



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 06:31 PM BST

PDB ID : 4U3U
Title : Crystal structure of Cycloheximide bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-22
Resolution : 2.90 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

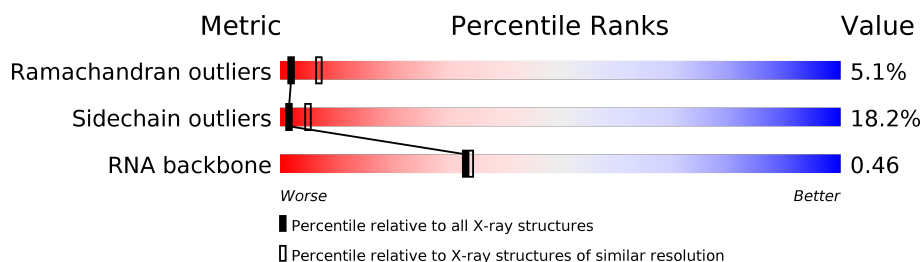
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)


























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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

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















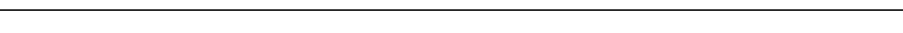




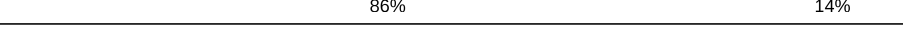
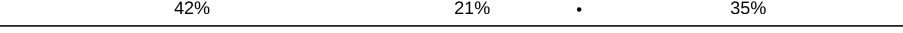




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Mol	Chain	Length	Quality of chain
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3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

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


























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















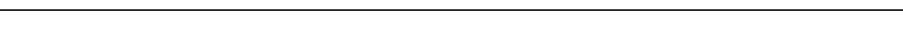




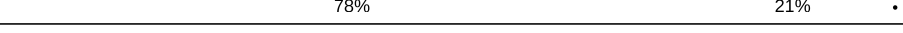





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Mol	Chain	Length	Quality of chain
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7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















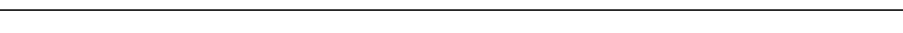




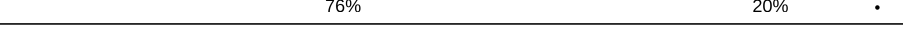





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Mol	Chain	Length	Quality of chain
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9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

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Mol	Chain	Length	Quality of chain
68	o2	129	 78%19% ..
69	O3	106	 88%11% .
69	o3	106	 85%14% .
70	O4	119	 76%17% . 6%
70	o4	119	 81%13% . 6%
71	O5	119	 80%18% .
71	o5	119	 82%18%
72	O6	99	 78%19% .
72	o6	99	 71%26% .
73	O7	87	 85%13% .
73	o7	87	 80%20%
74	O8	77	 79%19% .
74	o8	77	 83%16% .
75	O9	50	 88%12%
75	o9	50	 84%16%
76	Q0	52	 88%10% .
76	q0	52	 81%19%
77	Q1	25	 68%32%
77	q1	25	 76%20% .
78	Q2	105	 79%20% .
78	q2	105	 81%18% .
79	Q3	91	 82%18%
79	q3	91	 81%18% .
80	e0	62	 76%24%
81	e1	76	 58%34%7% .

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

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411205 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	0	0	0
			1111	711	204	196			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1764	1131	316	314	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O		0	0	0
			1521	935	326	260				
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 Ubiquitin-40S ribosomal protein S31.

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

- Molecule 82 is a protein called UNKNOWN PROTEIN 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 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 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	3	Total	Mg	0	0
			3	3		
86	m7	4	Total	Mg	0	0
			4	4		
86	n8	3	Total	Mg	0	0
			3	3		
86	o1	2	Total	Mg	0	0
			2	2		
86	N5	1	Total	Mg	0	0
			1	1		
86	6	147	Total	Mg	0	0
			147	147		
86	sM	2	Total	Mg	0	0
			2	2		
86	O4	2	Total	Mg	0	0
			2	2		
86	m5	2	Total	Mg	0	0
			2	2		
86	l3	1	Total	Mg	0	0
			1	1		
86	M1	1	Total	Mg	0	0
			1	1		
86	n0	2	Total	Mg	0	0
			2	2		
86	d6	1	Total	Mg	0	0
			1	1		
86	2	122	Total	Mg	0	0
			122	122		
86	O3	1	Total	Mg	0	0
			1	1		
86	L4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	l7	1	Total 1	Mg 1	0	0
86	M5	2	Total 2	Mg 2	0	0
86	l4	2	Total 2	Mg 2	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	o4	2	Total 2	Mg 2	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	c8	2	Total 2	Mg 2	0	0
86	M0	2	Total 2	Mg 2	0	0
86	c1	1	Total 1	Mg 1	0	0
86	5	505	Total 505	Mg 505	0	0
86	L5	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	s6	1	Total 1	Mg 1	0	0
86	Q2	1	Total 1	Mg 1	0	0
86	1	471	Total 471	Mg 471	0	0
86	c4	1	Total 1	Mg 1	0	0
86	D0	1	Total 1	Mg 1	0	0

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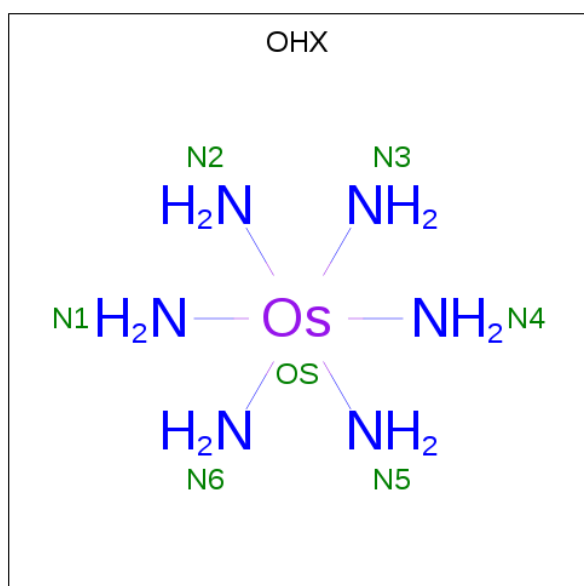
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	S8	1	Total 1	Mg 1	0	0
86	m1	2	Total 2	Mg 2	0	0
86	d3	1	Total 1	Mg 1	0	0
86	q3	2	Total 2	Mg 2	0	0
86	o3	1	Total 1	Mg 1	0	0
86	M3	4	Total 4	Mg 4	0	0
86	N3	3	Total 3	Mg 3	0	0
86	4	22	Total 22	Mg 22	0	0
86	n6	2	Total 2	Mg 2	0	0
86	S4	1	Total 1	Mg 1	0	0
86	L2	1	Total 1	Mg 1	0	0
86	o7	1	Total 1	Mg 1	0	0
86	l5	2	Total 2	Mg 2	0	0
86	C3	1	Total 1	Mg 1	0	0
86	M7	6	Total 6	Mg 6	0	0
86	N8	4	Total 4	Mg 4	0	0
86	s1	1	Total 1	Mg 1	0	0
86	m6	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	s8	1	Total 1	Mg 1	0	0
86	l8	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	c7	2	Total 2	Mg 2	0	0
86	7	15	Total 15	Mg 15	0	0
86	n3	2	Total 2	Mg 2	0	0
86	L3	3	Total 3	Mg 3	0	0
86	d4	1	Total 1	Mg 1	0	0
86	l2	2	Total 2	Mg 2	0	0
86	8	13	Total 13	Mg 13	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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		
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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	3	1	Total	N	Os	0	0
			7	6	1		
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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			7	6	1		
87	3	1	Total	N	Os	0	0
			7	6	1		
87	3	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M7	1	Total	N	Os	0	0
			7	6	1		
87	M9	1	Total	N	Os	0	0
			7	6	1		
87	N1	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	O9	1	Total	N	Os	0	0
			7	6	1		
87	Q2	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		
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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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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		
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
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			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
			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
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			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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			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
			7	6	1		
87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
			7	6	1		
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
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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		
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		
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	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
87	s9	1	Total 7	N 6	Os 1	0	0
87	c1	1	Total 7	N 6	Os 1	0	0
87	c3	1	Total 7	N 6	Os 1	0	0
87	c5	1	Total 7	N 6	Os 1	0	0
87	c8	1	Total 7	N 6	Os 1	0	0
87	d4	1	Total 7	N 6	Os 1	0	0
87	d9	1	Total 7	N 6	Os 1	0	0
87	sR	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	0	0

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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		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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	7	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	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	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		

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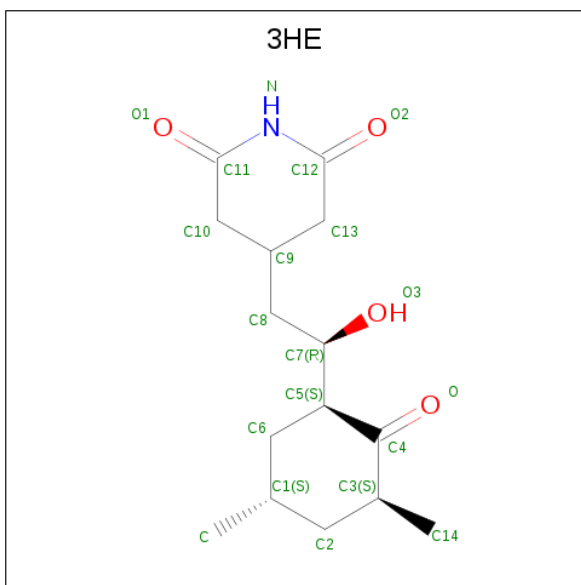
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l5	1	Total	N	Os	0	0
			7	6	1		
87	l9	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		
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	n3	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	o9	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 1	Zn 1	0	0
88	D6	1	Total 1	Zn 1	0	0
88	Q2	1	Total 1	Zn 1	0	0
88	e1	1	Total 1	Zn 1	0	0
88	Q3	1	Total 1	Zn 1	0	0
88	D9	1	Total 1	Zn 1	0	0
88	E1	1	Total 1	Zn 1	0	0
88	Q0	1	Total 1	Zn 1	0	0
88	d7	1	Total 1	Zn 1	0	0
88	q3	1	Total 1	Zn 1	0	0
88	d9	1	Total 1	Zn 1	0	0
88	D7	1	Total 1	Zn 1	0	0
88	d6	1	Total 1	Zn 1	0	0
88	o7	1	Total 1	Zn 1	0	0
88	O7	1	Total 1	Zn 1	0	0
88	q2	1	Total 1	Zn 1	0	0

- Molecule 89 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: C₁₅H₂₃NO₄).



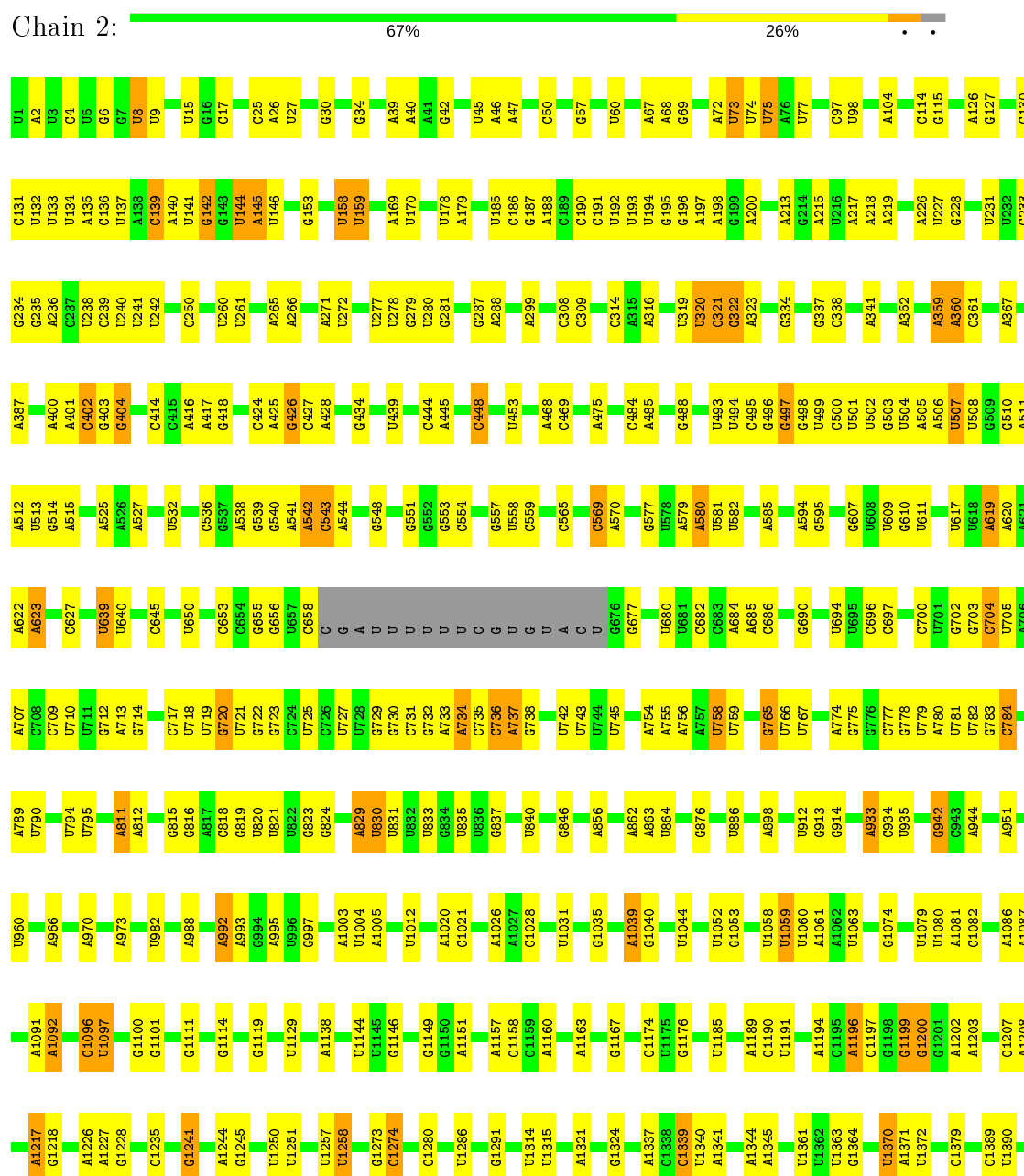
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			20	15	1	4		
89	5	1	Total	C	N	O	0	0
			20	15	1	4		

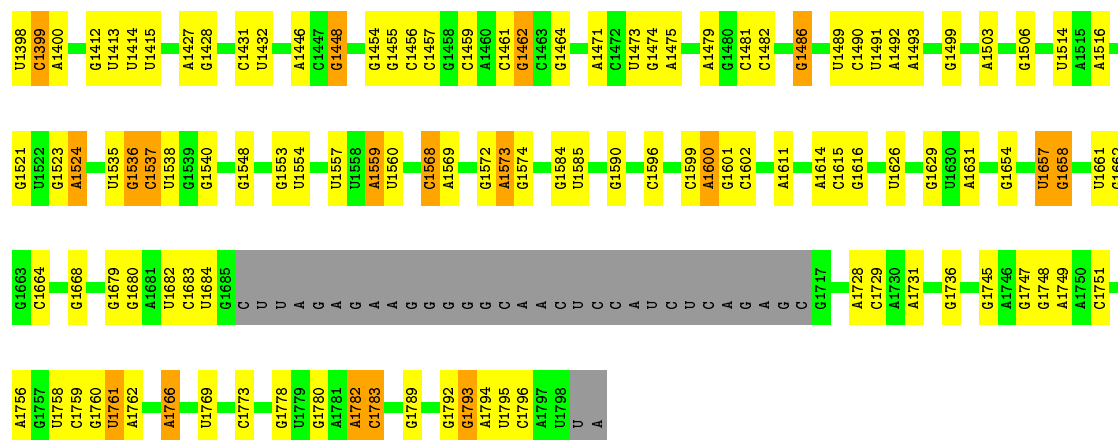
3 Residue-property plots

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.

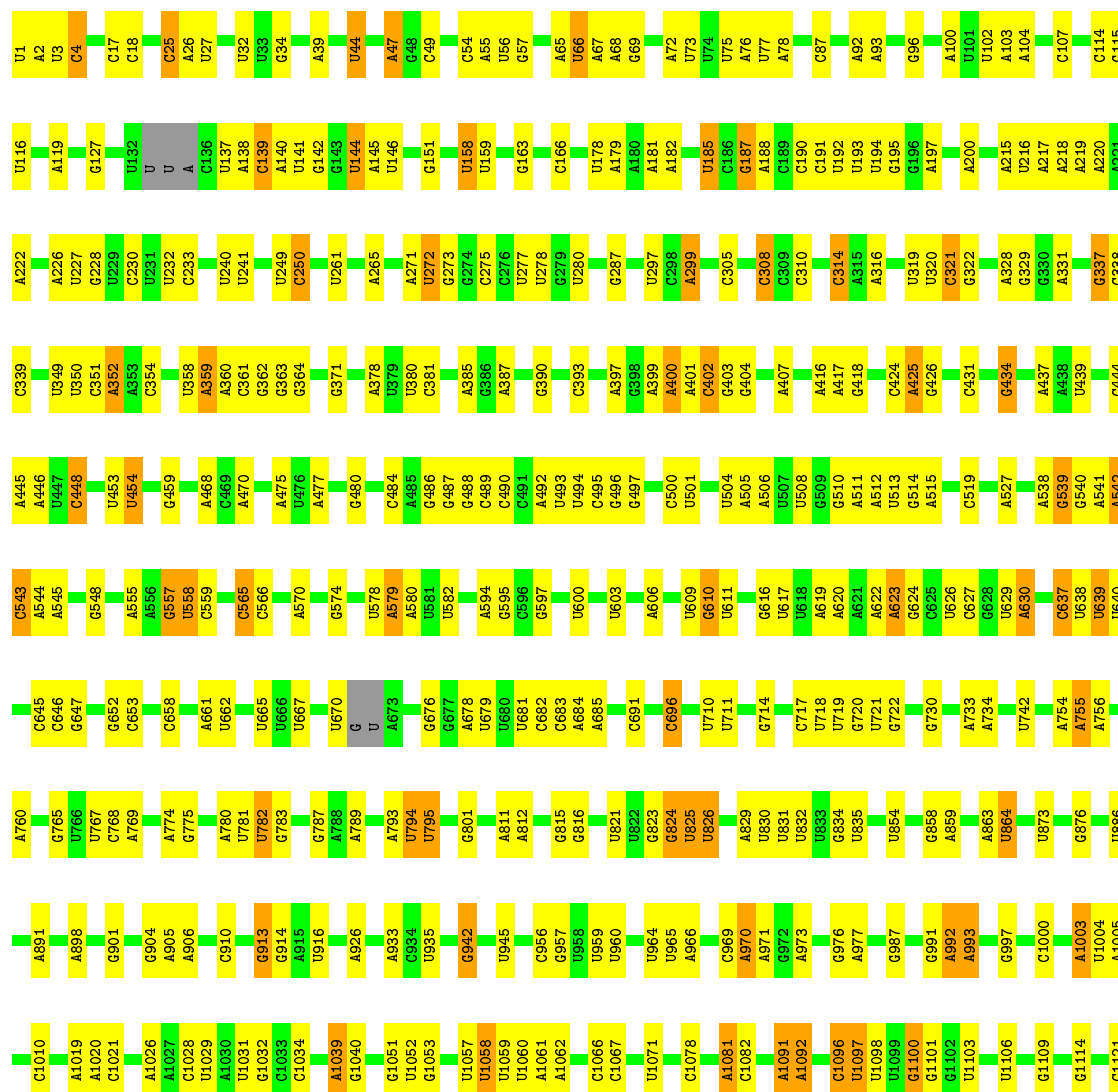
- Molecule 1: 18S ribosomal RNA

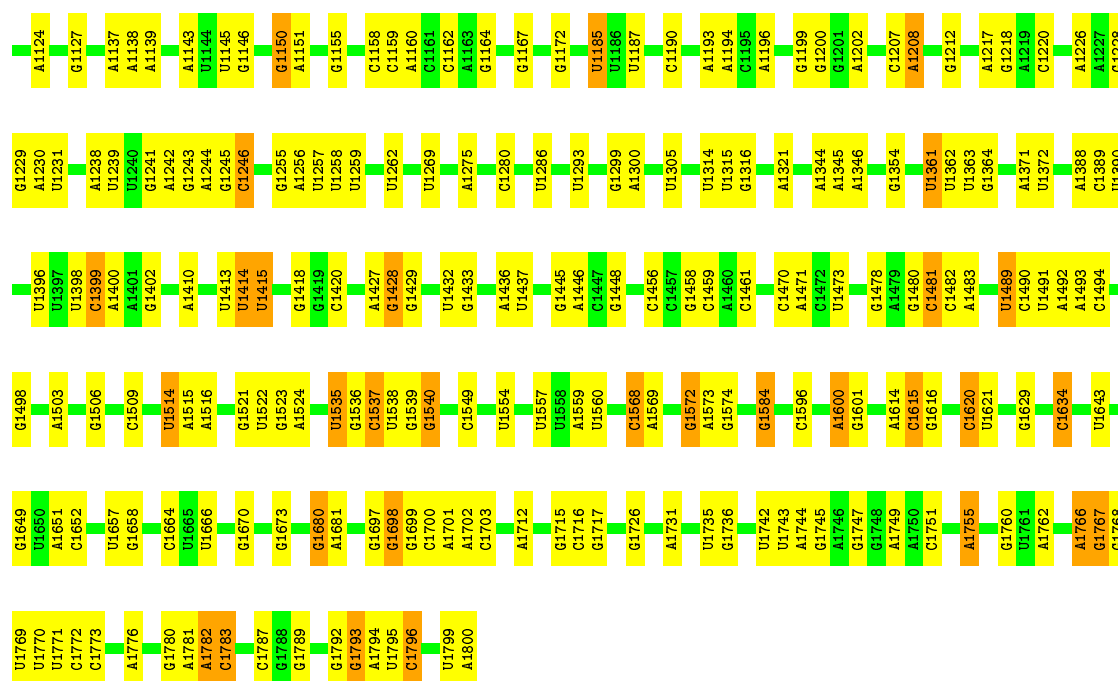




• Molecule 1: 18S ribosomal RNA

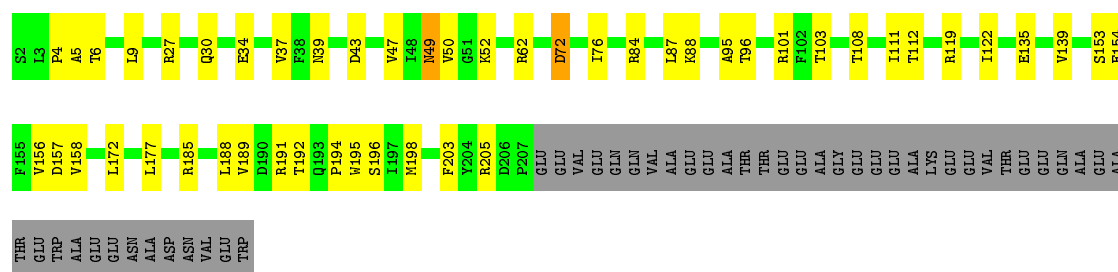
Chain 6: 66% 29% 5%





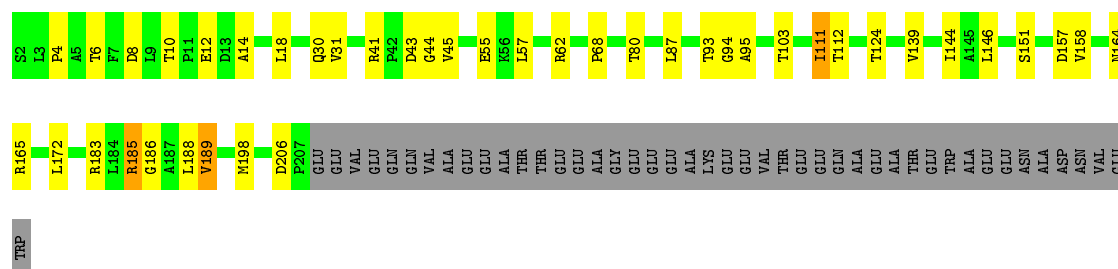
• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 63% 19% 18%



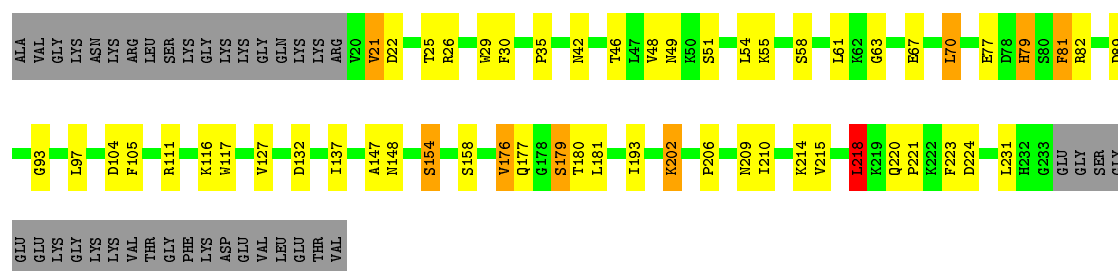
• Molecule 2: 40S ribosomal protein S0-A

