



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 11:25 am BST

PDB ID : 5NDG
Title : Crystal structure of geneticin (G418) bound to the yeast 80S ribosome
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2017-03-08
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

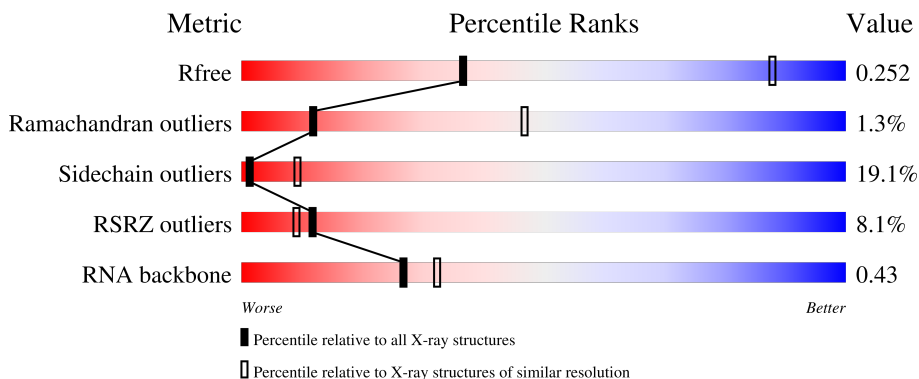
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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))
R_{free}	130704	1049 (3.88-3.52)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1800	
1	6	1800	
2	S0	206	
2	s0	206	
3	S1	216	

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Mol	Chain	Length	Quality of chain
3	s1	216	19% 83% 17%
4	S2	217	1% 79% 21%
4	s2	217	4% 83% 17%
5	S3	223	3% 83% 17%
5	s3	223	6% 79% 19%
6	S4	260	21% 83% 16%
6	s4	260	9% 87% 13%
7	S5	206	11% 81% 19%
7	s5	206	28% 82% 17%
8	S6	236	16% 79% 17%
8	s6	236	11% 78% 14% 8%
9	S7	185	18% 78% 19%
9	s7	185	14% 77% 21%
10	S8	200	26% 82% 12% 6%
10	s8	200	10% 80% 14% 6%
11	S9	185	36% 82% 17%
11	s9	185	42% 87% 13%
12	C0	105	20% 72% 14% 12%
12	c0	105	39% 70% 16% 12%
13	C1	156	11% 79% 12% 9%
13	c1	156	4% 77% 15% 6%
14	C2	143	31% 64% 16% 16%
14	c2	143	55% 63% 23% 13%
15	C3	150	3% 85% 15%
15	c3	150	2% 80% 19%

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Mol	Chain	Length	Quality of chain
16	C4	128	4% 81% 16% ..
16	c4	128	5% 84% 16%
17	C5	141	5% 70% 16% • 13%
17	c5	141	14% 70% 15% 16%
18	C6	141	16% 79% 19% ..
18	c6	141	56% 84% 16% •
19	C7	136	12% 70% 15% • 14%
19	c7	136	6% 72% 12% • 14%
20	C8	145	6% 77% 21% •
20	c8	145	19% 81% 19% •
21	C9	143	11% 83% 16% •
21	c9	143	43% 84% 15% •
22	D0	107	19% 79% 19% •
22	d0	107	25% 77% 16% .. 6%
23	D1	87	5% 82% 17% •
23	d1	87	3% 84% 16%
24	D2	129	9% 85% 13% ..
24	d2	129	5% 87% 12% •
25	D3	144	2% 80% 20%
25	d3	144	92% 8%
26	D4	134	22% 81% 17% •
26	d4	134	11% 81% 19%
27	D5	70	20% 67% 30% •
27	d5	70	36% 86% 13% •
28	D6	97	5% 65% 31% •





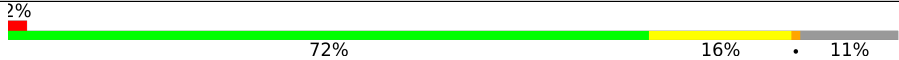
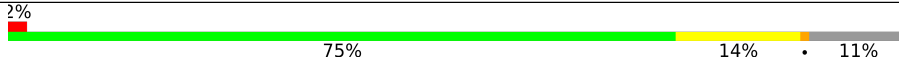
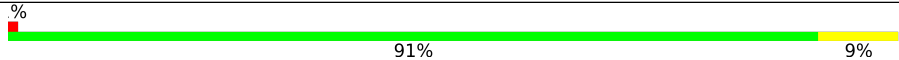
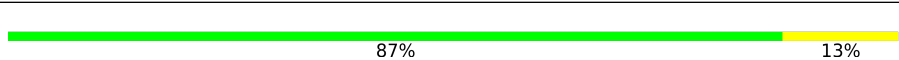
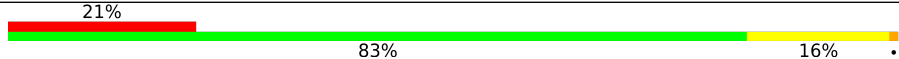
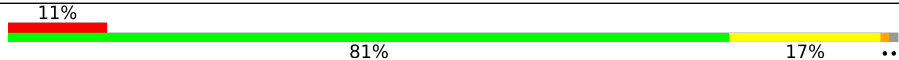
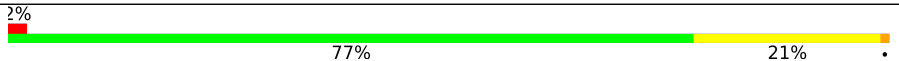
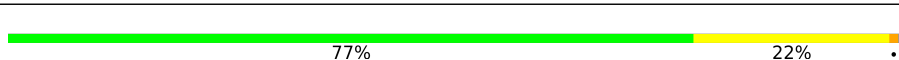


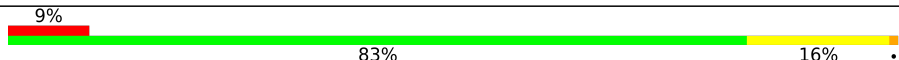
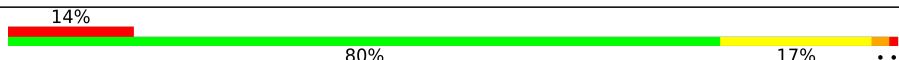
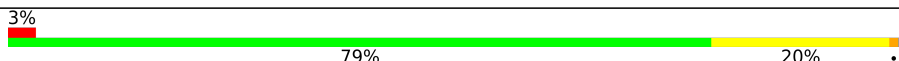
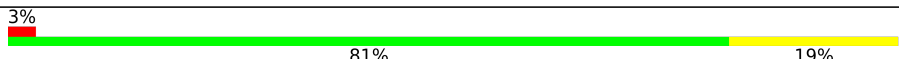
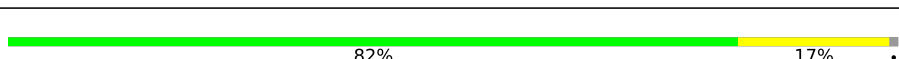

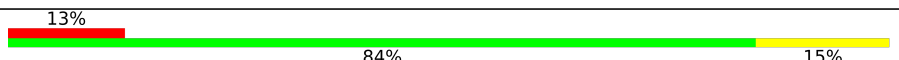
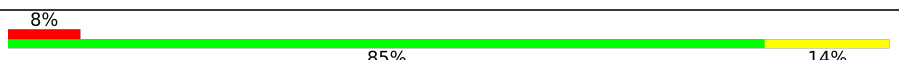
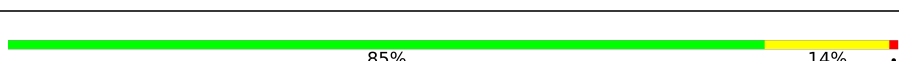
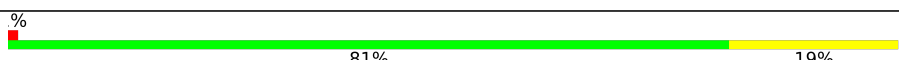
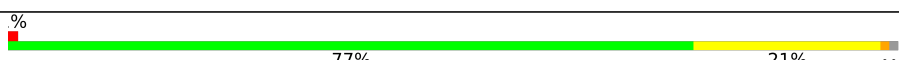
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Mol	Chain	Length	Quality of chain
28	d6	97	8% 87% 13%
29	D7	81	7% 85% 15%
29	d7	81	2% 83% 17%
30	D8	63	13% 73% 27%
30	d8	63	2% 71% 27% .
31	D9	53	17% 81% 17% .
31	d9	53	28% 81% 19%
32	E0	60	18% 82% 17% .
32	e0	60	17% 67% 32% .
33	E1	152	21% 30% 12% 5% 53%
33	e1	152	16% 22% 5% . 70%
34	SR	318	19% 90% 10%
34	sR	318	13% 90% 8% .
35	SM	272	2% 41% 8% 50%
35	sM	272	9% 33% 8% . 58%
36	1	3396	% 59% 27% 5% 9%
36	5	3396	% 61% 26% 5% 8%
37	3	121	74% 26% .
37	7	121	82% 17% .
38	4	158	3% 56% 41% .
38	8	158	% 61% 30% 8% .
39	L2	252	5% 86% 14%
39	l2	252	4% 81% 18% .
40	L3	386	3% 83% 16% .
40	l3	386	80% 19% .

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Mol	Chain	Length	Quality of chain
41	L4	361	 % 86% 14%
41	l4	361	 2% 82% 18%
42	L5	296	 24% 81% 18%
42	l5	296	 17% 84% 15%
43	L6	176	 2% 72% 16% 11%
43	l6	176	 2% 75% 14% 11%
44	L7	223	 % 91% 9%
44	l7	223	 87% 13%
45	L8	233	 21% 83% 16%
45	l8	233	 11% 81% 17%
46	L9	191	 2% 77% 21%
46	l9	191	 77% 22%
47	M0	221	 % 83% 11% 6%
47	m0	221	 4% 78% 16% 5%
48	M1	169	 9% 83% 16%
48	m1	169	 14% 80% 17%
49	M3	194	 3% 79% 20%
49	m3	194	 3% 81% 19%
50	M4	137	 82% 17%
50	m4	137	 84% 15%
51	M5	203	 13% 84% 15%
51	m5	203	 8% 85% 14%
52	M6	197	 85% 14%
52	m6	197	 % 81% 19%
53	M7	184	 % 77% 21%

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Mol	Chain	Length	Quality of chain
53	m7	184	2% 75% 20% 5%
54	M8	185	4% 86% 14%
54	m8	185	% 86% 14%
55	M9	188	11% 80% 20% .
55	m9	188	10% 77% 20% .
56	N0	172	81% 16% ..
56	n0	172	81% 19%
57	N1	159	16% 82% 17% .
57	n1	159	5% 82% 18%
58	N2	98	23% 88% 12%
58	n2	98	9% 83% 17%
59	N3	135	12% 89% 11%
59	n3	135	2% 88% 10% ..
60	N4	155	11% 70% 9% 21%
60	n4	155	12% 68% 8% 24%
61	N5	121	11% 82% 18%
61	n5	121	2% 82% 17% ..
62	N6	126	24% 81% 18% .
62	n6	126	12% 79% 19% ..
63	N7	135	35% 84% 14% .
63	n7	135	18% 79% 19% .
64	N8	148	11% 80% 19% .
64	n8	148	% 82% 17% .
65	N9	58	17% 86% 14%
65	n9	58	14% 84% 16%

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Mol	Chain	Length	Quality of chain
66	O0	100	18% 77% 19%
66	o0	100	5% 87% 13%
67	O1	109	15% 81% 18%
67	o1	109	8% 80% 18%
68	O2	127	5% 87% 13%
68	o2	127	86% 14%
69	O3	106	2% 86% 14%
69	o3	106	2% 82% 18%
70	O4	112	11% 79% 21%
70	o4	112	6% 84% 16%
71	O5	119	4% 82% 18%
71	o5	119	3% 82% 18%
72	O6	99	14% 75% 24%
72	o6	99	7% 77% 22%
73	O7	84	76% 24%
73	o7	84	82% 14%
74	O8	77	19% 81% 19%
74	o8	77	21% 83% 16%
75	O9	50	80% 18%
75	o9	50	84% 16%
76	Q0	52	4% 79% 21%
76	q0	52	4% 81% 19%
77	Q1	25	12% 88% 12%
77	q1	25	4% 60% 40%
78	Q2	105	23% 80% 20%

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Mol	Chain	Length	Quality of chain
78	q2	105	
79	Q3	91	
79	q3	91	
80	p0	312	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	1	3404	-	-	-	X
81	MG	1	3423	-	-	-	X
81	MG	1	3425	-	-	-	X
81	MG	1	3429	-	-	-	X
81	MG	1	3431	-	-	-	X
81	MG	1	3441	-	-	-	X
81	MG	1	3485	-	-	-	X
81	MG	1	3486	-	-	-	X
81	MG	1	3487	-	-	-	X
81	MG	1	3505	-	-	-	X
81	MG	1	3523	-	-	-	X
81	MG	1	3540	-	-	-	X
81	MG	1	3543	-	-	-	X
81	MG	1	3547	-	-	-	X
81	MG	1	3553	-	-	-	X
81	MG	1	3565	-	-	-	X
81	MG	1	3578	-	-	-	X
81	MG	1	3579	-	-	-	X
81	MG	1	3582	-	-	-	X
81	MG	1	3609	-	-	-	X
81	MG	1	3612	-	-	-	X
81	MG	1	3620	-	-	-	X
81	MG	1	3630	-	-	-	X
81	MG	1	3634	-	-	-	X
81	MG	1	3635	-	-	-	X
81	MG	1	3641	-	-	-	X
81	MG	1	3643	-	-	-	X
81	MG	1	3645	-	-	-	X
81	MG	1	3659	-	-	-	X
81	MG	1	3660	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	1	3663	-	-	-	X
81	MG	1	3668	-	-	-	X
81	MG	1	3673	-	-	-	X
81	MG	1	3676	-	-	-	X
81	MG	1	3687	-	-	-	X
81	MG	1	3688	-	-	-	X
81	MG	1	3690	-	-	-	X
81	MG	1	3692	-	-	-	X
81	MG	1	3693	-	-	-	X
81	MG	1	3695	-	-	-	X
81	MG	1	3700	-	-	-	X
81	MG	1	3704	-	-	-	X
81	MG	1	3712	-	-	-	X
81	MG	1	3720	-	-	-	X
81	MG	1	3721	-	-	-	X
81	MG	1	3723	-	-	-	X
81	MG	1	3724	-	-	-	X
81	MG	1	3725	-	-	-	X
81	MG	1	3726	-	-	-	X
81	MG	1	3727	-	-	-	X
81	MG	1	3733	-	-	-	X
81	MG	1	3744	-	-	-	X
81	MG	1	3745	-	-	-	X
81	MG	1	3748	-	-	-	X
81	MG	1	3761	-	-	-	X
81	MG	1	3762	-	-	-	X
81	MG	1	3763	-	-	-	X
81	MG	1	3769	-	-	-	X
81	MG	1	3771	-	-	-	X
81	MG	1	3773	-	-	-	X
81	MG	1	3780	-	-	-	X
81	MG	1	3781	-	-	-	X
81	MG	1	3782	-	-	-	X
81	MG	1	3783	-	-	-	X
81	MG	1	3784	-	-	-	X
81	MG	1	3785	-	-	-	X
81	MG	1	3788	-	-	-	X
81	MG	1	3789	-	-	-	X
81	MG	1	3791	-	-	-	X
81	MG	1	3792	-	-	-	X
81	MG	1	3795	-	-	-	X
81	MG	1	3800	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	1	3801	-	-	-	X
81	MG	1	3802	-	-	-	X
81	MG	1	3804	-	-	-	X
81	MG	1	3806	-	-	-	X
81	MG	2	1904	-	-	-	X
81	MG	2	1907	-	-	-	X
81	MG	2	1915	-	-	-	X
81	MG	2	1921	-	-	-	X
81	MG	2	1928	-	-	-	X
81	MG	2	1937	-	-	-	X
81	MG	2	1951	-	-	-	X
81	MG	2	1953	-	-	-	X
81	MG	2	1967	-	-	-	X
81	MG	2	1970	-	-	-	X
81	MG	2	1972	-	-	-	X
81	MG	2	1985	-	-	-	X
81	MG	2	1986	-	-	-	X
81	MG	2	1989	-	-	-	X
81	MG	2	1990	-	-	-	X
81	MG	2	1995	-	-	-	X
81	MG	2	1999	-	-	-	X
81	MG	2	2006	-	-	-	X
81	MG	3	201	-	-	-	X
81	MG	3	202	-	-	-	X
81	MG	3	205	-	-	-	X
81	MG	4	202	-	-	-	X
81	MG	4	206	-	-	-	X
81	MG	4	208	-	-	-	X
81	MG	4	210	-	-	-	X
81	MG	4	211	-	-	-	X
81	MG	4	215	-	-	-	X
81	MG	4	216	-	-	-	X
81	MG	4	222	-	-	-	X
81	MG	5	3412	-	-	-	X
81	MG	5	3426	-	-	-	X
81	MG	5	3465	-	-	-	X
81	MG	5	3488	-	-	-	X
81	MG	5	3491	-	-	-	X
81	MG	5	3493	-	-	-	X
81	MG	5	3500	-	-	-	X
81	MG	5	3514	-	-	-	X
81	MG	5	3516	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	5	3549	-	-	-	X
81	MG	5	3555	-	-	-	X
81	MG	5	3558	-	-	-	X
81	MG	5	3566	-	-	-	X
81	MG	5	3567	-	-	-	X
81	MG	5	3594	-	-	-	X
81	MG	5	3601	-	-	-	X
81	MG	5	3606	-	-	-	X
81	MG	5	3617	-	-	-	X
81	MG	5	3634	-	-	-	X
81	MG	5	3636	-	-	-	X
81	MG	5	3638	-	-	-	X
81	MG	5	3643	-	-	-	X
81	MG	5	3647	-	-	-	X
81	MG	5	3648	-	-	-	X
81	MG	5	3660	-	-	-	X
81	MG	5	3667	-	-	-	X
81	MG	5	3669	-	-	-	X
81	MG	5	3672	-	-	-	X
81	MG	5	3675	-	-	-	X
81	MG	5	3676	-	-	-	X
81	MG	5	3677	-	-	-	X
81	MG	5	3684	-	-	-	X
81	MG	5	3693	-	-	-	X
81	MG	5	3708	-	-	-	X
81	MG	5	3710	-	-	-	X
81	MG	5	3712	-	-	-	X
81	MG	5	3713	-	-	-	X
81	MG	5	3716	-	-	-	X
81	MG	5	3722	-	-	-	X
81	MG	5	3724	-	-	-	X
81	MG	5	3726	-	-	-	X
81	MG	5	3728	-	-	-	X
81	MG	5	3740	-	-	-	X
81	MG	5	3743	-	-	-	X
81	MG	5	3745	-	-	-	X
81	MG	5	3750	-	-	-	X
81	MG	5	3754	-	-	-	X
81	MG	5	3758	-	-	-	X
81	MG	5	3759	-	-	-	X
81	MG	5	3761	-	-	-	X
81	MG	5	3762	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	5	3765	-	-	-	X
81	MG	5	3771	-	-	-	X
81	MG	5	3779	-	-	-	X
81	MG	5	3787	-	-	-	X
81	MG	5	3788	-	-	-	X
81	MG	5	3789	-	-	-	X
81	MG	5	3790	-	-	-	X
81	MG	5	3792	-	-	-	X
81	MG	5	3793	-	-	-	X
81	MG	5	3794	-	-	-	X
81	MG	5	3800	-	-	-	X
81	MG	5	3803	-	-	-	X
81	MG	5	3806	-	-	-	X
81	MG	5	3807	-	-	-	X
81	MG	5	3811	-	-	-	X
81	MG	5	3812	-	-	-	X
81	MG	5	3818	-	-	-	X
81	MG	5	3819	-	-	-	X
81	MG	5	3820	-	-	-	X
81	MG	5	3822	-	-	-	X
81	MG	5	3823	-	-	-	X
81	MG	5	3825	-	-	-	X
81	MG	5	3826	-	-	-	X
81	MG	5	3832	-	-	-	X
81	MG	5	3833	-	-	-	X
81	MG	5	3834	-	-	-	X
81	MG	5	3837	-	-	-	X
81	MG	5	3838	-	-	-	X
81	MG	5	3839	-	-	-	X
81	MG	5	3840	-	-	-	X
81	MG	5	3841	-	-	-	X
81	MG	5	3842	-	-	-	X
81	MG	6	1910	-	-	-	X
81	MG	6	1911	-	-	-	X
81	MG	6	1916	-	-	-	X
81	MG	6	1918	-	-	-	X
81	MG	6	1919	-	-	-	X
81	MG	6	1922	-	-	-	X
81	MG	6	1939	-	-	-	X
81	MG	6	1952	-	-	-	X
81	MG	6	1958	-	-	-	X
81	MG	6	1972	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	6	1978	-	-	-	X
81	MG	6	1980	-	-	-	X
81	MG	6	1985	-	-	-	X
81	MG	6	1997	-	-	-	X
81	MG	6	2000	-	-	-	X
81	MG	6	2003	-	-	-	X
81	MG	6	2006	-	-	-	X
81	MG	6	2008	-	-	-	X
81	MG	6	2009	-	-	-	X
81	MG	6	2011	-	-	-	X
81	MG	6	2012	-	-	-	X
81	MG	7	206	-	-	-	X
81	MG	7	207	-	-	-	X
81	MG	8	204	-	-	-	X
81	MG	8	205	-	-	-	X
81	MG	8	206	-	-	-	X
81	MG	8	210	-	-	-	X
81	MG	8	213	-	-	-	X
81	MG	M6	201	-	-	-	X
81	MG	M7	201	-	-	-	X
81	MG	M7	205	-	-	-	X
81	MG	N8	202	-	-	-	X
81	MG	O2	202	-	-	-	X
81	MG	O3	201	-	-	-	X
81	MG	O9	101	-	-	-	X
81	MG	S1	301	-	-	-	X
81	MG	S8	301	-	-	-	X
81	MG	d3	201	-	-	-	X
81	MG	l2	301	-	-	-	X
81	MG	l3	403	-	-	-	X
81	MG	m6	201	-	-	-	X
81	MG	n0	201	-	-	-	X
81	MG	n0	202	-	-	-	X
81	MG	n5	201	-	-	-	X
81	MG	o2	202	-	-	-	X
81	MG	o3	201	-	-	-	X
81	MG	o3	203	-	-	-	X
81	MG	o5	201	-	-	-	X
81	MG	o7	505	-	-	-	X
81	MG	q2	503	-	-	-	X
81	MG	q2	504	-	-	-	X
81	MG	s8	302	-	-	-	X

2 Entry composition [i](#)

There are 84 unique types of molecules in this entry. The entry contains 397710 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
			Total	C	N	O	P			
1	2	1688	Total	C	N	O	P	0	0	0
			35985	16089	6386	11822	1688			
1	6	1700	Total	C	N	O	P	0	0	0
			36234	16201	6426	11907	1700			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	185	Total	C	N	O	0	0	0
			1486	954	266	266			

- 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	92	Total	C	N	O	S	0	0	0
			752	487	122	141	2			
12	c0	92	Total	C	N	O	S	0	0	0
			741	478	121	140	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	142	Total	C	N	O	S	0	0	0
			1146	735	217	191	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	120	Total	C	N	O	S	0	0	0
			870	548	152	168	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- 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
			Total	C	N	O	S			
16	C4	127	Total 891	C 545	N 182	O 163	S 1	0	0	0
16	c4	128	Total 949	C 582	N 188	O 176	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	C5	122	Total 967	C 616	N 180	O 164	S 7	0	0	0
17	c5	119	Total 939	C 595	N 176	O 161	S 7	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	C7	117	Total 911	C 568	N 174	O 167	S 2	0	0	0
19	c7	117	Total 906	C 563	N 174	O 167	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	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	105	Total	C	N	O	S	0	0	0
			837	529	152	155	1			
22	d0	101	Total	C	N	O	S	0	0	0
			805	512	145	147	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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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
			Total	C	N	O	S			
32	E0	60	475	299	98	77	1	0	0	0
32	e0	60	475	299	98	77	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	E1	71	566	362	106	94	4	0	0	0
33	e1	45	352	222	66	60	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	SR	318	2437	1541	418	470	8	0	0	0
34	sR	313	2403	1521	411	463	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SR	161	ALA	LYS	conflict	UNP P38011
sR	161	ALA	LYS	conflict	UNP P38011

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
35	SM	135	985	581	197	207	0	0	0
35	sM	115	874	514	177	183	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	1	3078	65838	29408	11870	21482	3078	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	5	3127	66891	29878	12066	21820	3127	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
38	4	158	3353	1500	586	1109	158	0	0	0
38	8	157	3333	1491	584	1101	157	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	L3	386	3075	1950	584	533	8	0	0	0
40	l3	386	3075	1950	584	533	8	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	L5	294	Total	C	N	O	S	0	0	0
			2357	1491	410	454	2			
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	18	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	19	190	Total	C	N	O	S	0	0	0
			1510	957	273	276	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	M0	208	Total 1690	C 1074	N 319	O 291	S 6	0	0	0
47	m0	209	Total 1696	C 1077	N 321	O 293	S 5	0	0	0

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O			
53	M7	183	Total	C	N	O	0	0	0
			1420	882	281	257			
53	m7	175	Total	C	N	O	0	0	0
			1378	856	273	249			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O			
55	M9	188	Total	C	N	O	0	0	0
			1521	935	326	260			
55	m9	183	Total	C	N	O	0	0	0
			1482	911	320	251			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	N0	170	Total	C	N	O	S	0	0	0
			1432	922	265	242	3			
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	
			Total	C	N	O				
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
			Total	C	N	O			
58	N2	98	778	505	127	146	0	0	0
58	n2	98	778	505	127	146	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	N3	135	997	625	188	177	7	0	0	0
59	n3	134	993	623	187	176	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
60	N4	122	925	582	184	158	1	0	0	0
60	n4	118	946	597	188	160	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
62	N6	126	993	625	192	176	0	0	0
62	n6	124	976	614	190	172	0	0	0

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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	84	Total	C	N	O	S	0	0	0
			665	405	145	110	5			
73	o7	82	Total	C	N	O	S	0	0	0
			650	396	142	107	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	49	Total	C	N	O	S	0	0	0
			431	269	96	64	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 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	p0	138	Total	C	N	O	S	0	0	0
			1052	672	187	190	3			

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	2	111	Total	Mg	0	0
			111	111		
81	S1	1	Total	Mg	0	0
			1	1		
81	S8	1	Total	Mg	0	0
			1	1		
81	C0	1	Total	Mg	0	0
			1	1		
81	C4	2	Total	Mg	0	0
			2	2		
81	C8	1	Total	Mg	0	0
			1	1		
81	D2	2	Total	Mg	0	0
			2	2		
81	D9	1	Total	Mg	0	0
			1	1		
81	SM	1	Total	Mg	0	0
			1	1		
81	1	407	Total	Mg	0	0
			407	407		
81	3	9	Total	Mg	0	0
			9	9		
81	4	25	Total	Mg	1	0
			25	25		
81	L2	3	Total	Mg	0	0
			3	3		
81	L3	2	Total	Mg	0	0
			2	2		
81	L5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	L6	1	Total Mg 1 1	0	0
81	L8	1	Total Mg 1 1	0	0
81	M0	2	Total Mg 2 2	0	0
81	M4	1	Total Mg 1 1	0	0
81	M5	1	Total Mg 1 1	0	0
81	M6	1	Total Mg 1 1	0	0
81	M7	6	Total Mg 6 6	0	0
81	N2	1	Total Mg 1 1	0	0
81	N7	1	Total Mg 1 1	0	0
81	N8	2	Total Mg 2 2	0	0
81	O2	3	Total Mg 3 3	0	0
81	O3	2	Total Mg 2 2	0	0
81	O5	1	Total Mg 1 1	0	0
81	O6	2	Total Mg 2 2	0	0
81	O7	1	Total Mg 1 1	0	0
81	O8	1	Total Mg 1 1	0	0
81	O9	1	Total Mg 1 1	0	0
81	Q2	1	Total Mg 1 1	0	0
81	6	112	Total Mg 112 112	0	0
81	s8	2	Total Mg 2 2	0	0
81	c3	1	Total Mg 1 1	0	0

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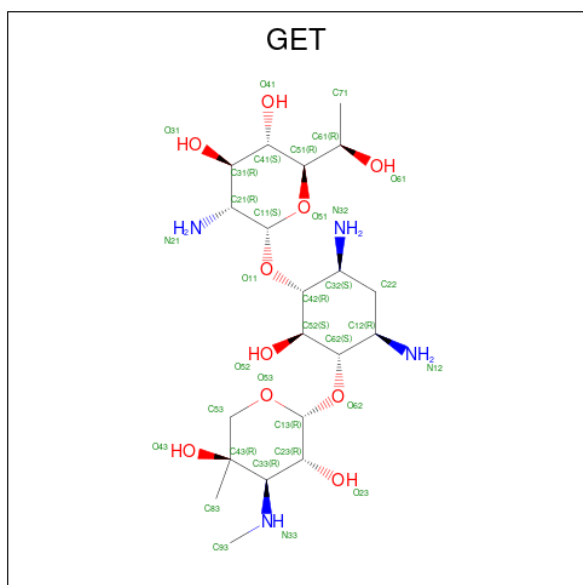
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	d3	2	Total 2	Mg 2	0	0
81	sM	1	Total 1	Mg 1	0	0
81	5	443	Total 443	Mg 443	1	0
81	7	8	Total 8	Mg 8	0	0
81	8	14	Total 14	Mg 14	0	0
81	l2	4	Total 4	Mg 4	0	0
81	l3	4	Total 4	Mg 4	0	0
81	l4	1	Total 1	Mg 1	0	0
81	l7	2	Total 2	Mg 2	0	0
81	l9	1	Total 1	Mg 1	0	0
81	m0	1	Total 1	Mg 1	0	0
81	m6	1	Total 1	Mg 1	0	0
81	m7	5	Total 5	Mg 5	0	0
81	n0	2	Total 2	Mg 2	0	0
81	n3	2	Total 2	Mg 2	0	0
81	n4	1	Total 1	Mg 1	0	0
81	n5	1	Total 1	Mg 1	0	0
81	n7	1	Total 1	Mg 1	0	0
81	o2	2	Total 2	Mg 2	0	0
81	o3	3	Total 3	Mg 3	0	0
81	o5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	o7	5	Total Mg 5 5	0	0
81	q2	4	Total Mg 4 4	0	0

- Molecule 82 is GENETICIN (three-letter code: GET) (formula: C₂₀H₄₀N₄O₁₀).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	2	1	Total C N O 34 20 4 10	0	0
82	2	1	Total C N O 34 20 4 10	0	0
82	2	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0
82	1	1	Total C N O 34 20 4 10	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
82	6	1	Total	C	N	O	0	0
			34	20	4	10		
82	6	1	Total	C	N	O	0	0
			34	20	4	10		
82	6	1	Total	C	N	O	0	0
			34	20	4	10		
82	5	1	Total	C	N	O	0	0
			34	20	4	10		
82	5	1	Total	C	N	O	0	0
			34	20	4	10		
82	5	1	Total	C	N	O	0	0
			34	20	4	10		
82	5	1	Total	C	N	O	0	0
			34	20	4	10		
82	5	1	Total	C	N	O	0	0
			34	20	4	10		
82	5	1	Total	C	N	O	0	0
			34	20	4	10		
82	n6	1	Total	C	N	O	0	0
			34	20	4	10		

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	D6	1	Total	Zn	0	0
			1	1		
83	D7	1	Total	Zn	0	0
			1	1		
83	D9	1	Total	Zn	0	0
			1	1		
83	E1	1	Total	Zn	0	0
			1	1		
83	O4	1	Total	Zn	0	0
			1	1		
83	O7	1	Total	Zn	0	0
			1	1		
83	Q0	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	Q2	1	Total 1	Zn 1	0	0
83	Q3	1	Total 1	Zn 1	0	0
83	d6	1	Total 1	Zn 1	0	0
83	d7	1	Total 1	Zn 1	0	0
83	d9	1	Total 1	Zn 1	0	0
83	e1	1	Total 1	Zn 1	0	0
83	o4	1	Total 1	Zn 1	0	0
83	o7	1	Total 1	Zn 1	0	0
83	q0	1	Total 1	Zn 1	0	0
83	q2	1	Total 1	Zn 1	0	0
83	q3	1	Total 1	Zn 1	0	0

- Molecule 84 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	2	99	Total 99	O 99	0	0
84	S4	1	Total 1	O 1	0	0
84	C1	1	Total 1	O 1	0	0
84	C3	1	Total 1	O 1	0	0
84	C6	1	Total 1	O 1	0	0
84	C9	2	Total 2	O 2	0	0
84	D3	1	Total 1	O 1	0	0
84	D9	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	SM	1	Total O 1 1	0	0
84	1	367	Total O 367 367	2	0
84	3	18	Total O 18 18	0	0
84	4	7	Total O 7 7	0	0
84	L2	1	Total O 1 1	0	0
84	L3	1	Total O 1 1	0	0
84	L4	1	Total O 1 1	0	0
84	M0	2	Total O 2 2	0	0
84	M5	1	Total O 1 1	0	0
84	M6	2	Total O 2 2	0	0
84	M7	4	Total O 4 4	0	0
84	N1	3	Total O 3 3	0	0
84	N3	3	Total O 3 3	0	0
84	N5	1	Total O 1 1	0	0
84	N8	1	Total O 1 1	0	0
84	O1	2	Total O 2 2	0	0
84	O2	2	Total O 2 2	0	0
84	6	111	Total O 111 111	0	0
84	c3	1	Total O 1 1	0	0
84	c8	1	Total O 1 1	0	0
84	c9	2	Total O 2 2	0	0

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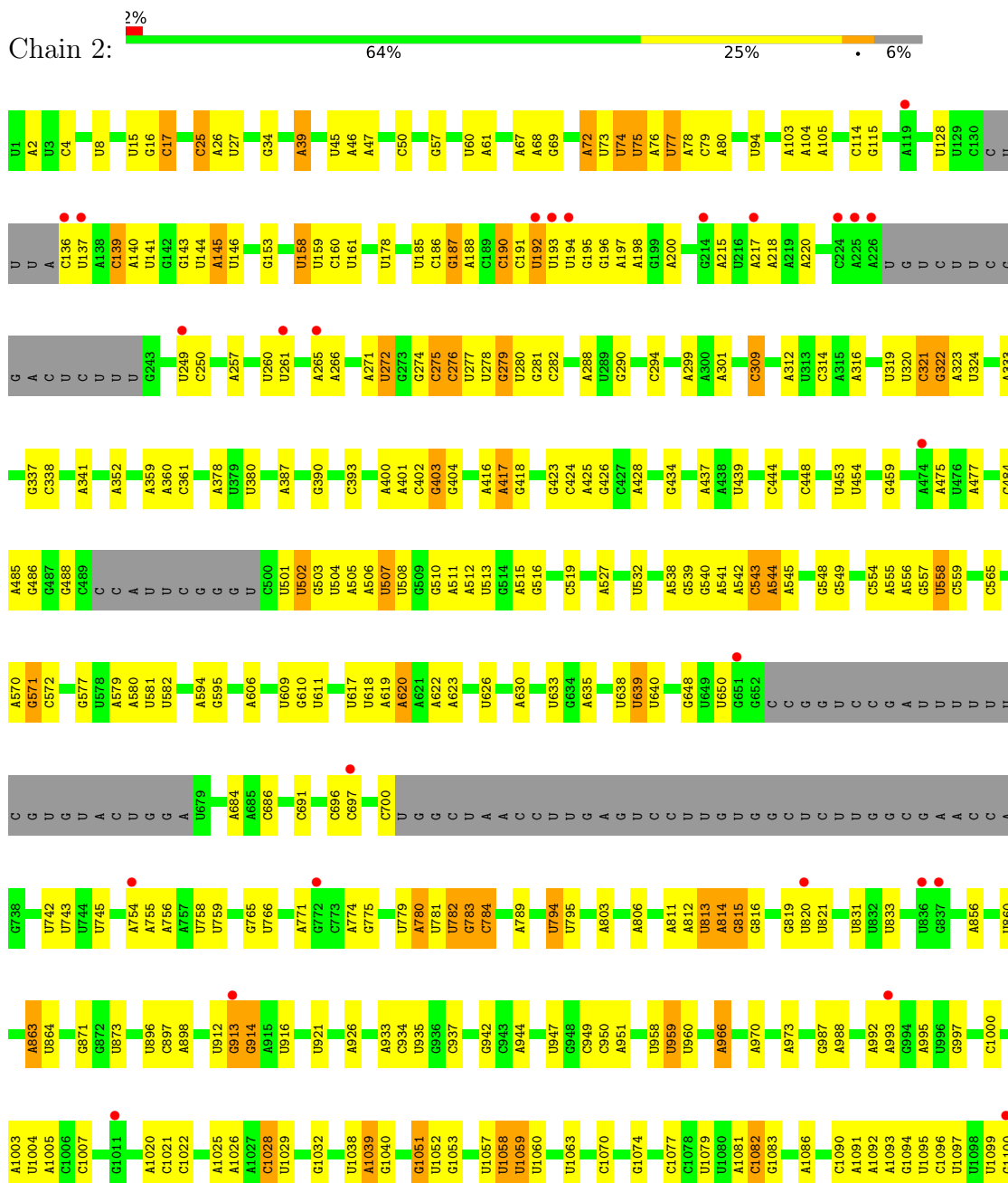
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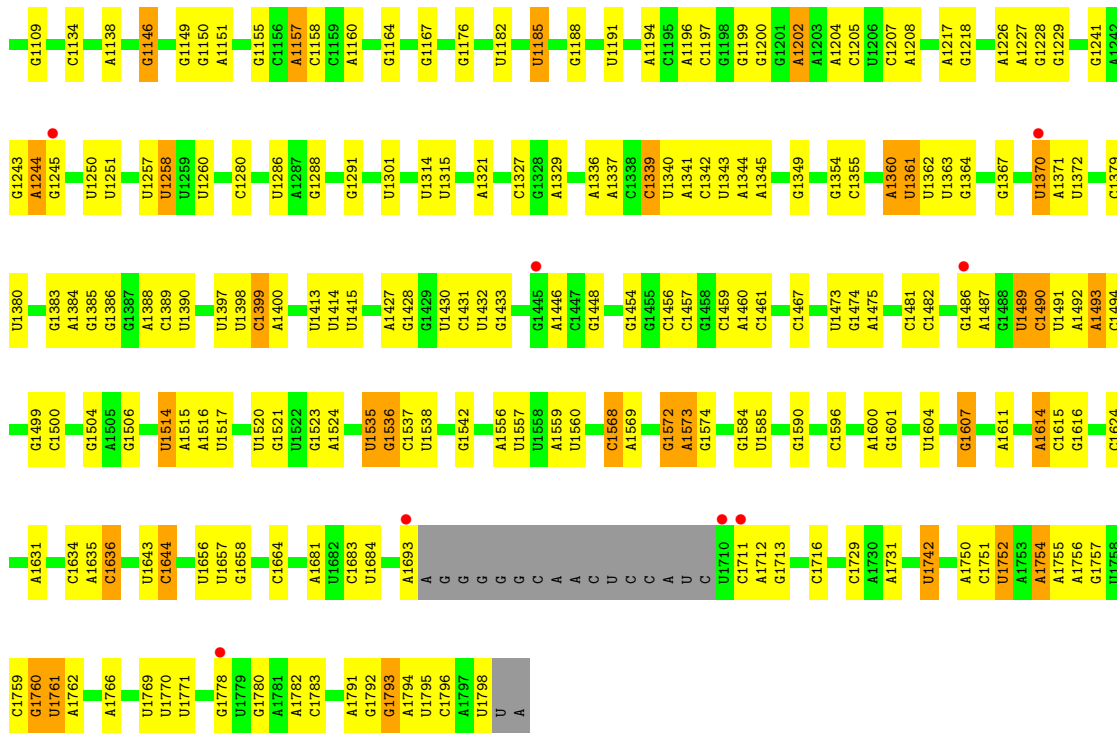
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84	d3	2	Total O 2 2	0	0
84	5	365	Total O 365 365	1	0
84	7	11	Total O 11 11	0	0
84	8	7	Total O 7 7	0	0
84	l2	1	Total O 1 1	0	0
84	l3	4	Total O 4 4	0	0
84	l4	2	Total O 2 2	0	0
84	l9	1	Total O 1 1	0	0
84	m0	1	Total O 1 1	0	0
84	m5	3	Total O 3 3	0	0
84	m6	1	Total O 1 1	0	0
84	m7	2	Total O 2 2	0	0
84	m9	2	Total O 2 2	0	0
84	n1	3	Total O 3 3	0	0
84	n3	3	Total O 3 3	0	0
84	o2	3	Total O 3 3	0	0
84	o4	2	Total O 2 2	0	0
84	o7	1	Total O 1 1	0	0
84	q2	1	Total O 1 1	0	0

