein S22-A

Chain D2:  83% 14% •



- Molecule 24: 40S ribosomal protein S22-A

Chain d2:  87% 11% •





- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 67% 27% 6%



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 71% 29%



- Molecule 29: 40S ribosomal protein S27-A

Chain D7: 81% 16% •



- Molecule 29: 40S ribosomal protein S27-A

Chain d7: 83% 15% •



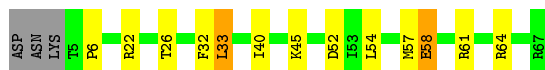
- Molecule 30: 40S ribosomal protein S28-A

Chain D8: 70% 23% • 5%



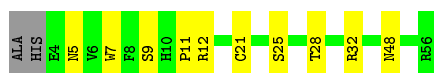
- Molecule 30: 40S ribosomal protein S28-A

Chain d8: 76% 17% • 5%



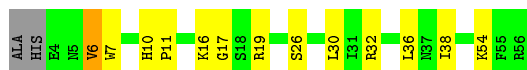
- Molecule 31: 40S ribosomal protein S29-A

Chain D9: 78% 18% •



- Molecule 31: 40S ribosomal protein S29-A

Chain d9: 73% 22% . .



- Molecule 32: 40S ribosomal protein S30-A

Chain E0: 77% 22% .



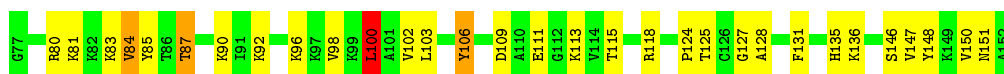
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 51% 36% 7% 7%



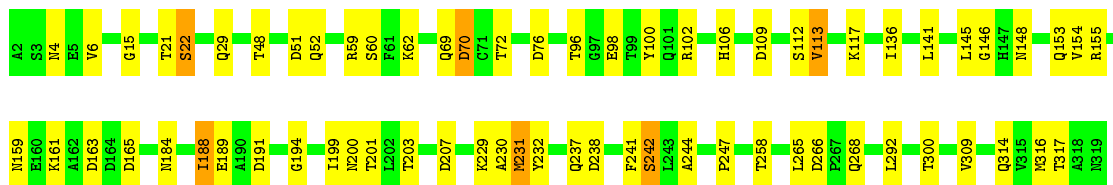
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1: 59% 36% . .



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

Chain SR: 79% 19% .



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

Chain sR: 87% 13% .





A1589	A1593	A1603	G1417	U1351	A1278	U1191	U1124	A1036	U954	A884	U797	G685	G610	C435	
A1604	G1605	A1606	A1418	A1352	C1279	C1192	U1124	C1037	U955	U885	G798	A691	A611	A438	
G1607	G1608	A1609	A1419	U1353	C1280	A1193	G1127	U1041	U956	C886	G799	A692	U612	C439	
A1609	G1510	G1510	C1420	G1354	G1285	G1194	A1128	U1042	U957	C887	G800	A693	G613	A440	
G1511	G1512	G1513	G1421	U1355	A1286	C1195	A1129	C1043	C958	C890	A801	C694	U614	U	
G1514	A1515	G1515	G1422	U1356	A1287	C1196	A1130	U1044	C959	C891	C802		C615	G	
G1616	G1617	G1617	U1425	C1360	C1292	C1198	G1131	A1045	U960	C893	C803		G616	G	
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G1655	G1656	G1656	U1450	C1383	C1317	G1235	A1153	U1072	A986	A830			A645	U	
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G1657	G1658	G1658	U1452	G1385	U1319	G1237	U1155	U1081	A988	U833			A647	U	
G1658	G1659	G1659	U1453	U1386	C1320	U1241	U1156	U1082	A989	U834			A648	G	
G1659	G1660	G1660	U1454	G1387	G1321	G1242	C1159	G1083	A990	U835			A649	G	
G1660	G1661	G1661	U1455	G1388	U1322	G1243	C1160	G1084	A991	A836			G650	U	
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G1664	G1665	G1665	U1459	G1392	A1326	A1245	G1164	U1094	A995	U764			C654	G	
G1665	G1666	G1666	U1460	A1393	C1327	G1246	A1165	U1095	A996	C765			G655	U	
G1666	G1667	G1667	U1461	G1394	C1328	U1247	A1166	U1096	A997	U766			G656	G	
G1667	G1668	G1668	U1462	C1395	U1329	C1248	G1167	U1097	A998	U767			G657	A	
G1668	G1669	G1669	U1463	G1396	A1330	G1249	A1168	A1098	A999	G768			A660	U	
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G1670	G1671	G1671	U1465	A1398	A1332	A1251	A1170	U1100	A1001	G770			U662	U	
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G1677	G1678	G1678	U1472	A1406	C1339	G1266	A1180	G1112	A1008	U777			U669	U	
G1678	G1679	G1679	U1473	A1407	C1340	U1267	A1181	G1113	A1009	G778			A670	C	
G1679	G1680	G1680	U1474	G1408	A1341	G1268	A1182	G1114	A1010	U779			G671	U	
G1680	G1681	G1681	U1475	U1409	G1342	U1269	A1183	U1115	A1011	A780			A672	C	
G1681	G1682	G1682	U1476	G1410	A1343	A1270	A1184	G1116	A1012	G781			G600	A	
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G1687	G1688	G1688	U1482	U1415	G1349	A1275	U1190	G1122	U1018	U787			A608	U	
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G1689	G1690	G1690	U1484						U1019	A883			G495	U	
G1690	G1691	G1691	U1485						A1020						
G1691	G1692	G1692	U1486						A1021						
G1692	G1693	G1693	U1487						A1022						
G1693	G1694	G1694	U1488						A1023						
G1694	G1695	G1695	U1489						A1024						
G1695	G1696	G1696	U1490						A1025						
G1696	G1697	G1697	U1491						A1026						
G1697	G1698	G1698	U1492						A1027						
G1698	G1699	G1699	U1493						A1028						
G1699	G1700	G1700	U1494						A1029						
G1700	G1701	G1701	U1495						A1030						
G1701	G1702	G1702	U1496						A1031						
G1702	G1703	G1703	U1497						A1032						
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G1725	G1726	G1726	U1520						A1055						
G1726	G1727	G1727	U1521						A1056						
G1727	G1728	G1728	U1522						A1057						
G1728	G1729	G1729	U1523						A1058						
G1729	G1730	G1730	U1524						A1059						
G1730	G1731	G1731	U1525						A1060						
G1731	G1732	G1732	U1526						A1061						
G1732	G1733	G1733	U1527						A1062						
G1733	G1734	G1734	U1528						A1063						
G1734	G1735	G1735	U1529						A1064						
G1735	G1736	G1736	U1530						A1065						
G1736	G1737	G1737	U1531												





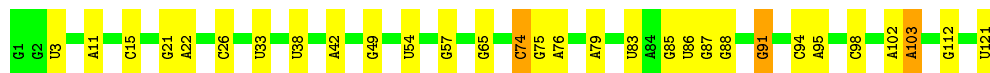


C	A2126	G	G1838	A1696	G1573	G1488	C1403	G	U1208	G1142	A1055	G971	G902
C	A2131	G	A1839	C1701	C1574	G1489	G1403	G	G1209	G1143	U1056	A972	G907
U	A2132	A	U1840	G	G1575	A1490	U1405	G	C1219	U1144	A1057	A973	G908
U	A2133	U	A1841	A1704	G1576	U1495	C1328	G	C1219	G1147	U1060	G974	G909
G	U2133	G	G1843	U1716	G1578	C1496	U1329	U	G1222	U1148	U	U979	G910
G	U2134	C	C1844	U1717	C1579	G1497	U1330	U	A1223	G1149	U	A980	G911
A	U2135	U	G1845	U1717	A1580	C1498	U1331	U	U	G1150	A1063	U981	G912
G	C2136	U	C1846	U1721	G1581	C1499	C1333	G	C1232	U1151	A1065	U	A913
G	U2137	G	A1847	U1721	C1582	G1500	G1412	U	U	G1152	U	G984	A914
U	A2138	U	G1848	U1724	U1583	A1504	G1413	U	U1235	A1153	G1072	A985	A915
U	U2140	U	C1849	C1725	C1585	A1505	G1416	U	G1236	U985	U	U986	A916
U	U2141	C	U1850	G	G1586	A1506	G1417	U	G1237	U986	A1075	U987	A917
C	U2142	G	U1851	G1736	A1587	A1507	G1418	U	C1238	U988	U1077	U989	C918
U	A2143	U	C1852	G	A1588	C1508	U1419	U	C1239	A1159	U	A990	U919
U	A2144	U	U1853	U1750	A1589	G1509	C1420	U	U1241	C1160	A1080	G991	A921
U	A2145	U	C1854	G1751	G1592	U1511	U1426	U	G1242	G1161	U1081	A992	U922
U	A2146	U	U1855	C1761	U1595	U1512	U1427	U	A1245	G1164	U1082	G993	C923
A	C2146	U	G1856	C1762	U1596	G1513	U1428	U	G1246	A1165	A1085	G994	G924
G	A2147	C	U1857	U1763	U1597	A1514	G1429	U	U	U1168	C1086	A997	C928
G	U2148	C	G1863	U1764	G1598	A1515	U1430	U	A1252	U1169	G1087	A998	A929
U	A2149	U	A1864	U1765	G1599	C1516	G1431	U	U1253	A1170	U1088	G999	U930
U	G2150	U	G1865	G1766	G1604	G1519	C1432	U	U1258	G1171	A1093	C1000	C931
U	C2156	C	A1866	G	A1605	G1520	A1433	U	U	G1174	U	G1001	U932
G	G2157	U	A1867	G1770	U1606	G1521	G1434	U	G1262	G1175	U1094	A1002	A933
U	U2159	C	C1868	G1780	U1607	G1522	C1437	U	A1263	C1176	U1095	A1003	G934
U	C2163	U	C1869	C1788	C1608	U1526	G1440	U	G1264	G1177	U1096	U1004	U
U	A2164	C	U1872	G1789	C1609	G1527	G1443	U	U1265	G1178	G1097	G1005	G937
U	G2165	C	U1873	G1794	U1620	C1528	U1444	U	G1266	G1179	A1098	U1006	C938
U	A2166	U	G1875	U1795	A1621	G1529	U1445	U	U1267	U	A1099	U1007	U
C	A2167	A	U1876	G1796	C1628	C1532	U1446	U	G1268	U1180	A1103	U1008	G941
U	G2168	C	U1877	U1797	U1629	U1533	A1447	U	U1181	G1182	G1104	A1009	U942
A	G2169	U	G1878	A1798	G1635	A1534	G1448	U	C1292	C1183	U	U1014	C944
A	U2170	U	A1879	U1799	U1636	G1536	U1449	U	U1293	A1184	G1107	U1015	U946
U	U2176	U	U1880	C1803	A1637	G1537	G1450	U	C1297	U	U1110	C1016	U947
U	G2177	U	A1881	U1810	C1639	G1541	C1451	U	U	G1187	U	C1017	C948
U	A2178	A	A1886	A1813	A1643	C1547	A1452	U	G1300	U1188	U	G1018	C949
U	G2180	U	A1891	A1814	C1644	C1548	U1462	U	A1301	C1189	U	G1019	G950
U	A2183	U	G1892	U1815	U1645	U1554	U1463	U	G1302	U1190	G1115	G1020	A951
U	G2184	C	A1893	A1816	U1657	C1556	G1464	U	A1303	C1191	G1116	G1021	A952
U	U2186	C	G1897	G1817	C1657	C1556	A1465	U	A1304	C1192	G1117	U	G953
U	G2187	U	G1898	U1818	G1661	G1560	A1468	U	G1307	U1194	C1119	G1024	U954
U	U2191	U	G1899	U1819	G1662	G1561	G1476	U	A1308	A1195	U1124	A1025	C957
U	C2192	U	U1902	U1820	G1663	C1562	A1477	U	U1309	C1196	U	A1026	C958
U	U2198	U	C1904	U1821	G1664	G1563	C1478	U	G1311	C1199	U1128	A1027	U959
U	G2199	U	G1905	G1829	G1665	U1565	U1479	U	C1312	A1200	A1129	U1028	C961
U	A2199	A	G1906	G1833	G1666	A1566	G1480	U	G1313	C1201	A1130	G1035	A962
U	C2204	U	A1909	U1834	A1667	U1567	A1481	U	C1314	A1202	G1131	U1044	G963
U	U2205	U	U1910	U1837	G1667	U1570	A1482	U	U1315	A1203	C1137	U	A964
U	G2122	G	A1911	U1837	A1683	U1571	G1483	U	C1316	A1204	U1138	A1047	U965
U	G2123	G	U1912	U1837	U1684	U1572	U1484	U	A1317	G1206	G1139	A1048	U966
U	A2208	U	U1912	U1837	U1684	U1572	U1484	U	G1321	G1207	C1141	C1049	A970



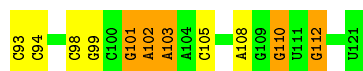
- Molecule 37: 5S ribosomal RNA

Chain 3:  75% 22%



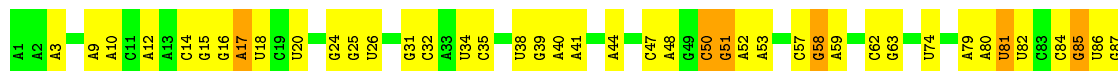
- Molecule 37: 5S ribosomal RNA

Chain 7:  60% 34% 7%



- Molecule 38: 5.8S ribosomal RNA

Chain 4:  56% 37% 7%




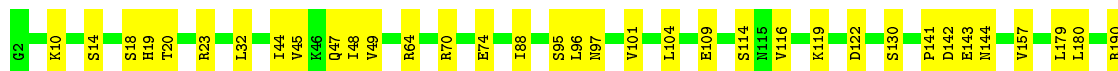
- Molecule 38: 5.8S ribosomal RNA

Chain 8:  63% 29% 8%




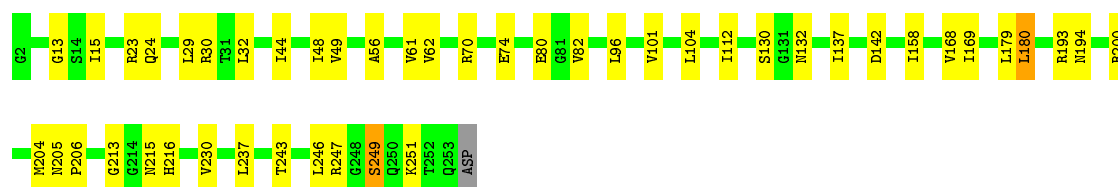
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:  82% 17%



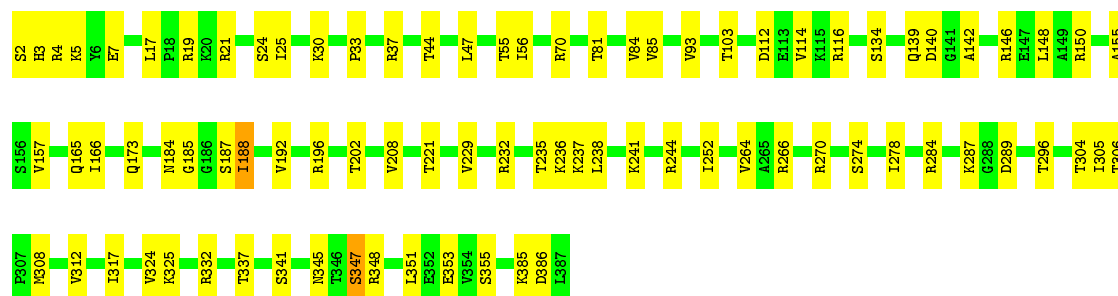
- Molecule 39: 60S ribosomal protein L2-A

Chain l2:  81% 17%



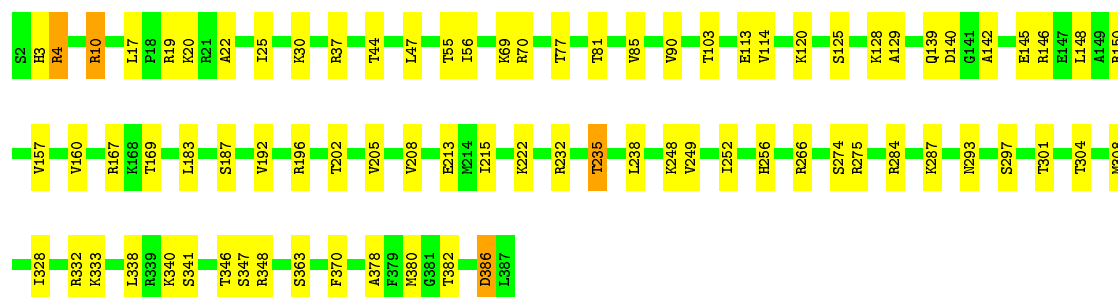
- Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 21% .



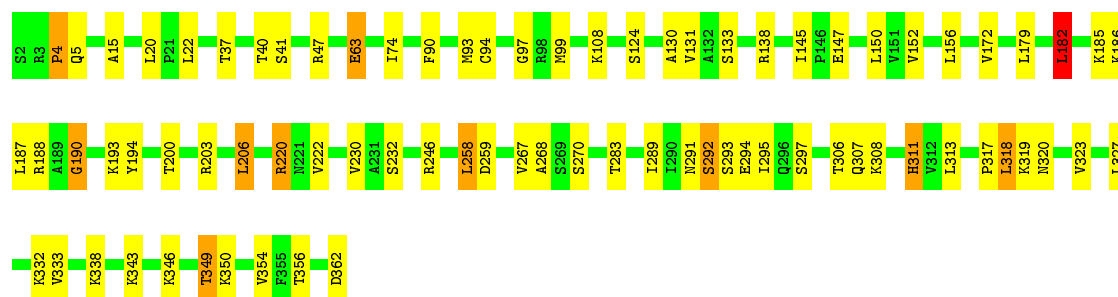
- Molecule 40: 60S ribosomal protein L3

Chain l3: 79% 20% .