Chain s0: 65% 16% 18%

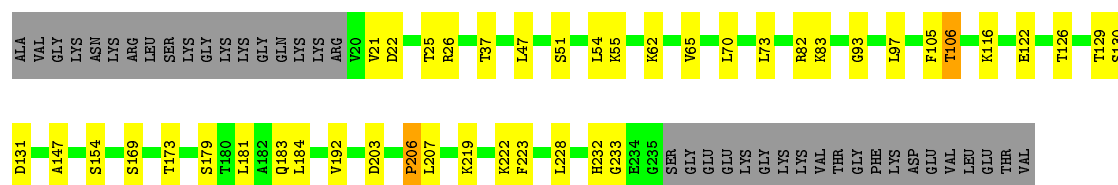


• Molecule 3: 40S ribosomal protein S1-A

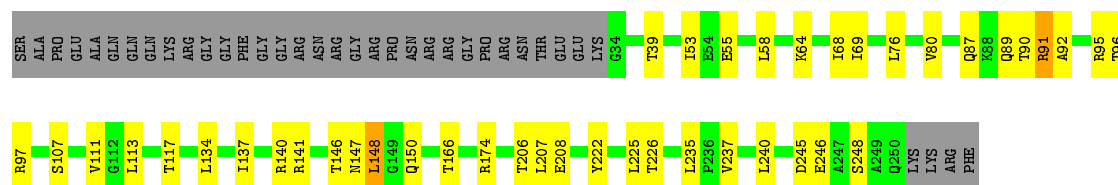
Chain S1: 62% 19% 16%



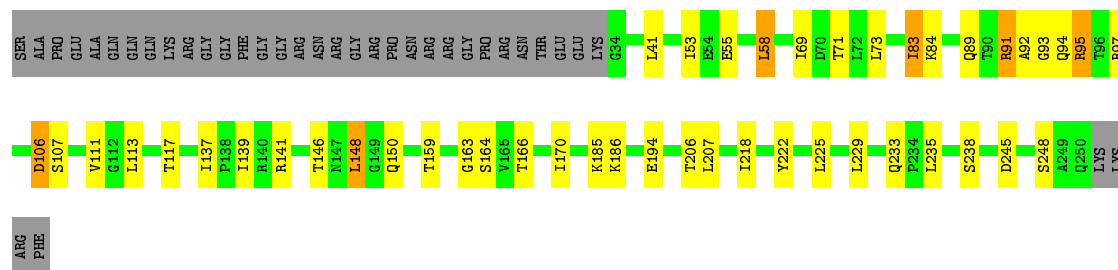
- Molecule 3: 40S ribosomal protein S1-A



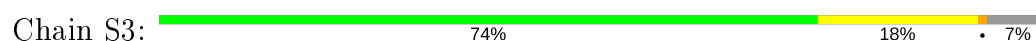
- Molecule 4: 40S ribosomal protein S2



- Molecule 4: 40S ribosomal protein S2



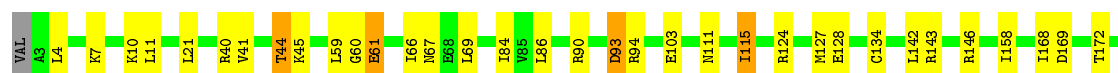
- Molecule 5: 40S ribosomal protein S3





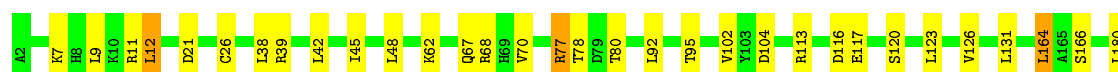
- Molecule 5: 40S ribosomal protein S3

Chain s3: 73% 18% 7%



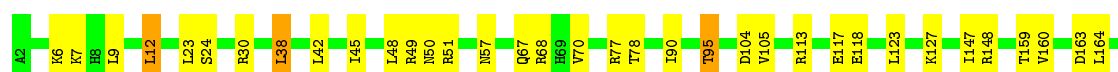
- Molecule 6: 40S ribosomal protein S4-A

Chain S4: 80% 19% 1%



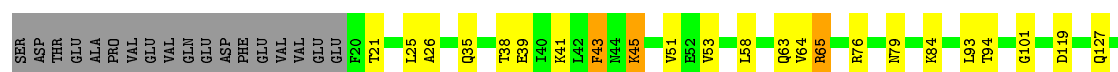
- Molecule 6: 40S ribosomal protein S4-A

Chain s4: 79% 20% 1%



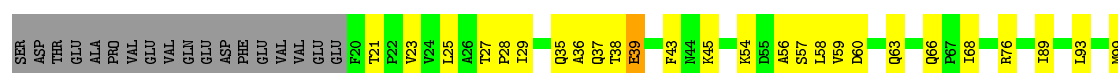
- Molecule 7: 40S ribosomal protein S5

Chain S5: 75% 16% 8%



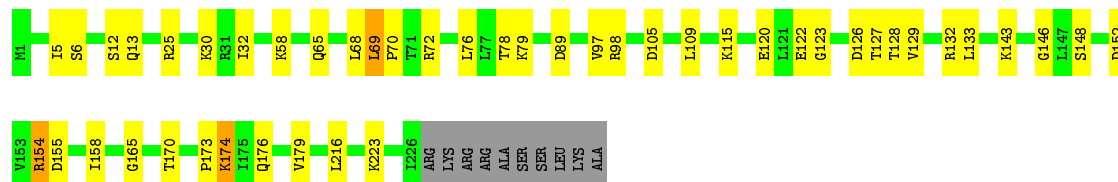
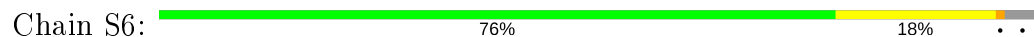
- Molecule 7: 40S ribosomal protein S5

Chain s5: 71% 21% 8%

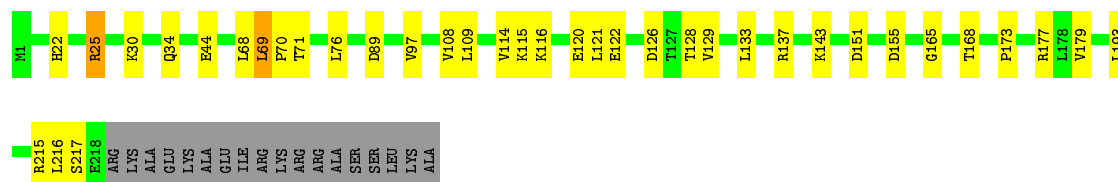
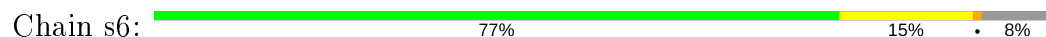




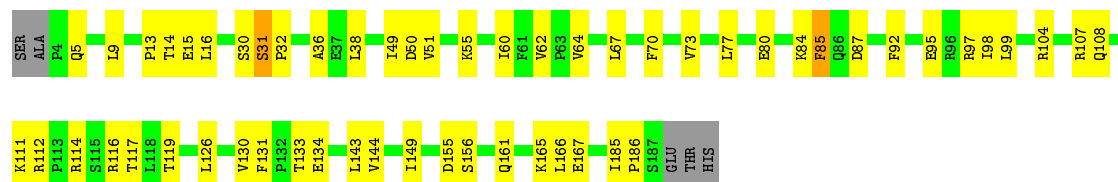
- Molecule 8: 40S ribosomal protein S6-A



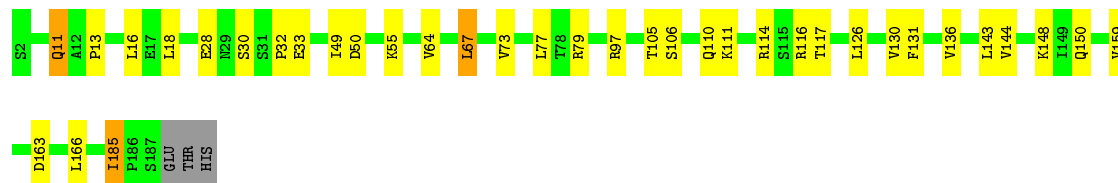
- Molecule 8: 40S ribosomal protein S6-A



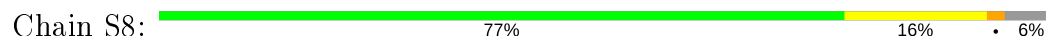
- Molecule 9: 40S ribosomal protein S7-A



- Molecule 9: 40S ribosomal protein S7-A



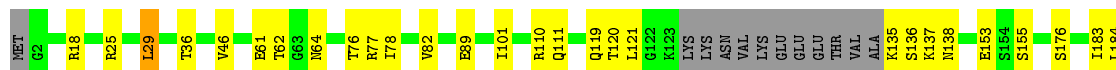
- Molecule 10: 40S ribosomal protein S8-A





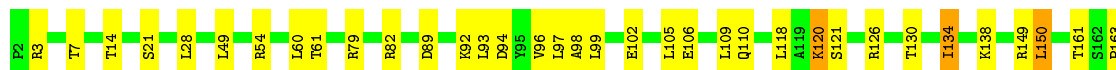
- Molecule 10: 40S ribosomal protein S8-A

Chain s8: 80% 14% 6%



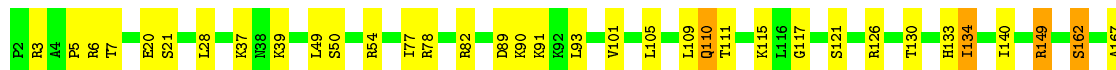
- Molecule 11: 40S ribosomal protein S9-A

Chain S9: 73% 20% 6%



- Molecule 11: 40S ribosomal protein S9-A

Chain s9: 73% 18% 6%



- Molecule 12: 40S ribosomal protein S10-A

Chain C0: 71% 18% 9%



- Molecule 12: 40S ribosomal protein S10-A

Chain c0: 72% 14% 5% 9%



- Molecule 13: 40S ribosomal protein S11-A

- Molecule 13: 40S ribosomal protein S11-A

ALA
ASN
LYS
GLN
PHE
ALA
LYS
PHE

- Molecule 14: 40S ribosomal protein S12

A101
G102
L103
I106
D107
R108
A112
V115
S119
W126
G127
A128
E129
T130
D131
E132
H139
F140
Q143

- Molecule 14: 40S ribosomal protein S12

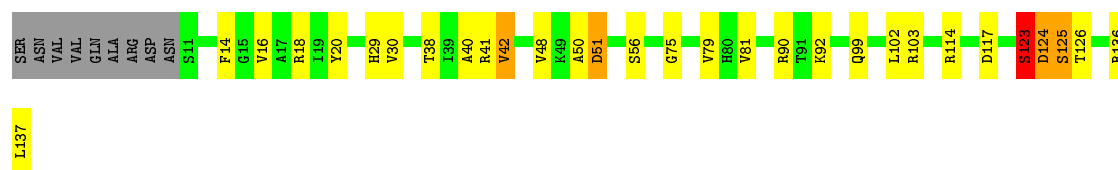
- Molecule 15: 40S ribosomal protein S13

- Molecule 15: 40S ribosomal protein S13

G2	S12	S13	I16	S19	R20	R21	A22	K27	L28	S29	E35	Q36	I37	V38	K39	V60	V65	I66	T67	K70	L80	I84	D87	L88	K93	L102	F103	R104	R105	R106	L115	L125	A126	R127	T131	N138	W139	K140	S147	V151
----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 



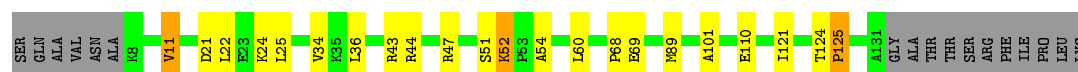
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 



- Molecule 17: 40S ribosomal protein S15

Chain C5: 




- Molecule 17: 40S ribosomal protein S15

Chain c5: 




- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 



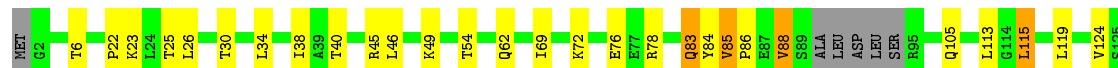
- Molecule 18: 40S ribosomal protein S16-A

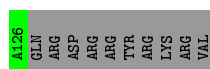
Chain c6: 



- Molecule 19: 40S ribosomal protein S17-A

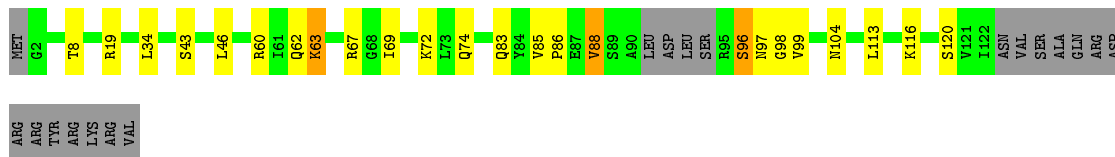
Chain C7: 






- Molecule 19: 40S ribosomal protein S17-A

Chain c7:  68% 15% 14%




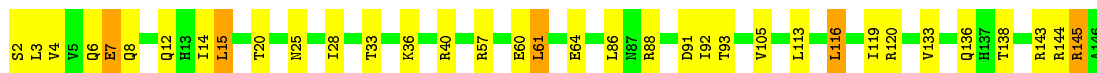
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:  77% 19%




- Molecule 20: 40S ribosomal protein S18-A

Chain c8:  76% 21%




- Molecule 21: 40S ribosomal protein S19-A

Chain C9:  83% 16%



- Molecule 21: 40S ribosomal protein S19-A

Chain c9:  83% 15%

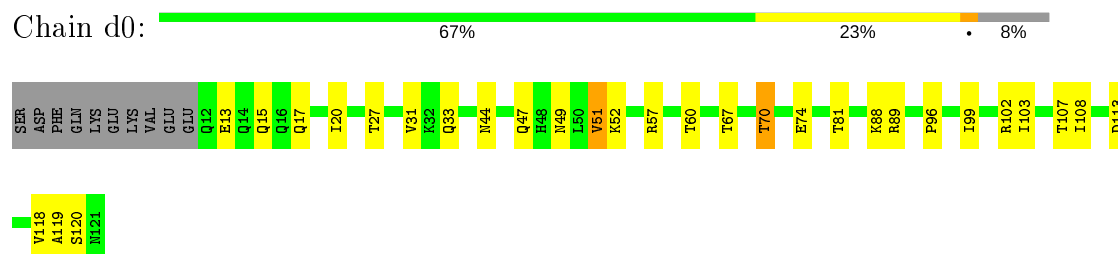


- Molecule 22: 40S ribosomal protein S20

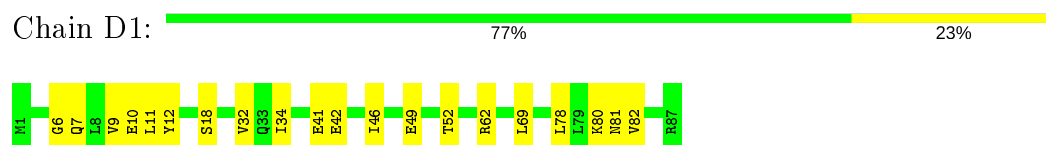
Chain D0:  67% 22% 11%



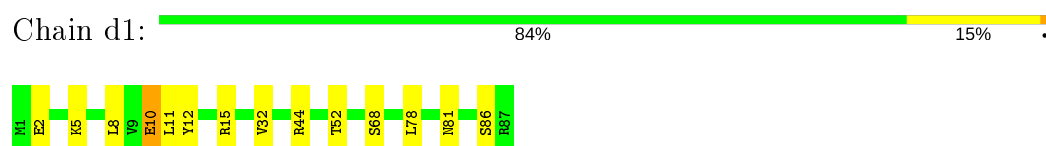
- Molecule 22: 40S ribosomal protein S20



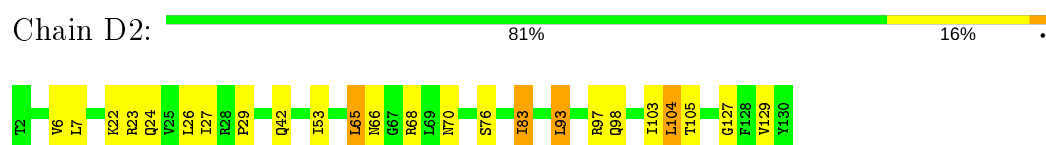
- Molecule 23: 40S ribosomal protein S21-A



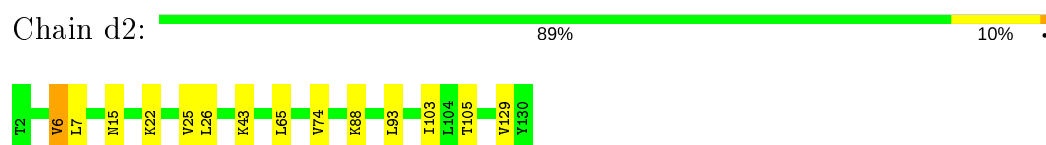
- Molecule 23: 40S ribosomal protein S21-A



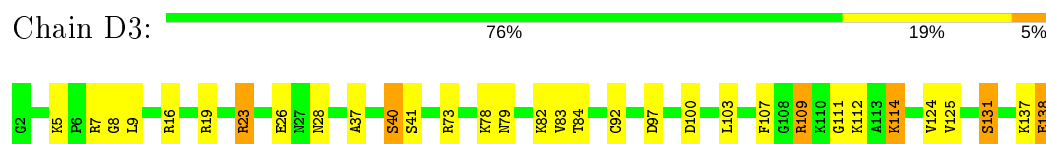
- Molecule 24: 40S ribosomal protein S22-A



- Molecule 24: 40S ribosomal protein S22-A

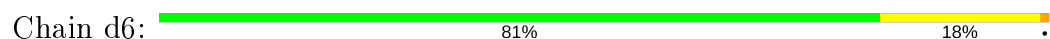


- Molecule 25: 40S ribosomal protein S23-A



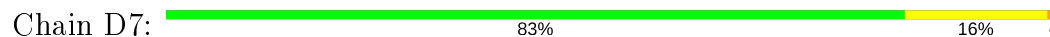
- Molecule 25: 40S ribosomal protein S23-A



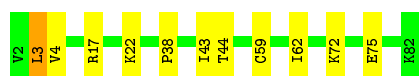
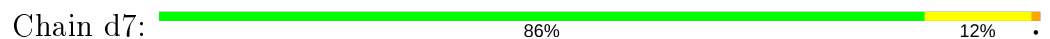




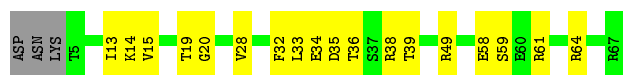
- Molecule 29: 40S ribosomal protein S27-A



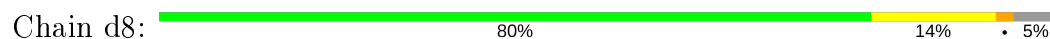
- Molecule 29: 40S ribosomal protein S27-A



- Molecule 30: 40S ribosomal protein S28-A



- Molecule 30: 40S ribosomal protein S28-A



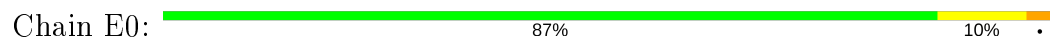
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A



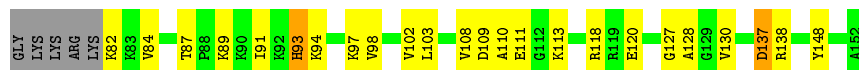
- Molecule 32: 40S ribosomal protein S30-A





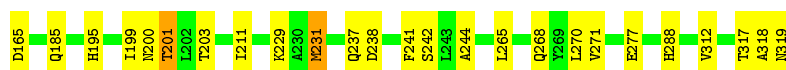
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1: 62% 29% 7%



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

Chain SR: 81% 18% 1%



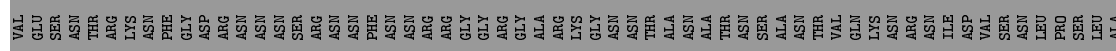
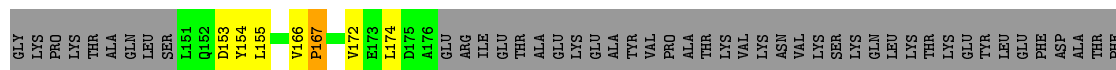
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 87% 13% 0%