3 Residue-property plots

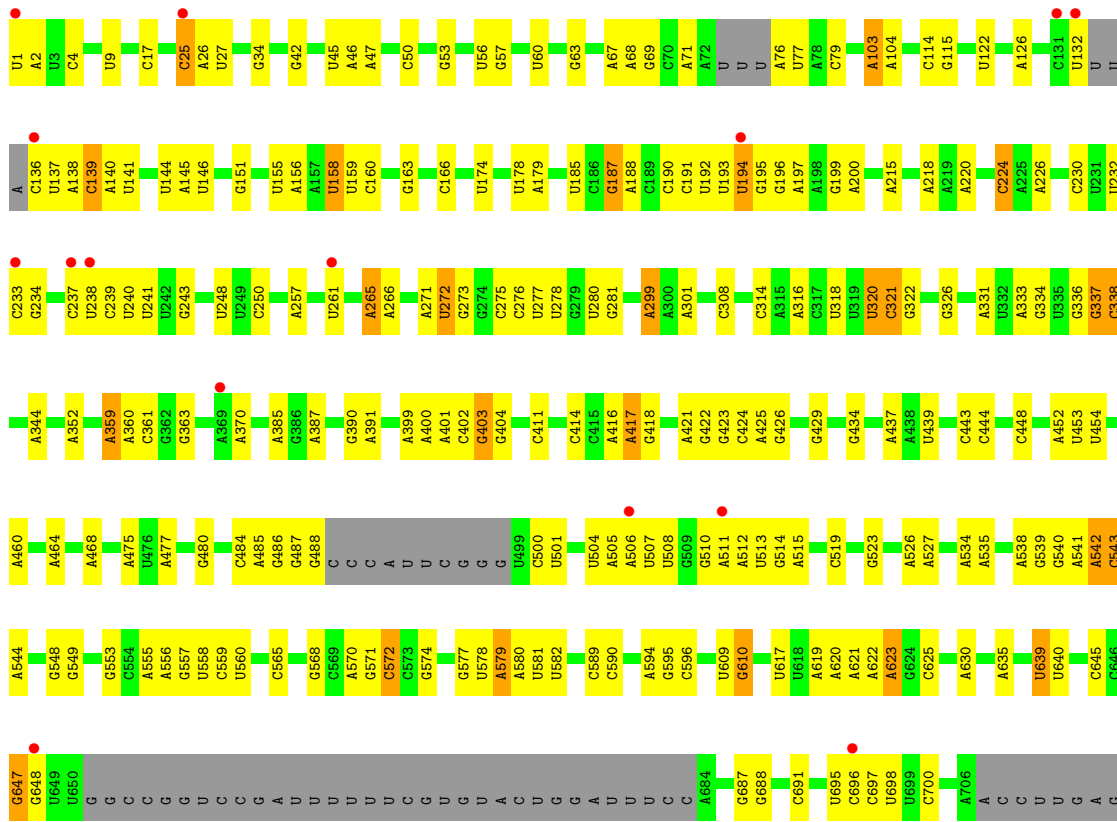
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

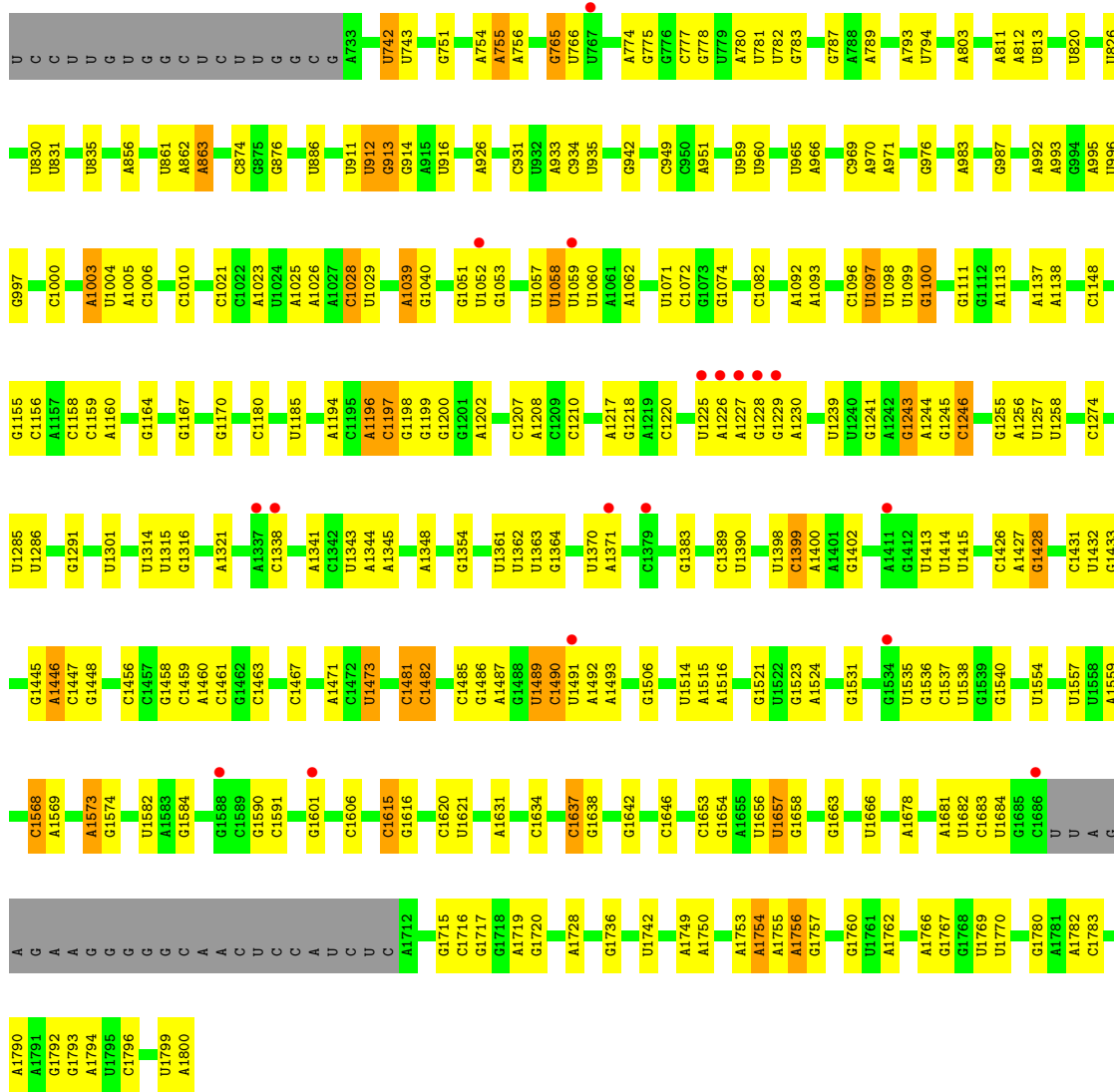
- Molecule 1: 18S ribosomal RNA



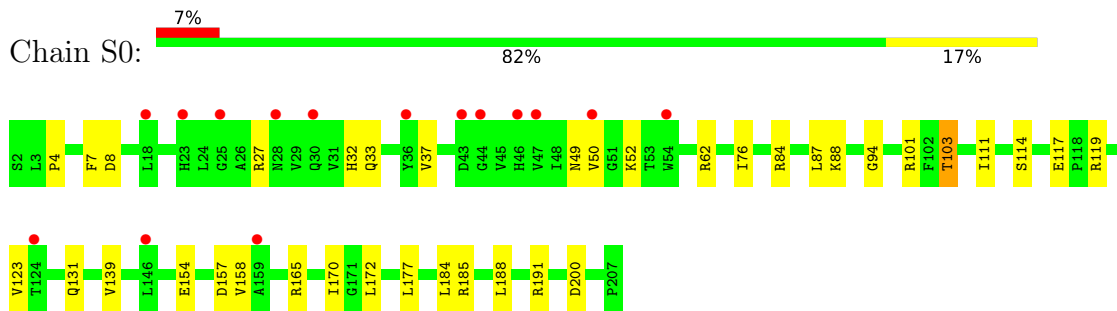


• Molecule 1: 18S ribosomal RNA

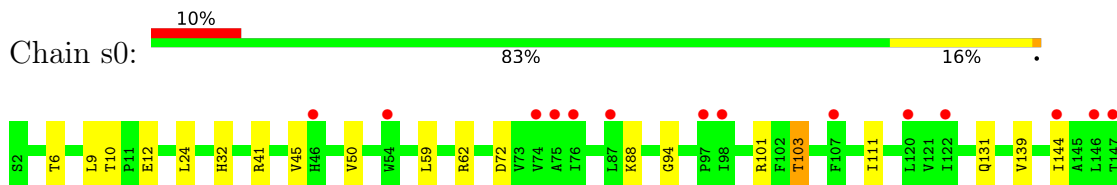




• Molecule 2: 40S ribosomal protein S0-A

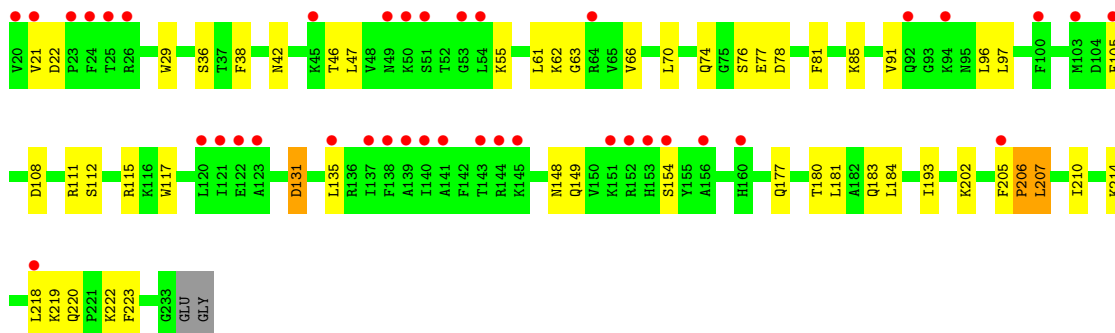
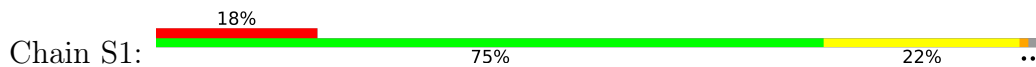


• Molecule 2: 40S ribosomal protein S0-A

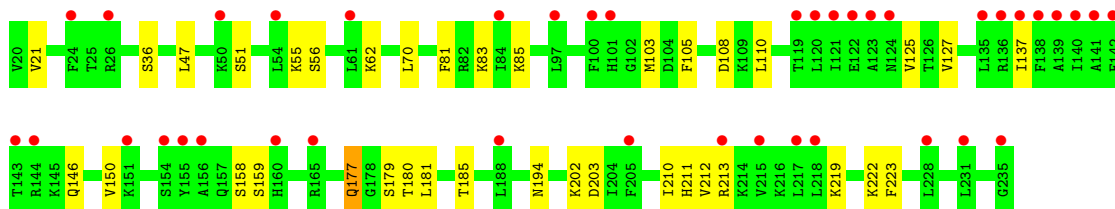
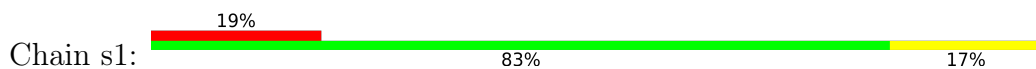




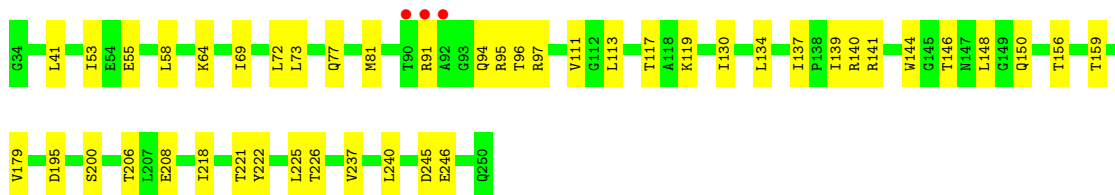
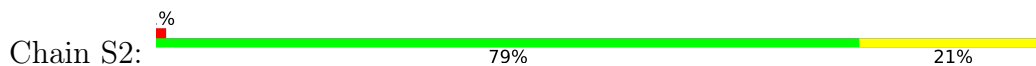
- Molecule 3: 40S ribosomal protein S1-A



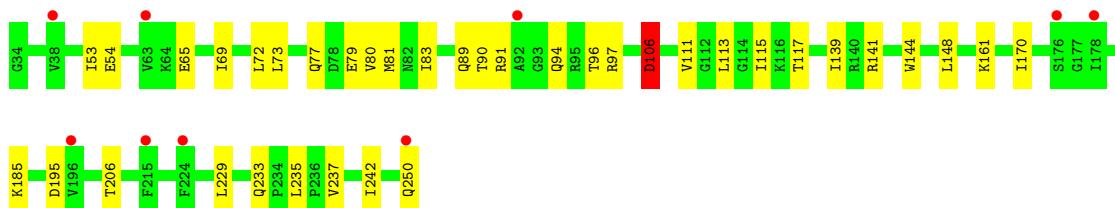
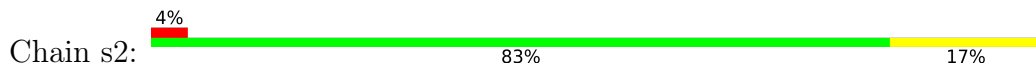
- Molecule 3: 40S ribosomal protein S1-A



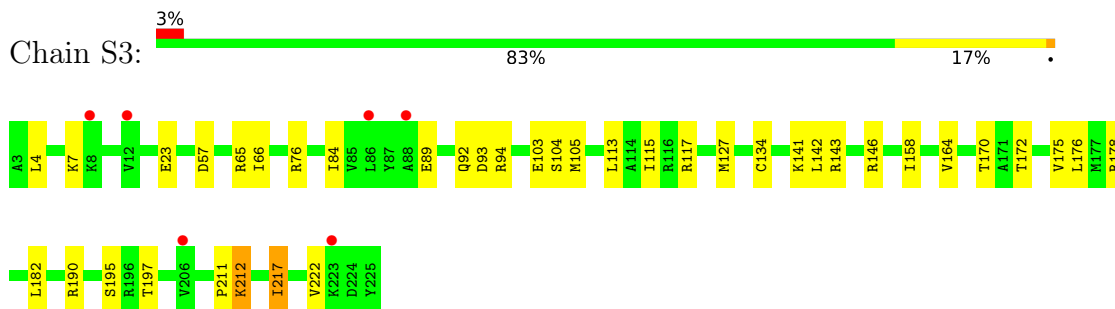
- Molecule 4: 40S ribosomal protein S2



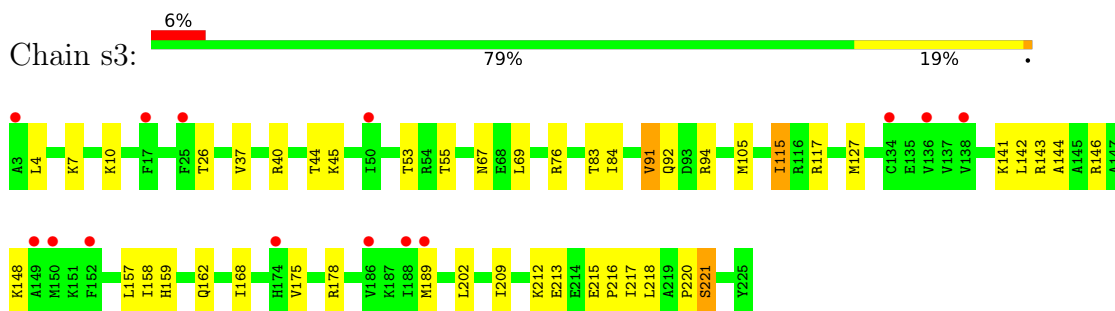
- Molecule 4: 40S ribosomal protein S2



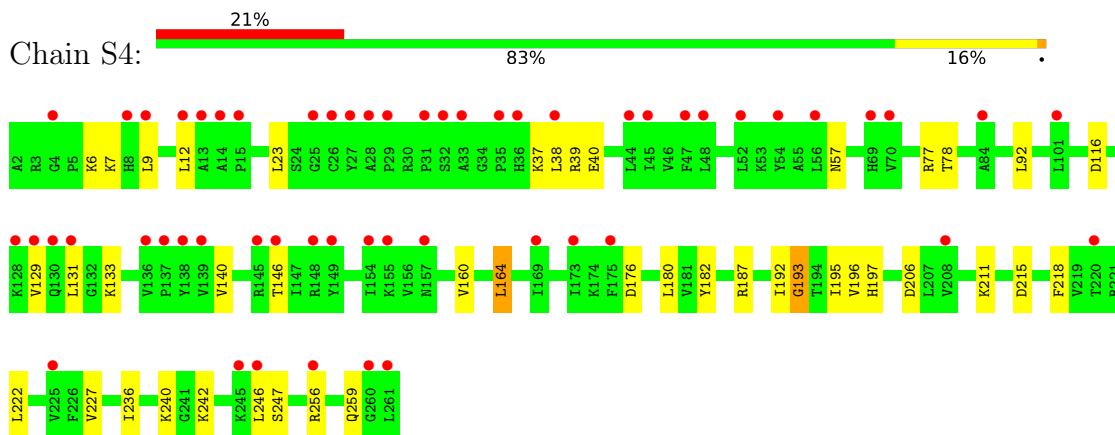
- Molecule 5: 40S ribosomal protein S3



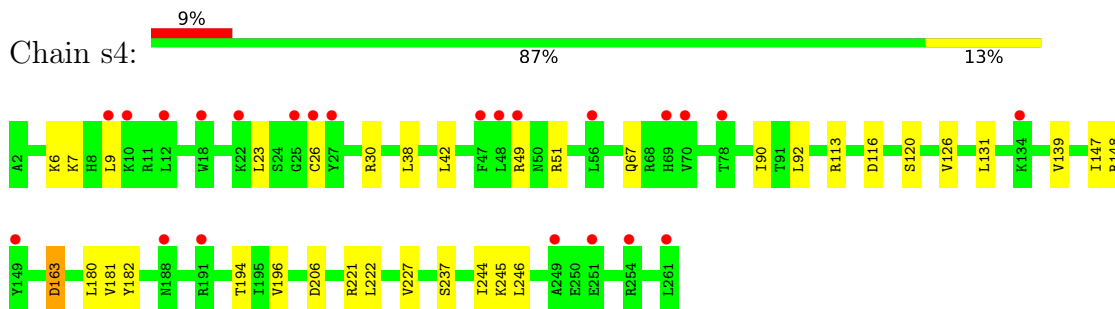
- Molecule 5: 40S ribosomal protein S3



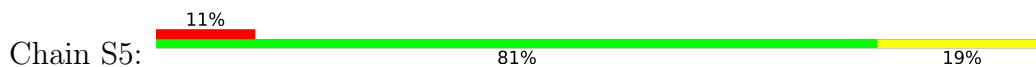
- Molecule 6: 40S ribosomal protein S4-A

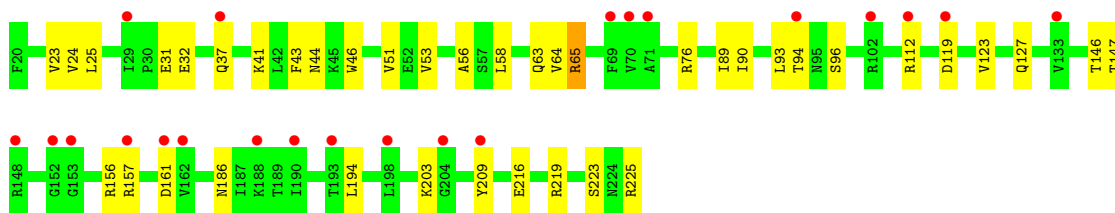


- Molecule 6: 40S ribosomal protein S4-A

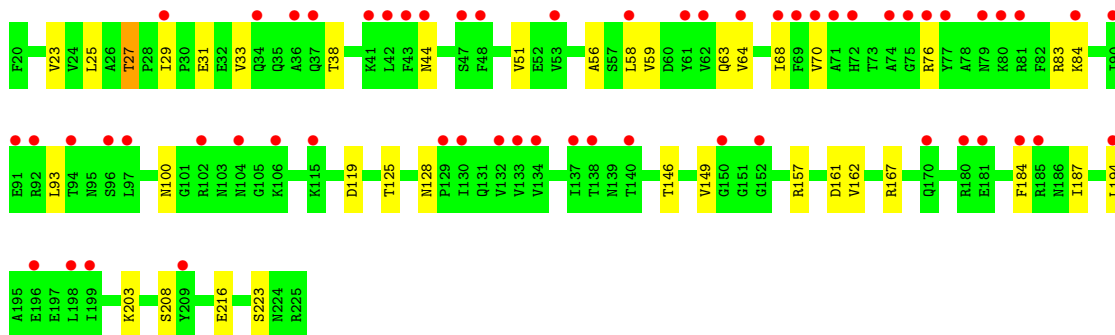
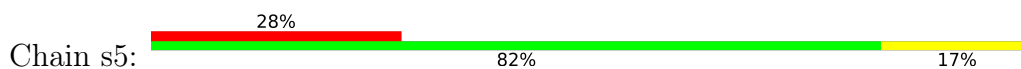


- Molecule 7: 40S ribosomal protein S5

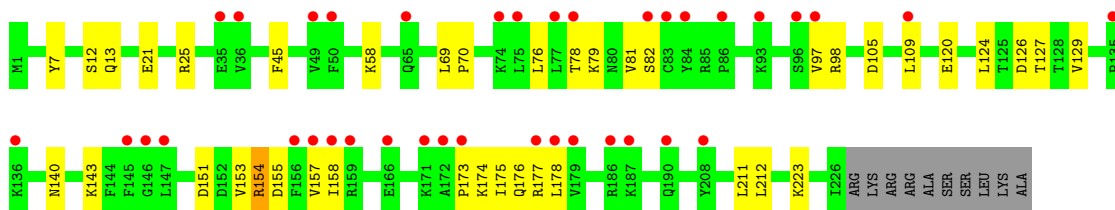
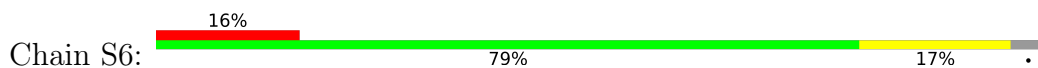




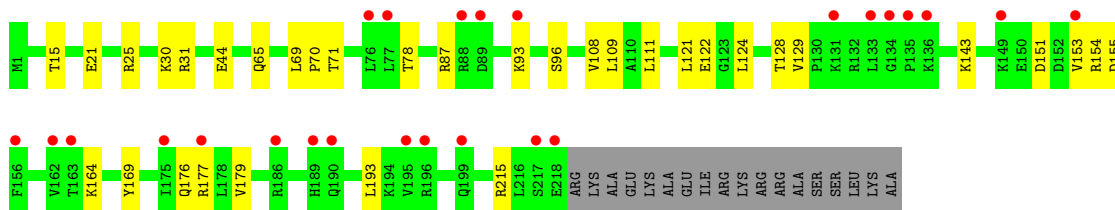
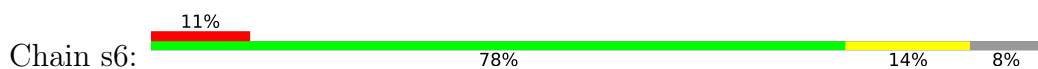
• Molecule 7: 40S ribosomal protein S5



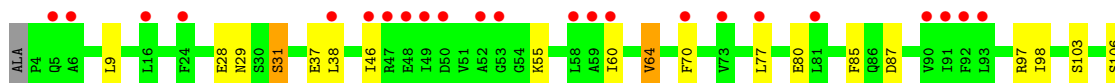
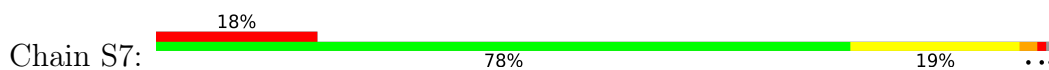
• Molecule 8: 40S ribosomal protein S6-A

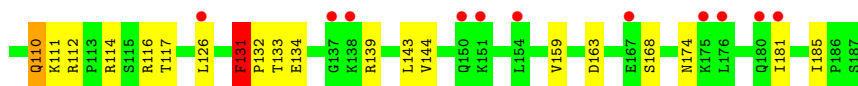


• Molecule 8: 40S ribosomal protein S6-A

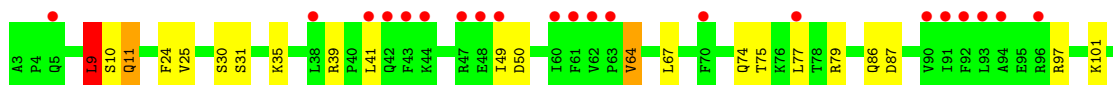
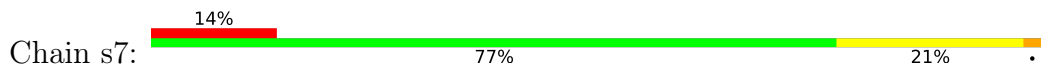


• Molecule 9: 40S ribosomal protein S7-A

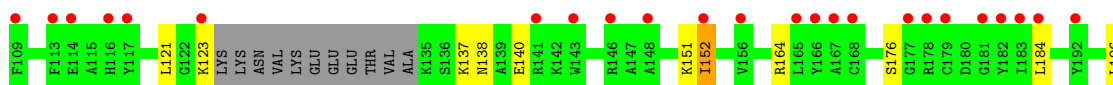
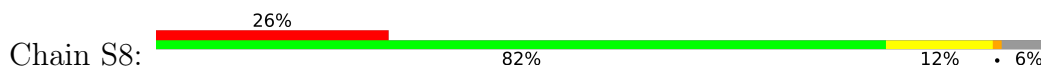




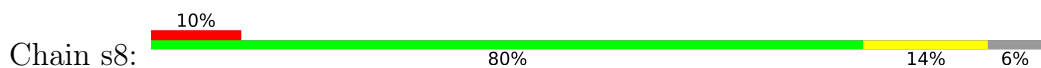
- Molecule 9: 40S ribosomal protein S7-A



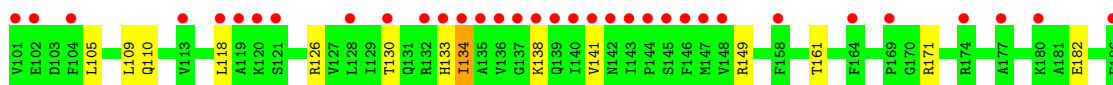
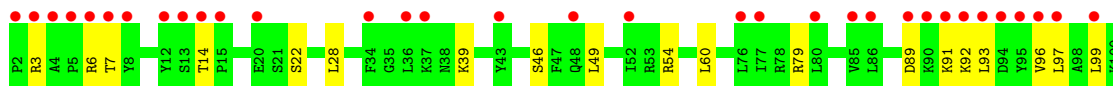
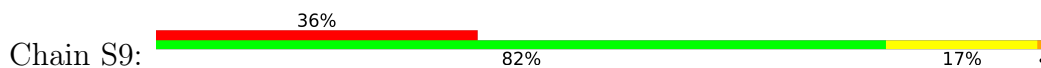
- Molecule 10: 40S ribosomal protein S8-A



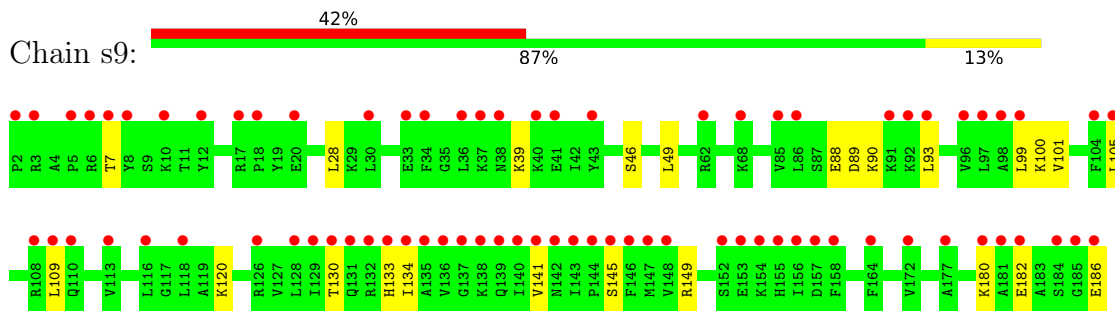
- Molecule 10: 40S ribosomal protein S8-A



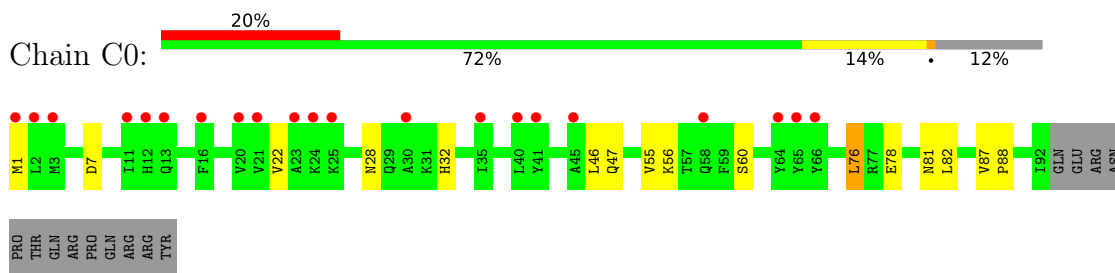
- Molecule 11: 40S ribosomal protein S9-A



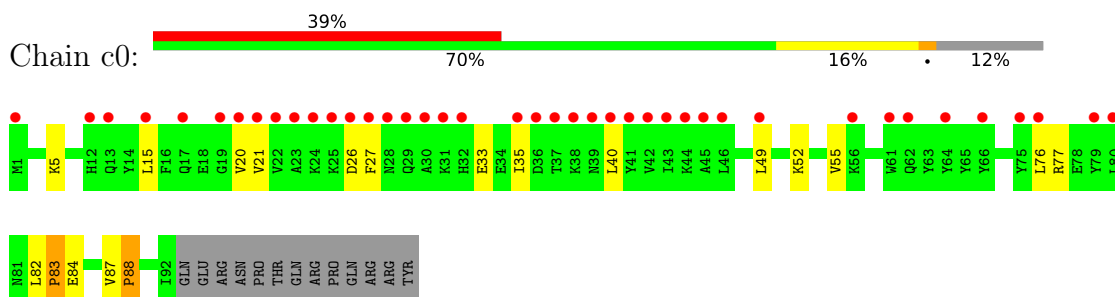
• Molecule 11: 40S ribosomal protein S9-A



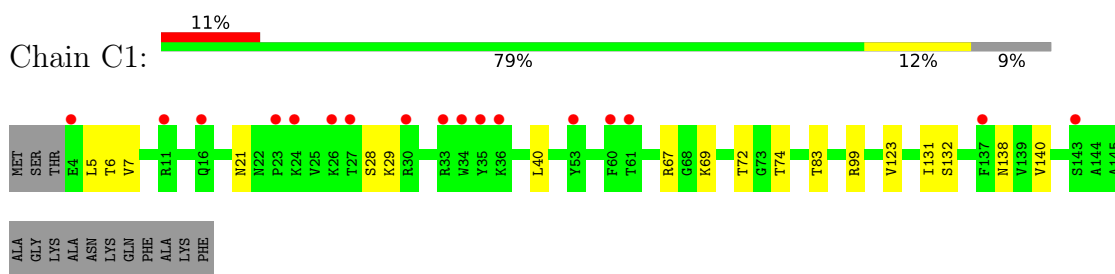
• Molecule 12: 40S ribosomal protein S10-A



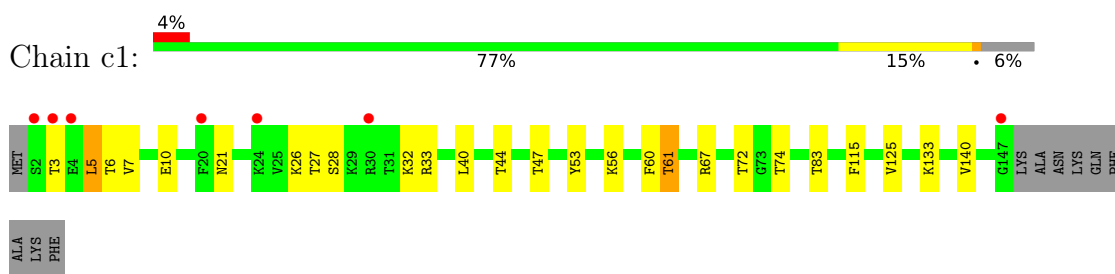
• Molecule 12: 40S ribosomal protein S10-A



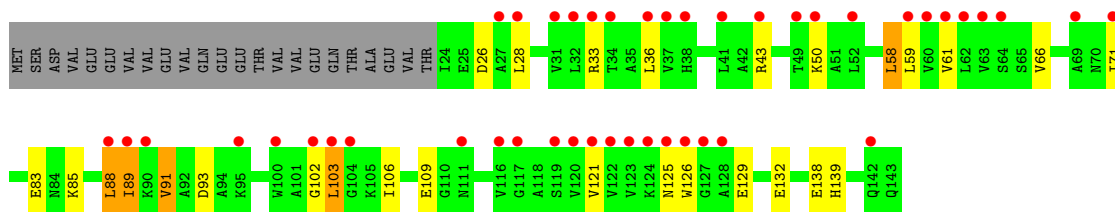
• Molecule 13: 40S ribosomal protein S11-A



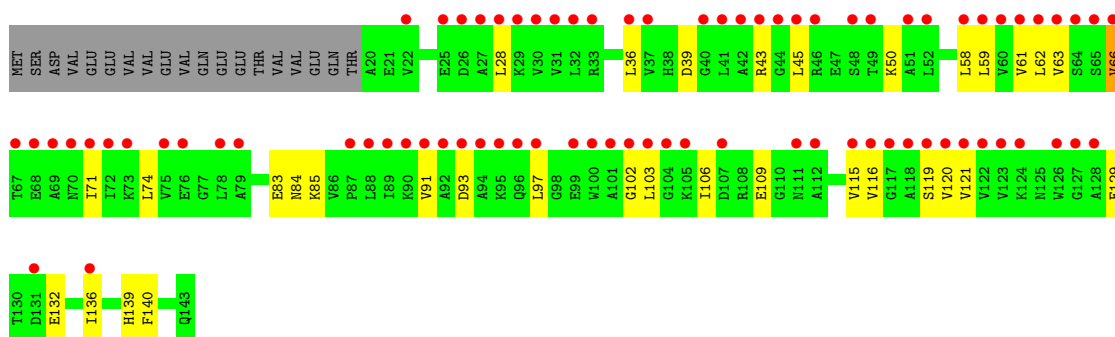
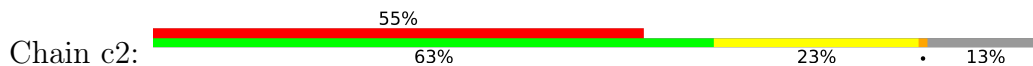
• Molecule 13: 40S ribosomal protein S11-A



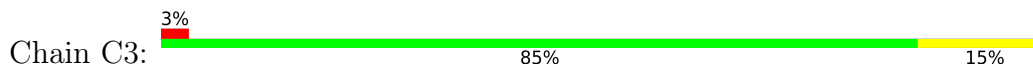
• Molecule 14: 40S ribosomal protein S12



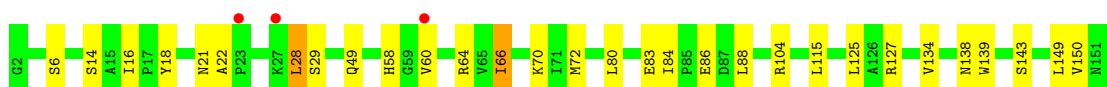
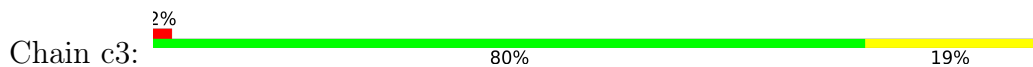
• Molecule 14: 40S ribosomal protein S12



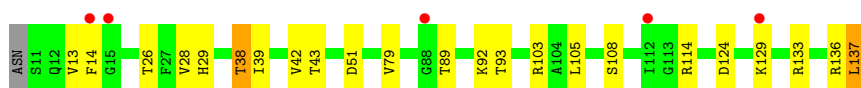
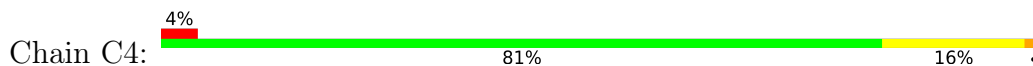
• Molecule 15: 40S ribosomal protein S13



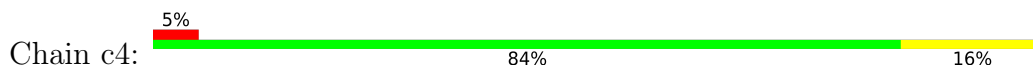
• Molecule 15: 40S ribosomal protein S13



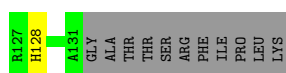
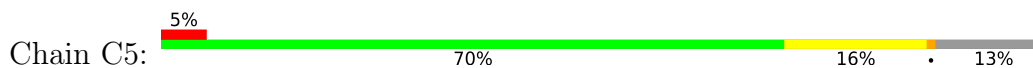
• Molecule 16: 40S ribosomal protein S14-A



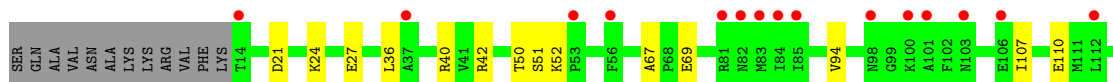
• Molecule 16: 40S ribosomal protein S14-A



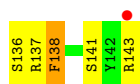
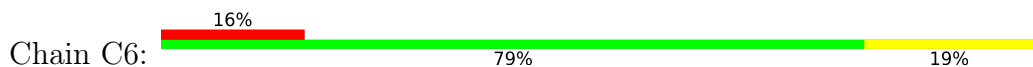
- Molecule 17: 40S ribosomal protein S15



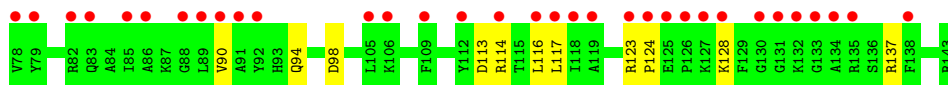
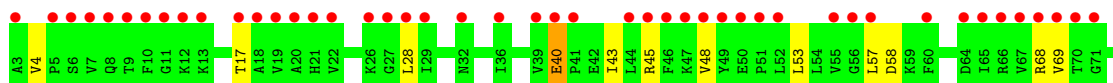
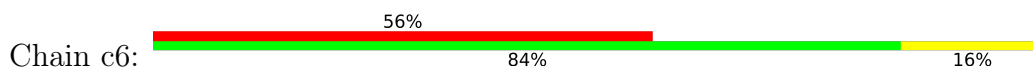
- Molecule 17: 40S ribosomal protein S15



