



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 07:41 AM BST

PDB ID : 4U4U  
Title : Crystal structure of Lycorine bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
Resolution : 3.00 Å(reported)

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

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

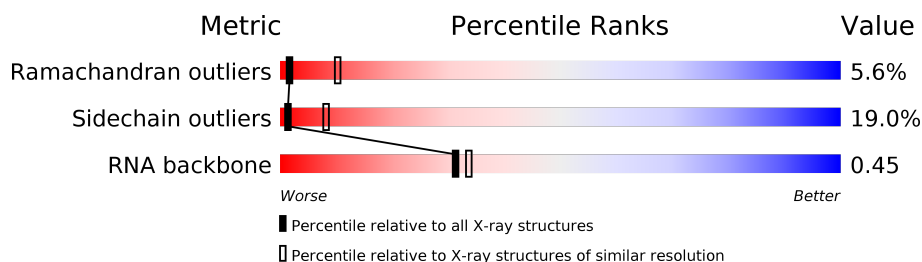
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



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















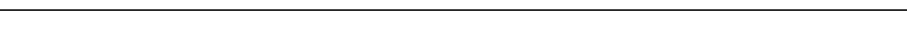




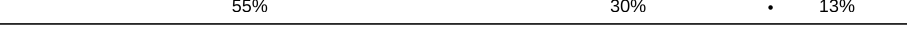





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	2	1800	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	




















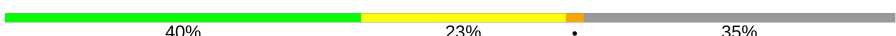





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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3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















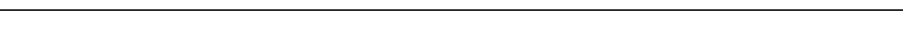




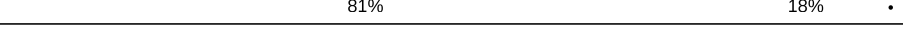





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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107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


























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Mol	Chain	Length	Quality of chain
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	


























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















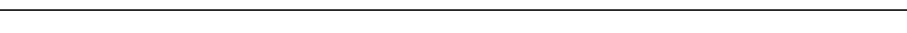




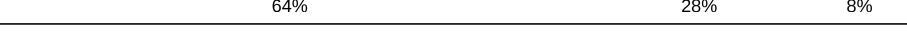





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Mol	Chain	Length	Quality of chain
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9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

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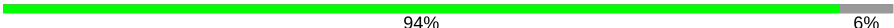

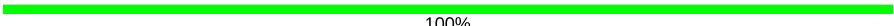

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Mol	Chain	Length	Quality of chain
68	o2	129	 78% 18% ...
69	O3	106	 89% 10% .
69	o3	106	 84% 16%
70	O4	119	 76% 16% . 6%
70	o4	119	 73% 20% . 6%
71	O5	119	 79% 20% .
71	o5	119	 80% 19% .
72	O6	99	 81% 17% .
72	o6	99	 72% 25% .
73	O7	87	 84% 15% .
73	o7	87	 84% 15% .
74	O8	77	 77% 23%
74	o8	77	 78% 21% .
75	O9	50	 86% 14%
75	o9	50	 82% 16% .
76	Q0	52	 75% 23% .
76	q0	52	 75% 23% .
77	Q1	25	 68% 28% .
77	q1	25	 64% 28% 8%
78	Q2	105	 73% 24% .
78	q2	105	 83% 16% .
79	Q3	91	 81% 16% .
79	q3	91	 90% 10%
80	e0	62	 74% 24% .
81	sM	273	 29% 8% 62%

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Mol	Chain	Length	Quality of chain
82	m2	160	 94% 6%
83	p0	311	 37% 9% 54%
84	p1	47	 100%
85	p2	46	 100%

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411211 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			

- 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				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	c6	142	Total	C	N	O			
			1111	711	204	196	0	0	0

- 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		
			926	577	177	170	2	0	0
19	c7	117	Total	C	N	O	S		
			906	563	174	167	2	0	0

- 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		
			1192	743	237	210	2	0	0
20	c8	145	Total	C	N	O	S		
			1192	743	237	210	2	0	0

- 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		
			1112	694	208	208	2	0	0
21	c9	143	Total	C	N	O	S		
			1112	694	208	208	2	0	0

- 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		
			855	539	156	159	1	0	0
22	d0	110	Total	C	N	O	S		
			882	554	161	166	1	0	0

- 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		
			684	420	125	137	2	0	0
23	d1	87	Total	C	N	O	S		
			684	420	125	137	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein 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 Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	sM	104	Total	C	N	O	0	0	0
			681	404	140	137			

- Molecule 82 is a protein called unknown protein chain m2.

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	2	Total	Mg	0	0
			2	2		
86	m6	1	Total	Mg	0	0
			1	1		
86	n8	5	Total	Mg	0	0
			5	5		
86	o1	2	Total	Mg	0	0
			2	2		
86	N5	1	Total	Mg	0	0
			1	1		
86	6	149	Total	Mg	0	0
			149	149		
86	sM	2	Total	Mg	0	0
			2	2		
86	O4	1	Total	Mg	0	0
			1	1		
86	m5	3	Total	Mg	0	0
			3	3		
86	l3	2	Total	Mg	0	0
			2	2		
86	M1	1	Total	Mg	0	0
			1	1		
86	l4	1	Total	Mg	0	0
			1	1		
86	2	123	Total	Mg	0	0
			123	123		
86	n0	1	Total	Mg	0	0
			1	1		
86	L4	2	Total	Mg	0	0
			2	2		
86	l7	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	M5	1	Total 1	Mg 1	0	0
86	S2	1	Total 1	Mg 1	0	0
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	M9	1	Total 1	Mg 1	0	0
86	q0	1	Total 1	Mg 1	0	0
86	SM	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0
86	M0	2	Total 2	Mg 2	0	0
86	c1	1	Total 1	Mg 1	0	0
86	n6	1	Total 1	Mg 1	0	0
86	5	506	Total 506	Mg 506	0	0
86	L5	2	Total 2	Mg 2	0	0
86	O7	1	Total 1	Mg 1	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	1	477	Total 477	Mg 477	0	0
86	D0	1	Total 1	Mg 1	0	0
86	S8	1	Total 1	Mg 1	0	0
86	m1	1	Total 1	Mg 1	0	0
86	M8	1	Total 1	Mg 1	0	0
86	q3	1	Total 1	Mg 1	0	0

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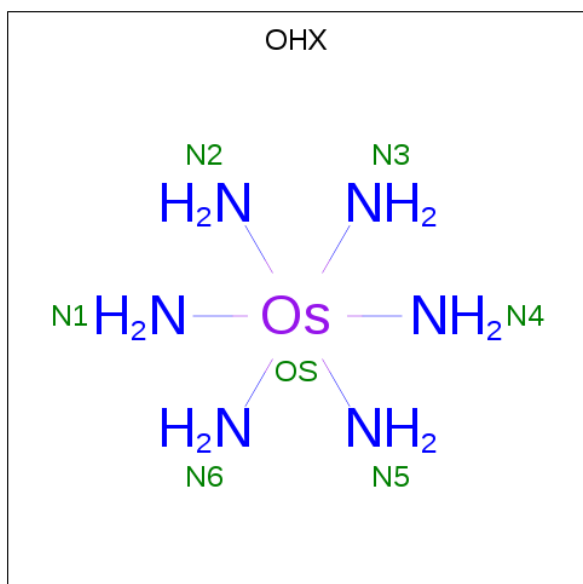
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	o3	2	Total 2	Mg 2	0	0
86	d3	2	Total 2	Mg 2	0	0
86	M3	3	Total 3	Mg 3	0	0
86	N3	3	Total 3	Mg 3	0	0
86	4	21	Total 21	Mg 21	0	0
86	D4	1	Total 1	Mg 1	0	0
86	L2	1	Total 1	Mg 1	0	0
86	l5	2	Total 2	Mg 2	0	0
86	m7	5	Total 5	Mg 5	0	0
86	M7	6	Total 6	Mg 6	0	0
86	N8	3	Total 3	Mg 3	0	0
86	s1	1	Total 1	Mg 1	0	0
86	l9	1	Total 1	Mg 1	0	0
86	s8	2	Total 2	Mg 2	0	0
86	O8	1	Total 1	Mg 1	0	0
86	c7	1	Total 1	Mg 1	0	0
86	7	16	Total 16	Mg 16	0	0
86	n3	2	Total 2	Mg 2	0	0
86	q1	1	Total 1	Mg 1	0	0
86	L3	2	Total 2	Mg 2	0	0
86	d4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	s4	1	Total 1	Mg 1	0	0
86	l2	2	Total 2	Mg 2	0	0
86	8	14	Total 14	Mg 14	0	0
86	M6	1	Total 1	Mg 1	0	0
86	N0	1	Total 1	Mg 1	0	0
86	3	14	Total 14	Mg 14	0	0

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



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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	2	1	Total 7	N 6	Os 1	0	0
87	2	1	Total 7	N 6	Os 1	0	0
87	2	1	Total 7	N 6	Os 1	0	0
87	2	1	Total 7	N 6	Os 1	0	0
87	2	1	Total 7	N 6	Os 1	0	0
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87	C3	1	Total 7	N 6	Os 1	0	0
87	C5	1	Total 7	N 6	Os 1	0	0
87	C8	1	Total 7	N 6	Os 1	0	0
87	D3	1	Total 7	N 6	Os 1	0	0
87	D9	1	Total 7	N 6	Os 1	0	0
87	SR	1	Total 7	N 6	Os 1	0	0
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87	1	1	Total 7	N 6	Os 1	0	0
87	1	1	Total 7	N 6	Os 1	0	0
87	1	1	Total 7	N 6	Os 1	0	0
87	1	1	Total 7	N 6	Os 1	0	0
87	1	1	Total 7	N 6	Os 1	0	0
87	1	1	Total 7	N 6	Os 1	0	0
87	1	1	Total 7	N 6	Os 1	0	0
87	1	1	Total 7	N 6	Os 1	0	0

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
			7	6	1		
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87	4	1	Total	N	Os	0	0
			7	6	1		
87	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
			7	6	1		
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87	4	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L3	1	Total	N	Os	0	0
			7	6	1		
87	L4	1	Total	N	Os	0	0
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87	M0	1	Total	N	Os	0	0
			7	6	1		
87	M5	1	Total	N	Os	0	0
			7	6	1		
87	M6	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M8	1	Total	N	Os	0	0
			7	6	1		
87	M9	1	Total	N	Os	0	0
			7	6	1		
87	N1	1	Total	N	Os	0	0
			7	6	1		
87	N9	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	O2	1	Total	N	Os	0	0
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87	O3	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
			7	6	1		
87	O9	1	Total	N	Os	0	0
			7	6	1		
87	Q2	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	s1	1	Total 7	N 6	Os 1	0	0
87	s1	1	Total 7	N 6	Os 1	0	0
87	s4	1	Total 7	N 6	Os 1	0	0
87	s8	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	c1	1	Total	N	Os	0	0
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87	c5	1	Total	N	Os	0	0
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87	c8	1	Total	N	Os	0	0
			7	6	1		
87	d4	1	Total	N	Os	0	0
			7	6	1		
87	d9	1	Total	N	Os	0	0
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87	sR	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m6	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m8	1	Total	N	Os	0	0
			7	6	1		
87	m9	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n6	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o2	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

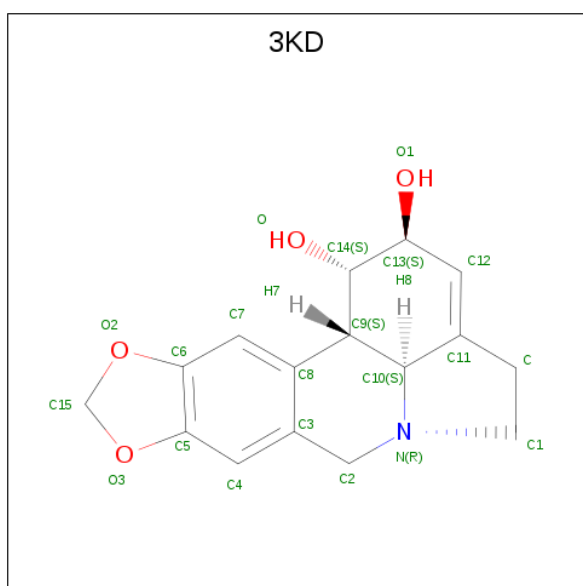
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		

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

- Molecule 89 is (1S,2S,12bS,12cS)-2,4,5,7,12b,12c-hexahydro-1H-[1,3]dioxolo[4,5-j]pyrrolo[3,2,1-de]phenanthridine-1,2-diol (three-letter code: 3KD) (formula: C<sub>16</sub>H<sub>17</sub>NO<sub>4</sub>).



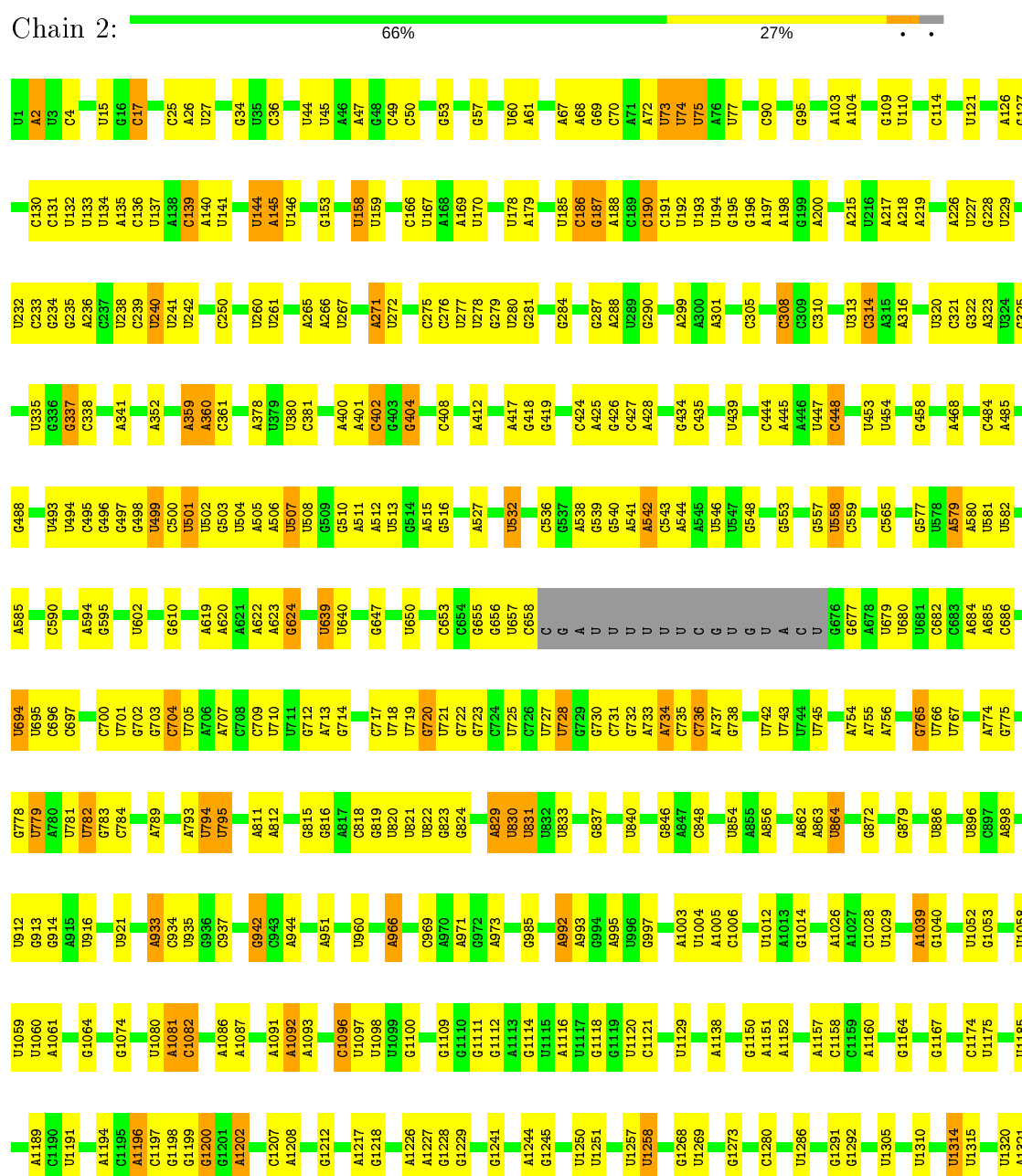
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			21	16	1	4		
89	5	1	Total	C	N	O	0	0
			21	16	1	4		

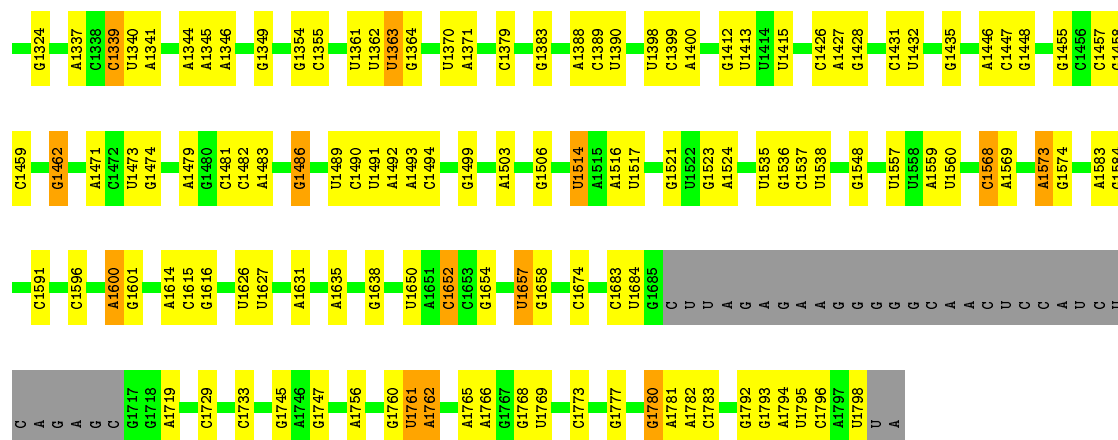
### 3 Residue-property plots

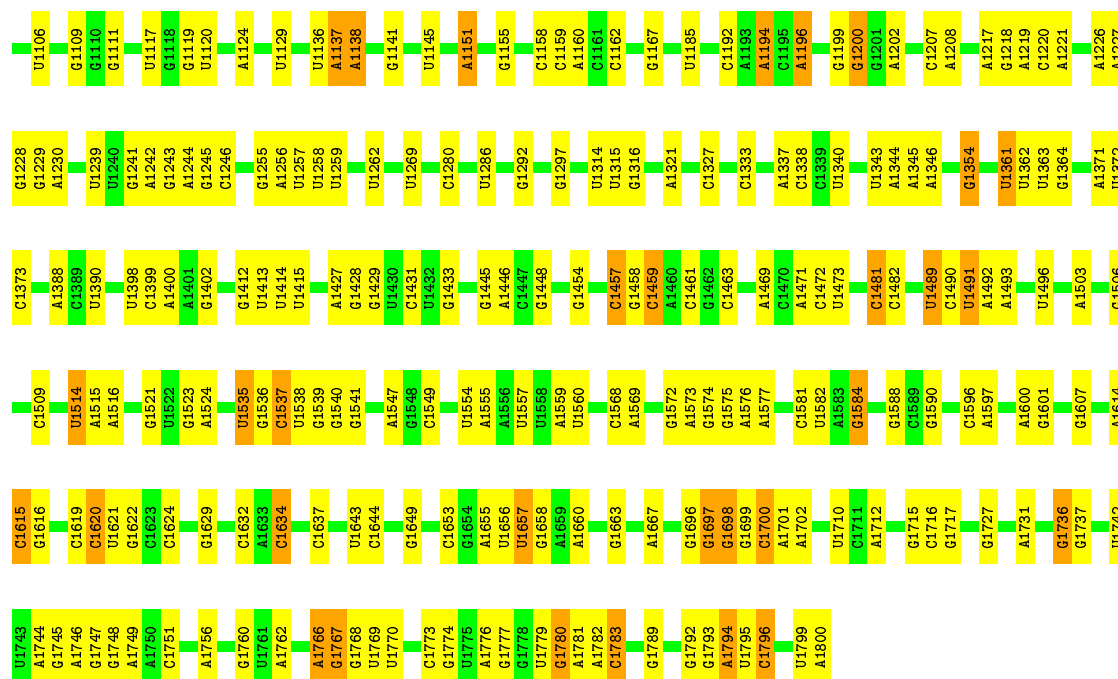
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

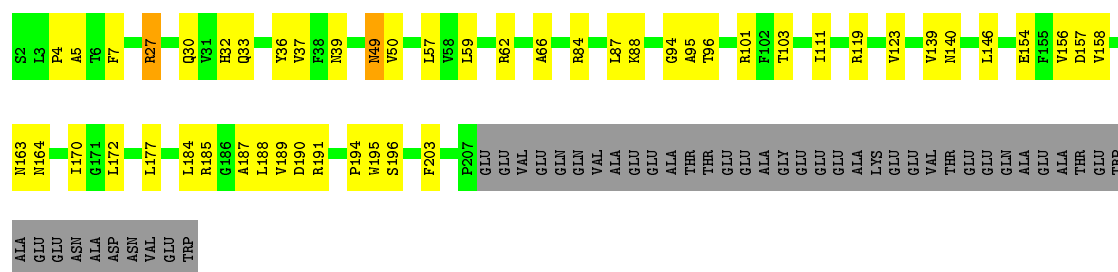
#### • Molecule 1: 18S ribosomal RNA







- Molecule 2: 40S ribosomal protein S0-A



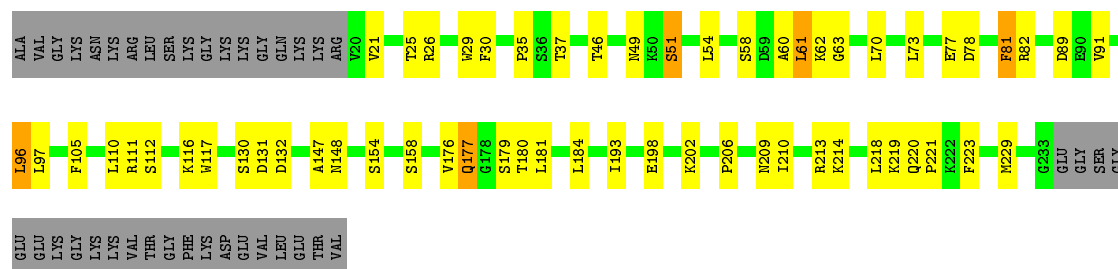
- Molecule 2: 40S ribosomal protein S0-A



- Molecule 3: 40S ribosomal protein S1-A

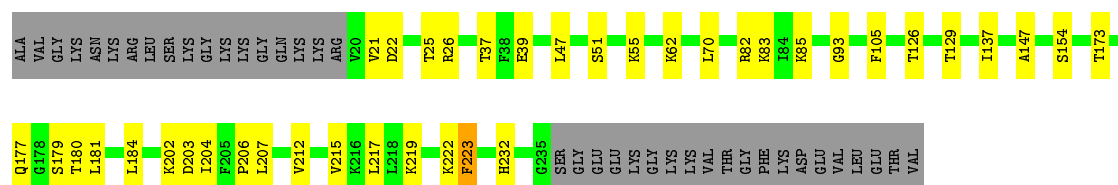






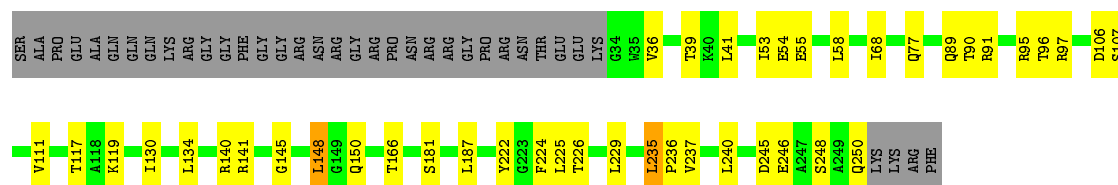
- Molecule 3: 40S ribosomal protein S1-A

Chain s1: 70% 15% 15%



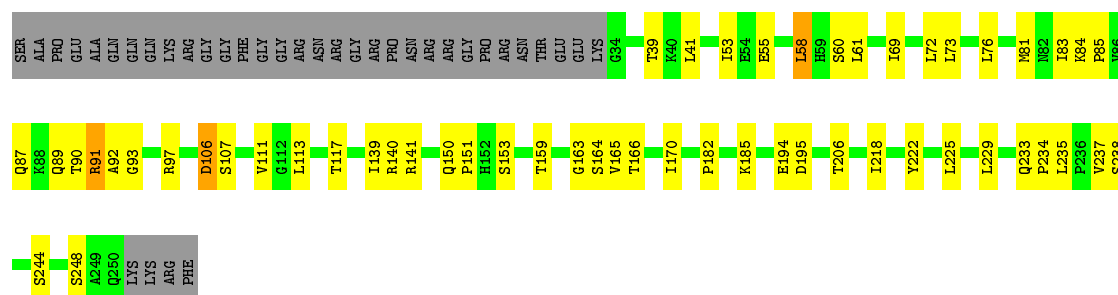
- Molecule 4: 40S ribosomal protein S2

Chain S2: 69% 16% 14%



- Molecule 4: 40S ribosomal protein S2

Chain s2: 64% 21% 14%



- Molecule 5: 40S ribosomal protein S3

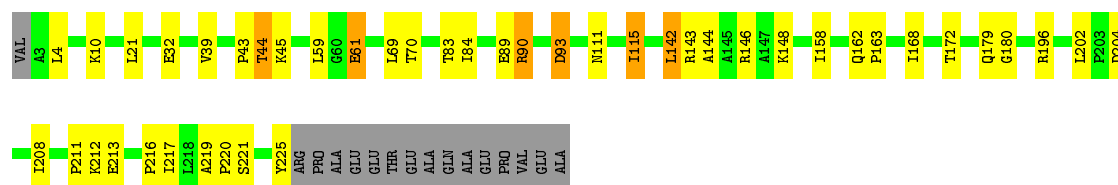
Chain S3: 74% 18% 7%





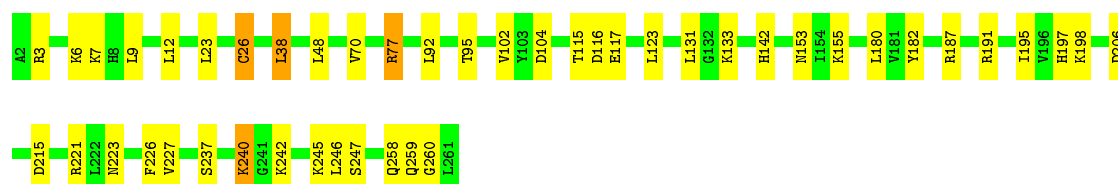
- Molecule 5: 40S ribosomal protein S3

Chain s3:  75% 16% 7%



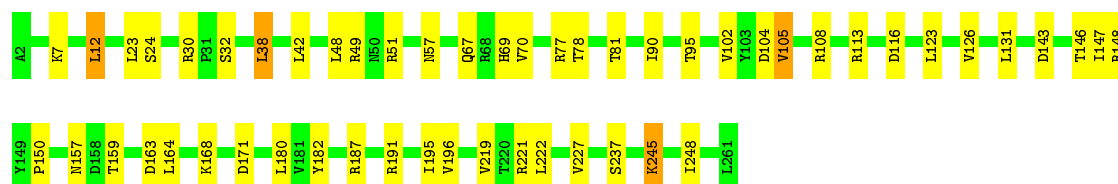
- Molecule 6: 40S ribosomal protein S4-A