- Molecule 35: Suppressor protein STM1

Chain SM: 44% 13% 42%

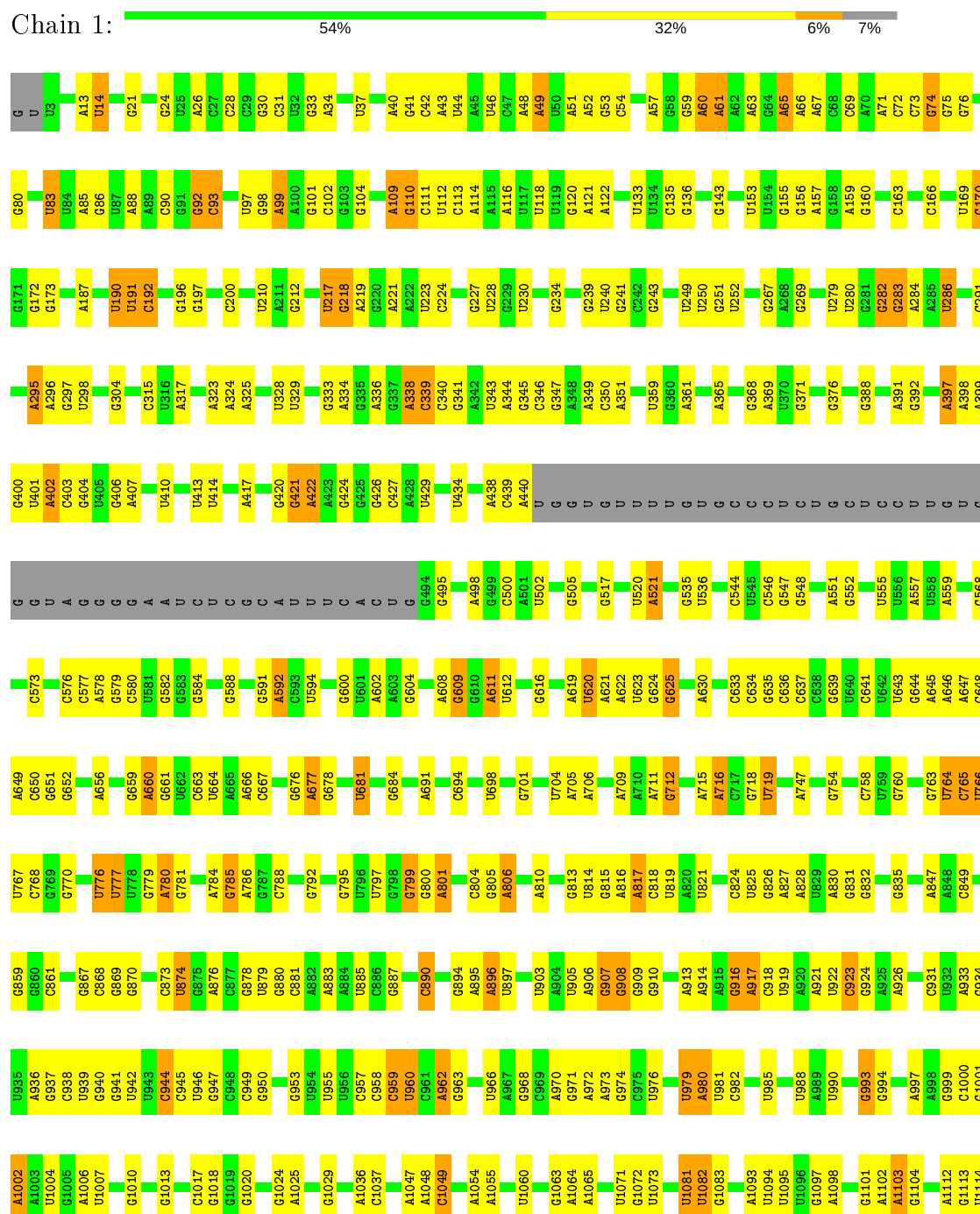


- Molecule 35: Suppressor protein STM1

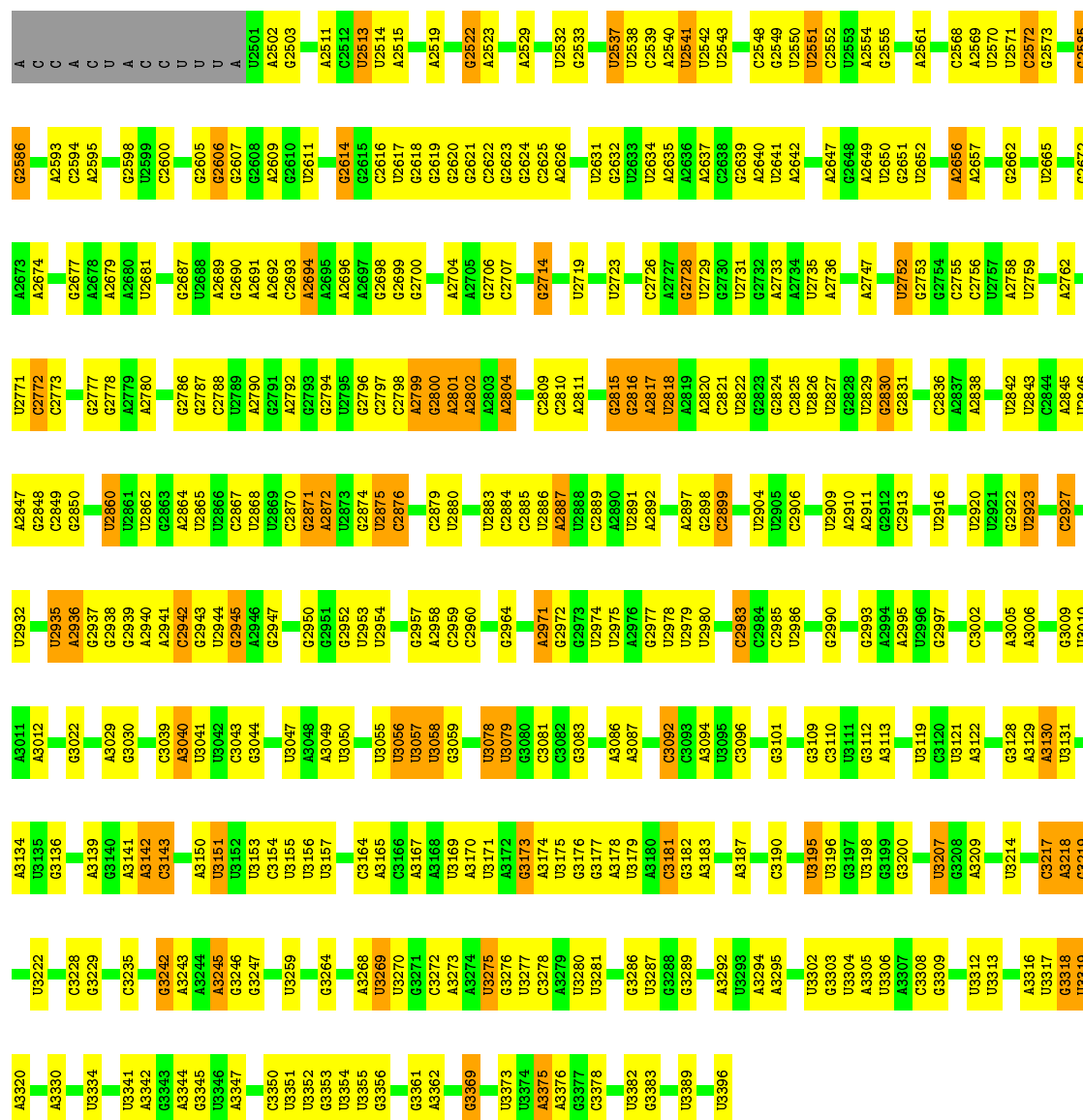
Chain sM: 28% 9% 62%



- Molecule 36: 25S ribosomal RNA

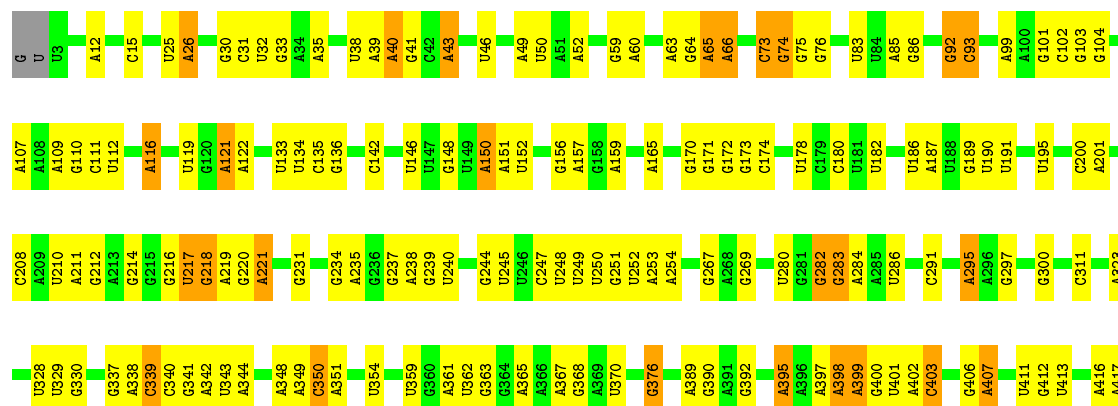






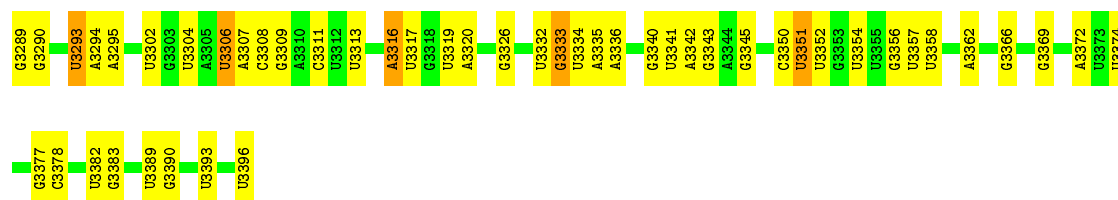
• Molecule 36: 25S ribosomal RNA

Chain 5: 54% 32% 6% 7%



U	C1872	G1736	U1569	G1380	A1294	G1171	U1094	U988	A914	C804	A690	U587	A418
G	U1876	G1741	A1571	A1381	U1299	G1172	U1095	A989	A915	G805	A691	G588	G419
U	U1877	G1747	A1572	C1385	G1300	G1174	U1096	A992	G916	A806	A692	A589	G420
C	A1878	G1750	G1573	A1386	A1301	G1177	A1098	G994	C918	G815	C696	A592	G421
A	A1879	G1751	A1575	A1387	A1302	G1178	A1101	G994	U919	A816	A697	C593	A423
Q	U1880	G1757	A1576	U1388	A1303	G1179	A1102	U995	A920	A817	U698	U594	A424
Q	A1881	C1762	G1577	G1389	A1304	G1180	A1103	G1001	A921	C818	C702	G600	A425
C	A1882	C1767	A1577	A1390	U1305	A1181	G1104	A1003	U922	U824	G701	G604	G426
C	A1883	U1765	C1578	G1391	G1306	U1181	A1105	A1003	G924	U825	C702	C	C427
C	A1884	G1766	C1579	G1392	G1307	A1182	G1108	A1004	G924	U825	C	A	A428
A	U1885	U1484	U1484	C1397	A1308	C1189	U1108	G1005	A925	A830	A705	G609	C491
C	A1886	U1484	U1484	U1397	A1309	A1190	A1112	A1006	A926	C927	U492	G610	U431
C	A1887	G1769	C1582	U1398	C1312	U1191	G1113	G1010	C928	G835	G708	A611	U434
G	U1888	G1770	A1583	A1399	G1313	U1191	G1113	G1010	C928	G835	G708	A611	U434
G	A1889	G1770	A1583	A1399	G1313	U1191	G1113	G1010	C928	G835	G708	A611	U434
G	U1890	G1770	A1583	A1399	G1313	U1191	G1113	G1010	C928	G835	G708	A611	U434
C	A1891	G1778	G1586	A1401	A1316	C1197	U1116	U1015	G931	G838	G712	G613	C497
C	U1892	G1779	A1587	C1402	A1317	C1198	G1117	U1016	G937	C839	A715	A619	C503
U	A1893	G1780	A1588	C1403	A1318	C1199	G1117	C1017	C938	C840	A716	U620	A504
U	A1894	G1781	A1589	C1404	A1319	C1200	U1121	C1018	U942	U852	C719	A621	G505
Q	A1895	G1782	A1590	C1405	G1320	C1201	U1122	G1019	U943	G859	A516	A630	U441
Q	A1896	G1783	A1591	U1406	G1321	C1202	U1123	G1020	C944	G860	A516	U631	G442
G	A1897	G1784	A1592	U1407	U1322	A1202	U1124	G1021	C945	C861	G725	U631	G443
C	A1898	G1785	A1593	C1408	U1323	A1203	U1125	G1022	C946	G862	G726	A519	U
U	A1900	G1786	A1594	C1409	C1324	A1204	U1126	G1023	U947	G863	A735	U632	G
U	A1901	G1787	A1595	C1410	U1325	A1205	U1127	A1024	C948	G864	A736	G635	U
U	A1902	G1788	A1596	C1411	U1326	A1206	U1128	A1025	C949	G865	A737	G636	U
G	A1903	G1789	A1597	C1412	U1327	A1207	U1129	A1026	C950	G866	A738	C637	U
G	A1904	G1790	A1598	C1413	U1328	A1208	U1130	A1027	C951	G867	A739	U638	U
G	A1905	G1791	A1599	C1414	U1329	A1209	U1131	A1028	C952	G868	A740	U639	U
C	A1906	G1792	A1600	C1415	U1330	A1210	U1132	A1029	C953	G869	A741	C641	G
C	A1907	G1793	A1601	C1416	U1331	A1211	U1133	A1030	C954	G870	C753	U642	U
A	A1908	G1794	A1602	C1417	U1332	A1212	U1134	A1031	C955	G871	C754	U643	G
C	A1909	G1795	A1603	C1418	U1333	A1213	U1135	A1032	C956	G872	C755	U644	C
U	A1910	G1796	A1604	C1419	U1334	A1214	U1136	A1033	C957	G873	C756	G645	C
U	A1911	G1797	A1605	C1420	U1335	A1215	U1137	A1034	C958	G874	C757	A646	U
C	A1912	G1798	A1606	C1421	U1336	A1216	U1138	A1035	C959	G875	C758	C647	C
C	A1913	G1799	A1607	C1422	U1337	A1217	U1139	A1036	C960	G876	C759	C648	U
C	A1914	G1800	A1608	C1423	U1338	A1218	U1140	A1037	C961	G877	C760	C649	U
U	A1915	G1801	A1609	C1424	U1339	A1219	U1141	A1038	C962	G878	C761	C650	G
U	A1916	G1802	A1610	C1425	U1340	A1220	U1142	A1039	C963	G879	C762	C651	U
U	A1917	G1803	A1611	C1426	U1341	A1221	U1143	A1040	C964	G880	C763	C652	C
U	A1918	G1804	A1612	C1427	U1342	A1222	U1144	A1041	C965	G881	C764	C653	U
U	A1919	G1805	A1613	C1428	U1343	A1223	U1145	A1042	C966	G882	C765	C654	C
U	A1920	G1806	A1614	C1429	U1344	A1224	U1146	A1043	C967	G883	C766	C655	C
G	A1921	G1807	A1615	C1430	U1345	A1225	U1147	A1044	C968	G884	C767	C656	U
G	A1922	G1808	A1616	C1431	U1346	A1226	U1148	A1045	C969	G885	C768	C657	U
G	A1923	G1809	A1617	C1432	U1347	A1227	U1149	A1046	C970	G886	C769	C658	U
C	A1924	G1810	A1618	C1433	U1348	A1228	U1150	A1047	C971	G887	C770	C659	C
C	A1925	G1811	A1619	C1434	U1349	A1229	U1151	A1048	C972	G888	C771	C660	U
U	A1926	G1812	A1620	C1435	U1350	A1230	U1152	A1049	C973	G889	C772	C661	U
U	A1927	G1813	A1621	C1436	U1351	A1231	U1153	A1050	C974	G890	C773	C662	U
U	A1928	G1814	A1622	C1437	U1352	A1232	U1154	A1051	C975	G891	C774	C663	U
U	A1929	G1815	A1623	C1438	U1353	A1233	U1155	A1052	C976	G892	C775	C664	U
U	A1930	G1816	A1624	C1439	U1354	A1234	U1156	A1053	C977	G893	C776	C665	U
U	A1931	G1817	A1625	C1440	U1355	A1235	U1157	A1054	C978	G894	C777	C666	U
U	A1932	G1818	A1626	C1441	U1356	A1236	U1158	A1055	C979	G895	C778	C667	U
U	A1933	G1819	A1627	C1442	U1357	A1237	U1159	A1056	C980	G896	C779	C668	U
U	A1934	G1820	A1628	C1443	U1358	A1238	U1160	A1057	C981	G897	C780	C669	U
U	A1935	G1821	A1629	C1444	U1359	A1239	U1161	A1058	C982	G898	C781	C670	U
U	A1936	G1822	A1630	C1445	U1360	A1240	U1162	A1059	C983	G899	C782	C671	U
U	A1937	G1823	A1631	C1446	U1361	A1241	U1163	A1060	C984	G900	C783	C672	U
U	A1938	G1824	A1632	C1447	U1362	A1242	U1164	A1061	C985	G901	C784	C673	U
U	A1939	G1825	A1633	C1448	U1363	A1243	U1165	A1062	C986	G902	C785	C674	U
U	A1940	G1826	A1634	C1449	U1364	A1244	U1166	A1063	C987	G903	C786	C675	U
U	A1941	G1827	A1635	C1450	U1365	A1245	U1167	A1064	C988	G904	C787	C676	U
U	A1942	G1828	A1636	C1451	U1366	A1246	U1168	A1065	C989	G905	C788	C677	U
U	A1943	G1829	A1637	C1452	U1367	A1247	U1169	A1066	C990	G906	C789	C678	U
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U	A1945	G1831	A1639	C1454	U1369	A1249	U1171	A1068	C992	G908	C791	C680	U
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U	A1947	G1833	A1641	C1456	U1371	A1251	U1173	A1070	C994	G910	C793	C682	U
U	A1948	G1834	A1642	C1457	U1372	A1252	U1174	A1071	C995	G911	C794	C683	U
U	A1949	G1835	A1643	C1458	U1373	A1253	U1175	A1072	C996	G912	C795	C684	U
U	A1950	G1836	A1644	C1459	U1374	A1254	U1176	A1073	C997	G913	C796	C685	U
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U	A1952	G1838	A1646	C1461	U1376	A1256	U1178	A1075	C999	G915	C798	C687	U
U	A1953	G1839	A1647	C1462	U1377	A1257	U1179	A1076	C1000	G916	C799	C688	U
U	A1954	G1840	A1648	C1463	U1378	A1258	U1180	A1077	C1001	G917	C800	C689	U
U	A1955	G1841	A1649	C1464	U1379	A1259	U1181	A1078	C1002	G918	C801	C690	U
U	A1956	G1842	A1650	C1465	U1380	A1260	U1182	A1079	C1003	G919	C802	C691	U
U	A1957	G1843	A1651	C1466	U1381	A1261	U1183	A1080	C1004	G920	C803	C692	U
U	A1958	G1844	A1652	C1467	U1382	A1262	U1184	A1081	C1005	G921	C804	C693	U
U	A1959	G1845	A1653	C1468	U1383	A1263	U1185	A1082	C1006	G922	C805	C694	U
U	A1960	G1846	A1654	C1469	U1384	A1264	U1186	A1083	C1007	G923	C806	C695	U
U	A1961	G1847	A1655	C1470	U1385	A1265	U1187	A1084	C1008	G924	C807	C696	U
U	A1962	G1848	A1656	C1471	U1386	A1266	U1188	A1085	C1009	G925	C808	C697	U
U	A1963	G1849	A1657	C1472	U1387	A1267	U1189	A1086	C1010	G926	C809	C698	U
U	A1964	G1850	A1658	C1473	U1388	A1268	U1190	A1087	C1011	G927	C810	C699	U
U	A1965	G1851	A1659	C1474	U1389	A1269	U1191	A1088	C1012	G928	C811	C700	U
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U	A1967	G1853	A1661	C1476	U1391	A1271	U1193	A1090	C1014	G930	C813	C702	U
U	A1968	G1854	A1662	C1477	U1392	A1272	U1194	A1091	C1015	G931	C814	C703	U
U	A1969	G1855	A1663	C1478	U1393	A1273	U1195	A1092	C1016	G932	C815	C704	U
U	A1970	G1856	A1664	C1479	U1394	A1274	U1196	A1093	C1017	G933	C816	C705	U
U	A1971	G1857	A1665	C1480	U1395	A1275	U1197	A1094	C1018	G934	C817	C706	U
U	A1972	G1858	A1666	C1481	U1396	A1276	U1198	A1095	C1019	G935	C818	C707	U
U	A1973	G1859	A1667	C1482	U1397	A1277	U1199	A1096	C1020	G936	C819	C708	U
U	A1974	G1860	A1668	C1483	U1398	A1278	U1200	A1097	C1021	G937	C820	C709	U
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G3208	U3125	A3020	A2940	C3870	G2794	G2677	A2593	U	A2438	C2367	C2293	U2190	A
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C3217	G3140	C3043	G2950	U2881	A2803	A2687	G2606	U	U	G2375	A2303	C2205	U
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C3222	C3145	G3051	G2957	U2888	A2811	A2692	G2611	U	U	G2382	G2308	U2210	G
G3223	A3150	C3052	G2964	A2889	C2812	A2693	G2612	U	U	G2383	A2309	U2211	A
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G3237	A3164	C3068	U2978	A2903	C2826	A2712	G2626	U	U	U2397	U2325	U2234	U
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C3245	C3172	C3076	U2986	U2911	A2834	A2720	G2634	U	C	G2404	U2333	U2242	C
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C3253	C3180	U3084	U2994	G2919	G2842	A2728	G2642	U	C	U2412	U2341	U2250	C
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C3255	C3182	U3086	U2996	U2921	G2844	A2730	G2644	U	U	U2414	U2343	U2252	C
U3256	U3183	C3087	U2997	U2922	U2845	A2731	G2645	U	C	U2415	U2344	U2253	C
C3257	C3184	U3088	U2998	U2923	U2846	A2732	G2646	U	C	U2416	U2345	U2254	C
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C3259	C3186	U3090	U3000	U2925	U2848	A2734	G2648	U	U	U2418	U2347	U2256	C
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C3261	C3188	U3092	A3002	U2927	G2850	A2736	G2650	U	U	U2420	U2349	U2258	C
U3262	U3189	C3093	A3003	U2928	U2851	A2737	G2651	U	C	U2421	U2350	U2259	C
C3263	C3190	U3094	U3004	C2928	C2852	A2738	G2652	U	U	U2422	U2351	U2260	C
U3264	U3191	C3095	U3005	C2929	U2853	A2739	G2653	U	C	U2423	U2352	U2261	C
C3265	C3192	U3096	A3006	U2930	U2854	A2740	G2654	U	U	U2424	U2353	U2262	C
U3266	U3193	C3097	A3007	U2931	U2855	A2741	G2655	U	C	U2425	U2354	U2263	C
C3267	C3194	U3098	U3008	U2932	U2856	A2742	G2656	U	U	U2426	U2355	U2264	C
U3268	U3195	C3099	A3009	U2933	G2857	A2743	G2657	U	U	U2427	U2356	U2265	C
C3269	C3196	U3100	A3010	C2934	U2858	A2744	G2658	U	C	U2428	U2357	U2266	C
U3270	U3197	C3101	U3011	U2935	U2859	A2745	G2659	U	U	U2429	U2358	U2267	C
C3271	C3198	C3102	A3012	U2936	G2860	A2746	G2660	U	C	U2430	U2359	U2268	C
U3272	U3199	C3103	U3013	U2937	U2861	A2747	G2661	U	U	U2431	U2360	U2269	C
C3273	C3200	U3104	A3014	C2936	U2862	A2748	G2662	U	U	U2432	U2361	U2270	C
U3274	U3201	C3105	U3015	U2938	U2863	A2749	G2663	U	C	U2433	U2362	U2271	C
C3275	C3202	U3106	A3016	U2939	U2864	A2750	G2664	U	U	U2434	U2363	U2272	C
U3276	U3203	C3107	U3017	U2940	U2865	A2751	G2665	U	C	U2435	U2364	U2273	C
C3277	C3204	U3108	A3018	U2941	U2866	A2752	G2666	U	U	U2436	U2365	U2274	C
U3278	U3205	C3109	U3019	U2942	U2867	A2753	G2667	U	U	U2437	U2366	U2275	C
C3279	C3206	U3110	A3020	U2943	U2868	A2754	G2668	U	C	U2438	U2367	U2276	C
U3280	U3207	C3111	U3021	U2944	U2869	A2755	G2669	U	U	U2439	U2368	U2277	C
C3281	C3208	U3112	A3022	U2945	U2870	A2756	G2670	U	C	U2440	U2369	U2278	C
U3282	U3209	C3113	U3023	U2946	U2871	A2757	G2671	U	U	U2441	U2370	U2279	C
C3283	C3210	U3114	A3024	U2947	U2872	A2758	G2672	U	U	U2442	U2371	U2280	C
U3284	U3211	C3115	U3025	U2948	U2873	A2759	G2673	U	C	U2443	U2372	U2281	C
C3285	C3212	U3116	A3026	U2949	U2874	A2760	G2674	U	U	U2444	U2373	U2282	C
U3286	U3213	C3117	U3027	U2950	U2875	A2761	G2675	U	C	U2445	U2374	U2283	C
C3287	C3214	U3118	A3028	U2951	U2876	A2762	G2676	U	U	U2446	U2375	U2284	C
U3288	U3215	C3119	U3029	U2952	U2877	A2763	G2677	U	C	U2447	U2376	U2285	C
C3289	C3216	U3120	A3030	U2953	U2878	A2764	G2678	U	U	U2448	U2377	U2286	C
U3290	U3217	C3121	U3031	U2954	U2879	A2765	G2679	U	C	U2449	U2378	U2287	C
C3291	C3218	U3122	A3032	U2955	U2880	A2766	G2680	U	U	U2450	U2379	U2288	C
U3292	U3219	C3123	U3033	U2956	U2881	A2767	G2681	U	C	U2451	U2380	U2289	C
C3293	C3220	U3124	A3034	U2957	U2882	A2768	G2682	U	U	U2452	U2381	U2290	C
U3294	U3221	C3125	U3035	U2958	U2883	A2769	G2683	U	C	U2453	U2382	U2291	C
C3295	C3222	U3126	A3036	U2959	U2884	A2770	G2684	U	U	U2454	U2383	U2292	C
U3296	U3223	C3127	U3037	U2960	U2885	A2771	G2685	U	C	U2455	U2384	U2293	C
C3297	C3224	U3128	A3038	U2961	U2886	A2772	G2686	U	U	U2456	U2385	U2294	C
U3298	U3225	C3129	U3039	U2962	U2887	A2773	G2687	U	C	U2457	U2386	U2295	C
C3299	C3226	U3130	A3040	U2963	U2888	A2774	G2688	U	U	U2458	U2387	U2296	C
U3300	U3227	C3131	U3041	U2964	U2889	A2775	G2689	U	C	U2459	U2388	U2297	C
C3301	C3228	U3132	A3042	U2965	U2890	A2776	G2690	U	U	U2460			



- Molecule 37: 5S ribosomal RNA

Chain 3: 76% 23%



- Molecule 37: 5S ribosomal RNA

Chain 7: 60% 34% 7%



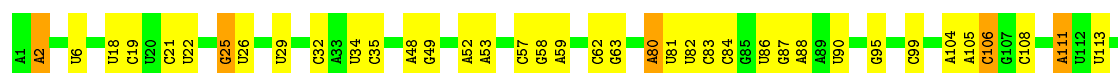
- Molecule 38: 5.8S ribosomal RNA

Chain 4: 64% 30% 6%



- Molecule 38: 5.8S ribosomal RNA

Chain 8: 70% 27%



- Molecule 39: 60S ribosomal protein L2-A

Chain L2: 83% 16%





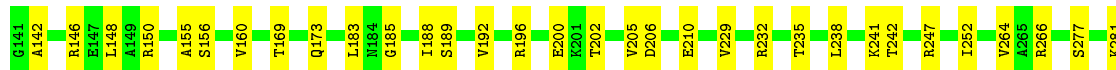
• Molecule 39: 60S ribosomal protein L2-A

Chain l2: 84% 15%



• Molecule 40: 60S ribosomal protein L3

Chain L3: 78% 20%



• Molecule 40: 60S ribosomal protein L3



Chain l3: 78% 21%




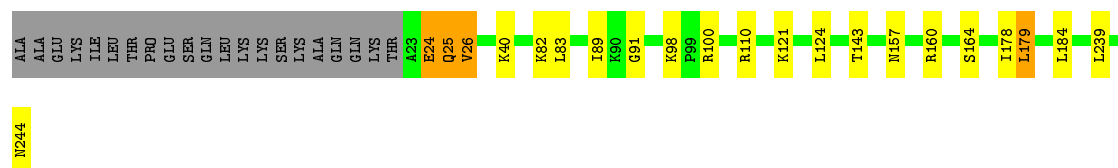
• Molecule 41: 60S ribosomal protein L4-A

Chain L4: 82% 17%


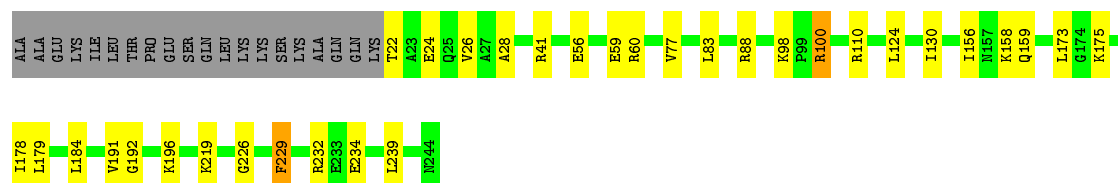


- Chain 16: 
- 


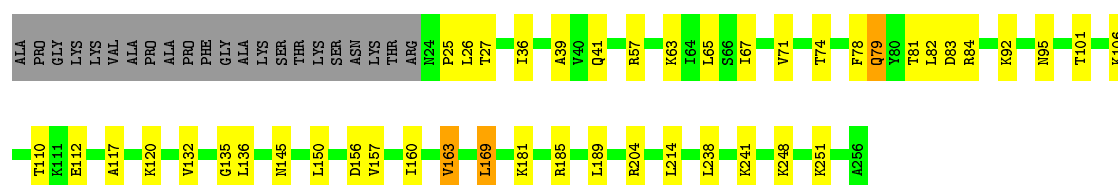
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:  82% 7% 9%

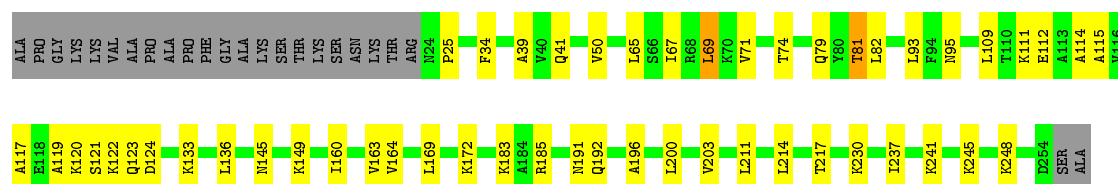
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:  78% 13% 8%


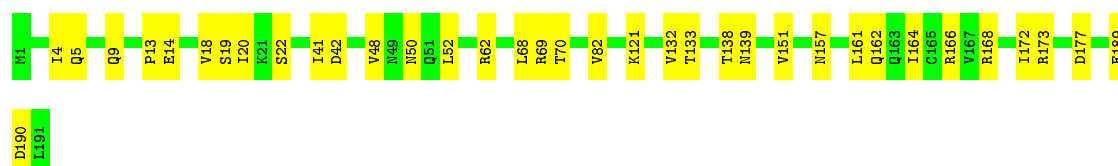
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:  74% 16% 9%

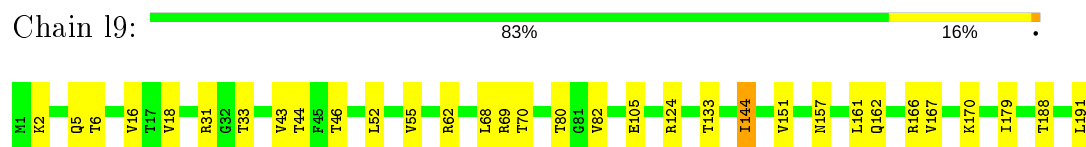
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:  71% 19% 9%

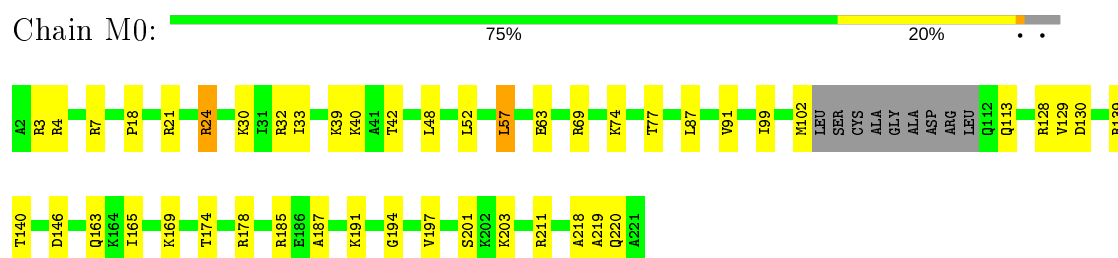
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:  81% 19%