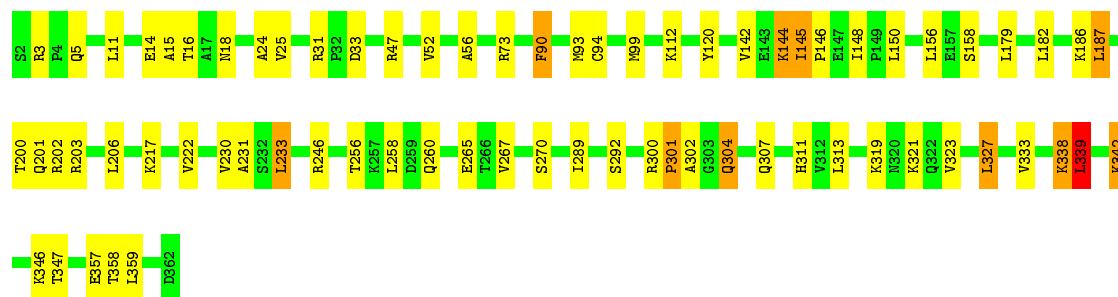
- Molecule 41: 60S ribosomal protein L4-A

Chain L4: 78% 19% .



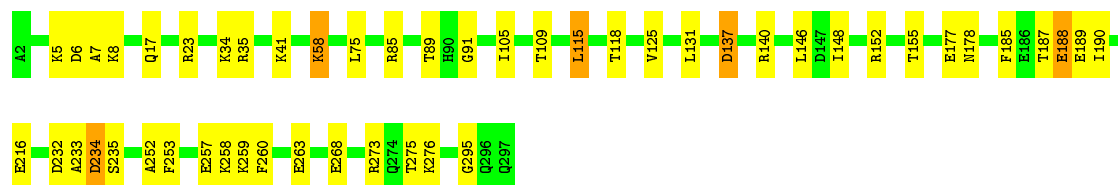
- Molecule 41: 60S ribosomal protein L4-A

Chain l4: 80% 17% .



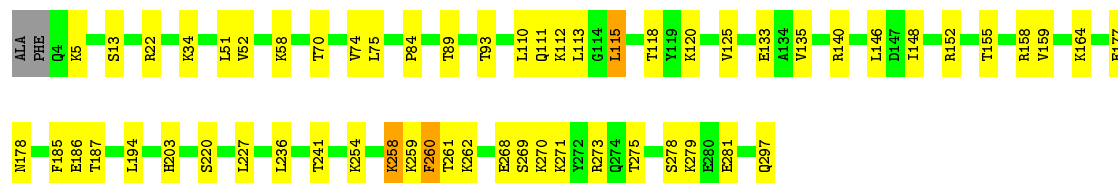
- Molecule 42: 60S ribosomal protein L5

Chain L5: 83% 15% .



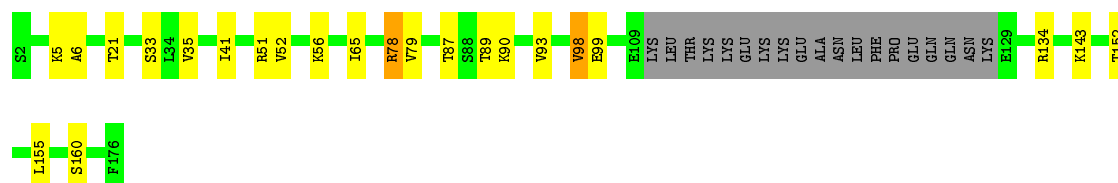
- Molecule 42: 60S ribosomal protein L5

Chain L5: 80% 19% ..



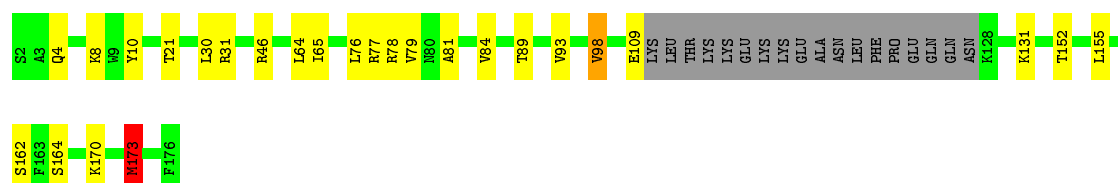
- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 76% 12% . 11%




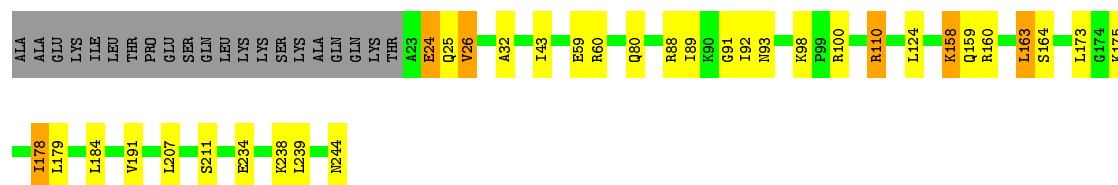
- Molecule 43: 60S ribosomal protein L6-A

Chain L6: 75% 14% .. 10%




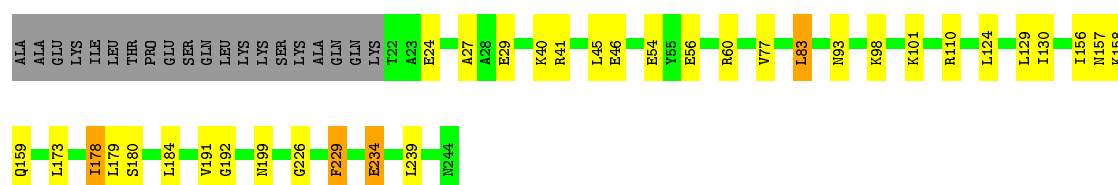
- Molecule 44: 60S ribosomal protein L7-A

Chain L7:  77% 12% 9%




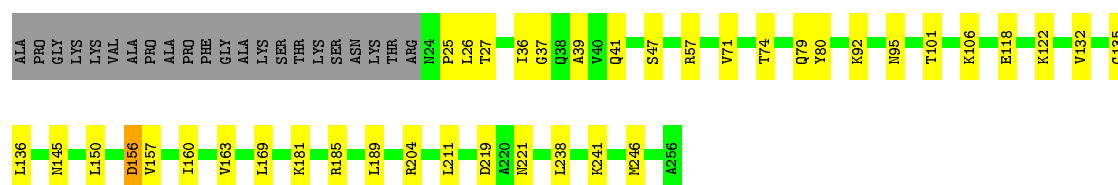
- Molecule 44: 60S ribosomal protein L7-A

Chain l7:  77% 13% 8%



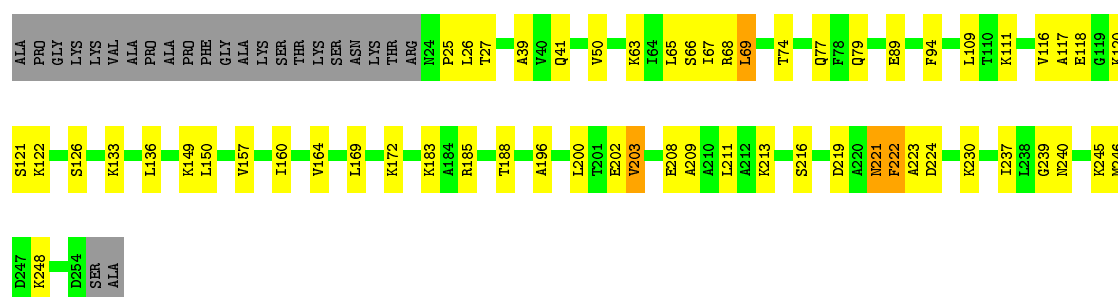
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:  76% 15% 9%




- Molecule 45: 60S ribosomal protein L8-A

Chain l8:  67% 22% 9%



- Molecule 46: 60S ribosomal protein L9-A

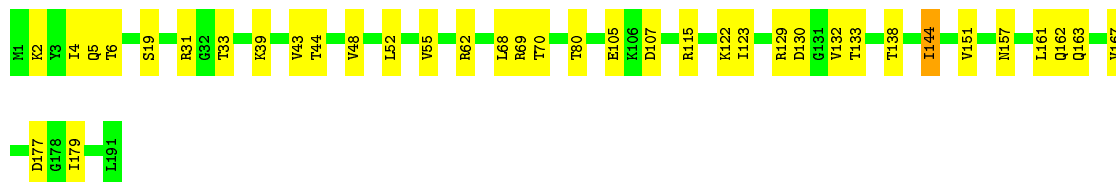
Chain L9:  75% 24% 1%





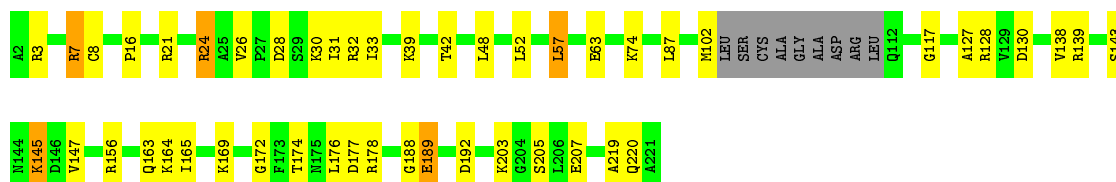
- Molecule 46: 60S ribosomal protein L9-A

Chain l9: 81% 19%



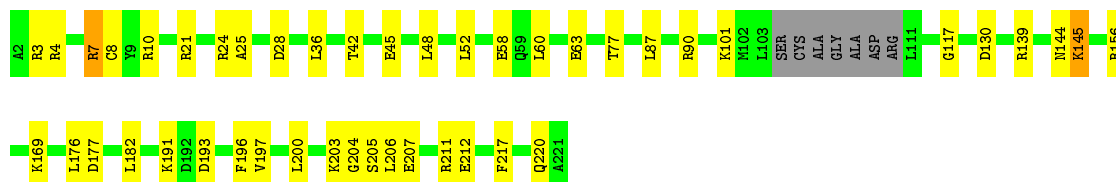
- Molecule 47: 60S ribosomal protein L10

Chain M0: 74% 20%



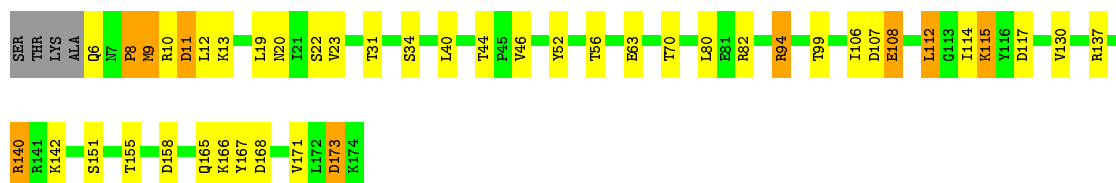
- Molecule 47: 60S ribosomal protein L10

Chain m0: 76% 20%



- Molecule 48: 60S ribosomal protein L11-B

Chain M1: 72% 20% 5%



- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 73% 23%





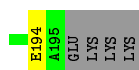
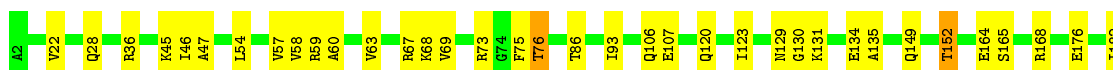
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 78% 18%



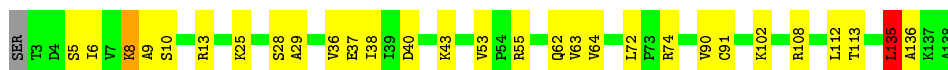
- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 79% 18%



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 78% 20%



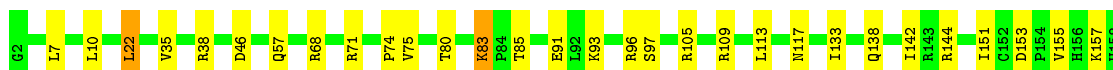
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 85% 13%



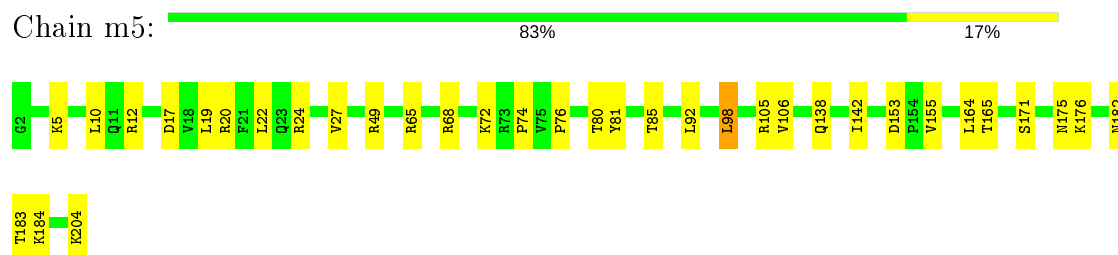
- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 80% 19%

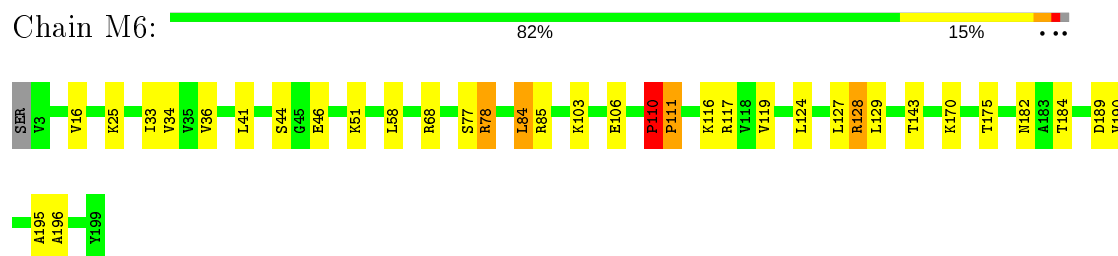


- Molecule 51: 60S ribosomal protein L15-A

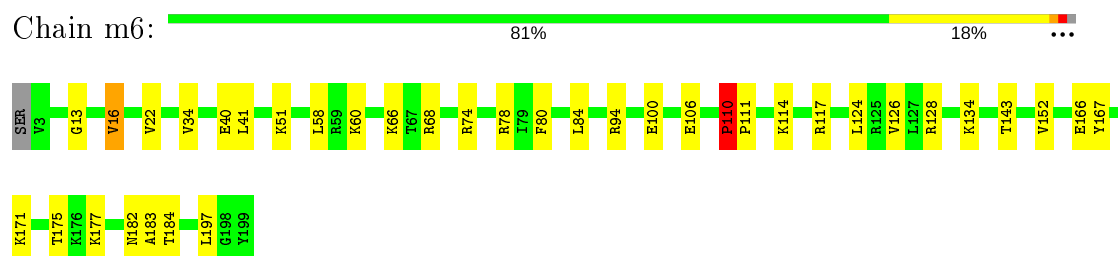




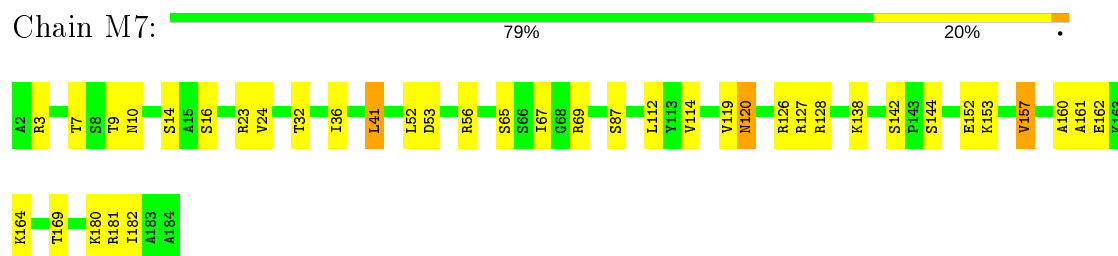
- Molecule 52: 60S ribosomal protein L16-A



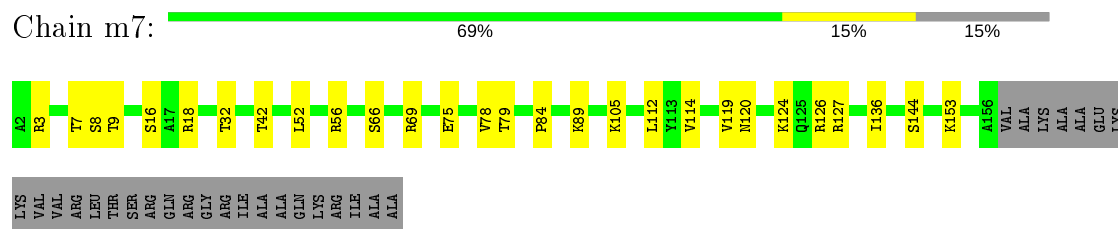
- Molecule 52: 60S ribosomal protein L16-A