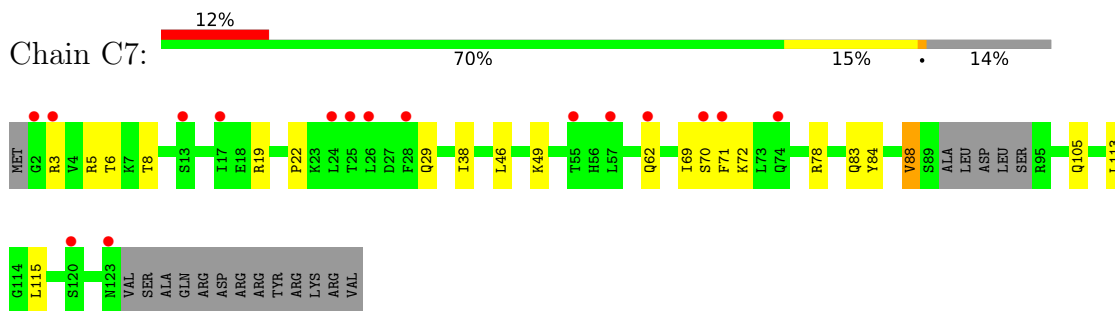
- Molecule 18: 40S ribosomal protein S16-A



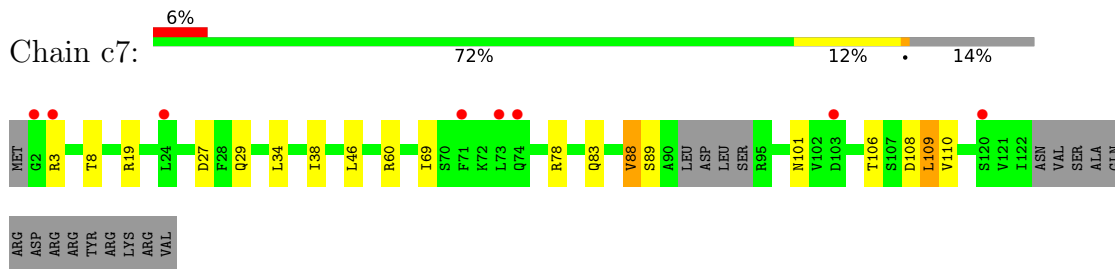
- Molecule 18: 40S ribosomal protein S16-A



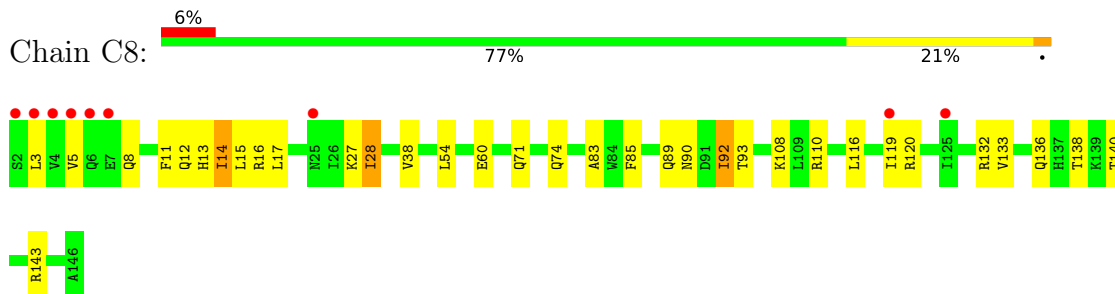
- Molecule 19: 40S ribosomal protein S17-A



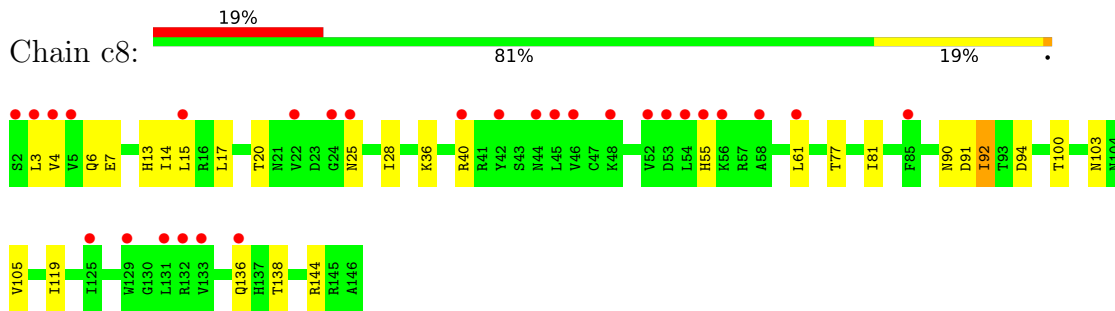
• Molecule 19: 40S ribosomal protein S17-A



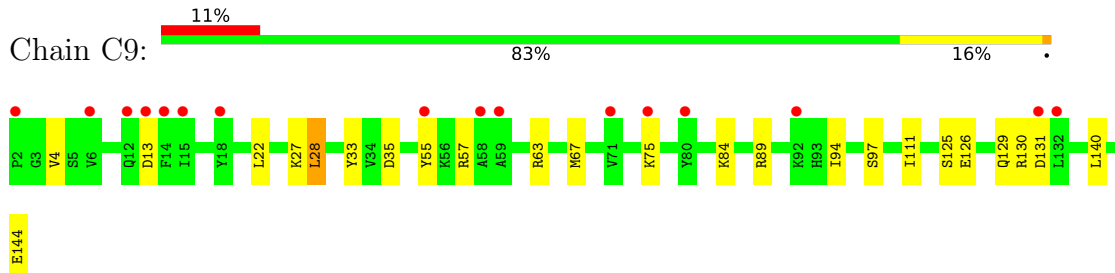
• Molecule 20: 40S ribosomal protein S18-A



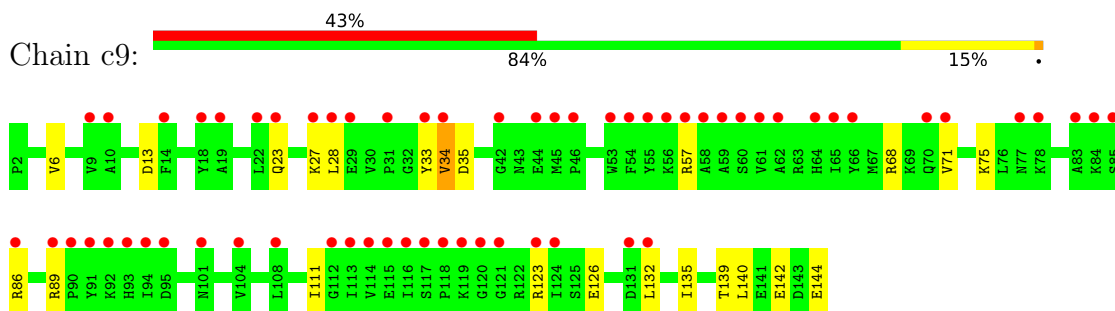
• Molecule 20: 40S ribosomal protein S18-A



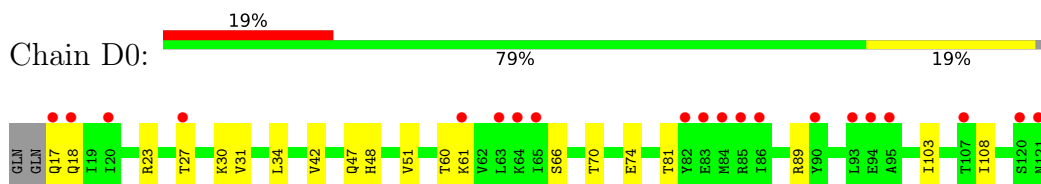
• Molecule 21: 40S ribosomal protein S19-A



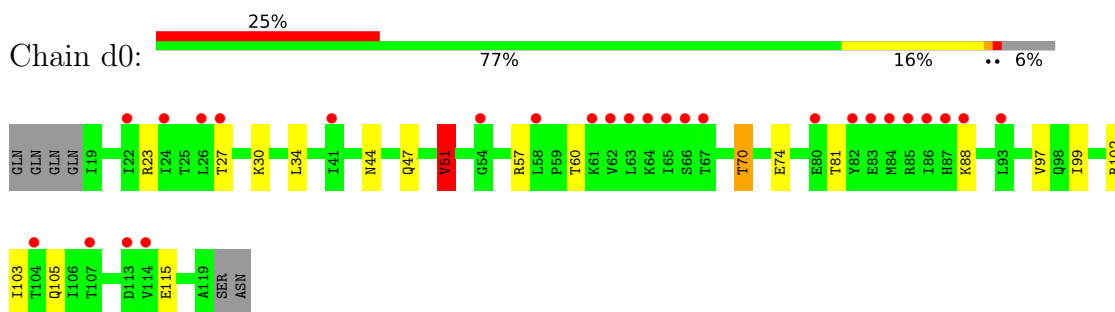
- Molecule 21: 40S ribosomal protein S19-A



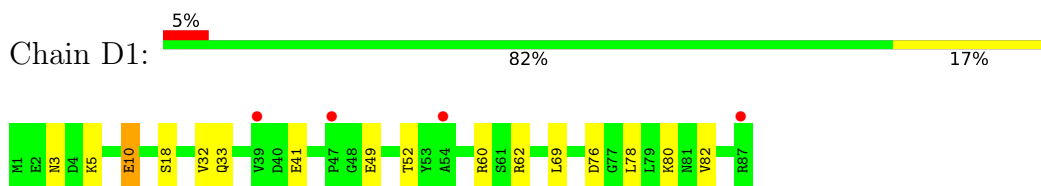
- Molecule 22: 40S ribosomal protein S20



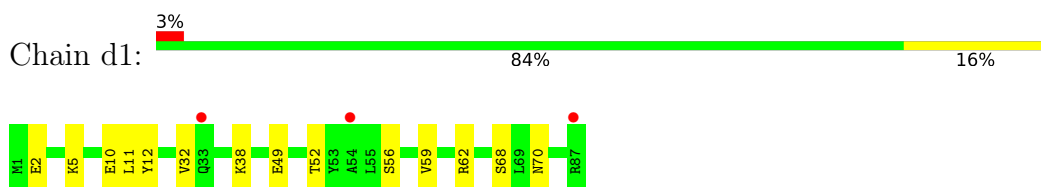
- Molecule 22: 40S ribosomal protein S20



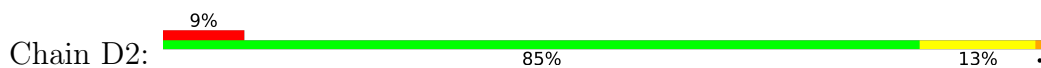
- Molecule 23: 40S ribosomal protein S21-A



- Molecule 23: 40S ribosomal protein S21-A

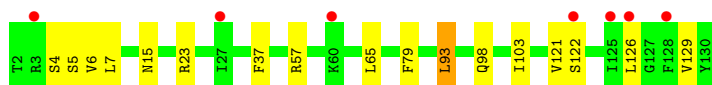
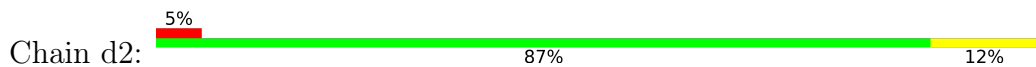


- Molecule 24: 40S ribosomal protein S22-A

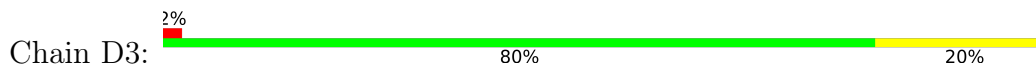




- Molecule 24: 40S ribosomal protein S22-A



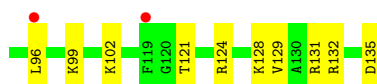
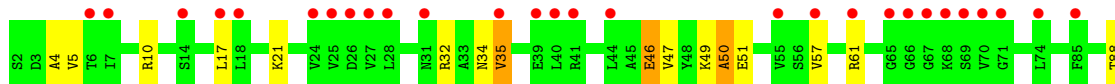
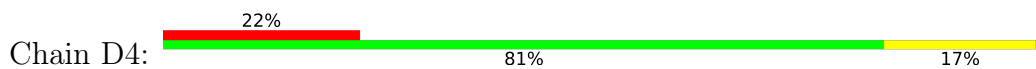
- Molecule 25: 40S ribosomal protein S23-A



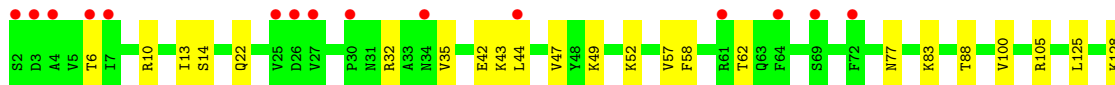
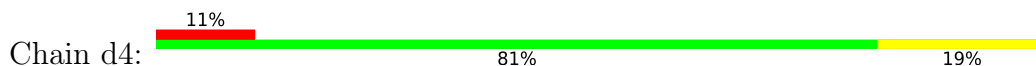
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A

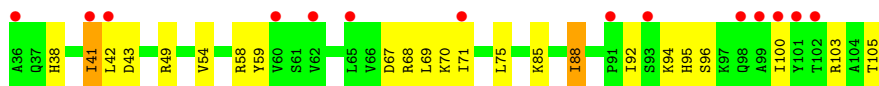


- Molecule 26: 40S ribosomal protein S24-A

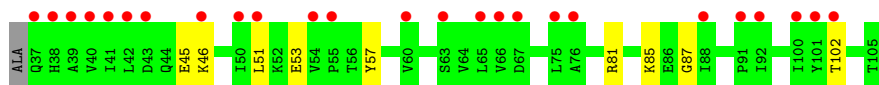
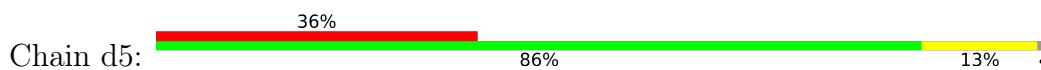


- Molecule 27: 40S ribosomal protein S25-A

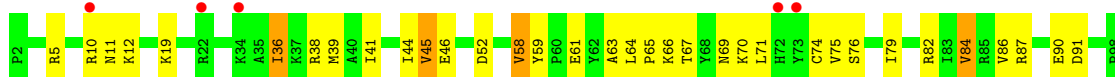




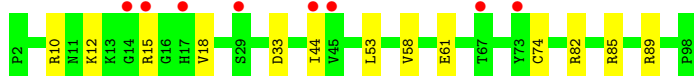
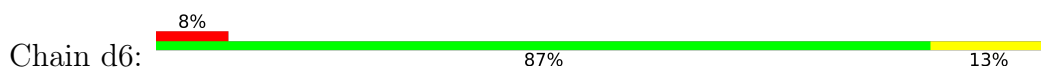
- Molecule 27: 40S ribosomal protein S25-A



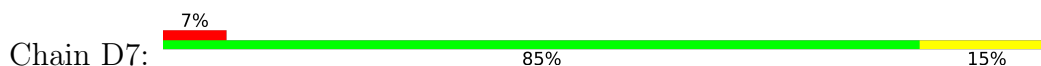
- Molecule 28: 40S ribosomal protein S26-B



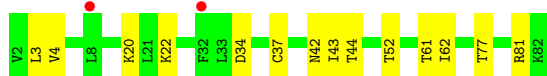
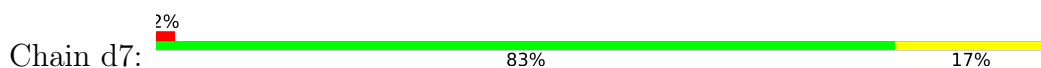
- Molecule 28: 40S ribosomal protein S26-B



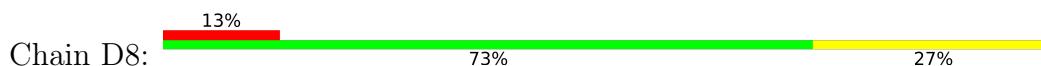
- Molecule 29: 40S ribosomal protein S27-A



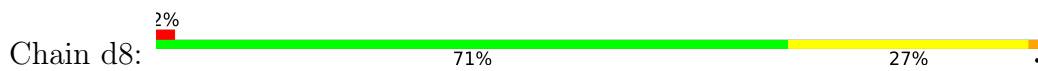
- Molecule 29: 40S ribosomal protein S27-A



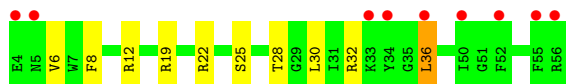
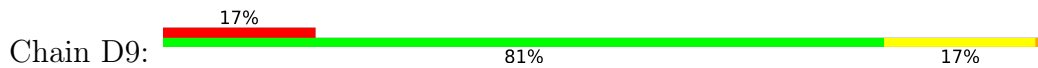
- Molecule 30: 40S ribosomal protein S28-A



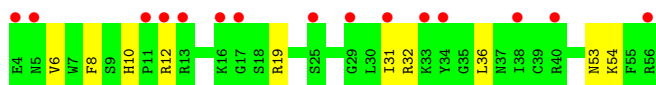
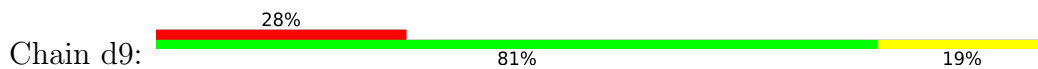
- Molecule 30: 40S ribosomal protein S28-A



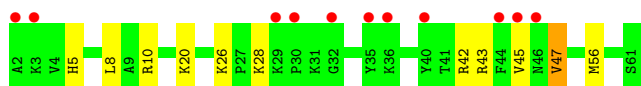
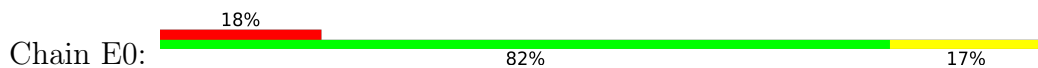
• Molecule 31: 40S ribosomal protein S29-A



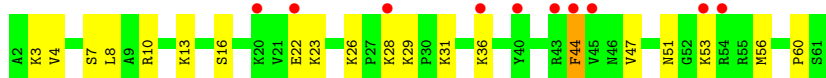
• Molecule 31: 40S ribosomal protein S29-A



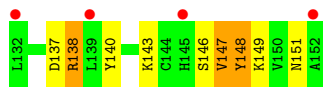
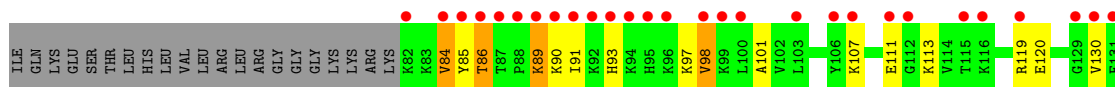
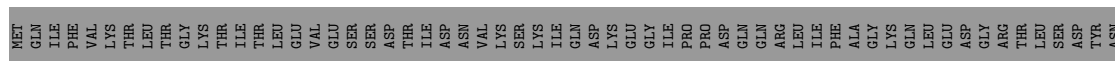
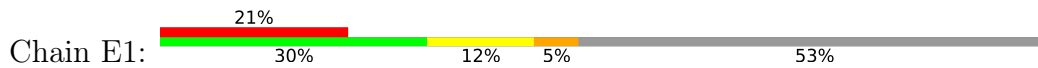
• Molecule 32: 40S ribosomal protein S30-A



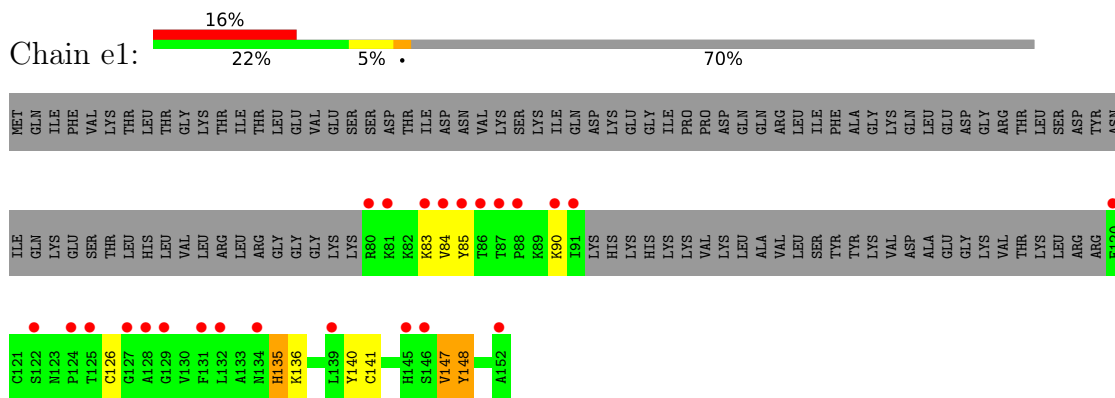
• Molecule 32: 40S ribosomal protein S30-A



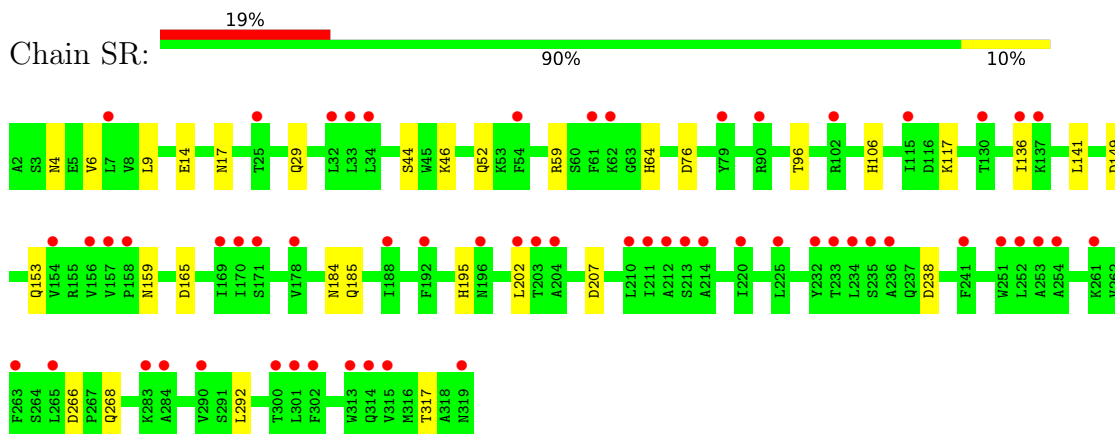
• Molecule 33: Ubiquitin-40S ribosomal protein S31



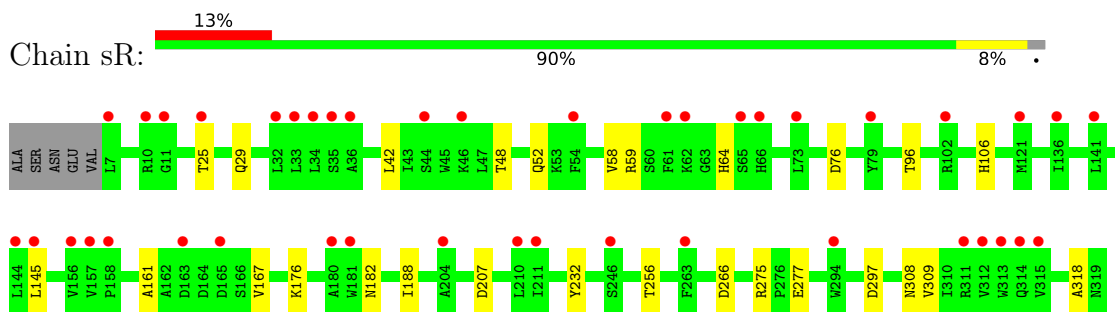
• Molecule 33: Ubiquitin-40S ribosomal protein S31



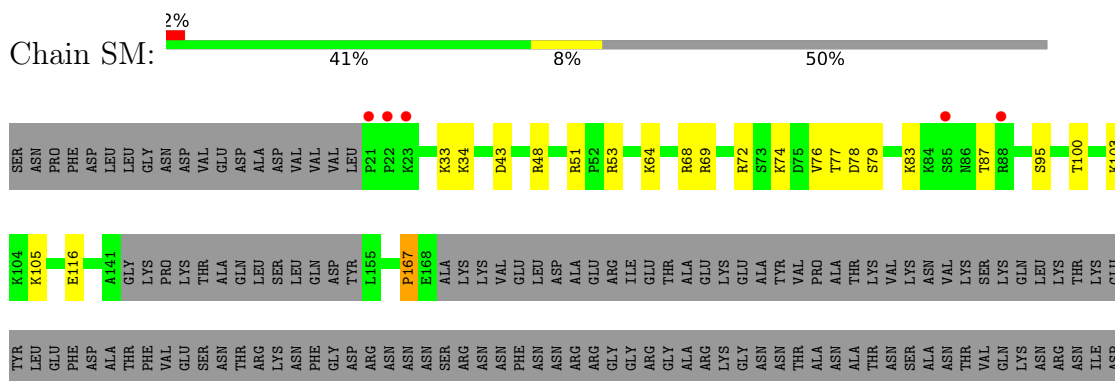
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

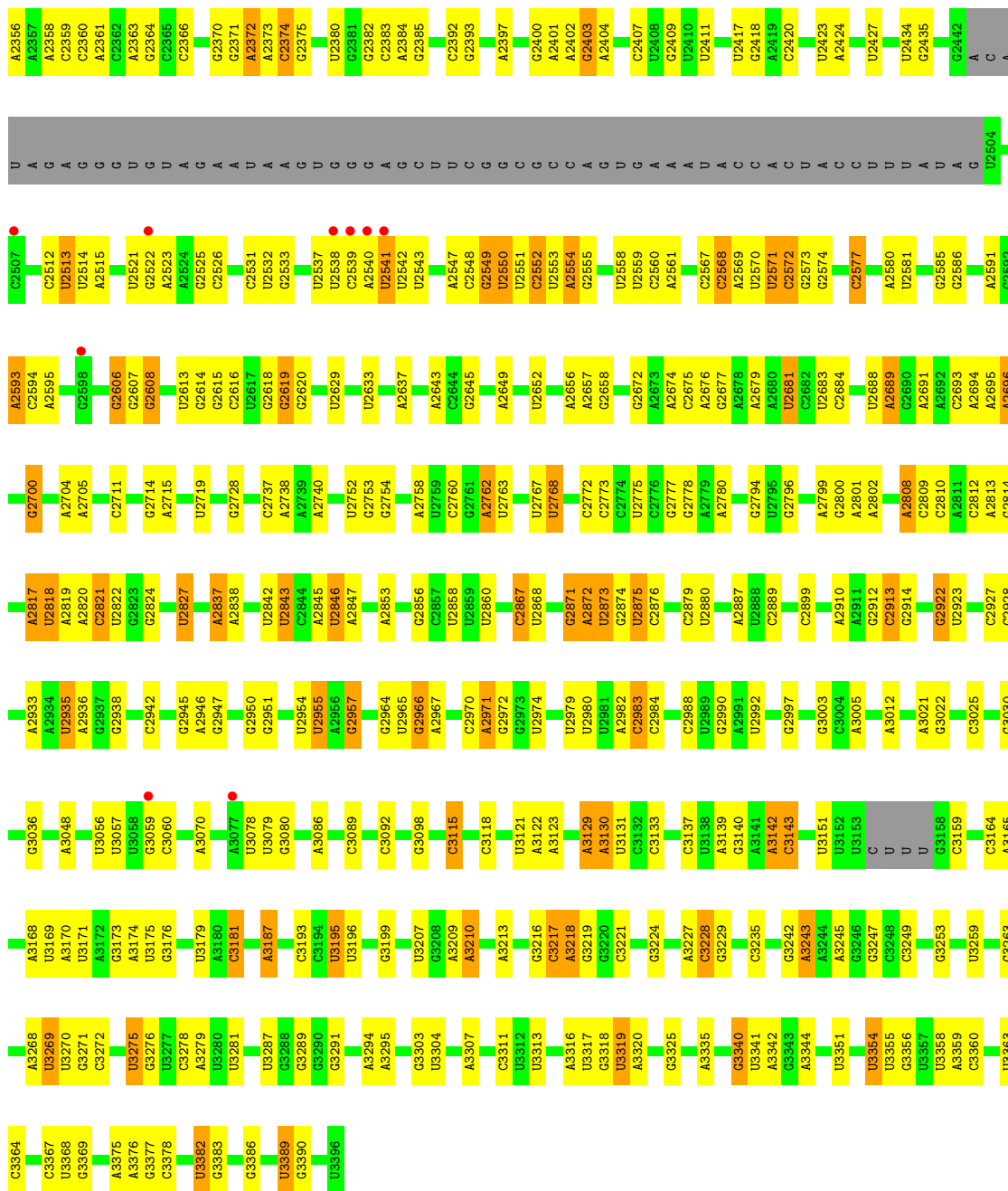


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

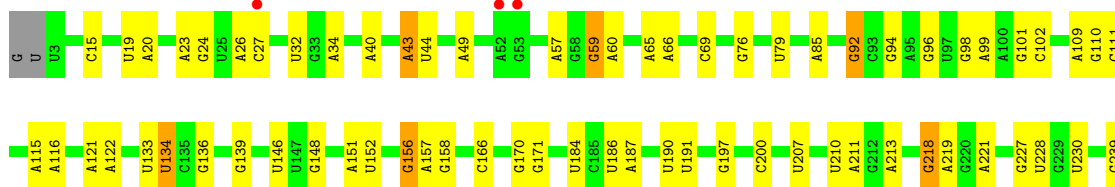


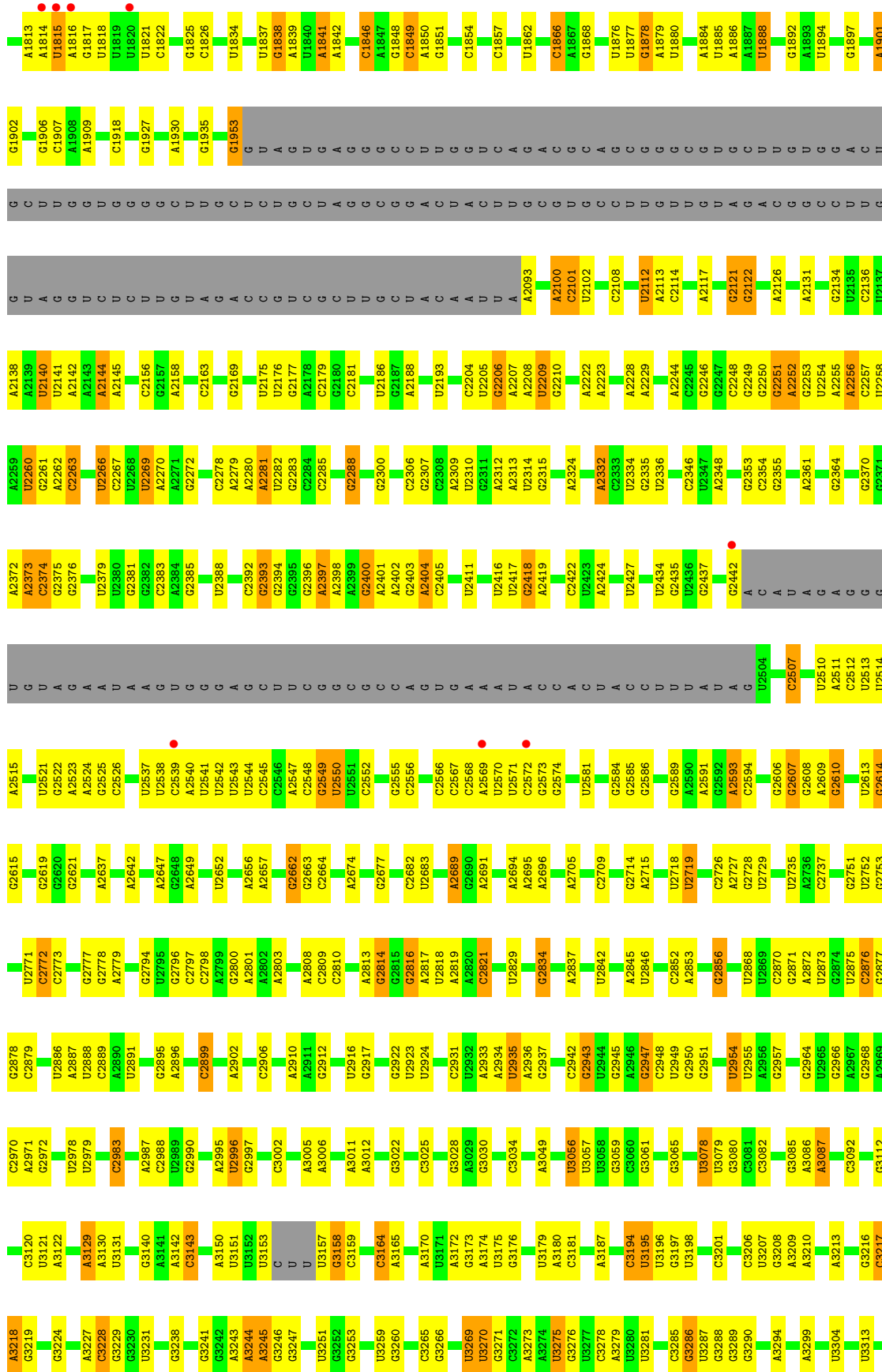
• Molecule 35: Suppressor protein STM1





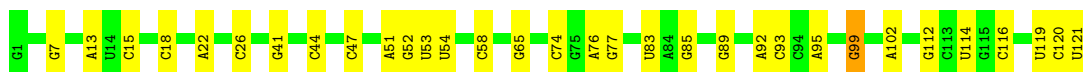
● Molecule 36: 25S ribosomal RNA



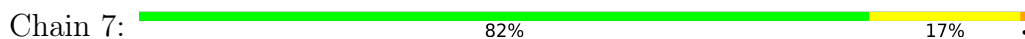




- Molecule 37: 5S ribosomal RNA



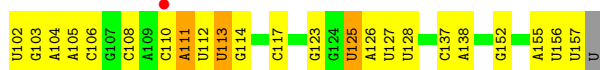
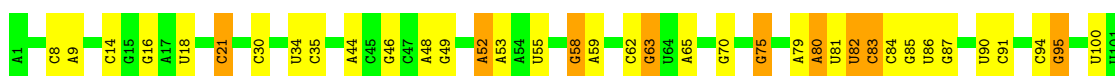
- Molecule 37: 5S ribosomal RNA



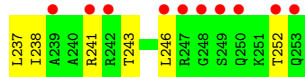
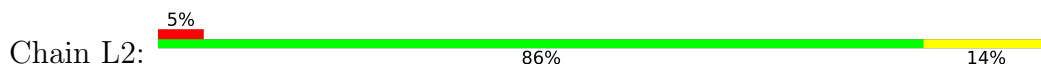
- Molecule 38: 5.8S ribosomal RNA



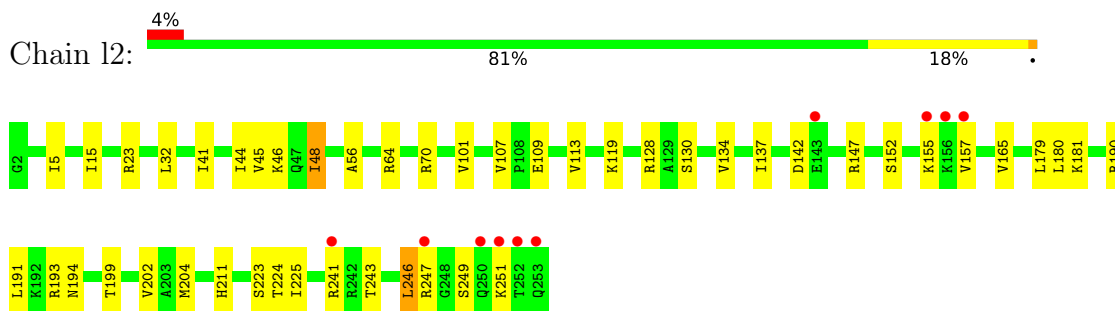
- Molecule 38: 5.8S ribosomal RNA



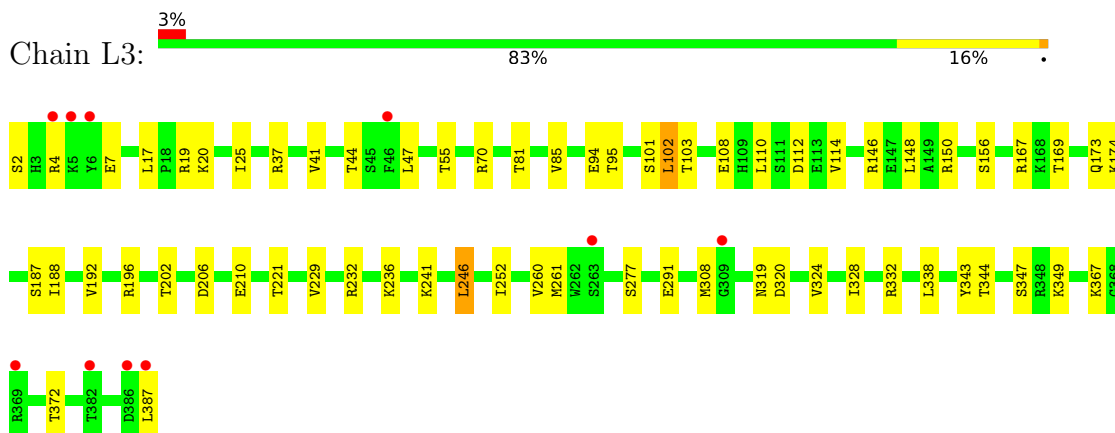
- Molecule 39: 60S ribosomal protein L2-A



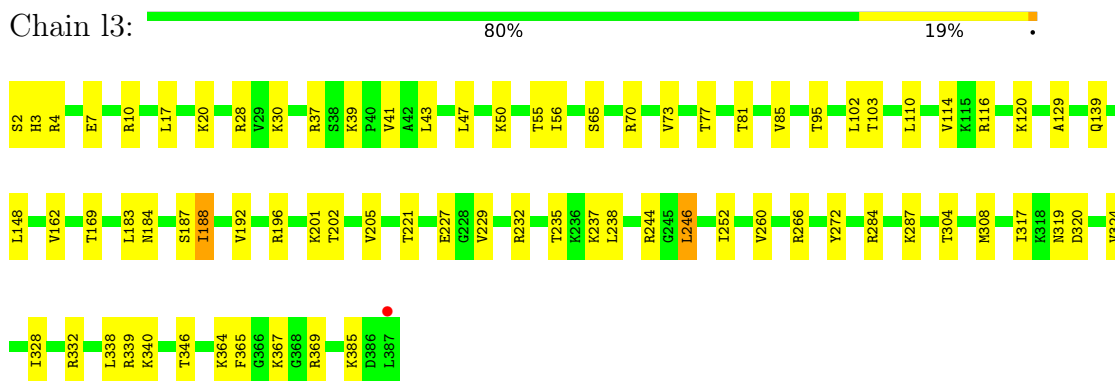
- Molecule 39: 60S ribosomal protein L2-A