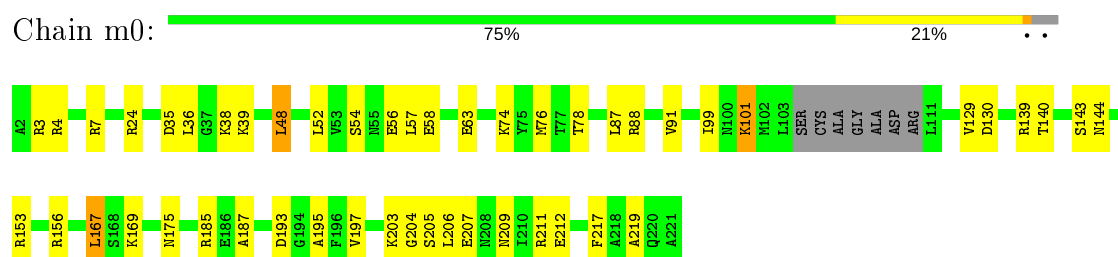
- Molecule 46: 60S ribosomal protein L9-A



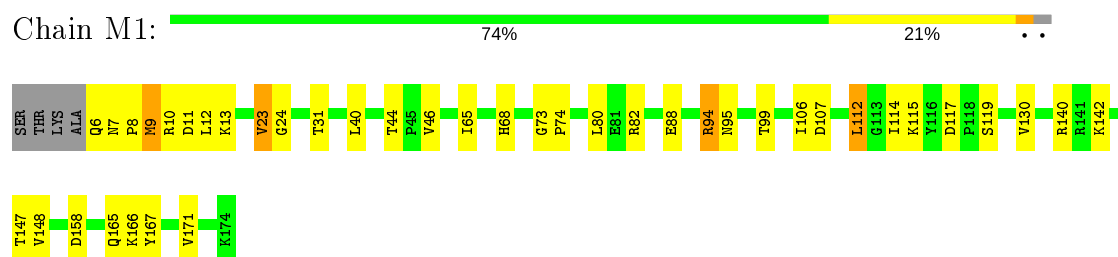
- Molecule 47: 60S ribosomal protein L10



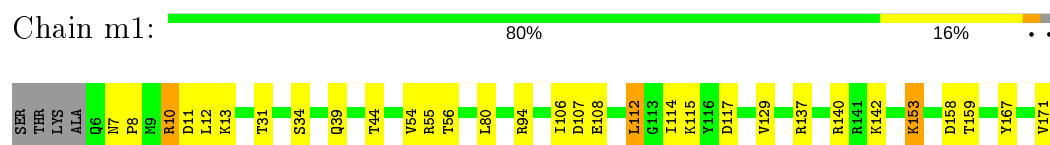
- Molecule 47: 60S ribosomal protein L10



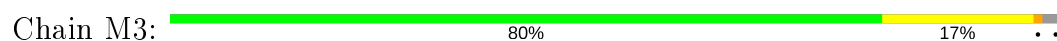
- Molecule 48: 60S ribosomal protein L11-B

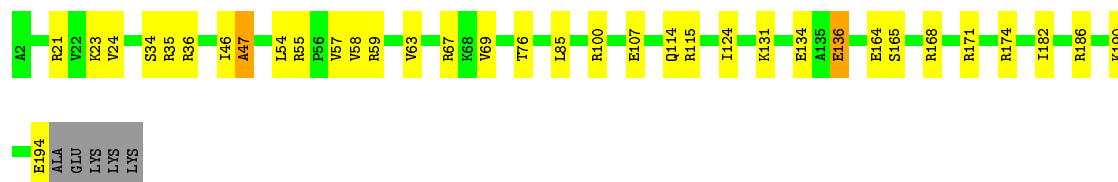


- Molecule 48: 60S ribosomal protein L11-B



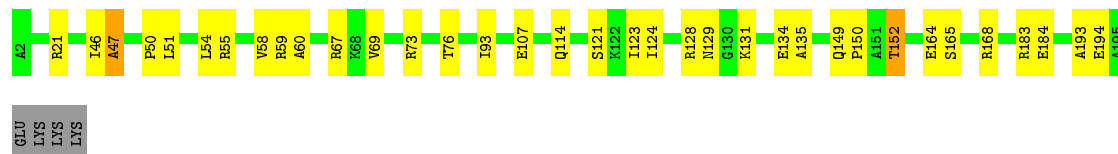
- Molecule 49: 60S ribosomal protein L13-A





- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 80% 17% ..



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 82% 15% ...



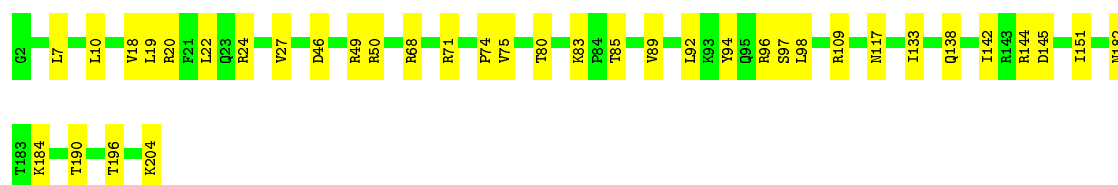
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 85% 14% .



- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 82% 18%



- Molecule 51: 60S ribosomal protein L15-A

Chain m5: 84% 14% .



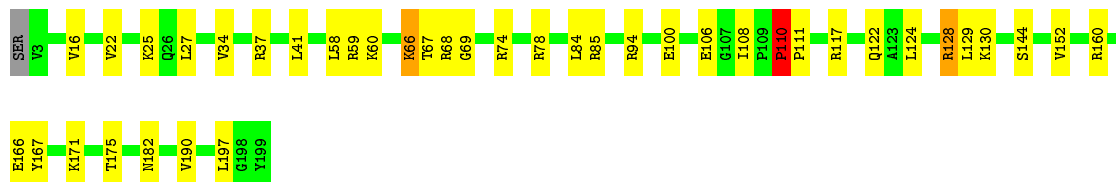
- Molecule 52: 60S ribosomal protein L16-A

Chain M6: 86% 12% ...



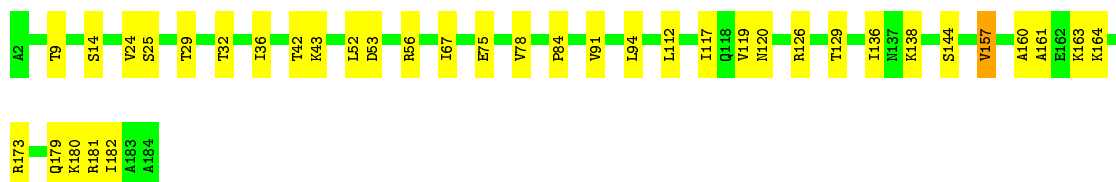
- Molecule 52: 60S ribosomal protein L16-A

Chain m6: 79% 19% ...



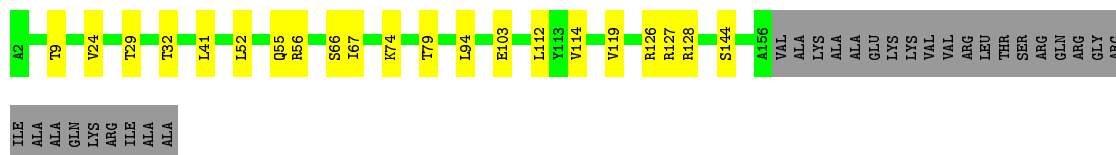
- Molecule 53: 60S ribosomal protein L17-A

Chain M7: 80% 20% .



- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 73% 11% 15%



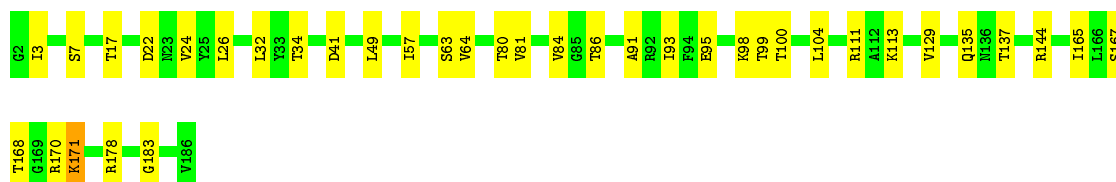
- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 84% 15% .



- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 80% 19% .



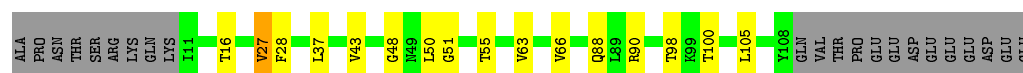
- Molecule 58: 60S ribosomal protein L22-A

Chain N2: 



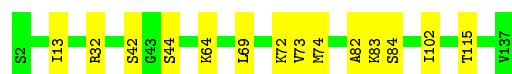
- Molecule 58: 60S ribosomal protein L22-A

Chain n2: 



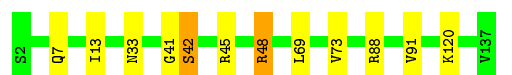
- Molecule 59: 60S ribosomal protein L23-A

Chain N3: 



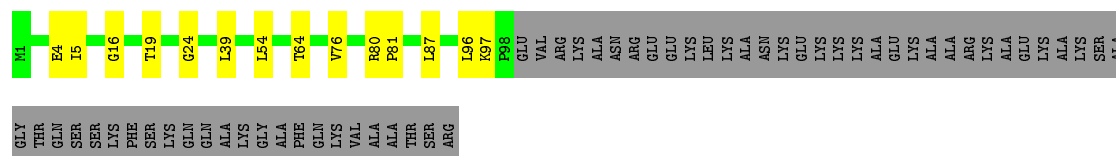
- Molecule 59: 60S ribosomal protein L23-A

Chain n3: 



- Molecule 60: 60S ribosomal protein L24-A

Chain N4: 



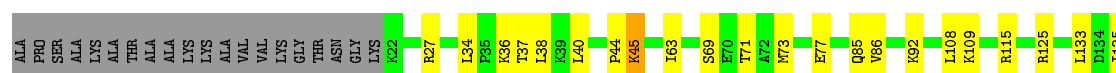
- Molecule 60: 60S ribosomal protein L24-A

Chain n4: 



- Molecule 61: 60S ribosomal protein L25

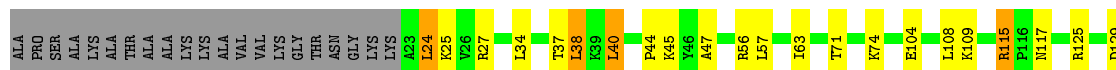
Chain N5: 





- Molecule 61: 60S ribosomal protein L25

Chain n5: 67% 15% 15%



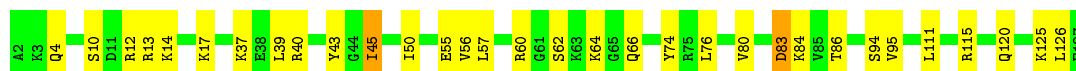
- Molecule 62: 60S ribosomal protein L26-A

Chain N6: 77% 21%



- Molecule 62: 60S ribosomal protein L26-A

Chain n6: 75% 24%



- Molecule 63: 60S ribosomal protein L27-A

Chain N7: 80% 19%



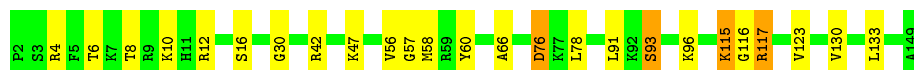
- Molecule 63: 60S ribosomal protein L27-A

Chain n7: 78% 21%




- Molecule 64: 60S ribosomal protein L28

Chain N8: 83% 14%




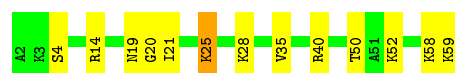
- Molecule 64: 60S ribosomal protein L28

Chain n8:  82% 18%



- Molecule 65: 60S ribosomal protein L29

Chain N9:  78% 21%




- Molecule 65: 60S ribosomal protein L29

Chain n9:  78% 21%




- Molecule 66: 60S ribosomal protein L30

Chain O0:  82% 11% 7%




- Molecule 66: 60S ribosomal protein L30

Chain o0:  80% 15%



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:  79% 18%




- Molecule 67: 60S ribosomal protein L31-A

Chain o1:  71% 27%




- Molecule 68: 60S ribosomal protein L32

Chain O2:  84% 14% ..



- Molecule 68: 60S ribosomal protein L32

Chain o2:  78% 19% ..




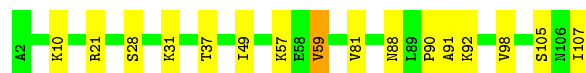
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  88% 11% .




- Molecule 69: 60S ribosomal protein L33-A

Chain o3:  85% 14% .




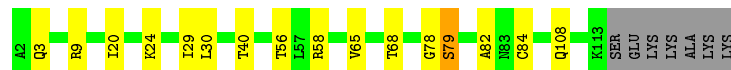
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  76% 17% • 6%



- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  81% 13% • 6%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  80% 18% .




- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  82% 18%



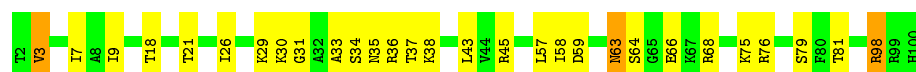
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:  78% 19%




- Molecule 72: 60S ribosomal protein L36-A

Chain o6:  71% 26%




- Molecule 73: 60S ribosomal protein L37-A

Chain O7:  85% 13%




- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  80% 20%




- Molecule 74: 60S ribosomal protein L38

Chain O8:  79% 19%




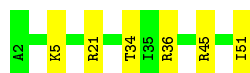
- Molecule 74: 60S ribosomal protein L38

Chain o8:  83% 16%




- Molecule 75: 60S ribosomal protein L39

Chain O9:  88% 12%




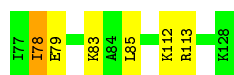
- Molecule 75: 60S ribosomal protein L39

Chain o9:  84% 16%




- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  88% 10%



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:  81% 19%



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:  68% 32%




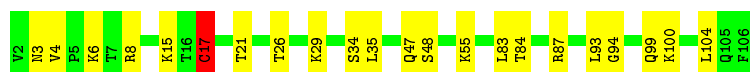
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:  76% 20%




- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:  79% 20%




- Molecule 78: 60S ribosomal protein L42-A

Chain q2:  81% 18% .




- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:  82% 18%



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:  81% 18% .



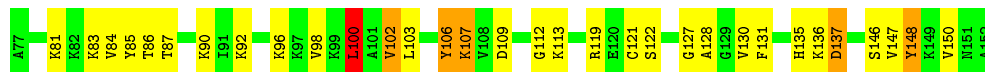
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:  76% 24%



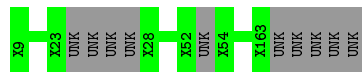
- Molecule 81: Ubiquitin-40S ribosomal protein S31

Chain e1:  58% 34% 7% .




- Molecule 82: UNKNOWN PROTEIN m2

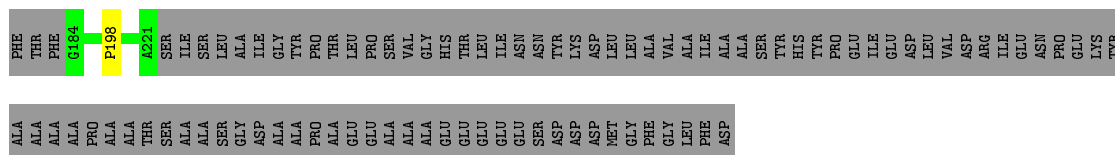
Chain m2:  94% 6%



- Molecule 83: 60S acidic ribosomal protein P0

Chain p0:  38% 8% 54%





- Molecule 84: UNKNOWN PROTEIN p1

Chain p1: 100%

There are no outlier residues recorded for this chain.

- Molecule 85: UNKNOWN PROTEIN p2

Chain p2: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.43Å 288.22Å 305.08Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	267.37 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (267.37-2.90)	Depositor
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.204 , 0.245	Depositor
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.213	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	411205	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OHX, MG, 3HE

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	0.69	3/41698 (0.0%)	1.25	259/64972 (0.4%)
1	6	0.83	9/42765 (0.0%)	1.36	416/66634 (0.6%)
2	S0	0.45	0/1617	0.63	0/2215
2	s0	0.50	0/1623	0.70	0/2222
3	S1	0.35	0/1735	0.63	2/2335 (0.1%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.49	0/1665	0.66	1/2263 (0.0%)
4	s2	0.60	0/1665	0.76	2/2263 (0.1%)
5	S3	0.49	0/1759	0.62	0/2368
5	s3	0.47	0/1759	0.60	0/2368
6	S4	0.48	0/2109	0.71	1/2839 (0.0%)
6	s4	0.57	0/2109	0.77	1/2839 (0.0%)
7	S5	0.39	0/1629	0.58	0/2202
7	s5	0.45	0/1629	0.63	0/2202
8	S6	0.45	0/1823	0.64	0/2439
8	s6	0.55	0/1779	0.69	0/2379
9	S7	0.43	0/1506	0.63	0/2028
9	s7	0.49	0/1516	0.68	0/2043
10	S8	0.53	0/1514	0.74	1/2021 (0.0%)
10	s8	0.62	0/1514	0.76	1/2021 (0.0%)
11	S9	0.46	0/1519	0.64	0/2035
11	s9	0.56	0/1519	0.72	1/2035 (0.0%)
12	C0	0.42	0/790	0.67	1/1069 (0.1%)
12	c0	0.39	0/777	0.63	3/1049 (0.3%)
13	C1	0.61	0/1240	0.80	1/1675 (0.1%)
13	c1	0.63	0/1194	0.78	0/1610
14	C2	0.36	0/900	0.63	0/1224
14	c2	0.30	0/900	0.56	0/1224
15	C3	0.46	0/1215	0.66	3/1638 (0.2%)
15	c3	0.56	0/1215	0.73	1/1638 (0.1%)
16	C4	0.36	0/901	0.63	0/1217
16	c4	0.51	0/960	0.72	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.46	0/998	0.65	0/1341
17	c5	0.51	0/1060	0.66	1/1426 (0.1%)
18	C6	0.45	0/1125	0.66	2/1510 (0.1%)
18	c6	0.49	0/1131	0.71	0/1518
19	C7	0.43	0/935	0.63	0/1254
19	c7	0.51	0/914	0.73	0/1224
20	C8	0.46	0/1211	0.64	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.46	0/1130	0.67	1/1517 (0.1%)
21	c9	0.51	0/1130	0.74	2/1517 (0.1%)
22	D0	0.46	0/865	0.65	0/1169
22	d0	0.51	0/892	0.68	0/1205
23	D1	0.43	0/693	0.60	0/935
23	d1	0.54	0/693	0.71	0/935
24	D2	0.53	0/1038	0.73	3/1395 (0.2%)
24	d2	0.62	0/1038	0.74	0/1395
25	D3	0.60	0/1139	0.81	3/1518 (0.2%)
25	d3	0.70	0/1139	0.79	1/1518 (0.1%)
26	D4	0.45	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.68	0/1449
27	D5	0.40	0/571	0.71	1/768 (0.1%)
27	d5	0.44	0/566	0.63	0/761
28	D6	0.44	0/782	0.67	0/1047
28	d6	0.54	0/782	0.72	0/1047
29	D7	0.43	0/620	0.67	1/838 (0.1%)
29	d7	0.49	0/620	0.68	0/838
30	D8	0.34	0/499	0.55	0/670
30	d8	0.42	0/499	0.66	0/670
31	D9	0.52	0/452	0.73	1/600 (0.2%)
31	d9	0.54	0/452	0.67	0/600
32	E0	0.46	0/483	0.61	0/643
33	E1	0.45	0/577	0.73	0/770
34	SR	0.89	2/2494 (0.1%)	1.42	4/3393 (0.1%)
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.52	0/1113	0.68	2/1502 (0.1%)
35	sM	0.50	0/683	0.66	1/923 (0.1%)
36	1	1.08	69/75394 (0.1%)	1.60	1618/117545 (1.4%)
36	5	1.10	113/75414 (0.1%)	1.60	1498/117575 (1.3%)
37	3	0.87	1/2883 (0.0%)	1.39	30/4491 (0.7%)
37	7	1.10	5/2883 (0.2%)	1.61	64/4491 (1.4%)
38	4	1.01	0/3746	1.51	61/5832 (1.0%)
38	8	0.87	0/3746	1.37	23/5832 (0.4%)
39	L2	0.72	0/1948	0.87	4/2617 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	l2	0.72	1/1946 (0.1%)	0.86	2/2614 (0.1%)
40	L3	0.73	0/3146	0.83	3/4228 (0.1%)
40	l3	0.82	2/3146 (0.1%)	0.89	7/4228 (0.2%)
41	L4	0.79	0/2800	0.94	6/3790 (0.2%)
41	l4	0.73	0/2800	0.88	3/3790 (0.1%)
42	L5	0.58	0/2425	0.70	0/3271
42	l5	0.71	0/2408	0.76	0/3248
43	L6	0.77	0/1260	0.84	1/1694 (0.1%)
43	l6	0.72	0/1269	0.82	1/1705 (0.1%)
44	L7	0.79	0/1821	0.85	1/2451 (0.0%)
44	l7	0.82	0/1828	0.86	3/2461 (0.1%)
45	L8	0.55	0/1836	0.67	1/2481 (0.0%)
45	l8	0.52	0/1796	0.69	1/2431 (0.0%)
46	L9	0.64	0/1539	0.76	1/2073 (0.0%)
46	l9	0.78	0/1539	0.82	0/2073
47	M0	0.72	0/1741	0.83	3/2335 (0.1%)
47	m0	0.77	1/1758 (0.1%)	0.85	3/2358 (0.1%)
48	M1	0.52	0/1374	0.71	1/1842 (0.1%)
48	m1	0.64	0/1374	0.79	1/1842 (0.1%)
49	M3	0.73	0/1568	0.84	3/2106 (0.1%)
49	m3	0.66	0/1573	0.82	3/2113 (0.1%)
50	M4	0.70	0/1068	0.80	1/1438 (0.1%)
50	m4	0.77	0/1074	0.81	1/1446 (0.1%)
51	M5	0.76	0/1757	0.82	0/2354
51	m5	0.65	0/1757	0.78	1/2354 (0.0%)
52	M6	0.83	1/1585 (0.1%)	0.92	3/2128 (0.1%)
52	m6	0.98	1/1585 (0.1%)	0.98	8/2128 (0.4%)
53	M7	0.78	1/1443 (0.1%)	0.83	0/1944
53	m7	0.84	0/1250	0.81	0/1683
54	M8	0.76	0/1465	0.91	4/1965 (0.2%)
54	m8	0.71	0/1465	0.87	1/1965 (0.1%)
55	M9	0.54	0/1538	0.66	0/2050
55	m9	0.59	0/1538	0.66	0/2050
56	N0	0.76	0/1481	0.83	1/1990 (0.1%)
56	n0	0.86	0/1481	0.83	0/1990
57	N1	0.78	1/1300 (0.1%)	0.81	0/1743
57	n1	0.82	1/1300 (0.1%)	0.81	0/1743
58	N2	0.44	0/812	0.61	0/1099
58	n2	0.51	0/794	0.67	0/1076
59	N3	0.72	0/1018	0.80	0/1369
59	n3	0.83	0/1018	0.94	3/1369 (0.2%)
60	N4	0.60	0/712	0.66	0/958
60	n4	0.66	0/1052	0.75	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	N5	0.61	0/979	0.77	1/1321 (0.1%)
61	n5	0.62	0/974	0.75	1/1314 (0.1%)
62	N6	0.70	0/1004	0.88	3/1341 (0.2%)
62	n6	0.63	0/1004	0.80	1/1341 (0.1%)
63	N7	0.50	0/1118	0.65	0/1497
63	n7	0.45	0/1118	0.61	0/1497
64	N8	0.82	0/1204	0.92	2/1612 (0.1%)
64	n8	0.76	0/1204	0.95	3/1612 (0.2%)
65	N9	0.73	0/473	0.80	1/629 (0.2%)
65	n9	0.81	0/473	1.00	1/629 (0.2%)
66	O0	0.45	0/751	0.63	0/1008
66	o0	0.49	0/775	0.66	0/1040
67	O1	0.61	0/890	0.72	0/1196
67	o1	0.77	0/897	0.82	0/1205
68	O2	0.83	0/1041	0.92	2/1394 (0.1%)
68	o2	0.82	0/1041	0.92	3/1394 (0.2%)
69	O3	0.89	0/868	0.88	1/1168 (0.1%)
69	o3	0.89	0/868	0.84	0/1168
70	O4	0.59	0/890	0.75	1/1189 (0.1%)
70	o4	0.61	1/890 (0.1%)	0.73	0/1189
71	O5	0.67	0/978	0.78	0/1301
71	o5	0.58	0/974	0.66	0/1297
72	O6	0.63	0/778	0.82	1/1034 (0.1%)
72	o6	0.52	0/777	0.68	0/1033
73	O7	0.81	1/696 (0.1%)	0.95	2/923 (0.2%)
73	o7	0.70	0/696	0.79	0/923
74	O8	0.51	0/618	0.63	0/826
74	o8	0.44	0/614	0.61	0/822
75	O9	0.77	0/443	0.89	0/588
75	o9	0.69	0/443	0.76	1/588 (0.2%)
76	Q0	0.67	0/423	0.76	0/562
76	q0	0.81	0/423	0.90	0/562
77	Q1	0.68	0/234	1.04	0/300
77	q1	0.83	0/234	0.94	1/300 (0.3%)
78	Q2	0.93	1/860 (0.1%)	0.87	2/1136 (0.2%)
78	q2	0.86	1/860 (0.1%)	0.81	0/1136
79	Q3	0.77	0/701	0.82	0/934
79	q3	0.70	0/701	0.85	2/934 (0.2%)
80	e0	0.52	0/499	0.72	0/665
81	e1	0.39	0/619	0.73	1/822 (0.1%)
83	p0	0.43	0/1092	0.60	0/1474
All	All	0.85	215/430075 (0.0%)	1.27	4114/631366 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	s0	0	1
3	s1	0	1
6	s4	0	1
7	s5	0	1
9	S7	0	1
9	s7	0	1
10	S8	0	1
13	C1	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	2
19	c7	0	1
20	c8	0	1
22	d0	0	1
25	d3	0	1
27	D5	0	3
28	D6	0	3
34	SR	0	2
39	L2	0	1
39	l2	0	2
42	l5	0	1
43	L6	0	1
44	L7	0	1
44	l7	0	2
52	M6	0	1
52	m6	0	1
53	M7	0	1
53	m7	0	1
56	n0	0	1
59	n3	0	1
62	n6	0	1
64	N8	0	2
64	n8	0	1
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
75	o9	0	1
78	Q2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
81	e1	0	1
All	All	0	50