Chain S4:  82% 16%



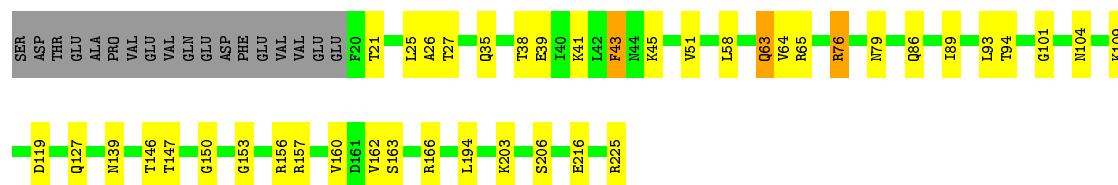
- Molecule 6: 40S ribosomal protein S4-A

Chain s4:  80% 19%



- Molecule 7: 40S ribosomal protein S5

Chain S5:  73% 17% 8%



- Molecule 7: 40S ribosomal protein S5

Chain s5:  68% 22% 8%





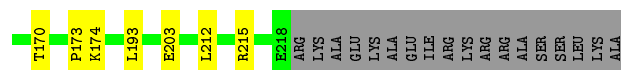
- Molecule 8: 40S ribosomal protein S6-A

Chain S6: 74% 21% • •



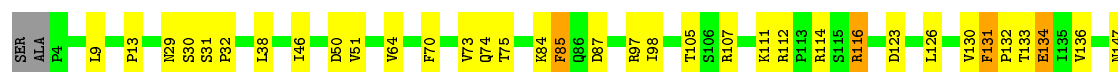
- Molecule 8: 40S ribosomal protein S6-A

Chain s6: 74% 17% • 8%



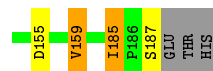
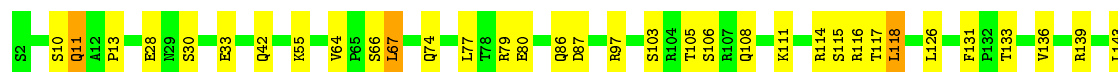
- Molecule 9: 40S ribosomal protein S7-A

Chain S7: 75% 20% • •



- Molecule 9: 40S ribosomal protein S7-A

Chain s7: 78% 17% • •



- Molecule 10: 40S ribosomal protein S8-A

Chain S8: 80% 14% • 6%





- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 81% 13% 6%



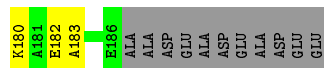
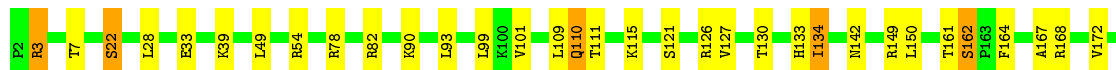
- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 72% 21% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 76% 16% 6%



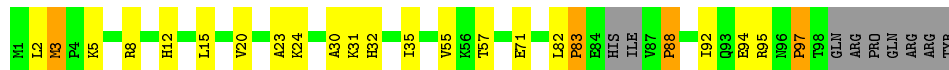
- Molecule 12: 40S ribosomal protein S10-A

Chain C0: 71% 19% 9%

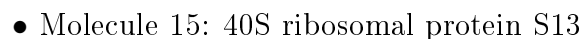


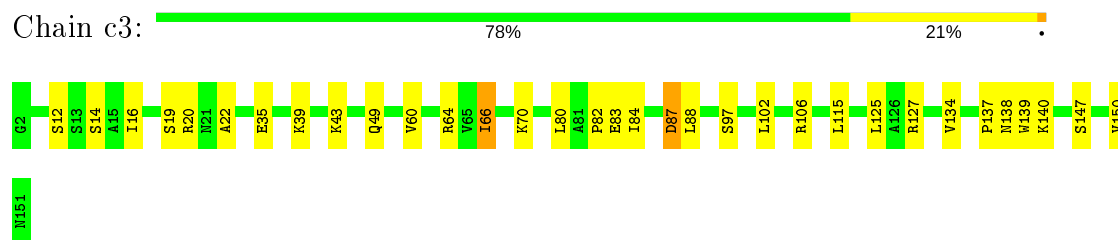
- Molecule 12: 40S ribosomal protein S10-A

Chain c0: 70% 18% 9%

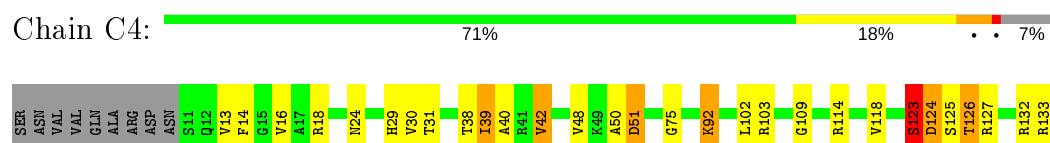


- Molecule 13: 40S ribosomal protein S11-A

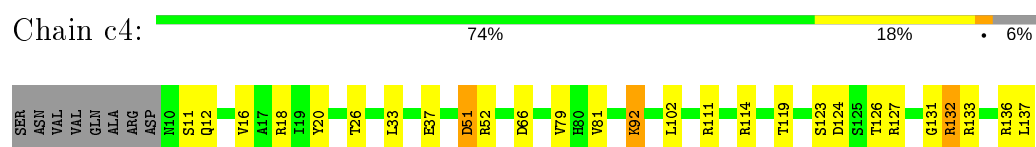




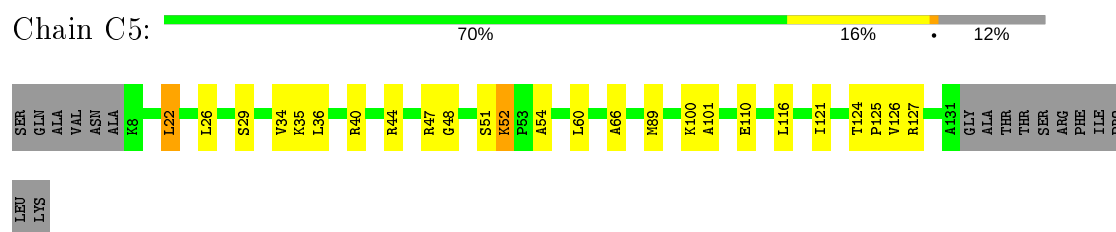
- Molecule 16: 40S ribosomal protein S14-A



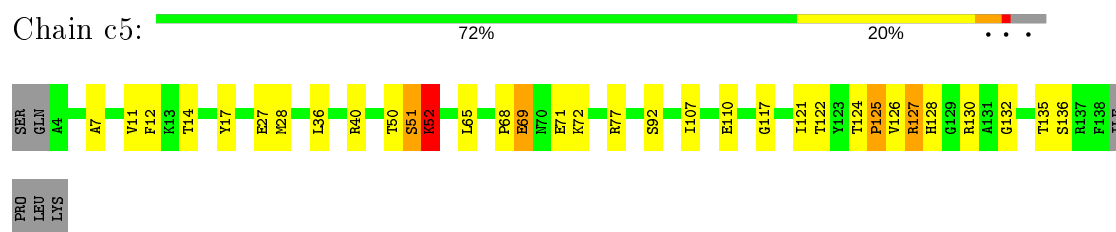
- Molecule 16: 40S ribosomal protein S14-A



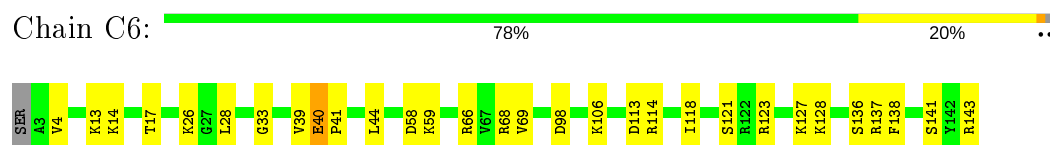
- Molecule 17: 40S ribosomal protein S15




- Molecule 17: 40S ribosomal protein S15



- Molecule 18: 40S ribosomal protein S16-A



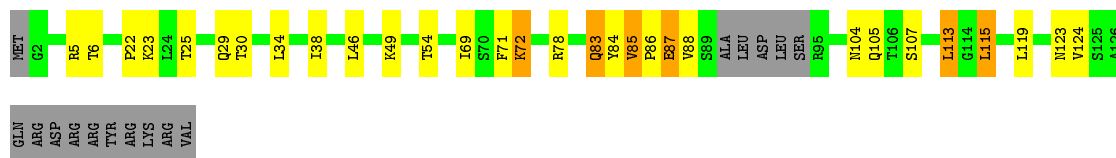
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:  77% 21% .



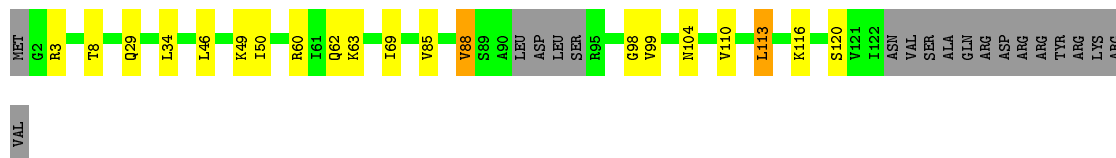
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:  66% 18% . 12%



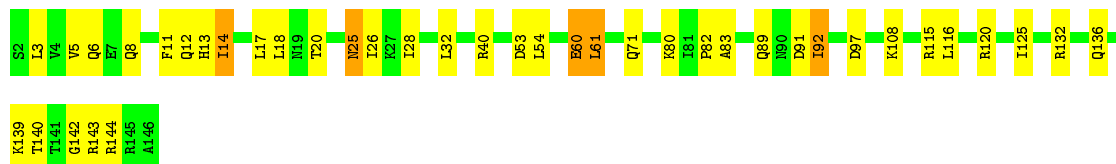
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  71% 13% . 14%



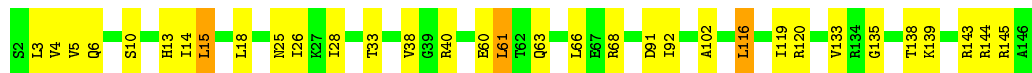
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  72% 24% .




- Molecule 20: 40S ribosomal protein S18-A

Chain c8:  77% 21% .




- Molecule 21: 40S ribosomal protein S19-A

Chain C9:  81% 19%



- Molecule 21: 40S ribosomal protein S19-A

Chain c9:  81% 17%



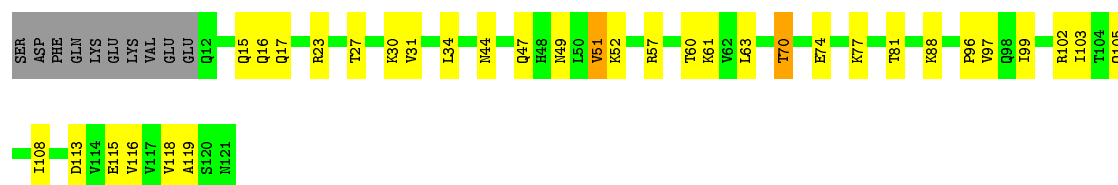
- Molecule 22: 40S ribosomal protein S20

Chain D0:  68% 22% 11%




- Molecule 22: 40S ribosomal protein S20

Chain d0:  63% 27% 8%




- Molecule 23: 40S ribosomal protein S21-A

Chain D1:  76% 24%



- Molecule 23: 40S ribosomal protein S21-A

Chain d1:  75% 24%




- Molecule 24: 40S ribosomal protein S22-A

Chain D2:  86% 12%




- Molecule 24: 40S ribosomal protein S22-A

Chain d2:  86% 13%





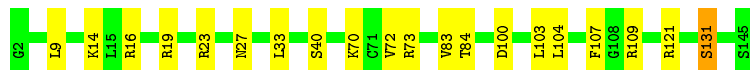
- Molecule 25: 40S ribosomal protein S23-A

Chain D3:  81% 17%




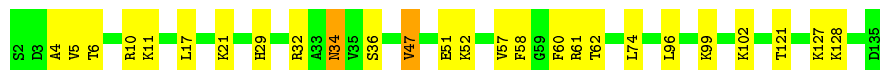
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:  86% 13%




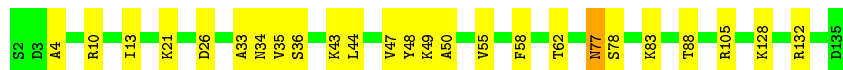
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:  81% 18%



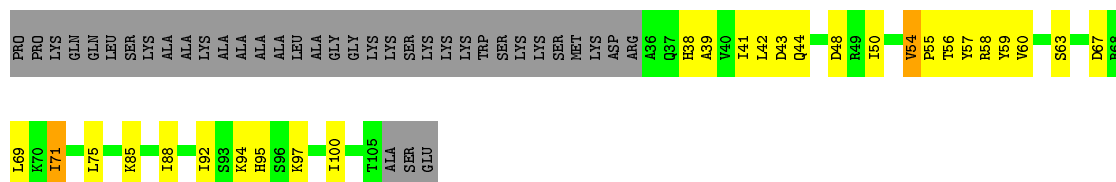
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:  81% 18%



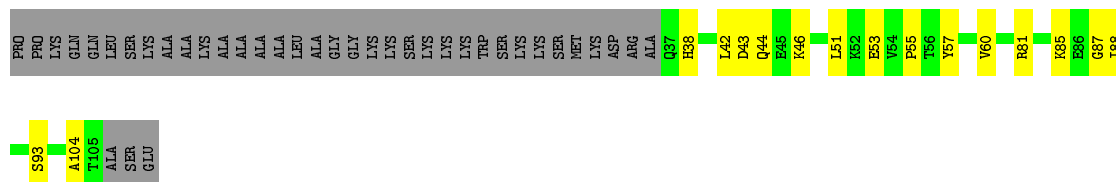
- Molecule 27: 40S ribosomal protein S25-A

Chain D5:  40% 23% 35%



- Molecule 27: 40S ribosomal protein S25-A

Chain d5:  50% 15% 36%




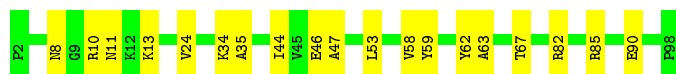
- Molecule 28: 40S ribosomal protein S26-B

Chain D6:  72% 20% 8%




- Molecule 28: 40S ribosomal protein S26-B

Chain d6:  80% 20%




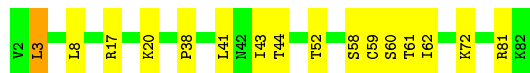
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:  86% 14%



- Molecule 29: 40S ribosomal protein S27-A

Chain d7:  80% 19% .



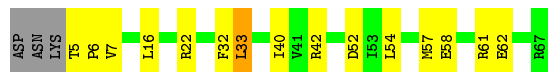
- Molecule 30: 40S ribosomal protein S28-A

Chain D8:  73% 21% . 5%




- Molecule 30: 40S ribosomal protein S28-A

Chain d8:  73% 21% . 5%



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:  78% 16% . .




- Molecule 31: 40S ribosomal protein S29-A

Chain d9:  71% 25% .



- Molecule 32: 40S ribosomal protein S30-A

Chain E0:  82% 17% .



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:  53% 38% . 7%




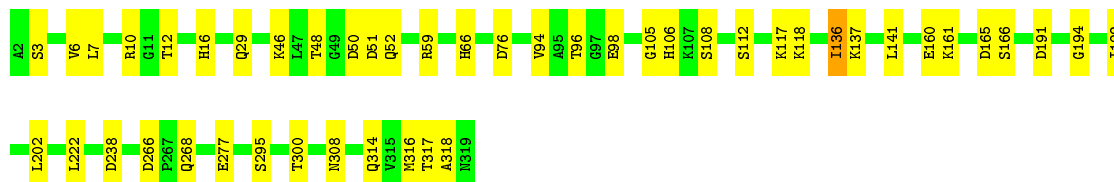
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:  59% 34% 7%




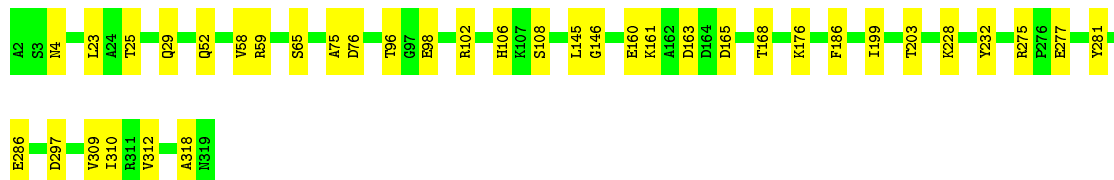
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:  85% 14%



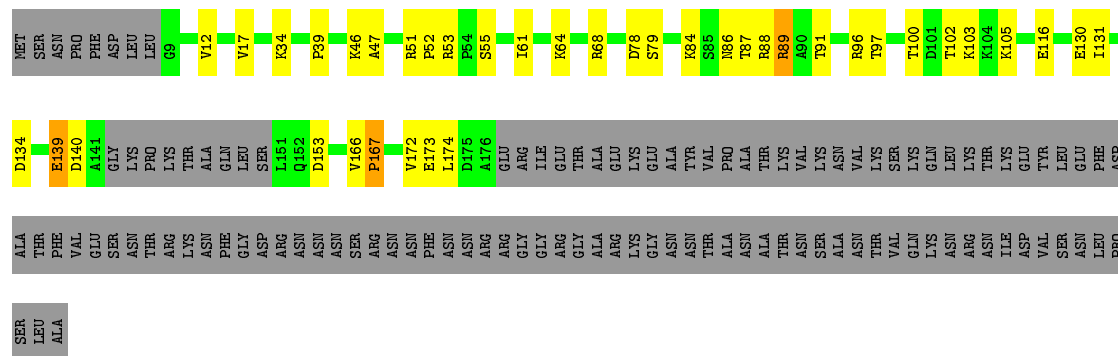
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:  88% 12%



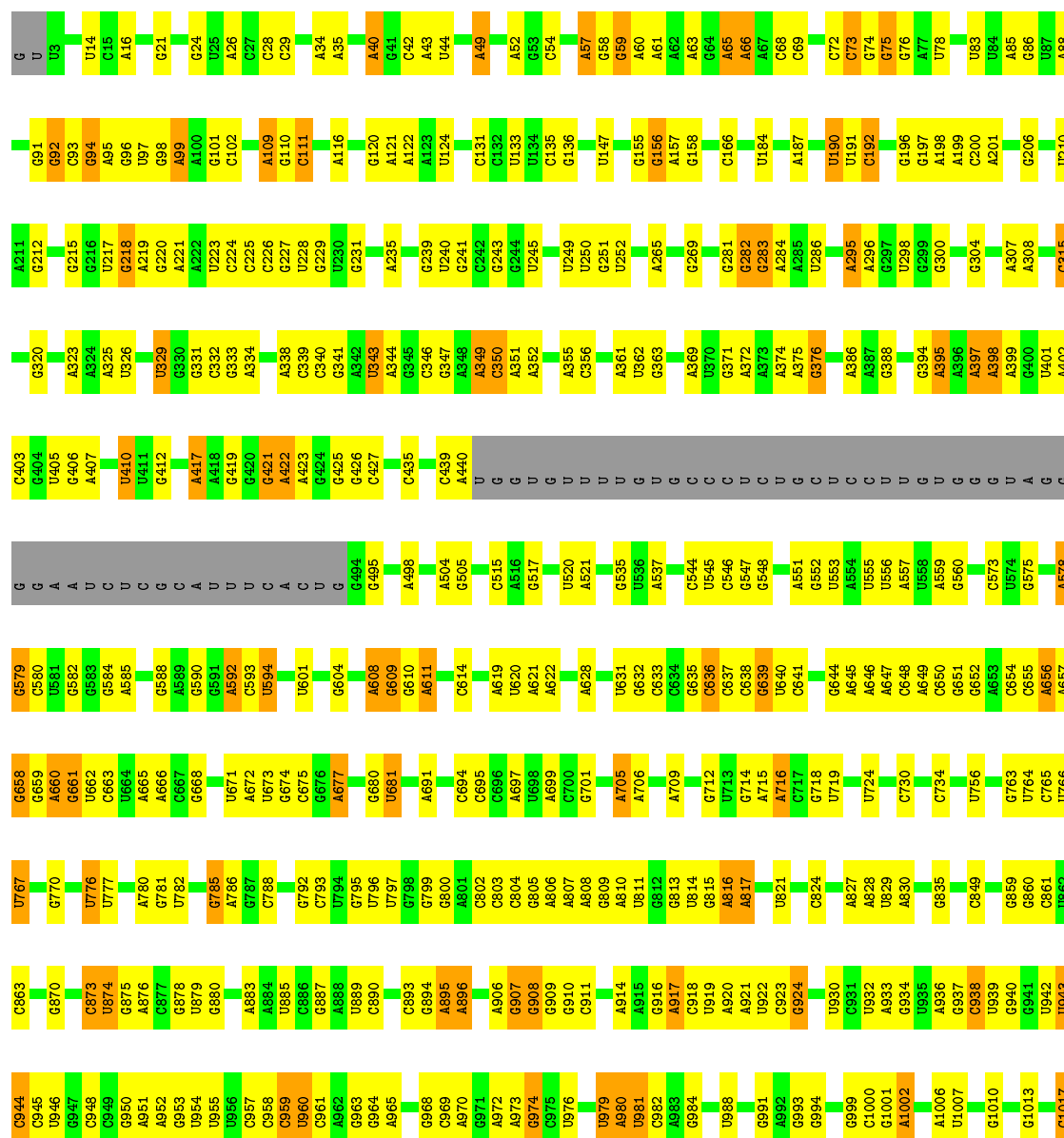
- Molecule 35: Suppressor protein STM1

Chain SM:  44% 13% 42%



### • Molecule 36: 25S ribosomal RNA

Chain 1: 52% 34% 7% 7%





A3310	A3311	A3312	A3313	A3314	A3315	A3316	A3317	A3318	A3319	A3320	A3323	A3326	A3330	A3335	A3336	A3341	A3342	A3343	A3344	A3345	A3346	A3347	A3350	A3351	A3352	A3353	A3354	A3355	A3356	A3361	A3362	A3368	A3369	A3375	A3376	A3377	A3378	A3382	A3383	A3389	A3396																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A3210	C3211	A3212	A3213	U3214	C3217	A3218	G3219	G3228	G3229	C3235	G3242	A3243	A3244	A3245	G3246	G3247	G3253	U3259	C3265	G3266	A3267	A3268	U3269	U3270	G3271	C3272	A3273	U3274	A3275	G3276	U3277	C3278	U3281	G3286	U3287	G3288	G3289	U3293	A3294	A3295	C3298	U3302	G3303	U3304	A3305	U3306																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
U3121	A3122	G3128	A3129	A3130	U3131	C3132	C3133	A3134	U3135	G3136	C3137	U3138	A3139	G3140	A3141	A3142	C3143	A3150	U3151	U3152	U3153	C3154	U3155	U3156	U3157	G3158	C3164	A3165	U3169	A3170	U3171	A3172	G3173	A3174	U3175	G3176	G3177	A3178	U3179	A3180	C3181	A3187	U3195	U3196	G3197	U3198	C3201	U3207	G3208	A3209																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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U2846	C2849	G2850	A2851	C2852	A2853	U2854	U2855	C2856	C2857	U2858	U2859	U2860	U2861	U2862	U2865	U2866	C2867	U2868	U2869	C2870	A2871	A2872	U2873	U2874	U2875	C2876	G2877	G2878	C2879	U2882	U2883	C2884	C2885	U2886	U2887	U2888	C2889	A2890	U2891	A2892	G2898	C2899	A2900	G2901	A2910	A2911	G2912	U2916	G2917	U2920	U2923																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C2772	C2773	G2777	G2778	A2779	G2787	C2788	U2789	A2790	G2791	A2792	G2793	U2794	U2795	G2796	C2797	C2798	A2799	G2800	A2801	U2802	A2803	A2804	G2805	U2806	U2807	A2808	C2809	C2810	A2811	C2812	G2815	G2816	A2817	U2818	U2819	A2820	C2821	U2822	G2823	G2824	C2825	U2826	U2827	G2828	U2829	G2830	G2831	C2832	A2833	C2836	U2842	U2843	A2845																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
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U2494	G2495	U2496	G2497	A2443	A2444	A2445	U	A	G	A	G	G	G	U	U	A	G	A	U	A	A	U	G	G	G	C	U	U	C	U	C	G	A	A	C	A	U	C	A	C	U	A	C	C	C	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	

• Molecule 36: 25S ribosomal RNA

Chain 5:

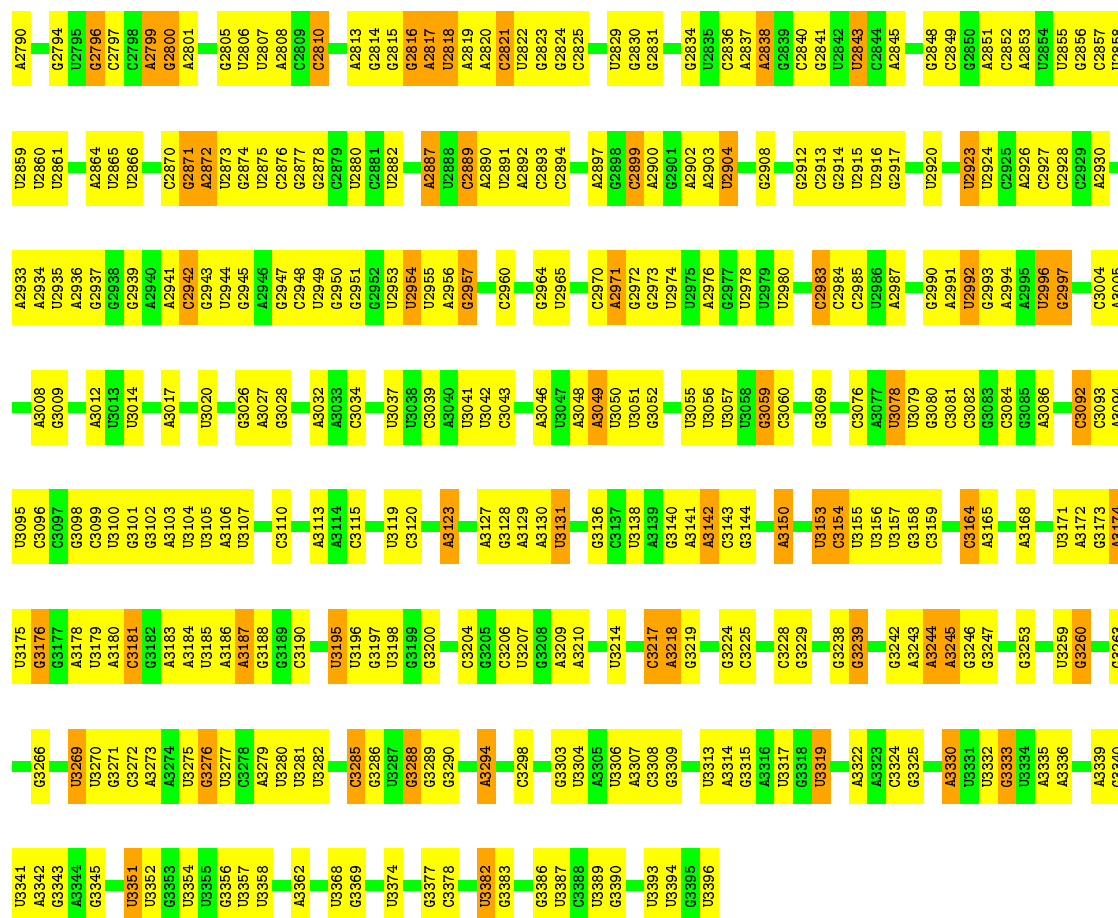


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U97	G98	A99	A100	G101	C102	A109	G110	C113	A116	A121	A122	U133	U134	C135	G136	C141	C142	A150	A151	U152	G156	A157	G158	A159	G160	G161	G162	A165	C166	G170	G171	G172	G173	C174	U178	C179	G180	U181	U182	A187	U188	G189	U190	U191	C192	G200				