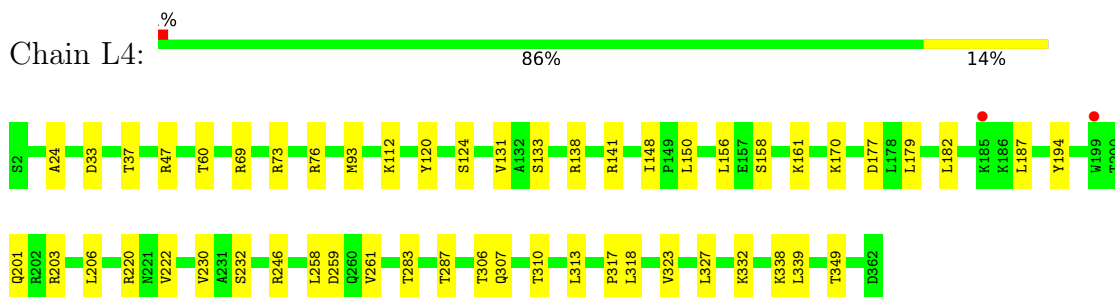
- Molecule 40: 60S ribosomal protein L3



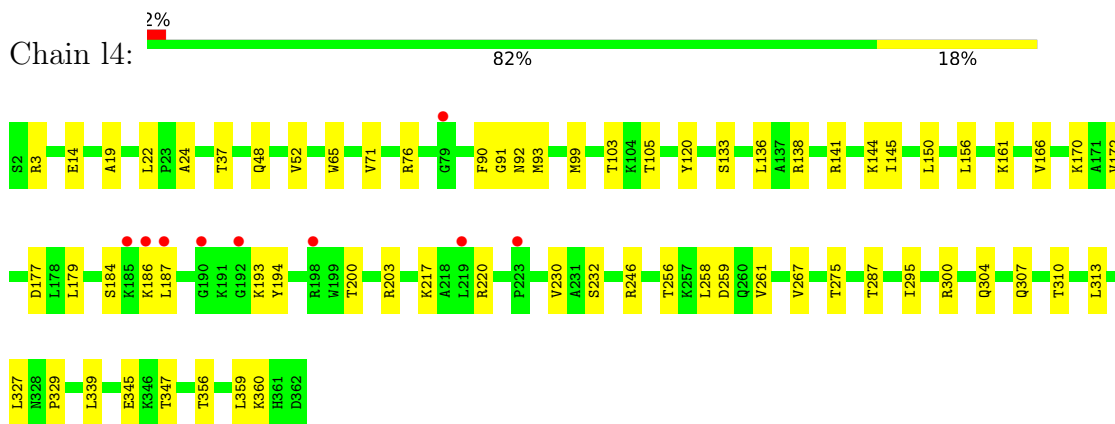
- Molecule 40: 60S ribosomal protein L3



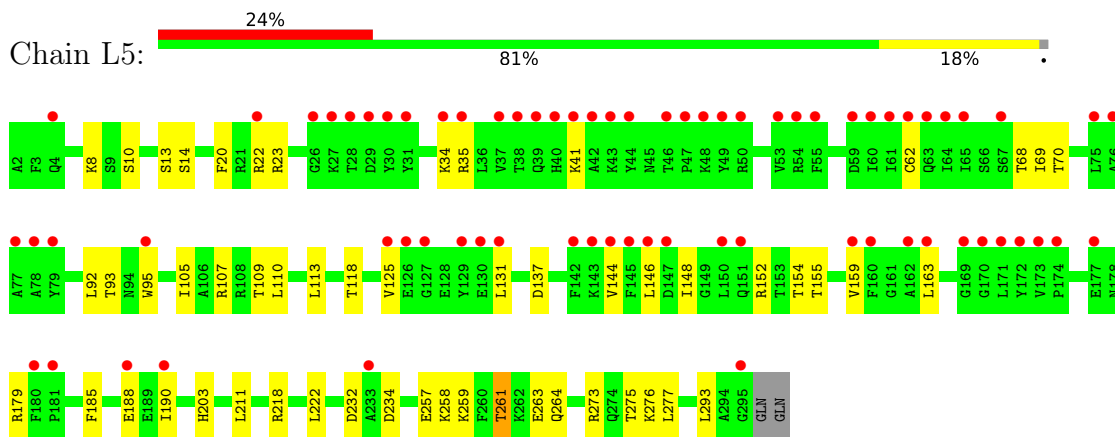
- Molecule 41: 60S ribosomal protein L4-A



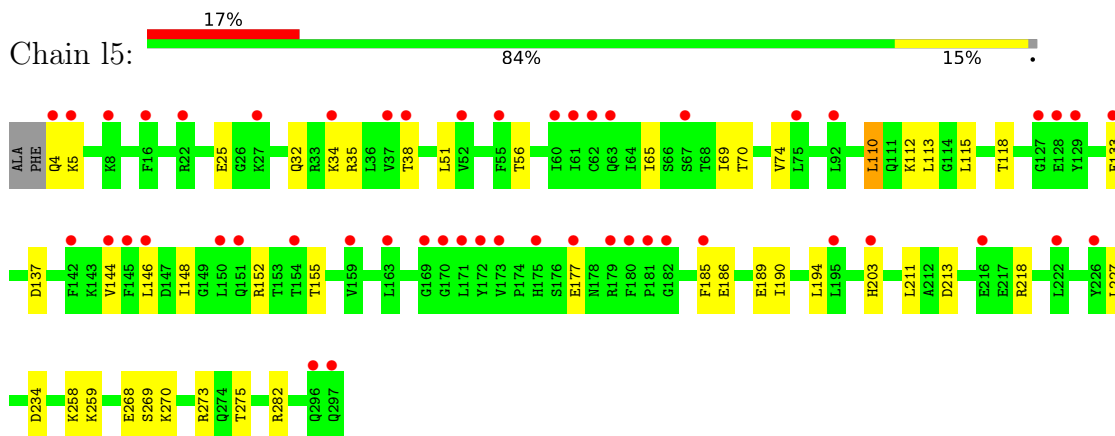
- Molecule 41: 60S ribosomal protein L4-A



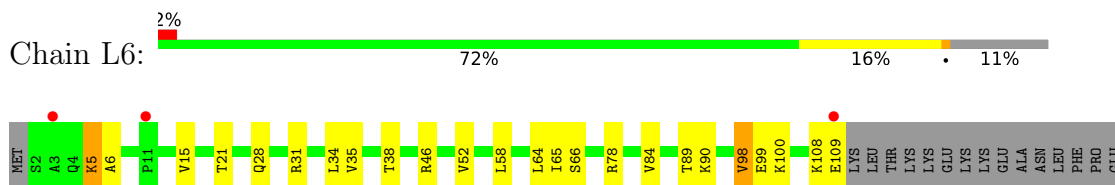
- Molecule 42: 60S ribosomal protein L5

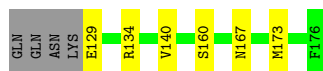


- Molecule 42: 60S ribosomal protein L5

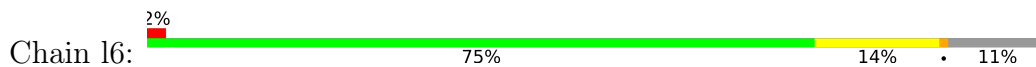


- Molecule 43: 60S ribosomal protein L6-A

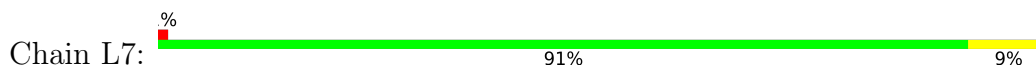




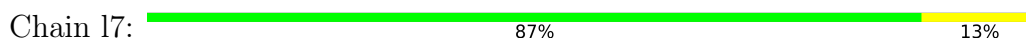
- Molecule 43: 60S ribosomal protein L6-A



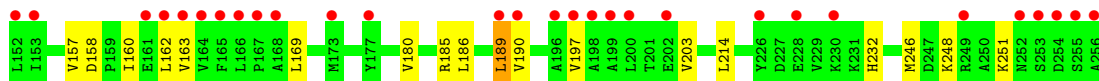
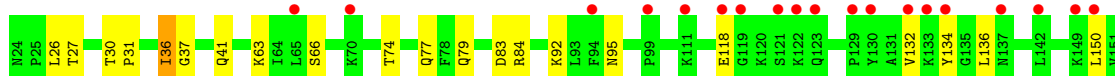
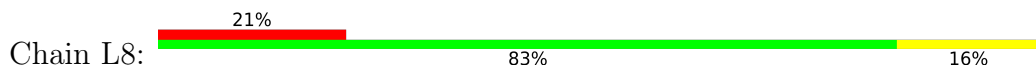
- Molecule 44: 60S ribosomal protein L7-A



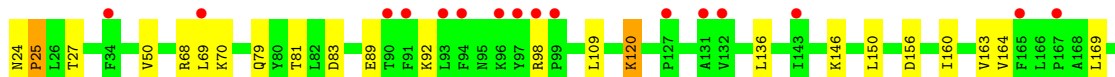
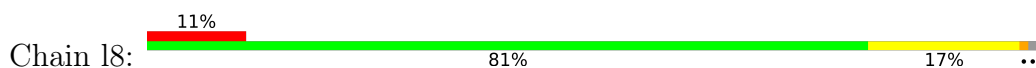
- Molecule 44: 60S ribosomal protein L7-A



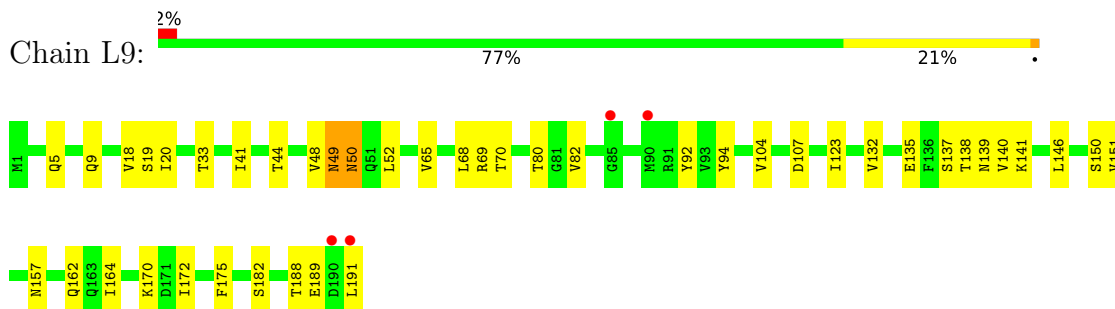
- Molecule 45: 60S ribosomal protein L8-A



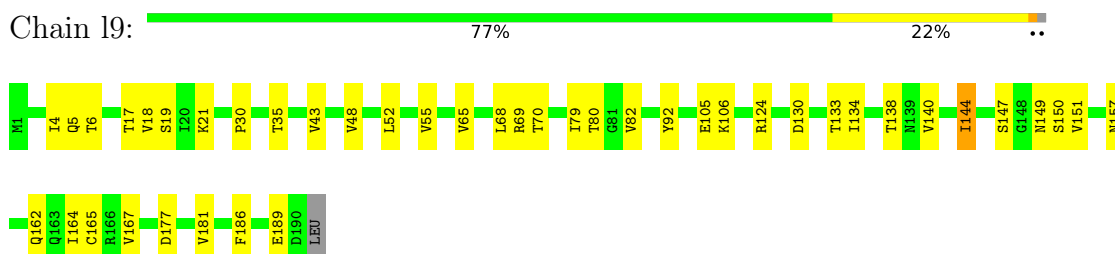
- Molecule 45: 60S ribosomal protein L8-A



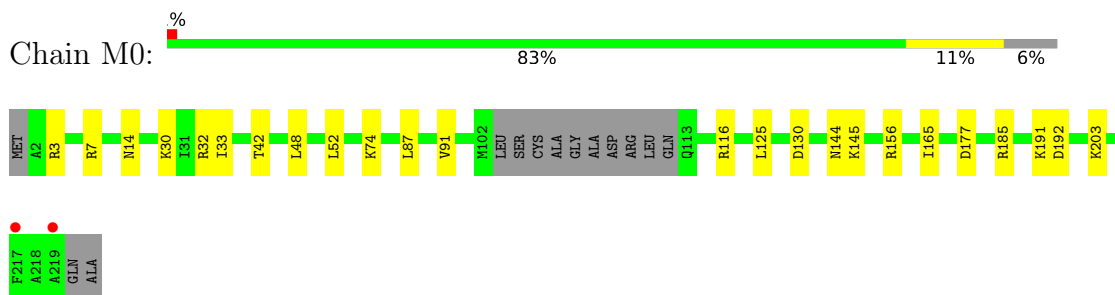
- Molecule 46: 60S ribosomal protein L9-A



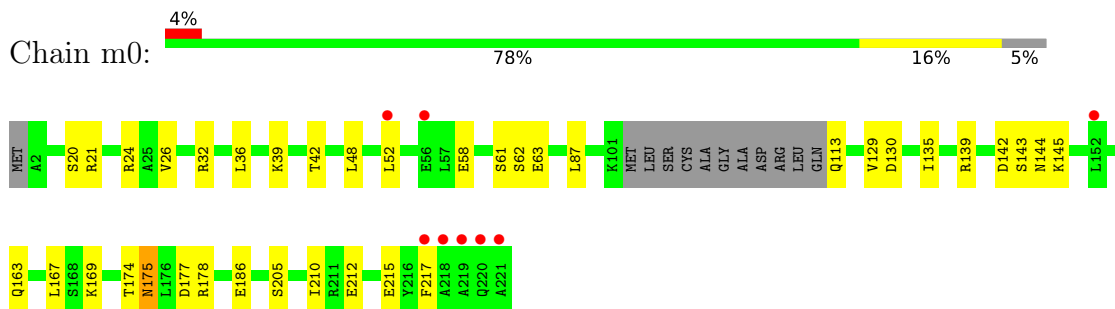
- Molecule 46: 60S ribosomal protein L9-A



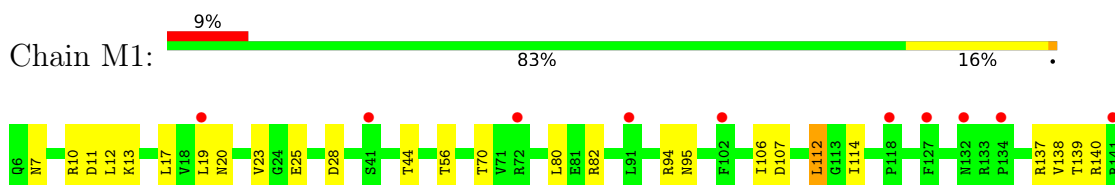
- Molecule 47: 60S ribosomal protein L10

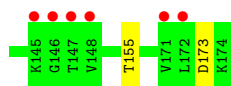


- Molecule 47: 60S ribosomal protein L10

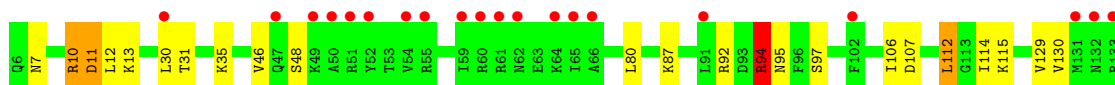
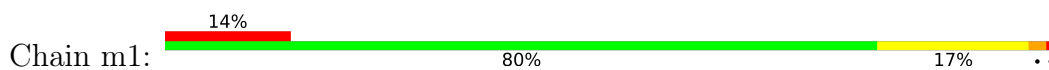


- Molecule 48: 60S ribosomal protein L11-A

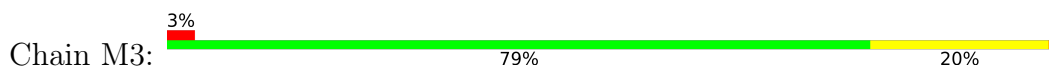




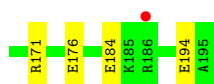
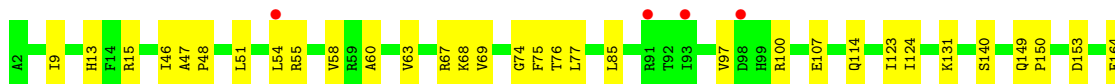
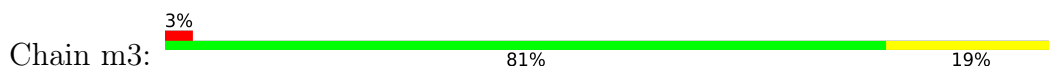
- Molecule 48: 60S ribosomal protein L11-A



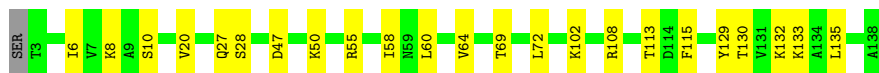
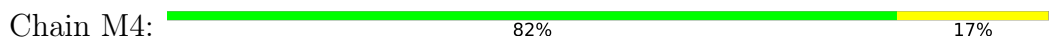
- Molecule 49: 60S ribosomal protein L13-A



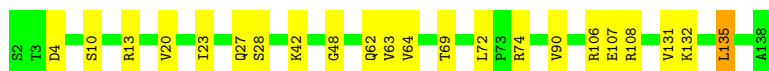
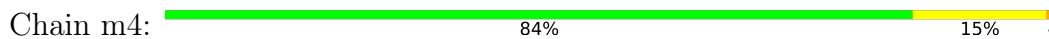
- Molecule 49: 60S ribosomal protein L13-A



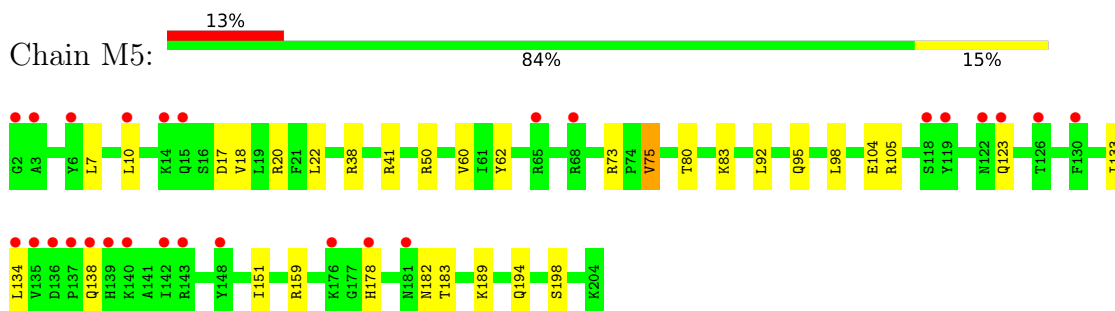
- Molecule 50: 60S ribosomal protein L14-A



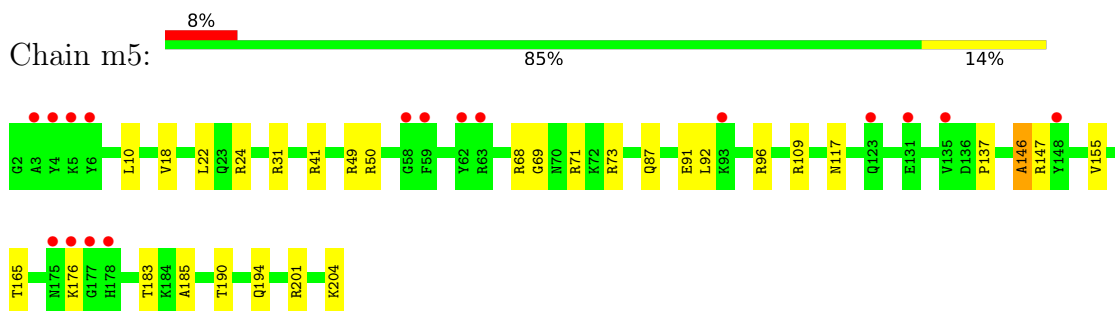
- Molecule 50: 60S ribosomal protein L14-A



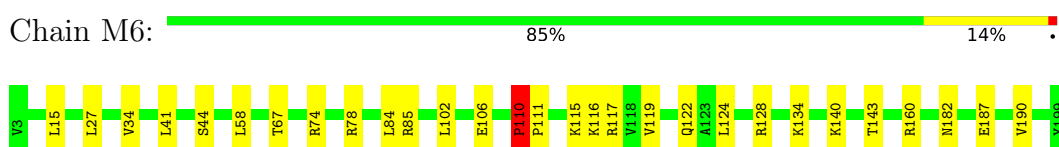
- Molecule 51: 60S ribosomal protein L15-A



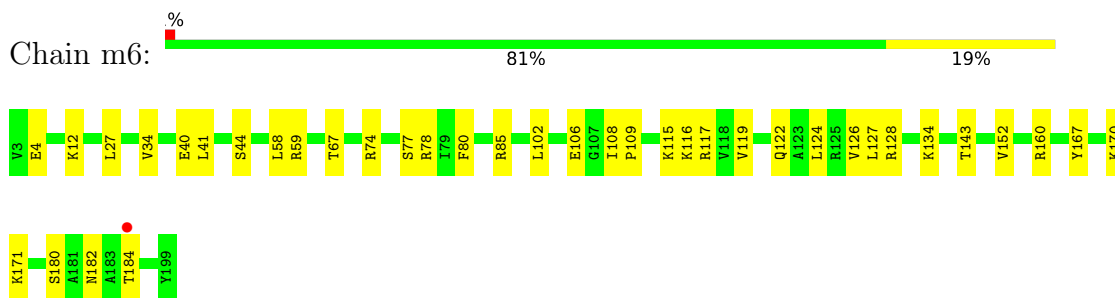
- Molecule 51: 60S ribosomal protein L15-A



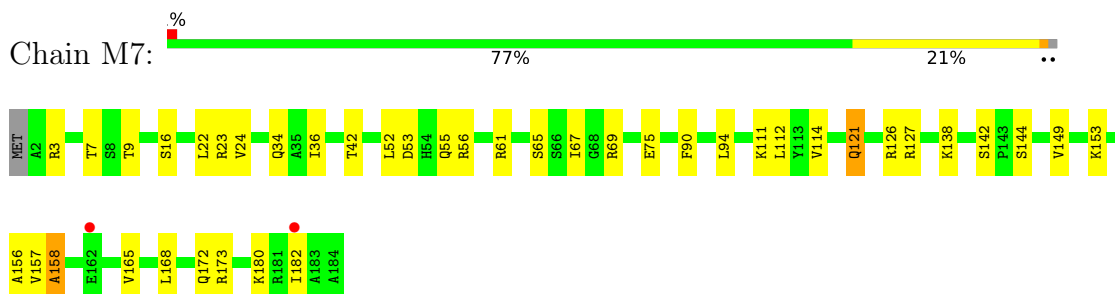
- Molecule 52: 60S ribosomal protein L16-A



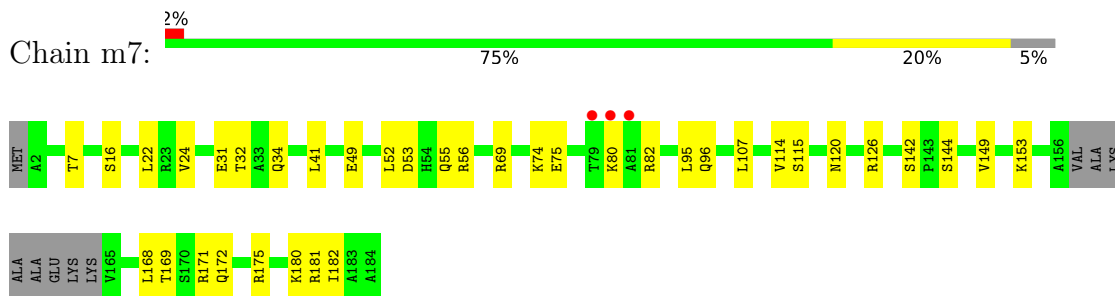
- Molecule 52: 60S ribosomal protein L16-A



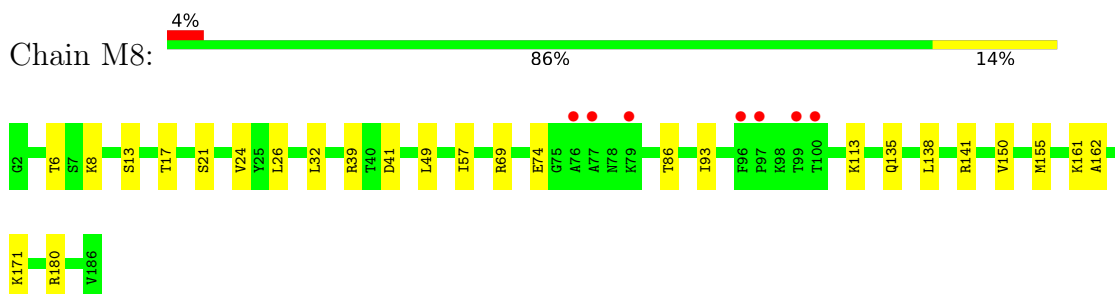
- Molecule 53: 60S ribosomal protein L17-A



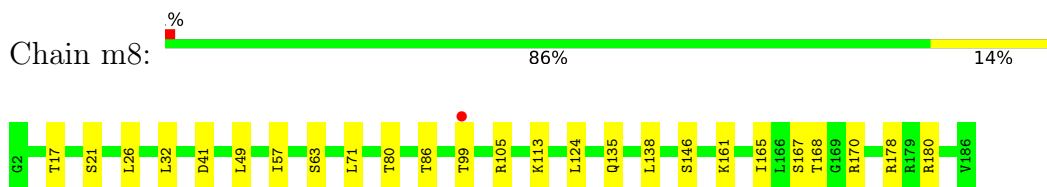
- Molecule 53: 60S ribosomal protein L17-A



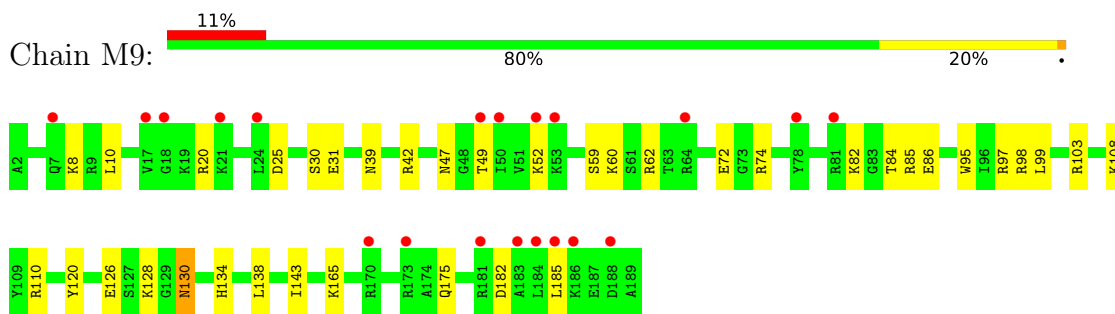
- Molecule 54: 60S ribosomal protein L18-A



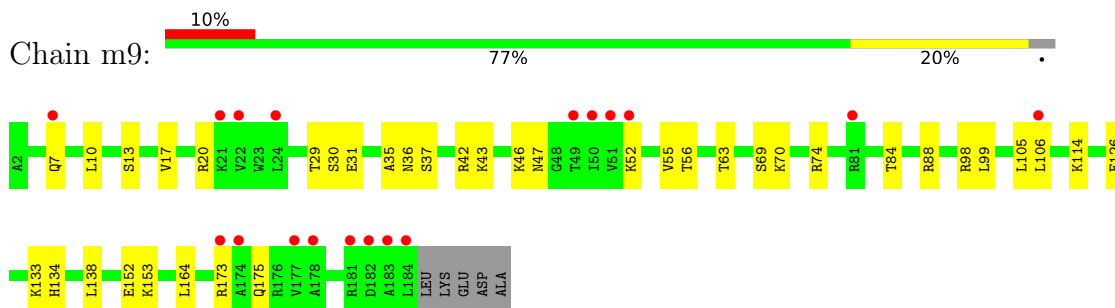
- Molecule 54: 60S ribosomal protein L18-A



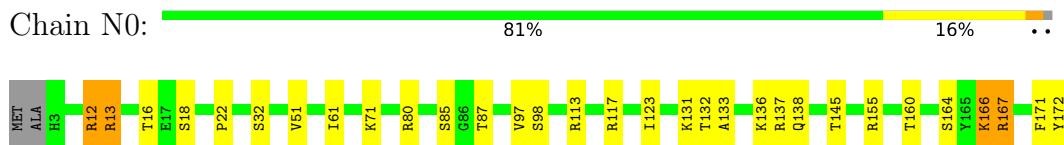
- Molecule 55: 60S ribosomal protein L19-A



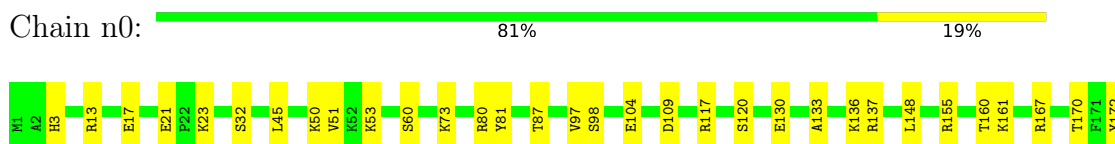
- Molecule 55: 60S ribosomal protein L19-A



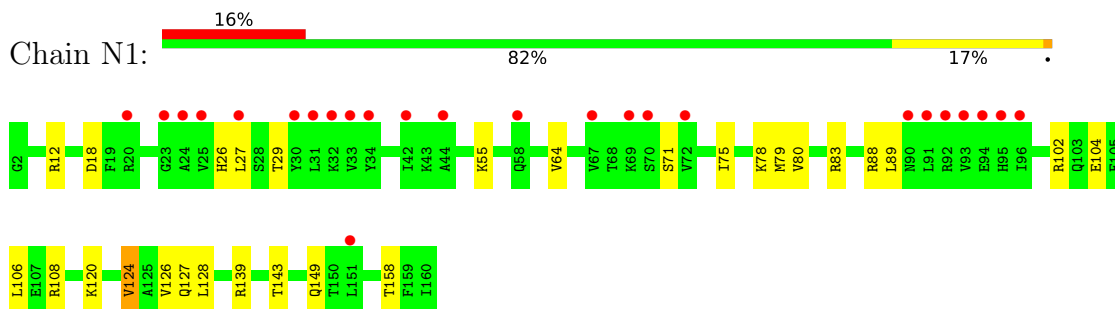
- Molecule 56: 60S ribosomal protein L20-A



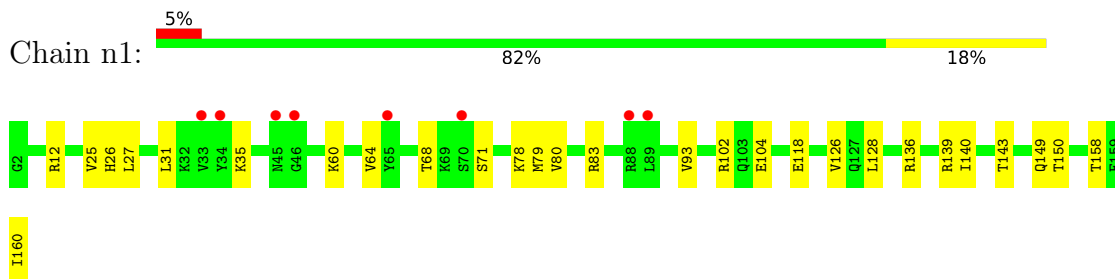
- Molecule 56: 60S ribosomal protein L20-A



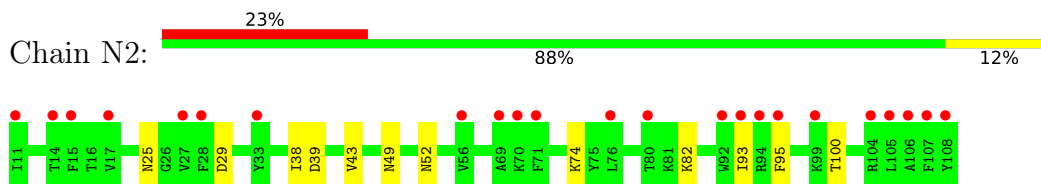
- Molecule 57: 60S ribosomal protein L21-A



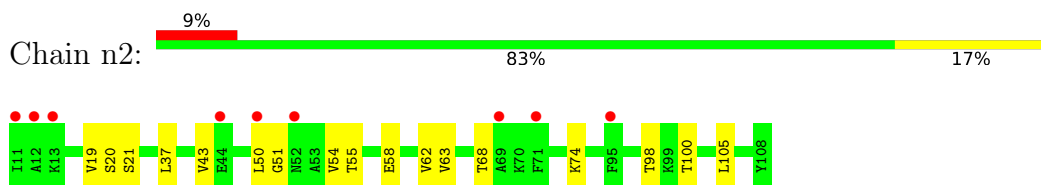
- Molecule 57: 60S ribosomal protein L21-A



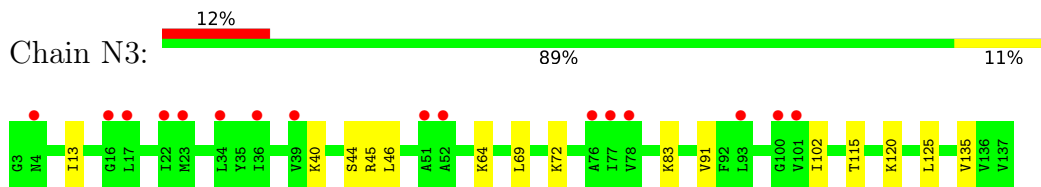
- Molecule 58: 60S ribosomal protein L22-A



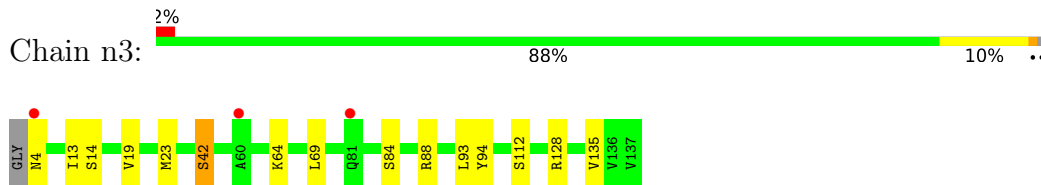
- Molecule 58: 60S ribosomal protein L22-A



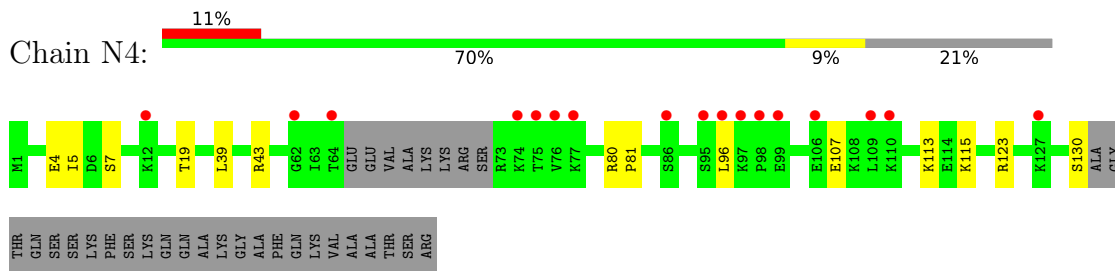
• Molecule 59: 60S ribosomal protein L23-A



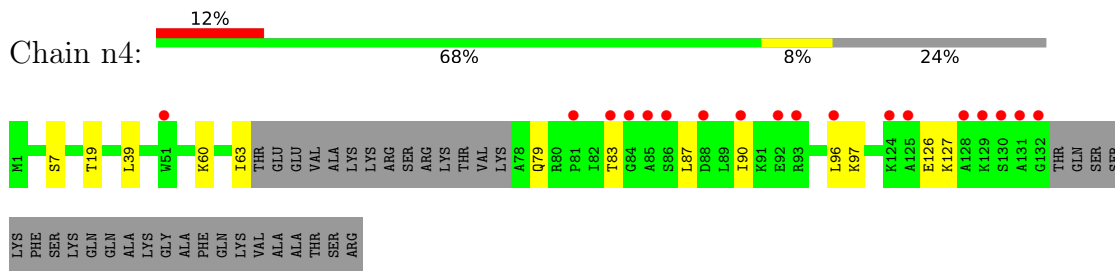
• Molecule 59: 60S ribosomal protein L23-A



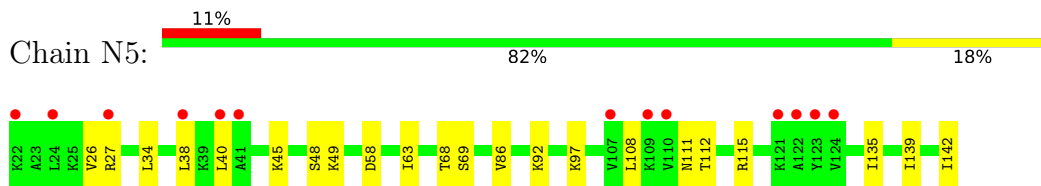
• Molecule 60: 60S ribosomal protein L24-A



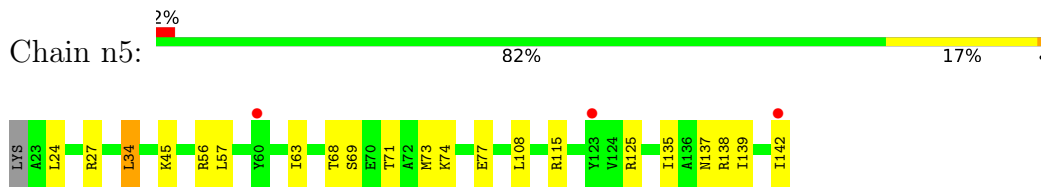
• Molecule 60: 60S ribosomal protein L24-A



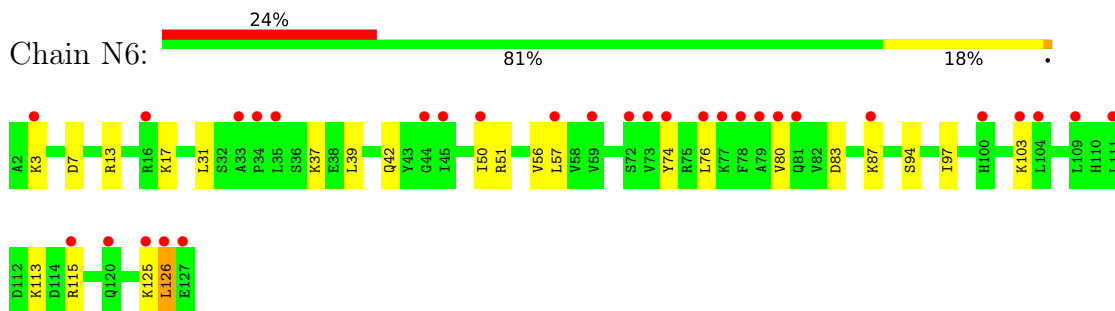
• Molecule 61: 60S ribosomal protein L25



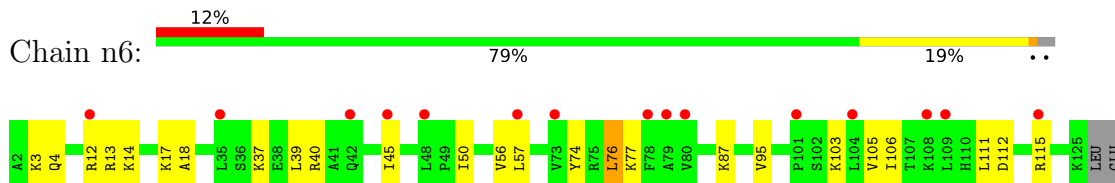
• Molecule 61: 60S ribosomal protein L25



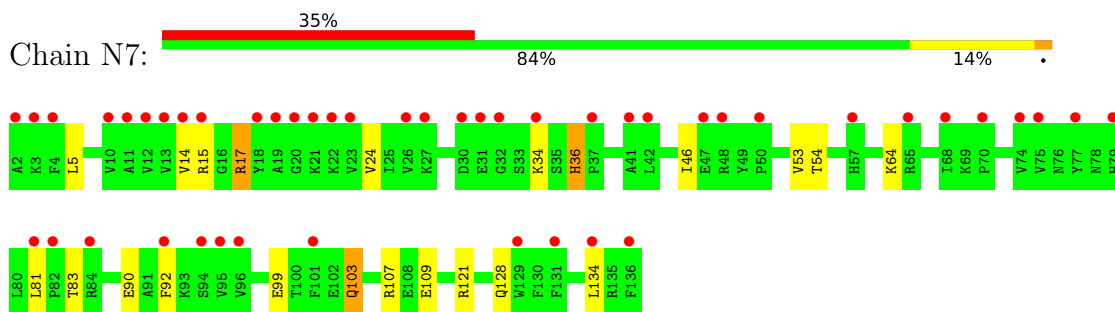
• Molecule 62: 60S ribosomal protein L26-A



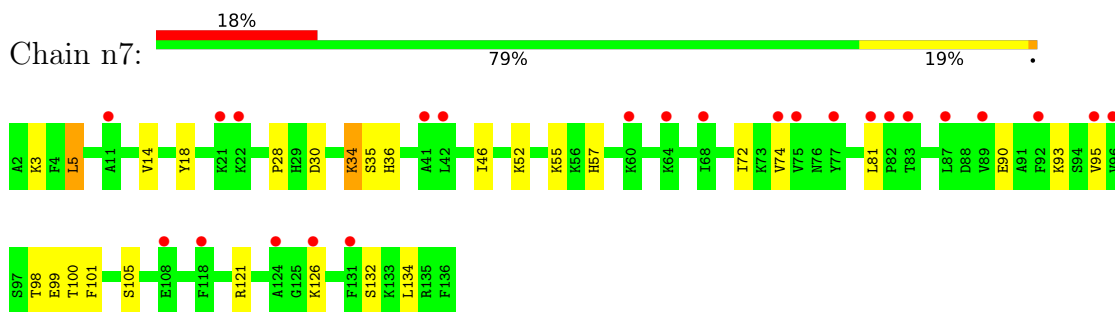
- Molecule 62: 60S ribosomal protein L26-A