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-30.25	0.64	1.34
34	SR	161	LYS	C-N	-24.97	0.76	1.34
78	Q2	17	CYS	CB-SG	16.00	2.09	1.82
36	5	1152	G	N9-C4	-13.57	1.27	1.38
78	q2	17	CYS	CB-SG	12.94	2.04	1.82

The worst 5 of 4114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	SR	161	LYS	O-C-N	-44.54	51.44	122.70
34	SR	160	GLU	C-N-CA	-39.83	22.12	121.70
34	SR	160	GLU	CA-C-N	-34.85	40.53	117.20
36	5	1152	G	N3-C4-C5	27.52	142.36	128.60
36	5	1152	G	N3-C4-N9	-27.23	109.66	126.00

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	88	ARG	Peptide
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
9	S7	31	SER	Peptide
10	S8	79	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	151 (74%)	36 (18%)	17 (8%)	1	2
2	s0	204/251 (81%)	157 (77%)	30 (15%)	17 (8%)	1	2
3	S1	212/254 (84%)	145 (68%)	35 (16%)	32 (15%)	0	0
3	s1	214/254 (84%)	179 (84%)	21 (10%)	14 (6%)	1	3
4	S2	215/253 (85%)	190 (88%)	17 (8%)	8 (4%)	3	13
4	s2	215/253 (85%)	184 (86%)	20 (9%)	11 (5%)	2	7
5	S3	221/239 (92%)	194 (88%)	19 (9%)	8 (4%)	3	14
5	s3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	1	3
6	S4	258/260 (99%)	213 (83%)	34 (13%)	11 (4%)	2	10
6	s4	258/260 (99%)	224 (87%)	19 (7%)	15 (6%)	1	5
7	S5	204/224 (91%)	166 (81%)	20 (10%)	18 (9%)	1	2
7	s5	204/224 (91%)	167 (82%)	18 (9%)	19 (9%)	0	1
8	S6	224/236 (95%)	194 (87%)	19 (8%)	11 (5%)	2	8
8	s6	216/236 (92%)	189 (88%)	20 (9%)	7 (3%)	4	16
9	S7	182/189 (96%)	137 (75%)	26 (14%)	19 (10%)	0	1
9	s7	184/189 (97%)	154 (84%)	21 (11%)	9 (5%)	2	8
10	S8	184/200 (92%)	156 (85%)	13 (7%)	15 (8%)	1	2
10	s8	184/200 (92%)	163 (89%)	15 (8%)	6 (3%)	4	15
11	S9	183/196 (93%)	153 (84%)	21 (12%)	9 (5%)	2	8
11	s9	183/196 (93%)	154 (84%)	19 (10%)	10 (6%)	2	5
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	2
12	c0	92/105 (88%)	65 (71%)	15 (16%)	12 (13%)	0	0
13	C1	153/155 (99%)	125 (82%)	14 (9%)	14 (9%)	1	1
13	c1	144/155 (93%)	123 (85%)	14 (10%)	7 (5%)	2	8
14	C2	122/142 (86%)	76 (62%)	24 (20%)	22 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	74 (61%)	30 (25%)	18 (15%)	0	0
15	C3	148/150 (99%)	129 (87%)	13 (9%)	6 (4%)	3	11
15	c3	148/150 (99%)	124 (84%)	14 (10%)	10 (7%)	1	3
16	C4	125/136 (92%)	98 (78%)	16 (13%)	11 (9%)	1	2
16	c4	126/136 (93%)	102 (81%)	12 (10%)	12 (10%)	0	1
17	C5	122/141 (86%)	91 (75%)	21 (17%)	10 (8%)	1	2
17	c5	133/141 (94%)	97 (73%)	22 (16%)	14 (10%)	0	1
18	C6	139/142 (98%)	122 (88%)	11 (8%)	6 (4%)	2	10
18	c6	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	2	10
19	C7	116/136 (85%)	87 (75%)	20 (17%)	9 (8%)	1	2
19	c7	113/136 (83%)	92 (81%)	10 (9%)	11 (10%)	0	1
20	C8	143/145 (99%)	117 (82%)	14 (10%)	12 (8%)	1	2
20	c8	143/145 (99%)	120 (84%)	16 (11%)	7 (5%)	2	8
21	C9	141/143 (99%)	121 (86%)	14 (10%)	6 (4%)	2	10
21	c9	141/143 (99%)	117 (83%)	17 (12%)	7 (5%)	2	7
22	D0	105/120 (88%)	87 (83%)	14 (13%)	4 (4%)	3	13
22	d0	108/120 (90%)	86 (80%)	13 (12%)	9 (8%)	1	2
23	D1	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1	2
23	d1	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	13	40
24	D2	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	6	22
24	d2	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
25	D3	142/144 (99%)	109 (77%)	17 (12%)	16 (11%)	0	1
25	d3	142/144 (99%)	124 (87%)	17 (12%)	1 (1%)	22	54
26	D4	132/134 (98%)	111 (84%)	14 (11%)	7 (5%)	2	6
26	d4	132/134 (98%)	109 (83%)	18 (14%)	5 (4%)	3	13
27	D5	68/107 (64%)	48 (71%)	10 (15%)	10 (15%)	0	0
27	d5	67/107 (63%)	52 (78%)	10 (15%)	5 (8%)	1	2
28	D6	95/97 (98%)	66 (70%)	10 (10%)	19 (20%)	0	0
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	2
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	3	13
29	d7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	51 (84%)	6 (10%)	4 (7%)	1	3
30	d8	61/66 (92%)	46 (75%)	13 (21%)	2 (3%)	4	15
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	3	12
31	d9	51/55 (93%)	43 (84%)	4 (8%)	4 (8%)	1	2
32	E0	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	6
33	E1	69/76 (91%)	35 (51%)	19 (28%)	15 (22%)	0	0
34	SR	316/318 (99%)	252 (80%)	36 (11%)	28 (9%)	1	1
34	sR	316/318 (99%)	274 (87%)	30 (10%)	12 (4%)	3	13
35	SM	155/273 (57%)	112 (72%)	22 (14%)	21 (14%)	0	0
35	sM	98/273 (36%)	65 (66%)	18 (18%)	15 (15%)	0	0
39	L2	250/253 (99%)	222 (89%)	25 (10%)	3 (1%)	13	40
39	l2	250/253 (99%)	219 (88%)	25 (10%)	6 (2%)	6	22
40	L3	384/386 (100%)	339 (88%)	31 (8%)	14 (4%)	3	14
40	l3	384/386 (100%)	343 (89%)	31 (8%)	10 (3%)	5	20
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	2	6
41	l4	359/361 (99%)	309 (86%)	31 (9%)	19 (5%)	2	6
42	L5	294/296 (99%)	249 (85%)	27 (9%)	18 (6%)	1	4
42	l5	292/296 (99%)	256 (88%)	32 (11%)	4 (1%)	11	36
43	L6	152/175 (87%)	140 (92%)	10 (7%)	2 (1%)	12	37
43	l6	153/175 (87%)	130 (85%)	19 (12%)	4 (3%)	5	20
44	L7	220/243 (90%)	202 (92%)	11 (5%)	7 (3%)	4	16
44	l7	221/243 (91%)	204 (92%)	14 (6%)	3 (1%)	11	36
45	L8	231/255 (91%)	189 (82%)	30 (13%)	12 (5%)	2	6
45	l8	229/255 (90%)	185 (81%)	23 (10%)	21 (9%)	1	1
46	L9	189/191 (99%)	170 (90%)	15 (8%)	4 (2%)	7	26
46	l9	189/191 (99%)	173 (92%)	13 (7%)	3 (2%)	9	32
47	M0	207/220 (94%)	182 (88%)	18 (9%)	7 (3%)	3	15
47	m0	209/220 (95%)	175 (84%)	25 (12%)	9 (4%)	2	10
48	M1	167/173 (96%)	127 (76%)	26 (16%)	14 (8%)	1	2
48	m1	167/173 (96%)	143 (86%)	15 (9%)	9 (5%)	2	6
49	M3	191/198 (96%)	170 (89%)	17 (9%)	4 (2%)	7	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	m3	192/198 (97%)	162 (84%)	18 (9%)	12 (6%)	1	4
50	M4	134/137 (98%)	116 (87%)	11 (8%)	7 (5%)	2	6
50	m4	135/137 (98%)	126 (93%)	7 (5%)	2 (2%)	10	34
51	M5	201/203 (99%)	186 (92%)	8 (4%)	7 (4%)	3	14
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	4	17
52	M6	195/198 (98%)	183 (94%)	7 (4%)	5 (3%)	5	20
52	m6	195/198 (98%)	184 (94%)	8 (4%)	3 (2%)	10	34
53	M7	181/183 (99%)	156 (86%)	17 (9%)	8 (4%)	2	10
53	m7	153/183 (84%)	136 (89%)	16 (10%)	1 (1%)	22	54
54	M8	183/185 (99%)	166 (91%)	12 (7%)	5 (3%)	5	19
54	m8	183/185 (99%)	161 (88%)	15 (8%)	7 (4%)	3	13
55	M9	186/188 (99%)	177 (95%)	7 (4%)	2 (1%)	14	42
55	m9	186/188 (99%)	169 (91%)	14 (8%)	3 (2%)	9	32
56	N0	170/172 (99%)	156 (92%)	10 (6%)	4 (2%)	6	22
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	25	58
57	N1	157/159 (99%)	137 (87%)	14 (9%)	6 (4%)	3	13
57	n1	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	8	28
58	N2	98/120 (82%)	73 (74%)	19 (19%)	6 (6%)	1	4
58	n2	96/120 (80%)	79 (82%)	13 (14%)	4 (4%)	3	10
59	N3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	22	54
59	n3	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	10	34
60	N4	96/155 (62%)	72 (75%)	15 (16%)	9 (9%)	0	1
60	n4	133/155 (86%)	113 (85%)	11 (8%)	9 (7%)	1	3
61	N5	119/141 (84%)	108 (91%)	9 (8%)	2 (2%)	9	31
61	n5	118/141 (84%)	97 (82%)	15 (13%)	6 (5%)	2	7
62	N6	124/126 (98%)	111 (90%)	7 (6%)	6 (5%)	2	8
62	n6	124/126 (98%)	109 (88%)	10 (8%)	5 (4%)	3	11
63	N7	133/135 (98%)	115 (86%)	11 (8%)	7 (5%)	2	6
63	n7	133/135 (98%)	109 (82%)	11 (8%)	13 (10%)	0	1
64	N8	146/148 (99%)	120 (82%)	18 (12%)	8 (6%)	2	5
64	n8	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	N9	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	3	14
65	n9	56/58 (97%)	44 (79%)	9 (16%)	3 (5%)	2	6
66	O0	95/104 (91%)	89 (94%)	4 (4%)	2 (2%)	7	26
66	o0	98/104 (94%)	88 (90%)	8 (8%)	2 (2%)	7	27
67	O1	107/112 (96%)	96 (90%)	7 (6%)	4 (4%)	3	13
67	o1	107/112 (96%)	89 (83%)	10 (9%)	8 (8%)	1	2
68	O2	125/129 (97%)	113 (90%)	11 (9%)	1 (1%)	19	51
68	o2	125/129 (97%)	108 (86%)	14 (11%)	3 (2%)	6	22
69	O3	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	15	45
69	o3	104/106 (98%)	95 (91%)	6 (6%)	3 (3%)	4	18
70	O4	110/119 (92%)	102 (93%)	7 (6%)	1 (1%)	17	48
70	o4	110/119 (92%)	102 (93%)	5 (4%)	3 (3%)	5	19
71	O5	117/119 (98%)	104 (89%)	9 (8%)	4 (3%)	3	15
71	o5	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	9	31
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	4
72	o6	97/99 (98%)	84 (87%)	5 (5%)	8 (8%)	1	2
73	O7	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
73	o7	85/87 (98%)	74 (87%)	9 (11%)	2 (2%)	6	22
74	O8	75/77 (97%)	65 (87%)	8 (11%)	2 (3%)	5	19
74	o8	75/77 (97%)	67 (89%)	5 (7%)	3 (4%)	3	11
75	O9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	26
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	11
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	7	27
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	89 (86%)	9 (9%)	5 (5%)	2	8
78	q2	103/105 (98%)	94 (91%)	7 (7%)	2 (2%)	8	28
79	Q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	6	24
79	q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	6	24
80	e0	60/62 (97%)	51 (85%)	5 (8%)	4 (7%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	e1	74/76 (97%)	37 (50%)	18 (24%)	19 (26%)	0	0
83	p0	139/311 (45%)	114 (82%)	21 (15%)	4 (3%)	4	18
All	All	22333/24141 (92%)	18964 (85%)	2226 (10%)	1143 (5%)	2	7

5 of 1143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN
2	S0	39	ASN
2	S0	95	ALA
2	S0	158	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	130 (79%)	34 (21%)	1	3
2	s0	165/209 (79%)	138 (84%)	27 (16%)	2	7
3	S1	191/223 (86%)	159 (83%)	32 (17%)	2	6
3	s1	192/223 (86%)	162 (84%)	30 (16%)	2	8
4	S2	176/204 (86%)	140 (80%)	36 (20%)	1	3
4	s2	176/204 (86%)	137 (78%)	39 (22%)	1	3
5	S3	182/194 (94%)	142 (78%)	40 (22%)	1	3
5	s3	182/194 (94%)	145 (80%)	37 (20%)	1	3
6	S4	221/221 (100%)	178 (80%)	43 (20%)	1	4
6	s4	221/221 (100%)	179 (81%)	42 (19%)	1	4
7	S5	173/190 (91%)	148 (86%)	25 (14%)	3	9
7	s5	173/190 (91%)	144 (83%)	29 (17%)	2	6
8	S6	188/201 (94%)	150 (80%)	38 (20%)	1	4
8	s6	187/201 (93%)	155 (83%)	32 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S7	165/169 (98%)	127 (77%)	38 (23%)	1	2
9	s7	165/169 (98%)	136 (82%)	29 (18%)	2	5
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	9
10	s8	150/161 (93%)	126 (84%)	24 (16%)	2	7
11	S9	158/165 (96%)	122 (77%)	36 (23%)	1	2
11	s9	158/165 (96%)	123 (78%)	35 (22%)	1	3
12	C0	77/98 (79%)	62 (80%)	15 (20%)	1	4
12	c0	73/98 (74%)	63 (86%)	10 (14%)	3	11
13	C1	129/136 (95%)	108 (84%)	21 (16%)	2	7
13	c1	129/136 (95%)	105 (81%)	24 (19%)	1	5
14	C2	88/118 (75%)	67 (76%)	21 (24%)	0	2
14	c2	88/118 (75%)	70 (80%)	18 (20%)	1	3
15	C3	127/127 (100%)	106 (84%)	21 (16%)	2	7
15	c3	127/127 (100%)	103 (81%)	24 (19%)	1	4
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	1
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	2
17	C5	101/117 (86%)	86 (85%)	15 (15%)	3	9
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	6
18	C6	117/118 (99%)	97 (83%)	20 (17%)	2	6
18	c6	118/118 (100%)	95 (80%)	23 (20%)	1	4
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	3
19	c7	92/124 (74%)	77 (84%)	15 (16%)	2	7
20	C8	128/128 (100%)	102 (80%)	26 (20%)	1	3
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	2
21	C9	115/115 (100%)	95 (83%)	20 (17%)	2	6
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	7
22	D0	100/113 (88%)	76 (76%)	24 (24%)	0	2
22	d0	103/113 (91%)	81 (79%)	22 (21%)	1	3
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	5
23	d1	74/74 (100%)	60 (81%)	14 (19%)	1	4
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	d2	110/110 (100%)	96 (87%)	14 (13%)	4	13
25	D3	119/119 (100%)	96 (81%)	23 (19%)	1	4
25	d3	119/119 (100%)	102 (86%)	17 (14%)	3	10
26	D4	112/112 (100%)	95 (85%)	17 (15%)	3	8
26	d4	112/112 (100%)	98 (88%)	14 (12%)	4	14
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	2
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	9
28	D6	83/83 (100%)	68 (82%)	15 (18%)	1	5
28	d6	83/83 (100%)	72 (87%)	11 (13%)	4	11
29	D7	70/70 (100%)	59 (84%)	11 (16%)	2	8
29	d7	70/70 (100%)	63 (90%)	7 (10%)	7	23
30	D8	56/59 (95%)	42 (75%)	14 (25%)	0	2
30	d8	56/59 (95%)	47 (84%)	9 (16%)	2	7
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	6
31	d9	47/48 (98%)	41 (87%)	6 (13%)	4	13
32	E0	51/51 (100%)	44 (86%)	7 (14%)	3	11
33	E1	62/66 (94%)	51 (82%)	11 (18%)	2	5
34	SR	260/261 (100%)	223 (86%)	37 (14%)	3	10
34	sR	260/261 (100%)	230 (88%)	30 (12%)	5	17
35	SM	97/228 (42%)	79 (81%)	18 (19%)	1	5
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	1
39	L2	193/195 (99%)	156 (81%)	37 (19%)	1	4
39	l2	192/195 (98%)	160 (83%)	32 (17%)	2	6
40	L3	321/322 (100%)	250 (78%)	71 (22%)	1	3
40	l3	319/322 (99%)	250 (78%)	69 (22%)	1	3
41	L4	288/288 (100%)	241 (84%)	47 (16%)	2	7
41	l4	288/288 (100%)	239 (83%)	49 (17%)	2	6
42	L5	244/244 (100%)	206 (84%)	38 (16%)	2	8
42	l5	243/244 (100%)	198 (82%)	45 (18%)	1	5
43	L6	134/152 (88%)	115 (86%)	19 (14%)	3	10
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	L7	186/204 (91%)	169 (91%)	17 (9%)	9	28
44	l7	187/204 (92%)	160 (86%)	27 (14%)	3	9
45	L8	187/207 (90%)	152 (81%)	35 (19%)	1	5
45	l8	177/207 (86%)	146 (82%)	31 (18%)	2	6
46	L9	171/171 (100%)	140 (82%)	31 (18%)	1	5
46	l9	171/171 (100%)	141 (82%)	30 (18%)	2	6
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	3
47	m0	179/186 (96%)	140 (78%)	39 (22%)	1	3
48	M1	147/150 (98%)	117 (80%)	30 (20%)	1	3
48	m1	147/150 (98%)	123 (84%)	24 (16%)	2	7
49	M3	154/158 (98%)	124 (80%)	30 (20%)	1	4
49	m3	154/158 (98%)	132 (86%)	22 (14%)	3	10
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	6
50	m4	108/108 (100%)	88 (82%)	20 (18%)	1	5
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	6
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2	7
52	M6	160/161 (99%)	138 (86%)	22 (14%)	3	10
52	m6	160/161 (99%)	127 (79%)	33 (21%)	1	3
53	M7	140/145 (97%)	112 (80%)	28 (20%)	1	4
53	m7	125/145 (86%)	106 (85%)	19 (15%)	3	8
54	M8	150/150 (100%)	126 (84%)	24 (16%)	2	7
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	4
55	M9	153/153 (100%)	128 (84%)	25 (16%)	2	7
55	m9	153/153 (100%)	123 (80%)	30 (20%)	1	4
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1	4
56	n0	156/156 (100%)	125 (80%)	31 (20%)	1	4
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	2
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	4
58	N2	87/106 (82%)	79 (91%)	8 (9%)	9	27
58	n2	85/106 (80%)	72 (85%)	13 (15%)	2	8
59	N3	104/104 (100%)	91 (88%)	13 (12%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	n3	104/104 (100%)	96 (92%)	8 (8%)	13	35
60	N4	57/129 (44%)	52 (91%)	5 (9%)	10	30
60	n4	100/129 (78%)	84 (84%)	16 (16%)	2	7
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	3
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	3
62	N6	109/109 (100%)	86 (79%)	23 (21%)	1	3
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	2
63	N7	115/115 (100%)	93 (81%)	22 (19%)	1	4
63	n7	115/115 (100%)	96 (84%)	19 (16%)	2	7
64	N8	118/118 (100%)	101 (86%)	17 (14%)	3	9
64	n8	118/118 (100%)	96 (81%)	22 (19%)	1	5
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	3
65	n9	46/46 (100%)	36 (78%)	10 (22%)	1	3
66	O0	81/87 (93%)	70 (86%)	11 (14%)	3	11
66	o0	84/87 (97%)	68 (81%)	16 (19%)	1	4
67	O1	92/96 (96%)	75 (82%)	17 (18%)	1	5
67	o1	94/96 (98%)	73 (78%)	21 (22%)	1	3
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2	7
68	o2	109/110 (99%)	88 (81%)	21 (19%)	1	4
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	11
69	o3	90/90 (100%)	76 (84%)	14 (16%)	2	8
70	O4	95/101 (94%)	75 (79%)	20 (21%)	1	3
70	o4	95/101 (94%)	82 (86%)	13 (14%)	3	11
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	3
71	o5	103/104 (99%)	83 (81%)	20 (19%)	1	4
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	3
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	6
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	3
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	3
74	o8	67/68 (98%)	56 (84%)	11 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	O9	45/45 (100%)	39 (87%)	6 (13%)	4	11
75	o9	45/45 (100%)	40 (89%)	5 (11%)	6	19
76	Q0	47/47 (100%)	42 (89%)	5 (11%)	6	20
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1	4
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	1
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	5
78	q2	90/90 (100%)	72 (80%)	18 (20%)	1	4
79	Q3	71/71 (100%)	57 (80%)	14 (20%)	1	4
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	3
80	e0	53/53 (100%)	42 (79%)	11 (21%)	1	3
81	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
83	p0	105/253 (42%)	83 (79%)	22 (21%)	1	3
All	All	18728/20239 (92%)	15327 (82%)	3401 (18%)	1	5

5 of 3401 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	O2	41	VAL
8	s6	22	HIS
64	n8	26	ARG
71	O5	15	GLU
3	s1	25	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	s1	209	ASN
8	s6	197	ASN
51	m5	194	GLN
3	s1	211	HIS
6	s4	231	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	451 (25%)	57 (3%)
1	6	1792/1800 (99%)	435 (24%)	48 (2%)
36	1	3145/3396 (92%)	619 (19%)	91 (2%)
36	5	3146/3396 (92%)	623 (19%)	88 (2%)
37	3	120/121 (99%)	10 (8%)	2 (1%)
37	7	120/121 (99%)	17 (14%)	0
38	4	157/158 (99%)	33 (21%)	3 (1%)
38	8	157/158 (99%)	38 (24%)	2 (1%)
All	All	10384/10950 (94%)	2226 (21%)	291 (2%)

5 of 2226 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	8	U
1	2	17	C
1	2	25	C