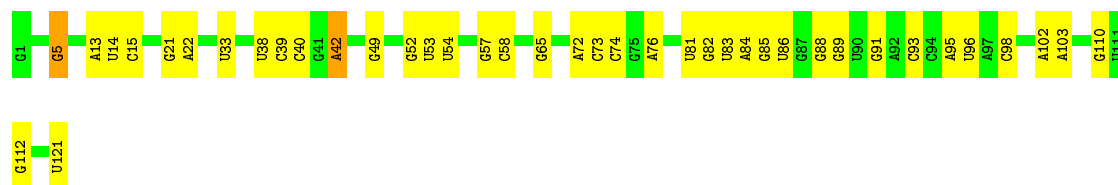
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C2708	G2623	A2529	G2391	U2319	A2243	A2145	U	G	A1841	A1842	U1717	U1569	G1489
C2709	C2627	G2530	C2392	U2319	A2244	A2146	U	G	U1722	U1723	U1722	U1570	A1490
C2710	A2628	C2531	C2393	G2323	C2245	A2147	U	C	A1935	A1846	A1723	U1571	A1491
C2711	U2631	U2532	G2394	G2323	C2246	G2150	A	U	U1937	A1847	U1724	G1492	G1493
U2712	G2632	G2533	G2395	U2327	C2248	U2153	G	U	G1953	C1848	C1725	C1574	U1494
G2714	U2633	G2534	G2396	U2327	G2249	G2154	A	C	G	C1849	U1733	G1576	U1495
U2719	U2634	U2537	A2397	C2331	G2250	G2155	C	U	U	A1850	G1733	U1577	C1496
U2724	A2635	U2538	C2398	A2332	G2253	A2158	U	U	A	C1856	G1736	C1578	C1499
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C2726	A2637	A2540	A2401	U2334	A2285	G2165	C	U	U	A1858	G1751	C1581	U1501
C2727	C2638	U2541	A2402	U2336	A2286	G2174	G	U	G	A1859	C1756	C1582	C1502
A2727	G2639	U2542	G2403	U2336	C2287	U2176	A	U	A	G1863	U1766	A1583	A1503
G2728	U2543	C2543	G2404	C2337	U2288	G2181	U	G	G	U1875	U1766	G1592	G1513
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A2733	G2645	U2644	C2406	C2339	U2290	U2186	U	C	U	C1866	A1760	G1586	A1505
C2737	U2650	C2651	C2407	U2340	A2270	G2187	U	C	C	A1867	C1761	A1586	A1506
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C2747	U2657	C2657	U2411	U2344	C2277	U2191	A	U	G	U1876	U1766	G1592	G1513
G2748	G2660	C2661	C2412	A2345	C2278	U2192	U	C	U	C1877	G1766	A1593	G1514
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C2753	G2674	C2674	U2433	A2358	A2279	U2199	A	U	C	A1879	G1770	A1605	A1516
G2754	U2674	C2675	U2434	C2359	U2280	U2200	A	U	C	U1880	G1770	U1606	G1517
C2755	C2675	C2675	U2434	C2360	U2281	G2201	U	C	U	A1881	G1780	U1607	U1518
U2757	A2593	C2594	G2437	A2361	C2290	G2204	U	C	G	U1882	G1780	G1608	G1519
A2758	C2594	C2594	A2438	C2362	A2291	U2205	U	C	U	U1883	G1790	G1620	G1520
U2759	U2599	C2599	A2439	C2363	U2292	G2206	U	C	U	A1884	C1791	A1620	G1521
A2762	C2682	U2601	G2440	G2364	C2293	U2207	U	C	U	U1885	C1792	U1522	U1522
C2763	U2683	C2602	A2441	C2365	U2294	G2210	U	C	U	A1886	C1793	U1523	A1524
C2764	C2684	G2602	G2442	C2366	A2295	G2211	A	C	G	A1891	U1795	G1639	G1528
C2765	A2685	G2602	A2443	C2367	U2296	U2209	U	C	U	U1894	G1796	G1640	A1529
U2766	C2686	C2602	C2444	A2368	U2297	G2212	U	C	U	G1897	A1797	A1641	U1533
U2767	G2687	G2606	C2444	A2368	U2298	G2213	U	C	U	G1898	A1799	C1644	U1533
G2770	U2688	G2607	A	G2371	A2299	G2214	A	C	U	G1902	A1813	U1645	G1536
U2771	C2689	G2608	U	A2372	G2300	U2211	U	C	U	U1906	A1814	C1657	G1541
C2772	U2690	C2609	G	A2373	G2301	G2212	U	C	U	G1907	A1816	G1658	G1547
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U2774	C2692	U2611	G	G2375	G2303	A2215	U	C	U	U1911	U1820	C1670	U1555
G2775	C2693	U2612	U	G2376	G2305	A2222	U	C	U	U1912	U1821	G1678	C1556
C2776	U2613	G2614	G	G2377	C2306	A2223	U	C	U	G1914	G1825	G1678	G1560
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C2778	U2615	G2616	U	U2379	C2308	U2225	U	C	U	G1918	G1833	U1684	C1562
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U2782	G2617	G2618	A	U2383	U2310	A2229	U	C	U	U1925	U1837	U1687	U1564
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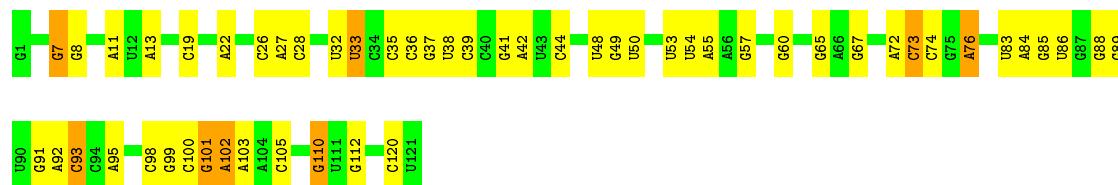
• Molecule 37: 5S ribosomal RNA

Chain 3: 67% 31%



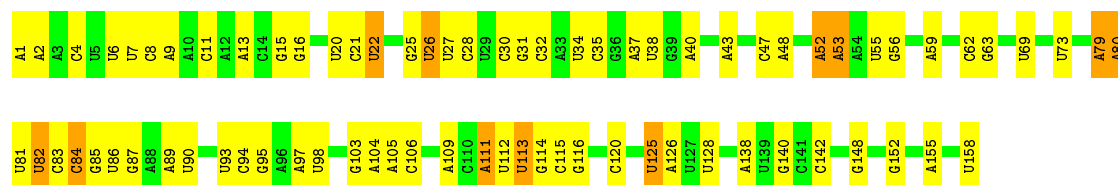
• Molecule 37: 5S ribosomal RNA

Chain 7: 56% 37% 7%



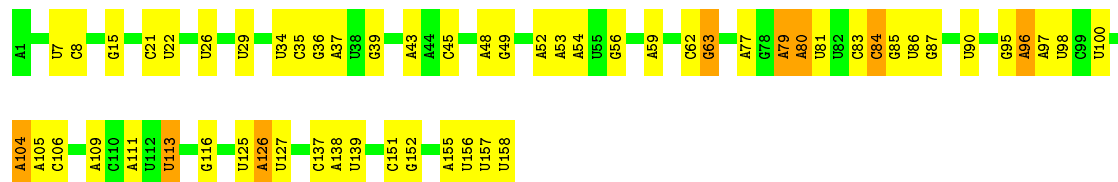
• Molecule 38: 5.8S ribosomal RNA

Chain 4: 52% 41% 7%



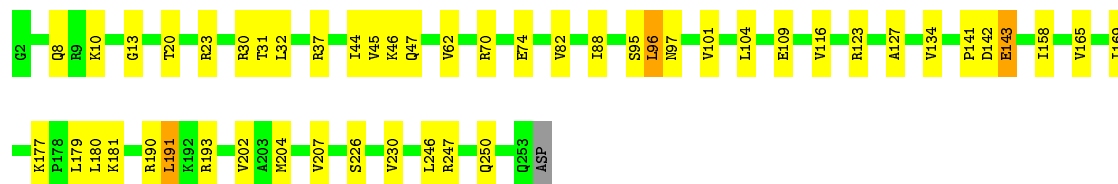
• Molecule 38: 5.8S ribosomal RNA

Chain 8: 64% 31% 5%



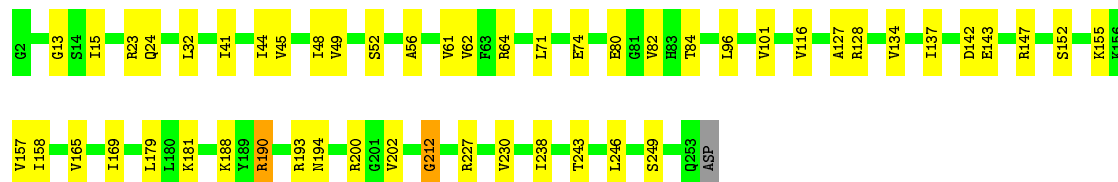
• Molecule 39: 60S ribosomal protein L2-A

Chain L2: 80% 18%



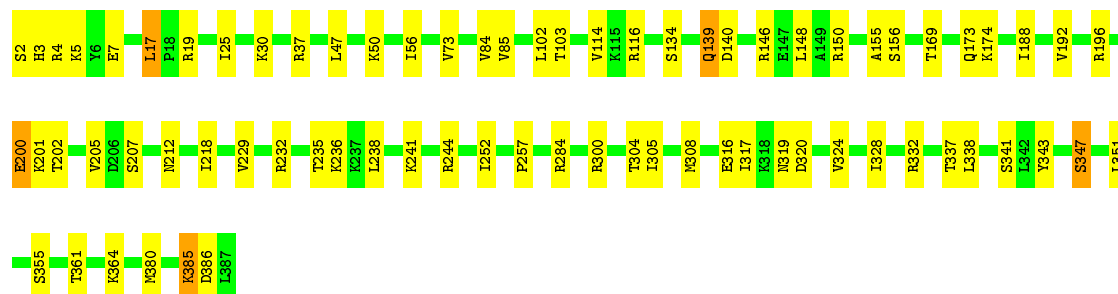
• Molecule 39: 60S ribosomal protein L2-A

Chain 12: 79% 19%

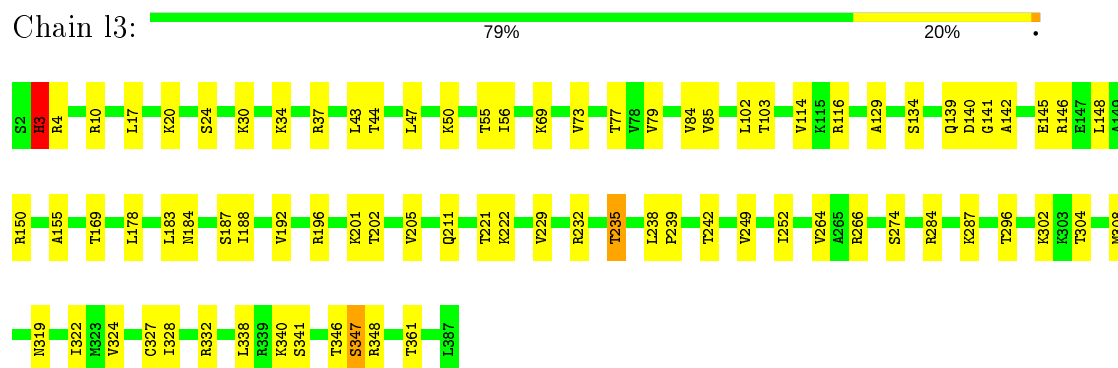


• Molecule 40: 60S ribosomal protein L3

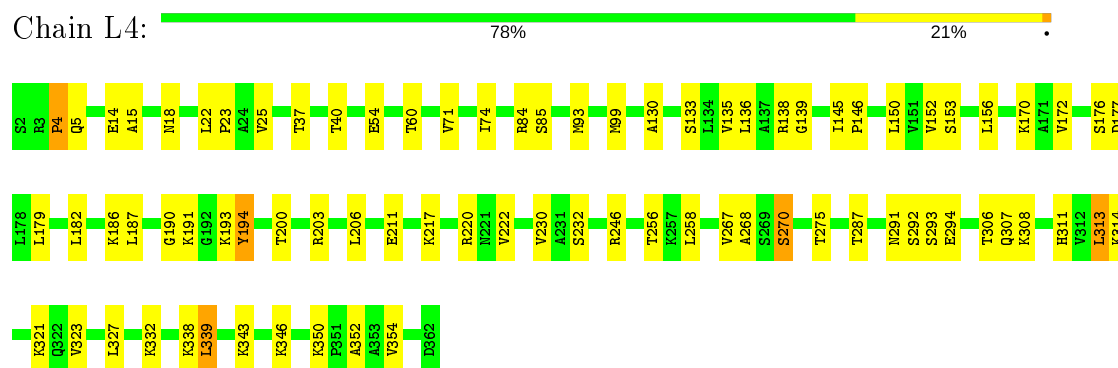
Chain L3: 81% 18%



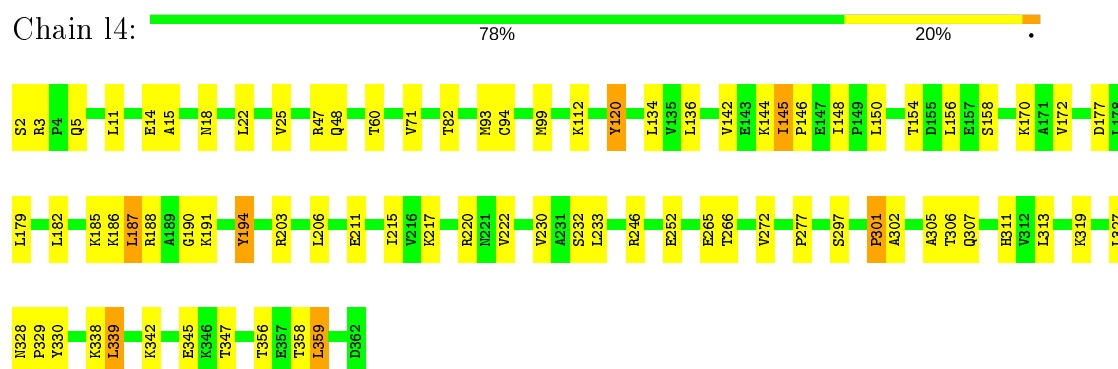
- Molecule 40: 60S ribosomal protein L3



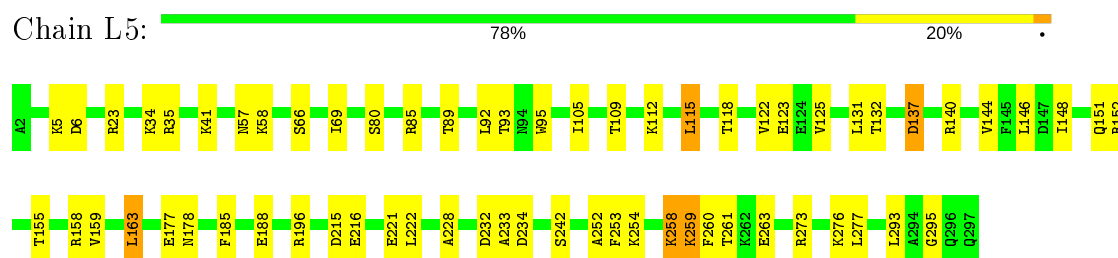
- Molecule 41: 60S ribosomal protein L4-A



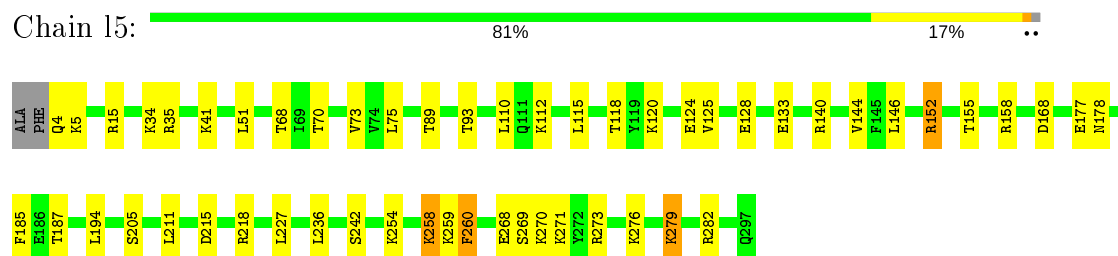
- Molecule 41: 60S ribosomal protein L4-A



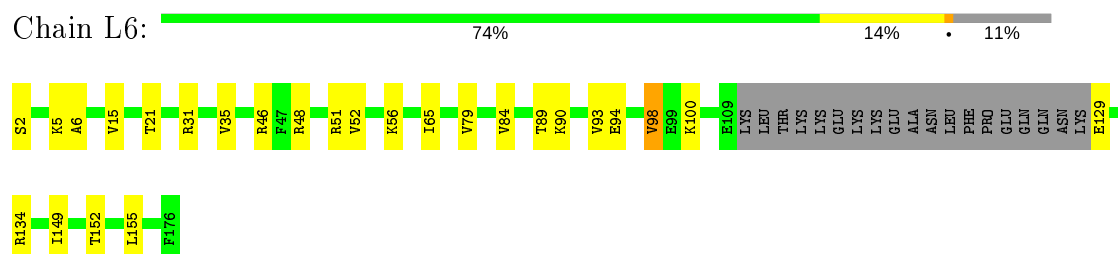
- Molecule 42: 60S ribosomal protein L5



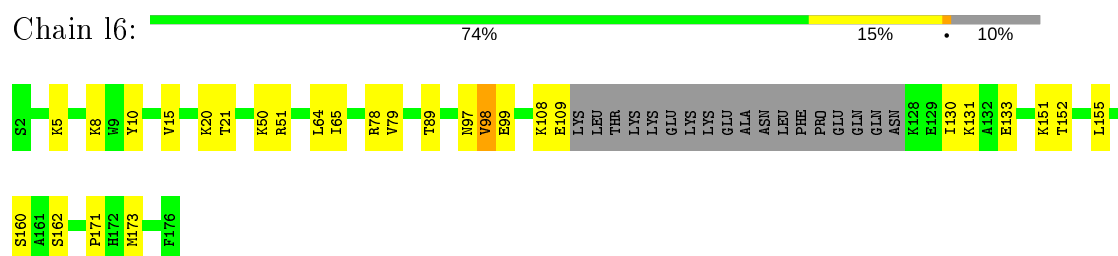
- Molecule 42: 60S ribosomal protein L5



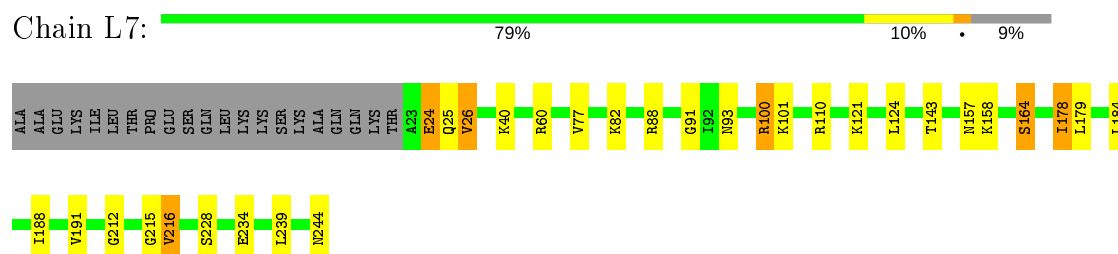
- Molecule 43: 60S ribosomal protein L6-A



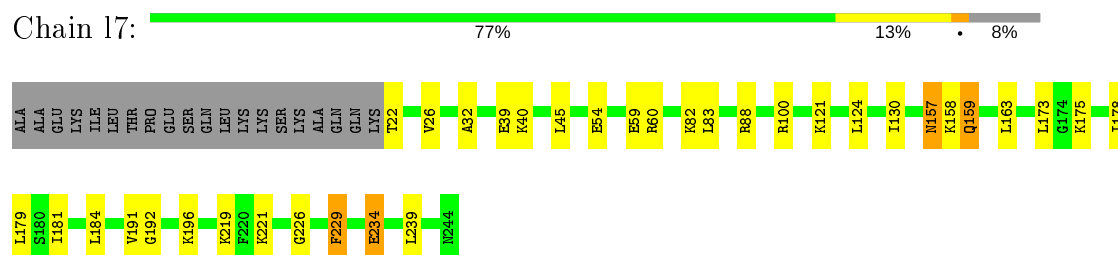
- Molecule 43: 60S ribosomal protein L6-A



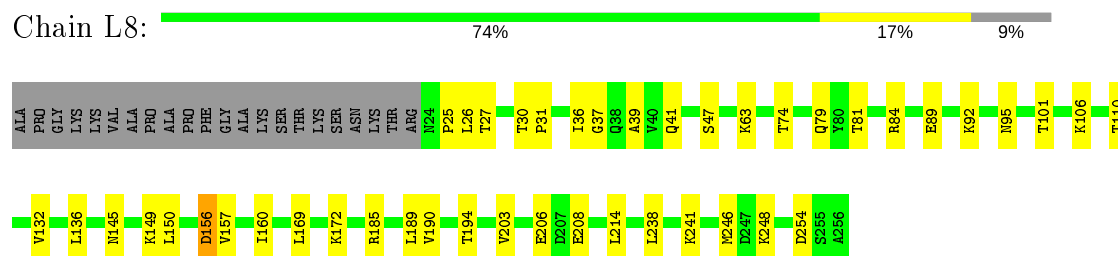
- Molecule 44: 60S ribosomal protein L7-A



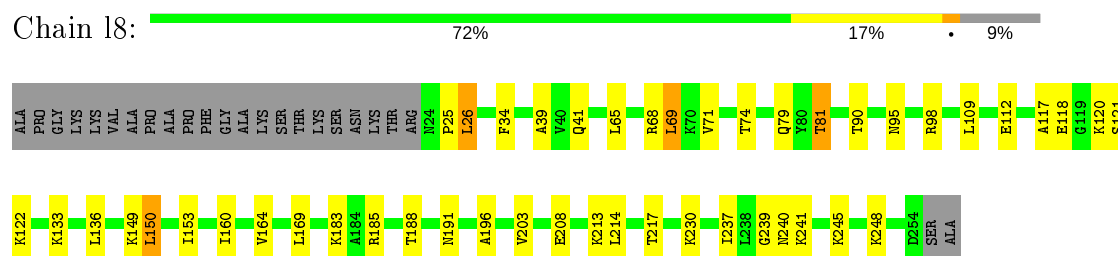
- Molecule 44: 60S ribosomal protein L7-A



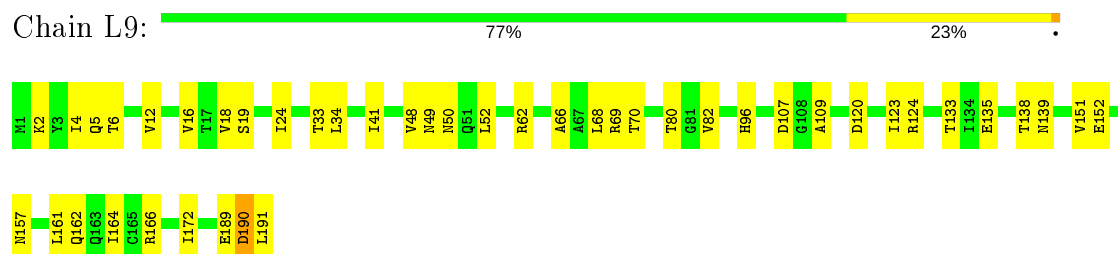
- Molecule 45: 60S ribosomal protein L8-A



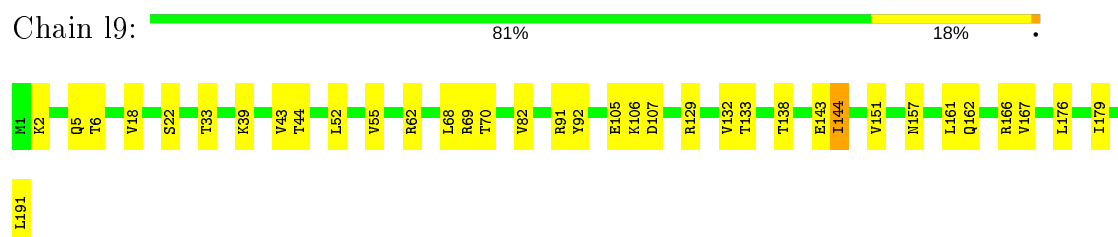
- Molecule 45: 60S ribosomal protein L8-A



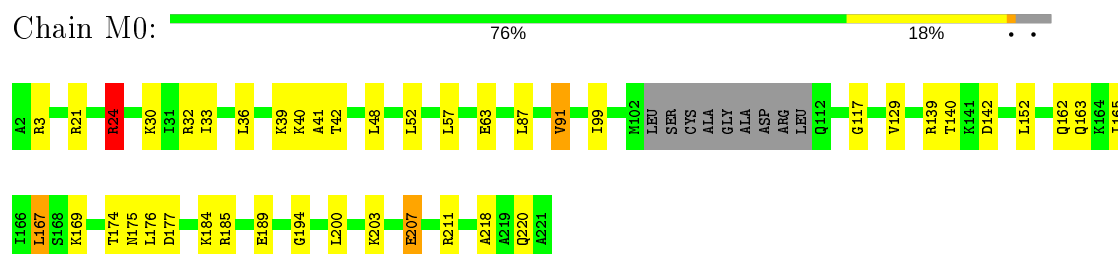
- Molecule 46: 60S ribosomal protein L9-A



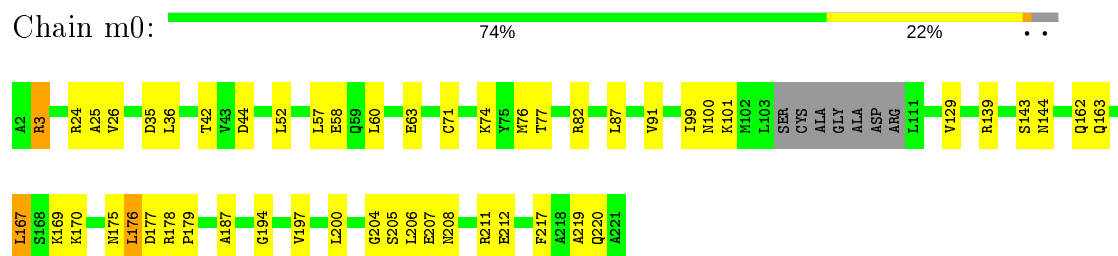
- Molecule 46: 60S ribosomal protein L9-A



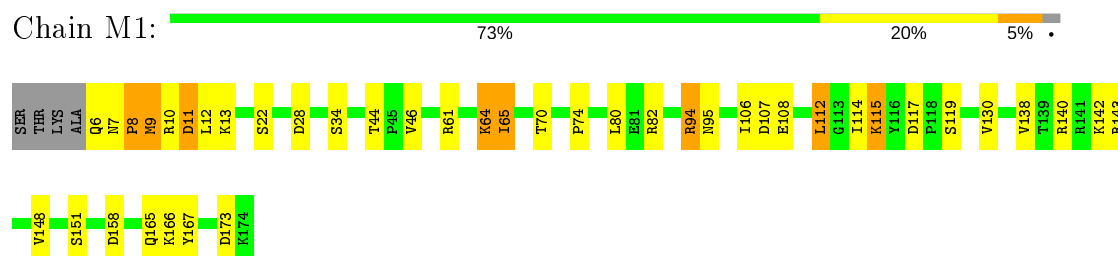
- Molecule 47: 60S ribosomal protein L10



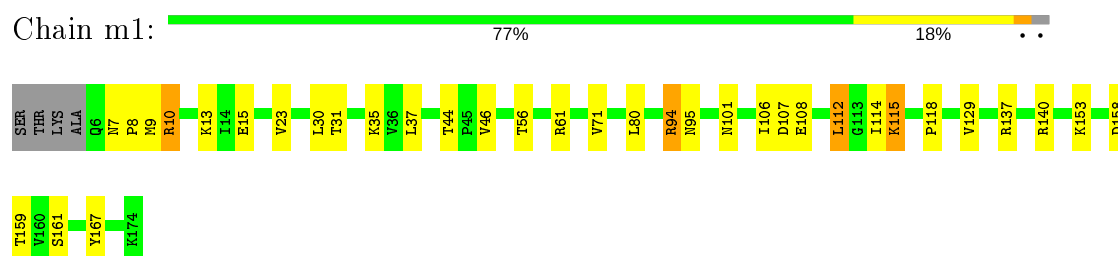
- Molecule 47: 60S ribosomal protein L10



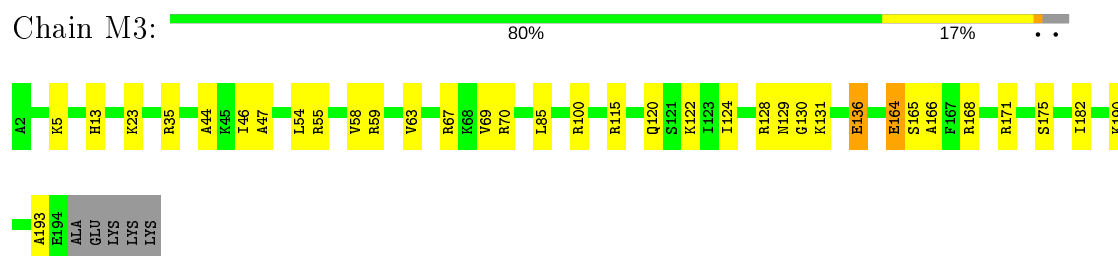
- Molecule 48: 60S ribosomal protein L11-B



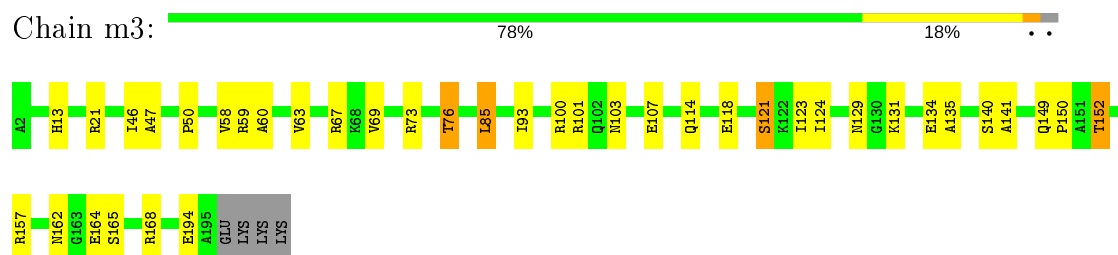
- Molecule 48: 60S ribosomal protein L11-B




- Molecule 49: 60S ribosomal protein L13-A



- Molecule 49: 60S ribosomal protein L13-A




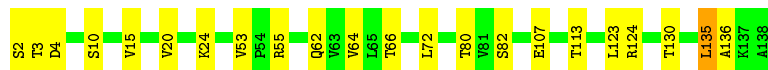
- Molecule 50: 60S ribosomal protein L14-A

Chain M4:  80% 18% ..