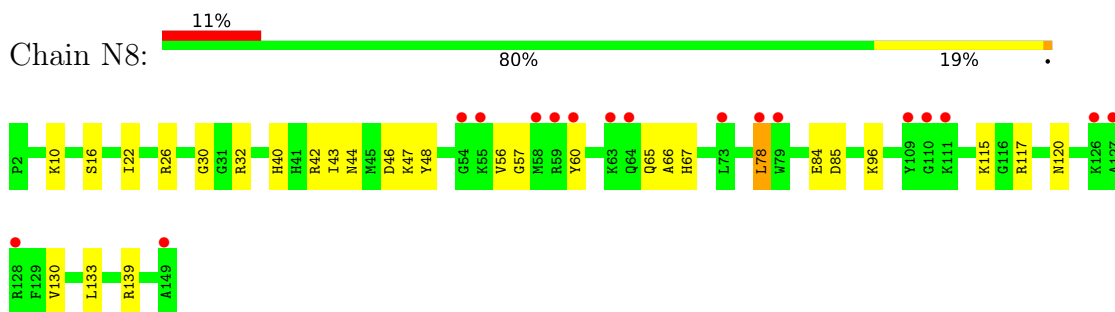
- Molecule 63: 60S ribosomal protein L27-A



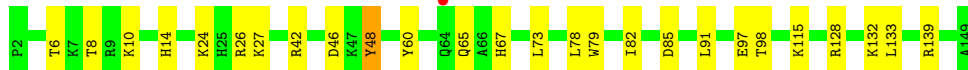
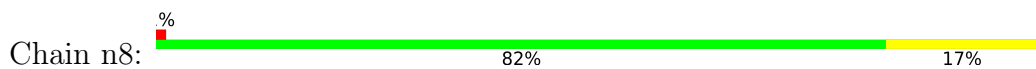
- Molecule 63: 60S ribosomal protein L27-A



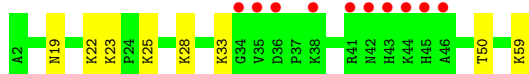
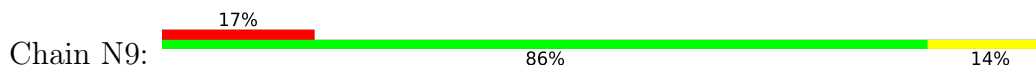
- Molecule 64: 60S ribosomal protein L28



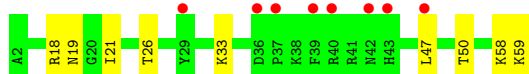
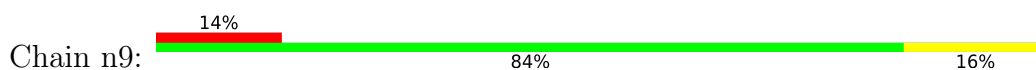
- Molecule 64: 60S ribosomal protein L28



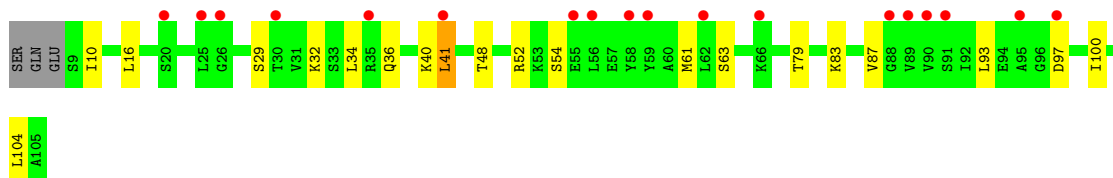
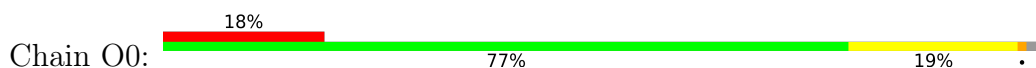
- Molecule 65: 60S ribosomal protein L29



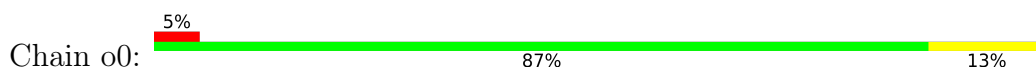
- Molecule 65: 60S ribosomal protein L29



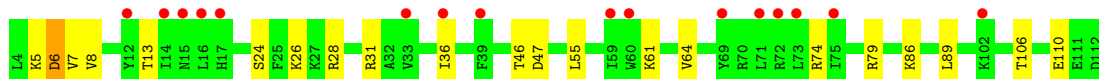
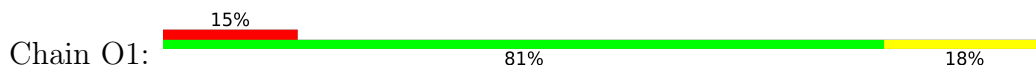
- Molecule 66: 60S ribosomal protein L30



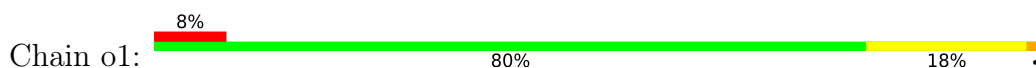
- Molecule 66: 60S ribosomal protein L30

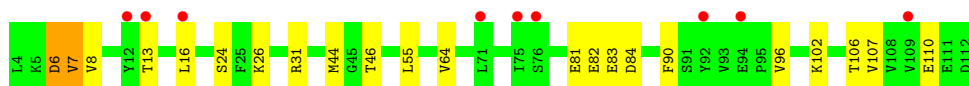


- Molecule 67: 60S ribosomal protein L31-A

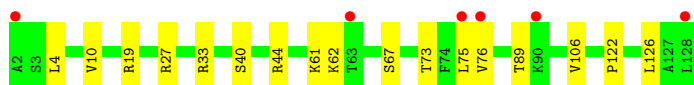
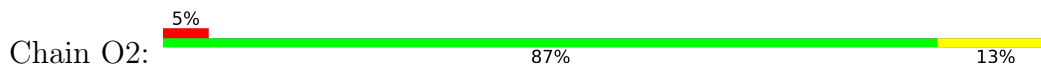


- Molecule 67: 60S ribosomal protein L31-A

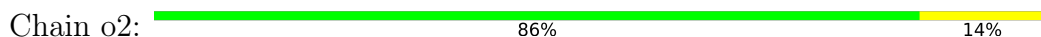




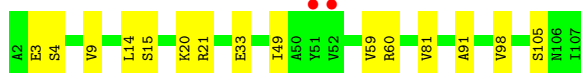
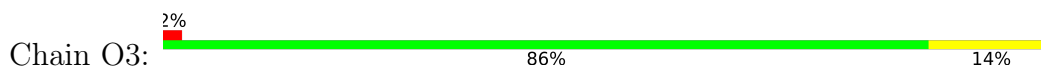
- Molecule 68: 60S ribosomal protein L32



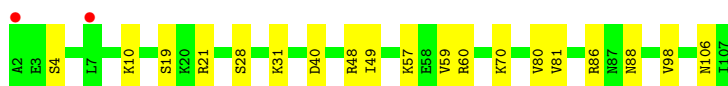
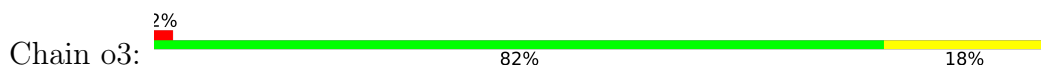
- Molecule 68: 60S ribosomal protein L32



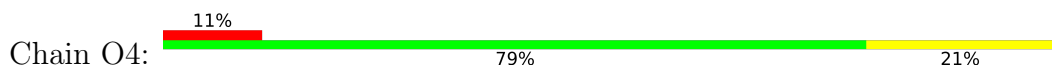
- Molecule 69: 60S ribosomal protein L33-A



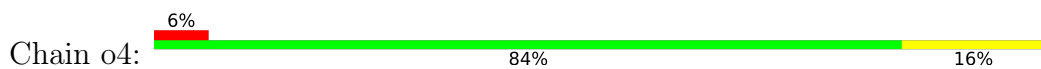
- Molecule 69: 60S ribosomal protein L33-A



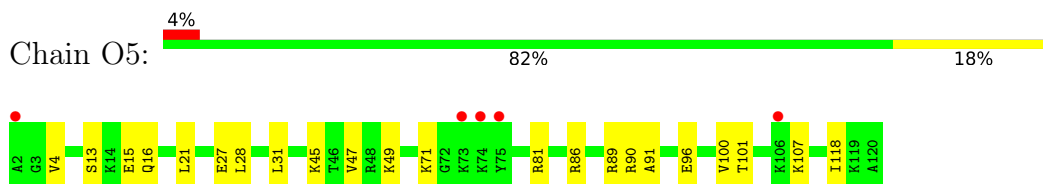
- Molecule 70: 60S ribosomal protein L34-A



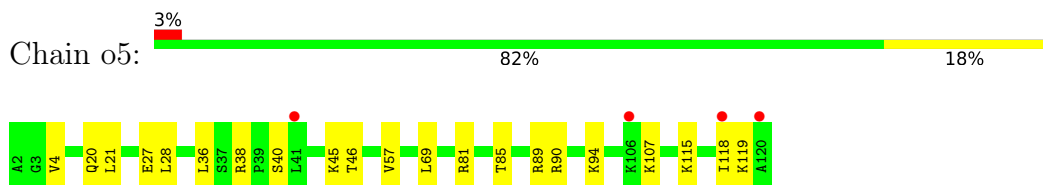
- Molecule 70: 60S ribosomal protein L34-A



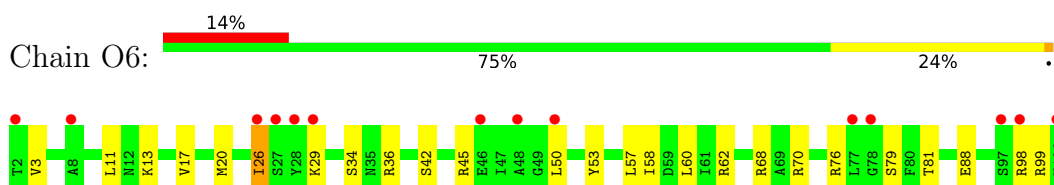
- Molecule 71: 60S ribosomal protein L35-A



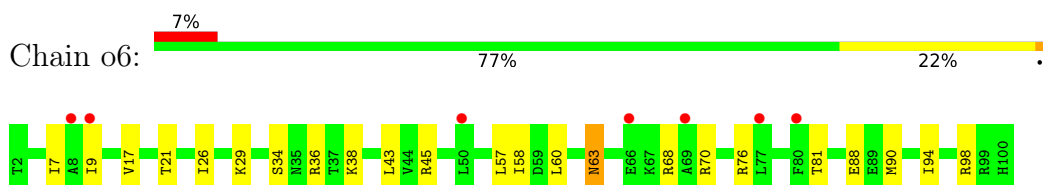
- Molecule 71: 60S ribosomal protein L35-A



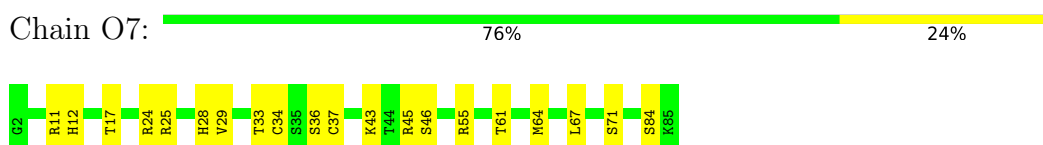
- Molecule 72: 60S ribosomal protein L36-A



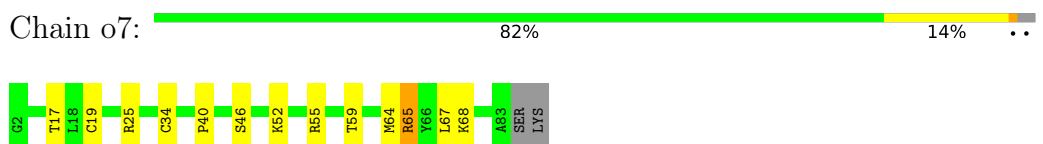
- Molecule 72: 60S ribosomal protein L36-A



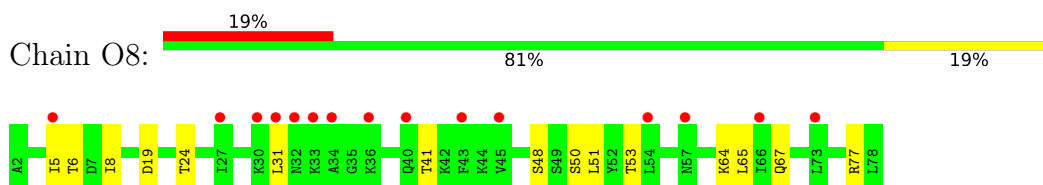
- Molecule 73: 60S ribosomal protein L37-A



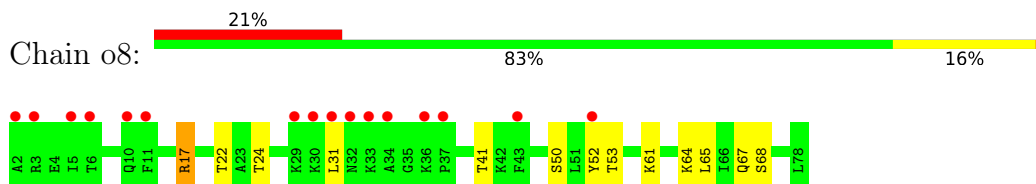
- Molecule 73: 60S ribosomal protein L37-A



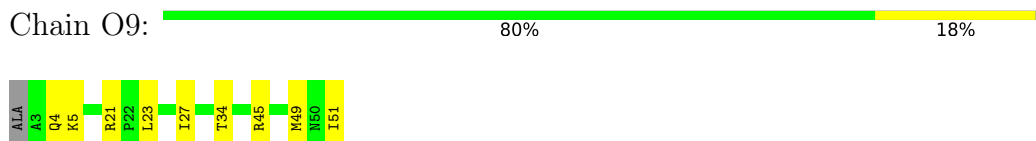
- Molecule 74: 60S ribosomal protein L38



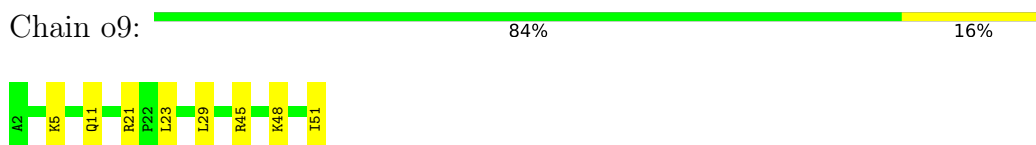
- Molecule 74: 60S ribosomal protein L38



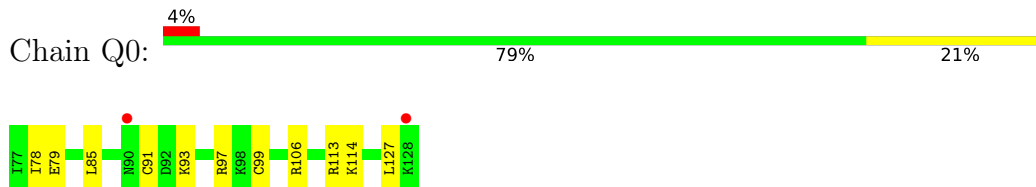
- Molecule 75: 60S ribosomal protein L39



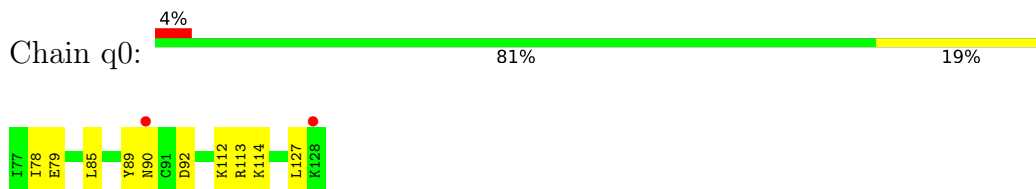
- Molecule 75: 60S ribosomal protein L39



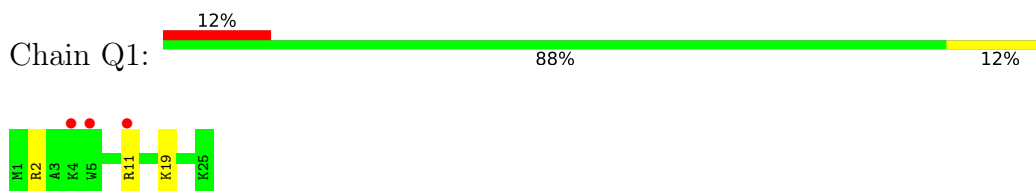
- Molecule 76: Ubiquitin-60S ribosomal protein L40



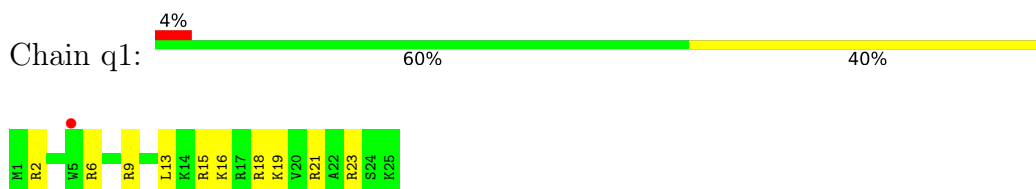
- Molecule 76: Ubiquitin-60S ribosomal protein L40



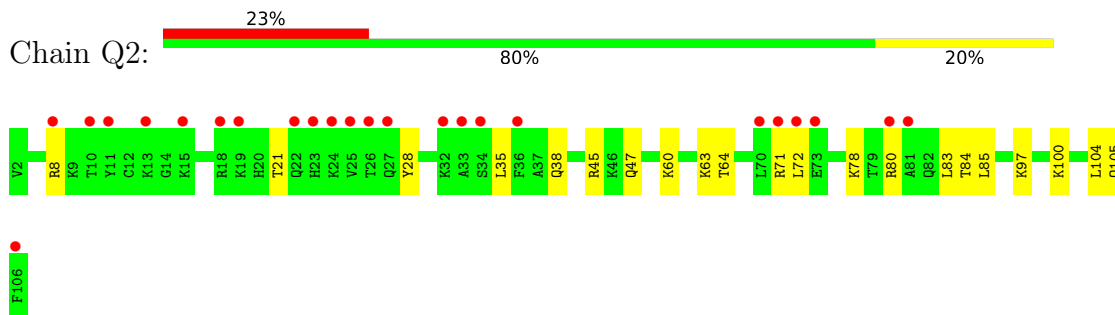
- Molecule 77: 60S ribosomal protein L41-A



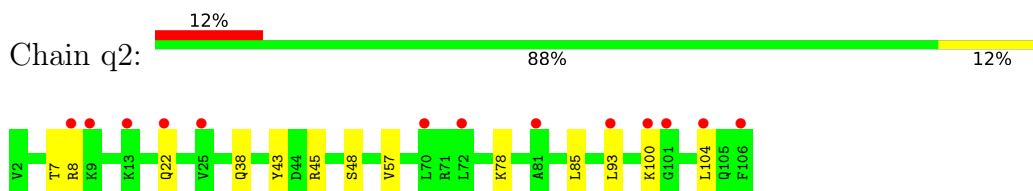
- Molecule 77: 60S ribosomal protein L41-A



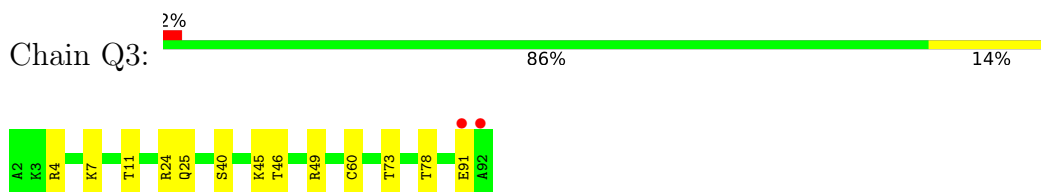
• Molecule 78: 60S ribosomal protein L42-A



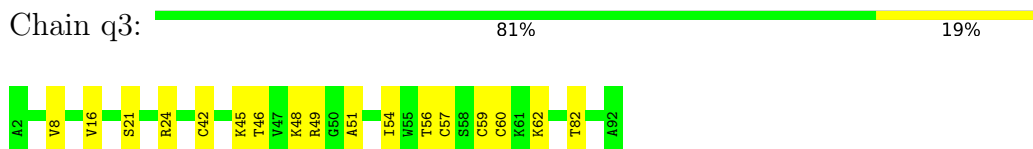
• Molecule 78: 60S ribosomal protein L42-A



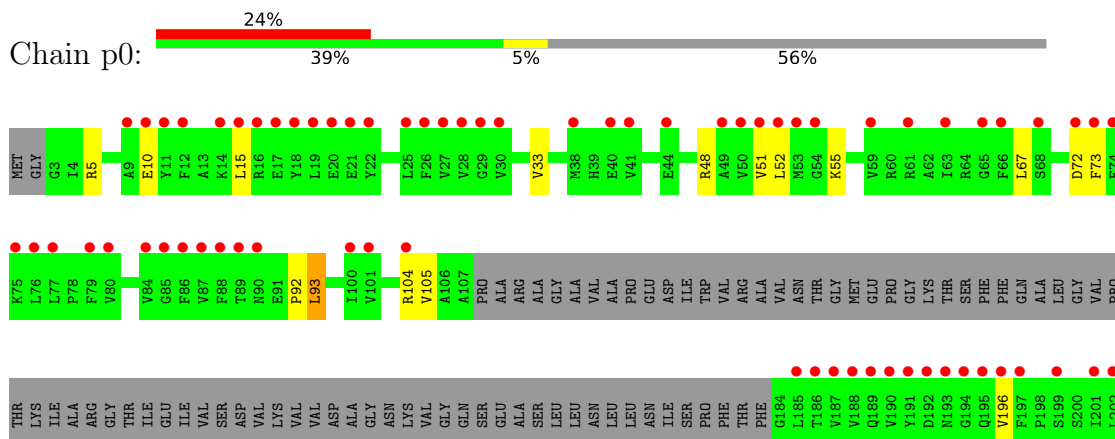
• Molecule 79: 60S ribosomal protein L43-A



• Molecule 79: 60S ribosomal protein L43-A



• Molecule 80: 60S acidic ribosomal protein P0



ASN	V210	VAL
PRO	S211	THR
GLU	H212	ILE
LYS	F213	ALA
TYR	V214	SER
ALA	S215	ILE
ALA	A216	GLY
ALA		TYR
PRO		PRO
ALA		THR
THR		LEU
SER		PRO
ALA		SER
ALA		VAL
ALA		GLY
THR		HIS
SER		THR
ALA		LEU
GLY		ILE
ASP		ASN
ALA		ASN
ALA		TYR
ALA		LYS
PRO		ASP
ALA		LEU
GLU		LEU
ALA		ALA
ALA		VAL
ALA		ALA
GLU		ILE
GLU		ALA
GLU		ALA
GLU		SER
GLU		TYR
GLU		HIS
GLU		TYR
GLU		PRO
GLU		GLU
GLU		ILE
GLU		GLU
GLU		ASP
GLU		VAL
GLU		ASP
GLU		ARG
GLU		ILE
GLU		GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	443.59Å 297.32Å 300.15Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	91.75 – 3.70 101.93 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (91.75-3.70) 89.5 (101.93-3.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 3.67Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.253 0.210 , 0.252	Depositor DCC
R_{free} test set	16296 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	120.7	Xtrriage
Anisotropy	0.428	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 113.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	397710	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.58	1/40250 (0.0%)	1.19	219/62707 (0.3%)
1	6	0.60	8/40528 (0.0%)	1.18	200/63141 (0.3%)
2	S0	0.36	0/1617	0.61	0/2215
2	s0	0.35	0/1623	0.60	0/2222
3	S1	0.34	0/1735	0.68	2/2335 (0.1%)
3	s1	0.34	0/1748	0.59	0/2352
4	S2	0.37	0/1665	0.65	1/2263 (0.0%)
4	s2	0.39	0/1665	0.65	1/2263 (0.0%)
5	S3	0.42	0/1759	0.61	0/2368
5	s3	0.36	0/1759	0.61	0/2368
6	S4	0.37	0/2109	0.64	3/2839 (0.1%)
6	s4	0.41	1/2109 (0.0%)	0.66	0/2839
7	S5	0.35	0/1629	0.59	0/2202
7	s5	0.34	0/1629	0.60	0/2202
8	S6	0.36	0/1823	0.56	0/2439
8	s6	0.40	0/1779	0.61	0/2379
9	S7	0.38	0/1506	0.64	0/2028
9	s7	0.39	0/1511	0.70	2/2036 (0.1%)
10	S8	0.40	0/1514	0.64	2/2021 (0.1%)
10	s8	0.47	0/1514	0.65	0/2021
11	S9	0.36	0/1519	0.62	0/2035
11	s9	0.39	0/1519	0.61	1/2035 (0.0%)
12	C0	0.37	0/769	0.71	1/1039 (0.1%)
12	c0	0.36	0/757	0.73	1/1022 (0.1%)
13	C1	0.40	0/1172	0.69	1/1580 (0.1%)
13	c1	0.47	0/1194	0.68	1/1610 (0.1%)
14	C2	0.33	0/878	0.71	3/1192 (0.3%)
14	c2	0.32	0/898	0.70	0/1220
15	C3	0.39	0/1215	0.65	0/1638
15	c3	0.40	0/1215	0.63	1/1638 (0.1%)
16	C4	0.37	0/901	0.65	1/1217 (0.1%)
16	c4	0.34	0/960	0.63	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.50	1/988 (0.1%)	0.69	0/1327
17	c5	0.40	0/959	0.67	0/1288
18	C6	0.43	0/1125	0.65	0/1510
18	c6	0.68	2/1125 (0.2%)	0.62	0/1510
19	C7	0.35	0/920	0.61	0/1233
19	c7	0.34	0/915	0.64	1/1227 (0.1%)
20	C8	0.40	0/1211	0.68	0/1628
20	c8	0.35	0/1211	0.63	0/1628
21	C9	0.45	0/1130	0.65	1/1517 (0.1%)
21	c9	0.37	0/1130	0.64	0/1517
22	D0	0.41	0/847	0.64	0/1145
22	d0	0.37	0/815	0.58	0/1102
23	D1	0.40	0/693	0.66	0/935
23	d1	0.37	0/693	0.61	0/935
24	D2	0.37	0/1038	0.70	2/1395 (0.1%)
24	d2	0.40	0/1038	0.64	1/1395 (0.1%)
25	D3	0.46	0/1139	0.73	1/1518 (0.1%)
25	d3	0.48	0/1139	0.68	0/1518
26	D4	0.32	0/1087	0.59	1/1449 (0.1%)
26	d4	0.39	0/1087	0.66	0/1449
27	D5	0.37	0/571	0.72	0/768
27	d5	0.34	0/566	0.58	0/761
28	D6	0.70	1/782 (0.1%)	0.73	1/1047 (0.1%)
28	d6	0.36	0/782	0.64	0/1047
29	D7	0.33	0/620	0.62	0/838
29	d7	0.36	0/620	0.68	0/838
30	D8	1.18	1/499 (0.2%)	0.61	0/670
30	d8	0.84	1/499 (0.2%)	0.61	0/670
31	D9	0.49	0/452	0.77	1/600 (0.2%)
31	d9	0.44	0/452	0.64	0/600
32	E0	0.42	0/483	0.68	0/643
32	e0	0.43	0/483	0.72	0/643
33	E1	0.44	0/577	0.89	0/770
33	e1	0.37	0/358	0.68	0/477
34	SR	0.31	0/2490	0.56	0/3389
34	sR	0.32	0/2456	0.57	0/3343
35	SM	0.41	0/994	0.70	1/1335 (0.1%)
35	sM	0.43	0/882	0.65	0/1180
36	1	0.76	18/73692 (0.0%)	1.39	806/114882 (0.7%)
36	5	0.79	25/74873 (0.0%)	1.40	785/116727 (0.7%)
37	3	0.64	0/2883	1.23	21/4491 (0.5%)
37	7	0.60	0/2883	1.11	9/4491 (0.2%)
38	4	0.74	0/3746	1.38	36/5832 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	8	0.80	0/3724	1.47	46/5798 (0.8%)
39	L2	0.45	0/1948	0.71	2/2617 (0.1%)
39	l2	0.53	1/1946 (0.1%)	0.77	1/2614 (0.0%)
40	L3	0.51	0/3146	0.70	2/4228 (0.0%)
40	l3	0.56	0/3146	0.72	1/4228 (0.0%)
41	L4	0.46	0/2800	0.71	3/3790 (0.1%)
41	l4	0.54	2/2800 (0.1%)	0.72	1/3790 (0.0%)
42	L5	0.42	0/2407	0.65	0/3247
42	l5	0.37	0/2408	0.58	1/3248 (0.0%)
43	L6	0.51	0/1260	0.70	0/1694
43	l6	0.58	0/1269	0.73	0/1705
44	L7	0.51	0/1821	0.66	0/2451
44	l7	0.52	0/1828	0.68	0/2461
45	L8	0.44	1/1836 (0.1%)	0.62	1/2481 (0.0%)
45	l8	0.43	1/1795 (0.1%)	0.65	1/2429 (0.0%)
46	L9	0.48	0/1539	0.66	0/2073
46	l9	0.49	0/1531	0.71	0/2062
47	M0	0.51	0/1726	0.68	0/2314
47	m0	0.47	0/1732	0.72	0/2323
48	M1	0.42	0/1374	0.66	1/1842 (0.1%)
48	m1	0.37	0/1374	0.62	1/1842 (0.1%)
49	M3	0.46	1/1568 (0.1%)	0.68	1/2106 (0.0%)
49	m3	0.47	0/1573	0.71	0/2113
50	M4	0.48	0/1068	0.68	0/1438
50	m4	0.55	0/1074	0.74	1/1446 (0.1%)
51	M5	0.46	0/1757	0.68	0/2354
51	m5	0.50	0/1757	0.75	1/2354 (0.0%)
52	M6	0.59	0/1585	0.74	2/2128 (0.1%)
52	m6	0.62	0/1585	0.76	1/2128 (0.0%)
53	M7	0.53	0/1443	0.72	1/1944 (0.1%)
53	m7	0.56	0/1400	0.77	1/1882 (0.1%)
54	M8	0.40	0/1465	0.62	0/1965
54	m8	0.45	0/1465	0.69	2/1965 (0.1%)
55	M9	0.40	0/1538	0.60	0/2050
55	m9	0.43	0/1499	0.61	0/1998
56	N0	0.51	0/1468	0.68	0/1973
56	n0	0.52	0/1481	0.70	0/1990
57	N1	0.48	0/1300	0.67	0/1743
57	n1	0.43	0/1300	0.61	0/1743
58	N2	0.40	0/794	0.63	0/1076
58	n2	0.39	0/794	0.57	0/1076
59	N3	0.49	0/1012	0.71	1/1361 (0.1%)
59	n3	0.58	0/1008	0.79	0/1356

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	N4	0.44	0/937	0.56	0/1243
60	n4	0.47	1/959 (0.1%)	0.66	2/1267 (0.2%)
61	N5	0.44	0/979	0.72	0/1321
61	n5	0.53	0/974	0.78	1/1314 (0.1%)
62	N6	0.45	0/1004	0.75	2/1341 (0.1%)
62	n6	0.48	0/987	0.82	2/1318 (0.2%)
63	N7	0.47	1/1118 (0.1%)	0.63	0/1497
63	n7	0.49	0/1118	0.63	1/1497 (0.1%)
64	N8	0.43	0/1204	0.73	1/1612 (0.1%)
64	n8	0.47	0/1204	0.72	1/1612 (0.1%)
65	N9	0.41	0/473	0.60	0/629
65	n9	0.44	0/473	0.72	0/629
66	O0	0.40	0/751	0.61	1/1008 (0.1%)
66	o0	0.45	0/775	0.62	0/1040
67	O1	0.47	0/890	0.71	0/1196
67	o1	0.52	0/897	0.71	1/1205 (0.1%)
68	O2	0.50	0/1041	0.72	0/1394
68	o2	0.53	0/1041	0.73	0/1394
69	O3	0.56	0/868	0.72	0/1168
69	o3	0.59	0/868	0.79	1/1168 (0.1%)
70	O4	0.43	0/890	0.71	1/1189 (0.1%)
70	o4	0.48	0/890	0.73	1/1189 (0.1%)
71	O5	0.44	0/978	0.66	0/1301
71	o5	0.51	0/974	0.69	0/1297
72	O6	0.45	1/778 (0.1%)	0.70	1/1034 (0.1%)
72	o6	0.43	0/777	0.67	0/1033
73	O7	0.54	1/680 (0.1%)	0.75	0/901
73	o7	0.63	0/665	0.84	1/882 (0.1%)
74	O8	0.38	0/618	0.60	0/826
74	o8	0.42	0/614	0.62	0/822
75	O9	0.45	0/438	0.66	0/581
75	o9	0.52	0/443	0.67	0/588
76	Q0	0.55	0/423	0.78	0/562
76	q0	0.66	0/423	0.76	0/562
77	Q1	0.41	0/234	0.67	0/300
77	q1	0.48	0/234	0.74	0/300
78	Q2	0.48	0/860	0.67	0/1136
78	q2	0.47	0/860	0.68	0/1136
79	Q3	0.45	0/701	0.62	0/934
79	q3	0.43	0/701	0.68	0/934
80	p0	0.34	0/1067	0.58	1/1439 (0.1%)
All	All	0.62	69/423555 (0.0%)	1.11	2197/621249 (0.4%)

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
2	s0	0	1
3	S1	0	4
4	S2	0	1
4	s2	0	2
5	s3	0	1
6	S4	0	1
7	S5	0	3
7	s5	0	4
8	s6	0	1
9	S7	0	4
9	s7	0	6
11	s9	0	2
12	c0	0	1
13	C1	0	1
14	C2	0	3
14	c2	0	1
15	c3	0	1
16	C4	0	1
17	C5	0	2
17	c5	0	4
18	C6	0	3
18	c6	0	1
19	C7	0	1
20	C8	0	3
20	c8	0	1
22	d0	0	2
24	D2	0	1
25	D3	0	1
26	D4	0	2
27	D5	0	2
27	d5	0	2
28	D6	0	2
29	D7	0	1
32	e0	0	2
33	E1	0	5
33	e1	0	3
34	SR	0	1
34	sR	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	sM	0	1
39	l2	0	2
40	L3	0	2
40	l3	0	1
41	l4	0	1
42	L5	0	3
42	l5	0	2
43	L6	0	2
43	l6	0	1
44	l7	0	2
45	L8	0	2
45	l8	0	3
46	L9	0	1
48	m1	0	1
49	m3	0	2
50	m4	0	1
51	M5	0	1
51	m5	0	2
52	M6	0	1
52	m6	0	1
53	M7	0	2
56	N0	0	4
56	n0	0	2
58	n2	0	1
60	N4	0	2
62	N6	0	1
63	n7	0	2
64	N8	0	2
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	2
69	O3	0	1
70	o4	0	1
71	O5	0	1
71	o5	0	1
72	O6	0	1
72	o6	0	1
79	q3	0	2
80	p0	0	1
All	All	0	141

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D8	5	THR	C-N	25.28	1.82	1.34
18	c6	4	VAL	C-N	18.52	1.69	1.34
30	d8	5	THR	C-N	17.27	1.67	1.34
28	D6	59	TYR	C-N	16.33	1.65	1.34
17	C5	67	ALA	C-N	9.82	1.52	1.34
45	L8	158	ASP	C-N	8.96	1.51	1.34
1	6	1756	A	N9-C4	8.52	1.43	1.37
36	1	1858	A	N9-C4	8.28	1.42	1.37
39	l2	204	MET	C-N	-7.68	1.16	1.34
36	5	1152	G	N9-C4	-7.43	1.32	1.38
18	c6	124	PRO	C-N	7.08	1.50	1.34
36	1	807	A	N9-C4	-6.94	1.33	1.37
36	5	23	A	N9-C4	-6.54	1.33	1.37
41	l4	65	TRP	CB-CG	-6.48	1.38	1.50
1	6	803	A	N9-C4	6.46	1.41	1.37
36	5	336	A	N9-C4	-6.43	1.33	1.37
36	5	3006	A	N9-C4	-6.20	1.34	1.37
36	1	1153	A	N9-C4	-6.19	1.34	1.37
36	1	2348	A	N9-C4	-6.18	1.34	1.37
1	6	623	A	N9-C4	-6.06	1.34	1.37
36	5	3129	A	N9-C4	-5.96	1.34	1.37
1	6	385	A	N9-C4	5.92	1.41	1.37
36	1	970	A	N9-C4	-5.89	1.34	1.37
36	1	2821	C	N1-C2	5.88	1.46	1.40
1	6	359	A	N9-C4	-5.83	1.34	1.37
6	s4	237	SER	C-N	-5.77	1.20	1.34
36	5	2902	A	N9-C4	-5.77	1.34	1.37
60	n4	96	LEU	C-N	5.73	1.47	1.34
36	5	2404	A	N9-C4	-5.71	1.34	1.37
36	5	1587	A	N9-C4	-5.71	1.34	1.37
36	1	1589	A	N9-C4	-5.70	1.34	1.37
36	1	2403	G	N7-C5	-5.70	1.35	1.39
36	5	1152	G	C8-N7	5.68	1.34	1.30
36	1	2875	U	N1-C2	5.62	1.43	1.38
36	1	806	A	N9-C4	-5.59	1.34	1.37
36	5	2933	A	N9-C4	-5.58	1.34	1.37
1	6	1023	A	N9-C4	5.55	1.41	1.37
49	M3	125	VAL	C-N	-5.54	1.21	1.34
36	5	630	A	N9-C4	-5.50	1.34	1.37
41	l4	19	ALA	C-N	5.45	1.46	1.34
36	5	3011	A	N9-C4	-5.43	1.34	1.37
36	5	2100	A	N9-C4	5.42	1.41	1.37
36	5	1355	A	N9-C4	5.38	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	O7	37	CYS	CB-SG	-5.37	1.73	1.81
36	5	2397	A	N9-C4	-5.34	1.34	1.37
36	5	1304	A	N9-C4	-5.34	1.34	1.37
63	N7	36	HIS	C-N	5.33	1.44	1.34
36	1	2207	A	N9-C4	5.33	1.41	1.37
36	5	1909	A	N9-C4	-5.26	1.34	1.37
1	2	1614	A	N9-C4	5.24	1.41	1.37
36	1	2093	A	N9-C4	5.19	1.41	1.37
36	5	2837	A	N9-C4	-5.19	1.34	1.37
36	5	2934	A	N9-C4	-5.17	1.34	1.37
36	1	2820	A	N9-C4	-5.16	1.34	1.37
1	6	1756	A	C5-C4	5.15	1.42	1.38
36	1	1302	A	N9-C4	-5.13	1.34	1.37
36	5	439	C	N1-C2	5.13	1.45	1.40
36	1	2348	A	N3-C4	-5.12	1.31	1.34
36	1	3129	A	N9-C4	-5.12	1.34	1.37
36	5	27	C	N1-C6	-5.12	1.34	1.37
36	5	1813	A	N9-C4	5.10	1.41	1.37
36	5	864	G	C2-N3	5.10	1.36	1.32
72	O6	50	LEU	C-N	5.09	1.45	1.34
36	1	718	G	N9-C4	-5.06	1.33	1.38
36	5	2397	A	N3-C4	-5.05	1.31	1.34
45	18	190	VAL	CB-CG1	-5.05	1.42	1.52
36	5	960	U	N1-C2	5.03	1.43	1.38
1	6	265	A	N9-C4	-5.03	1.34	1.37
36	1	3291	G	N9-C4	-5.00	1.33	1.38