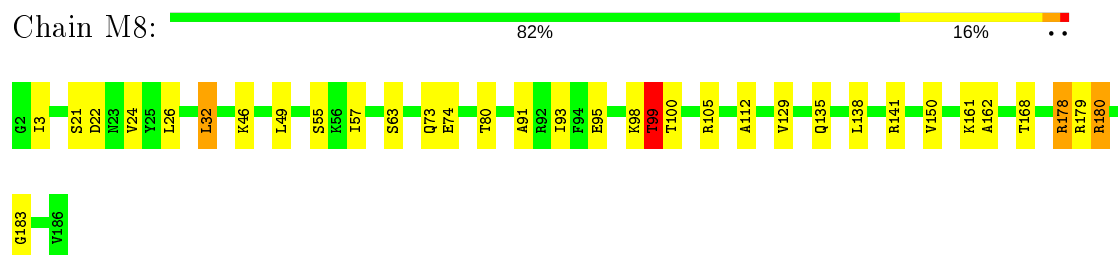
- Molecule 53: 60S ribosomal protein L17-A



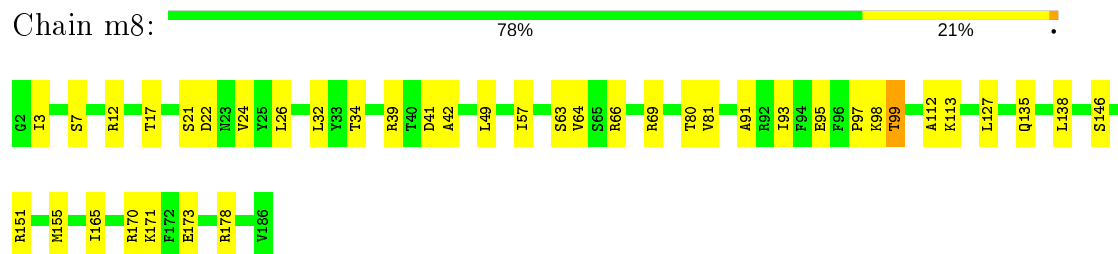
- Molecule 53: 60S ribosomal protein L17-A



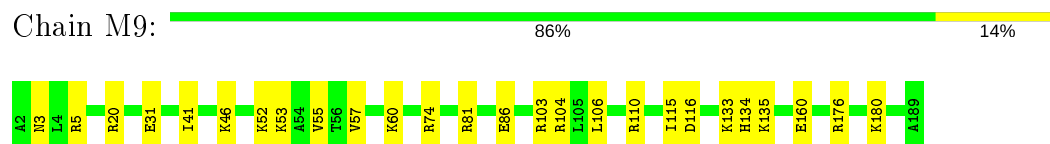
- Molecule 54: 60S ribosomal protein L18-A



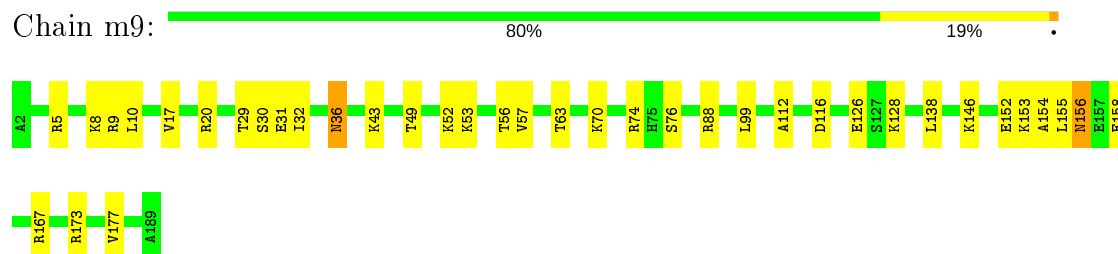
- Molecule 54: 60S ribosomal protein L18-A



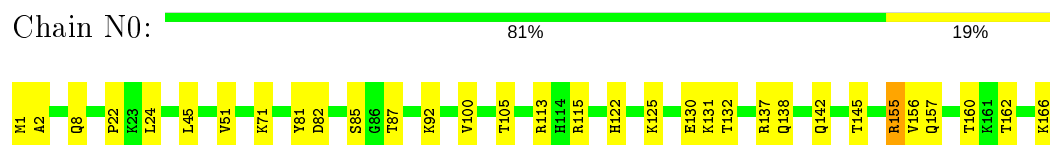
- Molecule 55: 60S ribosomal protein L19-A



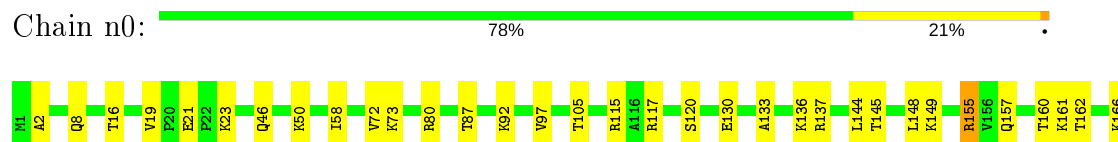
- Molecule 55: 60S ribosomal protein L19-A

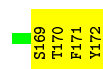


- Molecule 56: 60S ribosomal protein L20-A



- Molecule 56: 60S ribosomal protein L20-A





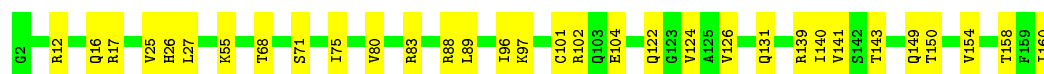
- Molecule 57: 60S ribosomal protein L21-A

Chain N1: 81% 16%



- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 80% 20%



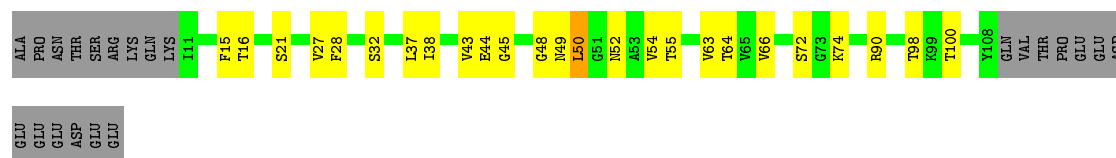
- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 68% 14% 17%



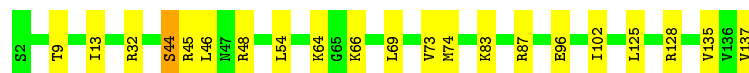
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 61% 20% 18%



- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 85% 15%



- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 88% 11%



- Molecule 60: 60S ribosomal protein L24-A


LYS	SER	ALA	GLY	THR	GLN	SER	SER	LYS	PHE	SER	LYS	GLN	GLN	ALA	LYS	GLY	ALA	PHE	GLN	LYS	VAL	ALA	ALA	THR	SER	ARG										
R1	E4	I5	G10	T19	K27	L39	P46	R47	T64	R69	V76	K77	P81	S86	L96	K97	P98	GLU	VAL	ARG	LYS	ALA	ASN	ARG	GLU	LYS	LYS	LYS	ALA	ALA	ARG	ALA	GLU	LYS	LYS	ALA

- |  |    |     |            |     |     |     |     |     |            |     |                          |                   |                             |      |      |      |  |
|--|----|-----|------------|-----|-----|-----|-----|-----|------------|-----|--------------------------|-------------------|-----------------------------|------|------|------|--|
|  | M1 | T19 | D25<br>S26 | S34 | L39 | L54 | K57 | I63 | V76<br>K77 | T83 | L89<br><b>E90</b><br>R91 | L96<br>R97<br>P98 | R105<br><b>E106</b><br>E107 | E119 | E126 | G132 | <b>S135</b><br>SER<br>LYS<br>PRE<br>SER<br>LYS<br>GLN<br>GLN<br>ALA<br>LYS<br>GLY<br>ALA<br>PRE<br>GLN<br>LYS<br>VAL<br>ALA<br>ALA<br>THR<br>SER |
|--|----|-----|------------|-----|-----|-----|-----|-----|------------|-----|--------------------------|-------------------|-----------------------------|------|------|------|--|

- |      |      |   |            |                          |  |            |            |            |            |            |            |            |             |                            |   |                            |             |                            |
|------|------|---|------------|--------------------------|--|------------|------------|------------|------------|------------|------------|------------|-------------|----------------------------|---|----------------------------|-------------|----------------------------|
| I139 | I142 | ALA<br>PRO<br>SER<br>ALA<br>LYS<br>ALA<br>THR<br>ALA<br>ALA<br>LYS<br>LYS<br>LYS<br>ALA<br>VAL<br>VAL<br>LYS<br>GLY<br>THR<br>ASN<br>GLY<br>LYS<br><b>R22</b> | <b>R27</b> | <b>R33</b><br><b>L34</b> | <b>T37</b><br><b>L38</b><br><b>K39</b> | <b>K45</b> | <b>S59</b> | <b>I63</b> | <b>K74</b> | <b>V86</b> | <b>K92</b> | <b>K96</b> | <b>V105</b> | <b>L108</b><br><b>K109</b> | <b>L113</b><br><b>V114</b><br><b>R115</b> | <b>R125</b><br><b>L126</b> | <b>T127</b> | <b>D134</b><br><b>I135</b> |
|------|------|---|------------|--------------------------|--|------------|------------|------------|------------|------------|------------|------------|-------------|----------------------------|---|----------------------------|-------------|----------------------------|

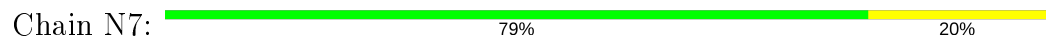
- |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|
| D134 | ALA | PRO | ALA | LYS | ALA | THR | ALA | LYS | LYS | VAL | LYS | GLY | THR | ASN | GLY | LYS | LYS | A23 | L24 | K25 | V26 | R27 | T37 | L38 | K39 | L40 | P44 | K45 | Y46 | A47 | M55 | R56 | L57 | I63 | E64 | V86 | K86 | E104 | L108 | K109 | R115 | P116 | M117 | R125 | I132 |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|

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

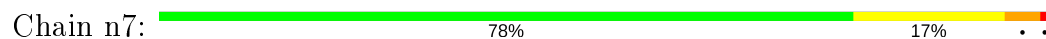
- Chain n6:  80% 19% .



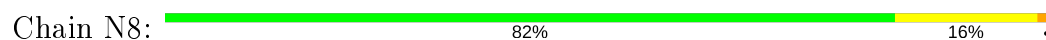
- Molecule 63: 60S ribosomal protein L27-A



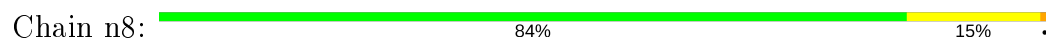
- Molecule 63: 60S ribosomal protein L27-A



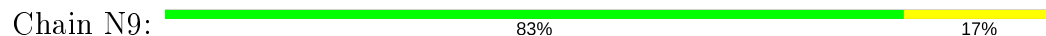
- Molecule 64: 60S ribosomal protein L28



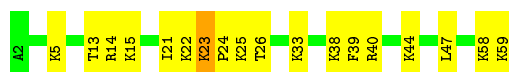
- Molecule 64: 60S ribosomal protein L28



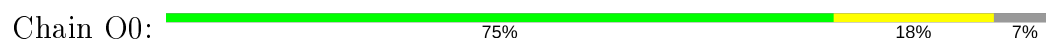
- Molecule 65: 60S ribosomal protein L29

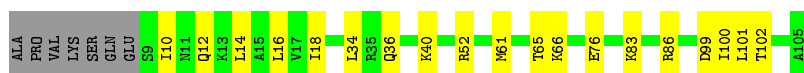


- Molecule 65: 60S ribosomal protein L29

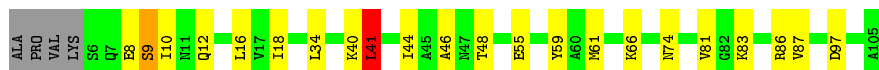


- Molecule 66: 60S ribosomal protein L30

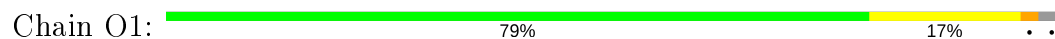




- Molecule 66: 60S ribosomal protein L30



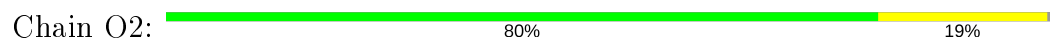
- Molecule 67: 60S ribosomal protein L31-A



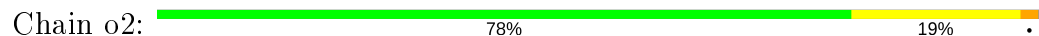
- Molecule 67: 60S ribosomal protein L31-A



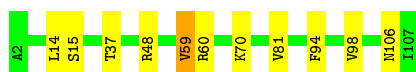
- Molecule 68: 60S ribosomal protein L32



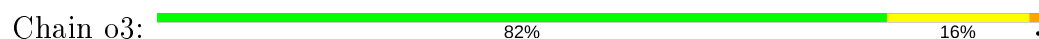
- Molecule 68: 60S ribosomal protein L32

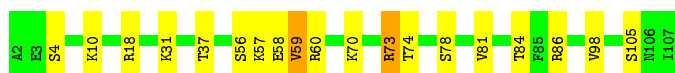


- Molecule 69: 60S ribosomal protein L33-A

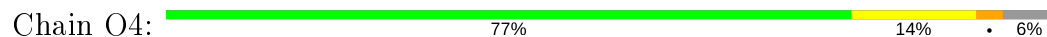


- Molecule 69: 60S ribosomal protein L33-A

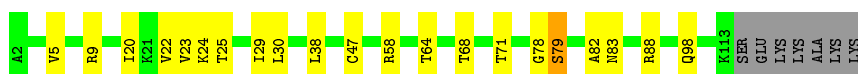
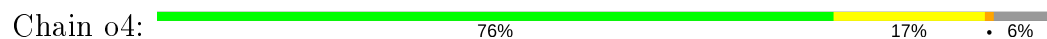




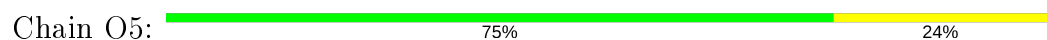
- Molecule 70: 60S ribosomal protein L34-A



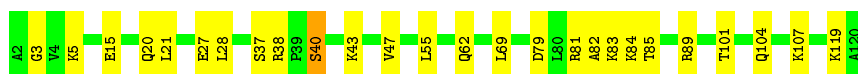
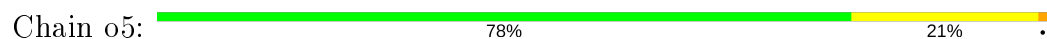
- Molecule 70: 60S ribosomal protein L34-A



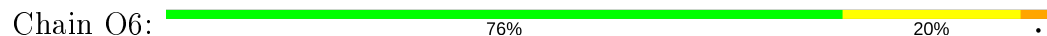
- Molecule 71: 60S ribosomal protein L35-A



- Molecule 71: 60S ribosomal protein L35-A



- Molecule 72: 60S ribosomal protein L36-A

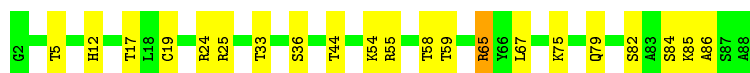


- Molecule 72: 60S ribosomal protein L36-A

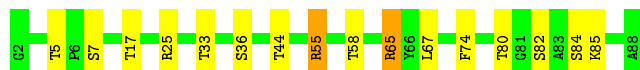
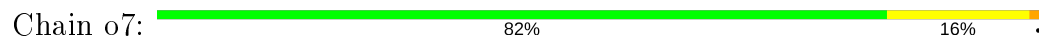


- Molecule 73: 60S ribosomal protein L37-A

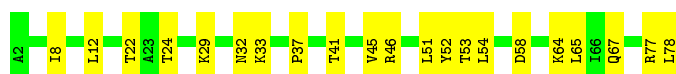
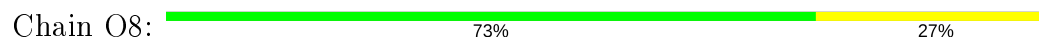




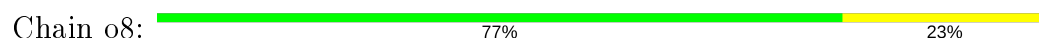
- Molecule 73: 60S ribosomal protein L37-A



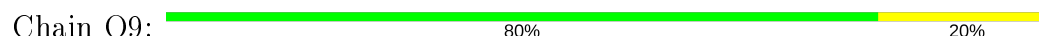
- Molecule 74: 60S ribosomal protein L38



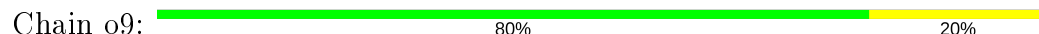
- Molecule 74: 60S ribosomal protein L38



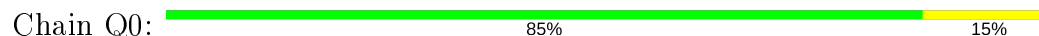
- Molecule 75: 60S ribosomal protein L39



- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



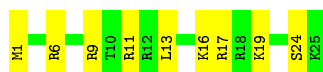
- Molecule 76: Ubiquitin-60S ribosomal protein L40







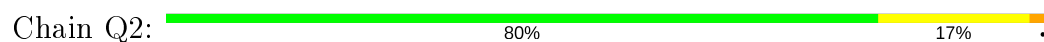
- Molecule 77: 60S ribosomal protein L41-A