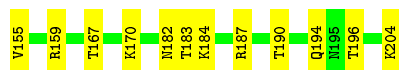
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:  84% 15% .




- Molecule 51: 60S ribosomal protein L15-A

Chain M5:  78% 22%




- Molecule 51: 60S ribosomal protein L15-A

Chain m5:  85% 14% .




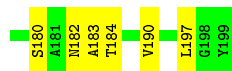
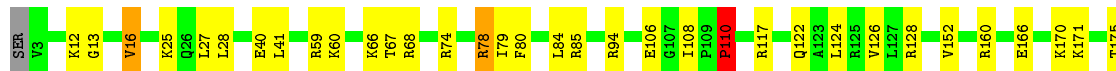
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:  83% 15% ..

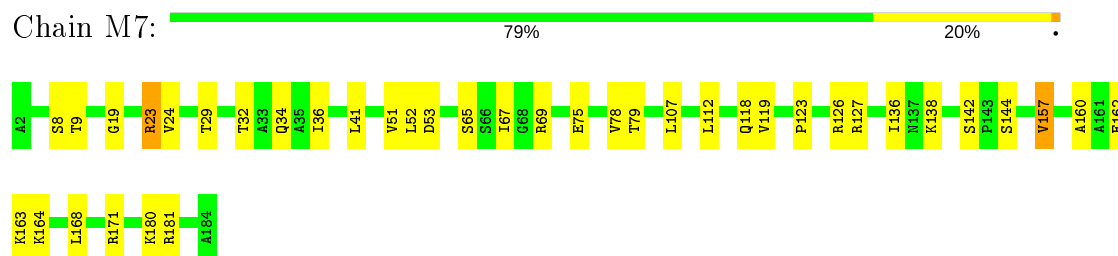


- Molecule 52: 60S ribosomal protein L16-A

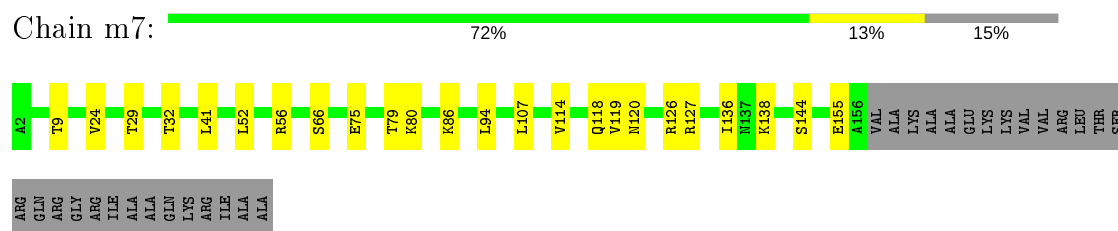
Chain m6:  79% 19% ...



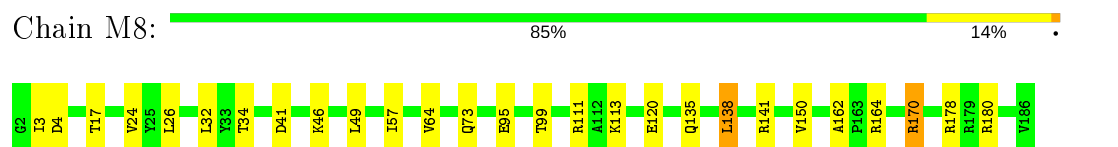
- Molecule 53: 60S ribosomal protein L17-A



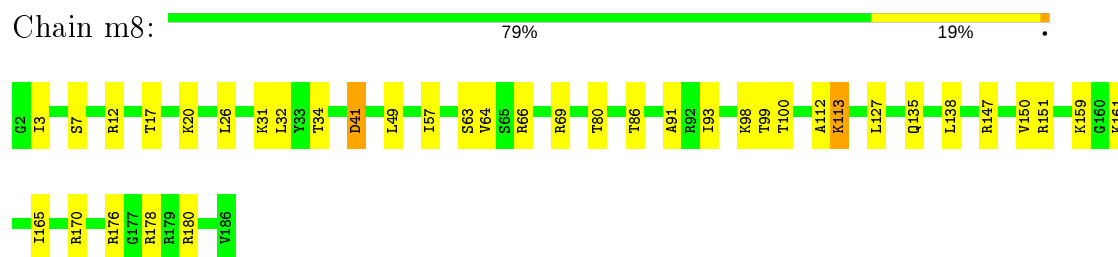
- Molecule 53: 60S ribosomal protein L17-A



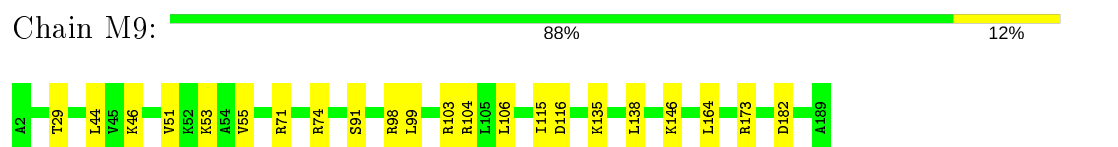
- Molecule 54: 60S ribosomal protein L18-A



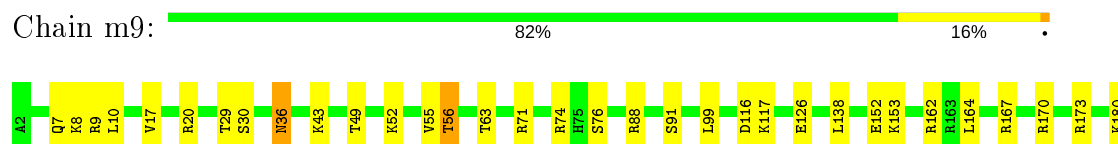
- Molecule 54: 60S ribosomal protein L18-A



- Molecule 55: 60S ribosomal protein L19-A



- Molecule 55: 60S ribosomal protein L19-A

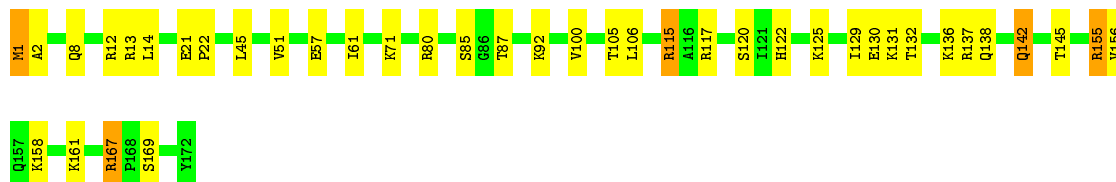






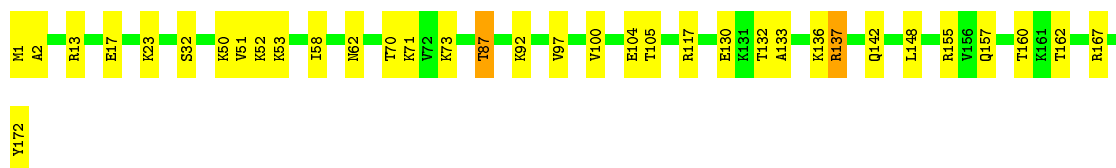
- Molecule 56: 60S ribosomal protein L20-A

Chain N0: 77% 20% .



- Molecule 56: 60S ribosomal protein L20-A

Chain n0: 80% 19% .



- Molecule 57: 60S ribosomal protein L21-A

Chain N1: 81% 17% .



- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 80% 19% .



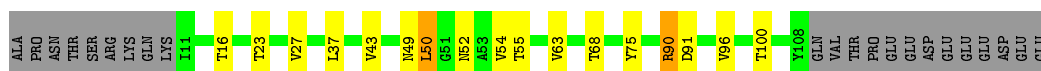
- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 69% 13% 17% .



- Molecule 58: 60S ribosomal protein L22-A

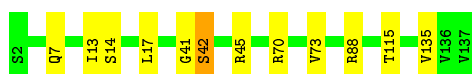
Chain n2: 68% 13% 18% .



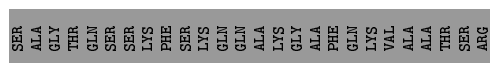
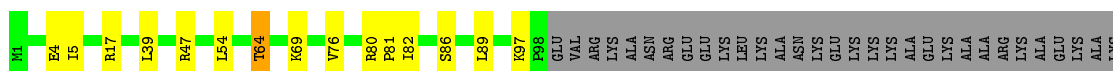
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 59: 60S ribosomal protein L23-A



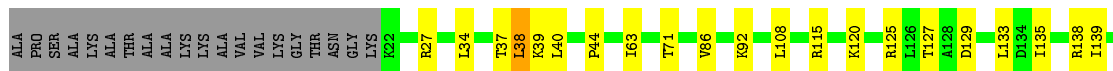
- Molecule 60: 60S ribosomal protein L24-A



- Molecule 60: 60S ribosomal protein L24-A

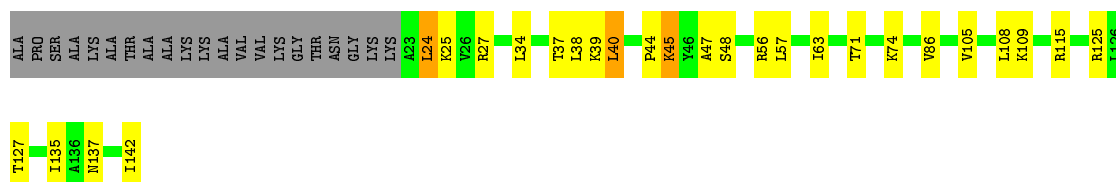


- Molecule 61: 60S ribosomal protein L25



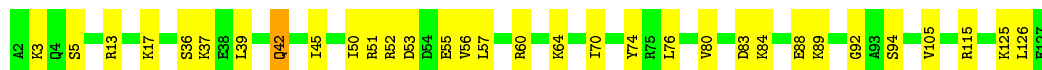
- Molecule 61: 60S ribosomal protein L25





- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 75% 25%



- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 75% 25%



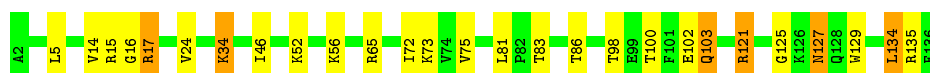
- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 81% 19%



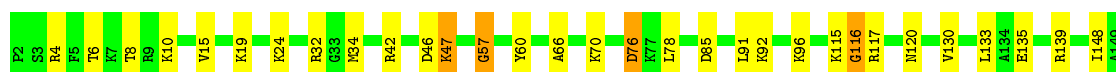
- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 80% 16%



- Molecule 64: 60S ribosomal protein L28

Chain N8: 79% 18%




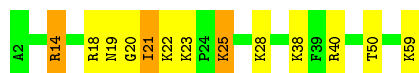
- Molecule 64: 60S ribosomal protein L28

Chain n8: 80% 18%




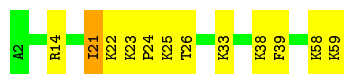
- Molecule 65: 60S ribosomal protein L29

Chain N9:  78% 17% 5%




- Molecule 65: 60S ribosomal protein L29

Chain n9:  79% 19% .




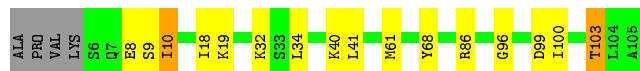
- Molecule 66: 60S ribosomal protein L30

Chain O0:  80% 13% . 7%




- Molecule 66: 60S ribosomal protein L30

Chain o0:  81% 13% . .



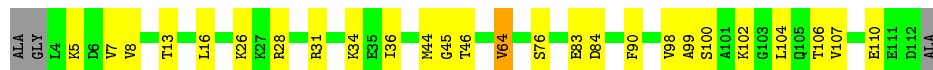
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  76% 19% . .




- Molecule 67: 60S ribosomal protein L31-A

Chain o1:  74% 22% . .




- Molecule 68: 60S ribosomal protein L32

Chain O2:  79% 18% . .



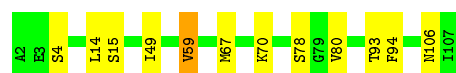
- Molecule 68: 60S ribosomal protein L32

Chain o2:  78% 18% ...




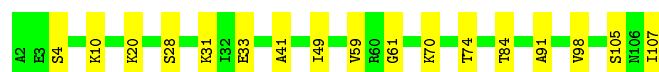
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  89% 10% .



- Molecule 69: 60S ribosomal protein L33-A

Chain o3:  84% 16%



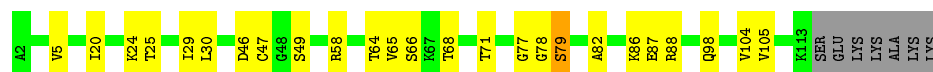
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  76% 16% . 6%




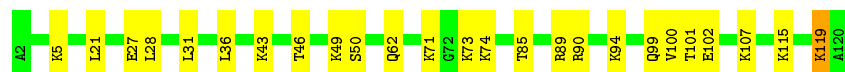
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  73% 20% . 6%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  79% 20% .




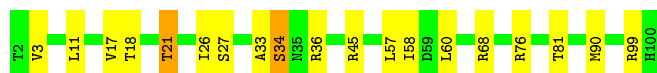
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  80% 19% .



- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  81% 17%




- Molecule 72: 60S ribosomal protein L36-A

Chain o6:  72% 25%




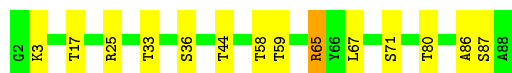
- Molecule 73: 60S ribosomal protein L37-A

Chain O7:  84% 15%




- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  84% 15%




- Molecule 74: 60S ribosomal protein L38

Chain O8:  77% 23%




- Molecule 74: 60S ribosomal protein L38

Chain o8:  78% 21%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  86% 14%




- Molecule 75: 60S ribosomal protein L39

Chain o9:  82% 16% .




- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  75% 23% .



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  75% 23% .



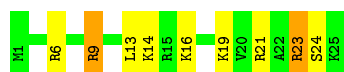
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  68% 28% .




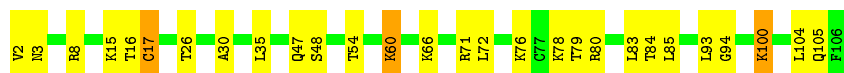
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  64% 28% 8% .




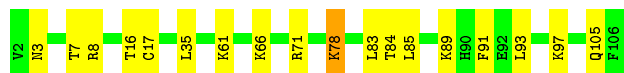
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  73% 24% .



- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  83% 16% .



- Molecule 79: 60S ribosomal protein L43-A

- 

- |    |  |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| A2 |  | K13 | E22 | K23 | K26 | K29 | L38 | T41 | R42 | R43 | F44 | V47 | T48 | L49 | V50 | N51 | R54 | R55 | P60 | S61 | V62 | Q63 |
|----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- |     |     |       |     |
|-----|-----|-------|-----|
| ARG | ALA | S85   | MET |
| ARG | GLU | ASN   | SER |
| ARG | ARG | THR   | ASN |
| GLY | ILE | ARG   | PRO |
| ARG | GLU | ARG   | PRO |
| GLY | THR | ALA   | ASP |
| ALA | ALA | THR   | LEU |
| ARG | GLU | ASP   | LEU |
| GLY | LYS | ARG   | ALA |
| GLY | GLU | HIS   | ASN |
| ASN | ALA | SER   | ASP |
| ASN | TYR | ARG   | VAL |
| THR | VAL | THR   | GLU |
| ALA | PRO | GLY   | ASP |
| ASN | ALA | LYS   | ALA |
| ALA | THR | THR   | ASP |
| THR | LYS | ASP   | VAL |
| ASN | VAL | THR   | VAL |
| SER | LYS | LYS   | VAL |
| ALA | ASN | LYS   | LEU |
| ASN | VAL | LYS   | PRO |
| THR | LYS | VAL   | PRO |
| VAL | SER | ASN   | K23 |
| GLN | LYS | GLN   |     |
| ASN | GLN | GLY   | T30 |
| ASN | LEU | THR   |     |
| ARG | LYS | GLY   | K33 |
| ASN | THR | ASP   |     |
| ILE | LYS | ASP   | A42 |
| ASP | GLU | LYS   | D43 |
| VAL | TYR | LYS   | P44 |
| SER | LEU | GLY   | S45 |
| ASN | GLU | LEU   | K46 |
| LEU | PHE | SER   | A47 |
| PRO | ASP | A119  | R48 |
| SER | ALA |       | K49 |
| LEU | THR | E139  | N50 |
| ALA | PHE | ASP   | R51 |
| VAL | VAL | ALA   | P52 |
| GLU | GLU | LYS   | R53 |
| SER | SER | GLY   | P54 |
| ASN | ASN | PRO   | S55 |
| THR | THR | LYS   |     |
| ARG | ARG | THR   | I61 |
| LYS | LYS | ALA   | R62 |
| ASN | ASN | GLN   | D63 |
| PHE | PHE | LEU   | K64 |
| GLY | GLY | SER   | T65 |
| ASP | ASP | LEU   | A66 |
| ARG | ARG | GLN   | G67 |
| ASN | ASN | ASP   | R68 |
| ASN | ASN | TYR   |     |
| ASN | ASN | L1455 | K74 |
| SER | SER |       | D75 |
| ARG | ARG | P167  | V76 |
| ASN | ASN |       | T77 |
| PHE | PHE | V172  | D78 |
| ASN | ASN | E173  |     |
| ASN | ASN | L174  | T82 |
| ASN | ASN | ASP   |     |

- [illegible]

- [illegible]





- Molecule 84: unknown protein chain p1

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 85: unknown protein chain p2

Chain p2:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	435.26Å 287.54Å 304.02Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	73.99 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (73.99-3.00)	Depositor
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.211 , 0.259	Depositor
Wilson B-factor (Å <sup>2</sup> )	64.9	Xtriage
Anisotropy	0.199	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	411211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

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

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3KD, 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	0.71	1/41698 (0.0%)	1.27	275/64972 (0.4%)
1	6	0.88	13/42765 (0.0%)	1.38	436/66634 (0.7%)
2	S0	0.43	0/1617	0.66	0/2215
2	s0	0.49	0/1623	0.71	0/2222
3	S1	0.35	0/1735	0.63	1/2335 (0.0%)
3	s1	0.48	0/1748	0.66	0/2352
4	S2	0.49	0/1665	0.67	0/2263
4	s2	0.57	0/1665	0.75	2/2263 (0.1%)
5	S3	0.48	0/1759	0.66	1/2368 (0.0%)
5	s3	0.42	0/1759	0.60	0/2368
6	S4	0.46	0/2109	0.73	1/2839 (0.0%)
6	s4	0.55	0/2109	0.78	1/2839 (0.0%)
7	S5	0.36	0/1629	0.58	0/2202
7	s5	0.44	0/1629	0.64	0/2202
8	S6	0.44	0/1823	0.64	0/2439
8	s6	0.54	0/1779	0.70	0/2379
9	S7	0.42	0/1506	0.65	0/2028
9	s7	0.45	0/1516	0.67	1/2043 (0.0%)
10	S8	0.54	0/1514	0.72	1/2021 (0.0%)
10	s8	0.60	0/1514	0.76	1/2021 (0.0%)
11	S9	0.47	0/1519	0.64	0/2035
11	s9	0.55	0/1519	0.76	2/2035 (0.1%)
12	C0	0.42	0/790	0.70	1/1069 (0.1%)
12	c0	0.36	0/777	0.63	3/1049 (0.3%)
13	C1	0.55	0/1240	0.66	0/1675
13	c1	0.61	0/1194	0.77	0/1610
14	C2	0.38	0/900	0.62	0/1224
14	c2	0.28	0/900	0.56	0/1224
15	C3	0.47	0/1215	0.68	2/1638 (0.1%)
15	c3	0.56	0/1215	0.73	0/1638
16	C4	0.36	0/901	0.63	0/1217
16	c4	0.52	0/960	0.72	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.44	0/998	0.68	0/1341
17	c5	0.45	0/1060	0.66	0/1426
18	C6	0.41	0/1125	0.69	2/1510 (0.1%)
18	c6	0.49	0/1131	0.69	0/1518
19	C7	0.41	0/935	0.62	0/1254
19	c7	0.48	0/914	0.71	0/1224
20	C8	0.42	0/1211	0.63	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.41	0/1130	0.63	0/1517
21	c9	0.50	0/1130	0.70	2/1517 (0.1%)
22	D0	0.45	0/865	0.64	0/1169
22	d0	0.46	0/892	0.65	0/1205
23	D1	0.44	0/693	0.62	0/935
23	d1	0.54	0/693	0.71	0/935
24	D2	0.48	0/1038	0.73	3/1395 (0.2%)
24	d2	0.59	0/1038	0.74	1/1395 (0.1%)
25	D3	0.60	0/1139	0.77	1/1518 (0.1%)
25	d3	0.70	0/1139	0.89	3/1518 (0.2%)
26	D4	0.44	0/1087	0.63	0/1449
26	d4	0.53	0/1087	0.73	0/1449
27	D5	0.39	0/571	0.68	0/768
27	d5	0.41	0/566	0.63	0/761
28	D6	0.43	0/782	0.67	0/1047
28	d6	0.56	0/782	0.71	0/1047
29	D7	0.42	0/620	0.66	0/838
29	d7	0.46	0/620	0.66	0/838
30	D8	0.35	0/499	0.57	0/670
30	d8	0.44	0/499	0.64	0/670
31	D9	0.50	0/452	0.70	1/600 (0.2%)
31	d9	0.50	0/452	0.64	0/600
32	E0	0.46	0/483	0.63	0/643
33	E1	0.42	0/577	0.78	0/770
33	e1	0.39	0/619	0.72	0/822
34	SR	0.37	0/2494	0.57	0/3393
34	sR	0.38	0/2495	0.56	0/3395
35	SM	0.48	0/1113	0.70	2/1502 (0.1%)
36	1	1.16	153/75394 (0.2%)	1.66	1837/117545 (1.6%)
36	5	1.20	178/75414 (0.2%)	1.67	1863/117575 (1.6%)
37	3	0.95	2/2883 (0.1%)	1.47	39/4491 (0.9%)
37	7	1.16	5/2883 (0.2%)	1.62	57/4491 (1.3%)
38	4	1.13	5/3746 (0.1%)	1.66	86/5832 (1.5%)
38	8	0.98	2/3746 (0.1%)	1.48	42/5832 (0.7%)
39	L2	0.74	0/1948	0.84	3/2617 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	l2	0.71	0/1946	0.86	2/2614 (0.1%)
40	L3	0.74	1/3146 (0.0%)	0.82	1/4228 (0.0%)
40	l3	0.88	1/3146 (0.0%)	0.89	2/4228 (0.0%)
41	L4	0.84	1/2800 (0.0%)	0.94	7/3790 (0.2%)
41	l4	0.74	1/2800 (0.0%)	0.90	6/3790 (0.2%)
42	L5	0.57	0/2425	0.69	1/3271 (0.0%)
42	l5	0.73	0/2408	0.82	1/3248 (0.0%)
43	L6	0.76	0/1260	0.84	0/1694
43	l6	0.78	0/1269	0.84	1/1705 (0.1%)
44	L7	0.78	1/1821 (0.1%)	0.90	2/2451 (0.1%)
44	l7	0.85	1/1828 (0.1%)	0.90	4/2461 (0.2%)
45	L8	0.55	0/1836	0.70	1/2481 (0.0%)
45	l8	0.51	0/1795	0.65	1/2429 (0.0%)
46	L9	0.65	0/1539	0.77	1/2073 (0.0%)
46	l9	0.77	0/1539	0.85	0/2073
47	M0	0.71	0/1741	0.84	3/2335 (0.1%)
47	m0	0.75	0/1758	0.87	2/2358 (0.1%)
48	M1	0.54	0/1374	0.73	1/1842 (0.1%)
48	m1	0.65	0/1374	0.82	2/1842 (0.1%)
49	M3	0.75	0/1568	0.86	0/2106
49	m3	0.69	0/1573	0.85	3/2113 (0.1%)
50	M4	0.73	0/1068	0.80	1/1438 (0.1%)
50	m4	0.82	0/1074	0.85	0/1446
51	M5	0.77	0/1757	0.85	0/2354
51	m5	0.66	0/1757	0.79	0/2354
52	M6	0.86	1/1585 (0.1%)	0.92	3/2128 (0.1%)
52	m6	1.02	5/1585 (0.3%)	0.98	7/2128 (0.3%)
53	M7	0.80	0/1443	0.85	2/1944 (0.1%)
53	m7	0.89	0/1250	0.89	0/1683
54	M8	0.79	0/1465	0.92	3/1965 (0.2%)
54	m8	0.73	0/1465	0.95	2/1965 (0.1%)
55	M9	0.57	0/1538	0.69	0/2050
55	m9	0.61	0/1538	0.70	0/2050
56	N0	0.78	0/1481	0.87	4/1990 (0.2%)
56	n0	0.87	0/1481	0.91	2/1990 (0.1%)
57	N1	0.78	0/1300	0.82	0/1743
57	n1	0.85	1/1300 (0.1%)	0.86	1/1743 (0.1%)
58	N2	0.42	0/812	0.62	0/1099
58	n2	0.51	0/794	0.65	0/1076
59	N3	0.70	0/1018	0.81	0/1369
59	n3	0.87	0/1018	0.98	1/1369 (0.1%)
60	N4	0.56	0/712	0.68	0/958
60	n4	0.69	0/1052	0.75	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	N5	0.63	0/979	0.80	2/1321 (0.2%)
61	n5	0.65	0/974	0.77	0/1314
62	N6	0.68	0/1004	0.90	1/1341 (0.1%)
62	n6	0.71	1/1004 (0.1%)	0.84	0/1341
63	N7	0.52	0/1118	0.66	0/1497
63	n7	0.46	0/1118	0.63	0/1497
64	N8	0.82	0/1204	0.92	2/1612 (0.1%)
64	n8	0.79	0/1204	0.90	0/1612
65	N9	0.67	0/473	0.83	2/629 (0.3%)
65	n9	0.80	0/473	0.97	0/629
66	O0	0.48	0/751	0.66	0/1008
66	o0	0.49	0/775	0.65	0/1040
67	O1	0.60	0/890	0.72	0/1196
67	o1	0.76	0/897	0.86	0/1205
68	O2	0.85	0/1041	0.89	2/1394 (0.1%)
68	o2	0.82	0/1041	0.94	2/1394 (0.1%)
69	O3	0.95	0/868	0.91	1/1168 (0.1%)
69	o3	0.92	0/868	0.84	0/1168
70	O4	0.58	0/890	0.82	4/1189 (0.3%)
70	o4	0.59	0/890	0.78	0/1189
71	O5	0.70	0/978	0.81	1/1301 (0.1%)
71	o5	0.59	0/974	0.72	0/1297
72	O6	0.64	0/778	0.79	0/1034
72	o6	0.54	0/777	0.73	0/1033
73	O7	0.78	0/696	0.90	1/923 (0.1%)
73	o7	0.75	0/696	0.85	1/923 (0.1%)
74	O8	0.51	0/618	0.64	0/826
74	o8	0.42	0/614	0.61	0/822
75	O9	0.83	1/443 (0.2%)	0.90	0/588
75	o9	0.76	0/443	0.83	0/588
76	Q0	0.73	0/423	0.84	0/562
76	q0	0.95	0/423	1.03	1/562 (0.2%)
77	Q1	0.72	0/234	0.96	1/300 (0.3%)
77	q1	0.82	0/234	1.05	2/300 (0.7%)
78	Q2	0.93	1/860 (0.1%)	0.85	1/1136 (0.1%)
78	q2	0.82	1/860 (0.1%)	0.83	0/1136
79	Q3	0.74	0/701	0.85	0/934
79	q3	0.72	0/701	0.81	0/934
80	e0	0.56	0/499	0.74	0/665
81	sM	0.50	0/684	0.69	1/925 (0.1%)
83	p0	0.46	0/1092	0.61	0/1474
All	All	0.90	376/430075 (0.1%)	1.30	4764/631366 (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
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
18	c6	0	1
19	C7	0	2
22	d0	0	1
27	D5	0	2
28	D6	0	1
33	E1	0	1
39	l2	0	1
42	l5	0	2
43	L6	0	1
43	l6	0	1
44	l7	0	2
45	L8	0	1
48	M1	0	2
51	M5	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
55	m9	0	1
56	N0	0	2
56	n0	0	2
57	N1	0	1
62	n6	0	1
64	N8	0	1
64	n8	0	2
65	N9	0	1
67	O1	0	1
67	o1	0	2
All	All	0	43