All (2197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	C4-N9-C1'	-16.36	105.24	126.50
36	5	1152	G	N3-C4-N9	-16.24	116.26	126.00
36	5	1152	G	C8-N9-C1'	15.84	147.59	127.00
36	5	1152	G	N3-C4-C5	14.71	135.96	128.60
36	1	2392	C	C6-N1-C2	13.33	125.63	120.30
36	5	2138	A	O5'-P-OP2	-13.27	93.76	105.70
36	5	1437	C	C6-N1-C2	-12.56	115.28	120.30
36	5	1063	G	C4-N9-C1'	11.81	141.85	126.50
36	5	1063	G	N7-C8-N9	11.64	118.92	113.10
36	5	1143	A	O5'-P-OP2	-11.32	95.52	105.70
36	1	1858	A	C2-N3-C4	11.11	116.15	110.60
1	2	1025	A	O5'-P-OP2	-11.02	95.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	340	C	O5'-P-OP1	-10.64	96.13	105.70
1	2	1754	A	N7-C8-N9	10.55	119.08	113.80
36	1	1858	A	N3-C4-C5	-10.54	119.42	126.80
36	1	1581	C	N1-C2-O2	10.32	125.09	118.90
36	5	1152	G	C6-C5-N7	10.32	136.59	130.40
36	5	2609	A	O5'-P-OP2	-10.28	96.45	105.70
36	5	2548	C	N1-C2-O2	10.25	125.05	118.90
36	5	420	G	N3-C4-N9	9.96	131.98	126.00
36	5	439	C	N1-C2-O2	9.95	124.87	118.90
36	5	1152	G	C4-C5-C6	-9.92	112.85	118.80
36	1	984	G	N3-C4-N9	9.78	131.87	126.00
36	5	2269	U	C5-C6-N1	9.68	127.54	122.70
1	6	1490	C	C6-N1-C2	-9.63	116.45	120.30
36	5	1495	U	C6-N1-C2	-9.63	115.22	121.00
36	5	1115	G	C8-N9-C4	-9.52	102.59	106.40
36	5	864	G	N3-C4-C5	-9.52	123.84	128.60
36	5	863	C	C6-N1-C2	-9.50	116.50	120.30
1	6	453	U	C2-N1-C1'	9.49	129.09	117.70
36	5	1308	A	C8-N9-C4	-9.48	102.01	105.80
1	2	620	A	O5'-P-OP2	-9.48	97.17	105.70
36	5	1063	G	C8-N9-C4	-9.48	102.61	106.40
36	1	1581	C	C2-N1-C1'	9.47	129.21	118.80
72	O6	50	LEU	C-N-CA	9.45	145.33	121.70
36	5	2548	C	N3-C2-O2	-9.43	115.30	121.90
36	5	2931	C	C6-N1-C2	9.42	124.07	120.30
36	1	644	G	N3-C4-C5	-9.40	123.90	128.60
36	5	1496	C	C6-N1-C2	-9.39	116.55	120.30
36	1	3217	C	N1-C2-O2	9.37	124.52	118.90
1	2	1490	C	O5'-P-OP1	-9.35	97.28	105.70
36	5	1607	U	P-O3'-C3'	9.35	130.92	119.70
36	1	1866	C	C2-N1-C1'	9.35	129.08	118.80
36	1	2400	G	C5-C6-O6	-9.34	123.00	128.60
36	5	439	C	N3-C2-O2	-9.30	115.39	121.90
36	1	2145	A	N1-C6-N6	9.20	124.12	118.60
36	1	1306	G	N1-C6-O6	9.18	125.41	119.90
36	5	2572	C	N1-C2-O2	9.15	124.39	118.90
36	5	1495	U	C5-C6-N1	9.11	127.26	122.70
1	6	1467	C	C6-N1-C2	-9.10	116.66	120.30
36	1	2552	C	O5'-P-OP1	-9.05	97.55	105.70
36	1	1526	U	O5'-P-OP2	-8.99	97.61	105.70
36	1	1589	A	C8-N9-C4	8.98	109.39	105.80
36	5	1496	C	C2-N1-C1'	8.96	128.65	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1763	U	C2-N1-C1'	8.93	128.41	117.70
50	m4	135	LEU	CA-CB-CG	8.90	135.77	115.30
36	1	2966	G	N3-C4-N9	8.89	131.34	126.00
36	5	1556	C	C2-N1-C1'	8.87	128.56	118.80
36	1	635	G	N3-C4-N9	8.84	131.30	126.00
36	5	1063	G	C8-N9-C1'	-8.84	115.51	127.00
36	1	1444	G	C5-C6-O6	-8.84	123.30	128.60
36	1	1581	C	N3-C2-O2	-8.82	115.72	121.90
1	2	626	U	C5-C6-N1	8.82	127.11	122.70
36	5	1482	A	O5'-P-OP2	-8.82	97.76	105.70
1	2	947	U	C5-C6-N1	8.80	127.10	122.70
36	5	420	G	N3-C4-C5	-8.79	124.21	128.60
1	6	1756	A	C4-C5-C6	8.76	121.38	117.00
36	1	2966	G	N3-C4-C5	-8.75	124.22	128.60
36	1	2400	G	N1-C6-O6	8.75	125.15	119.90
36	1	3278	C	C6-N1-C2	-8.74	116.80	120.30
36	1	1192	C	C5-C6-N1	8.74	125.37	121.00
36	1	1556	C	C2-N1-C1'	8.73	128.41	118.80
36	5	1531	C	C6-N1-C2	8.70	123.78	120.30
36	1	1765	U	O4'-C1'-N1	8.66	115.13	108.20
36	5	360	G	N3-C4-C5	-8.66	124.27	128.60
36	1	1759	C	O5'-P-OP1	8.63	121.05	110.70
36	1	371	G	N3-C4-C5	8.61	132.90	128.60
36	1	3217	C	N3-C2-O2	-8.59	115.89	121.90
36	1	884	A	O5'-P-OP1	-8.59	97.97	105.70
36	5	1196	C	C6-N1-C2	8.57	123.73	120.30
36	5	1014	U	C2-N1-C1'	8.55	127.96	117.70
36	1	638	C	O5'-P-OP2	-8.54	98.01	105.70
36	5	635	G	N9-C4-C5	-8.53	101.99	105.40
36	5	1092	C	C6-N1-C2	-8.51	116.89	120.30
36	1	2696	A	O5'-P-OP2	-8.51	98.04	105.70
36	1	1444	G	N1-C6-O6	8.50	125.00	119.90
1	6	1756	A	C8-N9-C4	-8.47	102.41	105.80
36	5	1115	G	N7-C8-N9	8.47	117.34	113.10
36	5	1841	A	O5'-P-OP1	-8.46	98.08	105.70
36	5	1303	A	O5'-P-OP1	-8.46	98.08	105.70
36	1	2821	C	N1-C2-O2	8.44	123.96	118.90
9	s7	9	LEU	CA-CB-CG	8.43	134.68	115.30
36	1	635	G	N9-C4-C5	-8.42	102.03	105.40
1	2	1754	A	C8-N9-C4	-8.42	102.43	105.80
36	5	360	G	N3-C4-N9	8.39	131.04	126.00
36	1	981	U	C5-C6-N1	8.38	126.89	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	309	C	C6-N1-C2	-8.35	116.96	120.30
36	1	875	G	O5'-P-OP2	-8.35	98.19	105.70
36	5	424	G	O5'-P-OP1	-8.35	98.19	105.70
36	5	2263	C	O5'-P-OP1	-8.34	98.20	105.70
36	5	2664	C	C6-N1-C2	-8.34	116.97	120.30
36	5	827	A	O5'-P-OP1	-8.33	98.20	105.70
36	5	2548	C	C6-N1-C2	-8.31	116.97	120.30
36	5	864	G	N3-C4-N9	8.30	130.98	126.00
36	5	3270	U	O5'-P-OP1	-8.30	98.23	105.70
1	2	1560	U	N3-C2-O2	-8.29	116.40	122.20
36	1	919	U	O5'-P-OP2	-8.29	98.24	105.70
36	5	329	U	C2-N1-C1'	8.28	127.64	117.70
36	5	1437	C	C5-C6-N1	8.28	125.14	121.00
36	1	1589	A	N9-C4-C5	-8.26	102.50	105.80
36	1	3278	C	N1-C2-O2	8.25	123.85	118.90
36	1	1589	A	N1-C6-N6	8.25	123.55	118.60
1	6	156	A	C8-N9-C4	8.25	109.10	105.80
36	1	1495	U	C4-C5-C6	8.24	124.65	119.70
36	5	3143	C	C6-N1-C2	8.22	123.59	120.30
36	1	1000	C	C6-N1-C2	8.21	123.58	120.30
36	1	1607	U	P-O3'-C3'	8.21	129.55	119.70
36	1	3278	C	N3-C2-O2	-8.21	116.16	121.90
36	1	2132	C	C6-N1-C2	-8.20	117.02	120.30
36	1	651	G	C8-N9-C4	-8.17	103.13	106.40
36	5	835	G	N3-C4-C5	8.16	132.68	128.60
36	5	2572	C	N3-C2-O2	-8.16	116.19	121.90
36	5	3005	A	C8-N9-C4	-8.14	102.54	105.80
36	5	824	C	N3-C2-O2	-8.13	116.21	121.90
36	5	939	U	C5-C6-N1	8.11	126.75	122.70
36	1	1556	C	P-O3'-C3'	8.10	129.42	119.70
9	s7	118	LEU	CA-CB-CG	8.07	133.87	115.30
36	1	1493	G	N3-C4-C5	-8.07	124.56	128.60
1	6	1485	C	C6-N1-C2	-8.07	117.07	120.30
36	5	3129	A	C8-N9-C4	8.07	109.03	105.80
38	4	17	A	O5'-P-OP2	-8.06	98.44	105.70
36	5	1437	C	N3-C4-C5	-8.05	118.68	121.90
36	1	863	C	C5-C6-N1	8.04	125.02	121.00
36	1	1866	C	C6-N1-C1'	-8.04	111.15	120.80
36	5	368	G	C8-N9-C4	8.04	109.62	106.40
36	5	2608	G	C8-N9-C4	8.03	109.61	106.40
60	n4	96	LEU	C-N-CA	8.02	141.75	121.70
1	6	1657	U	N3-C2-O2	8.01	127.81	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3022	G	O4'-C1'-N9	8.01	114.61	108.20
1	2	1389	C	N3-C2-O2	-8.01	116.29	121.90
38	8	14	C	C6-N1-C2	8.01	123.50	120.30
36	1	2392	C	C5-C6-N1	-8.00	117.00	121.00
1	2	934	C	C2-N1-C1'	7.99	127.59	118.80
36	1	1415	U	C5-C4-O4	7.98	130.69	125.90
38	4	126	A	N1-C2-N3	7.97	133.28	129.30
1	6	1756	A	N3-C4-C5	-7.94	121.24	126.80
36	5	1445	U	O5'-P-OP1	-7.94	98.56	105.70
36	5	402	A	O5'-P-OP1	-7.94	98.56	105.70
36	1	315	C	C6-N1-C2	-7.92	117.13	120.30
36	5	1772	U	C5-C6-N1	-7.92	118.74	122.70
36	1	3137	C	C6-N1-C2	-7.92	117.13	120.30
36	1	1639	C	C5-C6-N1	7.92	124.96	121.00
36	1	1858	A	N3-C4-N9	7.91	133.73	127.40
1	2	1754	A	C5-N7-C8	-7.89	99.95	103.90
36	1	1512	U	C6-N1-C2	-7.87	116.28	121.00
1	6	1606	C	C6-N1-C2	-7.86	117.16	120.30
36	5	27	C	O5'-P-OP1	-7.86	98.62	105.70
36	1	984	G	N3-C4-C5	-7.86	124.67	128.60
36	5	2400	G	OP2-P-O3'	7.86	122.49	105.20
36	1	1329	U	P-O3'-C3'	7.85	129.12	119.70
1	2	1389	C	C6-N1-C2	-7.84	117.16	120.30
36	5	1592	G	C5-C6-O6	-7.84	123.90	128.60
36	5	1585	C	C6-N1-C2	-7.83	117.17	120.30
36	1	3228	C	C4-C5-C6	7.83	121.31	117.40
38	8	100	U	C2-N1-C1'	7.83	127.09	117.70
37	3	47	C	C6-N1-C2	-7.83	117.17	120.30
1	6	1274	C	C2-N1-C1'	7.83	127.41	118.80
36	1	873	C	P-O3'-C3'	7.82	129.09	119.70
36	1	2145	A	N9-C4-C5	-7.82	102.67	105.80
36	1	2616	C	C6-N1-C2	7.82	123.43	120.30
36	5	2996	U	C5-C6-N1	-7.81	118.80	122.70
36	1	55	G	C8-N9-C4	7.80	109.52	106.40
36	1	312	C	C6-N1-C2	-7.80	117.18	120.30
1	6	1653	C	C6-N1-C2	-7.78	117.19	120.30
36	5	2283	G	O5'-P-OP2	-7.76	98.71	105.70
36	5	835	G	N3-C4-N9	-7.74	121.36	126.00
36	1	3367	C	C6-N1-C2	7.70	123.38	120.30
1	2	934	C	N1-C2-O2	7.70	123.52	118.90
36	5	2988	C	C2-N1-C1'	7.68	127.25	118.80
1	6	1756	A	N7-C8-N9	7.67	117.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2967	A	N1-C6-N6	7.67	123.20	118.60
36	5	1516	C	C6-N1-C2	7.66	123.36	120.30
36	1	2568	C	C2-N1-C1'	7.64	127.21	118.80
1	6	1463	C	C6-N1-C2	7.64	123.36	120.30
36	5	924	G	O5'-P-OP1	-7.63	98.83	105.70
36	5	2906	C	C6-N1-C2	-7.62	117.25	120.30
36	5	1609	C	C6-N1-C2	7.62	123.35	120.30
36	1	644	G	O5'-P-OP2	7.62	119.84	110.70
36	1	3217	C	C2-N1-C1'	7.61	127.17	118.80
38	8	94	C	C6-N1-C2	7.59	123.34	120.30
36	5	3278	C	N1-C2-O2	7.58	123.45	118.90
36	5	1556	C	C6-N1-C1'	-7.58	111.71	120.80
1	2	1752	U	C5-C6-N1	7.57	126.49	122.70
36	1	2132	C	C5-C6-N1	7.57	124.79	121.00
36	5	1495	U	C2-N1-C1'	7.57	126.79	117.70
36	5	2548	C	C2-N1-C1'	7.57	127.13	118.80
36	5	2281	A	O4'-C1'-N9	7.56	114.25	108.20
36	5	2572	C	C2-N1-C1'	7.56	127.12	118.80
36	5	3269	U	C5-C6-N1	7.56	126.48	122.70
36	1	2145	A	C4-C5-N7	7.54	114.47	110.70
36	1	1493	G	C4-N9-C1'	7.54	136.31	126.50
36	5	1152	G	N1-C2-N2	7.53	122.98	116.20
1	6	1654	G	C4-N9-C1'	7.53	136.29	126.50
36	5	1593	A	C8-N9-C4	-7.53	102.79	105.80
36	5	2837	A	C8-N9-C4	7.53	108.81	105.80
36	5	406	G	O4'-C1'-N9	7.52	114.22	108.20
1	2	1028	C	C6-N1-C2	7.52	123.31	120.30
38	4	119	C	C5-C6-N1	7.52	124.76	121.00
1	2	1280	C	C6-N1-C2	-7.52	117.29	120.30
36	5	1149	G	N3-C4-N9	7.52	130.51	126.00
1	2	1389	C	N1-C2-O2	7.51	123.41	118.90
36	1	1589	A	C5-C6-N6	-7.51	117.69	123.70
36	1	2407	C	C2-N1-C1'	7.50	127.05	118.80
36	5	635	G	C5-C6-O6	-7.50	124.10	128.60
36	1	3382	U	N1-C2-O2	7.49	128.04	122.80
36	5	1561	G	O4'-C1'-N9	7.48	114.19	108.20
36	5	1063	G	O4'-C1'-N9	7.47	114.18	108.20
1	6	813	U	N1-C2-O2	7.47	128.03	122.80
36	1	822	G	O5'-P-OP2	-7.47	98.98	105.70
36	5	2381	G	O5'-P-OP2	-7.47	98.98	105.70
39	12	246	LEU	CA-CB-CG	7.46	132.45	115.30
1	2	1751	C	C6-N1-C2	7.45	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	205	C	C6-N1-C2	7.45	123.28	120.30
36	5	939	U	N3-C2-O2	-7.45	116.98	122.20
36	1	2922	G	N9-C4-C5	-7.45	102.42	105.40
38	8	9	A	C8-N9-C4	7.45	108.78	105.80
36	1	591	G	N1-C6-O6	-7.44	115.44	119.90
36	1	959	C	C6-N1-C2	7.44	123.28	120.30
36	1	1639	C	C6-N1-C2	-7.42	117.33	120.30
36	5	1063	G	N3-C4-C5	-7.41	124.89	128.60
4	S2	113	LEU	CA-CB-CG	7.41	132.33	115.30
37	7	69	C	C6-N1-C2	-7.41	117.34	120.30
36	5	1312	C	C6-N1-C2	-7.40	117.34	120.30
36	5	1866	C	C2-N1-C1'	7.39	126.93	118.80
36	1	1086	C	C6-N1-C2	-7.39	117.34	120.30
37	3	85	G	N3-C4-C5	7.39	132.29	128.60
36	5	426	G	N3-C4-N9	-7.38	121.57	126.00
36	1	1541	G	N3-C2-N2	-7.38	114.74	119.90
36	1	2403	G	C6-C5-N7	-7.37	125.98	130.40
36	5	297	G	C4-N9-C1'	7.37	136.08	126.50
36	5	432	G	N1-C6-O6	7.37	124.32	119.90
1	6	1591	C	C6-N1-C2	-7.36	117.36	120.30
36	5	726	G	N7-C8-N9	7.35	116.78	113.10
1	6	1654	G	N3-C4-C5	-7.34	124.93	128.60
1	6	572	C	C6-N1-C2	-7.34	117.36	120.30
36	1	2407	C	C5-C6-N1	7.33	124.67	121.00
36	1	1531	C	C6-N1-C2	7.33	123.23	120.30
1	6	1137	A	C8-N9-C4	7.33	108.73	105.80
62	n6	76	LEU	CA-CB-CG	7.33	132.15	115.30
36	1	2427	U	O5'-P-OP2	-7.31	99.12	105.70
36	5	19	U	C2-N1-C1'	-7.31	108.93	117.70
36	1	98	G	N3-C4-N9	7.30	130.38	126.00
1	2	577	G	N1-C6-O6	7.30	124.28	119.90
36	1	371	G	N3-C4-N9	-7.30	121.62	126.00
1	2	145	A	N1-C6-N6	-7.29	114.22	118.60
36	5	92	G	C8-N9-C4	7.29	109.31	106.40
36	5	1633	C	C2-N1-C1'	7.29	126.81	118.80
36	5	1389	G	O5'-P-OP1	-7.28	99.15	105.70
36	1	1001	G	N3-C4-N9	7.28	130.37	126.00
36	5	1348	U	C6-N1-C2	-7.28	116.64	121.00
36	1	1001	G	N3-C4-C5	-7.27	124.96	128.60
36	1	2980	U	O5'-P-OP2	-7.27	99.15	105.70
36	1	406	G	O4'-C1'-N9	7.27	114.02	108.20
36	5	354	U	C2-N1-C1'	7.27	126.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3278	C	N3-C2-O2	-7.27	116.81	121.90
36	5	510	G	N1-C6-O6	7.26	124.26	119.90
36	1	3278	C	C2-N1-C1'	7.26	126.79	118.80
1	6	156	A	N9-C4-C5	-7.26	102.89	105.80
36	1	1115	G	C4-C5-N7	7.26	113.70	110.80
36	1	1886	A	N1-C6-N6	-7.25	114.25	118.60
38	4	14	C	C6-N1-C2	7.25	123.20	120.30
1	2	1157	A	C8-N9-C4	-7.24	102.90	105.80
1	6	1389	C	C2-N1-C1'	7.23	126.75	118.80
36	1	2549	G	N3-C4-N9	-7.22	121.67	126.00
36	5	3217	C	C6-N1-C2	7.22	123.19	120.30
1	6	1657	U	N1-C2-O2	-7.21	117.75	122.80
36	5	1014	U	C5-C6-N1	7.21	126.31	122.70
36	5	939	U	C2-N1-C1'	7.21	126.35	117.70
36	5	3269	U	P-O3'-C3'	7.20	128.34	119.70
36	1	1047	A	O5'-P-OP2	-7.20	99.22	105.70
36	5	345	G	N3-C4-N9	7.19	130.31	126.00
36	1	1773	C	C6-N1-C2	7.19	123.17	120.30
36	5	3078	U	N3-C2-O2	-7.18	117.18	122.20
1	6	1003	A	C8-N9-C4	7.17	108.67	105.80
36	5	518	G	N3-C4-C5	-7.17	125.01	128.60
36	5	3338	C	C6-N1-C2	7.17	123.17	120.30
36	1	1780	G	C4-N9-C1'	7.17	135.82	126.50
36	5	676	G	C4-N9-C1'	7.17	135.82	126.50
36	5	1151	U	N3-C4-C5	-7.17	110.30	114.60
36	1	3139	A	N7-C8-N9	7.16	117.38	113.80
36	5	927	C	C6-N1-C2	-7.16	117.44	120.30
36	1	1525	G	C4-N9-C1'	7.15	135.80	126.50
36	1	2966	G	C8-N9-C1'	-7.15	117.70	127.00
36	1	1859	A	OP1-P-O3'	7.14	120.91	105.20
36	1	2762	A	N1-C6-N6	-7.13	114.32	118.60
36	5	518	G	C4-N9-C1'	7.13	135.77	126.50
38	4	102	U	O5'-P-OP2	-7.12	99.29	105.70
36	5	2988	C	C6-N1-C2	-7.12	117.45	120.30
36	1	877	C	C6-N1-C2	7.12	123.15	120.30
36	1	1303	A	C8-N9-C4	7.10	108.64	105.80
36	1	2118	C	C2-N1-C1'	7.10	126.61	118.80
36	1	729	C	C6-N1-C2	-7.10	117.46	120.30
36	1	635	G	C6-C5-N7	-7.10	126.14	130.40
36	1	1858	A	C8-N9-C4	-7.10	102.96	105.80
36	5	922	U	C5-C6-N1	-7.09	119.15	122.70
36	1	1134	G	N9-C4-C5	7.09	108.24	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1909	A	C8-N9-C4	7.09	108.64	105.80
1	6	194	U	C2-N1-C1'	7.08	126.20	117.70
36	1	1585	C	C6-N1-C2	-7.08	117.47	120.30
36	5	939	U	C6-N1-C2	-7.08	116.75	121.00
36	5	1455	U	C6-N1-C2	7.07	125.25	121.00
36	1	718	G	N3-C4-C5	7.07	132.13	128.60
36	5	635	G	C4-C5-N7	7.07	113.63	110.80
38	8	137	C	C6-N1-C2	7.07	123.13	120.30
36	5	2572	C	C6-N1-C2	-7.06	117.48	120.30
36	5	2996	U	C6-N1-C2	7.05	125.23	121.00
36	1	2760	C	C6-N1-C2	7.04	123.12	120.30
36	5	1556	C	N1-C2-O2	7.04	123.12	118.90
1	2	1291	G	N3-C4-N9	-7.04	121.78	126.00
1	6	453	U	C6-N1-C1'	-7.04	111.35	121.20
36	5	676	G	N3-C4-N9	7.04	130.22	126.00
36	5	3278	C	C2-N1-C1'	7.02	126.53	118.80
36	5	635	G	C8-N9-C4	7.02	109.21	106.40
1	2	507	U	N3-C2-O2	-7.01	117.29	122.20
36	1	1907	C	C6-N1-C2	-7.01	117.49	120.30
36	5	1897	G	N9-C4-C5	-7.01	102.59	105.40
1	2	581	U	C2-N1-C1'	-7.01	109.28	117.70
36	1	2966	G	C4-N9-C1'	7.01	135.61	126.50
36	5	1329	U	P-O3'-C3'	7.01	128.11	119.70
36	5	909	G	N3-C4-N9	7.01	130.21	126.00
36	1	1807	G	C8-N9-C4	-7.01	103.60	106.40
36	1	546	C	C2-N1-C1'	7.00	126.50	118.80
36	1	639	G	C8-N9-C4	7.00	109.20	106.40
36	1	1820	U	P-O3'-C3'	7.00	128.10	119.70
36	5	1527	C	N3-C2-O2	-6.99	117.01	121.90
1	6	194	U	N3-C2-O2	-6.99	117.31	122.20
1	2	863	A	O4'-C1'-N9	6.98	113.79	108.20
36	1	2827	U	C2-N1-C1'	-6.98	109.32	117.70
36	5	1762	C	C6-N1-C2	-6.97	117.51	120.30
36	5	283	G	C4-N9-C1'	6.97	135.56	126.50
36	5	2978	U	O4'-C1'-N1	6.97	113.77	108.20
36	1	1493	G	N3-C4-N9	6.96	130.18	126.00
36	5	2256	A	C4-C5-C6	-6.96	113.52	117.00
36	5	639	G	C8-N9-C4	6.96	109.18	106.40
36	5	2988	C	N1-C2-O2	6.96	123.07	118.90
13	c1	5	LEU	CA-CB-CG	6.96	131.30	115.30
36	5	2138	A	C8-N9-C4	6.95	108.58	105.80
36	5	510	G	C4-C5-N7	6.95	113.58	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1146	C	C6-N1-C2	6.95	123.08	120.30
37	3	58	C	C6-N1-C2	-6.94	117.52	120.30
38	8	75	G	C4-N9-C1'	-6.93	117.48	126.50
36	5	2772	C	P-O3'-C3'	6.93	128.02	119.70
36	1	2311	G	O5'-P-OP1	-6.93	99.46	105.70
36	1	3291	G	N3-C4-N9	-6.92	121.85	126.00
36	1	1389	G	C8-N9-C4	6.92	109.17	106.40
36	1	2306	C	C2-N1-C1'	6.92	126.41	118.80
1	2	784	C	C5-C6-N1	6.91	124.45	121.00
36	1	2541	U	C2-N1-C1'	6.91	125.99	117.70
36	5	868	C	N1-C2-O2	-6.91	114.76	118.90
36	1	1788	C	C5-C6-N1	6.90	124.45	121.00
1	6	1568	C	C6-N1-C2	-6.90	117.54	120.30
36	5	824	C	N1-C2-O2	6.90	123.04	118.90
36	5	79	U	C5-C6-N1	6.89	126.15	122.70
36	5	1822	C	C6-N1-C2	-6.89	117.54	120.30
36	5	297	G	C8-N9-C1'	-6.89	118.04	127.00
38	8	113	U	C2-N1-C1'	6.88	125.96	117.70
36	1	2145	A	C5-N7-C8	-6.88	100.46	103.90
36	5	1308	A	N9-C4-C5	6.88	108.55	105.80
36	1	1017	C	C6-N1-C2	-6.87	117.55	120.30
36	5	1897	G	C5-C6-O6	-6.87	124.48	128.60
36	1	639	G	N9-C4-C5	-6.87	102.65	105.40
36	1	1740	U	C5-C6-N1	-6.87	119.27	122.70
45	18	69	LEU	CA-CB-CG	6.87	131.10	115.30
1	2	1258	U	N3-C2-O2	-6.85	117.41	122.20
36	5	1081	U	P-O3'-C3'	6.84	127.91	119.70
1	2	1644	C	C6-N1-C2	-6.84	117.56	120.30
36	1	91	G	N3-C4-C5	-6.84	125.18	128.60
36	5	824	C	OP1-P-O3'	6.84	120.25	105.20
36	1	2971	A	C8-N9-C4	6.84	108.53	105.80
36	5	1176	C	C6-N1-C2	6.83	123.03	120.30
36	5	297	G	N3-C4-N9	6.83	130.10	126.00
1	2	192	U	C2-N1-C1'	6.83	125.90	117.70
36	5	1580	A	N7-C8-N9	6.83	117.22	113.80
36	5	2842	U	C2-N1-C1'	6.83	125.90	117.70
36	5	2912	G	N3-C4-C5	6.82	132.01	128.60
1	6	1749	A	C8-N9-C4	6.82	108.53	105.80
36	1	824	C	C6-N1-C2	-6.81	117.58	120.30
36	1	219	A	P-O3'-C3'	6.81	127.87	119.70
36	5	518	G	C8-N9-C4	-6.80	103.68	106.40
1	6	321	C	P-O3'-C3'	6.80	127.86	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1604	G	C4-N9-C1'	6.80	135.34	126.50
36	5	1496	C	C5-C6-N1	6.80	124.40	121.00
36	5	1445	U	C2-N1-C1'	-6.80	109.54	117.70
36	1	2407	C	C6-N1-C2	-6.80	117.58	120.30
36	5	510	G	C5-C6-O6	-6.79	124.52	128.60
36	5	3299	A	O5'-P-OP2	-6.79	99.59	105.70
36	1	1556	C	C6-N1-C1'	-6.78	112.67	120.80
36	1	3382	U	C2-N1-C1'	6.77	125.83	117.70
36	1	1307	G	P-O3'-C3'	6.77	127.83	119.70
36	5	345	G	C6-C5-N7	-6.77	126.34	130.40
36	5	2988	C	N3-C2-O2	-6.77	117.16	121.90
36	1	2633	U	O5'-P-OP2	6.77	118.82	110.70
36	1	2371	G	C8-N9-C4	6.76	109.10	106.40
36	5	3065	G	N3-C4-C5	6.76	131.98	128.60
36	5	394	G	N3-C4-C5	6.76	131.98	128.60
36	1	2971	A	N9-C4-C5	-6.75	103.10	105.80
37	3	83	U	C2-N1-C1'	-6.75	109.60	117.70
1	2	783	G	C5-C6-O6	-6.75	124.55	128.60
37	3	89	G	C8-N9-C4	6.75	109.10	106.40
36	5	2355	G	N1-C6-O6	6.75	123.95	119.90
36	5	3278	C	C6-N1-C2	-6.74	117.60	120.30
1	2	39	A	O4'-C1'-N9	6.73	113.58	108.20
36	1	1103	A	P-O3'-C3'	6.73	127.77	119.70
36	5	2138	A	N1-C6-N6	6.72	122.64	118.60
36	1	2403	G	C8-N9-C4	-6.72	103.71	106.40
36	1	2335	G	N3-C4-C5	-6.72	125.24	128.60
1	6	103	A	P-O3'-C3'	6.72	127.76	119.70
35	SM	167	PRO	N-CA-CB	6.71	111.36	103.30
36	1	1742	U	C5-C6-N1	6.71	126.06	122.70
36	1	116	A	C8-N9-C4	-6.71	103.12	105.80
36	1	2808	A	O4'-C1'-N9	-6.71	102.83	108.20
36	1	1472	U	O5'-P-OP2	-6.70	99.67	105.70
36	1	2221	G	N3-C4-N9	-6.70	121.98	126.00
1	2	1399	C	N1-C2-O2	6.70	122.92	118.90
1	2	937	C	C6-N1-C2	-6.70	117.62	120.30
36	5	1429	G	N3-C4-N9	6.70	130.02	126.00
1	6	156	A	N1-C6-N6	6.69	122.62	118.60
36	1	1604	G	N3-C4-C5	-6.69	125.25	128.60
36	1	2871	G	N3-C4-N9	6.69	130.01	126.00
36	1	2359	C	C6-N1-C2	-6.69	117.63	120.30
36	5	1174	G	C4-N9-C1'	6.68	135.19	126.50
36	1	1306	G	C6-C5-N7	-6.68	126.39	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1258	U	C4-C5-C6	6.68	123.71	119.70
36	1	1495	U	C5-C6-N1	-6.68	119.36	122.70
36	1	1201	C	C6-N1-C2	-6.67	117.63	120.30
52	M6	15	LEU	CA-CB-CG	-6.67	99.96	115.30
1	2	1490	C	C2-N1-C1'	6.67	126.14	118.80
36	1	916	G	N3-C4-C5	-6.66	125.27	128.60
36	5	240	U	C5-C6-N1	6.66	126.03	122.70
36	1	2335	G	C8-N9-C4	-6.65	103.74	106.40
1	6	813	U	N3-C2-O2	-6.65	117.54	122.20
36	5	1416	C	N1-C2-O2	6.65	122.89	118.90
37	3	18	C	C5-C6-N1	6.64	124.32	121.00
1	2	577	G	C4-C5-N7	6.64	113.46	110.80
36	5	2138	A	N9-C4-C5	-6.64	103.14	105.80
36	5	2966	G	N3-C4-C5	-6.64	125.28	128.60
36	5	525	C	C6-N1-C2	-6.64	117.64	120.30
36	5	1332	A	C8-N9-C4	-6.64	103.14	105.80
38	4	24	G	N3-C4-C5	6.64	131.92	128.60
1	2	1022	C	C6-N1-C2	6.63	122.95	120.30
36	1	637	C	P-O3'-C3'	6.63	127.66	119.70
1	2	1291	G	N3-C4-C5	6.63	131.91	128.60
36	5	1389	G	N3-C4-N9	6.62	129.97	126.00
36	5	2878	G	N3-C4-C5	-6.62	125.29	128.60
38	4	117	C	C6-N1-C2	6.62	122.95	120.30
1	6	1568	C	P-O3'-C3'	6.62	127.64	119.70
1	6	194	U	N1-C2-O2	6.61	127.43	122.80
36	5	329	U	C6-N1-C1'	-6.61	111.94	121.20
36	5	1848	G	O5'-P-OP2	-6.61	99.75	105.70
36	1	1581	C	C6-N1-C1'	-6.61	112.87	120.80
36	1	3354	U	C2-N1-C1'	6.61	125.63	117.70
36	5	282	G	P-O3'-C3'	6.61	127.63	119.70
36	5	1308	A	N7-C8-N9	6.61	117.10	113.80
36	5	1902	G	C6-C5-N7	-6.61	126.44	130.40
36	1	3115	C	C6-N1-C2	6.60	122.94	120.30
36	5	240	U	C2-N1-C1'	6.60	125.62	117.70
36	1	644	G	C4-N9-C1'	6.60	135.08	126.50
36	1	1521	G	O5'-P-OP1	-6.60	99.76	105.70
1	6	1	U	C2-N1-C1'	6.60	125.62	117.70
36	1	1607	U	C6-N1-C2	-6.59	117.04	121.00
36	1	635	G	C5-C6-O6	-6.59	124.64	128.60
36	5	2615	G	N3-C4-C5	6.59	131.90	128.60
36	5	881	C	C6-N1-C2	6.58	122.93	120.30
36	1	227	G	N3-C4-N9	6.58	129.95	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2572	C	C6-N1-C2	-6.58	117.67	120.30
36	1	993	G	C8-N9-C4	-6.58	103.77	106.40
36	5	24	G	C8-N9-C4	6.58	109.03	106.40
36	1	282	G	C8-N9-C4	-6.58	103.77	106.40
36	1	718	G	N3-C4-N9	-6.58	122.05	126.00
36	5	3078	U	C5-C4-O4	6.58	129.84	125.90
1	6	1634	C	N1-C2-O2	6.57	122.84	118.90
36	1	3291	G	N3-C4-C5	6.57	131.88	128.60
36	5	439	C	C2-N1-C1'	6.57	126.03	118.80
1	2	507	U	C2-N1-C1'	6.57	125.58	117.70
36	5	1639	C	C6-N1-C2	-6.57	117.67	120.30
36	5	562	C	C6-N1-C2	-6.56	117.67	120.30
1	2	1514	U	N3-C4-O4	-6.56	114.81	119.40
36	1	2935	U	C5-C6-N1	6.56	125.98	122.70
36	1	2356	A	C8-N9-C4	6.56	108.42	105.80
36	1	2392	C	C2-N1-C1'	-6.55	111.59	118.80
36	1	2821	C	N3-C2-O2	-6.55	117.31	121.90
36	1	371	G	C4-N9-C1'	-6.55	117.99	126.50
1	2	139	C	P-O3'-C3'	6.54	127.55	119.70
36	1	2403	G	O5'-P-OP2	-6.54	99.81	105.70
36	5	2917	G	N1-C6-O6	-6.54	115.98	119.90
36	5	2607	G	N1-C6-O6	6.54	123.82	119.90
36	5	909	G	N3-C4-C5	-6.54	125.33	128.60
36	5	979	U	C6-N1-C2	-6.53	117.08	121.00
36	5	1429	G	C8-N9-C1'	-6.53	118.51	127.00
36	1	898	U	C2-N1-C1'	6.53	125.54	117.70
1	6	1756	A	N3-C4-N9	6.52	132.62	127.40
36	5	3275	U	OP1-P-O3'	6.52	119.55	105.20
36	5	609	G	O5'-P-OP2	-6.52	99.83	105.70
36	1	2711	C	C6-N1-C2	-6.52	117.69	120.30
1	2	934	C	C6-N1-C1'	-6.52	112.98	120.80
36	1	282	G	P-O3'-C3'	6.52	127.52	119.70
36	1	1306	G	N9-C4-C5	-6.52	102.79	105.40
1	2	1568	C	P-O3'-C3'	6.51	127.51	119.70
36	5	2621	G	C8-N9-C1'	-6.51	118.54	127.00
36	1	2403	G	N3-C4-C5	-6.50	125.35	128.60
36	5	1228	C	C6-N1-C2	-6.50	117.70	120.30
38	4	54	A	N7-C8-N9	6.50	117.05	113.80
36	1	2608	G	N7-C8-N9	-6.50	109.85	113.10
36	5	3065	G	N3-C4-N9	-6.50	122.10	126.00
36	5	1307	G	P-O3'-C3'	6.50	127.50	119.70
36	5	2396	G	N1-C6-O6	6.50	123.80	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	803	C	C2-N1-C1'	6.50	125.95	118.80
36	5	3245	A	N7-C8-N9	6.50	117.05	113.80
36	1	1886	A	N9-C4-C5	6.50	108.40	105.80
36	1	593	C	C6-N1-C2	6.49	122.90	120.30
36	5	1671	C	C6-N1-C2	6.49	122.90	120.30
36	5	2181	C	C6-N1-C2	6.49	122.90	120.30
36	1	1451	C	C6-N1-C2	6.49	122.89	120.30
36	5	1480	G	N9-C4-C5	-6.49	102.81	105.40
36	1	354	U	C5-C6-N1	6.48	125.94	122.70
1	6	385	A	C8-N9-C4	-6.48	103.21	105.80
36	1	2142	A	N1-C2-N3	6.48	132.54	129.30
36	5	1149	G	C6-C5-N7	-6.48	126.51	130.40
36	5	2947	G	C8-N9-C4	-6.48	103.81	106.40
36	5	3078	U	N3-C4-O4	-6.48	114.86	119.40
36	5	360	G	C4-N9-C1'	6.47	134.92	126.50
73	o7	65	ARG	NE-CZ-NH1	6.47	123.54	120.30
36	5	1016	C	C2-N1-C1'	6.47	125.92	118.80
1	6	1180	C	C5-C6-N1	6.47	124.23	121.00
36	5	2876	C	N3-C2-O2	-6.47	117.37	121.90
36	1	2913	C	C5-C6-N1	6.46	124.23	121.00
36	5	1902	G	C4-N9-C1'	6.46	134.90	126.50
36	1	867	G	C4-C5-N7	6.46	113.39	110.80
36	1	3269	U	P-O3'-C3'	6.46	127.46	119.70
1	6	813	U	C2-N1-C1'	6.46	125.45	117.70
36	5	726	G	C8-N9-C4	-6.46	103.82	106.40
36	5	1581	C	C4-C5-C6	6.46	120.63	117.40
36	1	715	A	P-O3'-C3'	6.46	127.45	119.70
1	2	453	U	C2-N1-C1'	6.45	125.43	117.70
36	1	3139	A	C8-N9-C4	-6.45	103.22	105.80
36	5	2983	C	O4'-C1'-N1	6.45	113.36	108.20
36	5	1527	C	N1-C2-O2	6.44	122.77	118.90
1	6	158	U	P-O3'-C3'	6.44	127.43	119.70
36	5	3164	C	O4'-C1'-N1	6.44	113.35	108.20
37	3	26	C	C6-N1-C2	-6.44	117.72	120.30
36	5	939	U	N1-C2-O2	6.44	127.31	122.80
36	1	2950	G	O4'-C1'-N9	6.43	113.35	108.20
1	6	1399	C	C6-N1-C2	-6.43	117.73	120.30
36	5	422	A	C8-N9-C4	-6.43	103.23	105.80
36	5	635	G	N1-C6-O6	6.43	123.76	119.90