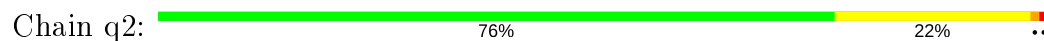
- Molecule 77: 60S ribosomal protein L41-A



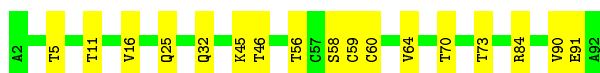
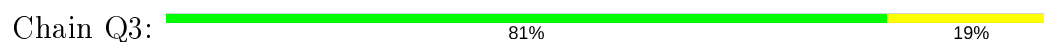
- Molecule 78: 60S ribosomal protein L42-A



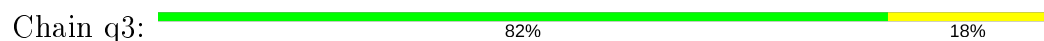
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



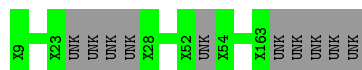
- Molecule 80: 40S ribosomal protein S30-A





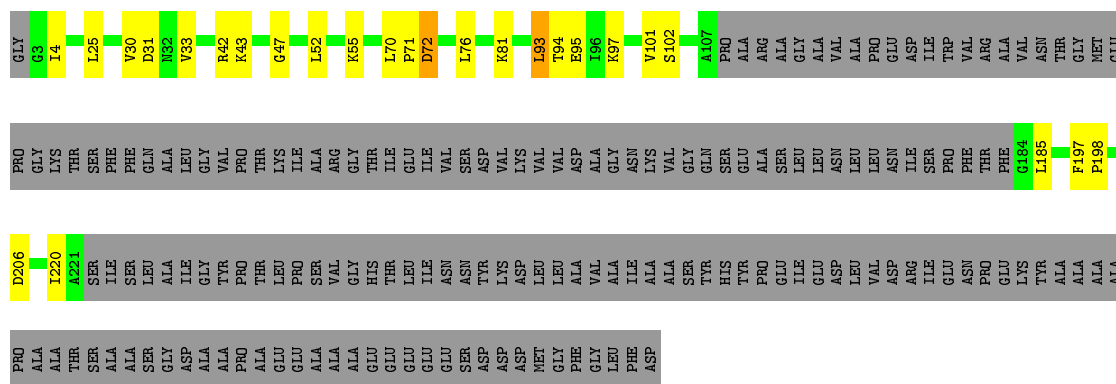
- Molecule 81: Unknown protein m2

Chain m2: 94% 6%



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0: 38% 8% 54%



- Molecule 83: Unknown protein p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	434.98Å 287.50Å 303.22Å 90.00° 98.85° 90.00°	Depositor
Resolution (Å)	299.60 – 3.10	Depositor
% Data completeness (in resolution range)	100.0 (299.60-3.10)	Depositor
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.202 , 0.252	Depositor
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.178	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: 3K5, 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	0.73	5/41698 (0.0%)	1.28	279/64972 (0.4%)
1	6	0.89	29/42765 (0.1%)	1.39	455/66634 (0.7%)
2	S0	0.48	0/1617	0.67	0/2215
2	s0	0.50	0/1623	0.68	0/2222
3	S1	0.37	0/1735	0.68	1/2335 (0.0%)
3	s1	0.53	0/1748	0.70	0/2352
4	S2	0.51	0/1665	0.66	0/2263
4	s2	0.59	0/1665	0.77	0/2263
5	S3	0.51	0/1759	0.70	1/2368 (0.0%)
5	s3	0.47	0/1759	0.61	0/2368
6	S4	0.50	0/2109	0.72	0/2839
6	s4	0.56	0/2109	0.76	1/2839 (0.0%)
7	S5	0.41	0/1629	0.61	0/2202
7	s5	0.47	0/1629	0.66	0/2202
8	S6	0.49	0/1823	0.67	0/2439
8	s6	0.57	0/1779	0.71	0/2379
9	S7	0.44	0/1506	0.67	0/2028
9	s7	0.49	0/1516	0.72	1/2043 (0.0%)
10	S8	0.56	0/1514	0.74	2/2021 (0.1%)
10	s8	0.65	0/1514	0.78	0/2021
11	S9	0.49	0/1519	0.68	1/2035 (0.0%)
11	s9	0.59	0/1519	0.74	0/2035
12	C0	0.42	0/790	0.64	1/1069 (0.1%)
12	c0	0.40	0/777	0.64	3/1049 (0.3%)
13	C1	0.61	0/1240	0.75	0/1675
13	c1	0.65	0/1194	0.77	0/1610
14	C2	0.38	0/900	0.64	0/1224
14	c2	0.30	0/900	0.59	1/1224 (0.1%)
15	C3	0.51	0/1215	0.72	3/1638 (0.2%)
15	c3	0.60	0/1215	0.73	0/1638
16	C4	0.38	0/901	0.63	0/1217
16	c4	0.54	0/960	0.78	1/1290 (0.1%)

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

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

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

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

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

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



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

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

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

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

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

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

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

## 5.3 Torsion angles [i](#)

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

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

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

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

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

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

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

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

5 of 1310 Ramachandran outliers are listed below:

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

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

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

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

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

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

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

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

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

Mol	Chain	Res	Type
68	O2	126	LEU
7	s5	216	GLU
64	n8	60	TYR
71	O5	100	VAL
3	s1	25	THR

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

Mol	Chain	Res	Type
57	N1	26	HIS
3	s1	74	GLN
61	n5	111	ASN
59	N3	98	ASN
64	N8	64	GLN

### 5.3.3 RNA ⓘ

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

5 of 2400 RNA backbone outliers are listed below:

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

5 of 269 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	2688	U
1	6	139	C
36	5	2585	G
36	1	2817	A
36	1	3269	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 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	OHX	6	2139	-	0,6,6	0.00	-	-		
86	OHX	2	2042	-	0,6,6	0.00	-	-		
86	OHX	5	4045	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	15	303	-	0,6,6	0.00	-	-		
86	OHX	5	4008	-	0,6,6	0.00	-	-		
86	OHX	6	2153	-	0,6,6	0.00	-	-		
86	OHX	1	3952	-	0,6,6	0.00	-	-		
86	OHX	6	2129	-	0,6,6	0.00	-	-		
86	OHX	6	2144	-	0,6,6	0.00	-	-		
86	OHX	5	4100	-	0,6,6	0.00	-	-		
86	OHX	4	227	-	0,6,6	0.00	-	-		
86	OHX	M5	302	-	0,6,6	0.00	-	-		
86	OHX	6	2114	-	0,6,6	0.00	-	-		
86	OHX	6	2105	-	0,6,6	0.00	-	-		
86	OHX	1	3915	-	0,6,6	0.00	-	-		
86	OHX	1	4041	-	0,6,6	0.00	-	-		
86	OHX	5	3913	-	0,6,6	0.00	-	-		
86	OHX	5	4185	-	0,6,6	0.00	-	-		
86	OHX	1	4131	-	0,6,6	0.00	-	-		
86	OHX	5	4118	-	0,6,6	0.00	-	-		
86	OHX	2	2086	-	0,6,6	0.00	-	-		
86	OHX	5	4236	-	0,6,6	0.00	-	-		
86	OHX	5	4014	-	0,6,6	0.00	-	-		
86	OHX	1	4138	-	0,6,6	0.00	-	-		
86	OHX	M7	205	-	0,6,6	0.00	-	-		
86	OHX	1	3932	-	0,6,6	0.00	-	-		
86	OHX	1	3913	-	0,6,6	0.00	-	-		
86	OHX	1	4109	-	0,6,6	0.00	-	-		
86	OHX	5	3992	-	0,6,6	0.00	-	-		
86	OHX	1	4006	-	0,6,6	0.00	-	-		
86	OHX	1	4135	-	0,6,6	0.00	-	-		
86	OHX	5	4175	-	0,6,6	0.00	-	-		
86	OHX	6	2082	-	0,6,6	0.00	-	-		
86	OHX	5	4126	-	0,6,6	0.00	-	-		
86	OHX	5	3995	-	0,6,6	0.00	-	-		
86	OHX	5	3899	-	0,6,6	0.00	-	-		
86	OHX	5	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2069	-	0,6,6	0.00	-	-		
86	OHX	6	2074	-	0,6,6	0.00	-	-		
86	OHX	5	4129	-	0,6,6	0.00	-	-		
86	OHX	1	4011	-	0,6,6	0.00	-	-		
86	OHX	1	3978	-	0,6,6	0.00	-	-		
86	OHX	5	4202	-	0,6,6	0.00	-	-		
86	OHX	6	2156	-	0,6,6	0.00	-	-		
86	OHX	6	2159	-	0,6,6	0.00	-	-		
86	OHX	2	2081	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4086	-	0,6,6	0.00	-	-		
86	OHX	1	4013	-	0,6,6	0.00	-	-		
86	OHX	2	2035	-	0,6,6	0.00	-	-		
86	OHX	5	4226	-	0,6,6	0.00	-	-		
86	OHX	s8	303	-	0,6,6	0.00	-	-		
86	OHX	1	4127	-	0,6,6	0.00	-	-		
86	OHX	5	4108	-	0,6,6	0.00	-	-		
86	OHX	1	3943	-	0,6,6	0.00	-	-		
86	OHX	5	4114	-	0,6,6	0.00	-	-		
86	OHX	5	4167	-	0,6,6	0.00	-	-		
86	OHX	1	3908	-	0,6,6	0.00	-	-		
86	OHX	6	2151	-	0,6,6	0.00	-	-		
86	OHX	6	2175	-	0,6,6	0.00	-	-		
86	OHX	5	3981	-	0,6,6	0.00	-	-		
86	OHX	5	4095	-	0,6,6	0.00	-	-		
86	OHX	5	4180	-	0,6,6	0.00	-	-		
86	OHX	2	2072	-	0,6,6	0.00	-	-		
86	OHX	5	3975	-	0,6,6	0.00	-	-		
86	OHX	1	4100	-	0,6,6	0.00	-	-		
86	OHX	5	3920	-	0,6,6	0.00	-	-		
86	OHX	1	3927	-	0,6,6	0.00	-	-		
86	OHX	5	4231	-	0,6,6	0.00	-	-		
86	OHX	1	3934	-	0,6,6	0.00	-	-		
86	OHX	5	3986	-	0,6,6	0.00	-	-		
86	OHX	6	2096	-	0,6,6	0.00	-	-		
86	OHX	5	4156	-	0,6,6	0.00	-	-		
86	OHX	6	2066	-	0,6,6	0.00	-	-		
86	OHX	8	228	-	0,6,6	0.00	-	-		
86	OHX	1	4007	-	0,6,6	0.00	-	-		
86	OHX	1	4149	-	0,6,6	0.00	-	-		
86	OHX	2	2048	-	0,6,6	0.00	-	-		
86	OHX	5	4240	-	0,6,6	0.00	-	-		
86	OHX	5	4233	-	0,6,6	0.00	-	-		
86	OHX	5	4232	-	0,6,6	0.00	-	-		
86	OHX	5	4172	-	0,6,6	0.00	-	-		
86	OHX	5	4168	-	0,6,6	0.00	-	-		
86	OHX	5	3994	-	0,6,6	0.00	-	-		
86	OHX	5	3923	-	0,6,6	0.00	-	-		
86	OHX	2	2070	-	0,6,6	0.00	-	-		
86	OHX	5	3944	-	0,6,6	0.00	-	-		
86	OHX	2	2137	-	0,6,6	0.00	-	-		
86	OHX	5	4085	-	0,6,6	0.00	-	-		
86	OHX	5	4072	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4097	-	0,6,6	0.00	-	-		
86	OHX	1	4175	-	0,6,6	0.00	-	-		
86	OHX	6	2166	-	0,6,6	0.00	-	-		
86	OHX	6	2168	-	0,6,6	0.00	-	-		
86	OHX	1	4061	-	0,6,6	0.00	-	-		
86	OHX	1	4186	-	0,6,6	0.00	-	-		
86	OHX	5	4198	-	0,6,6	0.00	-	-		
86	OHX	2	2064	-	0,6,6	0.00	-	-		
86	OHX	2	2061	-	0,6,6	0.00	-	-		
86	OHX	6	2085	-	0,6,6	0.00	-	-		
86	OHX	5	4217	-	0,6,6	0.00	-	-		
86	OHX	2	2055	-	0,6,6	0.00	-	-		
86	OHX	6	2101	-	0,6,6	0.00	-	-		
86	OHX	1	4025	-	0,6,6	0.00	-	-		
86	OHX	1	4196	-	0,6,6	0.00	-	-		
86	OHX	6	2134	-	0,6,6	0.00	-	-		
86	OHX	5	3999	-	0,6,6	0.00	-	-		
86	OHX	2	2024	-	0,6,6	0.00	-	-		
86	OHX	6	2116	-	0,6,6	0.00	-	-		
86	OHX	1	4213	-	0,6,6	0.00	-	-		
86	OHX	6	2064	-	0,6,6	0.00	-	-		
86	OHX	6	2051	-	0,6,6	0.00	-	-		
86	OHX	4	238	-	0,6,6	0.00	-	-		
86	OHX	6	2076	-	0,6,6	0.00	-	-		
86	OHX	1	3967	-	0,6,6	0.00	-	-		
86	OHX	L4	403	-	0,6,6	0.00	-	-		
86	OHX	5	3949	-	0,6,6	0.00	-	-		
86	OHX	2	2066	-	0,6,6	0.00	-	-		
86	OHX	5	4021	-	0,6,6	0.00	-	-		
86	OHX	5	4243	-	0,6,6	0.00	-	-		
86	OHX	1	3949	-	0,6,6	0.00	-	-		
86	OHX	2	2057	-	0,6,6	0.00	-	-		
86	OHX	5	4020	-	0,6,6	0.00	-	-		
86	OHX	5	4142	-	0,6,6	0.00	-	-		
86	OHX	5	4219	-	0,6,6	0.00	-	-		
86	OHX	2	2171	-	0,6,6	0.00	-	-		
86	OHX	1	4015	-	0,6,6	0.00	-	-		
86	OHX	6	2192	-	0,6,6	0.00	-	-		
86	OHX	1	4046	-	0,6,6	0.00	-	-		
86	OHX	3	214	-	0,6,6	0.00	-	-		
86	OHX	2	2043	-	0,6,6	0.00	-	-		
86	OHX	4	226	-	0,6,6	0.00	-	-		
86	OHX	1	3986	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3957	-	0,6,6	0.00	-	-		
86	OHX	1	4120	-	0,6,6	0.00	-	-		
86	OHX	5	4170	-	0,6,6	0.00	-	-		
86	OHX	1	3879	-	0,6,6	0.00	-	-		
86	OHX	2	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4086	-	0,6,6	0.00	-	-		
86	OHX	1	3907	-	0,6,6	0.00	-	-		
86	OHX	5	4068	-	0,6,6	0.00	-	-		
86	OHX	1	3910	-	0,6,6	0.00	-	-		
86	OHX	1	3980	-	0,6,6	0.00	-	-		
86	OHX	6	2109	-	0,6,6	0.00	-	-		
86	OHX	1	3959	-	0,6,6	0.00	-	-		
86	OHX	C8	201	-	0,6,6	0.00	-	-		
86	OHX	4	230	-	0,6,6	0.00	-	-		
86	OHX	6	2061	-	0,6,6	0.00	-	-		
86	OHX	5	4018	-	0,6,6	0.00	-	-		
86	OHX	1	4206	-	0,6,6	0.00	-	-		
86	OHX	q1	102	-	0,6,6	0.00	-	-		
86	OHX	5	4196	-	0,6,6	0.00	-	-		
86	OHX	2	2040	-	0,6,6	0.00	-	-		
86	OHX	2	2131	-	0,6,6	0.00	-	-		
86	OHX	1	4195	-	0,6,6	0.00	-	-		
86	OHX	2	2166	-	0,6,6	0.00	-	-		
86	OHX	1	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4103	-	0,6,6	0.00	-	-		
86	OHX	5	4076	-	0,6,6	0.00	-	-		
86	OHX	6	2079	-	0,6,6	0.00	-	-		
86	OHX	1	4023	-	0,6,6	0.00	-	-		
86	OHX	1	3951	-	0,6,6	0.00	-	-		
86	OHX	5	3993	-	0,6,6	0.00	-	-		
86	OHX	1	4125	-	0,6,6	0.00	-	-		
86	OHX	1	3882	-	0,6,6	0.00	-	-		
86	OHX	5	4070	-	0,6,6	0.00	-	-		
86	OHX	1	3888	-	0,6,6	0.00	-	-		
86	OHX	1	4176	-	0,6,6	0.00	-	-		
86	OHX	6	2048	-	0,6,6	0.00	-	-		
86	OHX	2	2132	-	0,6,6	0.00	-	-		
86	OHX	1	3975	-	0,6,6	0.00	-	-		
86	OHX	5	4139	-	0,6,6	0.00	-	-		
86	OHX	5	3976	-	0,6,6	0.00	-	-		
86	OHX	1	3935	-	0,6,6	0.00	-	-		
86	OHX	6	2152	-	0,6,6	0.00	-	-		
86	OHX	6	2157	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	n9	101	-	0,6,6	0.00	-	-		
86	OHX	7	222	-	0,6,6	0.00	-	-		
86	OHX	5	4087	-	0,6,6	0.00	-	-		
86	OHX	1	4037	-	0,6,6	0.00	-	-		
86	OHX	5	3950	-	0,6,6	0.00	-	-		
86	OHX	1	3881	-	0,6,6	0.00	-	-		
86	OHX	5	4190	-	0,6,6	0.00	-	-		
86	OHX	2	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4207	-	0,6,6	0.00	-	-		
86	OHX	5	4047	-	0,6,6	0.00	-	-		
86	OHX	6	2130	-	0,6,6	0.00	-	-		
86	OHX	1	4169	-	0,6,6	0.00	-	-		
86	OHX	2	2163	-	0,6,6	0.00	-	-		
86	OHX	1	4215	-	0,6,6	0.00	-	-		
86	OHX	2	2108	-	0,6,6	0.00	-	-		
86	OHX	1	3894	-	0,6,6	0.00	-	-		
86	OHX	2	2153	-	0,6,6	0.00	-	-		
86	OHX	5	4225	-	0,6,6	0.00	-	-		
86	OHX	1	3973	-	0,6,6	0.00	-	-		
86	OHX	2	2179	-	0,6,6	0.00	-	-		
86	OHX	1	4009	-	0,6,6	0.00	-	-		
86	OHX	6	2172	-	0,6,6	0.00	-	-		
86	OHX	6	2113	-	0,6,6	0.00	-	-		
86	OHX	1	4177	-	0,6,6	0.00	-	-		
86	OHX	2	2104	-	0,6,6	0.00	-	-		
86	OHX	5	3984	-	0,6,6	0.00	-	-		
86	OHX	5	3924	-	0,6,6	0.00	-	-		
86	OHX	5	4223	-	0,6,6	0.00	-	-		
86	OHX	1	4064	-	0,6,6	0.00	-	-		
86	OHX	1	3962	-	0,6,6	0.00	-	-		
86	OHX	5	4063	-	0,6,6	0.00	-	-		
86	OHX	3	221	-	0,6,6	0.00	-	-		
86	OHX	6	2087	-	0,6,6	0.00	-	-		
86	OHX	1	4146	-	0,6,6	0.00	-	-		
86	OHX	6	2104	-	0,6,6	0.00	-	-		
86	OHX	5	4052	-	0,6,6	0.00	-	-		
86	OHX	5	3898	-	0,6,6	0.00	-	-		
86	OHX	6	2190	-	0,6,6	0.00	-	-		
86	OHX	5	4189	-	0,6,6	0.00	-	-		
86	OHX	2	2045	-	0,6,6	0.00	-	-		
86	OHX	2	2044	-	0,6,6	0.00	-	-		
86	OHX	6	2119	-	0,6,6	0.00	-	-		
86	OHX	5	4177	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	m5	305	-	0,6,6	0.00	-	-		
86	OHX	4	231	-	0,6,6	0.00	-	-		
86	OHX	6	2164	-	0,6,6	0.00	-	-		
86	OHX	o2	201	-	0,6,6	0.00	-	-		
86	OHX	6	2054	-	0,6,6	0.00	-	-		
86	OHX	5	4036	-	0,6,6	0.00	-	-		
86	OHX	5	4193	-	0,6,6	0.00	-	-		
86	OHX	1	3982	-	0,6,6	0.00	-	-		
86	OHX	5	4239	-	0,6,6	0.00	-	-		
86	OHX	5	4211	-	0,6,6	0.00	-	-		
86	OHX	1	4191	-	0,6,6	0.00	-	-		
86	OHX	1	3939	-	0,6,6	0.00	-	-		
86	OHX	1	4143	-	0,6,6	0.00	-	-		
86	OHX	5	3958	-	0,6,6	0.00	-	-		
86	OHX	6	2203	-	0,6,6	0.00	-	-		
86	OHX	5	3952	-	0,6,6	0.00	-	-		
86	OHX	1	3987	-	0,6,6	0.00	-	-		
86	OHX	6	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4117	-	0,6,6	0.00	-	-		
86	OHX	2	2065	-	0,6,6	0.00	-	-		
86	OHX	1	3912	-	0,6,6	0.00	-	-		
86	OHX	5	3912	-	0,6,6	0.00	-	-		
86	OHX	1	4102	-	0,6,6	0.00	-	-		
86	OHX	1	4183	-	0,6,6	0.00	-	-		
86	OHX	5	3972	-	0,6,6	0.00	-	-		
86	OHX	1	4185	-	0,6,6	0.00	-	-		
86	OHX	3	219	-	0,6,6	0.00	-	-		
86	OHX	1	4010	-	0,6,6	0.00	-	-		
86	OHX	1	4018	-	0,6,6	0.00	-	-		
86	OHX	1	3905	-	0,6,6	0.00	-	-		
86	OHX	1	4053	-	0,6,6	0.00	-	-		
86	OHX	1	3958	-	0,6,6	0.00	-	-		
86	OHX	2	2135	-	0,6,6	0.00	-	-		
86	OHX	1	3933	-	0,6,6	0.00	-	-		
86	OHX	5	4144	-	0,6,6	0.00	-	-		
86	OHX	6	2204	-	0,6,6	0.00	-	-		
86	OHX	5	4112	-	0,6,6	0.00	-	-		
86	OHX	2	2080	-	0,6,6	0.00	-	-		
86	OHX	2	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4189	-	0,6,6	0.00	-	-		
86	OHX	5	4106	-	0,6,6	0.00	-	-		
86	OHX	7	221	-	0,6,6	0.00	-	-		
86	OHX	5	3945	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4200	-	0,6,6	0.00	-	-		
86	OHX	6	2089	-	0,6,6	0.00	-	-		
86	OHX	1	4182	-	0,6,6	0.00	-	-		
86	OHX	1	4044	-	0,6,6	0.00	-	-		
86	OHX	S8	302	-	0,6,6	0.00	-	-		
86	OHX	1	3960	-	0,6,6	0.00	-	-		
86	OHX	5	4120	-	0,6,6	0.00	-	-		
86	OHX	1	4049	-	0,6,6	0.00	-	-		
86	OHX	5	3967	-	0,6,6	0.00	-	-		
86	OHX	5	4143	-	0,6,6	0.00	-	-		
86	OHX	6	2182	-	0,6,6	0.00	-	-		
86	OHX	5	4218	-	0,6,6	0.00	-	-		
86	OHX	6	2097	-	0,6,6	0.00	-	-		
86	OHX	6	2199	-	0,6,6	0.00	-	-		
86	OHX	1	3969	-	0,6,6	0.00	-	-		
86	OHX	5	4116	-	0,6,6	0.00	-	-		
86	OHX	6	2112	-	0,6,6	0.00	-	-		
86	OHX	5	4088	-	0,6,6	0.00	-	-		
86	OHX	1	4197	-	0,6,6	0.00	-	-		
86	OHX	1	4158	-	0,6,6	0.00	-	-		
86	OHX	5	4013	-	0,6,6	0.00	-	-		
86	OHX	5	3985	-	0,6,6	0.00	-	-		
86	OHX	1	4134	-	0,6,6	0.00	-	-		
86	OHX	6	2091	-	0,6,6	0.00	-	-		
86	OHX	2	2159	-	0,6,6	0.00	-	-		
86	OHX	5	3929	-	0,6,6	0.00	-	-		
86	OHX	1	3930	-	0,6,6	0.00	-	-		
86	OHX	C3	201	-	0,6,6	0.00	-	-		
86	OHX	2	2083	-	0,6,6	0.00	-	-		
86	OHX	SR	401	-	0,6,6	0.00	-	-		
86	OHX	6	2171	-	0,6,6	0.00	-	-		
86	OHX	6	2145	-	0,6,6	0.00	-	-		
86	OHX	1	4091	-	0,6,6	0.00	-	-		
86	OHX	5	4011	-	0,6,6	0.00	-	-		
86	OHX	2	2116	-	0,6,6	0.00	-	-		
86	OHX	8	224	-	0,6,6	0.00	-	-		
86	OHX	2	2099	-	0,6,6	0.00	-	-		
86	OHX	5	3930	-	0,6,6	0.00	-	-		
86	OHX	1	3968	-	0,6,6	0.00	-	-		
88	3K5	5	4249	-	62,63,63	0.62	1 (1%)	82,95,95	1.38	11 (13%)
86	OHX	2	2140	-	0,6,6	0.00	-	-		
86	OHX	5	4038	-	0,6,6	0.00	-	-		
86	OHX	5	3939	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4096	-	0,6,6	0.00	-	-		
86	OHX	5	4133	-	0,6,6	0.00	-	-		
86	OHX	1	3909	-	0,6,6	0.00	-	-		
86	OHX	1	4104	-	0,6,6	0.00	-	-		
86	OHX	1	4099	-	0,6,6	0.00	-	-		
86	OHX	6	2099	-	0,6,6	0.00	-	-		
86	OHX	2	2151	-	0,6,6	0.00	-	-		
86	OHX	5	3997	-	0,6,6	0.00	-	-		
86	OHX	5	3934	-	0,6,6	0.00	-	-		
86	OHX	1	4116	-	0,6,6	0.00	-	-		
86	OHX	1	4030	-	0,6,6	0.00	-	-		
86	OHX	2	2160	-	0,6,6	0.00	-	-		
86	OHX	1	3895	-	0,6,6	0.00	-	-		
86	OHX	2	2050	-	0,6,6	0.00	-	-		
86	OHX	1	4209	-	0,6,6	0.00	-	-		
86	OHX	1	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4028	-	0,6,6	0.00	-	-		
86	OHX	1	4106	-	0,6,6	0.00	-	-		
86	OHX	1	3944	-	0,6,6	0.00	-	-		
86	OHX	1	4192	-	0,6,6	0.00	-	-		
86	OHX	1	4076	-	0,6,6	0.00	-	-		
86	OHX	5	4165	-	0,6,6	0.00	-	-		
86	OHX	5	4098	-	0,6,6	0.00	-	-		
86	OHX	5	4212	-	0,6,6	0.00	-	-		
86	OHX	6	2069	-	0,6,6	0.00	-	-		
86	OHX	5	4121	-	0,6,6	0.00	-	-		
86	OHX	6	2132	-	0,6,6	0.00	-	-		
86	OHX	6	2162	-	0,6,6	0.00	-	-		
86	OHX	2	2028	-	0,6,6	0.00	-	-		
86	OHX	4	236	-	0,6,6	0.00	-	-		
86	OHX	1	3897	-	0,6,6	0.00	-	-		
86	OHX	5	3926	-	0,6,6	0.00	-	-		
86	OHX	5	3980	-	0,6,6	0.00	-	-		
86	OHX	5	3937	-	0,6,6	0.00	-	-		
86	OHX	2	2133	-	0,6,6	0.00	-	-		
86	OHX	O3	202	-	0,6,6	0.00	-	-		
86	OHX	1	4032	-	0,6,6	0.00	-	-		
86	OHX	5	4135	-	0,6,6	0.00	-	-		
86	OHX	1	4068	-	0,6,6	0.00	-	-		
86	OHX	1	3874	-	0,6,6	0.00	-	-		
86	OHX	5	4186	-	0,6,6	0.00	-	-		
86	OHX	1	3917	-	0,6,6	0.00	-	-		
86	OHX	5	4157	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3915	-	0,6,6	0.00	-	-		
86	OHX	2	2150	-	0,6,6	0.00	-	-		
86	OHX	2	2038	-	0,6,6	0.00	-	-		
86	OHX	1	3963	-	0,6,6	0.00	-	-		
86	OHX	1	4002	-	0,6,6	0.00	-	-		
86	OHX	2	2090	-	0,6,6	0.00	-	-		
86	OHX	5	4237	-	0,6,6	0.00	-	-		
86	OHX	1	3875	-	0,6,6	0.00	-	-		
86	OHX	5	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2173	-	0,6,6	0.00	-	-		
86	OHX	1	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4148	-	0,6,6	0.00	-	-		
86	OHX	1	3965	-	0,6,6	0.00	-	-		
86	OHX	1	4123	-	0,6,6	0.00	-	-		
86	OHX	2	2145	-	0,6,6	0.00	-	-		
86	OHX	1	4045	-	0,6,6	0.00	-	-		
86	OHX	2	2063	-	0,6,6	0.00	-	-		
86	OHX	1	3884	-	0,6,6	0.00	-	-		
86	OHX	5	4208	-	0,6,6	0.00	-	-		
86	OHX	6	2068	-	0,6,6	0.00	-	-		
86	OHX	5	4174	-	0,6,6	0.00	-	-		
86	OHX	5	4073	-	0,6,6	0.00	-	-		
86	OHX	2	2073	-	0,6,6	0.00	-	-		