The worst 5 of 376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	15.91	2.09	1.82
36	5	1152	G	N9-C4	-12.55	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	11.87	2.02	1.82
36	1	3181	C	N3-C4	-9.25	1.27	1.33
36	5	2138	A	N7-C5	-8.87	1.33	1.39

The worst 5 of 4764 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	24.25	140.73	128.60
36	5	1152	G	N3-C4-N9	-22.33	112.60	126.00
36	5	1152	G	C2-N3-C4	-20.90	101.45	111.90
36	1	2945	G	O5'-P-OP2	-17.25	90.00	110.70
36	1	1308	A	O5'-P-OP2	-17.00	90.30	110.70

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
19	C7	22	PRO	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	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%)	152 (74%)	31 (15%)	21 (10%)	<b>0</b> <b>2</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	s0	204/251 (81%)	153 (75%)	26 (13%)	25 (12%)	0	1
3	S1	212/254 (84%)	146 (69%)	39 (18%)	27 (13%)	0	1
3	s1	214/254 (84%)	177 (83%)	26 (12%)	11 (5%)	2	12
4	S2	215/253 (85%)	187 (87%)	17 (8%)	11 (5%)	2	12
4	s2	215/253 (85%)	186 (86%)	16 (7%)	13 (6%)	1	9
5	S3	221/239 (92%)	179 (81%)	29 (13%)	13 (6%)	1	9
5	s3	221/239 (92%)	183 (83%)	19 (9%)	19 (9%)	1	3
6	S4	258/260 (99%)	206 (80%)	41 (16%)	11 (4%)	2	15
6	s4	258/260 (99%)	216 (84%)	24 (9%)	18 (7%)	1	6
7	S5	204/224 (91%)	158 (78%)	32 (16%)	14 (7%)	1	6
7	s5	204/224 (91%)	164 (80%)	25 (12%)	15 (7%)	1	5
8	S6	224/236 (95%)	194 (87%)	17 (8%)	13 (6%)	1	10
8	s6	216/236 (92%)	189 (88%)	15 (7%)	12 (6%)	2	10
9	S7	182/189 (96%)	137 (75%)	25 (14%)	20 (11%)	0	2
9	s7	184/189 (97%)	148 (80%)	21 (11%)	15 (8%)	1	4
10	S8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	2	13
10	s8	184/200 (92%)	163 (89%)	16 (9%)	5 (3%)	5	26
11	S9	183/196 (93%)	151 (82%)	23 (13%)	9 (5%)	2	13
11	s9	183/196 (93%)	140 (76%)	34 (19%)	9 (5%)	2	13
12	C0	94/105 (90%)	68 (72%)	15 (16%)	11 (12%)	0	1
12	c0	92/105 (88%)	64 (70%)	14 (15%)	14 (15%)	0	1
13	C1	153/155 (99%)	126 (82%)	16 (10%)	11 (7%)	1	5
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	1	7
14	C2	122/142 (86%)	70 (57%)	25 (20%)	27 (22%)	0	0
14	c2	122/142 (86%)	68 (56%)	32 (26%)	22 (18%)	0	0
15	C3	148/150 (99%)	123 (83%)	18 (12%)	7 (5%)	2	14
15	c3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	5
16	C4	125/136 (92%)	94 (75%)	15 (12%)	16 (13%)	0	1
16	c4	126/136 (93%)	101 (80%)	16 (13%)	9 (7%)	1	5
17	C5	122/141 (86%)	88 (72%)	23 (19%)	11 (9%)	1	3
17	c5	133/141 (94%)	92 (69%)	22 (16%)	19 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	116 (84%)	16 (12%)	7 (5%)	2	12
18	c6	140/142 (99%)	116 (83%)	16 (11%)	8 (6%)	1	10
19	C7	116/136 (85%)	91 (78%)	13 (11%)	12 (10%)	0	2
19	c7	113/136 (83%)	87 (77%)	18 (16%)	8 (7%)	1	5
20	C8	143/145 (99%)	115 (80%)	16 (11%)	12 (8%)	1	4
20	c8	143/145 (99%)	114 (80%)	20 (14%)	9 (6%)	1	7
21	C9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	5	25
21	c9	141/143 (99%)	119 (84%)	16 (11%)	6 (4%)	2	15
22	D0	105/120 (88%)	88 (84%)	13 (12%)	4 (4%)	3	18
22	d0	108/120 (90%)	82 (76%)	16 (15%)	10 (9%)	0	3
23	D1	85/87 (98%)	61 (72%)	16 (19%)	8 (9%)	0	3
23	d1	85/87 (98%)	72 (85%)	8 (9%)	5 (6%)	1	9
24	D2	127/129 (98%)	106 (84%)	19 (15%)	2 (2%)	9	40
24	d2	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	19	57
25	D3	142/144 (99%)	113 (80%)	19 (13%)	10 (7%)	1	6
25	d3	142/144 (99%)	123 (87%)	16 (11%)	3 (2%)	7	33
26	D4	132/134 (98%)	103 (78%)	20 (15%)	9 (7%)	1	6
26	d4	132/134 (98%)	103 (78%)	21 (16%)	8 (6%)	1	8
27	D5	68/107 (64%)	47 (69%)	9 (13%)	12 (18%)	0	0
27	d5	67/107 (63%)	52 (78%)	9 (13%)	6 (9%)	1	3
28	D6	95/97 (98%)	59 (62%)	18 (19%)	18 (19%)	0	0
28	d6	95/97 (98%)	74 (78%)	12 (13%)	9 (10%)	0	3
29	D7	79/81 (98%)	66 (84%)	8 (10%)	5 (6%)	1	7
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1	3
30	D8	61/66 (92%)	51 (84%)	6 (10%)	4 (7%)	1	6
30	d8	61/66 (92%)	42 (69%)	15 (25%)	4 (7%)	1	6
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	17
31	d9	51/55 (93%)	41 (80%)	6 (12%)	4 (8%)	1	4
32	E0	58/60 (97%)	44 (76%)	12 (21%)	2 (3%)	3	20
33	E1	69/76 (91%)	36 (52%)	17 (25%)	16 (23%)	0	0
33	e1	74/76 (97%)	36 (49%)	17 (23%)	21 (28%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	271 (86%)	35 (11%)	10 (3%)	4	22
34	sR	316/318 (99%)	270 (85%)	36 (11%)	10 (3%)	4	22
35	SM	155/273 (57%)	113 (73%)	23 (15%)	19 (12%)	0	1
39	L2	250/253 (99%)	223 (89%)	21 (8%)	6 (2%)	6	29
39	l2	250/253 (99%)	210 (84%)	30 (12%)	10 (4%)	3	17
40	L3	384/386 (100%)	326 (85%)	45 (12%)	13 (3%)	3	20
40	l3	384/386 (100%)	340 (88%)	32 (8%)	12 (3%)	4	23
41	L4	359/361 (99%)	299 (83%)	43 (12%)	17 (5%)	2	14
41	l4	359/361 (99%)	300 (84%)	39 (11%)	20 (6%)	2	10
42	L5	294/296 (99%)	242 (82%)	31 (10%)	21 (7%)	1	5
42	l5	292/296 (99%)	255 (87%)	30 (10%)	7 (2%)	6	29
43	L6	152/175 (87%)	132 (87%)	16 (10%)	4 (3%)	5	27
43	l6	153/175 (87%)	129 (84%)	20 (13%)	4 (3%)	5	27
44	L7	220/243 (90%)	198 (90%)	12 (6%)	10 (4%)	2	14
44	l7	221/243 (91%)	195 (88%)	20 (9%)	6 (3%)	5	26
45	L8	231/255 (91%)	188 (81%)	35 (15%)	8 (4%)	3	20
45	l8	229/255 (90%)	188 (82%)	21 (9%)	20 (9%)	1	3
46	L9	189/191 (99%)	167 (88%)	15 (8%)	7 (4%)	3	19
46	l9	189/191 (99%)	171 (90%)	15 (8%)	3 (2%)	9	40
47	M0	207/220 (94%)	178 (86%)	18 (9%)	11 (5%)	2	11
47	m0	209/220 (95%)	167 (80%)	27 (13%)	15 (7%)	1	5
48	M1	167/173 (96%)	131 (78%)	21 (13%)	15 (9%)	1	3
48	m1	167/173 (96%)	139 (83%)	16 (10%)	12 (7%)	1	5
49	M3	191/198 (96%)	164 (86%)	16 (8%)	11 (6%)	1	10
49	m3	192/198 (97%)	159 (83%)	17 (9%)	16 (8%)	1	4
50	M4	134/137 (98%)	117 (87%)	12 (9%)	5 (4%)	3	19
50	m4	135/137 (98%)	122 (90%)	10 (7%)	3 (2%)	6	31
51	M5	201/203 (99%)	181 (90%)	12 (6%)	8 (4%)	3	17
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	4	24
52	M6	195/198 (98%)	181 (93%)	11 (6%)	3 (2%)	10	42
52	m6	195/198 (98%)	179 (92%)	8 (4%)	8 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	M7	181/183 (99%)	152 (84%)	22 (12%)	7 (4%)	3	17
53	m7	153/183 (84%)	138 (90%)	13 (8%)	2 (1%)	12	45
54	M8	183/185 (99%)	165 (90%)	14 (8%)	4 (2%)	6	31
54	m8	183/185 (99%)	155 (85%)	22 (12%)	6 (3%)	4	21
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
55	m9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
56	N0	170/172 (99%)	150 (88%)	15 (9%)	5 (3%)	4	24
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	25	64
57	N1	157/159 (99%)	133 (85%)	18 (12%)	6 (4%)	3	18
57	n1	157/159 (99%)	141 (90%)	12 (8%)	4 (2%)	5	28
58	N2	98/120 (82%)	76 (78%)	17 (17%)	5 (5%)	2	12
58	n2	96/120 (80%)	77 (80%)	13 (14%)	6 (6%)	1	7
59	N3	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	22	60
59	n3	134/136 (98%)	121 (90%)	11 (8%)	2 (2%)	10	42
60	N4	96/155 (62%)	74 (77%)	13 (14%)	9 (9%)	0	3
60	n4	133/155 (86%)	107 (80%)	17 (13%)	9 (7%)	1	6
61	N5	119/141 (84%)	106 (89%)	12 (10%)	1 (1%)	19	57
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	1	5
62	N6	124/126 (98%)	110 (89%)	8 (6%)	6 (5%)	2	13
62	n6	124/126 (98%)	113 (91%)	7 (6%)	4 (3%)	4	22
63	N7	133/135 (98%)	109 (82%)	18 (14%)	6 (4%)	2	14
63	n7	133/135 (98%)	104 (78%)	18 (14%)	11 (8%)	1	4
64	N8	146/148 (99%)	121 (83%)	15 (10%)	10 (7%)	1	6
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	3	20
65	N9	56/58 (97%)	48 (86%)	6 (11%)	2 (4%)	3	19
65	n9	56/58 (97%)	40 (71%)	12 (21%)	4 (7%)	1	5
66	O0	95/104 (91%)	89 (94%)	4 (4%)	2 (2%)	7	33
66	o0	98/104 (94%)	88 (90%)	6 (6%)	4 (4%)	3	16
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	2	14
67	o1	107/112 (96%)	90 (84%)	12 (11%)	5 (5%)	2	14
68	O2	125/129 (97%)	112 (90%)	10 (8%)	3 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	o2	125/129 (97%)	106 (85%)	13 (10%)	6 (5%)	2	13
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	4	24
69	o3	104/106 (98%)	92 (88%)	8 (8%)	4 (4%)	3	18
70	O4	110/119 (92%)	97 (88%)	12 (11%)	1 (1%)	17	55
70	o4	110/119 (92%)	93 (84%)	11 (10%)	6 (6%)	2	10
71	O5	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	17	55
71	o5	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	9	39
72	O6	97/99 (98%)	77 (79%)	15 (16%)	5 (5%)	2	12
72	o6	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	5
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	3	20
73	o7	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	6	29
74	O8	75/77 (97%)	62 (83%)	11 (15%)	2 (3%)	5	26
74	o8	75/77 (97%)	60 (80%)	11 (15%)	4 (5%)	2	11
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	33
75	o9	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	33
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	34
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	15
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	1	10
78	q2	103/105 (98%)	92 (89%)	10 (10%)	1 (1%)	15	53
79	Q3	89/91 (98%)	77 (86%)	8 (9%)	4 (4%)	2	14
79	q3	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	14	50
80	e0	60/62 (97%)	43 (72%)	11 (18%)	6 (10%)	0	2
81	sM	98/273 (36%)	62 (63%)	22 (22%)	14 (14%)	0	1
83	p0	139/311 (45%)	120 (86%)	15 (11%)	4 (3%)	4	24
All	All	22333/24141 (92%)	18562 (83%)	2524 (11%)	1247 (6%)	2	10

5 of 1247 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%)	133 (81%)	31 (19%)	1	8
2	s0	165/209 (79%)	131 (79%)	34 (21%)	1	6
3	S1	191/223 (86%)	155 (81%)	36 (19%)	1	8
3	s1	192/223 (86%)	163 (85%)	29 (15%)	3	14
4	S2	176/204 (86%)	142 (81%)	34 (19%)	1	8
4	s2	176/204 (86%)	133 (76%)	43 (24%)	0	3
5	S3	182/194 (94%)	145 (80%)	37 (20%)	1	6
5	s3	182/194 (94%)	151 (83%)	31 (17%)	2	10
6	S4	221/221 (100%)	183 (83%)	38 (17%)	2	10
6	s4	221/221 (100%)	183 (83%)	38 (17%)	2	10
7	S5	173/190 (91%)	142 (82%)	31 (18%)	2	9
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1	4
8	S6	188/201 (94%)	148 (79%)	40 (21%)	1	5
8	s6	187/201 (93%)	151 (81%)	36 (19%)	1	8
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3	14
9	s7	165/169 (98%)	138 (84%)	27 (16%)	2	11
10	S8	150/161 (93%)	130 (87%)	20 (13%)	4	17
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	15
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	4
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	8
12	C0	77/98 (79%)	67 (87%)	10 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c0	73/98 (74%)	63 (86%)	10 (14%)	3	17
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2	10
13	c1	129/136 (95%)	106 (82%)	23 (18%)	2	9
14	C2	88/118 (75%)	66 (75%)	22 (25%)	0	3
14	c2	88/118 (75%)	66 (75%)	22 (25%)	0	3
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	5
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	8
16	C4	81/104 (78%)	60 (74%)	21 (26%)	0	2
16	c4	97/104 (93%)	76 (78%)	21 (22%)	1	5
17	C5	101/117 (86%)	85 (84%)	16 (16%)	2	12
17	c5	103/117 (88%)	84 (82%)	19 (18%)	1	9
18	C6	117/118 (99%)	94 (80%)	23 (20%)	1	7
18	c6	118/118 (100%)	93 (79%)	25 (21%)	1	5
19	C7	94/124 (76%)	72 (77%)	22 (23%)	1	4
19	c7	92/124 (74%)	78 (85%)	14 (15%)	3	14
20	C8	128/128 (100%)	95 (74%)	33 (26%)	0	2
20	c8	128/128 (100%)	103 (80%)	25 (20%)	1	7
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	7
21	c9	115/115 (100%)	93 (81%)	22 (19%)	1	8
22	D0	100/113 (88%)	78 (78%)	22 (22%)	1	4
22	d0	103/113 (91%)	78 (76%)	25 (24%)	0	3
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	10
23	d1	74/74 (100%)	56 (76%)	18 (24%)	0	3
24	D2	110/110 (100%)	94 (86%)	16 (14%)	3	15
24	d2	110/110 (100%)	93 (84%)	17 (16%)	2	13
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	10
25	d3	119/119 (100%)	104 (87%)	15 (13%)	4	20
26	D4	112/112 (100%)	93 (83%)	19 (17%)	2	10
26	d4	112/112 (100%)	94 (84%)	18 (16%)	2	12
27	D5	61/88 (69%)	46 (75%)	15 (25%)	0	3
27	d5	61/88 (69%)	51 (84%)	10 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	D6	83/83 (100%)	67 (81%)	16 (19%)	1	8
28	d6	83/83 (100%)	73 (88%)	10 (12%)	5	22
29	D7	70/70 (100%)	64 (91%)	6 (9%)	10	37
29	d7	70/70 (100%)	60 (86%)	10 (14%)	3	15
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	5
30	d8	56/59 (95%)	44 (79%)	12 (21%)	1	5
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	10
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	5
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1	7
33	E1	62/66 (94%)	46 (74%)	16 (26%)	0	2
33	e1	66/66 (100%)	51 (77%)	15 (23%)	1	4
34	SR	260/261 (100%)	222 (85%)	38 (15%)	3	15
34	sR	260/261 (100%)	233 (90%)	27 (10%)	7	27
35	SM	97/228 (42%)	76 (78%)	21 (22%)	1	5
39	L2	193/195 (99%)	150 (78%)	43 (22%)	1	4
39	l2	192/195 (98%)	152 (79%)	40 (21%)	1	5
40	L3	321/322 (100%)	257 (80%)	64 (20%)	1	7
40	l3	320/322 (99%)	251 (78%)	69 (22%)	1	5
41	L4	288/288 (100%)	228 (79%)	60 (21%)	1	5
41	l4	288/288 (100%)	229 (80%)	59 (20%)	1	6
42	L5	244/244 (100%)	197 (81%)	47 (19%)	1	8
42	l5	243/244 (100%)	196 (81%)	47 (19%)	1	8
43	L6	134/152 (88%)	112 (84%)	22 (16%)	2	11
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	10
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	19
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3	15
45	L8	187/207 (90%)	152 (81%)	35 (19%)	1	8
45	l8	177/207 (86%)	147 (83%)	30 (17%)	2	11
46	L9	171/171 (100%)	134 (78%)	37 (22%)	1	5
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	7
47	M0	177/186 (95%)	143 (81%)	34 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	6
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	5
48	m1	147/150 (98%)	122 (83%)	25 (17%)	2	10
49	M3	154/158 (98%)	128 (83%)	26 (17%)	2	11
49	m3	154/158 (98%)	130 (84%)	24 (16%)	2	13
50	M4	107/108 (99%)	84 (78%)	23 (22%)	1	5
50	m4	108/108 (100%)	88 (82%)	20 (18%)	1	8
51	M5	175/175 (100%)	138 (79%)	37 (21%)	1	5
51	m5	175/175 (100%)	149 (85%)	26 (15%)	3	14
52	M6	160/161 (99%)	133 (83%)	27 (17%)	2	11
52	m6	160/161 (99%)	132 (82%)	28 (18%)	2	10
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	4
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	10
54	M8	150/150 (100%)	128 (85%)	22 (15%)	3	15
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	5
55	M9	153/153 (100%)	132 (86%)	21 (14%)	3	17
55	m9	153/153 (100%)	120 (78%)	33 (22%)	1	5
56	N0	156/156 (100%)	121 (78%)	35 (22%)	1	4
56	n0	156/156 (100%)	124 (80%)	32 (20%)	1	6
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	6
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	6
58	N2	87/106 (82%)	74 (85%)	13 (15%)	3	14
58	n2	85/106 (80%)	72 (85%)	13 (15%)	2	13
59	N3	104/104 (100%)	86 (83%)	18 (17%)	2	10
59	n3	104/104 (100%)	94 (90%)	10 (10%)	8	32
60	N4	57/129 (44%)	50 (88%)	7 (12%)	4	21
60	n4	100/129 (78%)	82 (82%)	18 (18%)	1	9
61	N5	104/117 (89%)	84 (81%)	20 (19%)	1	8
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	6
62	N6	109/109 (100%)	83 (76%)	26 (24%)	0	3
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	N7	115/115 (100%)	94 (82%)	21 (18%)	1	9
63	n7	115/115 (100%)	93 (81%)	22 (19%)	1	8
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1	8
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1	5
65	N9	46/46 (100%)	35 (76%)	11 (24%)	0	3
65	n9	46/46 (100%)	37 (80%)	9 (20%)	1	7
66	O0	81/87 (93%)	68 (84%)	13 (16%)	2	12
66	o0	84/87 (97%)	70 (83%)	14 (17%)	2	11
67	O1	92/96 (96%)	71 (77%)	21 (23%)	1	4
67	o1	94/96 (98%)	74 (79%)	20 (21%)	1	5
68	O2	109/110 (99%)	87 (80%)	22 (20%)	1	6
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	4
69	O3	90/90 (100%)	81 (90%)	9 (10%)	7	29
69	o3	90/90 (100%)	77 (86%)	13 (14%)	3	15
70	O4	95/101 (94%)	74 (78%)	21 (22%)	1	4
70	o4	95/101 (94%)	75 (79%)	20 (21%)	1	5
71	O5	104/104 (100%)	80 (77%)	24 (23%)	1	4
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1	4
72	O6	81/81 (100%)	65 (80%)	16 (20%)	1	7
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	10
73	o7	70/70 (100%)	58 (83%)	12 (17%)	2	10
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	3
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1	5
75	O9	45/45 (100%)	40 (89%)	5 (11%)	6	25
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1	7
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
76	q0	47/47 (100%)	35 (74%)	12 (26%)	0	3
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	q2	90/90 (100%)	73 (81%)	17 (19%)	1	8
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	5
79	q3	71/71 (100%)	63 (89%)	8 (11%)	6	24
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	5
81	sM	54/228 (24%)	40 (74%)	14 (26%)	0	2
83	p0	105/253 (42%)	80 (76%)	25 (24%)	0	3
All	All	18729/20239 (92%)	15175 (81%)	3554 (19%)	1	8

5 of 3554 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	O2	61	LYS
7	s5	170	GLN
64	n8	46	ASP
71	O5	28	LEU
2	s0	119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
42	L5	40	HIS
74	O8	32	ASN
59	n3	33	ASN
42	L5	264	GLN
78	Q2	23	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	451 (25%)	62 (3%)
1	6	1793/1800 (99%)	468 (26%)	56 (3%)
36	1	3145/3396 (92%)	662 (21%)	85 (2%)
36	5	3145/3396 (92%)	673 (21%)	84 (2%)
37	3	120/121 (99%)	16 (13%)	3 (2%)
37	7	120/121 (99%)	21 (17%)	0
38	4	157/158 (99%)	39 (24%)	3 (1%)
38	8	157/158 (99%)	36 (22%)	3 (1%)
All	All	10384/10950 (94%)	2366 (22%)	296 (2%)

5 of 2366 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 296 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3121	U
1	6	277	U
36	5	2818	U
36	1	3217	C
38	4	85	G