5 of 291 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3121	U
1	6	217	A
36	5	2584	G
36	1	3217	C
36	1	3375	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	OHX	1	4122	-	0,6,6	0.00	-	-		
87	OHX	14	403	-	0,6,6	0.00	-	-		
87	OHX	5	3972	-	0,6,6	0.00	-	-		
87	OHX	6	2149	-	0,6,6	0.00	-	-		
87	OHX	1	4200	-	0,6,6	0.00	-	-		
87	OHX	5	4075	-	0,6,6	0.00	-	-		
87	OHX	1	4191	-	0,6,6	0.00	-	-		
87	OHX	5	3960	-	0,6,6	0.00	-	-		
87	OHX	5	3950	-	0,6,6	0.00	-	-		
87	OHX	2	2028	-	0,6,6	0.00	-	-		
87	OHX	5	4037	-	0,6,6	0.00	-	-		
87	OHX	1	4015	-	0,6,6	0.00	-	-		
87	OHX	1	4119	-	0,6,6	0.00	-	-		
87	OHX	O7	104	-	0,6,6	0.00	-	-		
87	OHX	5	4086	-	0,6,6	0.00	-	-		
87	OHX	1	3909	-	0,6,6	0.00	-	-		
87	OHX	1	3902	-	0,6,6	0.00	-	-		
87	OHX	1	3976	-	0,6,6	0.00	-	-		
87	OHX	6	2175	-	0,6,6	0.00	-	-		
87	OHX	5	4222	-	0,6,6	0.00	-	-		
87	OHX	1	4013	-	0,6,6	0.00	-	-		
87	OHX	1	4008	-	0,6,6	0.00	-	-		
87	OHX	1	4057	-	0,6,6	0.00	-	-		
87	OHX	5	4157	-	0,6,6	0.00	-	-		
87	OHX	1	4068	-	0,6,6	0.00	-	-		
87	OHX	5	3922	-	0,6,6	0.00	-	-		
87	OHX	1	3928	-	0,6,6	0.00	-	-		
87	OHX	2	2056	-	0,6,6	0.00	-	-		
87	OHX	6	2128	-	0,6,6	0.00	-	-		
87	OHX	1	4131	-	0,6,6	0.00	-	-		
87	OHX	1	3915	-	0,6,6	0.00	-	-		
87	OHX	5	4031	-	0,6,6	0.00	-	-		
87	OHX	2	2159	-	0,6,6	0.00	-	-		
87	OHX	6	2129	-	0,6,6	0.00	-	-		
87	OHX	6	2092	-	0,6,6	0.00	-	-		
87	OHX	5	4162	-	0,6,6	0.00	-	-		
87	OHX	1	3904	-	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	4138	-	0,6,6	0.00	-	-		
87	OHX	5	4169	-	0,6,6	0.00	-	-		
87	OHX	3	220	-	0,6,6	0.00	-	-		
87	OHX	6	2194	-	0,6,6	0.00	-	-		
87	OHX	5	4244	-	0,6,6	0.00	-	-		
87	OHX	1	4205	-	0,6,6	0.00	-	-		
87	OHX	6	2174	-	0,6,6	0.00	-	-		
87	OHX	2	2103	-	0,6,6	0.00	-	-		
87	OHX	1	3993	-	0,6,6	0.00	-	-		
87	OHX	5	4074	-	0,6,6	0.00	-	-		
87	OHX	5	4176	-	0,6,6	0.00	-	-		
87	OHX	1	3953	-	0,6,6	0.00	-	-		
87	OHX	5	4181	-	0,6,6	0.00	-	-		
87	OHX	5	3929	-	0,6,6	0.00	-	-		
87	OHX	6	2119	-	0,6,6	0.00	-	-		
87	OHX	19	600	-	0,6,6	0.00	-	-		
87	OHX	5	4093	-	0,6,6	0.00	-	-		
87	OHX	6	2058	-	0,6,6	0.00	-	-		
87	OHX	5	4018	-	0,6,6	0.00	-	-		
87	OHX	1	4202	-	0,6,6	0.00	-	-		
87	OHX	1	3967	-	0,6,6	0.00	-	-		
87	OHX	1	4194	-	0,6,6	0.00	-	-		
87	OHX	5	4058	-	0,6,6	0.00	-	-		
87	OHX	5	4112	-	0,6,6	0.00	-	-		
87	OHX	2	2136	-	0,6,6	0.00	-	-		
87	OHX	5	4227	-	0,6,6	0.00	-	-		
87	OHX	5	4042	-	0,6,6	0.00	-	-		
87	OHX	1	3921	-	0,6,6	0.00	-	-		
87	OHX	5	4101	-	0,6,6	0.00	-	-		
87	OHX	o9	101	-	0,6,6	0.00	-	-		
87	OHX	1	4172	-	0,6,6	0.00	-	-		
87	OHX	1	4106	-	0,6,6	0.00	-	-		
87	OHX	8	215	-	0,6,6	0.00	-	-		
87	OHX	5	3991	-	0,6,6	0.00	-	-		
87	OHX	6	2108	-	0,6,6	0.00	-	-		
87	OHX	6	2107	-	0,6,6	0.00	-	-		
87	OHX	5	4133	-	0,6,6	0.00	-	-		
87	OHX	2	2099	-	0,6,6	0.00	-	-		
87	OHX	1	3988	-	0,6,6	0.00	-	-		
87	OHX	2	2057	-	0,6,6	0.00	-	-		
87	OHX	7	216	-	0,6,6	0.00	-	-		
87	OHX	5	4206	-	0,6,6	0.00	-	-		
87	OHX	6	2155	-	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	4044	-	0,6,6	0.00	-	-		
87	OHX	1	4073	-	0,6,6	0.00	-	-		
87	OHX	6	2085	-	0,6,6	0.00	-	-		
87	OHX	1	4128	-	0,6,6	0.00	-	-		
87	OHX	5	3936	-	0,6,6	0.00	-	-		
87	OHX	5	4102	-	0,6,6	0.00	-	-		
87	OHX	5	4119	-	0,6,6	0.00	-	-		
87	OHX	1	4017	-	0,6,6	0.00	-	-		
87	OHX	5	4214	-	0,6,6	0.00	-	-		
87	OHX	5	4195	-	0,6,6	0.00	-	-		
87	OHX	2	2142	-	0,6,6	0.00	-	-		
87	OHX	6	2127	-	0,6,6	0.00	-	-		
87	OHX	1	4188	-	0,6,6	0.00	-	-		
87	OHX	2	2082	-	0,6,6	0.00	-	-		
87	OHX	2	2104	-	0,6,6	0.00	-	-		
87	OHX	1	4052	-	0,6,6	0.00	-	-		
87	OHX	5	4023	-	0,6,6	0.00	-	-		
87	OHX	8	223	-	0,6,6	0.00	-	-		
87	OHX	5	4124	-	0,6,6	0.00	-	-		
87	OHX	s4	301	-	0,6,6	0.00	-	-		
87	OHX	2	2145	-	0,6,6	0.00	-	-		
87	OHX	5	4054	-	0,6,6	0.00	-	-		
87	OHX	1	4165	-	0,6,6	0.00	-	-		
87	OHX	5	4067	-	0,6,6	0.00	-	-		
87	OHX	1	3944	-	0,6,6	0.00	-	-		
87	OHX	2	2116	-	0,6,6	0.00	-	-		
87	OHX	1	4186	-	0,6,6	0.00	-	-		
87	OHX	1	3985	-	0,6,6	0.00	-	-		
87	OHX	n9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4152	-	0,6,6	0.00	-	-		
87	OHX	5	4038	-	0,6,6	0.00	-	-		
87	OHX	5	4069	-	0,6,6	0.00	-	-		
87	OHX	6	2163	-	0,6,6	0.00	-	-		
87	OHX	5	4015	-	0,6,6	0.00	-	-		
87	OHX	6	2071	-	0,6,6	0.00	-	-		
87	OHX	2	2037	-	0,6,6	0.00	-	-		
87	OHX	6	2074	-	0,6,6	0.00	-	-		
87	OHX	6	2136	-	0,6,6	0.00	-	-		
87	OHX	5	4198	-	0,6,6	0.00	-	-		
87	OHX	1	4022	-	0,6,6	0.00	-	-		
87	OHX	1	4035	-	0,6,6	0.00	-	-		
87	OHX	5	4055	-	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	4205	-	0,6,6	0.00	-	-		
87	OHX	5	3905	-	0,6,6	0.00	-	-		
87	OHX	2	2179	-	0,6,6	0.00	-	-		
87	OHX	5	3990	-	0,6,6	0.00	-	-		
87	OHX	1	4056	-	0,6,6	0.00	-	-		
87	OHX	1	4170	-	0,6,6	0.00	-	-		
87	OHX	8	228	-	0,6,6	0.00	-	-		
87	OHX	5	4177	-	0,6,6	0.00	-	-		
87	OHX	6	2131	-	0,6,6	0.00	-	-		
87	OHX	5	4172	-	0,6,6	0.00	-	-		
87	OHX	1	3876	-	0,6,6	0.00	-	-		
87	OHX	1	3971	-	0,6,6	0.00	-	-		
87	OHX	6	2116	-	0,6,6	0.00	-	-		
87	OHX	2	2029	-	0,6,6	0.00	-	-		
87	OHX	2	2108	-	0,6,6	0.00	-	-		
87	OHX	6	2105	-	0,6,6	0.00	-	-		
87	OHX	3	221	-	0,6,6	0.00	-	-		
87	OHX	5	4139	-	0,6,6	0.00	-	-		
87	OHX	5	4159	-	0,6,6	0.00	-	-		
87	OHX	5	4156	-	0,6,6	0.00	-	-		
87	OHX	6	2087	-	0,6,6	0.00	-	-		
87	OHX	1	4032	-	0,6,6	0.00	-	-		
87	OHX	5	4026	-	0,6,6	0.00	-	-		
87	OHX	1	3992	-	0,6,6	0.00	-	-		
87	OHX	1	4155	-	0,6,6	0.00	-	-		
87	OHX	5	4220	-	0,6,6	0.00	-	-		
87	OHX	2	2025	-	0,6,6	0.00	-	-		
87	OHX	6	2187	-	0,6,6	0.00	-	-		
87	OHX	2	2100	-	0,6,6	0.00	-	-		
87	OHX	1	4059	-	0,6,6	0.00	-	-		
87	OHX	5	4179	-	0,6,6	0.00	-	-		
87	OHX	6	2089	-	0,6,6	0.00	-	-		
87	OHX	15	304	-	0,6,6	0.00	-	-		
87	OHX	14	404	-	0,6,6	0.00	-	-		
87	OHX	5	4230	-	0,6,6	0.00	-	-		
87	OHX	1	4178	-	0,6,6	0.00	-	-		
87	OHX	N9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4189	-	0,6,6	0.00	-	-		
87	OHX	6	2123	-	0,6,6	0.00	-	-		
87	OHX	8	221	-	0,6,6	0.00	-	-		
87	OHX	6	2073	-	0,6,6	0.00	-	-		
87	OHX	5	4142	-	0,6,6	0.00	-	-		
87	OHX	15	303	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	4234	-	0,6,6	0.00	-	-		
87	OHX	2	2081	-	0,6,6	0.00	-	-		
87	OHX	1	3941	-	0,6,6	0.00	-	-		
87	OHX	2	2115	-	0,6,6	0.00	-	-		
87	OHX	1	4055	-	0,6,6	0.00	-	-		
87	OHX	1	3949	-	0,6,6	0.00	-	-		
87	OHX	1	4201	-	0,6,6	0.00	-	-		
87	OHX	1	4204	-	0,6,6	0.00	-	-		
87	OHX	5	4120	-	0,6,6	0.00	-	-		
87	OHX	2	2044	-	0,6,6	0.00	-	-		
87	OHX	Q2	503	-	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	5	3970	-	0,6,6	0.00	-	-		
87	OHX	1	4125	-	0,6,6	0.00	-	-		
87	OHX	1	4198	-	0,6,6	0.00	-	-		
87	OHX	7	219	-	0,6,6	0.00	-	-		
87	OHX	5	3910	-	0,6,6	0.00	-	-		
87	OHX	1	3930	-	0,6,6	0.00	-	-		
87	OHX	N1	201	-	0,6,6	0.00	-	-		
87	OHX	1	4141	-	0,6,6	0.00	-	-		
87	OHX	5	4188	-	0,6,6	0.00	-	-		
87	OHX	5	4182	-	0,6,6	0.00	-	-		
87	OHX	2	2113	-	0,6,6	0.00	-	-		
87	OHX	2	2059	-	0,6,6	0.00	-	-		
87	OHX	1	4053	-	0,6,6	0.00	-	-		
87	OHX	6	2061	-	0,6,6	0.00	-	-		
87	OHX	2	2080	-	0,6,6	0.00	-	-		
87	OHX	6	2142	-	0,6,6	0.00	-	-		
87	OHX	5	4237	-	0,6,6	0.00	-	-		
87	OHX	7	215	-	0,6,6	0.00	-	-		
87	OHX	5	4105	-	0,6,6	0.00	-	-		
87	OHX	5	4184	-	0,6,6	0.00	-	-		
87	OHX	2	2139	-	0,6,6	0.00	-	-		
87	OHX	5	4197	-	0,6,6	0.00	-	-		
87	OHX	1	4173	-	0,6,6	0.00	-	-		
87	OHX	1	4021	-	0,6,6	0.00	-	-		
87	OHX	1	4130	-	0,6,6	0.00	-	-		
87	OHX	5	4081	-	0,6,6	0.00	-	-		
87	OHX	1	3979	-	0,6,6	0.00	-	-		
87	OHX	1	3912	-	0,6,6	0.00	-	-		
87	OHX	6	2047	-	0,6,6	0.00	-	-		
87	OHX	8	218	-	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	3893	-	0,6,6	0.00	-	-		
87	OHX	6	2138	-	0,6,6	0.00	-	-		
87	OHX	1	4007	-	0,6,6	0.00	-	-		
87	OHX	2	2161	-	0,6,6	0.00	-	-		
87	OHX	6	2080	-	0,6,6	0.00	-	-		
87	OHX	7	227	-	0,6,6	0.00	-	-		
87	OHX	5	4160	-	0,6,6	0.00	-	-		
87	OHX	1	4161	-	0,6,6	0.00	-	-		
87	OHX	1	4197	-	0,6,6	0.00	-	-		
87	OHX	5	4144	-	0,6,6	0.00	-	-		
87	OHX	6	2082	-	0,6,6	0.00	-	-		
87	OHX	1	4000	-	0,6,6	0.00	-	-		
87	OHX	2	2149	-	0,6,6	0.00	-	-		
87	OHX	4	232	-	0,6,6	0.00	-	-		
87	OHX	5	4098	-	0,6,6	0.00	-	-		
87	OHX	1	3885	-	0,6,6	0.00	-	-		
87	OHX	1	4081	-	0,6,6	0.00	-	-		
87	OHX	5	4076	-	0,6,6	0.00	-	-		
87	OHX	1	4207	-	0,6,6	0.00	-	-		
87	OHX	5	4072	-	0,6,6	0.00	-	-		
87	OHX	1	3896	-	0,6,6	0.00	-	-		
87	OHX	s1	302	-	0,6,6	0.00	-	-		
87	OHX	2	2109	-	0,6,6	0.00	-	-		
87	OHX	d4	202	-	0,6,6	0.00	-	-		
87	OHX	1	4090	-	0,6,6	0.00	-	-		
87	OHX	1	4126	-	0,6,6	0.00	-	-		
87	OHX	1	3923	-	0,6,6	0.00	-	-		
87	OHX	6	2132	-	0,6,6	0.00	-	-		
87	OHX	1	3908	-	0,6,6	0.00	-	-		
87	OHX	6	2112	-	0,6,6	0.00	-	-		
87	OHX	6	2099	-	0,6,6	0.00	-	-		
87	OHX	5	4146	-	0,6,6	0.00	-	-		
87	OHX	6	2100	-	0,6,6	0.00	-	-		
87	OHX	6	2076	-	0,6,6	0.00	-	-		
87	OHX	4	224	-	0,6,6	0.00	-	-		
87	OHX	1	4069	-	0,6,6	0.00	-	-		
87	OHX	M9	202	-	0,6,6	0.00	-	-		
87	OHX	5	4095	-	0,6,6	0.00	-	-		
87	OHX	5	4012	-	0,6,6	0.00	-	-		
87	OHX	1	3911	-	0,6,6	0.00	-	-		
87	OHX	1	3870	-	0,6,6	0.00	-	-		
87	OHX	5	3927	-	0,6,6	0.00	-	-		
87	OHX	2	2047	-	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	4004	-	0,6,6	0.00	-	-		
87	OHX	2	2133	-	0,6,6	0.00	-	-		
87	OHX	1	4124	-	0,6,6	0.00	-	-		
87	OHX	2	2062	-	0,6,6	0.00	-	-		
87	OHX	1	3973	-	0,6,6	0.00	-	-		
87	OHX	o2	201	-	0,6,6	0.00	-	-		
87	OHX	5	4073	-	0,6,6	0.00	-	-		
87	OHX	3	223	-	0,6,6	0.00	-	-		
87	OHX	5	4201	-	0,6,6	0.00	-	-		
87	OHX	5	3909	-	0,6,6	0.00	-	-		
87	OHX	6	2095	-	0,6,6	0.00	-	-		
87	OHX	7	224	-	0,6,6	0.00	-	-		
87	OHX	5	4091	-	0,6,6	0.00	-	-		
87	OHX	1	4199	-	0,6,6	0.00	-	-		
87	OHX	1	3916	-	0,6,6	0.00	-	-		
87	OHX	2	2066	-	0,6,6	0.00	-	-		
87	OHX	5	4175	-	0,6,6	0.00	-	-		
87	OHX	5	4053	-	0,6,6	0.00	-	-		
87	OHX	5	4207	-	0,6,6	0.00	-	-		
87	OHX	1	3900	-	0,6,6	0.00	-	-		
87	OHX	2	2118	-	0,6,6	0.00	-	-		
87	OHX	1	4014	-	0,6,6	0.00	-	-		
87	OHX	1	4050	-	0,6,6	0.00	-	-		
87	OHX	5	3946	-	0,6,6	0.00	-	-		
87	OHX	5	3918	-	0,6,6	0.00	-	-		
87	OHX	5	3947	-	0,6,6	0.00	-	-		
87	OHX	2	2106	-	0,6,6	0.00	-	-		
87	OHX	1	3934	-	0,6,6	0.00	-	-		
87	OHX	5	3902	-	0,6,6	0.00	-	-		
87	OHX	5	4001	-	0,6,6	0.00	-	-		
87	OHX	2	2098	-	0,6,6	0.00	-	-		
87	OHX	1	4181	-	0,6,6	0.00	-	-		
87	OHX	2	2137	-	0,6,6	0.00	-	-		
87	OHX	7	225	-	0,6,6	0.00	-	-		
87	OHX	2	2163	-	0,6,6	0.00	-	-		
87	OHX	5	4211	-	0,6,6	0.00	-	-		
87	OHX	5	4111	-	0,6,6	0.00	-	-		
87	OHX	1	4149	-	0,6,6	0.00	-	-		
87	OHX	1	4110	-	0,6,6	0.00	-	-		
87	OHX	1	3925	-	0,6,6	0.00	-	-		
87	OHX	l3	402	-	0,6,6	0.00	-	-		
87	OHX	6	2162	-	0,6,6	0.00	-	-		
87	OHX	6	2176	-	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	2151	-	0,6,6	0.00	-	-		
87	OHX	2	2048	-	0,6,6	0.00	-	-		
87	OHX	5	3930	-	0,6,6	0.00	-	-		
87	OHX	1	4091	-	0,6,6	0.00	-	-		
87	OHX	1	4140	-	0,6,6	0.00	-	-		
87	OHX	5	3906	-	0,6,6	0.00	-	-		
87	OHX	5	3908	-	0,6,6	0.00	-	-		
87	OHX	6	2078	-	0,6,6	0.00	-	-		
87	OHX	1	3927	-	0,6,6	0.00	-	-		
87	OHX	1	4054	-	0,6,6	0.00	-	-		
87	OHX	5	4003	-	0,6,6	0.00	-	-		
87	OHX	1	4080	-	0,6,6	0.00	-	-		
87	OHX	2	2088	-	0,6,6	0.00	-	-		
87	OHX	5	3998	-	0,6,6	0.00	-	-		
87	OHX	1	4129	-	0,6,6	0.00	-	-		
87	OHX	1	3960	-	0,6,6	0.00	-	-		
87	OHX	6	2048	-	0,6,6	0.00	-	-		
87	OHX	1	4120	-	0,6,6	0.00	-	-		
87	OHX	6	2094	-	0,6,6	0.00	-	-		
87	OHX	O3	202	-	0,6,6	0.00	-	-		
87	OHX	6	2164	-	0,6,6	0.00	-	-		
87	OHX	1	4180	-	0,6,6	0.00	-	-		
87	OHX	2	2164	-	0,6,6	0.00	-	-		
87	OHX	5	4212	-	0,6,6	0.00	-	-		
87	OHX	1	3961	-	0,6,6	0.00	-	-		
87	OHX	1	4196	-	0,6,6	0.00	-	-		
87	OHX	5	4085	-	0,6,6	0.00	-	-		
87	OHX	1	3989	-	0,6,6	0.00	-	-		
87	OHX	M7	208	-	0,6,6	0.00	-	-		
87	OHX	2	2175	-	0,6,6	0.00	-	-		
87	OHX	2	2039	-	0,6,6	0.00	-	-		
87	OHX	1	4142	-	0,6,6	0.00	-	-		
87	OHX	1	3865	-	0,6,6	0.00	-	-		
87	OHX	5	4107	-	0,6,6	0.00	-	-		
87	OHX	5	3917	-	0,6,6	0.00	-	-		
87	OHX	1	3910	-	0,6,6	0.00	-	-		
87	OHX	5	4059	-	0,6,6	0.00	-	-		
87	OHX	2	2132	-	0,6,6	0.00	-	-		
87	OHX	2	2035	-	0,6,6	0.00	-	-		
87	OHX	5	3956	-	0,6,6	0.00	-	-		
87	OHX	2	2141	-	0,6,6	0.00	-	-		
87	OHX	1	3883	-	0,6,6	0.00	-	-		
87	OHX	5	4071	-	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	3879	-	0,6,6	0.00	-	-		
87	OHX	6	2133	-	0,6,6	0.00	-	-		
89	3HE	5	4252	-	21,21,21	0.88	1 (4%)	19,30,30	0.76	0
87	OHX	1	4210	-	0,6,6	0.00	-	-		
87	OHX	o7	103	-	0,6,6	0.00	-	-		
87	OHX	3	222	-	0,6,6	0.00	-	-		
87	OHX	5	4221	-	0,6,6	0.00	-	-		
87	OHX	2	2140	-	0,6,6	0.00	-	-		
87	OHX	2	2052	-	0,6,6	0.00	-	-		
87	OHX	3	215	-	0,6,6	0.00	-	-		
87	OHX	6	2203	-	0,6,6	0.00	-	-		
87	OHX	2	2024	-	0,6,6	0.00	-	-		
87	OHX	1	4026	-	0,6,6	0.00	-	-		
87	OHX	1	3962	-	0,6,6	0.00	-	-		
87	OHX	8	222	-	0,6,6	0.00	-	-		
87	OHX	6	2079	-	0,6,6	0.00	-	-		
87	OHX	6	2098	-	0,6,6	0.00	-	-		
87	OHX	7	217	-	0,6,6	0.00	-	-		
87	OHX	5	4127	-	0,6,6	0.00	-	-		
87	OHX	5	4251	-	0,6,6	0.00	-	-		
87	OHX	6	2189	-	0,6,6	0.00	-	-		
87	OHX	L3	404	-	0,6,6	0.00	-	-		
87	OHX	6	2183	-	0,6,6	0.00	-	-		
87	OHX	5	4238	-	0,6,6	0.00	-	-		
87	OHX	2	2148	-	0,6,6	0.00	-	-		
87	OHX	6	2083	-	0,6,6	0.00	-	-		
87	OHX	6	2126	-	0,6,6	0.00	-	-		
87	OHX	5	4006	-	0,6,6	0.00	-	-		
87	OHX	1	3943	-	0,6,6	0.00	-	-		
87	OHX	5	4224	-	0,6,6	0.00	-	-		
87	OHX	1	3946	-	0,6,6	0.00	-	-		
87	OHX	6	2160	-	0,6,6	0.00	-	-		
87	OHX	1	3958	-	0,6,6	0.00	-	-		
87	OHX	6	2147	-	0,6,6	0.00	-	-		
87	OHX	5	4151	-	0,6,6	0.00	-	-		
87	OHX	5	4185	-	0,6,6	0.00	-	-		
87	OHX	S8	302	-	0,6,6	0.00	-	-		
87	OHX	5	3982	-	0,6,6	0.00	-	-		
87	OHX	1	3901	-	0,6,6	0.00	-	-		
87	OHX	5	4066	-	0,6,6	0.00	-	-		
87	OHX	1	3866	-	0,6,6	0.00	-	-		
87	OHX	1	3913	-	0,6,6	0.00	-	-		
87	OHX	5	4114	-	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	2036	-	0,6,6	0.00	-	-		
87	OHX	M5	303	-	0,6,6	0.00	-	-		
87	OHX	6	2122	-	0,6,6	0.00	-	-		
87	OHX	5	4183	-	0,6,6	0.00	-	-		
87	OHX	5	4046	-	0,6,6	0.00	-	-		
87	OHX	5	4161	-	0,6,6	0.00	-	-		
87	OHX	1	3956	-	0,6,6	0.00	-	-		
87	OHX	1	3935	-	0,6,6	0.00	-	-		
87	OHX	2	2120	-	0,6,6	0.00	-	-		
87	OHX	2	2051	-	0,6,6	0.00	-	-		
87	OHX	6	2193	-	0,6,6	0.00	-	-		
87	OHX	1	3894	-	0,6,6	0.00	-	-		
87	OHX	2	2092	-	0,6,6	0.00	-	-		
87	OHX	5	4158	-	0,6,6	0.00	-	-		
87	OHX	1	4108	-	0,6,6	0.00	-	-		
87	OHX	2	2058	-	0,6,6	0.00	-	-		
87	OHX	5	4106	-	0,6,6	0.00	-	-		
87	OHX	1	3881	-	0,6,6	0.00	-	-		
87	OHX	6	2202	-	0,6,6	0.00	-	-		
87	OHX	15	305	-	0,6,6	0.00	-	-		
87	OHX	5	4113	-	0,6,6	0.00	-	-		
87	OHX	1	3937	-	0,6,6	0.00	-	-		
87	OHX	6	2150	-	0,6,6	0.00	-	-		
87	OHX	5	4243	-	0,6,6	0.00	-	-		
87	OHX	1	3920	-	0,6,6	0.00	-	-		
87	OHX	1	3907	-	0,6,6	0.00	-	-		
87	OHX	1	4051	-	0,6,6	0.00	-	-		
87	OHX	6	2186	-	0,6,6	0.00	-	-		
87	OHX	5	4192	-	0,6,6	0.00	-	-		
87	OHX	1	3918	-	0,6,6	0.00	-	-		
87	OHX	1	3917	-	0,6,6	0.00	-	-		
87	OHX	6	2067	-	0,6,6	0.00	-	-		
87	OHX	1	4045	-	0,6,6	0.00	-	-		
87	OHX	5	4208	-	0,6,6	0.00	-	-		
87	OHX	2	2135	-	0,6,6	0.00	-	-		
87	OHX	2	2157	-	0,6,6	0.00	-	-		
87	OHX	1	4029	-	0,6,6	0.00	-	-		
87	OHX	1	4113	-	0,6,6	0.00	-	-		
87	OHX	5	4194	-	0,6,6	0.00	-	-		
87	OHX	5	3987	-	0,6,6	0.00	-	-		
87	OHX	2	2160	-	0,6,6	0.00	-	-		
87	OHX	5	4167	-	0,6,6	0.00	-	-		
87	OHX	5	3925	-	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	2143	-	0,6,6	0.00	-	-		
87	OHX	6	2111	-	0,6,6	0.00	-	-		
87	OHX	5	4209	-	0,6,6	0.00	-	-		
87	OHX	2	2128	-	0,6,6	0.00	-	-		
87	OHX	5	4096	-	0,6,6	0.00	-	-		
87	OHX	1	3889	-	0,6,6	0.00	-	-		
87	OHX	7	226	-	0,6,6	0.00	-	-		
87	OHX	5	4097	-	0,6,6	0.00	-	-		
87	OHX	5	3981	-	0,6,6	0.00	-	-		
87	OHX	2	2083	-	0,6,6	0.00	-	-		
87	OHX	2	2074	-	0,6,6	0.00	-	-		
87	OHX	8	224	-	0,6,6	0.00	-	-		
87	OHX	1	3970	-	0,6,6	0.00	-	-		
87	OHX	6	2177	-	0,6,6	0.00	-	-		
87	OHX	1	3929	-	0,6,6	0.00	-	-		
87	OHX	5	4030	-	0,6,6	0.00	-	-		
87	OHX	5	4082	-	0,6,6	0.00	-	-		
87	OHX	6	2106	-	0,6,6	0.00	-	-		
87	OHX	5	3965	-	0,6,6	0.00	-	-		
87	OHX	2	2061	-	0,6,6	0.00	-	-		
87	OHX	6	2101	-	0,6,6	0.00	-	-		
87	OHX	2	2111	-	0,6,6	0.00	-	-		
87	OHX	6	2118	-	0,6,6	0.00	-	-		
87	OHX	5	4040	-	0,6,6	0.00	-	-		
87	OHX	3	216	-	0,6,6	0.00	-	-		
87	OHX	5	4033	-	0,6,6	0.00	-	-		
87	OHX	D9	102	-	0,6,6	0.00	-	-		
87	OHX	1	4030	-	0,6,6	0.00	-	-		
87	OHX	6	2145	-	0,6,6	0.00	-	-		
87	OHX	1	4003	-	0,6,6	0.00	-	-		
87	OHX	2	2060	-	0,6,6	0.00	-	-		
87	OHX	5	3971	-	0,6,6	0.00	-	-		
87	OHX	5	4131	-	0,6,6	0.00	-	-		
87	OHX	2	2086	-	0,6,6	0.00	-	-		
87	OHX	s8	302	-	0,6,6	0.00	-	-		
87	OHX	4	228	-	0,6,6	0.00	-	-		
87	OHX	5	4223	-	0,6,6	0.00	-	-		
87	OHX	5	4178	-	0,6,6	0.00	-	-		
87	OHX	1	4067	-	0,6,6	0.00	-	-		
87	OHX	2	2176	-	0,6,6	0.00	-	-		
87	OHX	5	4141	-	0,6,6	0.00	-	-		
87	OHX	5	4215	-	0,6,6	0.00	-	-		
87	OHX	1	4212	-	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	4098	-	0,6,6	0.00	-	-		
87	OHX	5	4039	-	0,6,6	0.00	-	-		
87	OHX	4	234	-	0,6,6	0.00	-	-		
87	OHX	1	3895	-	0,6,6	0.00	-	-		
87	OHX	2	2079	-	0,6,6	0.00	-	-		
87	OHX	6	2077	-	0,6,6	0.00	-	-		
87	OHX	6	2096	-	0,6,6	0.00	-	-		
87	OHX	6	2181	-	0,6,6	0.00	-	-		
87	OHX	5	4051	-	0,6,6	0.00	-	-		
87	OHX	C8	201	-	0,6,6	0.00	-	-		
87	OHX	5	4013	-	0,6,6	0.00	-	-		
87	OHX	1	4096	-	0,6,6	0.00	-	-		
87	OHX	5	4170	-	0,6,6	0.00	-	-		
87	OHX	1	4016	-	0,6,6	0.00	-	-		
87	OHX	1	3926	-	0,6,6	0.00	-	-		
87	OHX	5	4024	-	0,6,6	0.00	-	-		
87	OHX	1	3882	-	0,6,6	0.00	-	-		
87	OHX	5	4002	-	0,6,6	0.00	-	-		
87	OHX	7	223	-	0,6,6	0.00	-	-		
87	OHX	7	222	-	0,6,6	0.00	-	-		
87	OHX	5	3926	-	0,6,6	0.00	-	-		
87	OHX	1	4136	-	0,6,6	0.00	-	-		
87	OHX	5	3962	-	0,6,6	0.00	-	-		
87	OHX	5	3924	-	0,6,6	0.00	-	-		
87	OHX	5	4249	-	0,6,6	0.00	-	-		
87	OHX	6	2081	-	0,6,6	0.00	-	-		
87	OHX	5	4204	-	0,6,6	0.00	-	-		
87	OHX	5	4196	-	0,6,6	0.00	-	-		
87	OHX	1	3968	-	0,6,6	0.00	-	-		
87	OHX	c5	201	-	0,6,6	0.00	-	-		
87	OHX	2	2168	-	0,6,6	0.00	-	-		
87	OHX	1	3965	-	0,6,6	0.00	-	-		
87	OHX	5	3985	-	0,6,6	0.00	-	-		
87	OHX	5	4047	-	0,6,6	0.00	-	-		
87	OHX	5	4104	-	0,6,6	0.00	-	-		
87	OHX	5	4020	-	0,6,6	0.00	-	-		
87	OHX	5	4218	-	0,6,6	0.00	-	-		
87	OHX	2	2063	-	0,6,6	0.00	-	-		
87	OHX	2	2166	-	0,6,6	0.00	-	-		
87	OHX	1	4111	-	0,6,6	0.00	-	-		
87	OHX	2	2034	-	0,6,6	0.00	-	-		
87	OHX	2	2076	-	0,6,6	0.00	-	-		
87	OHX	5	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	2	2110	-	0,6,6	0.00	-	-		
87	OHX	4	223	-	0,6,6	0.00	-	-		
87	OHX	1	4211	-	0,6,6	0.00	-	-		
87	OHX	2	2040	-	0,6,6	0.00	-	-		
87	OHX	1	3947	-	0,6,6	0.00	-	-		
87	OHX	2	2045	-	0,6,6	0.00	-	-		
87	OHX	6	2117	-	0,6,6	0.00	-	-		
87	OHX	1	4104	-	0,6,6	0.00	-	-		
87	OHX	2	2032	-	0,6,6	0.00	-	-		
87	OHX	5	3911	-	0,6,6	0.00	-	-		
87	OHX	2	2165	-	0,6,6	0.00	-	-		
87	OHX	6	2157	-	0,6,6	0.00	-	-		
87	OHX	5	4079	-	0,6,6	0.00	-	-		
87	OHX	1	4095	-	0,6,6	0.00	-	-		
87	OHX	1	3987	-	0,6,6	0.00	-	-		
87	OHX	1	3940	-	0,6,6	0.00	-	-		
87	OHX	5	3949	-	0,6,6	0.00	-	-		
87	OHX	1	3991	-	0,6,6	0.00	-	-		
87	OHX	5	4021	-	0,6,6	0.00	-	-		
87	OHX	5	3978	-	0,6,6	0.00	-	-		
87	OHX	5	4005	-	0,6,6	0.00	-	-		
87	OHX	1	4109	-	0,6,6	0.00	-	-		
87	OHX	2	2096	-	0,6,6	0.00	-	-		
87	OHX	1	3873	-	0,6,6	0.00	-	-		
87	OHX	1	3980	-	0,6,6	0.00	-	-		
87	OHX	2	2055	-	0,6,6	0.00	-	-		
87	OHX	6	2196	-	0,6,6	0.00	-	-		
87	OHX	1	3975	-	0,6,6	0.00	-	-		
87	OHX	1	4135	-	0,6,6	0.00	-	-		
87	OHX	5	3915	-	0,6,6	0.00	-	-		
87	OHX	2	2144	-	0,6,6	0.00	-	-		
87	OHX	1	4092	-	0,6,6	0.00	-	-		
87	OHX	6	2205	-	0,6,6	0.00	-	-		
87	OHX	5	3983	-	0,6,6	0.00	-	-		
87	OHX	1	3874	-	0,6,6	0.00	-	-		
87	OHX	6	2114	-	0,6,6	0.00	-	-		
87	OHX	1	4062	-	0,6,6	0.00	-	-		
87	OHX	2	2053	-	0,6,6	0.00	-	-		
87	OHX	5	3961	-	0,6,6	0.00	-	-		
87	OHX	1	4084	-	0,6,6	0.00	-	-		
87	OHX	1	3897	-	0,6,6	0.00	-	-		
87	OHX	1	3977	-	0,6,6	0.00	-	-		
87	OHX	5	4216	-	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	4002	-	0,6,6	0.00	-	-		
87	OHX	5	3919	-	0,6,6	0.00	-	-		
87	OHX	2	2147	-	0,6,6	0.00	-	-		
87	OHX	5	3939	-	0,6,6	0.00	-	-		
87	OHX	5	4099	-	0,6,6	0.00	-	-		
87	OHX	1	4154	-	0,6,6	0.00	-	-		
87	OHX	5	4135	-	0,6,6	0.00	-	-		
87	OHX	5	4129	-	0,6,6	0.00	-	-		
87	OHX	5	4110	-	0,6,6	0.00	-	-		
87	OHX	2	2101	-	0,6,6	0.00	-	-		
87	OHX	1	3995	-	0,6,6	0.00	-	-		
87	OHX	1	4134	-	0,6,6	0.00	-	-		
87	OHX	1	3880	-	0,6,6	0.00	-	-		
87	OHX	2	2129	-	0,6,6	0.00	-	-		
87	OHX	6	2191	-	0,6,6	0.00	-	-		
87	OHX	13	403	-	0,6,6	0.00	-	-		
87	OHX	2	2068	-	0,6,6	0.00	-	-		
87	OHX	6	2115	-	0,6,6	0.00	-	-		
87	OHX	5	4149	-	0,6,6	0.00	-	-		
87	OHX	6	2054	-	0,6,6	0.00	-	-		
87	OHX	1	4182	-	0,6,6	0.00	-	-		
87	OHX	5	4068	-	0,6,6	0.00	-	-		
87	OHX	1	3966	-	0,6,6	0.00	-	-		
87	OHX	2	2085	-	0,6,6	0.00	-	-		
87	OHX	1	4036	-	0,6,6	0.00	-	-		
87	OHX	6	2167	-	0,6,6	0.00	-	-		
87	OHX	1	4185	-	0,6,6	0.00	-	-		
87	OHX	1	4018	-	0,6,6	0.00	-	-		
87	OHX	13	404	-	0,6,6	0.00	-	-		
87	OHX	5	4232	-	0,6,6	0.00	-	-		
87	OHX	5	3999	-	0,6,6	0.00	-	-		
87	OHX	1	4025	-	0,6,6	0.00	-	-		
87	OHX	2	2114	-	0,6,6	0.00	-	-		
87	OHX	2	2119	-	0,6,6	0.00	-	-		
87	OHX	6	2104	-	0,6,6	0.00	-	-		
87	OHX	6	2200	-	0,6,6	0.00	-	-		
87	OHX	1	3869	-	0,6,6	0.00	-	-		
87	OHX	1	3887	-	0,6,6	0.00	-	-		
87	OHX	2	2153	-	0,6,6	0.00	-	-		
87	OHX	2	2131	-	0,6,6	0.00	-	-		
87	OHX	1	3875	-	0,6,6	0.00	-	-		
87	OHX	5	3901	-	0,6,6	0.00	-	-		
87	OHX	5	4118	-	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	3928	-	0,6,6	0.00	-	-		
87	OHX	6	2140	-	0,6,6	0.00	-	-		
87	OHX	5	3923	-	0,6,6	0.00	-	-		
87	OHX	5	4121	-	0,6,6	0.00	-	-		
87	OHX	1	3898	-	0,6,6	0.00	-	-		
87	OHX	1	3972	-	0,6,6	0.00	-	-		
87	OHX	1	4156	-	0,6,6	0.00	-	-		
87	OHX	3	219	-	0,6,6	0.00	-	-		
87	OHX	6	2066	-	0,6,6	0.00	-	-		
87	OHX	1	3986	-	0,6,6	0.00	-	-		
87	OHX	5	4108	-	0,6,6	0.00	-	-		
87	OHX	1	3950	-	0,6,6	0.00	-	-		
87	OHX	2	2138	-	0,6,6	0.00	-	-		
87	OHX	6	2069	-	0,6,6	0.00	-	-		
87	OHX	1	3990	-	0,6,6	0.00	-	-		
87	OHX	5	4228	-	0,6,6	0.00	-	-		
87	OHX	1	4012	-	0,6,6	0.00	-	-		
87	OHX	4	235	-	0,6,6	0.00	-	-		
87	OHX	5	4250	-	0,6,6	0.00	-	-		
87	OHX	2	2107	-	0,6,6	0.00	-	-		
87	OHX	5	3993	-	0,6,6	0.00	-	-		
87	OHX	2	2075	-	0,6,6	0.00	-	-		
87	OHX	5	3969	-	0,6,6	0.00	-	-		
87	OHX	1	3957	-	0,6,6	0.00	-	-		
87	OHX	5	4056	-	0,6,6	0.00	-	-		
87	OHX	5	4011	-	0,6,6	0.00	-	-		
87	OHX	2	2134	-	0,6,6	0.00	-	-		
87	OHX	1	4114	-	0,6,6	0.00	-	-		
87	OHX	2	2069	-	0,6,6	0.00	-	-		
87	OHX	1	4100	-	0,6,6	0.00	-	-		
87	OHX	6	2052	-	0,6,6	0.00	-	-		
87	OHX	5	3967	-	0,6,6	0.00	-	-		
87	OHX	6	2060	-	0,6,6	0.00	-	-		
87	OHX	1	4031	-	0,6,6	0.00	-	-		
87	OHX	1	4203	-	0,6,6	0.00	-	-		
87	OHX	2	2067	-	0,6,6	0.00	-	-		
87	OHX	1	4184	-	0,6,6	0.00	-	-		
87	OHX	4	236	-	0,6,6	0.00	-	-		
87	OHX	5	4048	-	0,6,6	0.00	-	-		
87	OHX	1	4139	-	0,6,6	0.00	-	-		
87	OHX	2	2171	-	0,6,6	0.00	-	-		
87	OHX	2	2124	-	0,6,6	0.00	-	-		
87	OHX	1	4038	-	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	2075	-	0,6,6	0.00	-	-		
87	OHX	5	4036	-	0,6,6	0.00	-	-		
87	OHX	5	4080	-	0,6,6	0.00	-	-		
87	OHX	1	3903	-	0,6,6	0.00	-	-		
87	OHX	m6	202	-	0,6,6	0.00	-	-		
87	OHX	1	4116	-	0,6,6	0.00	-	-		
87	OHX	m4	201	-	0,6,6	0.00	-	-		
87	OHX	6	2197	-	0,6,6	0.00	-	-		
87	OHX	5	4247	-	0,6,6	0.00	-	-		
87	OHX	1	4064	-	0,6,6	0.00	-	-		
87	OHX	2	2078	-	0,6,6	0.00	-	-		
87	OHX	1	4085	-	0,6,6	0.00	-	-		
87	OHX	5	4166	-	0,6,6	0.00	-	-		
87	OHX	1	4061	-	0,6,6	0.00	-	-		
87	OHX	2	2093	-	0,6,6	0.00	-	-		
87	OHX	5	3977	-	0,6,6	0.00	-	-		
87	OHX	1	4097	-	0,6,6	0.00	-	-		
87	OHX	2	2127	-	0,6,6	0.00	-	-		
87	OHX	2	2089	-	0,6,6	0.00	-	-		
87	OHX	n3	203	-	0,6,6	0.00	-	-		
87	OHX	6	2156	-	0,6,6	0.00	-	-		
87	OHX	1	4146	-	0,6,6	0.00	-	-		
87	OHX	1	4189	-	0,6,6	0.00	-	-		
87	OHX	1	4023	-	0,6,6	0.00	-	-		
87	OHX	2	2177	-	0,6,6	0.00	-	-		
87	OHX	1	4086	-	0,6,6	0.00	-	-		
87	OHX	5	4126	-	0,6,6	0.00	-	-		
87	OHX	1	4193	-	0,6,6	0.00	-	-		
87	OHX	5	4134	-	0,6,6	0.00	-	-		
87	OHX	5	4231	-	0,6,6	0.00	-	-		
87	OHX	1	4127	-	0,6,6	0.00	-	-		
87	OHX	m8	201	-	0,6,6	0.00	-	-		
87	OHX	5	4245	-	0,6,6	0.00	-	-		
87	OHX	1	4040	-	0,6,6	0.00	-	-		
87	OHX	6	2064	-	0,6,6	0.00	-	-		
87	OHX	1	3899	-	0,6,6	0.00	-	-		
87	OHX	6	2063	-	0,6,6	0.00	-	-		
87	OHX	6	2053	-	0,6,6	0.00	-	-		
87	OHX	sR	401	-	0,6,6	0.00	-	-		
87	OHX	5	4028	-	0,6,6	0.00	-	-		
87	OHX	5	4136	-	0,6,6	0.00	-	-		
87	OHX	m5	303	-	0,6,6	0.00	-	-		
87	OHX	1	3974	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	8	219	-	0,6,6	0.00	-	-		
87	OHX	1	4001	-	0,6,6	0.00	-	-		
87	OHX	2	2170	-	0,6,6	0.00	-	-		
87	OHX	6	2158	-	0,6,6	0.00	-	-		
87	OHX	5	3935	-	0,6,6	0.00	-	-		
87	OHX	1	4179	-	0,6,6	0.00	-	-		
87	OHX	5	4217	-	0,6,6	0.00	-	-		
87	OHX	6	2059	-	0,6,6	0.00	-	-		
87	OHX	6	2159	-	0,6,6	0.00	-	-		
87	OHX	2	2155	-	0,6,6	0.00	-	-		
87	OHX	1	4171	-	0,6,6	0.00	-	-		
87	OHX	2	2122	-	0,6,6	0.00	-	-		
87	OHX	5	4065	-	0,6,6	0.00	-	-		
87	OHX	1	4093	-	0,6,6	0.00	-	-		
87	OHX	1	4033	-	0,6,6	0.00	-	-		
87	OHX	6	2086	-	0,6,6	0.00	-	-		
87	OHX	5	4044	-	0,6,6	0.00	-	-		
87	OHX	5	4225	-	0,6,6	0.00	-	-		
87	OHX	1	4072	-	0,6,6	0.00	-	-		
87	OHX	5	4090	-	0,6,6	0.00	-	-		
87	OHX	1	3997	-	0,6,6	0.00	-	-		
87	OHX	5	4190	-	0,6,6	0.00	-	-		
87	OHX	6	2182	-	0,6,6	0.00	-	-		
87	OHX	5	4088	-	0,6,6	0.00	-	-		
87	OHX	1	3871	-	0,6,6	0.00	-	-		
87	OHX	1	4046	-	0,6,6	0.00	-	-		
87	OHX	5	4122	-	0,6,6	0.00	-	-		
87	OHX	1	4163	-	0,6,6	0.00	-	-		
87	OHX	6	2199	-	0,6,6	0.00	-	-		
87	OHX	5	3912	-	0,6,6	0.00	-	-		
87	OHX	6	2190	-	0,6,6	0.00	-	-		
87	OHX	1	3868	-	0,6,6	0.00	-	-		
87	OHX	5	3931	-	0,6,6	0.00	-	-		
87	OHX	6	2168	-	0,6,6	0.00	-	-		
87	OHX	5	4165	-	0,6,6	0.00	-	-		
87	OHX	1	4137	-	0,6,6	0.00	-	-		
87	OHX	5	3913	-	0,6,6	0.00	-	-		
87	OHX	5	4239	-	0,6,6	0.00	-	-		
87	OHX	6	2152	-	0,6,6	0.00	-	-		
87	OHX	5	4084	-	0,6,6	0.00	-	-		
87	OHX	5	3980	-	0,6,6	0.00	-	-		
87	OHX	5	4128	-	0,6,6	0.00	-	-		
87	OHX	1	4183	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	d9	102	-	0,6,6	0.00	-	-		
87	OHX	6	2180	-	0,6,6	0.00	-	-		
87	OHX	L3	405	-	0,6,6	0.00	-	-		
87	OHX	5	4035	-	0,6,6	0.00	-	-		
87	OHX	1	4074	-	0,6,6	0.00	-	-		
87	OHX	6	2144	-	0,6,6	0.00	-	-		
87	OHX	5	4180	-	0,6,6	0.00	-	-		
87	OHX	5	3944	-	0,6,6	0.00	-	-		
87	OHX	5	4153	-	0,6,6	0.00	-	-		
87	OHX	C3	202	-	0,6,6	0.00	-	-		
87	OHX	5	4145	-	0,6,6	0.00	-	-		
87	OHX	5	4063	-	0,6,6	0.00	-	-		
87	OHX	6	2201	-	0,6,6	0.00	-	-		
87	OHX	c8	203	-	0,6,6	0.00	-	-		
87	OHX	1	4103	-	0,6,6	0.00	-	-		
87	OHX	3	217	-	0,6,6	0.00	-	-		
87	OHX	5	4174	-	0,6,6	0.00	-	-		
87	OHX	1	3981	-	0,6,6	0.00	-	-		
87	OHX	5	4045	-	0,6,6	0.00	-	-		
87	OHX	5	4240	-	0,6,6	0.00	-	-		
87	OHX	8	217	-	0,6,6	0.00	-	-		
87	OHX	6	2102	-	0,6,6	0.00	-	-		
87	OHX	2	2172	-	0,6,6	0.00	-	-		
87	OHX	6	2195	-	0,6,6	0.00	-	-		
87	OHX	1	4070	-	0,6,6	0.00	-	-		
87	OHX	5	3940	-	0,6,6	0.00	-	-		
87	OHX	1	3963	-	0,6,6	0.00	-	-		
87	OHX	5	4029	-	0,6,6	0.00	-	-		
87	OHX	2	2030	-	0,6,6	0.00	-	-		
87	OHX	6	2091	-	0,6,6	0.00	-	-		
87	OHX	5	4200	-	0,6,6	0.00	-	-		
87	OHX	6	2057	-	0,6,6	0.00	-	-		
87	OHX	1	4063	-	0,6,6	0.00	-	-		
87	OHX	6	2188	-	0,6,6	0.00	-	-		
87	OHX	5	3996	-	0,6,6	0.00	-	-		
87	OHX	2	2042	-	0,6,6	0.00	-	-		
87	OHX	6	2103	-	0,6,6	0.00	-	-		
87	OHX	5	4034	-	0,6,6	0.00	-	-		
87	OHX	1	4099	-	0,6,6	0.00	-	-		
87	OHX	L3	406	-	0,6,6	0.00	-	-		
87	OHX	1	3955	-	0,6,6	0.00	-	-		
87	OHX	4	231	-	0,6,6	0.00	-	-		
87	OHX	1	3906	-	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	2022	-	0,6,6	0.00	-	-		
87	OHX	5	4100	-	0,6,6	0.00	-	-		
87	OHX	5	4154	-	0,6,6	0.00	-	-		
87	OHX	2	2094	-	0,6,6	0.00	-	-		
87	OHX	6	2125	-	0,6,6	0.00	-	-		
87	OHX	6	2161	-	0,6,6	0.00	-	-		
87	OHX	1	3877	-	0,6,6	0.00	-	-		
87	OHX	2	2154	-	0,6,6	0.00	-	-		
87	OHX	1	3999	-	0,6,6	0.00	-	-		
87	OHX	c3	201	-	0,6,6	0.00	-	-		
87	OHX	1	4027	-	0,6,6	0.00	-	-		
87	OHX	1	4132	-	0,6,6	0.00	-	-		
87	OHX	1	4133	-	0,6,6	0.00	-	-		
87	OHX	2	2070	-	0,6,6	0.00	-	-		
87	OHX	1	4034	-	0,6,6	0.00	-	-		
87	OHX	5	3937	-	0,6,6	0.00	-	-		
87	OHX	2	2150	-	0,6,6	0.00	-	-		
87	OHX	5	4008	-	0,6,6	0.00	-	-		
87	OHX	1	4177	-	0,6,6	0.00	-	-		
87	OHX	5	4087	-	0,6,6	0.00	-	-		
87	OHX	5	4025	-	0,6,6	0.00	-	-		
87	OHX	2	2167	-	0,6,6	0.00	-	-		
87	OHX	2	2050	-	0,6,6	0.00	-	-		
87	OHX	5	3953	-	0,6,6	0.00	-	-		
87	OHX	5	4092	-	0,6,6	0.00	-	-		
87	OHX	2	2143	-	0,6,6	0.00	-	-		
87	OHX	5	3948	-	0,6,6	0.00	-	-		
87	OHX	5	4062	-	0,6,6	0.00	-	-		
87	OHX	5	3964	-	0,6,6	0.00	-	-		
87	OHX	2	2162	-	0,6,6	0.00	-	-		
87	OHX	5	4125	-	0,6,6	0.00	-	-		
87	OHX	2	2095	-	0,6,6	0.00	-	-		
87	OHX	6	2049	-	0,6,6	0.00	-	-		
87	OHX	4	227	-	0,6,6	0.00	-	-		
87	OHX	2	2090	-	0,6,6	0.00	-	-		
87	OHX	1	3983	-	0,6,6	0.00	-	-		
87	OHX	5	4007	-	0,6,6	0.00	-	-		
87	OHX	6	2185	-	0,6,6	0.00	-	-		
87	OHX	5	4155	-	0,6,6	0.00	-	-		
87	OHX	6	2171	-	0,6,6	0.00	-	-		
87	OHX	5	3920	-	0,6,6	0.00	-	-		
87	OHX	1	4167	-	0,6,6	0.00	-	-		
87	OHX	5	3995	-	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	2146	-	0,6,6	0.00	-	-		
87	OHX	1	3892	-	0,6,6	0.00	-	-		
87	OHX	1	4209	-	0,6,6	0.00	-	-		
87	OHX	5	4057	-	0,6,6	0.00	-	-		
87	OHX	2	2091	-	0,6,6	0.00	-	-		
87	OHX	1	4065	-	0,6,6	0.00	-	-		
87	OHX	5	3989	-	0,6,6	0.00	-	-		
87	OHX	5	4187	-	0,6,6	0.00	-	-		
87	OHX	5	4163	-	0,6,6	0.00	-	-		
87	OHX	1	3936	-	0,6,6	0.00	-	-		
87	OHX	1	4101	-	0,6,6	0.00	-	-		
87	OHX	2	2097	-	0,6,6	0.00	-	-		
87	OHX	1	4019	-	0,6,6	0.00	-	-		
87	OHX	1	3886	-	0,6,6	0.00	-	-		
87	OHX	1	4175	-	0,6,6	0.00	-	-		
87	OHX	4	225	-	0,6,6	0.00	-	-		
87	OHX	1	4048	-	0,6,6	0.00	-	-		
87	OHX	2	2178	-	0,6,6	0.00	-	-		
87	OHX	1	4088	-	0,6,6	0.00	-	-		
87	OHX	5	4004	-	0,6,6	0.00	-	-		
87	OHX	5	4077	-	0,6,6	0.00	-	-		
87	OHX	8	227	-	0,6,6	0.00	-	-		
87	OHX	1	4107	-	0,6,6	0.00	-	-		
87	OHX	1	4066	-	0,6,6	0.00	-	-		
87	OHX	1	3872	-	0,6,6	0.00	-	-		
87	OHX	1	3933	-	0,6,6	0.00	-	-		
87	OHX	1	4006	-	0,6,6	0.00	-	-		
87	OHX	1	4078	-	0,6,6	0.00	-	-		
87	OHX	5	3945	-	0,6,6	0.00	-	-		
87	OHX	6	2093	-	0,6,6	0.00	-	-		
87	OHX	5	4043	-	0,6,6	0.00	-	-		
87	OHX	5	3934	-	0,6,6	0.00	-	-		
87	OHX	2	2065	-	0,6,6	0.00	-	-		
87	OHX	6	2151	-	0,6,6	0.00	-	-		
87	OHX	1	4118	-	0,6,6	0.00	-	-		
87	OHX	1	3954	-	0,6,6	0.00	-	-		
87	OHX	2	2043	-	0,6,6	0.00	-	-		
87	OHX	5	3963	-	0,6,6	0.00	-	-		
87	OHX	5	4009	-	0,6,6	0.00	-	-		
87	OHX	5	3958	-	0,6,6	0.00	-	-		
87	OHX	5	3974	-	0,6,6	0.00	-	-		
87	OHX	2	2146	-	0,6,6	0.00	-	-		
87	OHX	3	218	-	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	4010	-	0,6,6	0.00	-	-		
87	OHX	D3	202	-	0,6,6	0.00	-	-		
87	OHX	3	224	-	0,6,6	0.00	-	-		
87	OHX	5	4248	-	0,6,6	0.00	-	-		
87	OHX	2	2073	-	0,6,6	0.00	-	-		
87	OHX	5	4210	-	0,6,6	0.00	-	-		
87	OHX	2	2046	-	0,6,6	0.00	-	-		
87	OHX	5	4213	-	0,6,6	0.00	-	-		
87	OHX	2	2169	-	0,6,6	0.00	-	-		
87	OHX	1	4169	-	0,6,6	0.00	-	-		
87	OHX	1	3964	-	0,6,6	0.00	-	-		
87	OHX	2	2038	-	0,6,6	0.00	-	-		
87	OHX	1	4005	-	0,6,6	0.00	-	-		
87	OHX	5	4143	-	0,6,6	0.00	-	-		
87	OHX	5	4202	-	0,6,6	0.00	-	-		
87	OHX	1	4187	-	0,6,6	0.00	-	-		
87	OHX	1	3969	-	0,6,6	0.00	-	-		
87	OHX	m7	205	-	0,6,6	0.00	-	-		
87	OHX	7	220	-	0,6,6	0.00	-	-		
87	OHX	6	2065	-	0,6,6	0.00	-	-		
87	OHX	8	214	-	0,6,6	0.00	-	-		
87	OHX	1	3931	-	0,6,6	0.00	-	-		
87	OHX	2	2031	-	0,6,6	0.00	-	-		
87	OHX	6	2110	-	0,6,6	0.00	-	-		
87	OHX	5	4242	-	0,6,6	0.00	-	-		
87	OHX	1	3905	-	0,6,6	0.00	-	-		
87	OHX	6	2124	-	0,6,6	0.00	-	-		
87	OHX	5	4199	-	0,6,6	0.00	-	-		
87	OHX	8	220	-	0,6,6	0.00	-	-		
87	OHX	5	3986	-	0,6,6	0.00	-	-		
87	OHX	1	4024	-	0,6,6	0.00	-	-		
87	OHX	1	3939	-	0,6,6	0.00	-	-		
87	OHX	5	4010	-	0,6,6	0.00	-	-		
87	OHX	1	4121	-	0,6,6	0.00	-	-		
87	OHX	5	3952	-	0,6,6	0.00	-	-		
87	OHX	6	2148	-	0,6,6	0.00	-	-		
87	OHX	6	2051	-	0,6,6	0.00	-	-		
87	OHX	1	3891	-	0,6,6	0.00	-	-		
87	OHX	1	4148	-	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	4164	-	0,6,6	0.00	-	-		
87	OHX	1	4166	-	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	2113	-	0,6,6	0.00	-	-		
87	OHX	2	2152	-	0,6,6	0.00	-	-		
87	OHX	6	2056	-	0,6,6	0.00	-	-		
87	OHX	1	3951	-	0,6,6	0.00	-	-		
87	OHX	1	4195	-	0,6,6	0.00	-	-		
87	OHX	2	2041	-	0,6,6	0.00	-	-		
87	OHX	1	4176	-	0,6,6	0.00	-	-		
87	OHX	1	3919	-	0,6,6	0.00	-	-		
87	OHX	5	4022	-	0,6,6	0.00	-	-		
87	OHX	1	4144	-	0,6,6	0.00	-	-		
87	OHX	5	4193	-	0,6,6	0.00	-	-		
87	OHX	M7	207	-	0,6,6	0.00	-	-		
87	OHX	2	2064	-	0,6,6	0.00	-	-		
87	OHX	5	4064	-	0,6,6	0.00	-	-		
87	OHX	5	4078	-	0,6,6	0.00	-	-		
87	OHX	1	4192	-	0,6,6	0.00	-	-		
87	OHX	6	2120	-	0,6,6	0.00	-	-		
87	OHX	1	3932	-	0,6,6	0.00	-	-		
87	OHX	1	3996	-	0,6,6	0.00	-	-		
87	OHX	1	4115	-	0,6,6	0.00	-	-		
87	OHX	6	2070	-	0,6,6	0.00	-	-		
87	OHX	5	4203	-	0,6,6	0.00	-	-		
87	OHX	5	4103	-	0,6,6	0.00	-	-		
87	OHX	6	2192	-	0,6,6	0.00	-	-		
87	OHX	1	4076	-	0,6,6	0.00	-	-		
87	OHX	5	3900	-	0,6,6	0.00	-	-		
87	OHX	5	3954	-	0,6,6	0.00	-	-		
87	OHX	6	2121	-	0,6,6	0.00	-	-		
87	OHX	1	4089	-	0,6,6	0.00	-	-		
87	OHX	6	2141	-	0,6,6	0.00	-	-		
87	OHX	1	4060	-	0,6,6	0.00	-	-		
87	OHX	1	4047	-	0,6,6	0.00	-	-		
87	OHX	6	2135	-	0,6,6	0.00	-	-		
87	OHX	1	4011	-	0,6,6	0.00	-	-		
87	OHX	6	2072	-	0,6,6	0.00	-	-		
87	OHX	4	233	-	0,6,6	0.00	-	-		
87	OHX	5	3938	-	0,6,6	0.00	-	-		
87	OHX	1	4145	-	0,6,6	0.00	-	-		
87	OHX	2	2105	-	0,6,6	0.00	-	-		
87	OHX	5	4235	-	0,6,6	0.00	-	-		
87	OHX	1	4058	-	0,6,6	0.00	-	-		
87	OHX	1	4138	-	0,6,6	0.00	-	-		
87	OHX	5	3904	-	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	4037	-	0,6,6	0.00	-	-		
87	OHX	1	4087	-	0,6,6	0.00	-	-		
87	OHX	1	4039	-	0,6,6	0.00	-	-		
87	OHX	5	4229	-	0,6,6	0.00	-	-		
87	OHX	5	3988	-	0,6,6	0.00	-	-		
87	OHX	5	4117	-	0,6,6	0.00	-	-		
87	OHX	C5	201	-	0,6,6	0.00	-	-		
87	OHX	5	4052	-	0,6,6	0.00	-	-		
87	OHX	1	3948	-	0,6,6	0.00	-	-		
87	OHX	6	2184	-	0,6,6	0.00	-	-		
87	OHX	5	4070	-	0,6,6	0.00	-	-		
87	OHX	5	4050	-	0,6,6	0.00	-	-		
87	OHX	4	226	-	0,6,6	0.00	-	-		
87	OHX	5	4089	-	0,6,6	0.00	-	-		
87	OHX	1	4079	-	0,6,6	0.00	-	-		
87	OHX	1	4009	-	0,6,6	0.00	-	-		
87	OHX	5	4123	-	0,6,6	0.00	-	-		
87	OHX	O2	201	-	0,6,6	0.00	-	-		
87	OHX	6	2172	-	0,6,6	0.00	-	-		
87	OHX	1	4028	-	0,6,6	0.00	-	-		
87	OHX	5	3976	-	0,6,6	0.00	-	-		
87	OHX	1	4020	-	0,6,6	0.00	-	-		
87	OHX	5	4236	-	0,6,6	0.00	-	-		
87	OHX	5	3921	-	0,6,6	0.00	-	-		
87	OHX	5	4233	-	0,6,6	0.00	-	-		
87	OHX	1	4117	-	0,6,6	0.00	-	-		
87	OHX	1	4147	-	0,6,6	0.00	-	-		
87	OHX	5	3994	-	0,6,6	0.00	-	-		
87	OHX	6	2139	-	0,6,6	0.00	-	-		
87	OHX	5	4049	-	0,6,6	0.00	-	-		
87	OHX	2	2102	-	0,6,6	0.00	-	-		
87	OHX	6	2165	-	0,6,6	0.00	-	-		
87	OHX	6	2109	-	0,6,6	0.00	-	-		
87	OHX	1	4213	-	0,6,6	0.00	-	-		
87	OHX	5	4115	-	0,6,6	0.00	-	-		
87	OHX	3	225	-	0,6,6	0.00	-	-		
87	OHX	1	4162	-	0,6,6	0.00	-	-		
87	OHX	1	4168	-	0,6,6	0.00	-	-		
87	OHX	1	4150	-	0,6,6	0.00	-	-		
87	OHX	O7	103	-	0,6,6	0.00	-	-		
87	OHX	6	2068	-	0,6,6	0.00	-	-		
87	OHX	m0	301	-	0,6,6	0.00	-	-		
87	OHX	6	2097	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	o3	202	-	0,6,6	0.00	-	-		
87	OHX	8	226	-	0,6,6	0.00	-	-		
87	OHX	1	4151	-	0,6,6	0.00	-	-		
87	OHX	5	4137	-	0,6,6	0.00	-	-		
87	OHX	1	4157	-	0,6,6	0.00	-	-		
87	OHX	5	3957	-	0,6,6	0.00	-	-		
87	OHX	5	3951	-	0,6,6	0.00	-	-		
87	OHX	1	4071	-	0,6,6	0.00	-	-		
87	OHX	1	3888	-	0,6,6	0.00	-	-		
87	OHX	5	3959	-	0,6,6	0.00	-	-		
87	OHX	2	2027	-	0,6,6	0.00	-	-		
87	OHX	1	4214	-	0,6,6	0.00	-	-		
87	OHX	5	4130	-	0,6,6	0.00	-	-		
87	OHX	1	3938	-	0,6,6	0.00	-	-		
87	OHX	1	3978	-	0,6,6	0.00	-	-		
87	OHX	5	3975	-	0,6,6	0.00	-	-		
87	OHX	2	2130	-	0,6,6	0.00	-	-		
87	OHX	5	3914	-	0,6,6	0.00	-	-		
87	OHX	2	2173	-	0,6,6	0.00	-	-		
87	OHX	5	3955	-	0,6,6	0.00	-	-		
87	OHX	5	4191	-	0,6,6	0.00	-	-		
87	OHX	5	3997	-	0,6,6	0.00	-	-		
87	OHX	m1	203	-	0,6,6	0.00	-	-		
87	OHX	s9	201	-	0,6,6	0.00	-	-		
87	OHX	1	4112	-	0,6,6	0.00	-	-		
87	OHX	1	4158	-	0,6,6	0.00	-	-		
89	3HE	1	4215	-	21,21,21	0.53	0	19,30,30	0.62	0
87	OHX	1	4094	-	0,6,6	0.00	-	-		
87	OHX	1	4153	-	0,6,6	0.00	-	-		
87	OHX	1	3890	-	0,6,6	0.00	-	-		
87	OHX	2	2121	-	0,6,6	0.00	-	-		
87	OHX	1	4075	-	0,6,6	0.00	-	-		
87	OHX	1	3982	-	0,6,6	0.00	-	-		
87	OHX	1	3867	-	0,6,6	0.00	-	-		
87	OHX	1	4152	-	0,6,6	0.00	-	-		
87	OHX	5	4171	-	0,6,6	0.00	-	-		
87	OHX	6	2173	-	0,6,6	0.00	-	-		
87	OHX	L4	402	-	0,6,6	0.00	-	-		
87	OHX	6	2088	-	0,6,6	0.00	-	-		
87	OHX	2	2084	-	0,6,6	0.00	-	-		
87	OHX	5	4147	-	0,6,6	0.00	-	-		
87	OHX	2	2125	-	0,6,6	0.00	-	-		
87	OHX	5	4168	-	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	3959	-	0,6,6	0.00	-	-		
87	OHX	2	2049	-	0,6,6	0.00	-	-		
87	OHX	2	2174	-	0,6,6	0.00	-	-		
87	OHX	5	4061	-	0,6,6	0.00	-	-		
87	OHX	1	4123	-	0,6,6	0.00	-	-		
87	OHX	6	2055	-	0,6,6	0.00	-	-		
87	OHX	6	2050	-	0,6,6	0.00	-	-		
87	OHX	5	4164	-	0,6,6	0.00	-	-		
87	OHX	1	4102	-	0,6,6	0.00	-	-		
87	OHX	1	4105	-	0,6,6	0.00	-	-		
87	OHX	M0	303	-	0,6,6	0.00	-	-		
87	OHX	2	2087	-	0,6,6	0.00	-	-		
87	OHX	5	4083	-	0,6,6	0.00	-	-		
87	OHX	1	3984	-	0,6,6	0.00	-	-		
87	OHX	6	2084	-	0,6,6	0.00	-	-		
87	OHX	6	2090	-	0,6,6	0.00	-	-		
87	OHX	5	3984	-	0,6,6	0.00	-	-		
87	OHX	5	3942	-	0,6,6	0.00	-	-		
87	OHX	5	4019	-	0,6,6	0.00	-	-		
87	OHX	5	4140	-	0,6,6	0.00	-	-		
87	OHX	5	4094	-	0,6,6	0.00	-	-		
87	OHX	O9	101	-	0,6,6	0.00	-	-		
87	OHX	5	4032	-	0,6,6	0.00	-	-		
87	OHX	5	4017	-	0,6,6	0.00	-	-		
87	OHX	2	2112	-	0,6,6	0.00	-	-		
87	OHX	1	3994	-	0,6,6	0.00	-	-		
87	OHX	2	2054	-	0,6,6	0.00	-	-		
87	OHX	1	4043	-	0,6,6	0.00	-	-		
87	OHX	5	4219	-	0,6,6	0.00	-	-		
87	OHX	1	3864	-	0,6,6	0.00	-	-		
87	OHX	1	4083	-	0,6,6	0.00	-	-		
87	OHX	6	2179	-	0,6,6	0.00	-	-		
87	OHX	6	2134	-	0,6,6	0.00	-	-		
87	OHX	5	3973	-	0,6,6	0.00	-	-		
87	OHX	5	4014	-	0,6,6	0.00	-	-		
87	OHX	2	2126	-	0,6,6	0.00	-	-		
87	OHX	6	2198	-	0,6,6	0.00	-	-		
87	OHX	1	4190	-	0,6,6	0.00	-	-		
87	OHX	1	4082	-	0,6,6	0.00	-	-		
87	OHX	8	229	-	0,6,6	0.00	-	-		
87	OHX	7	221	-	0,6,6	0.00	-	-		
87	OHX	2	2077	-	0,6,6	0.00	-	-		
87	OHX	1	4041	-	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	2062	-	0,6,6	0.00	-	-		
87	OHX	1	4049	-	0,6,6	0.00	-	-		
87	OHX	1	3878	-	0,6,6	0.00	-	-		
87	OHX	2	2156	-	0,6,6	0.00	-	-		
87	OHX	SR	401	-	0,6,6	0.00	-	-		
87	OHX	5	3943	-	0,6,6	0.00	-	-		
87	OHX	m0	302	-	0,6,6	0.00	-	-		
87	OHX	1	4077	-	0,6,6	0.00	-	-		
87	OHX	7	218	-	0,6,6	0.00	-	-		
87	OHX	5	3933	-	0,6,6	0.00	-	-		
87	OHX	5	3932	-	0,6,6	0.00	-	-		
87	OHX	5	3979	-	0,6,6	0.00	-	-		
87	OHX	1	4042	-	0,6,6	0.00	-	-		
87	OHX	1	3952	-	0,6,6	0.00	-	-		
87	OHX	5	3903	-	0,6,6	0.00	-	-		
87	OHX	1	4206	-	0,6,6	0.00	-	-		
87	OHX	1	4160	-	0,6,6	0.00	-	-		
87	OHX	5	3992	-	0,6,6	0.00	-	-		
87	OHX	1	3998	-	0,6,6	0.00	-	-		
87	OHX	6	2153	-	0,6,6	0.00	-	-		
87	OHX	1	3884	-	0,6,6	0.00	-	-		
87	OHX	4	229	-	0,6,6	0.00	-	-		
87	OHX	2	2023	-	0,6,6	0.00	-	-		
87	OHX	5	3916	-	0,6,6	0.00	-	-		
87	OHX	1	4174	-	0,6,6	0.00	-	-		
87	OHX	5	4041	-	0,6,6	0.00	-	-		
87	OHX	1	3924	-	0,6,6	0.00	-	-		
87	OHX	c1	202	-	0,6,6	0.00	-	-		
87	OHX	5	3968	-	0,6,6	0.00	-	-		
87	OHX	4	230	-	0,6,6	0.00	-	-		
87	OHX	1	3942	-	0,6,6	0.00	-	-		
87	OHX	5	4109	-	0,6,6	0.00	-	-		
87	OHX	6	2204	-	0,6,6	0.00	-	-		
87	OHX	2	2026	-	0,6,6	0.00	-	-		
87	OHX	5	4016	-	0,6,6	0.00	-	-		
87	OHX	1	3914	-	0,6,6	0.00	-	-		
87	OHX	5	4116	-	0,6,6	0.00	-	-		
87	OHX	5	3941	-	0,6,6	0.00	-	-		
87	OHX	q2	502	-	0,6,6	0.00	-	-		
87	OHX	2	2072	-	0,6,6	0.00	-	-		
87	OHX	5	4148	-	0,6,6	0.00	-	-		
87	OHX	6	2178	-	0,6,6	0.00	-	-		
87	OHX	8	225	-	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	2137	-	0,6,6	0.00	-	-		
87	OHX	1	3922	-	0,6,6	0.00	-	-		
87	OHX	1	4208	-	0,6,6	0.00	-	-		
87	OHX	2	2158	-	0,6,6	0.00	-	-		
87	OHX	5	3966	-	0,6,6	0.00	-	-		
87	OHX	6	2170	-	0,6,6	0.00	-	-		
87	OHX	5	4186	-	0,6,6	0.00	-	-		
87	OHX	1	4143	-	0,6,6	0.00	-	-		
87	OHX	5	4060	-	0,6,6	0.00	-	-		
87	OHX	5	4150	-	0,6,6	0.00	-	-		
87	OHX	8	216	-	0,6,6	0.00	-	-		
87	OHX	5	4246	-	0,6,6	0.00	-	-		
87	OHX	5	4226	-	0,6,6	0.00	-	-		
87	OHX	1	3945	-	0,6,6	0.00	-	-		
87	OHX	6	2130	-	0,6,6	0.00	-	-		
87	OHX	5	4027	-	0,6,6	0.00	-	-		
87	OHX	1	4159	-	0,6,6	0.00	-	-		
87	OHX	6	2166	-	0,6,6	0.00	-	-		
87	OHX	5	4173	-	0,6,6	0.00	-	-		
87	OHX	2	2123	-	0,6,6	0.00	-	-		
87	OHX	6	2169	-	0,6,6	0.00	-	-		
87	OHX	6	2154	-	0,6,6	0.00	-	-		
87	OHX	5	4132	-	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	3HE	1	4215	-	-	1/8/36/36	0/2/2/2
89	3HE	5	4252	-	-	3/8/36/36	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4252	3HE	C5-C7	3.31	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