86	OHX	5	4183	-	0,6,6	0.00	-	-		
86	OHX	1	4155	-	0,6,6	0.00	-	-		
86	OHX	5	3979	-	0,6,6	0.00	-	-		
86	OHX	1	4150	-	0,6,6	0.00	-	-		
86	OHX	D3	202	-	0,6,6	0.00	-	-		
86	OHX	5	4056	-	0,6,6	0.00	-	-		
86	OHX	5	4222	-	0,6,6	0.00	-	-		
86	OHX	5	4140	-	0,6,6	0.00	-	-		
86	OHX	1	4024	-	0,6,6	0.00	-	-		
86	OHX	5	4191	-	0,6,6	0.00	-	-		
86	OHX	1	4193	-	0,6,6	0.00	-	-		
86	OHX	5	4019	-	0,6,6	0.00	-	-		
86	OHX	2	2169	-	0,6,6	0.00	-	-		
86	OHX	5	4093	-	0,6,6	0.00	-	-		
86	OHX	5	4155	-	0,6,6	0.00	-	-		
86	OHX	4	239	-	0,6,6	0.00	-	-		
86	OHX	5	4077	-	0,6,6	0.00	-	-		
86	OHX	5	4224	-	0,6,6	0.00	-	-		
86	OHX	6	2170	-	0,6,6	0.00	-	-		
86	OHX	1	4159	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4085	-	0,6,6	0.00	-	-		
86	OHX	6	2072	-	0,6,6	0.00	-	-		
86	OHX	1	4157	-	0,6,6	0.00	-	-		
86	OHX	5	4163	-	0,6,6	0.00	-	-		
86	OHX	1	3892	-	0,6,6	0.00	-	-		
86	OHX	1	4075	-	0,6,6	0.00	-	-		
86	OHX	1	4001	-	0,6,6	0.00	-	-		
86	OHX	1	4141	-	0,6,6	0.00	-	-		
86	OHX	1	3929	-	0,6,6	0.00	-	-		
86	OHX	5	4084	-	0,6,6	0.00	-	-		
86	OHX	5	3927	-	0,6,6	0.00	-	-		
86	OHX	2	2091	-	0,6,6	0.00	-	-		
86	OHX	5	4062	-	0,6,6	0.00	-	-		
86	OHX	6	2177	-	0,6,6	0.00	-	-		
86	OHX	5	4094	-	0,6,6	0.00	-	-		
86	OHX	6	2198	-	0,6,6	0.00	-	-		
86	OHX	6	2122	-	0,6,6	0.00	-	-		
86	OHX	5	3941	-	0,6,6	0.00	-	-		
86	OHX	1	4129	-	0,6,6	0.00	-	-		
86	OHX	5	4205	-	0,6,6	0.00	-	-		
86	OHX	1	4101	-	0,6,6	0.00	-	-		
86	OHX	5	3906	-	0,6,6	0.00	-	-		
86	OHX	L3	405	-	0,6,6	0.00	-	-		
86	OHX	1	3988	-	0,6,6	0.00	-	-		
86	OHX	1	3901	-	0,6,6	0.00	-	-		
86	OHX	5	4127	-	0,6,6	0.00	-	-		
86	OHX	6	2141	-	0,6,6	0.00	-	-		
86	OHX	5	3965	-	0,6,6	0.00	-	-		
86	OHX	1	4219	-	0,6,6	0.00	-	-		
86	OHX	8	230	-	0,6,6	0.00	-	-		
86	OHX	6	2163	-	0,6,6	0.00	-	-		
86	OHX	1	3997	-	0,6,6	0.00	-	-		
86	OHX	1	4083	-	0,6,6	0.00	-	-		
86	OHX	1	3984	-	0,6,6	0.00	-	-		
86	OHX	1	4187	-	0,6,6	0.00	-	-		
86	OHX	1	4094	-	0,6,6	0.00	-	-		
86	OHX	6	2106	-	0,6,6	0.00	-	-		
86	OHX	5	4104	-	0,6,6	0.00	-	-		
86	OHX	O7	104	-	0,6,6	0.00	-	-		
86	OHX	5	3971	-	0,6,6	0.00	-	-		
86	OHX	m8	201	-	0,6,6	0.00	-	-		
86	OHX	5	4111	-	0,6,6	0.00	-	-		
86	OHX	5	3942	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4235	-	0,6,6	0.00	-	-		
86	OHX	5	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4110	-	0,6,6	0.00	-	-		
86	OHX	5	4058	-	0,6,6	0.00	-	-		
86	OHX	1	4174	-	0,6,6	0.00	-	-		
86	OHX	5	4210	-	0,6,6	0.00	-	-		
86	OHX	5	4024	-	0,6,6	0.00	-	-		
86	OHX	6	2100	-	0,6,6	0.00	-	-		
86	OHX	15	306	-	0,6,6	0.00	-	-		
86	OHX	1	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4047	-	0,6,6	0.00	-	-		
86	OHX	1	4108	-	0,6,6	0.00	-	-		
86	OHX	m0	302	-	0,6,6	0.00	-	-		
86	OHX	1	4211	-	0,6,6	0.00	-	-		
86	OHX	2	2121	-	0,6,6	0.00	-	-		
86	OHX	5	3988	-	0,6,6	0.00	-	-		
86	OHX	5	3963	-	0,6,6	0.00	-	-		
86	OHX	O7	105	-	0,6,6	0.00	-	-		
86	OHX	5	4134	-	0,6,6	0.00	-	-		
86	OHX	5	3978	-	0,6,6	0.00	-	-		
86	OHX	5	3977	-	0,6,6	0.00	-	-		
86	OHX	1	4133	-	0,6,6	0.00	-	-		
86	OHX	5	4149	-	0,6,6	0.00	-	-		
86	OHX	6	2128	-	0,6,6	0.00	-	-		
86	OHX	6	2183	-	0,6,6	0.00	-	-		
86	OHX	m0	301	-	0,6,6	0.00	-	-		
86	OHX	5	3955	-	0,6,6	0.00	-	-		
86	OHX	1	3955	-	0,6,6	0.00	-	-		
86	OHX	6	2110	-	0,6,6	0.00	-	-		
86	OHX	5	4122	-	0,6,6	0.00	-	-		
86	OHX	6	2185	-	0,6,6	0.00	-	-		
86	OHX	5	4046	-	0,6,6	0.00	-	-		
86	OHX	6	2046	-	0,6,6	0.00	-	-		
86	OHX	1	4171	-	0,6,6	0.00	-	-		
86	OHX	2	2027	-	0,6,6	0.00	-	-		
86	OHX	5	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4025	-	0,6,6	0.00	-	-		
86	OHX	6	2149	-	0,6,6	0.00	-	-		
86	OHX	2	2095	-	0,6,6	0.00	-	-		
86	OHX	5	3901	-	0,6,6	0.00	-	-		
86	OHX	15	305	-	0,6,6	0.00	-	-		
86	OHX	1	4070	-	0,6,6	0.00	-	-		
86	OHX	5	4125	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3886	-	0,6,6	0.00	-	-		
86	OHX	1	4168	-	0,6,6	0.00	-	-		
86	OHX	1	3887	-	0,6,6	0.00	-	-		
86	OHX	1	4140	-	0,6,6	0.00	-	-		
86	OHX	5	4029	-	0,6,6	0.00	-	-		
86	OHX	1	4027	-	0,6,6	0.00	-	-		
86	OHX	2	2076	-	0,6,6	0.00	-	-		
86	OHX	19	202	-	0,6,6	0.00	-	-		
86	OHX	6	2071	-	0,6,6	0.00	-	-		
86	OHX	5	3961	-	0,6,6	0.00	-	-		
86	OHX	5	4141	-	0,6,6	0.00	-	-		
86	OHX	6	2090	-	0,6,6	0.00	-	-		
86	OHX	1	4111	-	0,6,6	0.00	-	-		
86	OHX	2	2037	-	0,6,6	0.00	-	-		
86	OHX	5	4053	-	0,6,6	0.00	-	-		
86	OHX	1	4107	-	0,6,6	0.00	-	-		
86	OHX	5	3943	-	0,6,6	0.00	-	-		
86	OHX	1	4066	-	0,6,6	0.00	-	-		
86	OHX	6	2195	-	0,6,6	0.00	-	-		
86	OHX	c8	203	-	0,6,6	0.00	-	-		
86	OHX	1	4167	-	0,6,6	0.00	-	-		
86	OHX	2	2088	-	0,6,6	0.00	-	-		
86	OHX	5	4131	-	0,6,6	0.00	-	-		
86	OHX	5	3983	-	0,6,6	0.00	-	-		
86	OHX	6	2176	-	0,6,6	0.00	-	-		
86	OHX	5	4176	-	0,6,6	0.00	-	-		
86	OHX	5	4188	-	0,6,6	0.00	-	-		
86	OHX	6	2205	-	0,6,6	0.00	-	-		
86	OHX	2	2129	-	0,6,6	0.00	-	-		
86	OHX	5	4242	-	0,6,6	0.00	-	-		
86	OHX	5	3956	-	0,6,6	0.00	-	-		
86	OHX	7	225	-	0,6,6	0.00	-	-		
86	OHX	5	4037	-	0,6,6	0.00	-	-		
86	OHX	1	3936	-	0,6,6	0.00	-	-		
86	OHX	5	4138	-	0,6,6	0.00	-	-		
86	OHX	5	3970	-	0,6,6	0.00	-	-		
86	OHX	5	3925	-	0,6,6	0.00	-	-		
86	OHX	5	4150	-	0,6,6	0.00	-	-		
86	OHX	2	2032	-	0,6,6	0.00	-	-		
86	OHX	2	2107	-	0,6,6	0.00	-	-		
86	OHX	1	4089	-	0,6,6	0.00	-	-		
86	OHX	6	2181	-	0,6,6	0.00	-	-		
86	OHX	2	2102	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3962	-	0,6,6	0.00	-	-		
86	OHX	1	4154	-	0,6,6	0.00	-	-		
86	OHX	4	235	-	0,6,6	0.00	-	-		
86	OHX	1	4096	-	0,6,6	0.00	-	-		
86	OHX	8	229	-	0,6,6	0.00	-	-		
86	OHX	6	2174	-	0,6,6	0.00	-	-		
86	OHX	1	3904	-	0,6,6	0.00	-	-		
86	OHX	5	4162	-	0,6,6	0.00	-	-		
86	OHX	7	226	-	0,6,6	0.00	-	-		
86	OHX	5	4215	-	0,6,6	0.00	-	-		
86	OHX	7	223	-	0,6,6	0.00	-	-		
86	OHX	6	2107	-	0,6,6	0.00	-	-		
86	OHX	8	221	-	0,6,6	0.00	-	-		
86	OHX	1	3996	-	0,6,6	0.00	-	-		
86	OHX	c5	201	-	0,6,6	0.00	-	-		
86	OHX	1	3925	-	0,6,6	0.00	-	-		
86	OHX	1	4092	-	0,6,6	0.00	-	-		
86	OHX	1	3924	-	0,6,6	0.00	-	-		
86	OHX	8	232	-	0,6,6	0.00	-	-		
86	OHX	1	4112	-	0,6,6	0.00	-	-		
86	OHX	2	2105	-	0,6,6	0.00	-	-		
86	OHX	6	2124	-	0,6,6	0.00	-	-		
86	OHX	1	3899	-	0,6,6	0.00	-	-		
86	OHX	1	4130	-	0,6,6	0.00	-	-		
86	OHX	1	4122	-	0,6,6	0.00	-	-		
86	OHX	2	2054	-	0,6,6	0.00	-	-		
86	OHX	1	3976	-	0,6,6	0.00	-	-		
86	OHX	2	2175	-	0,6,6	0.00	-	-		
86	OHX	4	233	-	0,6,6	0.00	-	-		
86	OHX	2	2113	-	0,6,6	0.00	-	-		
86	OHX	1	4063	-	0,6,6	0.00	-	-		
86	OHX	6	2083	-	0,6,6	0.00	-	-		
86	OHX	1	3947	-	0,6,6	0.00	-	-		
86	OHX	5	4247	-	0,6,6	0.00	-	-		
86	OHX	1	3928	-	0,6,6	0.00	-	-		
86	OHX	2	2103	-	0,6,6	0.00	-	-		
86	OHX	m6	203	-	0,6,6	0.00	-	-		
86	OHX	1	4059	-	0,6,6	0.00	-	-		
86	OHX	5	4089	-	0,6,6	0.00	-	-		
86	OHX	1	4084	-	0,6,6	0.00	-	-		
88	3K5	1	4221	-	62,63,63	1.22	2 (3%)	82,95,95	1.47	11 (13%)
86	OHX	1	4042	-	0,6,6	0.00	-	-		
86	OHX	o7	503	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4115	-	0,6,6	0.00	-	-		
86	OHX	2	2096	-	0,6,6	0.00	-	-		
86	OHX	d4	201	-	0,6,6	0.00	-	-		
86	OHX	1	3940	-	0,6,6	0.00	-	-		
86	OHX	1	4071	-	0,6,6	0.00	-	-		
86	OHX	1	4003	-	0,6,6	0.00	-	-		
86	OHX	5	4173	-	0,6,6	0.00	-	-		
86	OHX	1	4142	-	0,6,6	0.00	-	-		
86	OHX	5	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4051	-	0,6,6	0.00	-	-		
86	OHX	1	4147	-	0,6,6	0.00	-	-		
86	OHX	1	4212	-	0,6,6	0.00	-	-		
86	OHX	5	4012	-	0,6,6	0.00	-	-		
86	OHX	6	2065	-	0,6,6	0.00	-	-		
86	OHX	5	4229	-	0,6,6	0.00	-	-		
86	OHX	1	4198	-	0,6,6	0.00	-	-		
86	OHX	1	4205	-	0,6,6	0.00	-	-		
86	OHX	2	2078	-	0,6,6	0.00	-	-		
86	OHX	1	4017	-	0,6,6	0.00	-	-		
86	OHX	2	2127	-	0,6,6	0.00	-	-		
86	OHX	1	4098	-	0,6,6	0.00	-	-		
86	OHX	2	2062	-	0,6,6	0.00	-	-		
86	OHX	2	2068	-	0,6,6	0.00	-	-		
86	OHX	3	222	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	6	2142	-	0,6,6	0.00	-	-		
86	OHX	1	4164	-	0,6,6	0.00	-	-		
86	OHX	5	4010	-	0,6,6	0.00	-	-		
86	OHX	8	227	-	0,6,6	0.00	-	-		
86	OHX	2	2046	-	0,6,6	0.00	-	-		
86	OHX	6	2084	-	0,6,6	0.00	-	-		
86	OHX	1	4172	-	0,6,6	0.00	-	-		
86	OHX	6	2137	-	0,6,6	0.00	-	-		
86	OHX	5	3907	-	0,6,6	0.00	-	-		
86	OHX	1	4207	-	0,6,6	0.00	-	-		
86	OHX	1	4208	-	0,6,6	0.00	-	-		
86	OHX	5	4067	-	0,6,6	0.00	-	-		
86	OHX	2	2143	-	0,6,6	0.00	-	-		
86	OHX	1	3974	-	0,6,6	0.00	-	-		
86	OHX	6	2056	-	0,6,6	0.00	-	-		
86	OHX	1	3979	-	0,6,6	0.00	-	-		
86	OHX	5	4158	-	0,6,6	0.00	-	-		
86	OHX	1	3903	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2056	-	0,6,6	0.00	-	-		
86	OHX	2	2093	-	0,6,6	0.00	-	-		
86	OHX	1	3906	-	0,6,6	0.00	-	-		
86	OHX	5	4241	-	0,6,6	0.00	-	-		
86	OHX	2	2067	-	0,6,6	0.00	-	-		
86	OHX	1	4035	-	0,6,6	0.00	-	-		
86	OHX	5	3982	-	0,6,6	0.00	-	-		
86	OHX	2	2059	-	0,6,6	0.00	-	-		
86	OHX	5	3914	-	0,6,6	0.00	-	-		
86	OHX	1	3991	-	0,6,6	0.00	-	-		
86	OHX	5	4102	-	0,6,6	0.00	-	-		
86	OHX	6	2193	-	0,6,6	0.00	-	-		
86	OHX	N1	201	-	0,6,6	0.00	-	-		
86	OHX	6	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4146	-	0,6,6	0.00	-	-		
86	OHX	s1	303	-	0,6,6	0.00	-	-		
86	OHX	1	4113	-	0,6,6	0.00	-	-		
86	OHX	2	2094	-	0,6,6	0.00	-	-		
86	OHX	5	3919	-	0,6,6	0.00	-	-		
86	OHX	5	3911	-	0,6,6	0.00	-	-		
86	OHX	1	4065	-	0,6,6	0.00	-	-		
86	OHX	2	2079	-	0,6,6	0.00	-	-		
86	OHX	2	2174	-	0,6,6	0.00	-	-		
86	OHX	5	4031	-	0,6,6	0.00	-	-		
86	OHX	2	2120	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	1	4181	-	0,6,6	0.00	-	-		
86	OHX	3	224	-	0,6,6	0.00	-	-		
86	OHX	5	3960	-	0,6,6	0.00	-	-		
86	OHX	1	4069	-	0,6,6	0.00	-	-		
86	OHX	1	4093	-	0,6,6	0.00	-	-		
86	OHX	1	3916	-	0,6,6	0.00	-	-		
86	OHX	2	2155	-	0,6,6	0.00	-	-		
86	OHX	1	3921	-	0,6,6	0.00	-	-		
86	OHX	2	2089	-	0,6,6	0.00	-	-		
86	OHX	2	2123	-	0,6,6	0.00	-	-		
86	OHX	5	4002	-	0,6,6	0.00	-	-		
86	OHX	5	4039	-	0,6,6	0.00	-	-		
86	OHX	5	4228	-	0,6,6	0.00	-	-		
86	OHX	6	2136	-	0,6,6	0.00	-	-		
86	OHX	1	4210	-	0,6,6	0.00	-	-		
86	OHX	2	2039	-	0,6,6	0.00	-	-		
86	OHX	5	4054	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4012	-	0,6,6	0.00	-	-		
86	OHX	4	225	-	0,6,6	0.00	-	-		
86	OHX	1	4178	-	0,6,6	0.00	-	-		
86	OHX	1	3964	-	0,6,6	0.00	-	-		
86	OHX	1	3873	-	0,6,6	0.00	-	-		
86	OHX	1	4152	-	0,6,6	0.00	-	-		
86	OHX	5	4159	-	0,6,6	0.00	-	-		
86	OHX	5	3959	-	0,6,6	0.00	-	-		
86	OHX	1	4202	-	0,6,6	0.00	-	-		
86	OHX	14	402	-	0,6,6	0.00	-	-		
86	OHX	2	2060	-	0,6,6	0.00	-	-		
86	OHX	2	2141	-	0,6,6	0.00	-	-		
86	OHX	5	4119	-	0,6,6	0.00	-	-		
86	OHX	2	2106	-	0,6,6	0.00	-	-		
86	OHX	5	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4026	-	0,6,6	0.00	-	-		
86	OHX	5	4028	-	0,6,6	0.00	-	-		
86	OHX	5	4145	-	0,6,6	0.00	-	-		
86	OHX	5	3996	-	0,6,6	0.00	-	-		
86	OHX	5	3954	-	0,6,6	0.00	-	-		
86	OHX	1	3948	-	0,6,6	0.00	-	-		
86	OHX	1	4110	-	0,6,6	0.00	-	-		
86	OHX	1	4072	-	0,6,6	0.00	-	-		
86	OHX	8	223	-	0,6,6	0.00	-	-		
86	OHX	4	234	-	0,6,6	0.00	-	-		
86	OHX	1	4077	-	0,6,6	0.00	-	-		
86	OHX	1	3914	-	0,6,6	0.00	-	-		
86	OHX	7	219	-	0,6,6	0.00	-	-		
86	OHX	5	4061	-	0,6,6	0.00	-	-		
86	OHX	s1	302	-	0,6,6	0.00	-	-		
86	OHX	6	2123	-	0,6,6	0.00	-	-		
86	OHX	5	4040	-	0,6,6	0.00	-	-		
86	OHX	5	3909	-	0,6,6	0.00	-	-		
86	OHX	6	2133	-	0,6,6	0.00	-	-		
86	OHX	5	4209	-	0,6,6	0.00	-	-		
86	OHX	2	2030	-	0,6,6	0.00	-	-		
86	OHX	5	4203	-	0,6,6	0.00	-	-		
86	OHX	5	3900	-	0,6,6	0.00	-	-		
86	OHX	5	4033	-	0,6,6	0.00	-	-		
86	OHX	5	4003	-	0,6,6	0.00	-	-		
86	OHX	6	2179	-	0,6,6	0.00	-	-		
86	OHX	1	4034	-	0,6,6	0.00	-	-		
86	OHX	5	3910	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4099	-	0,6,6	0.00	-	-		
86	OHX	1	4043	-	0,6,6	0.00	-	-		
86	OHX	1	4126	-	0,6,6	0.00	-	-		
86	OHX	5	3917	-	0,6,6	0.00	-	-		
86	OHX	sR	401	-	0,6,6	0.00	-	-		
86	OHX	1	3876	-	0,6,6	0.00	-	-		
86	OHX	5	4166	-	0,6,6	0.00	-	-		
86	OHX	5	3966	-	0,6,6	0.00	-	-		
86	OHX	6	2184	-	0,6,6	0.00	-	-		
86	OHX	5	4048	-	0,6,6	0.00	-	-		
86	OHX	5	4016	-	0,6,6	0.00	-	-		
86	OHX	6	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4114	-	0,6,6	0.00	-	-		
86	OHX	6	2194	-	0,6,6	0.00	-	-		
86	OHX	1	3878	-	0,6,6	0.00	-	-		
86	OHX	5	4171	-	0,6,6	0.00	-	-		
86	OHX	5	3973	-	0,6,6	0.00	-	-		
86	OHX	5	4182	-	0,6,6	0.00	-	-		
86	OHX	1	4163	-	0,6,6	0.00	-	-		
86	OHX	2	2125	-	0,6,6	0.00	-	-		
86	OHX	2	2173	-	0,6,6	0.00	-	-		
86	OHX	6	2158	-	0,6,6	0.00	-	-		
86	OHX	1	3985	-	0,6,6	0.00	-	-		
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	1	3893	-	0,6,6	0.00	-	-		
86	OHX	5	4051	-	0,6,6	0.00	-	-		
86	OHX	1	3971	-	0,6,6	0.00	-	-		
86	OHX	1	3911	-	0,6,6	0.00	-	-		
86	OHX	6	2178	-	0,6,6	0.00	-	-		
86	OHX	1	4162	-	0,6,6	0.00	-	-		
86	OHX	6	2180	-	0,6,6	0.00	-	-		
86	OHX	1	3885	-	0,6,6	0.00	-	-		
86	OHX	1	3999	-	0,6,6	0.00	-	-		
86	OHX	1	3877	-	0,6,6	0.00	-	-		
86	OHX	5	4057	-	0,6,6	0.00	-	-		
86	OHX	5	4059	-	0,6,6	0.00	-	-		
86	OHX	2	2110	-	0,6,6	0.00	-	-		
86	OHX	8	226	-	0,6,6	0.00	-	-		
86	OHX	6	2191	-	0,6,6	0.00	-	-		
86	OHX	2	2161	-	0,6,6	0.00	-	-		
86	OHX	1	4097	-	0,6,6	0.00	-	-		
86	OHX	5	4227	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4248	-	0,6,6	0.00	-	-		
86	OHX	2	2097	-	0,6,6	0.00	-	-		
86	OHX	1	4021	-	0,6,6	0.00	-	-		
86	OHX	2	2092	-	0,6,6	0.00	-	-		
86	OHX	5	3932	-	0,6,6	0.00	-	-		
86	OHX	1	3922	-	0,6,6	0.00	-	-		
86	OHX	5	4148	-	0,6,6	0.00	-	-		
86	OHX	5	4060	-	0,6,6	0.00	-	-		
86	OHX	1	4058	-	0,6,6	0.00	-	-		
86	OHX	2	2162	-	0,6,6	0.00	-	-		
86	OHX	6	2186	-	0,6,6	0.00	-	-		
86	OHX	6	2161	-	0,6,6	0.00	-	-		
86	OHX	5	4206	-	0,6,6	0.00	-	-		
86	OHX	2	2053	-	0,6,6	0.00	-	-		
86	OHX	1	4190	-	0,6,6	0.00	-	-		
86	OHX	1	3945	-	0,6,6	0.00	-	-		