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2563 ligands modelled in this entry, 1428 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	$\# Z  > 2$
87	OHX	5	4223	-	0,6,6	0.00	-	-		
87	OHX	5	3942	-	0,6,6	0.00	-	-		
87	OHX	1	3997	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4249	-	0,6,6	0.00	-	-		
87	OHX	5	4237	-	0,6,6	0.00	-	-		
87	OHX	s8	303	-	0,6,6	0.00	-	-		
87	OHX	1	4120	-	0,6,6	0.00	-	-		
87	OHX	5	3933	-	0,6,6	0.00	-	-		
87	OHX	6	2088	-	0,6,6	0.00	-	-		
87	OHX	6	2207	-	0,6,6	0.00	-	-		
87	OHX	5	3923	-	0,6,6	0.00	-	-		
87	OHX	6	2072	-	0,6,6	0.00	-	-		
87	OHX	1	3971	-	0,6,6	0.00	-	-		
87	OHX	2	2121	-	0,6,6	0.00	-	-		
87	OHX	5	3991	-	0,6,6	0.00	-	-		
87	OHX	5	4023	-	0,6,6	0.00	-	-		
87	OHX	1	4090	-	0,6,6	0.00	-	-		
87	OHX	D9	102	-	0,6,6	0.00	-	-		
87	OHX	d4	202	-	0,6,6	0.00	-	-		
87	OHX	5	4137	-	0,6,6	0.00	-	-		
87	OHX	n6	202	-	0,6,6	0.00	-	-		
87	OHX	6	2113	-	0,6,6	0.00	-	-		
87	OHX	1	3982	-	0,6,6	0.00	-	-		
87	OHX	S8	302	-	0,6,6	0.00	-	-		
87	OHX	5	4106	-	0,6,6	0.00	-	-		
87	OHX	8	215	-	0,6,6	0.00	-	-		
87	OHX	2	2163	-	0,6,6	0.00	-	-		
87	OHX	1	3944	-	0,6,6	0.00	-	-		
87	OHX	6	2196	-	0,6,6	0.00	-	-		
87	OHX	4	229	-	0,6,6	0.00	-	-		
87	OHX	6	2097	-	0,6,6	0.00	-	-		
87	OHX	2	2125	-	0,6,6	0.00	-	-		
87	OHX	2	2090	-	0,6,6	0.00	-	-		
87	OHX	2	2080	-	0,6,6	0.00	-	-		
87	OHX	5	4206	-	0,6,6	0.00	-	-		
87	OHX	6	2203	-	0,6,6	0.00	-	-		
87	OHX	5	4070	-	0,6,6	0.00	-	-		
87	OHX	6	2163	-	0,6,6	0.00	-	-		
87	OHX	1	3980	-	0,6,6	0.00	-	-		
87	OHX	1	4065	-	0,6,6	0.00	-	-		
87	OHX	1	4080	-	0,6,6	0.00	-	-		
87	OHX	5	4186	-	0,6,6	0.00	-	-		
87	OHX	6	2142	-	0,6,6	0.00	-	-		
87	OHX	3	220	-	0,6,6	0.00	-	-		
87	OHX	1	3947	-	0,6,6	0.00	-	-		
87	OHX	2	2071	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3977	-	0,6,6	0.00	-	-		
87	OHX	6	2071	-	0,6,6	0.00	-	-		
87	OHX	5	4246	-	0,6,6	0.00	-	-		
87	OHX	1	4036	-	0,6,6	0.00	-	-		
87	OHX	5	4243	-	0,6,6	0.00	-	-		
87	OHX	5	4022	-	0,6,6	0.00	-	-		
87	OHX	c8	201	-	0,6,6	0.00	-	-		
87	OHX	5	3982	-	0,6,6	0.00	-	-		
87	OHX	5	4089	-	0,6,6	0.00	-	-		
87	OHX	1	3946	-	0,6,6	0.00	-	-		
87	OHX	1	4039	-	0,6,6	0.00	-	-		
87	OHX	2	2073	-	0,6,6	0.00	-	-		
87	OHX	1	4217	-	0,6,6	0.00	-	-		
87	OHX	1	4113	-	0,6,6	0.00	-	-		
87	OHX	5	4128	-	0,6,6	0.00	-	-		
87	OHX	2	2078	-	0,6,6	0.00	-	-		
87	OHX	1	3950	-	0,6,6	0.00	-	-		
87	OHX	6	2123	-	0,6,6	0.00	-	-		
87	OHX	5	4019	-	0,6,6	0.00	-	-		
87	OHX	1	3991	-	0,6,6	0.00	-	-		
87	OHX	1	3898	-	0,6,6	0.00	-	-		
87	OHX	5	4139	-	0,6,6	0.00	-	-		
87	OHX	5	4115	-	0,6,6	0.00	-	-		
87	OHX	1	4095	-	0,6,6	0.00	-	-		
87	OHX	6	2181	-	0,6,6	0.00	-	-		
87	OHX	1	4022	-	0,6,6	0.00	-	-		
87	OHX	2	2055	-	0,6,6	0.00	-	-		
87	OHX	5	3928	-	0,6,6	0.00	-	-		
87	OHX	1	4151	-	0,6,6	0.00	-	-		
87	OHX	6	2115	-	0,6,6	0.00	-	-		
87	OHX	1	4160	-	0,6,6	0.00	-	-		
87	OHX	5	4225	-	0,6,6	0.00	-	-		
87	OHX	5	4167	-	0,6,6	0.00	-	-		
87	OHX	5	4146	-	0,6,6	0.00	-	-		
87	OHX	1	3879	-	0,6,6	0.00	-	-		
87	OHX	1	3880	-	0,6,6	0.00	-	-		
87	OHX	5	3935	-	0,6,6	0.00	-	-		
87	OHX	1	4161	-	0,6,6	0.00	-	-		
87	OHX	2	2097	-	0,6,6	0.00	-	-		
87	OHX	4	222	-	0,6,6	0.00	-	-		
87	OHX	5	3990	-	0,6,6	0.00	-	-		
87	OHX	1	4049	-	0,6,6	0.00	-	-		
87	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
87	OHX	6	2182	-	0,6,6	0.00	-	-		
87	OHX	1	4064	-	0,6,6	0.00	-	-		
87	OHX	5	4043	-	0,6,6	0.00	-	-		
87	OHX	2	2138	-	0,6,6	0.00	-	-		
87	OHX	5	4169	-	0,6,6	0.00	-	-		
87	OHX	1	4182	-	0,6,6	0.00	-	-		
87	OHX	2	2155	-	0,6,6	0.00	-	-		
87	OHX	6	2070	-	0,6,6	0.00	-	-		
87	OHX	5	4091	-	0,6,6	0.00	-	-		
87	OHX	5	4200	-	0,6,6	0.00	-	-		
87	OHX	2	2144	-	0,6,6	0.00	-	-		
87	OHX	1	3964	-	0,6,6	0.00	-	-		
87	OHX	1	3961	-	0,6,6	0.00	-	-		
87	OHX	5	4230	-	0,6,6	0.00	-	-		
87	OHX	2	2031	-	0,6,6	0.00	-	-		
87	OHX	5	4194	-	0,6,6	0.00	-	-		
87	OHX	5	4199	-	0,6,6	0.00	-	-		
87	OHX	6	2106	-	0,6,6	0.00	-	-		
87	OHX	6	2122	-	0,6,6	0.00	-	-		
87	OHX	5	4053	-	0,6,6	0.00	-	-		
87	OHX	1	4133	-	0,6,6	0.00	-	-		
87	OHX	1	3992	-	0,6,6	0.00	-	-		
87	OHX	8	221	-	0,6,6	0.00	-	-		
87	OHX	6	2144	-	0,6,6	0.00	-	-		
87	OHX	2	2065	-	0,6,6	0.00	-	-		
87	OHX	5	4184	-	0,6,6	0.00	-	-		
87	OHX	5	4178	-	0,6,6	0.00	-	-		
87	OHX	5	3968	-	0,6,6	0.00	-	-		
87	OHX	1	3895	-	0,6,6	0.00	-	-		
87	OHX	1	3970	-	0,6,6	0.00	-	-		
87	OHX	1	4083	-	0,6,6	0.00	-	-		
87	OHX	2	2107	-	0,6,6	0.00	-	-		
87	OHX	1	4057	-	0,6,6	0.00	-	-		
87	OHX	1	3873	-	0,6,6	0.00	-	-		
87	OHX	1	3951	-	0,6,6	0.00	-	-		
87	OHX	2	2057	-	0,6,6	0.00	-	-		
87	OHX	1	3881	-	0,6,6	0.00	-	-		
87	OHX	1	4014	-	0,6,6	0.00	-	-		
87	OHX	1	3885	-	0,6,6	0.00	-	-		
87	OHX	1	3972	-	0,6,6	0.00	-	-		
87	OHX	2	2075	-	0,6,6	0.00	-	-		
87	OHX	6	2059	-	0,6,6	0.00	-	-		
87	OHX	5	4049	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	3987	-	0,6,6	0.00	-	-		
87	OHX	6	2124	-	0,6,6	0.00	-	-		
87	OHX	5	4001	-	0,6,6	0.00	-	-		
87	OHX	5	3989	-	0,6,6	0.00	-	-		
87	OHX	1	3892	-	0,6,6	0.00	-	-		
87	OHX	5	4095	-	0,6,6	0.00	-	-		
87	OHX	5	3958	-	0,6,6	0.00	-	-		
87	OHX	1	3999	-	0,6,6	0.00	-	-		
87	OHX	1	3996	-	0,6,6	0.00	-	-		
87	OHX	5	3916	-	0,6,6	0.00	-	-		
87	OHX	8	225	-	0,6,6	0.00	-	-		
87	OHX	6	2151	-	0,6,6	0.00	-	-		
87	OHX	2	2133	-	0,6,6	0.00	-	-		
87	OHX	1	4092	-	0,6,6	0.00	-	-		
87	OHX	5	3908	-	0,6,6	0.00	-	-		
87	OHX	1	4102	-	0,6,6	0.00	-	-		
87	OHX	7	219	-	0,6,6	0.00	-	-		
87	OHX	7	217	-	0,6,6	0.00	-	-		
87	OHX	5	4217	-	0,6,6	0.00	-	-		
87	OHX	5	3956	-	0,6,6	0.00	-	-		
87	OHX	6	2074	-	0,6,6	0.00	-	-		
87	OHX	5	4250	-	0,6,6	0.00	-	-		
87	OHX	1	3969	-	0,6,6	0.00	-	-		
87	OHX	1	4216	-	0,6,6	0.00	-	-		
87	OHX	5	4211	-	0,6,6	0.00	-	-		
87	OHX	5	4059	-	0,6,6	0.00	-	-		
87	OHX	5	3950	-	0,6,6	0.00	-	-		
87	OHX	1	3935	-	0,6,6	0.00	-	-		
87	OHX	1	3913	-	0,6,6	0.00	-	-		
87	OHX	5	4102	-	0,6,6	0.00	-	-		
87	OHX	5	4179	-	0,6,6	0.00	-	-		
87	OHX	5	4131	-	0,6,6	0.00	-	-		
87	OHX	2	2042	-	0,6,6	0.00	-	-		
87	OHX	N1	201	-	0,6,6	0.00	-	-		
87	OHX	6	2114	-	0,6,6	0.00	-	-		
87	OHX	5	4248	-	0,6,6	0.00	-	-		
87	OHX	1	4063	-	0,6,6	0.00	-	-		
87	OHX	1	3960	-	0,6,6	0.00	-	-		
87	OHX	2	2113	-	0,6,6	0.00	-	-		
87	OHX	6	2053	-	0,6,6	0.00	-	-		
87	OHX	6	2058	-	0,6,6	0.00	-	-		
87	OHX	s1	303	-	0,6,6	0.00	-	-		
87	OHX	1	4000	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4033	-	0,6,6	0.00	-	-		
87	OHX	5	4232	-	0,6,6	0.00	-	-		
87	OHX	5	3940	-	0,6,6	0.00	-	-		
87	OHX	sR	401	-	0,6,6	0.00	-	-		
87	OHX	1	4131	-	0,6,6	0.00	-	-		
87	OHX	5	4105	-	0,6,6	0.00	-	-		
87	OHX	5	4166	-	0,6,6	0.00	-	-		
87	OHX	2	2074	-	0,6,6	0.00	-	-		
87	OHX	2	2177	-	0,6,6	0.00	-	-		
87	OHX	4	223	-	0,6,6	0.00	-	-		
87	OHX	1	3921	-	0,6,6	0.00	-	-		
87	OHX	M5	302	-	0,6,6	0.00	-	-		
87	OHX	1	4110	-	0,6,6	0.00	-	-		
87	OHX	2	2044	-	0,6,6	0.00	-	-		
87	OHX	6	2162	-	0,6,6	0.00	-	-		
87	OHX	5	4006	-	0,6,6	0.00	-	-		
87	OHX	5	3985	-	0,6,6	0.00	-	-		
87	OHX	5	4189	-	0,6,6	0.00	-	-		
87	OHX	1	4139	-	0,6,6	0.00	-	-		
87	OHX	2	2157	-	0,6,6	0.00	-	-		
87	OHX	5	4145	-	0,6,6	0.00	-	-		
87	OHX	5	4161	-	0,6,6	0.00	-	-		
87	OHX	2	2106	-	0,6,6	0.00	-	-		
87	OHX	6	2185	-	0,6,6	0.00	-	-		
87	OHX	1	4116	-	0,6,6	0.00	-	-		
87	OHX	5	4205	-	0,6,6	0.00	-	-		
87	OHX	2	2141	-	0,6,6	0.00	-	-		
87	OHX	6	2107	-	0,6,6	0.00	-	-		
87	OHX	6	2159	-	0,6,6	0.00	-	-		
87	OHX	m0	302	-	0,6,6	0.00	-	-		
87	OHX	6	2206	-	0,6,6	0.00	-	-		
87	OHX	5	4149	-	0,6,6	0.00	-	-		
87	OHX	5	4191	-	0,6,6	0.00	-	-		
87	OHX	1	4147	-	0,6,6	0.00	-	-		
87	OHX	1	3981	-	0,6,6	0.00	-	-		
87	OHX	1	3939	-	0,6,6	0.00	-	-		
87	OHX	2	2087	-	0,6,6	0.00	-	-		
87	OHX	2	2054	-	0,6,6	0.00	-	-		
87	OHX	6	2140	-	0,6,6	0.00	-	-		
87	OHX	8	222	-	0,6,6	0.00	-	-		
87	OHX	5	3965	-	0,6,6	0.00	-	-		
87	OHX	6	2111	-	0,6,6	0.00	-	-		
87	OHX	6	2080	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	M7	208	-	0,6,6	0.00	-	-		
87	OHX	1	3988	-	0,6,6	0.00	-	-		
87	OHX	8	220	-	0,6,6	0.00	-	-		
87	OHX	O7	103	-	0,6,6	0.00	-	-		
87	OHX	1	4202	-	0,6,6	0.00	-	-		
87	OHX	2	2092	-	0,6,6	0.00	-	-		
87	OHX	2	2131	-	0,6,6	0.00	-	-		
87	OHX	5	4018	-	0,6,6	0.00	-	-		
87	OHX	1	4044	-	0,6,6	0.00	-	-		
87	OHX	2	2037	-	0,6,6	0.00	-	-		
87	OHX	1	3942	-	0,6,6	0.00	-	-		
87	OHX	5	4215	-	0,6,6	0.00	-	-		
87	OHX	6	2118	-	0,6,6	0.00	-	-		
87	OHX	1	3968	-	0,6,6	0.00	-	-		
87	OHX	1	4164	-	0,6,6	0.00	-	-		
87	OHX	1	3953	-	0,6,6	0.00	-	-		
87	OHX	1	4079	-	0,6,6	0.00	-	-		
87	OHX	2	2178	-	0,6,6	0.00	-	-		
87	OHX	1	3915	-	0,6,6	0.00	-	-		
87	OHX	6	2129	-	0,6,6	0.00	-	-		
87	OHX	6	2147	-	0,6,6	0.00	-	-		
87	OHX	5	3988	-	0,6,6	0.00	-	-		
87	OHX	5	4118	-	0,6,6	0.00	-	-		
87	OHX	6	2201	-	0,6,6	0.00	-	-		
87	OHX	1	4061	-	0,6,6	0.00	-	-		
87	OHX	5	4123	-	0,6,6	0.00	-	-		
87	OHX	5	4156	-	0,6,6	0.00	-	-		
87	OHX	6	2169	-	0,6,6	0.00	-	-		
87	OHX	1	4077	-	0,6,6	0.00	-	-		
87	OHX	O9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4208	-	0,6,6	0.00	-	-		
87	OHX	1	3949	-	0,6,6	0.00	-	-		
87	OHX	5	3957	-	0,6,6	0.00	-	-		
87	OHX	5	3998	-	0,6,6	0.00	-	-		
87	OHX	6	2112	-	0,6,6	0.00	-	-		
87	OHX	1	4051	-	0,6,6	0.00	-	-		
87	OHX	6	2085	-	0,6,6	0.00	-	-		
87	OHX	1	3919	-	0,6,6	0.00	-	-		
87	OHX	1	4010	-	0,6,6	0.00	-	-		
87	OHX	5	4034	-	0,6,6	0.00	-	-		
87	OHX	2	2110	-	0,6,6	0.00	-	-		
87	OHX	5	4042	-	0,6,6	0.00	-	-		
87	OHX	2	2084	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4061	-	0,6,6	0.00	-	-		
87	OHX	1	4099	-	0,6,6	0.00	-	-		
87	OHX	1	3902	-	0,6,6	0.00	-	-		
87	OHX	1	4056	-	0,6,6	0.00	-	-		
87	OHX	m4	201	-	0,6,6	0.00	-	-		
87	OHX	2	2079	-	0,6,6	0.00	-	-		
87	OHX	1	3930	-	0,6,6	0.00	-	-		
87	OHX	5	3966	-	0,6,6	0.00	-	-		
87	OHX	1	4027	-	0,6,6	0.00	-	-		
87	OHX	1	3886	-	0,6,6	0.00	-	-		
87	OHX	5	4213	-	0,6,6	0.00	-	-		
87	OHX	5	4157	-	0,6,6	0.00	-	-		
87	OHX	1	3893	-	0,6,6	0.00	-	-		
87	OHX	1	3878	-	0,6,6	0.00	-	-		
87	OHX	1	4197	-	0,6,6	0.00	-	-		
87	OHX	2	2104	-	0,6,6	0.00	-	-		
87	OHX	1	3932	-	0,6,6	0.00	-	-		
87	OHX	5	3986	-	0,6,6	0.00	-	-		
87	OHX	2	2101	-	0,6,6	0.00	-	-		
87	OHX	1	4130	-	0,6,6	0.00	-	-		
87	OHX	1	4024	-	0,6,6	0.00	-	-		
87	OHX	5	3953	-	0,6,6	0.00	-	-		
87	OHX	6	2174	-	0,6,6	0.00	-	-		
87	OHX	5	4092	-	0,6,6	0.00	-	-		
87	OHX	5	4231	-	0,6,6	0.00	-	-		
87	OHX	1	3931	-	0,6,6	0.00	-	-		
87	OHX	5	4121	-	0,6,6	0.00	-	-		
87	OHX	5	4229	-	0,6,6	0.00	-	-		
87	OHX	1	4109	-	0,6,6	0.00	-	-		
87	OHX	5	4065	-	0,6,6	0.00	-	-		
87	OHX	5	3967	-	0,6,6	0.00	-	-		
87	OHX	2	2056	-	0,6,6	0.00	-	-		
87	OHX	l3	403	-	0,6,6	0.00	-	-		
87	OHX	1	4062	-	0,6,6	0.00	-	-		
87	OHX	6	2194	-	0,6,6	0.00	-	-		
87	OHX	1	4183	-	0,6,6	0.00	-	-		
87	OHX	5	3978	-	0,6,6	0.00	-	-		
87	OHX	6	2172	-	0,6,6	0.00	-	-		
87	OHX	5	4076	-	0,6,6	0.00	-	-		
87	OHX	5	4096	-	0,6,6	0.00	-	-		
87	OHX	1	3870	-	0,6,6	0.00	-	-		
87	OHX	5	4020	-	0,6,6	0.00	-	-		
87	OHX	1	4074	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	3911	-	0,6,6	0.00	-	-		
87	OHX	6	2199	-	0,6,6	0.00	-	-		
87	OHX	5	3936	-	0,6,6	0.00	-	-		
87	OHX	6	2132	-	0,6,6	0.00	-	-		
87	OHX	6	2054	-	0,6,6	0.00	-	-		
87	OHX	1	4169	-	0,6,6	0.00	-	-		
87	OHX	m6	202	-	0,6,6	0.00	-	-		
87	OHX	6	2158	-	0,6,6	0.00	-	-		
87	OHX	5	4027	-	0,6,6	0.00	-	-		
87	OHX	5	4109	-	0,6,6	0.00	-	-		
87	OHX	5	4170	-	0,6,6	0.00	-	-		
87	OHX	2	2027	-	0,6,6	0.00	-	-		
87	OHX	1	4011	-	0,6,6	0.00	-	-		
87	OHX	8	230	-	0,6,6	0.00	-	-		
87	OHX	1	3965	-	0,6,6	0.00	-	-		
87	OHX	1	4123	-	0,6,6	0.00	-	-		
87	OHX	1	3889	-	0,6,6	0.00	-	-		
87	OHX	2	2086	-	0,6,6	0.00	-	-		
87	OHX	6	2164	-	0,6,6	0.00	-	-		
87	OHX	6	2051	-	0,6,6	0.00	-	-		
87	OHX	5	4228	-	0,6,6	0.00	-	-		
87	OHX	2	2051	-	0,6,6	0.00	-	-		
87	OHX	5	4247	-	0,6,6	0.00	-	-		
87	OHX	L3	405	-	0,6,6	0.00	-	-		
87	OHX	2	2089	-	0,6,6	0.00	-	-		
87	OHX	1	3959	-	0,6,6	0.00	-	-		
87	OHX	6	2082	-	0,6,6	0.00	-	-		
87	OHX	6	2187	-	0,6,6	0.00	-	-		
87	OHX	1	3937	-	0,6,6	0.00	-	-		
87	OHX	6	2100	-	0,6,6	0.00	-	-		
87	OHX	5	4245	-	0,6,6	0.00	-	-		
87	OHX	5	4155	-	0,6,6	0.00	-	-		
87	OHX	5	4134	-	0,6,6	0.00	-	-		
87	OHX	1	3899	-	0,6,6	0.00	-	-		
87	OHX	SR	401	-	0,6,6	0.00	-	-		
87	OHX	1	3911	-	0,6,6	0.00	-	-		
87	OHX	2	2022	-	0,6,6	0.00	-	-		
87	OHX	2	2139	-	0,6,6	0.00	-	-		
87	OHX	o3	203	-	0,6,6	0.00	-	-		
87	OHX	6	2056	-	0,6,6	0.00	-	-		
87	OHX	5	4067	-	0,6,6	0.00	-	-		
87	OHX	2	2167	-	0,6,6	0.00	-	-		
87	OHX	6	2133	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	14	402	-	0,6,6	0.00	-	-		
87	OHX	1	4093	-	0,6,6	0.00	-	-		
87	OHX	1	4069	-	0,6,6	0.00	-	-		
87	OHX	1	4191	-	0,6,6	0.00	-	-		
87	OHX	5	4162	-	0,6,6	0.00	-	-		
87	OHX	1	4209	-	0,6,6	0.00	-	-		
87	OHX	1	4208	-	0,6,6	0.00	-	-		
87	OHX	1	4078	-	0,6,6	0.00	-	-		
87	OHX	1	4103	-	0,6,6	0.00	-	-		
87	OHX	1	4001	-	0,6,6	0.00	-	-		
87	OHX	6	2139	-	0,6,6	0.00	-	-		
87	OHX	5	3981	-	0,6,6	0.00	-	-		
87	OHX	5	3934	-	0,6,6	0.00	-	-		
87	OHX	5	4026	-	0,6,6	0.00	-	-		
87	OHX	2	2021	-	0,6,6	0.00	-	-		
87	OHX	1	3967	-	0,6,6	0.00	-	-		
87	OHX	6	2078	-	0,6,6	0.00	-	-		
87	OHX	2	2082	-	0,6,6	0.00	-	-		
87	OHX	1	4087	-	0,6,6	0.00	-	-		
87	OHX	1	4106	-	0,6,6	0.00	-	-		
87	OHX	1	4167	-	0,6,6	0.00	-	-		
87	OHX	2	2091	-	0,6,6	0.00	-	-		
87	OHX	6	2120	-	0,6,6	0.00	-	-		
87	OHX	5	3910	-	0,6,6	0.00	-	-		
87	OHX	1	4096	-	0,6,6	0.00	-	-		
87	OHX	5	4013	-	0,6,6	0.00	-	-		
87	OHX	2	2148	-	0,6,6	0.00	-	-		
87	OHX	5	4016	-	0,6,6	0.00	-	-		
87	OHX	1	4119	-	0,6,6	0.00	-	-		
87	OHX	1	4143	-	0,6,6	0.00	-	-		
87	OHX	1	4117	-	0,6,6	0.00	-	-		
87	OHX	5	4220	-	0,6,6	0.00	-	-		
87	OHX	1	4055	-	0,6,6	0.00	-	-		
87	OHX	m7	206	-	0,6,6	0.00	-	-		
87	OHX	6	2103	-	0,6,6	0.00	-	-		
87	OHX	s1	302	-	0,6,6	0.00	-	-		
87	OHX	3	226	-	0,6,6	0.00	-	-		
87	OHX	1	4132	-	0,6,6	0.00	-	-		
87	OHX	6	2079	-	0,6,6	0.00	-	-		
87	OHX	1	4084	-	0,6,6	0.00	-	-		
87	OHX	1	4186	-	0,6,6	0.00	-	-		
87	OHX	1	4081	-	0,6,6	0.00	-	-		
87	OHX	2	2062	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4017	-	0,6,6	0.00	-	-		
87	OHX	1	4111	-	0,6,6	0.00	-	-		
87	OHX	6	2141	-	0,6,6	0.00	-	-		
87	OHX	2	2070	-	0,6,6	0.00	-	-		
87	OHX	5	4180	-	0,6,6	0.00	-	-		
87	OHX	1	3914	-	0,6,6	0.00	-	-		
87	OHX	5	4011	-	0,6,6	0.00	-	-		
87	OHX	5	3993	-	0,6,6	0.00	-	-		
87	OHX	5	4173	-	0,6,6	0.00	-	-		
87	OHX	2	2164	-	0,6,6	0.00	-	-		
87	OHX	2	2048	-	0,6,6	0.00	-	-		
87	OHX	2	2028	-	0,6,6	0.00	-	-		
87	OHX	5	3992	-	0,6,6	0.00	-	-		
87	OHX	5	3926	-	0,6,6	0.00	-	-		
87	OHX	5	4168	-	0,6,6	0.00	-	-		
87	OHX	6	2186	-	0,6,6	0.00	-	-		
87	OHX	1	3897	-	0,6,6	0.00	-	-		
87	OHX	5	3904	-	0,6,6	0.00	-	-		
87	OHX	L3	404	-	0,6,6	0.00	-	-		
87	OHX	C3	201	-	0,6,6	0.00	-	-		
87	OHX	1	3973	-	0,6,6	0.00	-	-		
87	OHX	m5	304	-	0,6,6	0.00	-	-		
87	OHX	1	3906	-	0,6,6	0.00	-	-		
87	OHX	5	4046	-	0,6,6	0.00	-	-		
87	OHX	5	4126	-	0,6,6	0.00	-	-		
87	OHX	1	4031	-	0,6,6	0.00	-	-		
87	OHX	5	3987	-	0,6,6	0.00	-	-		
87	OHX	1	4073	-	0,6,6	0.00	-	-		
87	OHX	1	4066	-	0,6,6	0.00	-	-		
87	OHX	5	4066	-	0,6,6	0.00	-	-		
87	OHX	1	3974	-	0,6,6	0.00	-	-		
87	OHX	5	4216	-	0,6,6	0.00	-	-		
87	OHX	4	224	-	0,6,6	0.00	-	-		
87	OHX	1	4003	-	0,6,6	0.00	-	-		
87	OHX	1	3877	-	0,6,6	0.00	-	-		
87	OHX	1	3916	-	0,6,6	0.00	-	-		
87	OHX	n9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4188	-	0,6,6	0.00	-	-		
87	OHX	6	2171	-	0,6,6	0.00	-	-		
87	OHX	5	4218	-	0,6,6	0.00	-	-		
87	OHX	1	3876	-	0,6,6	0.00	-	-		
87	OHX	5	4072	-	0,6,6	0.00	-	-		
87	OHX	1	3958	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2098	-	0,6,6	0.00	-	-		
87	OHX	5	3964	-	0,6,6	0.00	-	-		
87	OHX	2	2154	-	0,6,6	0.00	-	-		
87	OHX	2	2036	-	0,6,6	0.00	-	-		
87	OHX	1	4163	-	0,6,6	0.00	-	-		
87	OHX	5	4195	-	0,6,6	0.00	-	-		
87	OHX	5	4226	-	0,6,6	0.00	-	-		
87	OHX	5	4210	-	0,6,6	0.00	-	-		
87	OHX	5	4048	-	0,6,6	0.00	-	-		
87	OHX	5	4021	-	0,6,6	0.00	-	-		
87	OHX	5	4107	-	0,6,6	0.00	-	-		
87	OHX	6	2096	-	0,6,6	0.00	-	-		
87	OHX	6	2189	-	0,6,6	0.00	-	-		
87	OHX	5	4193	-	0,6,6	0.00	-	-		
87	OHX	1	3891	-	0,6,6	0.00	-	-		
87	OHX	6	2192	-	0,6,6	0.00	-	-		
87	OHX	1	4125	-	0,6,6	0.00	-	-		
87	OHX	3	218	-	0,6,6	0.00	-	-		
87	OHX	1	3887	-	0,6,6	0.00	-	-		
87	OHX	6	2165	-	0,6,6	0.00	-	-		
87	OHX	5	4236	-	0,6,6	0.00	-	-		
87	OHX	1	3926	-	0,6,6	0.00	-	-		
87	OHX	6	2095	-	0,6,6	0.00	-	-		
87	OHX	6	2153	-	0,6,6	0.00	-	-		
87	OHX	2	2128	-	0,6,6	0.00	-	-		
87	OHX	2	2076	-	0,6,6	0.00	-	-		
87	OHX	3	224	-	0,6,6	0.00	-	-		
87	OHX	5	4071	-	0,6,6	0.00	-	-		
87	OHX	2	2170	-	0,6,6	0.00	-	-		
87	OHX	5	3941	-	0,6,6	0.00	-	-		
87	OHX	5	4077	-	0,6,6	0.00	-	-		
87	OHX	5	4113	-	0,6,6	0.00	-	-		
87	OHX	5	4050	-	0,6,6	0.00	-	-		
87	OHX	1	4091	-	0,6,6	0.00	-	-		
87	OHX	5	3919	-	0,6,6	0.00	-	-		
87	OHX	5	3900	-	0,6,6	0.00	-	-		
87	OHX	6	2063	-	0,6,6	0.00	-	-		
87	OHX	2	2159	-	0,6,6	0.00	-	-		
87	OHX	4	221	-	0,6,6	0.00	-	-		
87	OHX	5	4110	-	0,6,6	0.00	-	-		
87	OHX	1	4192	-	0,6,6	0.00	-	-		
87	OHX	2	2029	-	0,6,6	0.00	-	-		
87	OHX	2	2026	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2125	-	0,6,6	0.00	-	-		
87	OHX	5	4028	-	0,6,6	0.00	-	-		
87	OHX	1	4171	-	0,6,6	0.00	-	-		
87	OHX	5	4183	-	0,6,6	0.00	-	-		
87	OHX	1	4054	-	0,6,6	0.00	-	-		
87	OHX	6	2135	-	0,6,6	0.00	-	-		
87	OHX	d9	102	-	0,6,6	0.00	-	-		
87	OHX	1	3910	-	0,6,6	0.00	-	-		
87	OHX	1	4215	-	0,6,6	0.00	-	-		
87	OHX	1	4146	-	0,6,6	0.00	-	-		
87	OHX	5	4108	-	0,6,6	0.00	-	-		
87	OHX	5	4044	-	0,6,6	0.00	-	-		
87	OHX	1	3918	-	0,6,6	0.00	-	-		
87	OHX	1	4013	-	0,6,6	0.00	-	-		
87	OHX	5	3961	-	0,6,6	0.00	-	-		
87	OHX	5	3960	-	0,6,6	0.00	-	-		
87	OHX	1	4004	-	0,6,6	0.00	-	-		
87	OHX	1	4122	-	0,6,6	0.00	-	-		
87	OHX	2	2093	-	0,6,6	0.00	-	-		
87	OHX	5	4101	-	0,6,6	0.00	-	-		
87	OHX	6	2119	-	0,6,6	0.00	-	-		
87	OHX	6	2084	-	0,6,6	0.00	-	-		
87	OHX	2	2114	-	0,6,6	0.00	-	-		
87	OHX	1	4020	-	0,6,6	0.00	-	-		
87	OHX	1	4203	-	0,6,6	0.00	-	-		
87	OHX	6	2117	-	0,6,6	0.00	-	-		
87	OHX	2	2119	-	0,6,6	0.00	-	-		
87	OHX	1	4149	-	0,6,6	0.00	-	-		
87	OHX	1	3941	-	0,6,6	0.00	-	-		
87	OHX	1	4045	-	0,6,6	0.00	-	-		
87	OHX	2	2108	-	0,6,6	0.00	-	-		
87	OHX	8	227	-	0,6,6	0.00	-	-		
87	OHX	2	2049	-	0,6,6	0.00	-	-		
87	OHX	6	2160	-	0,6,6	0.00	-	-		
87	OHX	1	3924	-	0,6,6	0.00	-	-		
87	OHX	5	3929	-	0,6,6	0.00	-	-		
87	OHX	5	4012	-	0,6,6	0.00	-	-		
87	OHX	5	4099	-	0,6,6	0.00	-	-		
87	OHX	6	2077	-	0,6,6	0.00	-	-		
87	OHX	1	4043	-	0,6,6	0.00	-	-		
87	OHX	6	2060	-	0,6,6	0.00	-	-		
87	OHX	5	4103	-	0,6,6	0.00	-	-		
87	OHX	1	3882	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4076	-	0,6,6	0.00	-	-		
87	OHX	2	2117	-	0,6,6	0.00	-	-		
87	OHX	2	2033	-	0,6,6	0.00	-	-		
87	OHX	1	4118	-	0,6,6	0.00	-	-		
87	OHX	2	2112	-	0,6,6	0.00	-	-		
87	OHX	5	4219	-	0,6,6	0.00	-	-		
87	OHX	5	3999	-	0,6,6	0.00	-	-		
87	OHX	5	3920	-	0,6,6	0.00	-	-		
87	OHX	1	3948	-	0,6,6	0.00	-	-		
87	OHX	2	2050	-	0,6,6	0.00	-	-		
87	OHX	1	3927	-	0,6,6	0.00	-	-		
87	OHX	4	226	-	0,6,6	0.00	-	-		
87	OHX	6	2136	-	0,6,6	0.00	-	-		
87	OHX	5	3979	-	0,6,6	0.00	-	-		
87	OHX	6	2148	-	0,6,6	0.00	-	-		
87	OHX	5	4124	-	0,6,6	0.00	-	-		
87	OHX	2	2069	-	0,6,6	0.00	-	-		
87	OHX	6	2202	-	0,6,6	0.00	-	-		
87	OHX	5	3948	-	0,6,6	0.00	-	-		
87	OHX	1	4058	-	0,6,6	0.00	-	-		
87	OHX	5	3927	-	0,6,6	0.00	-	-		
87	OHX	2	2038	-	0,6,6	0.00	-	-		
87	OHX	5	4037	-	0,6,6	0.00	-	-		
87	OHX	5	4056	-	0,6,6	0.00	-	-		
87	OHX	1	3874	-	0,6,6	0.00	-	-		
87	OHX	15	304	-	0,6,6	0.00	-	-		
87	OHX	5	4165	-	0,6,6	0.00	-	-		
87	OHX	1	3871	-	0,6,6	0.00	-	-		
87	OHX	1	4029	-	0,6,6	0.00	-	-		
87	OHX	1	4136	-	0,6,6	0.00	-	-		
87	OHX	6	2131	-	0,6,6	0.00	-	-		
87	OHX	1	4177	-	0,6,6	0.00	-	-		
87	OHX	1	4210	-	0,6,6	0.00	-	-		
87	OHX	5	4030	-	0,6,6	0.00	-	-		
87	OHX	5	3914	-	0,6,6	0.00	-	-		
87	OHX	1	3903	-	0,6,6	0.00	-	-		
87	OHX	5	4163	-	0,6,6	0.00	-	-		
87	OHX	5	3932	-	0,6,6	0.00	-	-		
87	OHX	1	4121	-	0,6,6	0.00	-	-		
87	OHX	7	224	-	0,6,6	0.00	-	-		
87	OHX	2	2066	-	0,6,6	0.00	-	-		
87	OHX	C5	201	-	0,6,6	0.00	-	-		
87	OHX	5	4148	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	3	225	-	0,6,6	0.00	-	-		
87	OHX	1	4025	-	0,6,6	0.00	-	-		
87	OHX	2	2143	-	0,6,6	0.00	-	-		
87	OHX	6	2101	-	0,6,6	0.00	-	-		
87	OHX	5	4196	-	0,6,6	0.00	-	-		
87	OHX	2	2083	-	0,6,6	0.00	-	-		
87	OHX	5	4197	-	0,6,6	0.00	-	-		
87	OHX	5	4201	-	0,6,6	0.00	-	-		
87	OHX	2	2172	-	0,6,6	0.00	-	-		
87	OHX	7	218	-	0,6,6	0.00	-	-		
87	OHX	2	2077	-	0,6,6	0.00	-	-		
87	OHX	5	4097	-	0,6,6	0.00	-	-		
87	OHX	1	3943	-	0,6,6	0.00	-	-		
87	OHX	5	4010	-	0,6,6	0.00	-	-		
87	OHX	m0	301	-	0,6,6	0.00	-	-		
87	OHX	5	4252	-	0,6,6	0.00	-	-		
87	OHX	6	2161	-	0,6,6	0.00	-	-		
87	OHX	5	4004	-	0,6,6	0.00	-	-		
87	OHX	5	4093	-	0,6,6	0.00	-	-		
87	OHX	3	216	-	0,6,6	0.00	-	-		
87	OHX	5	4130	-	0,6,6	0.00	-	-		
87	OHX	5	4198	-	0,6,6	0.00	-	-		
87	OHX	1	4007	-	0,6,6	0.00	-	-		
87	OHX	6	2205	-	0,6,6	0.00	-	-		
87	OHX	1	3909	-	0,6,6	0.00	-	-		
87	OHX	6	2155	-	0,6,6	0.00	-	-		
87	OHX	6	2126	-	0,6,6	0.00	-	-		
87	OHX	6	2052	-	0,6,6	0.00	-	-		
87	OHX	1	4009	-	0,6,6	0.00	-	-		
87	OHX	2	2137	-	0,6,6	0.00	-	-		
87	OHX	O7	104	-	0,6,6	0.00	-	-		
87	OHX	5	4207	-	0,6,6	0.00	-	-		
87	OHX	1	4159	-	0,6,6	0.00	-	-		
87	OHX	5	4133	-	0,6,6	0.00	-	-		
87	OHX	2	2043	-	0,6,6	0.00	-	-		
87	OHX	1	4188	-	0,6,6	0.00	-	-		
87	OHX	5	3976	-	0,6,6	0.00	-	-		
87	OHX	1	4178	-	0,6,6	0.00	-	-		
87	OHX	1	4172	-	0,6,6	0.00	-	-		
87	OHX	5	3909	-	0,6,6	0.00	-	-		
87	OHX	1	3888	-	0,6,6	0.00	-	-		
87	OHX	5	4031	-	0,6,6	0.00	-	-		
87	OHX	2	2151	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4132	-	0,6,6	0.00	-	-		
87	OHX	3	215	-	0,6,6	0.00	-	-		
87	OHX	2	2102	-	0,6,6	0.00	-	-		
87	OHX	6	2138	-	0,6,6	0.00	-	-		
87	OHX	5	4153	-	0,6,6	0.00	-	-		
87	OHX	2	2088	-	0,6,6	0.00	-	-		
87	OHX	1	4138	-	0,6,6	0.00	-	-		
87	OHX	2	2024	-	0,6,6	0.00	-	-		
87	OHX	2	2130	-	0,6,6	0.00	-	-		
87	OHX	1	4053	-	0,6,6	0.00	-	-		
87	OHX	6	2137	-	0,6,6	0.00	-	-		
87	OHX	1	4175	-	0,6,6	0.00	-	-		
87	OHX	6	2197	-	0,6,6	0.00	-	-		
87	OHX	6	2188	-	0,6,6	0.00	-	-		
87	OHX	2	2140	-	0,6,6	0.00	-	-		
87	OHX	q2	502	-	0,6,6	0.00	-	-		
87	OHX	7	226	-	0,6,6	0.00	-	-		
87	OHX	1	4193	-	0,6,6	0.00	-	-		
87	OHX	1	4205	-	0,6,6	0.00	-	-		
87	OHX	5	4075	-	0,6,6	0.00	-	-		
87	OHX	5	4233	-	0,6,6	0.00	-	-		
87	OHX	1	4129	-	0,6,6	0.00	-	-		
87	OHX	1	3896	-	0,6,6	0.00	-	-		
87	OHX	1	3977	-	0,6,6	0.00	-	-		
87	OHX	5	4164	-	0,6,6	0.00	-	-		
87	OHX	1	3917	-	0,6,6	0.00	-	-		
87	OHX	6	2176	-	0,6,6	0.00	-	-		
87	OHX	1	4068	-	0,6,6	0.00	-	-		
87	OHX	1	3954	-	0,6,6	0.00	-	-		
87	OHX	5	3980	-	0,6,6	0.00	-	-		
87	OHX	5	4007	-	0,6,6	0.00	-	-		
87	OHX	1	4127	-	0,6,6	0.00	-	-		
87	OHX	6	2152	-	0,6,6	0.00	-	-		
87	OHX	1	4174	-	0,6,6	0.00	-	-		
87	OHX	1	4052	-	0,6,6	0.00	-	-		
87	OHX	8	218	-	0,6,6	0.00	-	-		
87	OHX	1	4190	-	0,6,6	0.00	-	-		
87	OHX	2	2068	-	0,6,6	0.00	-	-		
87	OHX	2	2072	-	0,6,6	0.00	-	-		
87	OHX	m8	201	-	0,6,6	0.00	-	-		
87	OHX	5	4177	-	0,6,6	0.00	-	-		
87	OHX	1	4107	-	0,6,6	0.00	-	-		
87	OHX	5	4014	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2090	-	0,6,6	0.00	-	-		
87	OHX	2	2127	-	0,6,6	0.00	-	-		
87	OHX	6	2167	-	0,6,6	0.00	-	-		
87	OHX	1	4168	-	0,6,6	0.00	-	-		
87	OHX	1	4166	-	0,6,6	0.00	-	-		
87	OHX	1	3912	-	0,6,6	0.00	-	-		
87	OHX	M0	303	-	0,6,6	0.00	-	-		
87	OHX	1	4137	-	0,6,6	0.00	-	-		
87	OHX	1	4035	-	0,6,6	0.00	-	-		
87	OHX	6	2089	-	0,6,6	0.00	-	-		
87	OHX	5	3924	-	0,6,6	0.00	-	-		
87	OHX	6	2099	-	0,6,6	0.00	-	-		
87	OHX	1	4006	-	0,6,6	0.00	-	-		
87	OHX	1	4050	-	0,6,6	0.00	-	-		
87	OHX	M8	202	-	0,6,6	0.00	-	-		
87	OHX	5	4221	-	0,6,6	0.00	-	-		
87	OHX	5	3947	-	0,6,6	0.00	-	-		
87	OHX	5	3952	-	0,6,6	0.00	-	-		
87	OHX	5	4174	-	0,6,6	0.00	-	-		
87	OHX	1	3905	-	0,6,6	0.00	-	-		
87	OHX	6	2081	-	0,6,6	0.00	-	-		
87	OHX	1	3952	-	0,6,6	0.00	-	-		
87	OHX	1	4162	-	0,6,6	0.00	-	-		
87	OHX	5	3903	-	0,6,6	0.00	-	-		
87	OHX	L4	403	-	0,6,6	0.00	-	-		
87	OHX	1	4012	-	0,6,6	0.00	-	-		
87	OHX	1	3966	-	0,6,6	0.00	-	-		
87	OHX	1	3901	-	0,6,6	0.00	-	-		
87	OHX	7	227	-	0,6,6	0.00	-	-		
87	OHX	4	230	-	0,6,6	0.00	-	-		
87	OHX	5	4009	-	0,6,6	0.00	-	-		
87	OHX	1	4212	-	0,6,6	0.00	-	-		
87	OHX	Q2	503	-	0,6,6	0.00	-	-		
87	OHX	5	4159	-	0,6,6	0.00	-	-		
87	OHX	2	2025	-	0,6,6	0.00	-	-		
87	OHX	6	2134	-	0,6,6	0.00	-	-		
87	OHX	5	4080	-	0,6,6	0.00	-	-		
87	OHX	5	4182	-	0,6,6	0.00	-	-		
87	OHX	6	2050	-	0,6,6	0.00	-	-		
87	OHX	2	2060	-	0,6,6	0.00	-	-		
87	OHX	1	3900	-	0,6,6	0.00	-	-		
87	OHX	5	4073	-	0,6,6	0.00	-	-		
87	OHX	5	4140	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2123	-	0,6,6	0.00	-	-		
87	OHX	5	4129	-	0,6,6	0.00	-	-		
87	OHX	2	2081	-	0,6,6	0.00	-	-		
87	OHX	5	4078	-	0,6,6	0.00	-	-		
87	OHX	6	2105	-	0,6,6	0.00	-	-		
87	OHX	5	4114	-	0,6,6	0.00	-	-		
87	OHX	6	2130	-	0,6,6	0.00	-	-		
87	OHX	5	4098	-	0,6,6	0.00	-	-		
87	OHX	6	2150	-	0,6,6	0.00	-	-		
87	OHX	2	2094	-	0,6,6	0.00	-	-		
87	OHX	1	4097	-	0,6,6	0.00	-	-		
87	OHX	2	2169	-	0,6,6	0.00	-	-		
87	OHX	5	4212	-	0,6,6	0.00	-	-		
87	OHX	5	4242	-	0,6,6	0.00	-	-		
87	OHX	2	2023	-	0,6,6	0.00	-	-		
87	OHX	5	4074	-	0,6,6	0.00	-	-		
87	OHX	6	2062	-	0,6,6	0.00	-	-		
87	OHX	5	4251	-	0,6,6	0.00	-	-		
87	OHX	1	4144	-	0,6,6	0.00	-	-		
87	OHX	5	4035	-	0,6,6	0.00	-	-		
87	OHX	5	3913	-	0,6,6	0.00	-	-		
87	OHX	1	3962	-	0,6,6	0.00	-	-		
87	OHX	5	4002	-	0,6,6	0.00	-	-		
87	OHX	5	4104	-	0,6,6	0.00	-	-		
87	OHX	2	2103	-	0,6,6	0.00	-	-		
87	OHX	1	4082	-	0,6,6	0.00	-	-		
87	OHX	6	2075	-	0,6,6	0.00	-	-		
87	OHX	1	3925	-	0,6,6	0.00	-	-		
87	OHX	6	2116	-	0,6,6	0.00	-	-		
87	OHX	5	3996	-	0,6,6	0.00	-	-		
87	OHX	1	4142	-	0,6,6	0.00	-	-		
87	OHX	5	4127	-	0,6,6	0.00	-	-		
87	OHX	4	232	-	0,6,6	0.00	-	-		
87	OHX	1	3938	-	0,6,6	0.00	-	-		
87	OHX	8	223	-	0,6,6	0.00	-	-		
87	OHX	1	4086	-	0,6,6	0.00	-	-		
87	OHX	6	2093	-	0,6,6	0.00	-	-		
87	OHX	1	3945	-	0,6,6	0.00	-	-		
87	OHX	1	4112	-	0,6,6	0.00	-	-		
87	OHX	5	3974	-	0,6,6	0.00	-	-		
87	OHX	1	4128	-	0,6,6	0.00	-	-		
87	OHX	1	4176	-	0,6,6	0.00	-	-		
87	OHX	1	3989	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4173	-	0,6,6	0.00	-	-		
87	OHX	m1	202	-	0,6,6	0.00	-	-		
87	OHX	6	2145	-	0,6,6	0.00	-	-		
87	OHX	5	4057	-	0,6,6	0.00	-	-		
87	OHX	1	3923	-	0,6,6	0.00	-	-		
87	OHX	c3	201	-	0,6,6	0.00	-	-		
87	OHX	1	4032	-	0,6,6	0.00	-	-		
87	OHX	5	4214	-	0,6,6	0.00	-	-		
87	OHX	1	4134	-	0,6,6	0.00	-	-		
87	OHX	5	3945	-	0,6,6	0.00	-	-		
87	OHX	5	4068	-	0,6,6	0.00	-	-		
87	OHX	2	2061	-	0,6,6	0.00	-	-		
87	OHX	2	2063	-	0,6,6	0.00	-	-		
87	OHX	5	3997	-	0,6,6	0.00	-	-		
87	OHX	D3	202	-	0,6,6	0.00	-	-		
87	OHX	5	4084	-	0,6,6	0.00	-	-		
87	OHX	1	4098	-	0,6,6	0.00	-	-		
87	OHX	1	4156	-	0,6,6	0.00	-	-		
87	OHX	3	222	-	0,6,6	0.00	-	-		
87	OHX	1	3894	-	0,6,6	0.00	-	-		
87	OHX	6	2092	-	0,6,6	0.00	-	-		
87	OHX	5	4111	-	0,6,6	0.00	-	-		
87	OHX	1	4085	-	0,6,6	0.00	-	-		
87	OHX	1	3957	-	0,6,6	0.00	-	-		
87	OHX	1	4213	-	0,6,6	0.00	-	-		
87	OHX	5	4069	-	0,6,6	0.00	-	-		
87	OHX	C8	201	-	0,6,6	0.00	-	-		
87	OHX	2	2152	-	0,6,6	0.00	-	-		
87	OHX	1	4105	-	0,6,6	0.00	-	-		
87	OHX	6	2069	-	0,6,6	0.00	-	-		
87	OHX	5	4119	-	0,6,6	0.00	-	-		
87	OHX	1	3979	-	0,6,6	0.00	-	-		
87	OHX	5	3925	-	0,6,6	0.00	-	-		
87	OHX	4	227	-	0,6,6	0.00	-	-		
87	OHX	6	2110	-	0,6,6	0.00	-	-		
87	OHX	1	4170	-	0,6,6	0.00	-	-		
87	OHX	L3	403	-	0,6,6	0.00	-	-		
87	OHX	8	226	-	0,6,6	0.00	-	-		
87	OHX	5	3955	-	0,6,6	0.00	-	-		
87	OHX	1	4037	-	0,6,6	0.00	-	-		
87	OHX	1	4204	-	0,6,6	0.00	-	-		
87	OHX	5	4041	-	0,6,6	0.00	-	-		
87	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
87	OHX	2	2120	-	0,6,6	0.00	-	-		
87	OHX	1	4005	-	0,6,6	0.00	-	-		
87	OHX	1	3983	-	0,6,6	0.00	-	-		
87	OHX	2	2142	-	0,6,6	0.00	-	-		
87	OHX	2	2052	-	0,6,6	0.00	-	-		
87	OHX	2	2165	-	0,6,6	0.00	-	-		
87	OHX	1	3920	-	0,6,6	0.00	-	-		
87	OHX	5	4143	-	0,6,6	0.00	-	-		
87	OHX	1	4071	-	0,6,6	0.00	-	-		
87	OHX	1	3929	-	0,6,6	0.00	-	-		
87	OHX	5	4136	-	0,6,6	0.00	-	-		
87	OHX	2	2040	-	0,6,6	0.00	-	-		
87	OHX	1	4124	-	0,6,6	0.00	-	-		
87	OHX	5	3938	-	0,6,6	0.00	-	-		
87	OHX	5	4141	-	0,6,6	0.00	-	-		
87	OHX	6	2166	-	0,6,6	0.00	-	-		
87	OHX	5	4055	-	0,6,6	0.00	-	-		
87	OHX	1	3995	-	0,6,6	0.00	-	-		
87	OHX	1	4207	-	0,6,6	0.00	-	-		
87	OHX	5	4253	-	0,6,6	0.00	-	-		
87	OHX	6	2065	-	0,6,6	0.00	-	-		
87	OHX	6	2066	-	0,6,6	0.00	-	-		
87	OHX	1	4155	-	0,6,6	0.00	-	-		
87	OHX	1	3985	-	0,6,6	0.00	-	-		
87	OHX	1	4189	-	0,6,6	0.00	-	-		
87	OHX	5	4240	-	0,6,6	0.00	-	-		
87	OHX	3	219	-	0,6,6	0.00	-	-		
87	OHX	5	4138	-	0,6,6	0.00	-	-		
87	OHX	6	2083	-	0,6,6	0.00	-	-		
87	OHX	5	4062	-	0,6,6	0.00	-	-		
87	OHX	1	4145	-	0,6,6	0.00	-	-		
87	OHX	1	4115	-	0,6,6	0.00	-	-		
87	OHX	1	4198	-	0,6,6	0.00	-	-		
87	OHX	2	2136	-	0,6,6	0.00	-	-		
87	OHX	2	2175	-	0,6,6	0.00	-	-		
87	OHX	5	4116	-	0,6,6	0.00	-	-		
87	OHX	6	2143	-	0,6,6	0.00	-	-		
87	OHX	5	4079	-	0,6,6	0.00	-	-		
87	OHX	5	4175	-	0,6,6	0.00	-	-		
87	OHX	5	3906	-	0,6,6	0.00	-	-		
87	OHX	1	4158	-	0,6,6	0.00	-	-		
87	OHX	5	4032	-	0,6,6	0.00	-	-		
87	OHX	1	4152	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	l4	403	-	0,6,6	0.00	-	-		
87	OHX	c5	201	-	0,6,6	0.00	-	-		
87	OHX	n3	203	-	0,6,6	0.00	-	-		
87	OHX	5	4036	-	0,6,6	0.00	-	-		
87	OHX	5	4239	-	0,6,6	0.00	-	-		
87	OHX	2	2039	-	0,6,6	0.00	-	-		
87	OHX	5	4000	-	0,6,6	0.00	-	-		
87	OHX	5	4005	-	0,6,6	0.00	-	-		
87	OHX	5	3975	-	0,6,6	0.00	-	-		
87	OHX	5	4029	-	0,6,6	0.00	-	-		
87	OHX	5	4122	-	0,6,6	0.00	-	-		
87	OHX	2	2132	-	0,6,6	0.00	-	-		
87	OHX	3	223	-	0,6,6	0.00	-	-		
87	OHX	5	4087	-	0,6,6	0.00	-	-		
87	OHX	6	2073	-	0,6,6	0.00	-	-		
87	OHX	5	4039	-	0,6,6	0.00	-	-		
87	OHX	5	4090	-	0,6,6	0.00	-	-		
87	OHX	6	2198	-	0,6,6	0.00	-	-		
87	OHX	6	2178	-	0,6,6	0.00	-	-		
87	OHX	5	4203	-	0,6,6	0.00	-	-		
87	OHX	1	4211	-	0,6,6	0.00	-	-		
87	OHX	5	4120	-	0,6,6	0.00	-	-		
87	OHX	5	4033	-	0,6,6	0.00	-	-		
87	OHX	1	4214	-	0,6,6	0.00	-	-		
87	OHX	5	3944	-	0,6,6	0.00	-	-		
87	OHX	6	2149	-	0,6,6	0.00	-	-		
87	OHX	1	4141	-	0,6,6	0.00	-	-		
87	OHX	1	4021	-	0,6,6	0.00	-	-		
87	OHX	5	3915	-	0,6,6	0.00	-	-		
87	OHX	5	4063	-	0,6,6	0.00	-	-		
87	OHX	5	3939	-	0,6,6	0.00	-	-		
87	OHX	1	4140	-	0,6,6	0.00	-	-		
87	OHX	o7	502	-	0,6,6	0.00	-	-		
87	OHX	6	2121	-	0,6,6	0.00	-	-		
87	OHX	1	3933	-	0,6,6	0.00	-	-		
87	OHX	8	216	-	0,6,6	0.00	-	-		
87	OHX	m9	201	-	0,6,6	0.00	-	-		
87	OHX	2	2111	-	0,6,6	0.00	-	-		
87	OHX	o2	201	-	0,6,6	0.00	-	-		
87	OHX	1	4206	-	0,6,6	0.00	-	-		
87	OHX	1	4181	-	0,6,6	0.00	-	-		
87	OHX	1	4108	-	0,6,6	0.00	-	-		
87	OHX	2	2118	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4015	-	0,6,6	0.00	-	-		
87	OHX	6	2068	-	0,6,6	0.00	-	-		
87	OHX	1	4040	-	0,6,6	0.00	-	-		
87	OHX	1	3883	-	0,6,6	0.00	-	-		
87	OHX	6	2193	-	0,6,6	0.00	-	-		
87	OHX	6	2076	-	0,6,6	0.00	-	-		
87	OHX	2	2115	-	0,6,6	0.00	-	-		
87	OHX	5	4135	-	0,6,6	0.00	-	-		
87	OHX	5	3962	-	0,6,6	0.00	-	-		
87	OHX	4	231	-	0,6,6	0.00	-	-		
87	OHX	M7	207	-	0,6,6	0.00	-	-		
87	OHX	2	2166	-	0,6,6	0.00	-	-		
87	OHX	1	4030	-	0,6,6	0.00	-	-		
87	OHX	6	2128	-	0,6,6	0.00	-	-		
87	OHX	6	2127	-	0,6,6	0.00	-	-		
87	OHX	6	2184	-	0,6,6	0.00	-	-		
87	OHX	5	4187	-	0,6,6	0.00	-	-		
87	OHX	1	4179	-	0,6,6	0.00	-	-		
87	OHX	5	4152	-	0,6,6	0.00	-	-		
87	OHX	6	2190	-	0,6,6	0.00	-	-		
89	3KD	1	4218	-	24,25,25	0.80	0	30,39,39	1.10	1 (3%)
87	OHX	5	3931	-	0,6,6	0.00	-	-		
87	OHX	1	4067	-	0,6,6	0.00	-	-		
87	OHX	5	4088	-	0,6,6	0.00	-	-		
87	OHX	5	4082	-	0,6,6	0.00	-	-		
87	OHX	6	2200	-	0,6,6	0.00	-	-		
87	OHX	8	217	-	0,6,6	0.00	-	-		
87	OHX	1	4201	-	0,6,6	0.00	-	-		
87	OHX	1	4070	-	0,6,6	0.00	-	-		
87	OHX	5	4234	-	0,6,6	0.00	-	-		
87	OHX	6	2191	-	0,6,6	0.00	-	-		
87	OHX	5	3970	-	0,6,6	0.00	-	-		
87	OHX	5	4047	-	0,6,6	0.00	-	-		
87	OHX	c1	202	-	0,6,6	0.00	-	-		
87	OHX	2	2122	-	0,6,6	0.00	-	-		
87	OHX	5	4125	-	0,6,6	0.00	-	-		
87	OHX	4	233	-	0,6,6	0.00	-	-		
87	OHX	5	3922	-	0,6,6	0.00	-	-		
87	OHX	1	4072	-	0,6,6	0.00	-	-		
87	OHX	5	4085	-	0,6,6	0.00	-	-		
87	OHX	1	3940	-	0,6,6	0.00	-	-		
89	3KD	5	4254	-	24,25,25	1.04	2 (8%)	30,39,39	1.06	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	2	2116	-	0,6,6	0.00	-	-		
87	OHX	4	225	-	0,6,6	0.00	-	-		
87	OHX	5	4003	-	0,6,6	0.00	-	-		
87	OHX	1	3986	-	0,6,6	0.00	-	-		
87	OHX	1	3956	-	0,6,6	0.00	-	-		
87	OHX	1	4059	-	0,6,6	0.00	-	-		
87	OHX	6	2064	-	0,6,6	0.00	-	-		
87	OHX	1	4046	-	0,6,6	0.00	-	-		
87	OHX	2	2099	-	0,6,6	0.00	-	-		
87	OHX	1	3978	-	0,6,6	0.00	-	-		
87	OHX	1	4075	-	0,6,6	0.00	-	-		
87	OHX	6	2177	-	0,6,6	0.00	-	-		
87	OHX	2	2174	-	0,6,6	0.00	-	-		
87	OHX	19	202	-	0,6,6	0.00	-	-		
87	OHX	2	2149	-	0,6,6	0.00	-	-		
87	OHX	2	2059	-	0,6,6	0.00	-	-		
87	OHX	2	2058	-	0,6,6	0.00	-	-		
87	OHX	1	4038	-	0,6,6	0.00	-	-		
87	OHX	1	4048	-	0,6,6	0.00	-	-		
87	OHX	2	2098	-	0,6,6	0.00	-	-		
87	OHX	6	2087	-	0,6,6	0.00	-	-		
87	OHX	2	2047	-	0,6,6	0.00	-	-		
87	OHX	1	4126	-	0,6,6	0.00	-	-		
87	OHX	6	2173	-	0,6,6	0.00	-	-		
87	OHX	1	3955	-	0,6,6	0.00	-	-		
87	OHX	1	4195	-	0,6,6	0.00	-	-		
87	OHX	1	4023	-	0,6,6	0.00	-	-		
87	OHX	5	3984	-	0,6,6	0.00	-	-		
87	OHX	7	223	-	0,6,6	0.00	-	-		
87	OHX	1	4018	-	0,6,6	0.00	-	-		
87	OHX	6	2061	-	0,6,6	0.00	-	-		
87	OHX	1	4199	-	0,6,6	0.00	-	-		
87	OHX	5	3917	-	0,6,6	0.00	-	-		
87	OHX	6	2154	-	0,6,6	0.00	-	-		
87	OHX	5	4094	-	0,6,6	0.00	-	-		
87	OHX	1	3904	-	0,6,6	0.00	-	-		
87	OHX	6	2086	-	0,6,6	0.00	-	-		
87	OHX	2	2109	-	0,6,6	0.00	-	-		
87	OHX	1	4150	-	0,6,6	0.00	-	-		
87	OHX	5	4150	-	0,6,6	0.00	-	-		
87	OHX	1	4180	-	0,6,6	0.00	-	-		
87	OHX	1	4026	-	0,6,6	0.00	-	-		
87	OHX	6	2055	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	7	220	-	0,6,6	0.00	-	-		
87	OHX	O2	201	-	0,6,6	0.00	-	-		
87	OHX	2	2085	-	0,6,6	0.00	-	-		
87	OHX	5	3994	-	0,6,6	0.00	-	-		
87	OHX	5	3951	-	0,6,6	0.00	-	-		
87	OHX	2	2046	-	0,6,6	0.00	-	-		
87	OHX	1	3963	-	0,6,6	0.00	-	-		
87	OHX	5	4202	-	0,6,6	0.00	-	-		
87	OHX	5	3921	-	0,6,6	0.00	-	-		
87	OHX	5	4024	-	0,6,6	0.00	-	-		
87	OHX	1	3998	-	0,6,6	0.00	-	-		
87	OHX	1	3922	-	0,6,6	0.00	-	-		
87	OHX	5	4222	-	0,6,6	0.00	-	-		
87	OHX	5	3946	-	0,6,6	0.00	-	-		
87	OHX	5	4209	-	0,6,6	0.00	-	-		
87	OHX	2	2176	-	0,6,6	0.00	-	-		
87	OHX	3	217	-	0,6,6	0.00	-	-		
87	OHX	6	2175	-	0,6,6	0.00	-	-		
87	OHX	5	4142	-	0,6,6	0.00	-	-		
87	OHX	5	3901	-	0,6,6	0.00	-	-		
87	OHX	5	4181	-	0,6,6	0.00	-	-		
87	OHX	6	2156	-	0,6,6	0.00	-	-		
87	OHX	5	4158	-	0,6,6	0.00	-	-		
87	OHX	5	3983	-	0,6,6	0.00	-	-		
87	OHX	1	4016	-	0,6,6	0.00	-	-		
87	OHX	2	2168	-	0,6,6	0.00	-	-		
87	OHX	1	4187	-	0,6,6	0.00	-	-		
87	OHX	M6	202	-	0,6,6	0.00	-	-		
87	OHX	5	4171	-	0,6,6	0.00	-	-		
87	OHX	2	2126	-	0,6,6	0.00	-	-		
87	OHX	6	2179	-	0,6,6	0.00	-	-		
87	OHX	6	2104	-	0,6,6	0.00	-	-		
87	OHX	5	4017	-	0,6,6	0.00	-	-		
87	OHX	1	4194	-	0,6,6	0.00	-	-		
87	OHX	5	4060	-	0,6,6	0.00	-	-		
87	OHX	5	4235	-	0,6,6	0.00	-	-		
87	OHX	1	4153	-	0,6,6	0.00	-	-		
87	OHX	2	2171	-	0,6,6	0.00	-	-		
87	OHX	5	3912	-	0,6,6	0.00	-	-		
87	OHX	l3	404	-	0,6,6	0.00	-	-		
87	OHX	2	2145	-	0,6,6	0.00	-	-		
87	OHX	7	225	-	0,6,6	0.00	-	-		
87	OHX	1	3934	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	1	4154	-	0,6,6	0.00	-	-		
87	OHX	5	4160	-	0,6,6	0.00	-	-		
87	OHX	5	4204	-	0,6,6	0.00	-	-		
87	OHX	1	3875	-	0,6,6	0.00	-	-		
87	OHX	5	3995	-	0,6,6	0.00	-	-		
87	OHX	5	4244	-	0,6,6	0.00	-	-		
87	OHX	15	303	-	0,6,6	0.00	-	-		
87	OHX	s9	201	-	0,6,6	0.00	-	-		
87	OHX	1	4060	-	0,6,6	0.00	-	-		
87	OHX	1	3884	-	0,6,6	0.00	-	-		
87	OHX	5	4025	-	0,6,6	0.00	-	-		
87	OHX	5	4040	-	0,6,6	0.00	-	-		
87	OHX	5	4192	-	0,6,6	0.00	-	-		
87	OHX	1	4002	-	0,6,6	0.00	-	-		
87	OHX	5	4144	-	0,6,6	0.00	-	-		
87	OHX	2	2067	-	0,6,6	0.00	-	-		
87	OHX	1	4028	-	0,6,6	0.00	-	-		
87	OHX	1	4157	-	0,6,6	0.00	-	-		
87	OHX	1	4185	-	0,6,6	0.00	-	-		
87	OHX	5	3959	-	0,6,6	0.00	-	-		
87	OHX	5	4008	-	0,6,6	0.00	-	-		
87	OHX	6	2170	-	0,6,6	0.00	-	-		
87	OHX	2	2135	-	0,6,6	0.00	-	-		
87	OHX	5	4172	-	0,6,6	0.00	-	-		
87	OHX	5	4054	-	0,6,6	0.00	-	-		
87	OHX	2	2134	-	0,6,6	0.00	-	-		
87	OHX	6	2091	-	0,6,6	0.00	-	-		
87	OHX	1	3928	-	0,6,6	0.00	-	-		
87	OHX	8	219	-	0,6,6	0.00	-	-		
87	OHX	8	224	-	0,6,6	0.00	-	-		
87	OHX	N9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4045	-	0,6,6	0.00	-	-		
87	OHX	1	3908	-	0,6,6	0.00	-	-		
87	OHX	5	4176	-	0,6,6	0.00	-	-		
87	OHX	1	4089	-	0,6,6	0.00	-	-		
87	OHX	5	3937	-	0,6,6	0.00	-	-		
87	OHX	1	4047	-	0,6,6	0.00	-	-		
87	OHX	5	4086	-	0,6,6	0.00	-	-		
87	OHX	5	4100	-	0,6,6	0.00	-	-		
87	OHX	5	4224	-	0,6,6	0.00	-	-		
87	OHX	5	4083	-	0,6,6	0.00	-	-		
87	OHX	8	229	-	0,6,6	0.00	-	-		
87	OHX	1	4100	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	7	221	-	0,6,6	0.00	-	-		
87	OHX	1	3907	-	0,6,6	0.00	-	-		
87	OHX	5	4081	-	0,6,6	0.00	-	-		
87	OHX	2	2150	-	0,6,6	0.00	-	-		
87	OHX	2	2124	-	0,6,6	0.00	-	-		
87	OHX	5	4052	-	0,6,6	0.00	-	-		
87	OHX	2	2096	-	0,6,6	0.00	-	-		
87	OHX	2	2129	-	0,6,6	0.00	-	-		
87	OHX	1	4148	-	0,6,6	0.00	-	-		
87	OHX	3	221	-	0,6,6	0.00	-	-		
87	OHX	5	3972	-	0,6,6	0.00	-	-		
87	OHX	1	3990	-	0,6,6	0.00	-	-		
87	OHX	5	4151	-	0,6,6	0.00	-	-		
87	OHX	5	3969	-	0,6,6	0.00	-	-		
87	OHX	1	4135	-	0,6,6	0.00	-	-		
87	OHX	1	3975	-	0,6,6	0.00	-	-		
87	OHX	6	2094	-	0,6,6	0.00	-	-		
87	OHX	5	3918	-	0,6,6	0.00	-	-		
87	OHX	2	2045	-	0,6,6	0.00	-	-		
87	OHX	6	2204	-	0,6,6	0.00	-	-		
87	OHX	2	2161	-	0,6,6	0.00	-	-		
87	OHX	2	2147	-	0,6,6	0.00	-	-		
87	OHX	1	3872	-	0,6,6	0.00	-	-		
87	OHX	s4	302	-	0,6,6	0.00	-	-		
87	OHX	5	3943	-	0,6,6	0.00	-	-		
87	OHX	1	4088	-	0,6,6	0.00	-	-		
87	OHX	1	4008	-	0,6,6	0.00	-	-		
87	OHX	6	2180	-	0,6,6	0.00	-	-		
87	OHX	6	2183	-	0,6,6	0.00	-	-		
87	OHX	5	4058	-	0,6,6	0.00	-	-		
87	OHX	2	2095	-	0,6,6	0.00	-	-		
87	OHX	1	4015	-	0,6,6	0.00	-	-		
87	OHX	5	3963	-	0,6,6	0.00	-	-		
87	OHX	2	2041	-	0,6,6	0.00	-	-		
87	OHX	1	4165	-	0,6,6	0.00	-	-		
87	OHX	5	4117	-	0,6,6	0.00	-	-		
87	OHX	1	3993	-	0,6,6	0.00	-	-		
87	OHX	6	2057	-	0,6,6	0.00	-	-		
87	OHX	2	2100	-	0,6,6	0.00	-	-		
87	OHX	5	3954	-	0,6,6	0.00	-	-		
87	OHX	5	4190	-	0,6,6	0.00	-	-		
87	OHX	2	2173	-	0,6,6	0.00	-	-		
87	OHX	5	4154	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	5	4185	-	0,6,6	0.00	-	-		
87	OHX	5	3949	-	0,6,6	0.00	-	-		
87	OHX	5	4064	-	0,6,6	0.00	-	-		
87	OHX	1	4042	-	0,6,6	0.00	-	-		
87	OHX	5	3930	-	0,6,6	0.00	-	-		
87	OHX	6	2067	-	0,6,6	0.00	-	-		
87	OHX	2	2162	-	0,6,6	0.00	-	-		
87	OHX	5	3905	-	0,6,6	0.00	-	-		
87	OHX	7	222	-	0,6,6	0.00	-	-		
87	OHX	5	4051	-	0,6,6	0.00	-	-		
87	OHX	1	4104	-	0,6,6	0.00	-	-		
87	OHX	2	2146	-	0,6,6	0.00	-	-		
87	OHX	2	2053	-	0,6,6	0.00	-	-		
87	OHX	2	2156	-	0,6,6	0.00	-	-		
87	OHX	6	2195	-	0,6,6	0.00	-	-		
87	OHX	8	228	-	0,6,6	0.00	-	-		
87	OHX	1	4196	-	0,6,6	0.00	-	-		
87	OHX	2	2105	-	0,6,6	0.00	-	-		
87	OHX	2	2030	-	0,6,6	0.00	-	-		
87	OHX	5	3902	-	0,6,6	0.00	-	-		
87	OHX	2	2035	-	0,6,6	0.00	-	-		
87	OHX	1	4101	-	0,6,6	0.00	-	-		
87	OHX	5	4112	-	0,6,6	0.00	-	-		
87	OHX	4	228	-	0,6,6	0.00	-	-		
87	OHX	1	4184	-	0,6,6	0.00	-	-		
87	OHX	5	3971	-	0,6,6	0.00	-	-		
87	OHX	1	3984	-	0,6,6	0.00	-	-		
87	OHX	1	4019	-	0,6,6	0.00	-	-		
87	OHX	o7	503	-	0,6,6	0.00	-	-		
87	OHX	2	2064	-	0,6,6	0.00	-	-		
87	OHX	5	3907	-	0,6,6	0.00	-	-		
87	OHX	5	4241	-	0,6,6	0.00	-	-		
87	OHX	6	2168	-	0,6,6	0.00	-	-		
87	OHX	6	2146	-	0,6,6	0.00	-	-		
87	OHX	1	3994	-	0,6,6	0.00	-	-		
87	OHX	l5	305	-	0,6,6	0.00	-	-		
87	OHX	M9	202	-	0,6,6	0.00	-	-		
87	OHX	1	4114	-	0,6,6	0.00	-	-		
87	OHX	1	4041	-	0,6,6	0.00	-	-		
87	OHX	6	2108	-	0,6,6	0.00	-	-		
87	OHX	6	2102	-	0,6,6	0.00	-	-		
87	OHX	1	3890	-	0,6,6	0.00	-	-		
87	OHX	1	4200	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	OHX	6	2109	-	0,6,6	0.00	-	-		
87	OHX	2	2158	-	0,6,6	0.00	-	-		
87	OHX	5	4147	-	0,6,6	0.00	-	-		
87	OHX	2	2032	-	0,6,6	0.00	-	-		
87	OHX	O3	201	-	0,6,6	0.00	-	-		
87	OHX	1	4034	-	0,6,6	0.00	-	-		
87	OHX	1	4094	-	0,6,6	0.00	-	-		
87	OHX	5	3973	-	0,6,6	0.00	-	-		
87	OHX	1	3976	-	0,6,6	0.00	-	-		
87	OHX	1	3936	-	0,6,6	0.00	-	-		
87	OHX	5	4038	-	0,6,6	0.00	-	-		
87	OHX	2	2160	-	0,6,6	0.00	-	-		
87	OHX	2	2153	-	0,6,6	0.00	-	-		
87	OHX	2	2034	-	0,6,6	0.00	-	-		
87	OHX	5	4238	-	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
89	3KD	5	4254	-	-	-	0/5/5/5
89	3KD	1	4218	-	-	-	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4254	3KD	C13-C12	3.04	1.54	1.50
89	5	4254	3KD	C8-C9	-2.40	1.47	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	5	4254	3KD	O-C14-C9	-3.44	101.86	109.57
89	1	4218	3KD	O-C14-C9	-2.91	103.05	109.57