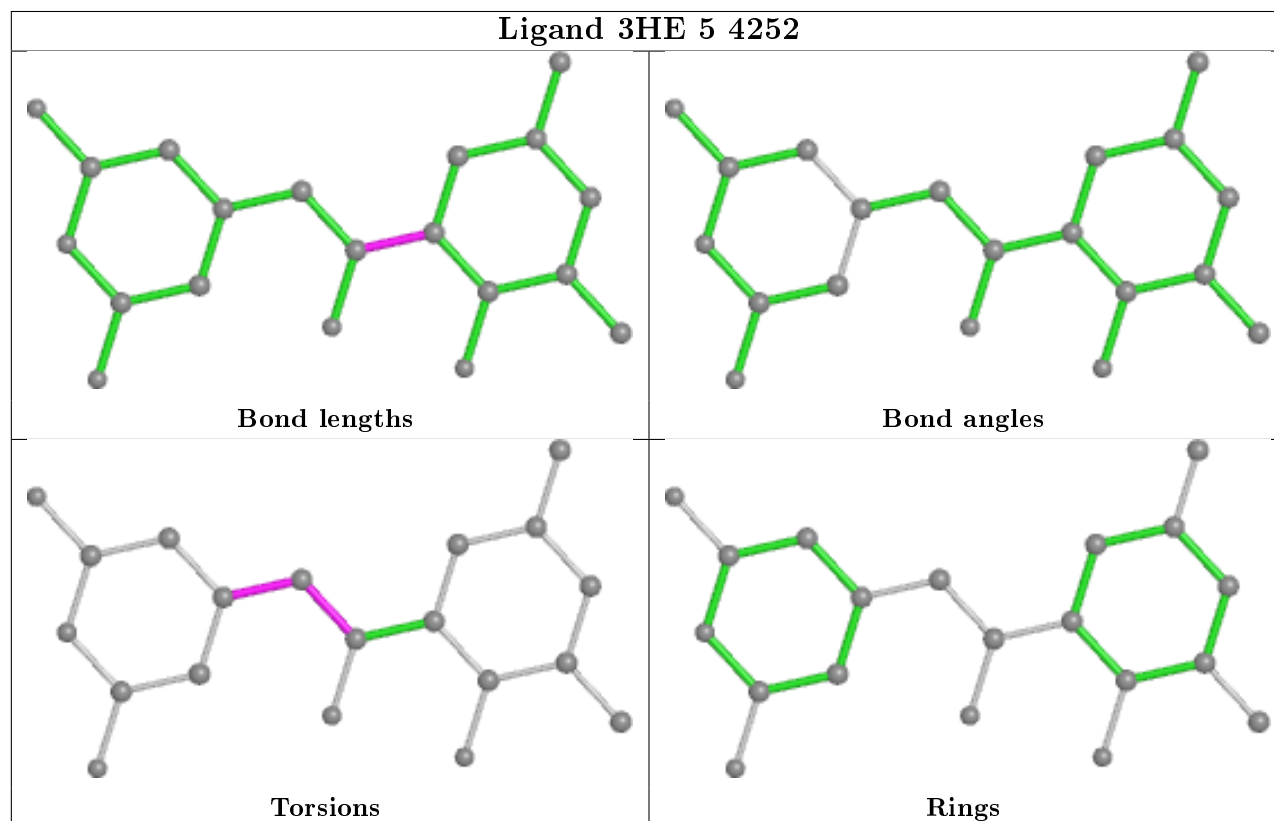
All (4) torsion outliers are listed below:

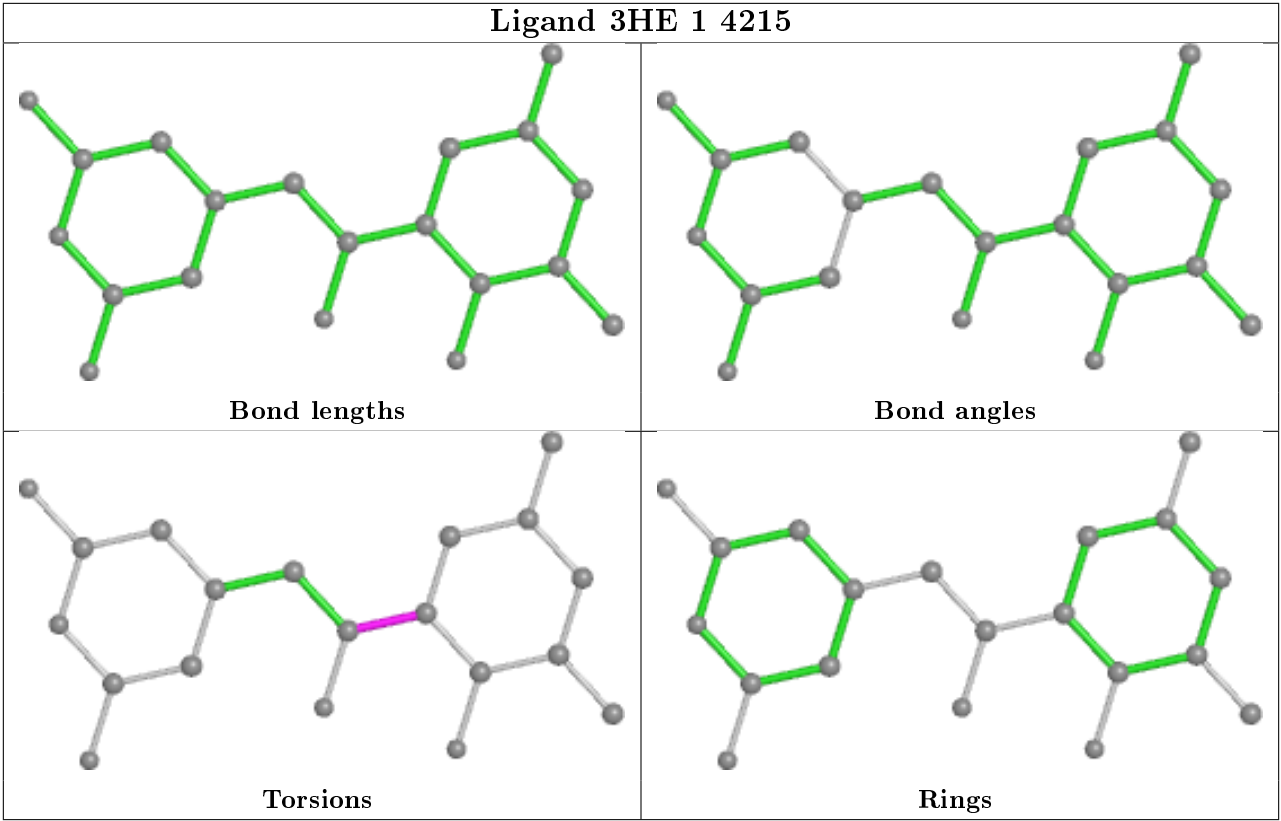
Mol	Chain	Res	Type	Atoms
89	5	4252	3HE	C7-C8-C9-C10
89	5	4252	3HE	C7-C8-C9-C13
89	5	4252	3HE	O3-C7-C8-C9
89	1	4215	3HE	C6-C5-C7-O3

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	SR	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SR	161:LYS	C	162:ALA	N	0.76
1	SR	160:GLU	C	161:LYS	N	0.64

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.