36	5	2314	U	C4-C5-C6	6.43	123.56	119.70
36	5	3194	C	C6-N1-C2	-6.43	117.73	120.30
36	5	218	G	N3-C4-N9	6.43	129.86	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	439	C	C6-N1-C2	-6.43	117.73	120.30
1	6	1426	C	C6-N1-C2	6.42	122.87	120.30
1	6	1458	G	N3-C4-N9	6.42	129.85	126.00
36	1	2227	C	P-O3'-C3'	6.41	127.39	119.70
36	5	1495	U	N3-C2-O2	-6.41	117.71	122.20
1	2	581	U	C5-C6-N1	-6.41	119.50	122.70
36	1	208	C	C5-C6-N1	6.41	124.20	121.00
36	5	1413	G	N1-C6-O6	6.41	123.74	119.90
36	5	1556	C	O4'-C1'-N1	-6.40	103.08	108.20
36	5	2922	G	N3-C4-N9	6.40	129.84	126.00
38	8	100	U	C6-N1-C1'	-6.40	112.24	121.20
1	6	1473	U	C2-N1-C1'	6.40	125.38	117.70
36	5	1354	G	C8-N9-C4	-6.40	103.84	106.40
1	6	1654	G	C8-N9-C4	-6.40	103.84	106.40
36	5	825	U	O5'-P-OP1	-6.40	99.94	105.70
1	6	151	G	N3-C4-N9	-6.40	122.16	126.00
36	1	1508	C	O5'-P-OP2	-6.39	99.94	105.70
36	5	283	G	C8-N9-C4	-6.39	103.84	106.40
36	5	2621	G	N3-C4-N9	6.39	129.84	126.00
36	5	1149	G	N9-C4-C5	-6.39	102.84	105.40
38	8	110	C	OP2-P-O3'	6.39	119.25	105.20
1	2	950	C	C6-N1-C2	-6.38	117.75	120.30
36	1	2221	G	N3-C4-C5	6.38	131.79	128.60
1	2	1514	U	C5-C4-O4	6.38	129.73	125.90
36	5	426	G	C8-N9-C4	-6.38	103.85	106.40
36	1	2719	U	C2-N1-C1'	-6.38	110.05	117.70
1	2	15	U	C5-C6-N1	6.37	125.89	122.70
36	1	1183	C	C6-N1-C2	6.37	122.85	120.30
36	1	3175	U	N1-C2-O2	6.37	127.26	122.80
36	5	1521	G	N3-C4-N9	-6.37	122.18	126.00
36	1	1327	C	O5'-P-OP1	-6.36	99.97	105.70
36	1	2645	G	C6-C5-N7	-6.36	126.58	130.40
1	6	1431	C	C6-N1-C2	6.36	122.84	120.30
1	2	1604	U	C6-N1-C2	-6.36	117.19	121.00
36	1	984	G	C8-N9-C1'	-6.36	118.74	127.00
36	5	676	G	C8-N9-C1'	-6.36	118.74	127.00
36	5	134	U	C2-N1-C1'	6.36	125.33	117.70
36	1	1780	G	N3-C4-C5	-6.35	125.42	128.60
1	2	190	C	O4'-C1'-N1	6.35	113.28	108.20
1	2	794	U	N1-C2-O2	6.34	127.24	122.80
69	o3	88	ASN	C-N-CA	-6.34	105.84	121.70
36	1	635	G	C4-C5-N7	6.34	113.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	352	A	O5'-P-OP1	-6.34	100.00	105.70
36	1	1484	U	P-O3'-C3'	6.34	127.30	119.70
36	1	2689	A	C8-N9-C4	-6.33	103.27	105.80
36	1	2549	G	C8-N9-C1'	6.33	135.23	127.00
36	1	765	C	OP1-P-O3'	6.33	119.11	105.20
36	1	984	G	C4-N9-C1'	6.33	134.72	126.50
36	1	1134	G	C8-N9-C4	-6.33	103.87	106.40
36	1	2964	G	O5'-P-OP1	-6.33	100.01	105.70
36	5	835	G	C4-N9-C1'	-6.33	118.28	126.50
36	5	1284	C	P-O3'-C3'	6.33	127.29	119.70
36	1	1115	G	C5-N7-C8	-6.32	101.14	104.30
36	1	1456	A	C8-N9-C4	-6.32	103.27	105.80
36	1	2967	A	C5-C6-N6	-6.32	118.64	123.70
36	1	546	C	N1-C2-O2	6.32	122.69	118.90
36	1	3221	C	C6-N1-C2	-6.32	117.77	120.30
1	2	322	G	O5'-P-OP1	-6.32	100.01	105.70
36	1	2400	G	C4-C5-N7	6.32	113.33	110.80
36	1	2615	G	O5'-P-OP1	-6.32	100.02	105.70
36	5	2396	G	C5-C6-O6	-6.31	124.81	128.60
36	1	3025	C	C6-N1-C2	6.31	122.82	120.30
40	l3	246	LEU	CA-CB-CG	6.31	129.81	115.30
1	2	1504	G	C4-N9-C1'	6.30	134.69	126.50
36	1	1201	C	C5-C6-N1	6.30	124.15	121.00
37	3	89	G	N9-C4-C5	-6.30	102.88	105.40
36	1	2983	C	O4'-C1'-N1	6.30	113.24	108.20
1	2	1399	C	N3-C2-O2	-6.30	117.49	121.90
36	5	1150	A	O5'-P-OP2	-6.30	100.03	105.70
36	1	1710	C	C6-N1-C2	6.29	122.82	120.30
36	1	3210	A	C8-N9-C4	6.29	108.32	105.80
31	D9	36	LEU	CA-CB-CG	6.29	129.77	115.30
36	1	2843	U	N3-C2-O2	-6.29	117.80	122.20
36	5	3354	U	O4'-C1'-N1	-6.29	103.17	108.20
36	1	2179	C	C6-N1-C2	6.29	122.82	120.30
36	1	2967	A	N9-C4-C5	-6.29	103.28	105.80
1	2	1389	C	C2-N1-C1'	6.29	125.71	118.80
36	5	1096	U	O5'-P-OP1	-6.29	100.04	105.70
36	5	1174	G	C8-N9-C1'	-6.29	118.83	127.00
36	1	708	G	N3-C4-N9	6.28	129.77	126.00
1	6	1039	A	O4'-C1'-N9	6.28	113.22	108.20
1	2	1070	C	C6-N1-C2	6.28	122.81	120.30
36	1	2554	A	P-O3'-C3'	6.28	127.23	119.70
36	1	1094	U	N3-C2-O2	-6.28	117.81	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	163	G	N3-C2-N2	-6.28	115.51	119.90
1	2	1600	A	C4-N9-C1'	6.27	137.59	126.30
36	1	312	C	C5-C6-N1	6.27	124.14	121.00
36	1	718	G	C5-N7-C8	-6.27	101.16	104.30
36	1	764	U	P-O3'-C3'	6.27	127.23	119.70
36	1	922	U	C6-N1-C1'	-6.27	112.42	121.20
36	1	1815	U	P-O3'-C3'	6.27	127.23	119.70
36	5	347	G	N1-C6-O6	6.27	123.66	119.90
36	5	2726	C	N3-C2-O2	-6.27	117.51	121.90
36	1	1306	G	C8-N9-C1'	-6.27	118.85	127.00
36	5	870	G	C8-N9-C4	6.27	108.91	106.40
38	4	100	U	C2-N1-C1'	6.27	125.22	117.70
36	1	635	G	C8-N9-C1'	-6.26	118.86	127.00
36	1	1114	U	N3-C4-C5	-6.26	110.84	114.60
36	5	1793	C	C6-N1-C2	6.26	122.81	120.30
36	1	2403	G	C4-C5-C6	6.26	122.56	118.80
1	6	1180	C	C6-N1-C2	-6.26	117.80	120.30
36	5	614	C	N3-C4-C5	6.26	124.40	121.90
36	5	1152	G	N3-C2-N2	-6.26	115.52	119.90
1	2	158	U	P-O3'-C3'	6.25	127.21	119.70
36	1	3048	A	N9-C4-C5	-6.25	103.30	105.80
1	2	1489	U	O5'-P-OP1	-6.25	100.08	105.70
36	5	3195	U	P-O3'-C3'	6.25	127.20	119.70
36	1	1556	C	OP2-P-O3'	6.25	118.94	105.20
38	4	144	G	C8-N9-C4	6.25	108.90	106.40
36	5	1149	G	N1-C6-O6	6.25	123.65	119.90
36	5	1838	G	OP1-P-O3'	6.25	118.94	105.20
36	5	1716	U	P-O3'-C3'	6.24	127.19	119.70
36	1	281	G	N3-C4-N9	6.24	129.75	126.00
41	L4	339	LEU	CA-CB-CG	6.24	129.65	115.30
1	6	1642	G	N3-C4-C5	-6.24	125.48	128.60
36	5	2252	A	O5'-P-OP2	-6.24	100.08	105.70
36	5	2163	C	C6-N1-C2	-6.24	117.81	120.30
36	1	2933	A	N9-C4-C5	6.24	108.30	105.80
36	1	1759	C	C6-N1-C1'	-6.24	113.32	120.80
1	2	275	C	C6-N1-C2	-6.23	117.81	120.30
1	6	1023	A	C8-N9-C4	-6.23	103.31	105.80
36	1	315	C	C5-C6-N1	6.23	124.12	121.00
1	6	338	C	C6-N1-C2	6.23	122.79	120.30
36	1	1355	A	P-O3'-C3'	6.23	127.17	119.70
36	5	1815	U	P-O3'-C3'	6.22	127.17	119.70
36	5	1772	U	C2-N1-C1'	-6.22	110.23	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2615	G	O5'-P-OP2	6.22	118.16	110.70
36	1	2827	U	C5-C6-N1	-6.22	119.59	122.70
36	5	2285	C	C6-N1-C2	-6.21	117.81	120.30
36	5	321	C	C6-N1-C2	6.21	122.78	120.30
36	1	2348	A	N1-C6-N6	-6.21	114.87	118.60
36	1	2319	U	C2-N1-C1'	-6.21	110.25	117.70
36	5	2916	U	C5-C6-N1	-6.21	119.60	122.70
38	8	30	C	C2-N1-C1'	-6.21	111.97	118.80
36	1	2711	C	C5-C6-N1	6.21	124.10	121.00
36	5	1902	G	N3-C4-N9	6.21	129.72	126.00
36	1	2935	U	C2-N1-C1'	6.20	125.14	117.70
36	1	1444	G	C4-C5-N7	6.20	113.28	110.80
36	1	3311	C	C2-N1-C1'	6.20	125.62	118.80
38	4	144	G	C4-N9-C1'	-6.20	118.44	126.50
36	5	1305	U	O5'-P-OP1	-6.20	100.12	105.70
36	5	2269	U	C6-N1-C2	-6.20	117.28	121.00
70	O4	51	LEU	CA-CB-CG	6.19	129.54	115.30
36	5	676	G	N3-C4-C5	-6.19	125.50	128.60
36	1	684	G	C8-N9-C4	6.19	108.88	106.40
36	1	3382	U	N3-C2-O2	-6.19	117.87	122.20
38	4	44	A	O5'-P-OP1	-6.19	100.13	105.70
62	N6	126	LEU	CA-CB-CG	6.19	129.53	115.30
36	5	432	G	C6-C5-N7	-6.19	126.69	130.40
36	1	384	A	C8-N9-C4	6.18	108.27	105.80
36	1	1115	G	C5-C6-O6	-6.18	124.89	128.60
36	1	1856	C	C5-C6-N1	6.18	124.09	121.00
36	1	304	G	O4'-C1'-N9	-6.18	103.26	108.20
42	15	110	LEU	CA-CB-CG	6.18	129.51	115.30
36	1	1300	G	N1-C6-O6	6.17	123.60	119.90
1	2	1793	G	N3-C4-C5	-6.17	125.52	128.60
36	5	1701	C	C6-N1-C2	-6.17	117.83	120.30
36	1	688	G	C8-N9-C4	-6.17	103.93	106.40
1	6	1000	C	C2-N1-C1'	6.17	125.58	118.80
36	1	304	G	N3-C4-C5	6.17	131.68	128.60
61	n5	34	LEU	CA-CB-CG	6.16	129.47	115.30
1	2	1504	G	N3-C4-N9	6.16	129.70	126.00
36	5	2392	C	C6-N1-C2	6.15	122.76	120.30
36	5	3213	A	N1-C6-N6	6.15	122.29	118.60
1	2	617	U	C2-N1-C1'	6.15	125.08	117.70
1	2	794	U	P-O3'-C3'	6.15	127.08	119.70
36	1	288	C	O5'-P-OP1	-6.15	100.17	105.70
36	1	797	U	C6-N1-C2	-6.15	117.31	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1389	G	N9-C4-C5	-6.15	102.94	105.40
1	6	453	U	N1-C2-O2	6.15	127.11	122.80
36	5	2206	G	O4'-C1'-N9	-6.15	103.28	108.20
36	1	1866	C	O4'-C1'-N1	-6.14	103.28	108.20
1	6	334	G	N3-C4-N9	-6.14	122.31	126.00
36	5	1308	A	O5'-P-OP2	-6.14	100.17	105.70
36	1	1197	A	N1-C6-N6	6.14	122.29	118.60
36	1	708	G	C4-N9-C1'	6.14	134.48	126.50
36	1	1495	U	N1-C2-N3	6.14	118.58	114.90
36	5	922	U	C2-N1-C1'	-6.14	110.33	117.70
36	5	2269	U	C5-C4-O4	-6.14	122.22	125.90
36	5	590	G	N1-C6-O6	-6.14	116.22	119.90
36	5	422	A	C4-N9-C1'	6.14	137.34	126.30
1	6	934	C	C2-N1-C1'	6.13	125.55	118.80
36	5	1657	C	C6-N1-C2	-6.13	117.85	120.30
36	1	834	U	C5-C6-N1	-6.13	119.63	122.70
36	1	2966	G	N3-C2-N2	6.13	124.19	119.90
36	5	875	G	N3-C4-N9	-6.13	122.32	126.00
36	5	1324	U	C5-C6-N1	-6.12	119.64	122.70
36	1	908	G	C4-N9-C1'	6.12	134.46	126.50
36	5	3005	A	N7-C8-N9	6.12	116.86	113.80
36	5	510	G	N9-C4-C5	-6.12	102.95	105.40
1	6	543	C	N1-C2-O2	6.12	122.57	118.90
36	1	1192	C	C4-C5-C6	-6.11	114.34	117.40
1	2	136	C	C2-N1-C1'	6.11	125.52	118.80
1	6	1389	C	C6-N1-C2	-6.11	117.86	120.30
36	5	2550	U	C5-C4-O4	6.11	129.56	125.90
60	n4	96	LEU	CA-CB-CG	6.11	129.34	115.30
36	1	1314	C	C6-N1-C2	6.10	122.74	120.30
1	6	326	G	C8-N9-C1'	6.10	134.93	127.00
36	5	1527	C	C6-N1-C2	-6.10	117.86	120.30
36	5	2404	A	C8-N9-C4	6.10	108.24	105.80
36	5	329	U	N1-C2-O2	6.10	127.07	122.80
36	1	2423	U	O5'-P-OP2	-6.10	100.21	105.70
1	2	453	U	C5-C6-N1	6.10	125.75	122.70
36	5	2816	G	N9-C4-C5	-6.10	102.96	105.40
16	C4	137	LEU	CA-CB-CG	6.09	129.31	115.30
36	1	765	C	P-O3'-C3'	6.09	127.01	119.70
36	1	1578	C	C2-N1-C1'	6.09	125.50	118.80
41	14	339	LEU	CA-CB-CG	6.09	129.32	115.30
36	5	2144	A	O5'-P-OP2	-6.09	100.22	105.70
1	6	326	G	N3-C4-N9	-6.09	122.35	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	347	G	C5-C6-O6	-6.09	124.95	128.60
37	3	99	G	N1-C6-O6	6.09	123.55	119.90
1	6	1637	C	C2-N1-C1'	6.08	125.49	118.80
37	3	15	C	C6-N1-C2	6.08	122.73	120.30
36	5	3209	A	N9-C4-C5	-6.08	103.37	105.80
36	1	644	G	N3-C4-N9	6.08	129.65	126.00
1	6	1642	G	N3-C4-N9	6.08	129.65	126.00
1	6	1756	A	C4-N9-C1'	6.07	137.23	126.30
36	5	2621	G	C6-C5-N7	-6.07	126.76	130.40
36	5	2393	G	C8-N9-C4	-6.07	103.97	106.40
1	2	639	U	N1-C2-O2	6.07	127.05	122.80
36	5	2324	A	C8-N9-C4	6.07	108.23	105.80
36	1	1763	U	C5-C6-N1	6.07	125.73	122.70
36	5	793	C	C2-N1-C1'	6.07	125.47	118.80
36	1	42	C	O5'-P-OP1	-6.07	100.24	105.70
36	1	1589	A	C4-C5-N7	6.07	113.73	110.70
36	1	703	G	O5'-P-OP2	-6.06	100.25	105.70
36	1	1493	G	C8-N9-C1'	-6.06	119.12	127.00
36	1	2118	C	C6-N1-C1'	-6.06	113.53	120.80
1	2	321	C	O4'-C1'-N1	6.06	113.05	108.20
36	1	2316	G	N3-C4-C5	-6.06	125.57	128.60
12	c0	88	PRO	N-CA-CB	6.06	110.57	103.30
36	1	2572	C	C5-C6-N1	6.05	124.03	121.00
36	1	1512	U	N3-C2-O2	-6.05	117.97	122.20
66	O0	41	LEU	CA-CB-CG	6.04	129.20	115.30
36	1	1602	A	N1-C6-N6	-6.04	114.97	118.60
36	1	2874	G	C5-C6-O6	6.04	132.22	128.60
1	6	1654	G	N3-C4-N9	6.04	129.62	126.00
36	5	942	U	C6-N1-C2	6.04	124.62	121.00
1	2	577	G	C5-C6-O6	-6.04	124.98	128.60
1	6	617	U	C2-N1-C1'	6.04	124.95	117.70
1	6	1028	C	C6-N1-C2	6.04	122.72	120.30
36	1	1854	C	C6-N1-C2	-6.04	117.89	120.30
38	4	144	G	N7-C8-N9	-6.04	110.08	113.10
36	5	197	G	C4-N9-C1'	6.04	134.34	126.50
36	5	3112	G	N3-C4-N9	6.03	129.62	126.00
38	8	63	G	N3-C4-N9	-6.03	122.38	126.00
36	5	3061	G	C5-C6-O6	-6.03	124.98	128.60
36	1	282	G	C2'-C3'-O3'	6.03	123.35	113.70
36	1	2837	A	N1-C6-N6	-6.03	114.98	118.60
1	6	163	G	C8-N9-C4	-6.03	103.99	106.40
36	1	332	C	O5'-P-OP2	-6.03	100.28	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1653	C	C5-C6-N1	6.03	124.01	121.00
36	1	1716	U	P-O3'-C3'	6.03	126.93	119.70
36	1	2818	U	C5-C6-N1	6.03	125.71	122.70
36	5	1482	A	O5'-P-OP1	6.03	117.93	110.70
36	5	2719	U	C2-N1-C1'	-6.03	110.47	117.70
36	1	1514	G	C4-N9-C1'	6.02	134.32	126.50
1	6	697	C	C6-N1-C2	-6.02	117.89	120.30
36	5	2324	A	C4-C5-C6	-6.02	113.99	117.00
36	1	1306	G	C5-C6-O6	-6.02	124.99	128.60
36	1	93	C	C6-N1-C2	6.01	122.71	120.30
38	8	44	A	N1-C6-N6	6.01	122.21	118.60
1	2	1490	C	C6-N1-C2	-6.01	117.89	120.30
36	1	2679	A	O4'-C1'-N9	6.01	113.01	108.20
36	5	1927	G	N3-C4-N9	6.01	129.61	126.00
36	1	641	C	C6-N1-C2	6.01	122.70	120.30
36	1	708	G	N3-C4-C5	-6.01	125.60	128.60
36	1	835	G	O4'-C1'-N9	6.00	113.00	108.20
1	6	56	U	O4'-C1'-N1	6.00	113.00	108.20
1	2	1146	G	C8-N9-C4	-6.00	104.00	106.40
28	D6	63	ALA	C-N-CA	6.00	136.69	121.70
37	7	114	U	C2-N1-C1'	-6.00	110.51	117.70
1	2	1536	G	C4-N9-C1'	5.99	134.29	126.50
1	2	1771	U	O5'-P-OP1	-5.99	100.31	105.70
6	S4	193	GLY	N-CA-C	5.99	128.08	113.10
36	5	1897	G	N1-C6-O6	5.99	123.49	119.90
36	1	546	C	C6-N1-C2	-5.99	117.91	120.30
36	1	1759	C	C2-N1-C1'	5.99	125.39	118.80
36	1	3159	C	C2-N1-C1'	-5.99	112.21	118.80
36	5	864	G	C4-N9-C1'	5.99	134.28	126.50
36	5	1803	C	C6-N1-C2	-5.99	117.91	120.30
37	3	85	G	N3-C4-N9	-5.99	122.41	126.00
36	1	101	G	N3-C4-C5	5.99	131.59	128.60
36	1	1631	C	C6-N1-C2	5.99	122.69	120.30
1	6	526	A	C8-N9-C4	-5.99	103.41	105.80
36	1	2719	U	C5-C6-N1	-5.98	119.71	122.70
36	1	199	A	O4'-C1'-N9	5.98	112.99	108.20
36	1	2356	A	N9-C4-C5	-5.98	103.41	105.80
36	5	2664	C	N3-C4-C5	-5.98	119.51	121.90
1	6	1654	G	C4-C5-C6	5.98	122.39	118.80
36	5	2899	C	C6-N1-C2	-5.97	117.91	120.30
38	8	94	C	C5-C6-N1	-5.97	118.01	121.00
36	1	2593	A	P-O3'-C3'	5.97	126.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1431	C	C6-N1-C2	5.97	122.69	120.30
38	8	58	G	C4-C5-N7	5.97	113.19	110.80
36	1	1179	A	O5'-P-OP1	-5.97	100.33	105.70
36	1	1581	C	C6-N1-C2	-5.97	117.91	120.30
36	1	3021	A	C8-N9-C4	5.97	108.19	105.80
1	2	1059	U	N3-C2-O2	-5.96	118.03	122.20
36	1	2613	U	O5'-P-OP2	-5.96	100.33	105.70
36	5	2206	G	P-O3'-C3'	5.96	126.86	119.70
36	5	3209	A	N1-C6-N6	5.96	122.18	118.60
36	5	1152	G	N9-C4-C5	5.96	107.78	105.40
36	1	34	A	O5'-P-OP2	-5.96	100.34	105.70
1	2	187	G	P-O3'-C3'	5.96	126.85	119.70
36	1	360	G	C8-N9-C4	-5.96	104.02	106.40
36	5	59	G	C5-C6-O6	-5.95	125.03	128.60
36	5	2376	G	C5-C6-O6	-5.95	125.03	128.60
36	5	186	U	O5'-P-OP1	-5.95	100.34	105.70
36	5	905	U	O5'-P-OP1	-5.95	100.34	105.70
38	8	105	A	N1-C6-N6	5.95	122.17	118.60
37	3	77	G	N3-C4-N9	-5.95	122.43	126.00
36	5	2613	U	O5'-P-OP2	-5.95	100.35	105.70
36	5	873	C	P-O3'-C3'	5.95	126.84	119.70
36	5	1589	A	O5'-P-OP2	-5.95	100.35	105.70
1	2	1572	G	C4-C5-N7	5.95	113.18	110.80
36	5	1177	G	N9-C4-C5	-5.95	103.02	105.40
36	5	1878	G	C8-N9-C4	-5.95	104.02	106.40
36	5	426	G	N9-C4-C5	5.94	107.78	105.40
36	1	2979	U	N3-C2-O2	-5.94	118.04	122.20
36	5	1331	U	C6-N1-C2	5.94	124.57	121.00
1	2	1504	G	N3-C4-C5	-5.94	125.63	128.60
36	5	2621	G	N1-C6-O6	5.94	123.46	119.90
36	1	2145	A	C5-C6-N6	-5.94	118.95	123.70
36	5	2353	G	N3-C4-C5	-5.94	125.63	128.60
36	1	688	G	N7-C8-N9	5.94	116.07	113.10
36	1	718	G	N1-C6-O6	5.94	123.46	119.90
36	5	800	G	C4-N9-C1'	5.94	134.22	126.50
1	6	337	G	N7-C8-N9	5.93	116.07	113.10
36	5	1049	C	C6-N1-C2	-5.93	117.93	120.30
36	1	208	C	C6-N1-C2	-5.93	117.93	120.30
36	1	2355	G	N1-C6-O6	5.93	123.46	119.90
36	5	355	A	O5'-P-OP1	-5.93	100.36	105.70
36	5	803	C	C6-N1-C2	-5.93	117.93	120.30
36	5	1772	U	C6-N1-C2	5.93	124.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	900	G	C8-N9-C4	-5.93	104.03	106.40
1	2	25	C	P-O3'-C3'	5.93	126.81	119.70
36	1	590	G	N3-C4-N9	-5.93	122.44	126.00
36	5	2878	G	N3-C4-N9	5.93	129.56	126.00
38	8	70	G	N9-C4-C5	-5.93	103.03	105.40
36	1	3133	C	C6-N1-C2	5.92	122.67	120.30
1	2	1370	U	P-O3'-C3'	5.92	126.81	119.70
1	6	1058	U	P-O3'-C3'	5.92	126.81	119.70
36	1	1763	U	C6-N1-C1'	-5.92	112.91	121.20
1	6	1754	A	OP2-P-O3'	5.92	118.22	105.20
36	5	1096	U	C2-N1-C1'	5.92	124.80	117.70
36	5	1239	C	C2-N1-C1'	5.92	125.31	118.80
36	1	2269	U	O5'-P-OP2	-5.92	100.38	105.70
36	1	2290	C	N3-C4-C5	5.91	124.27	121.90
36	1	283	G	N3-C4-N9	5.91	129.55	126.00
36	1	922	U	C2-N1-C1'	5.91	124.79	117.70
36	5	895	A	N1-C2-N3	5.91	132.25	129.30
36	5	2140	U	C4-C5-C6	5.91	123.25	119.70
36	1	900	G	N9-C4-C5	5.91	107.76	105.40
36	1	2541	U	P-O3'-C3'	5.91	126.79	119.70
1	2	1504	G	C8-N9-C1'	-5.91	119.32	127.00
36	1	2281	A	O4'-C1'-N9	5.91	112.93	108.20
36	1	2837	A	N9-C4-C5	5.91	108.16	105.80
36	1	2838	A	N1-C6-N6	-5.91	115.06	118.60
36	1	927	C	C6-N1-C2	-5.90	117.94	120.30
1	2	1433	G	N1-C6-O6	-5.90	116.36	119.90
36	1	635	G	N1-C6-O6	5.90	123.44	119.90
51	m5	185	ALA	C-N-CA	5.90	134.70	122.30
1	2	549	G	C4-N9-C1'	5.90	134.17	126.50
36	1	2846	U	N3-C2-O2	-5.90	118.07	122.20
36	5	2405	C	C6-N1-C2	5.90	122.66	120.30
36	1	2873	U	N1-C2-O2	5.90	126.93	122.80
36	1	929	A	OP1-P-O3'	5.90	118.17	105.20
36	1	1879	A	O4'-C1'-N9	5.90	112.92	108.20
36	1	2112	U	P-O3'-C3'	5.89	126.77	119.70
36	1	2568	C	N1-C2-O2	5.89	122.44	118.90
36	5	1429	G	C8-N9-C4	5.89	108.76	106.40
36	5	1032	C	C6-N1-C2	-5.89	117.94	120.30
36	1	435	C	C6-N1-C2	5.89	122.66	120.30
36	1	2643	A	O5'-P-OP1	-5.89	100.40	105.70
36	5	2943	G	N3-C4-N9	5.89	129.53	126.00
36	5	2398	A	C6-C5-N7	-5.89	128.18	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2258	U	P-O3'-C3'	5.88	126.76	119.70
36	5	966	U	C6-N1-C2	-5.88	117.47	121.00
36	5	3244	A	O5'-P-OP2	-5.88	100.41	105.70
38	8	30	C	C6-N1-C2	5.88	122.65	120.30
36	1	3140	G	N3-C4-N9	5.88	129.53	126.00
1	6	1654	G	C6-C5-N7	-5.88	126.87	130.40
36	5	2312	A	O5'-P-OP1	-5.88	100.41	105.70
36	5	2550	U	N3-C2-O2	-5.88	118.09	122.20
36	5	3120	C	C2-N1-C1'	5.87	125.26	118.80
36	5	910	G	C8-N9-C4	-5.87	104.05	106.40
36	5	2621	G	C4-N9-C1'	5.87	134.13	126.50
1	2	77	U	O4'-C1'-N1	-5.87	103.50	108.20
36	5	1304	A	O5'-P-OP1	-5.87	100.42	105.70
36	5	3317	U	N3-C2-O2	-5.87	118.09	122.20
1	6	1097	U	P-O3'-C3'	5.87	126.74	119.70
1	6	1274	C	C6-N1-C1'	-5.87	113.76	120.80
36	5	2912	G	N1-C6-O6	5.87	123.42	119.90
36	5	338	A	C8-N9-C4	-5.86	103.45	105.80
1	6	79	C	C6-N1-C2	-5.86	117.96	120.30
1	6	543	C	N3-C2-O2	-5.86	117.80	121.90
36	5	1854	C	C6-N1-C2	-5.86	117.96	120.30
25	D3	15	LEU	CA-CB-CG	5.86	128.77	115.30
36	1	2257	C	N1-C2-O2	5.86	122.41	118.90
36	1	2868	U	N1-C2-O2	5.86	126.90	122.80
36	1	1708	C	C5-C6-N1	5.85	123.93	121.00
36	5	800	G	N3-C4-N9	5.85	129.51	126.00
1	2	507	U	N1-C2-O2	5.85	126.90	122.80
36	5	765	C	C6-N1-C2	5.85	122.64	120.30
38	8	55	U	N3-C4-O4	5.85	123.50	119.40
36	5	2141	U	C6-N1-C2	5.85	124.51	121.00
36	1	3022	G	O4'-C1'-N9	5.85	112.88	108.20
36	5	2593	A	P-O3'-C3'	5.85	126.72	119.70
36	5	2876	C	C6-N1-C2	-5.85	117.96	120.30
36	5	3394	U	C2-N1-C1'	-5.84	110.69	117.70
36	5	1092	C	C5-C6-N1	5.84	123.92	121.00
1	2	1134	C	C6-N1-C2	5.84	122.64	120.30
36	1	2693	C	C6-N1-C2	5.84	122.64	120.30
36	1	1654	A	N1-C2-N3	5.84	132.22	129.30
1	6	863	A	C8-N9-C4	5.84	108.13	105.80
36	5	2383	C	C6-N1-C1'	5.84	127.80	120.80
1	2	294	C	C6-N1-C2	5.83	122.63	120.30
59	N3	46	LEU	CA-CB-CG	-5.83	101.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1355	C	C6-N1-C2	-5.83	117.97	120.30
36	1	627	U	N3-C4-C5	-5.83	111.10	114.60
36	1	1856	C	C6-N1-C2	-5.83	117.97	120.30
36	5	676	G	C6-C5-N7	-5.83	126.90	130.40
36	5	1488	G	C8-N9-C4	-5.83	104.07	106.40
1	2	321	C	C2-N1-C1'	5.83	125.21	118.80
1	6	639	U	N3-C2-O2	-5.83	118.12	122.20
1	6	1010	C	C6-N1-C2	5.83	122.63	120.30
1	6	1654	G	N7-C8-N9	5.83	116.01	113.10
36	5	667	C	C6-N1-C2	5.83	122.63	120.30
36	5	1014	U	C6-N1-C1'	-5.83	113.04	121.20
36	5	1806	A	C8-N9-C4	5.83	108.13	105.80
36	5	3180	A	C8-N9-C4	5.83	108.13	105.80
37	3	85	G	C8-N9-C4	5.83	108.73	106.40
1	2	1568	C	C2-N1-C1'	5.82	125.21	118.80
36	5	823	C	C5-C6-N1	5.82	123.91	121.00
36	5	864	G	N1-C2-N2	-5.82	110.96	116.20
38	8	112	U	C5-C6-N1	-5.82	119.79	122.70
36	1	860	G	O5'-P-OP2	-5.82	100.47	105.70
36	5	3354	U	C2-N1-C1'	5.82	124.68	117.70
1	2	949	C	C6-N1-C2	-5.81	117.97	120.30
36	1	54	C	C6-N1-C2	5.81	122.62	120.30
36	1	218	G	P-O3'-C3'	5.81	126.68	119.70
38	8	75	G	C8-N9-C4	5.81	108.72	106.40
36	1	1415	U	N3-C4-C5	-5.81	111.11	114.60
36	1	823	C	C6-N1-C2	-5.81	117.98	120.30
36	5	2821	C	N1-C2-O2	5.81	122.39	118.90
1	2	1185	U	C2-N1-C1'	5.81	124.67	117.70
36	5	345	G	C8-N9-C1'	-5.81	119.45	127.00
36	1	569	A	C8-N9-C4	5.80	108.12	105.80
36	1	2512	C	C6-N1-C2	5.80	122.62	120.30
36	5	1521	G	O5'-P-OP1	-5.80	100.48	105.70
1	2	959	U	N3-C2-O2	-5.80	118.14	122.20
38	8	8	C	C6-N1-C2	5.80	122.62	120.30
1	6	1196	A	P-O3'-C3'	5.80	126.66	119.70
10	S8	121	LEU	CA-CB-CG	5.80	128.63	115.30
36	1	156	G	C8-N9-C4	-5.80	104.08	106.40
36	1	1886	A	C8-N9-C4	-5.80	103.48	105.80
36	5	3245	A	N1-C6-N6	5.79	122.08	118.60
36	5	282	G	C2'-C3'-O3'	5.79	122.96	113.70
36	1	979	U	P-O3'-C3'	5.79	126.65	119.70
36	1	2874	G	N9-C4-C5	5.79	107.72	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3187	A	C8-N9-C4	5.79	108.11	105.80
36	5	1394	A	C8-N9-C4	5.79	108.11	105.80
36	5	3011	A	N3-C4-N9	-5.79	122.77	127.40
36	1	1294	A	C8-N9-C4	5.78	108.11	105.80
37	3	51	A	N1-C2-N3	5.78	132.19	129.30
36	5	1445	U	O5'-P-OP2	5.78	117.64	110.70
1	2	1600	A	N7-C8-N9	5.78	116.69	113.80
36	1	3291	G	C4-N9-C1'	-5.78	118.98	126.50
36	5	1063	G	N3-C4-N9	5.78	129.47	126.00
36	5	1797	A	C8-N9-C4	5.78	108.11	105.80
36	1	656	A	C8-N9-C4	-5.78	103.49	105.80
36	1	984	G	N3-C2-N2	5.78	123.94	119.90
36	1	2812	C	N3-C4-C5	5.78	124.21	121.90
36	1	1552	G	N3-C4-N9	5.78	129.47	126.00
1	6	477	A	C8-N9-C4	5.78	108.11	105.80
36	5	426	G	N3-C2-N2	-5.78	115.86	119.90
1	2	1568	C	C6-N1-C2	-5.77	117.99	120.30
36	1	2938	G	C5-C6-O6	-5.77	125.14	128.60
1	2	1077	C	C6-N1-C2	-5.77	117.99	120.30
1	6	9	U	C5-C6-N1	5.77	125.59	122.70
36	1	283	G	C8-N9-C1'	-5.77	119.50	127.00
36	1	2871	G	C6-C5-N7	-5.77	126.94	130.40
1	2	813	U	P-O3'-C3'	5.77	126.62	119.70
36	5	3245	A	C2-N3-C4	-5.77	107.72	110.60
36	1	863	C	C4-C5-C6	-5.76	114.52	117.40
36	1	898	U	C5-C6-N1	5.76	125.58	122.70
36	1	1635	G	N3-C4-N9	-5.76	122.55	126.00
36	5	1354	G	N7-C8-N9	5.76	115.98	113.10
1	2	697	C	C6-N1-C2	-5.76	118.00	120.30
36	1	620	U	C2-N1-C1'	-5.76	110.79	117.70
38	4	54	A	N1-C6-N6	5.76	122.05	118.60
36	5	2949	U	C5-C6-N1	-5.76	119.82	122.70
36	1	2549	G	C4-N9-C1'	-5.75	119.02	126.50
36	5	1548	C	C6-N1-C2	-5.75	118.00	120.30
1	2	322	G	O4'-C1'-N9	-5.75	103.60	108.20
1	6	949	C	C6-N1-C2	-5.75	118.00	120.30
36	5	1633	C	C6-N1-C1'	-5.75	113.90	120.80
36	5	3231	U	C2-N1-C1'	-5.75	110.80	117.70
36	1	2767	U	C5-C6-N1	-5.75	119.83	122.70
36	5	409	A	N1-C6-N6	5.75	122.05	118.60
1	2	913	G	P-O3'-C3'	5.75	126.59	119.70
36	1	715	A	C8-N9-C4	-5.75	103.50	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2922	G	C4-C5-N7	5.75	113.10	110.80
36	5	98	G	N3-C4-C5	5.75	131.47	128.60
36	1	1329	U	OP1-P-O3'	5.74	117.84	105.20
1	2	1051	G	P-O3'-C3'	5.74	126.59	119.70
36	1	92	G	N3-C4-C5	5.74	131.47	128.60
36	1	1183	C	C2-N1-C1'	-5.74	112.48	118.80
36	1	1740	U	C6-N1-C2	5.74	124.44	121.00
36	5	2917	G	C5-C6-O6	5.74	132.04	128.60
36	5	2954	U	N1-C2-O2	5.74	126.82	122.80
36	1	591	G	C5-C6-O6	5.74	132.04	128.60
1	6	610	G	O4'-C1'-N9	5.74	112.79	108.20
37	3	85	G	C4-N9-C1'	-5.74	119.04	126.50
36	5	2878	G	C4-N9-C1'	5.74	133.96	126.50
1	2	1243	G	C4-N9-C1'	5.73	133.95	126.50
36	1	1408	G	N3-C4-C5	5.73	131.47	128.60
38	8	108	C	C6-N1-C2	5.73	122.59	120.30
36	1	867	G	C5-C6-O6	-5.73	125.16	128.60
36	5	934	G	C4-N9-C1'	5.73	133.95	126.50
36	1	2982	A	C8-N9-C4	-5.73	103.51	105.80
36	5	405	U	OP2-P-O3'	5.73	117.80	105.20
38	8	114	G	C8-N9-C4	5.73	108.69	106.40
36	1	1300	G	C8-N9-C4	5.72	108.69	106.40
36	1	1879	A	N1-C6-N6	5.72	122.03	118.60
36	1	3275	U	OP1-P-O3'	5.72	117.79	105.20
36	5	1174	G	C6-C5-N7	-5.72	126.97	130.40
36	1	1866	C	N1-C2-O2	5.72	122.33	118.90
36	1	2645	G	N3-C4-N9	5.72	129.43	126.00
1	6	542	A	P-O3'-C3'	5.72	126.57	119.70
36	5	1866	C	C5-C6-N1	5.72	123.86	121.00
36	1	3181	C	N3-C2-O2	-5.72	117.90	121.90
37	3	99	G	C5-C6-O6	-5.72	125.17	128.60
36	5	1222	G	P-O3'-C3'	5.72	126.56	119.70
36	1	1300	G	N9-C4-C5	-5.72	103.11	105.40
37	3	99	G	N3-C4-C5	5.72	131.46	128.60
1	2	1761	U	C2-N1-C1'	5.71	124.56	117.70
36	1	547	G	P-O3'-C3'	5.71	126.56	119.70
36	1	1456	A	N9-C4-C5	5.71	108.09	105.80
36	1	340	C	O5'-P-OP2	5.71	117.55	110.70
36	1	1443	G	OP1-P-O3'	5.71	117.77	105.20
36	1	3036	G	C6-C5-N7	5.71	133.83	130.40
1	2	1535	U	O5'-P-OP1	5.71	117.55	110.70
14	C2	103	LEU	CA-CB-CG	5.71	128.43	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2403	G	C4-N9-C1'	5.71	133.92	126.50
36	5	609	G	O5'-P-OP1	5.71	117.55	110.70
1	6	320	U	C5-C6-N1	5.71	125.55	122.70
36	5	2383	C	N1-C2-O2	-5.71	115.48	118.90
13	C1	5	LEU	CA-CB-CG	5.70	128.40	115.30
36	1	497	C	C6-N1-C2	-5.70	118.02	120.30