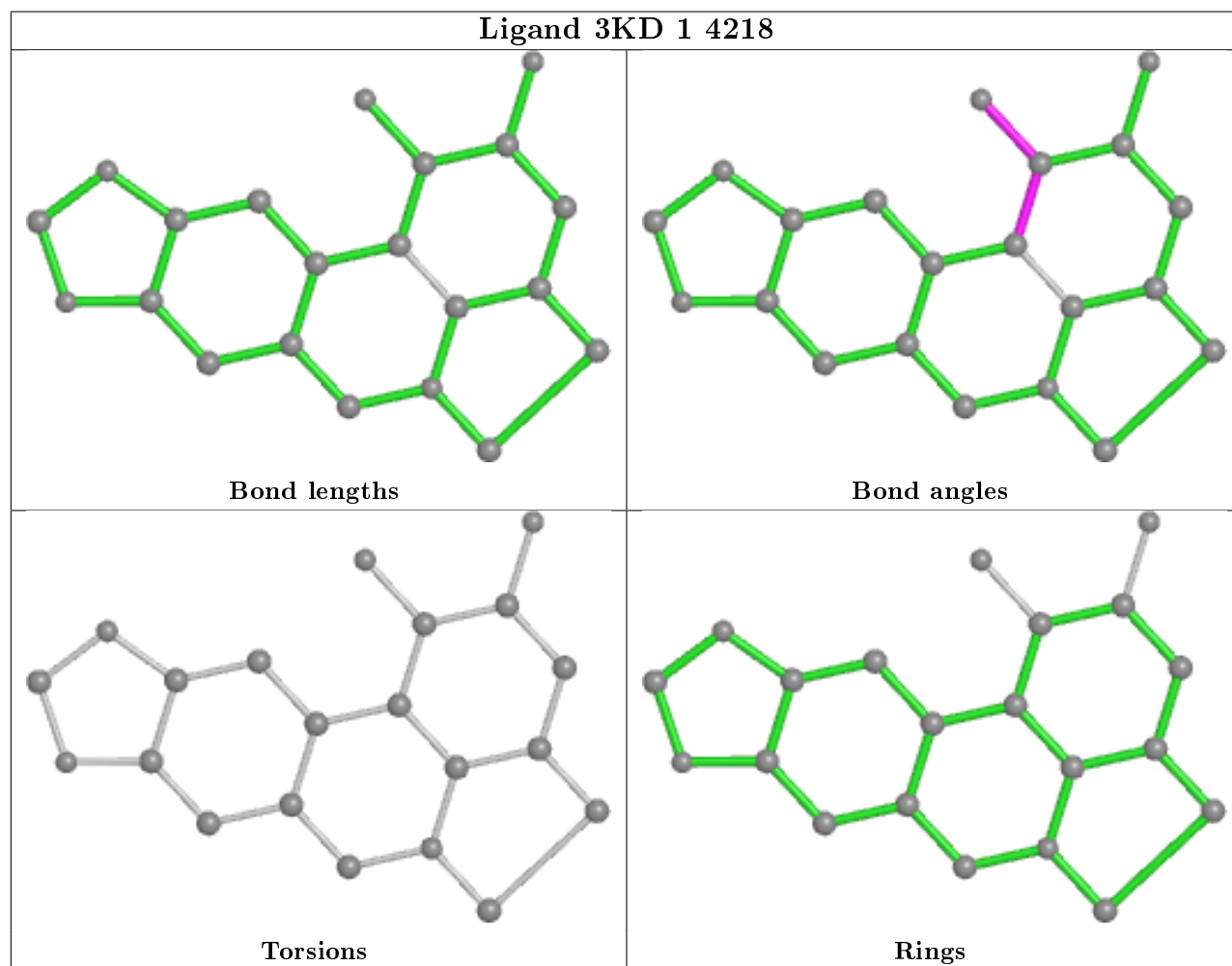
There are no chirality outliers.