86	OHX	5	4042	-	0,6,6	0.00	-	-		
86	OHX	6	2111	-	0,6,6	0.00	-	-		
86	OHX	5	3916	-	0,6,6	0.00	-	-		
86	OHX	1	3880	-	0,6,6	0.00	-	-		
86	OHX	5	4192	-	0,6,6	0.00	-	-		
86	OHX	1	3998	-	0,6,6	0.00	-	-		
86	OHX	5	4246	-	0,6,6	0.00	-	-		
86	OHX	1	3992	-	0,6,6	0.00	-	-		
86	OHX	8	222	-	0,6,6	0.00	-	-		
86	OHX	5	4007	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	1	3942	-	0,6,6	0.00	-	-		
86	OHX	2	2168	-	0,6,6	0.00	-	-		
86	OHX	6	2093	-	0,6,6	0.00	-	-		
86	OHX	2	2031	-	0,6,6	0.00	-	-		
86	OHX	2	2136	-	0,6,6	0.00	-	-		
86	OHX	6	2138	-	0,6,6	0.00	-	-		
86	OHX	2	2047	-	0,6,6	0.00	-	-		
86	OHX	5	4179	-	0,6,6	0.00	-	-		
86	OHX	l3	404	-	0,6,6	0.00	-	-		
86	OHX	m5	304	-	0,6,6	0.00	-	-		
86	OHX	n3	203	-	0,6,6	0.00	-	-		
86	OHX	1	4124	-	0,6,6	0.00	-	-		
86	OHX	2	2074	-	0,6,6	0.00	-	-		
86	OHX	5	4030	-	0,6,6	0.00	-	-		
86	OHX	5	3946	-	0,6,6	0.00	-	-		
86	OHX	5	4065	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	O1	201	-	0,6,6	0.00	-	-		
86	OHX	d9	102	-	0,6,6	0.00	-	-		
86	OHX	3	220	-	0,6,6	0.00	-	-		
86	OHX	1	4067	-	0,6,6	0.00	-	-		
86	OHX	m1	202	-	0,6,6	0.00	-	-		
86	OHX	1	4000	-	0,6,6	0.00	-	-		
86	OHX	2	2109	-	0,6,6	0.00	-	-		
86	OHX	5	4115	-	0,6,6	0.00	-	-		
86	OHX	1	4166	-	0,6,6	0.00	-	-		
86	OHX	2	2128	-	0,6,6	0.00	-	-		
86	OHX	5	4137	-	0,6,6	0.00	-	-		
86	OHX	2	2100	-	0,6,6	0.00	-	-		
86	OHX	1	4139	-	0,6,6	0.00	-	-		
86	OHX	1	3977	-	0,6,6	0.00	-	-		
86	OHX	1	4121	-	0,6,6	0.00	-	-		
86	OHX	1	3937	-	0,6,6	0.00	-	-		
86	OHX	c3	201	-	0,6,6	0.00	-	-		
86	OHX	1	3989	-	0,6,6	0.00	-	-		
86	OHX	1	4050	-	0,6,6	0.00	-	-		
86	OHX	5	4049	-	0,6,6	0.00	-	-		
86	OHX	2	2022	-	0,6,6	0.00	-	-		
86	OHX	6	2070	-	0,6,6	0.00	-	-		
86	OHX	2	2149	-	0,6,6	0.00	-	-		
86	OHX	14	403	-	0,6,6	0.00	-	-		
86	OHX	5	4101	-	0,6,6	0.00	-	-		
86	OHX	6	2062	-	0,6,6	0.00	-	-		
86	OHX	5	4105	-	0,6,6	0.00	-	-		
86	OHX	6	2140	-	0,6,6	0.00	-	-		
86	OHX	6	2050	-	0,6,6	0.00	-	-		
86	OHX	3	216	-	0,6,6	0.00	-	-		
86	OHX	1	4080	-	0,6,6	0.00	-	-		
86	OHX	1	4137	-	0,6,6	0.00	-	-		
86	OHX	2	2130	-	0,6,6	0.00	-	-		
86	OHX	5	4027	-	0,6,6	0.00	-	-		
86	OHX	1	4132	-	0,6,6	0.00	-	-		
86	OHX	5	4050	-	0,6,6	0.00	-	-		
86	OHX	2	2156	-	0,6,6	0.00	-	-		
86	OHX	3	223	-	0,6,6	0.00	-	-		
86	OHX	5	4109	-	0,6,6	0.00	-	-		
86	OHX	1	3920	-	0,6,6	0.00	-	-		
86	OHX	1	4119	-	0,6,6	0.00	-	-		
86	OHX	1	4052	-	0,6,6	0.00	-	-		
86	OHX	5	3931	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2075	-	0,6,6	0.00	-	-		
86	OHX	1	4199	-	0,6,6	0.00	-	-		
86	OHX	5	4107	-	0,6,6	0.00	-	-		
86	OHX	2	2082	-	0,6,6	0.00	-	-		
86	OHX	2	2178	-	0,6,6	0.00	-	-		
86	OHX	5	3964	-	0,6,6	0.00	-	-		
86	OHX	6	2118	-	0,6,6	0.00	-	-		
86	OHX	1	3926	-	0,6,6	0.00	-	-		
86	OHX	6	2092	-	0,6,6	0.00	-	-		
86	OHX	1	4054	-	0,6,6	0.00	-	-		
86	OHX	1	4039	-	0,6,6	0.00	-	-		
86	OHX	6	2127	-	0,6,6	0.00	-	-		
86	OHX	5	4194	-	0,6,6	0.00	-	-		
86	OHX	1	4160	-	0,6,6	0.00	-	-		
86	OHX	2	2152	-	0,6,6	0.00	-	-		
86	OHX	1	4165	-	0,6,6	0.00	-	-		
86	OHX	1	4026	-	0,6,6	0.00	-	-		
86	OHX	5	3974	-	0,6,6	0.00	-	-		
86	OHX	2	2115	-	0,6,6	0.00	-	-		
86	OHX	1	4088	-	0,6,6	0.00	-	-		
86	OHX	6	2120	-	0,6,6	0.00	-	-		
86	OHX	1	4036	-	0,6,6	0.00	-	-		
86	OHX	1	3931	-	0,6,6	0.00	-	-		
86	OHX	2	2154	-	0,6,6	0.00	-	-		
86	OHX	5	3908	-	0,6,6	0.00	-	-		
86	OHX	5	4082	-	0,6,6	0.00	-	-		
86	OHX	2	2033	-	0,6,6	0.00	-	-		
86	OHX	2	2117	-	0,6,6	0.00	-	-		
86	OHX	2	2036	-	0,6,6	0.00	-	-		
86	OHX	5	4043	-	0,6,6	0.00	-	-		
86	OHX	5	4022	-	0,6,6	0.00	-	-		
86	OHX	5	4147	-	0,6,6	0.00	-	-		
86	OHX	1	4040	-	0,6,6	0.00	-	-		
86	OHX	5	4154	-	0,6,6	0.00	-	-		
86	OHX	5	3969	-	0,6,6	0.00	-	-		
86	OHX	5	4023	-	0,6,6	0.00	-	-		
86	OHX	5	4055	-	0,6,6	0.00	-	-		
86	OHX	6	2200	-	0,6,6	0.00	-	-		
86	OHX	O2	201	-	0,6,6	0.00	-	-		
86	OHX	5	3991	-	0,6,6	0.00	-	-		
86	OHX	1	4161	-	0,6,6	0.00	-	-		
86	OHX	5	4164	-	0,6,6	0.00	-	-		
86	OHX	7	220	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	M9	203	-	0,6,6	0.00	-	-		
86	OHX	5	4032	-	0,6,6	0.00	-	-		
86	OHX	5	3938	-	0,6,6	0.00	-	-		
86	OHX	6	2103	-	0,6,6	0.00	-	-		
86	OHX	6	2143	-	0,6,6	0.00	-	-		
86	OHX	1	4153	-	0,6,6	0.00	-	-		
86	OHX	4	237	-	0,6,6	0.00	-	-		
86	OHX	5	4152	-	0,6,6	0.00	-	-		
86	OHX	2	2071	-	0,6,6	0.00	-	-		
86	OHX	5	4015	-	0,6,6	0.00	-	-		
86	OHX	5	3903	-	0,6,6	0.00	-	-		
86	OHX	6	2094	-	0,6,6	0.00	-	-		
86	OHX	6	2135	-	0,6,6	0.00	-	-		
86	OHX	7	224	-	0,6,6	0.00	-	-		
86	OHX	8	225	-	0,6,6	0.00	-	-		
86	OHX	6	2146	-	0,6,6	0.00	-	-		
86	OHX	1	3883	-	0,6,6	0.00	-	-		
86	OHX	6	2167	-	0,6,6	0.00	-	-		
86	OHX	5	4204	-	0,6,6	0.00	-	-		
86	OHX	5	4071	-	0,6,6	0.00	-	-		
86	OHX	5	4136	-	0,6,6	0.00	-	-		
86	OHX	1	4220	-	0,6,6	0.00	-	-		
86	OHX	6	2202	-	0,6,6	0.00	-	-		
86	OHX	1	4033	-	0,6,6	0.00	-	-		
86	OHX	5	4066	-	0,6,6	0.00	-	-		
86	OHX	1	4188	-	0,6,6	0.00	-	-		
86	OHX	2	2098	-	0,6,6	0.00	-	-		
86	OHX	1	4014	-	0,6,6	0.00	-	-		
86	OHX	1	4055	-	0,6,6	0.00	-	-		
86	OHX	5	4078	-	0,6,6	0.00	-	-		
86	OHX	2	2146	-	0,6,6	0.00	-	-		
86	OHX	1	3919	-	0,6,6	0.00	-	-		
86	OHX	1	4087	-	0,6,6	0.00	-	-		
86	OHX	6	2057	-	0,6,6	0.00	-	-		
86	OHX	5	4001	-	0,6,6	0.00	-	-		
86	OHX	5	4161	-	0,6,6	0.00	-	-		
86	OHX	5	3990	-	0,6,6	0.00	-	-		
86	OHX	5	4035	-	0,6,6	0.00	-	-		
86	OHX	2	2148	-	0,6,6	0.00	-	-		
86	OHX	1	3902	-	0,6,6	0.00	-	-		
86	OHX	6	2121	-	0,6,6	0.00	-	-		
86	OHX	6	2081	-	0,6,6	0.00	-	-		
86	OHX	5	4079	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2144	-	0,6,6	0.00	-	-		
86	OHX	1	4144	-	0,6,6	0.00	-	-		
86	OHX	7	217	-	0,6,6	0.00	-	-		
86	OHX	8	216	-	0,6,6	0.00	-	-		
86	OHX	2	2058	-	0,6,6	0.00	-	-		
86	OHX	5	4178	-	0,6,6	0.00	-	-		
86	OHX	2	2112	-	0,6,6	0.00	-	-		
86	OHX	1	3900	-	0,6,6	0.00	-	-		
86	OHX	5	4006	-	0,6,6	0.00	-	-		
86	OHX	o3	203	-	0,6,6	0.00	-	-		
86	OHX	7	227	-	0,6,6	0.00	-	-		
86	OHX	2	2077	-	0,6,6	0.00	-	-		
86	OHX	8	231	-	0,6,6	0.00	-	-		
86	OHX	5	4080	-	0,6,6	0.00	-	-		
86	OHX	1	3891	-	0,6,6	0.00	-	-		
86	OHX	3	215	-	0,6,6	0.00	-	-		
86	OHX	5	4117	-	0,6,6	0.00	-	-		
86	OHX	5	4187	-	0,6,6	0.00	-	-		
86	OHX	5	4075	-	0,6,6	0.00	-	-		
86	OHX	5	3940	-	0,6,6	0.00	-	-		
86	OHX	2	2172	-	0,6,6	0.00	-	-		
86	OHX	6	2148	-	0,6,6	0.00	-	-		
86	OHX	M0	304	-	0,6,6	0.00	-	-		
86	OHX	1	4020	-	0,6,6	0.00	-	-		
86	OHX	6	2095	-	0,6,6	0.00	-	-		
86	OHX	5	3922	-	0,6,6	0.00	-	-		
86	OHX	6	2155	-	0,6,6	0.00	-	-		
86	OHX	2	2126	-	0,6,6	0.00	-	-		
86	OHX	5	4074	-	0,6,6	0.00	-	-		
86	OHX	6	2160	-	0,6,6	0.00	-	-		
86	OHX	1	4184	-	0,6,6	0.00	-	-		
86	OHX	5	4124	-	0,6,6	0.00	-	-		
86	OHX	1	3970	-	0,6,6	0.00	-	-		
86	OHX	1	4022	-	0,6,6	0.00	-	-		
86	OHX	N9	101	-	0,6,6	0.00	-	-		
86	OHX	2	2118	-	0,6,6	0.00	-	-		
86	OHX	8	217	-	0,6,6	0.00	-	-		
86	OHX	1	3889	-	0,6,6	0.00	-	-		
86	OHX	1	3981	-	0,6,6	0.00	-	-		
86	OHX	6	2169	-	0,6,6	0.00	-	-		
86	OHX	2	2167	-	0,6,6	0.00	-	-		
86	OHX	1	3918	-	0,6,6	0.00	-	-		
86	OHX	1	4218	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3872	-	0,6,6	0.00	-	-		
86	OHX	2	2177	-	0,6,6	0.00	-	-		
86	OHX	5	4090	-	0,6,6	0.00	-	-		
86	OHX	1	4180	-	0,6,6	0.00	-	-		
86	OHX	1	4016	-	0,6,6	0.00	-	-		
86	OHX	1	4048	-	0,6,6	0.00	-	-		
86	OHX	1	4031	-	0,6,6	0.00	-	-		
86	OHX	5	3989	-	0,6,6	0.00	-	-		
86	OHX	2	2029	-	0,6,6	0.00	-	-		
86	OHX	2	2139	-	0,6,6	0.00	-	-		
86	OHX	1	3995	-	0,6,6	0.00	-	-		
86	OHX	5	3998	-	0,6,6	0.00	-	-		
86	OHX	1	3953	-	0,6,6	0.00	-	-		
86	OHX	5	4169	-	0,6,6	0.00	-	-		
86	OHX	6	2059	-	0,6,6	0.00	-	-		
86	OHX	6	2187	-	0,6,6	0.00	-	-		
86	OHX	6	2117	-	0,6,6	0.00	-	-		
86	OHX	5	4041	-	0,6,6	0.00	-	-		
86	OHX	1	4156	-	0,6,6	0.00	-	-		
86	OHX	M7	206	-	0,6,6	0.00	-	-		
86	OHX	1	4090	-	0,6,6	0.00	-	-		
86	OHX	7	218	-	0,6,6	0.00	-	-		
86	OHX	1	4082	-	0,6,6	0.00	-	-		
86	OHX	8	219	-	0,6,6	0.00	-	-		
86	OHX	6	2073	-	0,6,6	0.00	-	-		
86	OHX	1	3993	-	0,6,6	0.00	-	-		
86	OHX	5	4064	-	0,6,6	0.00	-	-		
86	OHX	5	3918	-	0,6,6	0.00	-	-		
86	OHX	5	3987	-	0,6,6	0.00	-	-		
86	OHX	6	2102	-	0,6,6	0.00	-	-		
86	OHX	5	4092	-	0,6,6	0.00	-	-		
86	OHX	5	3968	-	0,6,6	0.00	-	-		
86	OHX	1	4081	-	0,6,6	0.00	-	-		
86	OHX	l3	406	-	0,6,6	0.00	-	-		
86	OHX	2	2087	-	0,6,6	0.00	-	-		
86	OHX	6	2154	-	0,6,6	0.00	-	-		
86	OHX	6	2080	-	0,6,6	0.00	-	-		
86	OHX	2	2034	-	0,6,6	0.00	-	-		
86	OHX	1	4151	-	0,6,6	0.00	-	-		
86	OHX	1	4060	-	0,6,6	0.00	-	-		
86	OHX	2	2114	-	0,6,6	0.00	-	-		
86	OHX	5	4083	-	0,6,6	0.00	-	-		
86	OHX	s4	302	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2111	-	0,6,6	0.00	-	-		
86	OHX	2	2051	-	0,6,6	0.00	-	-		
86	OHX	5	4234	-	0,6,6	0.00	-	-		
86	OHX	4	228	-	0,6,6	0.00	-	-		
86	OHX	6	2047	-	0,6,6	0.00	-	-		
86	OHX	1	4217	-	0,6,6	0.00	-	-		
86	OHX	8	220	-	0,6,6	0.00	-	-		
86	OHX	5	3947	-	0,6,6	0.00	-	-		
86	OHX	1	4216	-	0,6,6	0.00	-	-		
86	OHX	5	3904	-	0,6,6	0.00	-	-		
86	OHX	5	4151	-	0,6,6	0.00	-	-		
86	OHX	2	2134	-	0,6,6	0.00	-	-		
86	OHX	1	3956	-	0,6,6	0.00	-	-		
86	OHX	2	2085	-	0,6,6	0.00	-	-		
86	OHX	6	2125	-	0,6,6	0.00	-	-		
86	OHX	1	4095	-	0,6,6	0.00	-	-		
86	OHX	5	3905	-	0,6,6	0.00	-	-		
86	OHX	1	4145	-	0,6,6	0.00	-	-		
86	OHX	1	4074	-	0,6,6	0.00	-	-		
86	OHX	L3	404	-	0,6,6	0.00	-	-		
86	OHX	1	3961	-	0,6,6	0.00	-	-		
86	OHX	2	2023	-	0,6,6	0.00	-	-		
86	OHX	1	3896	-	0,6,6	0.00	-	-		
86	OHX	1	3950	-	0,6,6	0.00	-	-		
86	OHX	2	2101	-	0,6,6	0.00	-	-		
86	OHX	1	4204	-	0,6,6	0.00	-	-		
86	OHX	6	2078	-	0,6,6	0.00	-	-		
86	OHX	8	218	-	0,6,6	0.00	-	-		
86	OHX	C5	201	-	0,6,6	0.00	-	-		
86	OHX	1	4173	-	0,6,6	0.00	-	-		
86	OHX	3	218	-	0,6,6	0.00	-	-		
86	OHX	1	4179	-	0,6,6	0.00	-	-		
86	OHX	2	2164	-	0,6,6	0.00	-	-		
86	OHX	5	4230	-	0,6,6	0.00	-	-		
86	OHX	6	2055	-	0,6,6	0.00	-	-		
86	OHX	5	4004	-	0,6,6	0.00	-	-		
86	OHX	1	3938	-	0,6,6	0.00	-	-		
86	OHX	5	4005	-	0,6,6	0.00	-	-		
86	OHX	15	304	-	0,6,6	0.00	-	-		
86	OHX	5	4000	-	0,6,6	0.00	-	-		
86	OHX	1	4128	-	0,6,6	0.00	-	-		
86	OHX	1	3923	-	0,6,6	0.00	-	-		
86	OHX	Q2	503	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4195	-	0,6,6	0.00	-	-		
86	OHX	1	4079	-	0,6,6	0.00	-	-		
86	OHX	6	2131	-	0,6,6	0.00	-	-		
86	OHX	1	4078	-	0,6,6	0.00	-	-		
86	OHX	l3	405	-	0,6,6	0.00	-	-		
86	OHX	5	4128	-	0,6,6	0.00	-	-		
86	OHX	1	4008	-	0,6,6	0.00	-	-		
86	OHX	6	2115	-	0,6,6	0.00	-	-		
86	OHX	1	3966	-	0,6,6	0.00	-	-		
86	OHX	5	4113	-	0,6,6	0.00	-	-		
86	OHX	6	2189	-	0,6,6	0.00	-	-		
86	OHX	5	4009	-	0,6,6	0.00	-	-		
86	OHX	6	2067	-	0,6,6	0.00	-	-		
86	OHX	1	3972	-	0,6,6	0.00	-	-		
86	OHX	5	3957	-	0,6,6	0.00	-	-		
86	OHX	2	2170	-	0,6,6	0.00	-	-		
86	OHX	q2	502	-	0,6,6	0.00	-	-		
86	OHX	1	4004	-	0,6,6	0.00	-	-		
86	OHX	5	4160	-	0,6,6	0.00	-	-		
86	OHX	6	2150	-	0,6,6	0.00	-	-		
86	OHX	1	4062	-	0,6,6	0.00	-	-		
86	OHX	4	224	-	0,6,6	0.00	-	-		
86	OHX	5	4069	-	0,6,6	0.00	-	-		
86	OHX	5	4044	-	0,6,6	0.00	-	-		
86	OHX	2	2165	-	0,6,6	0.00	-	-		
86	OHX	5	4245	-	0,6,6	0.00	-	-		
86	OHX	1	4073	-	0,6,6	0.00	-	-		
86	OHX	5	3921	-	0,6,6	0.00	-	-		
86	OHX	1	4136	-	0,6,6	0.00	-	-		
86	OHX	5	4244	-	0,6,6	0.00	-	-		
86	OHX	1	3983	-	0,6,6	0.00	-	-		
86	OHX	2	2049	-	0,6,6	0.00	-	-		
86	OHX	1	4118	-	0,6,6	0.00	-	-		
86	OHX	5	4130	-	0,6,6	0.00	-	-		
86	OHX	6	2088	-	0,6,6	0.00	-	-		
86	OHX	5	4081	-	0,6,6	0.00	-	-		
86	OHX	1	4214	-	0,6,6	0.00	-	-		
86	OHX	2	2084	-	0,6,6	0.00	-	-		
86	OHX	2	2119	-	0,6,6	0.00	-	-		
86	OHX	6	2077	-	0,6,6	0.00	-	-		
86	OHX	1	3990	-	0,6,6	0.00	-	-		
86	OHX	1	3946	-	0,6,6	0.00	-	-		
86	OHX	6	2165	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2041	-	0,6,6	0.00	-	-		
86	OHX	2	2122	-	0,6,6	0.00	-	-		
86	OHX	6	2108	-	0,6,6	0.00	-	-		
86	OHX	1	4105	-	0,6,6	0.00	-	-		
86	OHX	2	2075	-	0,6,6	0.00	-	-		
86	OHX	5	4238	-	0,6,6	0.00	-	-		
86	OHX	2	2157	-	0,6,6	0.00	-	-		
86	OHX	2	2026	-	0,6,6	0.00	-	-		
86	OHX	5	3935	-	0,6,6	0.00	-	-		
86	OHX	L3	406	-	0,6,6	0.00	-	-		
86	OHX	1	4057	-	0,6,6	0.00	-	-		
86	OHX	1	3994	-	0,6,6	0.00	-	-		
86	OHX	6	2147	-	0,6,6	0.00	-	-		
86	OHX	1	3954	-	0,6,6	0.00	-	-		
86	OHX	m4	202	-	0,6,6	0.00	-	-		
86	OHX	1	4203	-	0,6,6	0.00	-	-		
86	OHX	5	3928	-	0,6,6	0.00	-	-		
86	OHX	5	4216	-	0,6,6	0.00	-	-		
86	OHX	6	2052	-	0,6,6	0.00	-	-		
86	OHX	5	4197	-	0,6,6	0.00	-	-		
86	OHX	5	4213	-	0,6,6	0.00	-	-		
86	OHX	4	229	-	0,6,6	0.00	-	-		
86	OHX	5	4091	-	0,6,6	0.00	-	-		
86	OHX	5	4153	-	0,6,6	0.00	-	-		
86	OHX	1	3890	-	0,6,6	0.00	-	-		
86	OHX	3	217	-	0,6,6	0.00	-	-		
86	OHX	5	4017	-	0,6,6	0.00	-	-		
86	OHX	6	2201	-	0,6,6	0.00	-	-		
86	OHX	1	4103	-	0,6,6	0.00	-	-		
86	OHX	2	2147	-	0,6,6	0.00	-	-		
86	OHX	5	4199	-	0,6,6	0.00	-	-		
86	OHX	5	3936	-	0,6,6	0.00	-	-		
86	OHX	6	2188	-	0,6,6	0.00	-	-		
86	OHX	2	2138	-	0,6,6	0.00	-	-		
86	OHX	5	3933	-	0,6,6	0.00	-	-		
86	OHX	1	4019	-	0,6,6	0.00	-	-		
86	OHX	5	4221	-	0,6,6	0.00	-	-		
86	OHX	1	4038	-	0,6,6	0.00	-	-		
86	OHX	2	2124	-	0,6,6	0.00	-	-		
86	OHX	1	4201	-	0,6,6	0.00	-	-		
86	OHX	5	4034	-	0,6,6	0.00	-	-		
86	OHX	5	3951	-	0,6,6	0.00	-	-		
86	OHX	5	4214	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	4	232	-	0,6,6	0.00	-	-		
86	OHX	D9	102	-	0,6,6	0.00	-	-		
86	OHX	6	2196	-	0,6,6	0.00	-	-		
86	OHX	5	4200	-	0,6,6	0.00	-	-		
86	OHX	5	4181	-	0,6,6	0.00	-	-		
86	OHX	1	3898	-	0,6,6	0.00	-	-		
86	OHX	1	4005	-	0,6,6	0.00	-	-		
86	OHX	m7	206	-	0,6,6	0.00	-	-		
86	OHX	6	2197	-	0,6,6	0.00	-	-		
86	OHX	1	4170	-	0,6,6	0.00	-	-		
86	OHX	6	2126	-	0,6,6	0.00	-	-		
86	OHX	6	2098	-	0,6,6	0.00	-	-		
86	OHX	2	2158	-	0,6,6	0.00	-	-		
86	OHX	5	3902	-	0,6,6	0.00	-	-		