There are no torsion outliers.

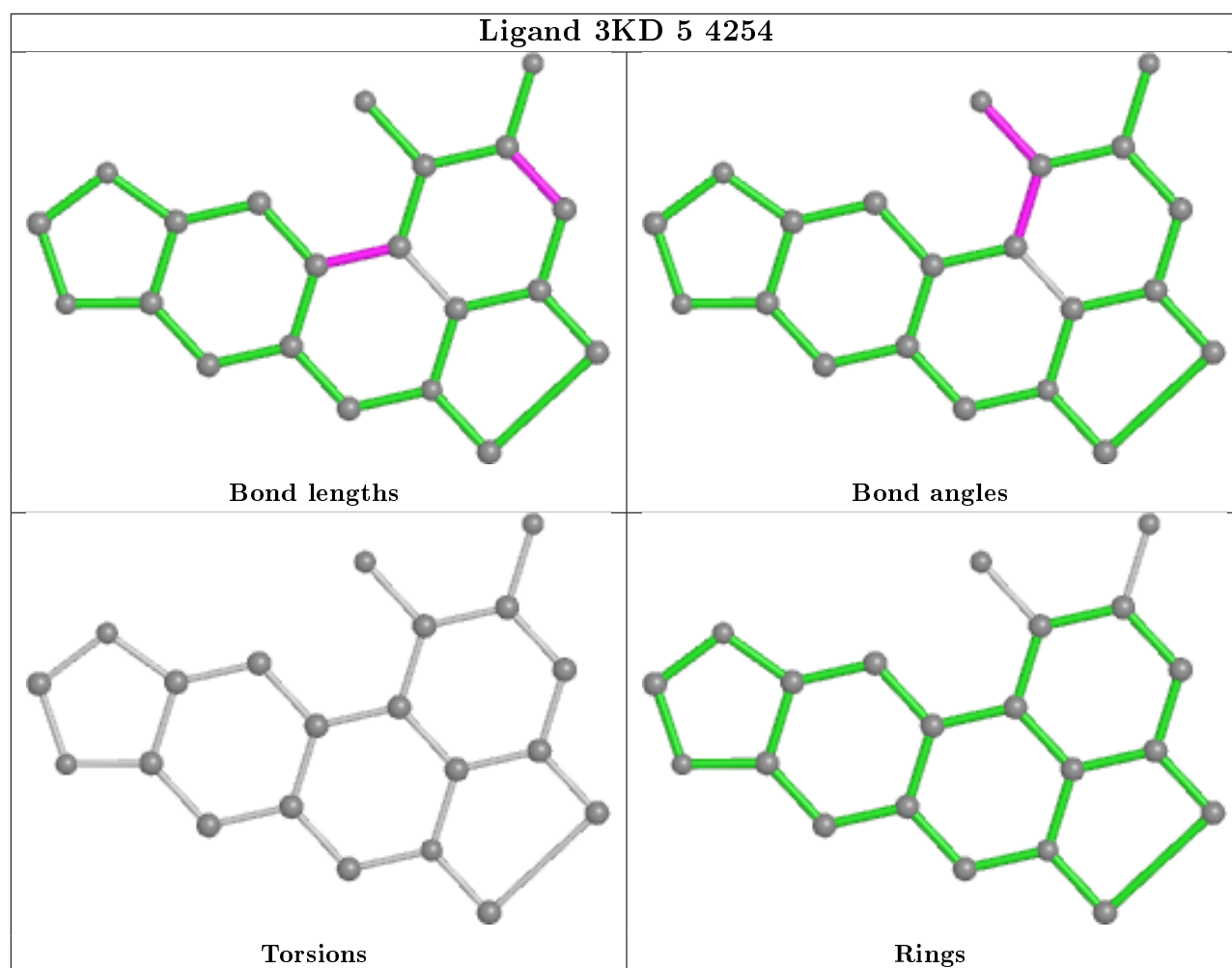
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

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

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