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

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

All (3) bond length outliers are listed below:

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

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

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

There are no chirality outliers.



5 of 9 torsion outliers are listed below:

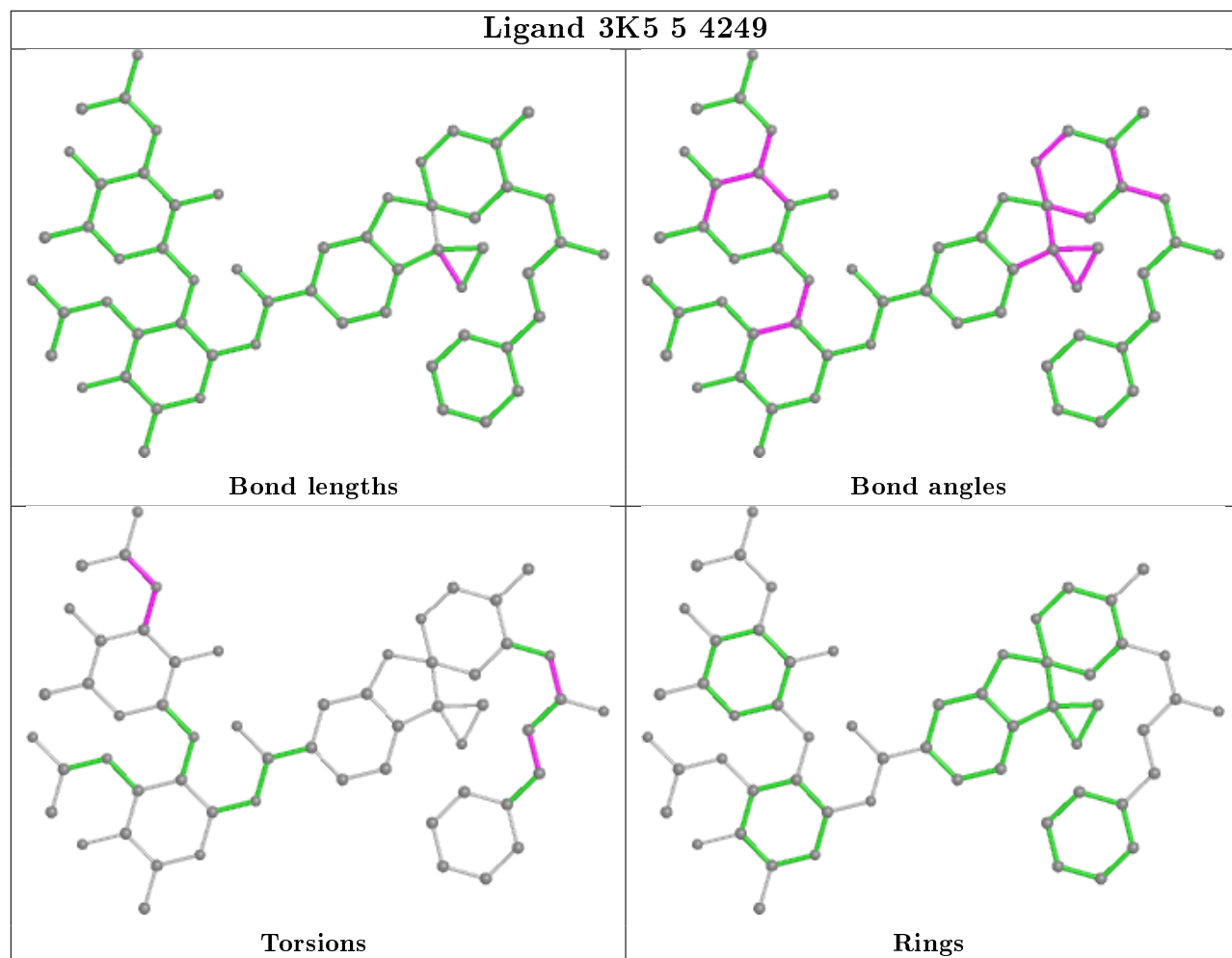
Mol	Chain	Res	Type	Atoms
88	5	4249	3K5	C6-C7-C8-C9
88	5	4249	3K5	C35-C34-O14-C38
88	5	4249	3K5	C39-C38-O14-C34
88	5	4249	3K5	C33-C34-O14-C38
88	5	4249	3K5	O15-C38-O14-C34

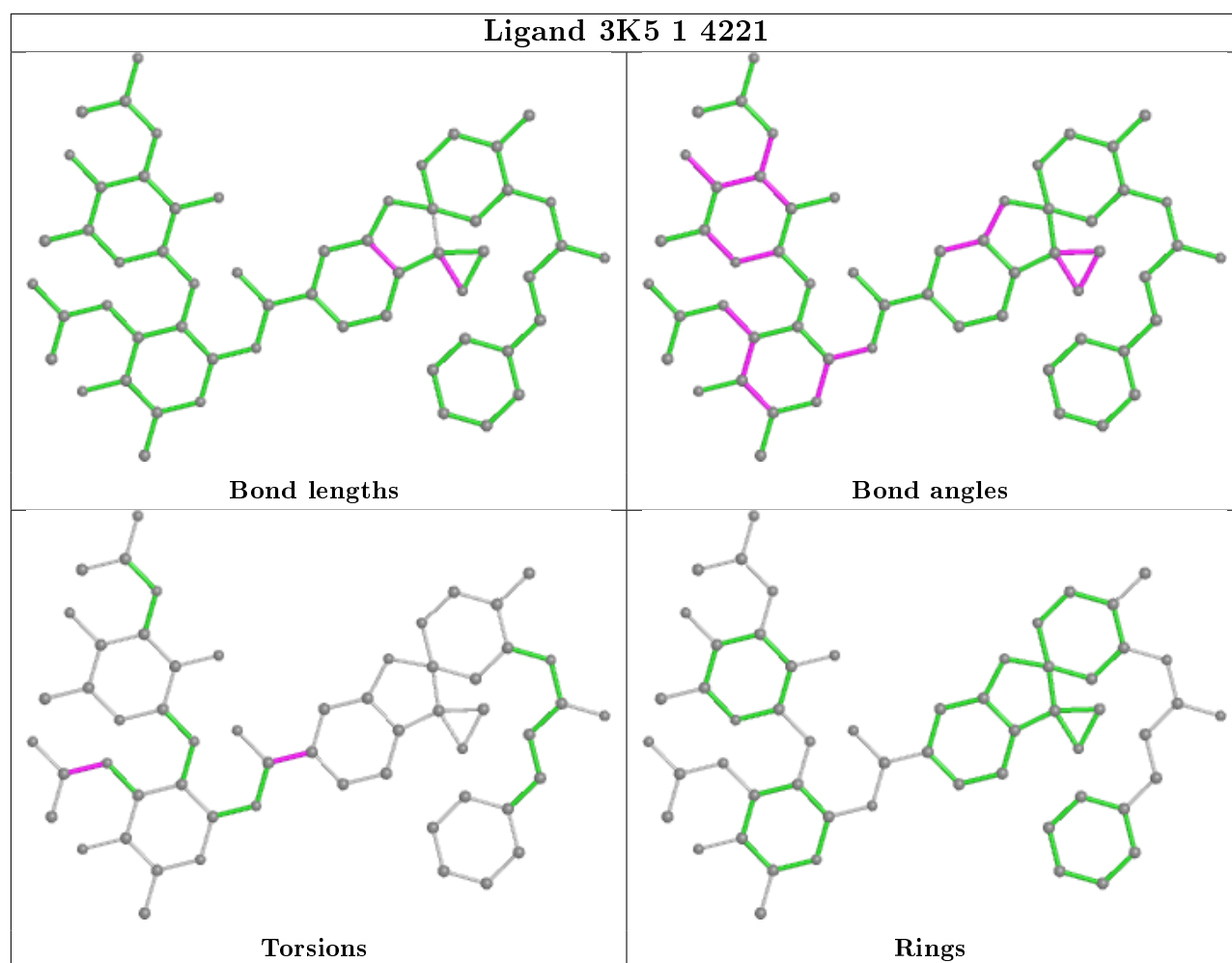
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand 3K5 5 4249





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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