36	1	3354	U	N3-C2-O2	-5.70	118.21	122.20
36	5	1302	A	O5'-P-OP1	-5.70	100.57	105.70
1	2	1573	A	P-O3'-C3'	5.70	126.54	119.70
36	5	1081	U	C6-N1-C2	-5.70	117.58	121.00
36	5	1329	U	N3-C2-O2	-5.70	118.21	122.20
36	5	1435	A	N1-C6-N6	-5.70	115.18	118.60
36	1	2142	A	C8-N9-C4	-5.69	103.52	105.80
36	5	1633	C	C5-C6-N1	5.69	123.85	121.00
36	5	3005	A	O5'-P-OP1	-5.69	100.58	105.70
36	1	278	U	C2-N1-C1'	-5.69	110.87	117.70
36	1	1858	A	C4-N9-C1'	5.69	136.54	126.30
36	1	41	G	C8-N9-C4	-5.69	104.12	106.40
36	1	2118	C	O5'-P-OP1	-5.69	100.58	105.70
36	5	1481	A	C4-N9-C1'	5.69	136.54	126.30
36	5	1878	G	N7-C8-N9	5.69	115.94	113.10
36	5	1902	G	C8-N9-C1'	-5.69	119.61	127.00
36	1	1115	G	N1-C6-O6	5.68	123.31	119.90
36	1	2321	A	O5'-P-OP2	-5.68	100.59	105.70
1	6	163	G	N3-C4-N9	-5.68	122.59	126.00
12	C0	76	LEU	CA-CB-CG	5.68	128.37	115.30
36	1	1444	G	C5-N7-C8	-5.68	101.46	104.30
36	1	2618	G	C5-C6-O6	5.68	132.01	128.60
36	5	860	G	N1-C6-O6	5.68	123.31	119.90
36	5	633	C	C6-N1-C2	-5.68	118.03	120.30
1	2	626	U	C6-N1-C2	-5.67	117.59	121.00
36	1	1432	C	C6-N1-C2	-5.67	118.03	120.30
36	1	1795	U	O5'-P-OP1	-5.67	100.59	105.70
36	5	92	G	N3-C4-C5	5.67	131.44	128.60
36	5	2662	G	N9-C1'-C2'	-5.67	105.76	112.00
36	5	2996	U	C2-N1-C1'	-5.67	110.89	117.70
36	1	316	U	O5'-P-OP1	-5.67	100.59	105.70
36	1	2715	A	O5'-P-OP1	-5.67	100.59	105.70
36	1	925	A	N9-C4-C5	-5.67	103.53	105.80
36	1	2305	G	C4-N9-C1'	5.67	133.87	126.50
36	5	3394	U	C5-C6-N1	-5.67	119.86	122.70
36	5	360	G	OP1-P-O3'	5.67	117.67	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	34	A	O5'-P-OP2	-5.66	100.60	105.70
36	5	3061	G	C8-N9-C4	5.66	108.67	106.40
1	2	1059	U	C2-N1-C1'	5.66	124.49	117.70
36	5	2922	G	C8-N9-C1'	-5.66	119.64	127.00
36	5	420	G	C2-N3-C4	5.66	114.73	111.90
37	3	83	U	C5-C6-N1	-5.66	119.87	122.70
1	6	755	A	C3'-C2'-C1'	5.66	106.03	101.50
1	6	1100	G	N9-C4-C5	-5.66	103.14	105.40
36	5	2715	A	C8-N9-C4	5.66	108.06	105.80
1	6	1615	C	P-O3'-C3'	5.66	126.49	119.70
36	5	896	A	O5'-P-OP2	-5.66	100.61	105.70
36	5	534	U	N1-C2-O2	5.65	126.76	122.80
36	1	2982	A	N9-C4-C5	5.65	108.06	105.80
1	2	192	U	C6-N1-C2	-5.65	117.61	121.00
36	5	3158	G	C8-N9-C4	-5.65	104.14	106.40
36	1	1902	G	N3-C4-N9	5.65	129.39	126.00
38	8	111	A	N1-C6-N6	5.65	121.99	118.60
1	2	74	U	OP1-P-O3'	5.65	117.62	105.20
36	1	1938	U	C5-C6-N1	-5.65	119.88	122.70
36	1	1654	A	O4'-C1'-N9	-5.64	103.68	108.20
38	8	44	A	O5'-P-OP1	-5.64	100.62	105.70
1	2	94	U	C5-C6-N1	-5.64	119.88	122.70
36	1	2982	A	N1-C6-N6	-5.64	115.22	118.60
36	1	3275	U	P-O3'-C3'	5.64	126.47	119.70
36	1	1783	U	O5'-P-OP1	-5.64	100.62	105.70
36	1	3389	U	P-O3'-C3'	5.64	126.47	119.70
36	5	1733	G	N1-C6-O6	5.64	123.28	119.90
36	5	2381	G	N1-C6-O6	5.64	123.28	119.90
1	2	1146	G	C4-N9-C1'	5.64	133.83	126.50
36	1	644	G	C5-C6-O6	5.64	131.98	128.60
1	2	75	U	O5'-P-OP1	-5.64	100.63	105.70
36	1	1780	G	C8-N9-C1'	-5.64	119.67	127.00
36	1	1943	C	C6-N1-C2	-5.64	118.05	120.30
36	1	2541	U	C6-N1-C1'	-5.64	113.31	121.20
1	6	639	U	N1-C2-O2	5.64	126.75	122.80
6	S4	12	LEU	CA-CB-CG	5.63	128.26	115.30
1	2	1399	C	C2-N1-C1'	5.63	125.00	118.80
36	5	1862	U	C2-N1-C1'	-5.63	110.95	117.70
1	2	1778	G	C8-N9-C4	-5.63	104.15	106.40
36	1	922	U	N1-C2-N3	-5.63	111.52	114.90
36	1	1127	G	C4-C5-N7	-5.63	108.55	110.80
38	4	39	G	N3-C4-C5	-5.63	125.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2315	G	O5'-P-OP1	-5.62	100.64	105.70
36	1	2867	C	C6-N1-C2	5.62	122.55	120.30
36	1	823	C	C5-C6-N1	5.62	123.81	121.00
62	N6	31	LEU	CA-CB-CG	-5.62	102.37	115.30
52	m6	27	LEU	CA-CB-CG	-5.62	102.38	115.30
36	1	1780	G	N3-C4-N9	5.62	129.37	126.00
36	5	1444	G	N1-C6-O6	5.62	123.27	119.90
36	5	2718	U	C2-N1-C1'	-5.62	110.96	117.70
36	5	2370	G	N3-C4-N9	-5.62	122.63	126.00
36	1	155	G	O5'-P-OP1	-5.62	100.65	105.70
36	1	2983	C	C4-C5-C6	5.62	120.21	117.40
64	n8	48	TYR	CA-CB-CG	5.62	124.07	113.40
36	1	1604	G	N3-C4-N9	5.61	129.37	126.00
38	4	108	C	C6-N1-C2	5.61	122.55	120.30
36	5	1849	C	C2-N3-C4	-5.61	117.09	119.90
36	5	2868	U	OP2-P-O3'	5.61	117.55	105.20
36	5	102	C	C2-N1-C1'	5.61	124.97	118.80
36	5	2416	U	O5'-P-OP2	-5.61	100.65	105.70
38	4	54	A	O5'-P-OP1	-5.61	100.65	105.70
36	5	800	G	C8-N9-C1'	-5.61	119.71	127.00
36	5	3317	U	C6-N1-C2	-5.61	117.64	121.00
36	1	1495	U	C6-N1-C1'	5.61	129.05	121.20
36	1	2278	C	OP2-P-O3'	5.61	117.54	105.20
38	8	46	G	C4-N9-C1'	5.61	133.79	126.50
1	6	9	U	C6-N1-C2	-5.60	117.64	121.00
1	6	589	C	C6-N1-C2	-5.60	118.06	120.30
36	5	1149	G	C8-N9-C1'	-5.60	119.72	127.00
36	1	1879	A	N9-C4-C5	-5.60	103.56	105.80
36	1	2420	C	C6-N1-C2	-5.60	118.06	120.30
36	1	670	C	C6-N1-C2	5.60	122.54	120.30
36	5	2101	C	O5'-P-OP1	-5.60	100.66	105.70
36	1	1158	A	N1-C6-N6	5.60	121.96	118.60
1	6	156	A	C5-C6-N6	-5.59	119.22	123.70
24	D2	104	LEU	CA-CB-CG	5.59	128.16	115.30
1	2	1059	U	P-O3'-C3'	5.59	126.41	119.70
36	1	639	G	N1-C6-O6	5.59	123.25	119.90
36	1	1303	A	N7-C8-N9	-5.59	111.00	113.80
36	1	925	A	N1-C6-N6	5.59	121.95	118.60
36	1	1843	C	C6-N1-C1'	-5.59	114.09	120.80
36	1	1525	G	C8-N9-C1'	-5.59	119.74	127.00
36	1	2407	C	N3-C4-N4	5.59	121.91	118.00
41	L4	182	LEU	CA-CB-CG	5.59	128.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2879	C	O5'-P-OP1	-5.59	100.67	105.70
36	1	3340	G	OP1-P-O3'	-5.58	92.91	105.20
36	5	69	C	O5'-P-OP1	-5.58	100.67	105.70
38	8	102	U	O5'-P-OP2	-5.58	100.67	105.70
36	1	1037	C	C2-N1-C1'	5.58	124.94	118.80
36	1	3098	G	N3-C4-C5	-5.58	125.81	128.60
1	6	590	C	C2-N1-C1'	5.58	124.94	118.80
36	5	2256	A	C8-N9-C4	5.58	108.03	105.80
36	5	659	G	C8-N9-C4	-5.58	104.17	106.40
36	1	887	G	O5'-P-OP1	-5.58	100.68	105.70
36	1	2817	A	C5-N7-C8	-5.58	101.11	103.90
36	5	652	G	O5'-P-OP2	-5.58	100.68	105.70
36	5	3112	G	C6-C5-N7	-5.58	127.05	130.40
36	5	2266	U	C2-N1-C1'	5.58	124.39	117.70
36	1	800	G	C8-N9-C4	5.58	108.63	106.40
36	5	3228	C	P-O3'-C3'	5.58	126.39	119.70
1	2	794	U	N3-C2-O2	-5.57	118.30	122.20
36	1	3070	A	C8-N9-C4	5.57	108.03	105.80
1	6	610	G	C4-N9-C1'	5.57	133.74	126.50
36	5	1525	G	C4-N9-C1'	5.57	133.74	126.50
36	1	3325	G	C8-N9-C4	5.57	108.63	106.40
1	2	276	C	C6-N1-C1'	5.57	127.48	120.80
1	2	1568	C	C5-C6-N1	5.57	123.78	121.00
36	5	920	A	N1-C6-N6	5.57	121.94	118.60
39	L2	150	LEU	CA-CB-CG	-5.56	102.50	115.30
38	8	111	A	C8-N9-C4	5.56	108.03	105.80
54	m8	71	LEU	CA-CB-CG	-5.56	102.51	115.30
1	2	321	C	C6-N1-C1'	-5.56	114.13	120.80
36	5	1592	G	N1-C6-O6	5.56	123.24	119.90
36	5	2117	A	O5'-P-OP1	-5.56	100.69	105.70
36	5	2398	A	C4-C5-C6	5.56	119.78	117.00
36	5	2418	G	O4'-C1'-N9	-5.56	103.75	108.20
36	1	546	C	N3-C2-O2	-5.56	118.01	121.90
36	1	647	A	C8-N9-C4	-5.56	103.58	105.80
36	1	2875	U	N1-C2-O2	5.56	126.69	122.80
1	6	53	G	N3-C4-C5	5.56	131.38	128.60
1	2	1585	U	C2-N3-C4	5.56	130.34	127.00
36	5	297	G	N3-C4-C5	-5.56	125.82	128.60
36	5	1170	A	O5'-P-OP1	-5.56	100.70	105.70
1	2	577	G	C5-N7-C8	-5.55	101.52	104.30
36	1	648	C	O5'-P-OP1	-5.55	100.70	105.70
36	1	1607	U	C5-C6-N1	5.55	125.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1907	C	OP2-P-O3'	5.55	117.42	105.20
36	1	1495	U	C2-N1-C1'	-5.55	111.04	117.70
36	1	2794	G	N3-C4-C5	5.55	131.37	128.60
36	1	2971	A	C4-C5-C6	-5.55	114.23	117.00
36	5	966	U	C2-N1-C1'	5.55	124.36	117.70
36	5	3241	G	N3-C4-N9	5.55	129.33	126.00
36	1	877	C	C5-C6-N1	-5.54	118.23	121.00
1	6	1683	C	N1-C2-O2	5.54	122.23	118.90
36	5	871	U	C5-C6-N1	-5.54	119.93	122.70
36	1	1486	G	O5'-P-OP2	-5.54	100.71	105.70
1	6	337	G	C8-N9-C4	-5.54	104.18	106.40
1	2	1572	G	C5-C6-O6	-5.54	125.28	128.60
1	2	1604	U	C5-C6-N1	5.54	125.47	122.70
36	1	3098	G	N3-C4-N9	5.54	129.32	126.00
36	5	1307	G	O5'-P-OP1	-5.54	100.72	105.70
36	5	1554	U	O4'-C1'-N1	5.54	112.63	108.20
36	5	1763	U	C2-N1-C1'	5.54	124.35	117.70
1	2	276	C	C2-N1-C1'	-5.54	112.71	118.80
36	5	1697	A	O5'-P-OP1	-5.54	100.72	105.70
36	5	1761	C	P-O3'-C3'	5.54	126.34	119.70
36	1	2808	A	N9-C4-C5	-5.54	103.59	105.80
38	8	21	C	C6-N1-C2	5.54	122.52	120.30
1	2	913	G	OP1-P-O3'	5.53	117.38	105.20
36	1	2131	A	C8-N9-C4	5.53	108.01	105.80
1	6	803	A	C8-N9-C4	-5.53	103.59	105.80
36	5	718	G	C4-N9-C1'	5.53	133.69	126.50
36	1	91	G	N3-C4-N9	5.53	129.32	126.00
36	1	807	A	C2-N3-C4	-5.53	107.83	110.60
36	5	326	U	C6-N1-C2	-5.53	117.68	121.00
36	1	2645	G	N1-C6-O6	5.53	123.22	119.90
36	1	218	G	N3-C4-C5	-5.53	125.84	128.60
36	1	2274	U	C5-C6-N1	5.53	125.46	122.70
36	1	2874	G	C4-C5-N7	-5.53	108.59	110.80
36	1	2875	U	C6-N1-C1'	-5.53	113.46	121.20
1	6	996	U	C5-C6-N1	5.53	125.46	122.70
1	2	782	U	P-O3'-C3'	5.53	126.33	119.70
36	1	2571	U	O4'-C1'-N1	5.53	112.62	108.20
38	4	103	G	N3-C4-N9	5.53	129.31	126.00
36	5	614	C	C6-N1-C2	5.52	122.51	120.30
36	1	116	A	N9-C4-C5	5.52	108.01	105.80
36	5	297	G	O4'-C1'-N9	5.52	112.61	108.20
36	5	3201	C	C6-N1-C2	5.52	122.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1875	G	N3-C4-C5	5.51	131.36	128.60
36	5	2614	G	N1-C6-O6	5.51	123.21	119.90
36	1	2980	U	O5'-P-OP1	5.51	117.31	110.70
36	5	354	U	C5-C6-N1	5.51	125.46	122.70
36	1	620	U	C6-N1-C1'	5.51	128.92	121.20
40	L3	246	LEU	CA-CB-CG	5.51	127.98	115.30
67	o1	81	GLU	C-N-CA	5.51	135.48	121.70
1	2	783	G	N1-C6-O6	5.51	123.21	119.90
36	1	2314	U	O4'-C1'-N1	5.51	112.61	108.20
36	1	2591	A	C8-N9-C4	5.51	108.00	105.80
1	6	911	U	C5-C6-N1	5.51	125.45	122.70
36	5	2621	G	N9-C4-C5	-5.51	103.20	105.40
36	5	2607	G	C5-C6-O6	-5.51	125.30	128.60
36	1	1198	C	C6-N1-C2	-5.51	118.10	120.30
36	1	2618	G	N9-C4-C5	5.51	107.60	105.40
38	4	105	A	N1-C6-N6	5.51	121.90	118.60
36	5	422	A	C4-C5-C6	5.51	119.75	117.00
36	5	1356	U	C6-N1-C2	-5.51	117.70	121.00
36	5	1901	A	N1-C6-N6	-5.51	115.30	118.60
36	5	406	G	N3-C4-N9	-5.50	122.70	126.00
36	5	422	A	N7-C8-N9	5.50	116.55	113.80
1	6	272	U	P-O3'-C3'	5.50	126.30	119.70
1	6	1389	C	C5-C6-N1	5.50	123.75	121.00
36	1	1742	U	C6-N1-C2	-5.50	117.70	121.00
36	1	2403	G	N1-C6-O6	5.50	123.20	119.90
36	1	2409	G	N3-C4-N9	5.50	129.30	126.00
36	5	2093	A	O4'-C1'-N9	5.50	112.60	108.20
36	5	3140	G	N9-C4-C5	-5.50	103.20	105.40
36	1	153	U	C6-N1-C2	-5.50	117.70	121.00
36	1	281	G	N3-C4-C5	-5.50	125.85	128.60
36	5	1148	G	N3-C4-N9	5.50	129.30	126.00
38	8	100	U	N3-C4-O4	5.50	123.25	119.40
36	1	970	A	C8-N9-C4	5.49	108.00	105.80
36	1	1735	G	C8-N9-C4	5.49	108.60	106.40
36	1	2568	C	C5-C6-N1	5.49	123.75	121.00
36	5	931	C	C6-N1-C2	-5.49	118.10	120.30
21	C9	28	LEU	CA-CB-CG	5.49	127.93	115.30
36	5	1826	C	C6-N1-C2	5.49	122.50	120.30
36	1	1306	G	N3-C4-N9	5.49	129.29	126.00
36	1	2355	G	C4-C5-N7	5.49	113.00	110.80
1	6	1654	G	C8-N9-C1'	-5.49	119.86	127.00
36	5	1306	G	C5-C6-O6	-5.49	125.31	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	95	G	N3-C4-N9	5.49	129.29	126.00
36	1	3218	A	N1-C6-N6	5.49	121.89	118.60
1	6	617	U	C5-C6-N1	5.49	125.44	122.70
36	5	424	G	OP1-P-OP2	5.49	127.83	119.60
36	5	1495	U	C2-N3-C4	5.49	130.29	127.00
36	5	1897	G	N3-C4-N9	5.49	129.29	126.00
36	1	2858	U	C6-N1-C2	-5.48	117.71	121.00
1	6	414	C	C6-N1-C2	5.48	122.49	120.30
1	2	1360	A	N1-C2-N3	5.48	132.04	129.30
36	5	1450	G	O4'-C1'-N9	-5.48	103.81	108.20
36	1	2794	G	C4-N9-C1'	-5.48	119.38	126.50
1	2	1572	G	N1-C6-O6	5.48	123.19	119.90
1	2	279	G	OP1-P-O3'	5.48	117.25	105.20
36	1	2221	G	C4-N9-C1'	-5.48	119.38	126.50
36	1	2767	U	C6-N1-C2	5.48	124.29	121.00
36	5	878	G	N3-C4-C5	-5.48	125.86	128.60
1	2	8	U	C6-N1-C2	5.47	124.28	121.00
1	2	784	C	C6-N1-C2	-5.47	118.11	120.30
36	1	283	G	C4-N9-C1'	5.47	133.62	126.50
36	1	1080	A	C8-N9-C4	5.47	107.99	105.80
36	1	1426	C	N1-C2-O2	5.47	122.18	118.90
36	5	655	C	O5'-P-OP2	5.47	117.27	110.70
36	5	835	G	C8-N9-C1'	5.47	134.12	127.00
1	2	1176	G	C8-N9-C4	-5.47	104.21	106.40
1	6	913	G	P-O3'-C3'	5.47	126.27	119.70
36	5	981	U	C6-N1-C2	-5.47	117.72	121.00
1	2	947	U	C6-N1-C2	-5.47	117.72	121.00
36	1	1017	C	C5-C6-N1	5.47	123.73	121.00
36	1	2868	U	N3-C2-O2	-5.47	118.37	122.20
36	1	770	G	O4'-C1'-N9	5.47	112.57	108.20
36	5	1145	G	O5'-P-OP2	-5.47	100.78	105.70
36	5	2256	A	P-O3'-C3'	5.46	126.26	119.70
36	5	2891	U	C6-N1-C2	5.46	124.28	121.00
36	5	3082	C	C6-N1-C2	5.46	122.48	120.30
36	5	2373	A	N1-C6-N6	-5.46	115.32	118.60
36	1	1856	C	OP1-P-O3'	5.46	117.21	105.20
36	5	1722	U	N3-C2-O2	-5.46	118.38	122.20
36	1	2938	G	N1-C6-O6	5.46	123.17	119.90
36	5	344	A	O5'-P-OP1	-5.46	100.79	105.70
36	5	1481	A	C8-N9-C4	-5.46	103.62	105.80
36	1	3193	C	C6-N1-C2	-5.46	118.12	120.30
36	5	1866	C	C6-N1-C1'	-5.46	114.25	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2374	C	O4'-C1'-N1	-5.46	103.83	108.20
36	5	3164	C	C6-N1-C2	5.46	122.48	120.30
36	5	518	G	N7-C8-N9	5.45	115.83	113.10
1	2	1146	G	N3-C4-C5	-5.45	125.88	128.60
36	1	2821	C	C2-N1-C1'	5.45	124.80	118.80
36	5	3231	U	C5-C6-N1	-5.45	119.97	122.70
36	1	3181	C	N1-C2-O2	5.45	122.17	118.90
36	1	3243	A	O4'-C1'-N9	-5.45	103.84	108.20
1	6	1006	C	C6-N1-C2	-5.45	118.12	120.30
36	1	2618	G	N1-C6-O6	-5.45	116.63	119.90
38	4	62	C	C6-N1-C2	5.45	122.48	120.30
1	6	1642	G	C6-C5-N7	-5.45	127.13	130.40
36	5	1481	A	N7-C8-N9	5.45	116.52	113.80
36	5	1139	G	O5'-P-OP1	-5.44	100.80	105.70
36	1	637	C	C2-N1-C1'	5.44	124.79	118.80
36	1	2194	G	C4-N9-C1'	5.44	133.58	126.50
36	1	2608	G	C8-N9-C4	5.44	108.58	106.40
36	1	2629	U	C6-N1-C2	5.44	124.27	121.00
36	5	3206	C	C6-N1-C2	-5.44	118.12	120.30
1	2	1756	A	C8-N9-C4	-5.44	103.62	105.80
36	5	959	C	N1-C2-O2	5.44	122.16	118.90
1	2	544	A	OP2-P-O3'	5.44	117.16	105.20
36	5	156	G	N3-C4-N9	5.44	129.26	126.00
36	5	1593	A	N9-C4-C5	5.44	107.97	105.80
36	1	3005	A	C8-N9-C4	-5.43	103.63	105.80
36	1	3118	C	C6-N1-C2	5.43	122.47	120.30
1	6	1446	A	C8-N9-C4	5.43	107.97	105.80
36	5	1115	G	C5-N7-C8	-5.43	101.58	104.30
36	5	2427	U	O5'-P-OP1	5.43	117.22	110.70
36	5	2719	U	C5-C6-N1	-5.43	119.98	122.70
36	1	41	G	N9-C4-C5	5.43	107.57	105.40
36	1	2137	U	C2-N1-C1'	-5.43	111.18	117.70
36	1	3142	A	C8-N9-C4	5.43	107.97	105.80
1	6	965	U	N3-C2-O2	-5.43	118.40	122.20
36	5	1063	G	C4-C5-C6	5.43	122.06	118.80
36	5	2816	G	C8-N9-C4	5.43	108.57	106.40
1	2	1536	G	C8-N9-C1'	-5.43	119.94	127.00
1	2	1572	G	N9-C4-C5	-5.43	103.23	105.40
1	2	1742	U	C5-C6-N1	5.43	125.41	122.70
36	5	1149	G	C4-N9-C1'	5.43	133.56	126.50
36	5	1190	A	O5'-P-OP1	-5.43	100.81	105.70
36	5	2931	C	C5-C6-N1	-5.43	118.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1442	U	C6-N1-C2	5.42	124.25	121.00
36	1	1713	G	N3-C4-N9	-5.42	122.75	126.00
4	s2	235	LEU	CA-CB-CG	5.42	127.77	115.30
36	5	3245	A	N1-C2-N3	5.42	132.01	129.30
36	1	315	C	C2-N1-C1'	5.42	124.76	118.80
1	6	874	C	C6-N1-C2	-5.42	118.13	120.30
36	5	3164	C	N3-C4-C5	5.42	124.07	121.90
36	1	380	U	C2-N1-C1'	5.42	124.20	117.70
36	5	353	G	C8-N9-C1'	5.42	134.04	127.00
36	5	2609	A	O5'-P-OP1	5.42	117.20	110.70
36	5	875	G	N3-C2-N2	-5.42	116.11	119.90
38	8	46	G	C8-N9-C1'	-5.42	119.96	127.00
36	1	916	G	N3-C4-N9	5.41	129.25	126.00
36	1	2384	A	C8-N9-C4	-5.41	103.63	105.80
1	6	1490	C	C2-N1-C1'	5.41	124.75	118.80
36	5	826	G	O5'-P-OP2	5.41	117.19	110.70
36	5	1582	C	N1-C2-O2	5.41	122.15	118.90
36	5	800	G	C6-C5-N7	-5.41	127.15	130.40
36	5	1183	C	C6-N1-C2	5.41	122.46	120.30
36	5	1348	U	C5-C6-N1	5.41	125.41	122.70
36	5	2608	G	N9-C4-C5	-5.41	103.24	105.40
1	2	1636	C	C6-N1-C2	-5.41	118.14	120.30
36	5	59	G	N1-C6-O6	5.41	123.14	119.90
36	5	934	G	C8-N9-C1'	-5.41	119.97	127.00
1	2	914	G	N1-C6-O6	-5.41	116.66	119.90
1	6	464	A	N1-C6-N6	5.41	121.84	118.60
38	8	117	C	O5'-P-OP2	-5.41	100.83	105.70
10	S8	29	LEU	CA-CB-CG	5.40	127.73	115.30
36	5	875	G	N3-C4-C5	5.40	131.30	128.60
36	1	282	G	N7-C8-N9	5.40	115.80	113.10
36	1	2872	A	C2-N3-C4	-5.40	107.90	110.60
36	5	3120	C	C6-N1-C2	-5.40	118.14	120.30
38	4	105	A	N9-C4-C5	-5.40	103.64	105.80
1	6	647	G	P-O3'-C3'	5.40	126.18	119.70
36	5	1878	G	C4-N9-C1'	5.40	133.52	126.50
1	2	1754	A	C6-C5-N7	-5.40	128.52	132.30
36	1	635	G	C4-N9-C1'	5.40	133.51	126.50
36	5	807	A	C5-N7-C8	-5.39	101.20	103.90
36	5	3208	G	N9-C4-C5	-5.39	103.24	105.40
36	1	2966	G	C4-C5-C6	5.39	122.04	118.80
1	6	1100	G	N3-C4-N9	5.39	129.24	126.00
36	5	406	G	N3-C4-C5	5.39	131.30	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2314	U	C2-N1-C1'	5.39	124.17	117.70
1	6	1458	G	N9-C4-C5	-5.39	103.24	105.40
36	1	1353	U	O4'-C1'-N1	-5.39	103.89	108.20
36	1	1820	U	OP2-P-O3'	5.39	117.05	105.20
37	3	18	C	C6-N1-C2	-5.39	118.14	120.30
19	c7	109	LEU	CA-CB-CG	5.39	127.69	115.30
36	5	915	A	C2-N3-C4	5.39	113.29	110.60
1	2	1560	U	N1-C2-O2	5.38	126.57	122.80
1	6	1447	C	C6-N1-C2	-5.38	118.15	120.30
36	5	360	G	C8-N9-C1'	-5.38	120.00	127.00
36	5	2870	C	C2-N1-C1'	-5.38	112.88	118.80
36	5	2943	G	C6-C5-N7	-5.38	127.17	130.40
36	1	893	C	C6-N1-C2	-5.38	118.15	120.30
36	1	1875	G	N3-C4-N9	-5.38	122.77	126.00
36	1	3263	G	OP1-P-O3'	5.38	117.04	105.20
36	1	2568	C	C6-N1-C2	-5.38	118.15	120.30
1	6	1756	A	C6-C5-N7	-5.38	128.53	132.30
36	5	345	G	C4-N9-C1'	5.38	133.49	126.50
36	5	2260	U	P-O3'-C3'	5.38	126.16	119.70
1	2	1433	G	C5-C6-O6	5.38	131.83	128.60
36	5	2332	A	N1-C6-N6	5.38	121.83	118.60
36	1	145	G	C8-N9-C4	-5.38	104.25	106.40
36	1	1578	C	C6-N1-C1'	-5.38	114.35	120.80
36	1	2858	U	OP2-P-O3'	5.38	117.03	105.20
36	1	2971	A	N3-C4-C5	5.37	130.56	126.80
36	1	3269	U	N3-C2-O2	-5.37	118.44	122.20
36	5	2314	U	C5-C6-N1	-5.37	120.01	122.70
36	5	2777	G	OP1-P-O3'	5.37	117.02	105.20
1	2	1760	G	C5-C6-O6	-5.37	125.38	128.60
36	1	836	A	N1-C6-N6	5.37	121.82	118.60
36	1	1480	G	O4'-C1'-N9	5.37	112.50	108.20
1	6	1058	U	OP1-P-O3'	5.37	117.01	105.20
1	6	1246	C	C2-N1-C1'	5.37	124.71	118.80
36	1	371	G	C8-N9-C1'	5.37	133.98	127.00
36	5	336	A	N3-C4-C5	5.37	130.56	126.80
38	8	65	A	C8-N9-C4	5.37	107.95	105.80
36	5	290	G	N3-C4-C5	-5.36	125.92	128.60
36	5	345	G	N9-C4-C5	-5.36	103.25	105.40
36	5	1696	A	O5'-P-OP1	-5.36	100.87	105.70
54	m8	124	LEU	CA-CB-CG	-5.36	102.97	115.30
1	2	1756	A	N7-C8-N9	5.36	116.48	113.80
1	6	421	A	C8-N9-C4	5.36	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	874	C	C5-C6-N1	5.36	123.68	121.00
36	5	1857	C	N1-C2-O2	5.36	122.12	118.90
36	1	1620	U	O5'-P-OP2	-5.36	100.88	105.70
38	4	115	C	C5-C6-N1	-5.36	118.32	121.00
36	5	2140	U	N1-C2-N3	5.36	118.12	114.90
1	2	72	A	OP1-P-O3'	5.36	116.98	105.20
1	2	309	C	C5-C6-N1	5.36	123.68	121.00
36	1	205	C	N3-C4-C5	5.36	124.04	121.90
36	1	547	G	OP1-P-O3'	5.36	116.99	105.20
36	1	2355	G	C5-N7-C8	-5.36	101.62	104.30
1	6	1170	G	N9-C4-C5	-5.36	103.26	105.40
36	1	2374	C	N1-C2-O2	-5.36	115.69	118.90
36	1	3089	C	C6-N1-C2	-5.36	118.16	120.30
36	5	283	G	C8-N9-C1'	-5.36	120.04	127.00
1	2	1039	A	O4'-C1'-N9	5.35	112.48	108.20
36	1	545	U	C2-N1-C1'	5.35	124.12	117.70
36	1	2409	G	N3-C4-C5	-5.35	125.92	128.60
1	6	1473	U	C5-C6-N1	5.35	125.38	122.70
36	5	387	A	N7-C8-N9	5.35	116.48	113.80
36	1	1858	A	C4-C5-C6	5.35	119.67	117.00
36	5	639	G	N9-C1'-C2'	-5.35	106.11	112.00
36	1	21	G	N1-C6-O6	-5.35	116.69	119.90
36	1	304	G	N3-C2-N2	-5.35	116.16	119.90
36	5	1192	C	C6-N1-C2	5.35	122.44	120.30
1	2	1760	G	N1-C6-O6	5.35	123.11	119.90
36	1	1490	A	O5'-P-OP1	-5.35	100.89	105.70
36	1	2392	C	O5'-P-OP1	-5.35	100.89	105.70
1	6	163	G	N9-C4-C5	5.35	107.54	105.40
1	6	623	A	O4'-C1'-N9	5.35	112.48	108.20
36	5	838	G	OP2-P-O3'	5.35	116.96	105.20
38	8	100	U	O5'-P-OP2	5.35	117.12	110.70
36	1	1938	U	C6-N1-C2	5.35	124.21	121.00
36	5	851	C	C6-N1-C2	-5.35	118.16	120.30
36	5	2964	G	N3-C4-N9	-5.35	122.79	126.00
36	1	1536	G	O5'-P-OP2	-5.34	100.89	105.70
36	5	297	G	C6-C5-N7	-5.34	127.19	130.40
38	4	4	C	C6-N1-C2	-5.34	118.16	120.30
36	1	2403	G	N3-C4-N9	5.34	129.21	126.00
36	5	1115	G	N3-C2-N2	-5.34	116.16	119.90
36	5	2727	A	N1-C6-N6	-5.34	115.40	118.60
36	1	2700	G	N9-C4-C5	-5.34	103.27	105.40
1	2	1751	C	C5-C6-N1	-5.34	118.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	M1	112	LEU	CA-CB-CG	5.34	127.57	115.30
1	6	765	G	C6-C5-N7	5.34	133.60	130.40
36	5	2121	G	C8-N9-C4	-5.34	104.27	106.40
36	1	2306	C	C6-N1-C1'	-5.33	114.40	120.80
36	1	2568	C	C6-N1-C1'	-5.33	114.40	120.80
36	5	338	A	N9-C4-C5	5.33	107.93	105.80
1	6	187	G	P-O3'-C3'	5.33	126.10	119.70
1	6	934	C	N1-C2-O2	5.33	122.10	118.90
36	1	725	G	C8-N9-C4	5.33	108.53	106.40
36	1	870	G	N3-C4-N9	5.33	129.20	126.00
36	1	908	G	C8-N9-C1'	-5.33	120.07	127.00
36	1	2808	A	C8-N9-C4	5.33	107.93	105.80
36	1	2933	A	N1-C6-N6	-5.33	115.40	118.60
36	1	908	G	O4'-C1'-N9	-5.33	103.94	108.20
36	1	2619	G	N3-C4-N9	5.33	129.20	126.00
36	5	1149	G	C5-C6-O6	-5.33	125.40	128.60
36	5	2968	G	N1-C6-O6	5.33	123.10	119.90
36	5	3285	C	N3-C2-O2	-5.33	118.17	121.90
1	2	1490	C	N3-C2-O2	-5.33	118.17	121.90
36	5	637	C	C5-C4-N4	-5.33	116.47	120.20
1	2	1493	A	P-O3'-C3'	5.33	126.09	119.70
36	1	369	A	C5-N7-C8	-5.32	101.24	103.90
36	5	207	U	C6-N1-C2	-5.32	117.81	121.00
36	5	655	C	N3-C4-C5	5.32	124.03	121.90
36	5	1580	A	C8-N9-C4	-5.32	103.67	105.80
1	2	1607	G	C8-N9-C4	-5.32	104.27	106.40
36	5	1148	G	O5'-P-OP1	5.32	117.09	110.70
36	5	3213	A	N9-C4-C5	-5.32	103.67	105.80
36	1	964	G	C6-C5-N7	-5.32	127.21	130.40
36	1	1331	U	N3-C2-O2	-5.32	118.47	122.20
36	1	1666	G	N1-C6-O6	5.32	123.09	119.90
36	1	1866	C	C5-C6-N1	5.32	123.66	121.00
36	1	2827	U	C6-N1-C1'	5.32	128.65	121.20
36	1	943	U	N1-C2-O2	-5.32	119.08	122.80
36	5	864	G	N3-C2-N2	5.32	123.62	119.90
36	5	2507	C	C6-N1-C2	-5.32	118.17	120.30
36	1	979	U	N3-C4-O4	-5.32	115.68	119.40
36	5	793	C	N1-C2-O2	5.32	122.09	118.90
36	5	1063	G	C6-C5-N7	-5.32	127.21	130.40
36	1	700	C	C5-C6-N1	5.31	123.66	121.00
36	1	1113	G	N3-C4-C5	-5.31	125.94	128.60
36	1	1902	G	C4-N9-C1'	5.31	133.41	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2987	A	N1-C2-N3	-5.31	126.64	129.30
38	8	125	U	C2-N1-C1'	5.31	124.08	117.70
36	5	1016	C	O4'-C1'-N1	-5.31	103.95	108.20
1	6	299	A	C8-N9-C4	-5.31	103.68	105.80
1	6	700	C	C6-N1-C2	-5.31	118.18	120.30
1	6	1428	G	O5'-P-OP1	-5.31	100.92	105.70
36	5	1112	A	C4-N9-C1'	5.31	135.85	126.30
36	5	2209	U	O4'-C1'-N1	5.31	112.44	108.20
36	1	890	C	C6-N1-C2	5.30	122.42	120.30
36	1	1001	G	C4-N9-C1'	5.30	133.40	126.50
36	1	1902	G	C6-C5-N7	-5.30	127.22	130.40
36	1	2768	U	O5'-P-OP2	-5.30	100.92	105.70
36	5	1953	G	N3-C4-N9	5.30	129.18	126.00
36	5	3394	U	C6-N1-C2	5.30	124.18	121.00
1	6	579	A	O4'-C1'-N9	5.30	112.44	108.20
36	5	1493	G	N1-C6-O6	-5.30	116.72	119.90
36	5	1511	U	C5-C6-N1	-5.30	120.05	122.70
36	5	2251	G	C4-N9-C1'	5.30	133.39	126.50
36	1	1115	G	N7-C8-N9	5.30	115.75	113.10
36	1	2577	C	C2-N1-C1'	5.30	124.63	118.80
36	5	336	A	C8-N9-C4	5.30	107.92	105.80
36	1	964	G	C4-N9-C1'	5.30	133.39	126.50
36	1	1187	C	C2-N1-C1'	5.29	124.62	118.80
1	6	1489	U	C5-C6-N1	5.29	125.35	122.70
1	2	453	U	C6-N1-C2	-5.29	117.82	121.00
1	2	1596	C	C6-N1-C2	5.29	122.42	120.30
1	2	192	U	C5-C6-N1	5.29	125.34	122.70
1	2	1490	C	N1-C2-O2	5.29	122.07	118.90
36	1	1604	G	C8-N9-C1'	-5.29	120.13	127.00
36	1	622	A	N1-C6-N6	5.28	121.77	118.60
36	5	875	G	N1-C2-N2	5.28	120.95	116.20
1	2	1514	U	N3-C2-O2	-5.28	118.50	122.20
6	S4	164	LEU	CA-CB-CG	5.28	127.44	115.30
1	6	987	G	N1-C6-O6	5.28	123.07	119.90
36	1	2571	U	O5'-P-OP2	-5.28	100.95	105.70
36	1	2197	C	C6-N1-C2	5.28	122.41	120.30
36	5	1480	G	C8-N9-C4	5.28	108.51	106.40
36	5	2922	G	C4-N9-C1'	5.28	133.36	126.50
1	2	8	U	C5-C6-N1	-5.28	120.06	122.70
36	1	2148	U	C5-C6-N1	-5.27	120.06	122.70
3	S1	207	LEU	CA-CB-CG	-5.27	103.17	115.30
36	1	1852	G	OP2-P-O3'	5.27	116.80	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2922	G	N3-C4-N9	5.27	129.16	126.00
36	5	2156	C	N3-C4-C5	5.27	124.01	121.90
1	2	1536	G	N3-C4-N9	5.27	129.16	126.00
36	1	3195	U	O4'-C1'-N1	5.27	112.42	108.20
37	7	86	U	C5-C4-O4	5.27	129.06	125.90
38	8	111	A	N9-C4-C5	-5.27	103.69	105.80
36	1	1113	G	C4-N9-C1'	5.27	133.35	126.50
38	4	31	G	C8-N9-C4	5.27	108.51	106.40
1	6	987	G	N3-C4-C5	5.27	131.23	128.60
36	5	2251	G	C8-N9-C1'	-5.27	120.15	127.00
36	5	3143	C	N3-C2-O2	5.27	125.59	121.90
1	2	276	C	O4'-C1'-N1	5.26	112.41	108.20
36	1	3130	A	N1-C6-N6	5.26	121.76	118.60
1	6	326	G	N9-C4-C5	5.26	107.51	105.40
36	1	1149	G	N9-C4-C5	-5.26	103.30	105.40
36	1	627	U	C5-C4-O4	5.26	129.06	125.90
36	1	2619	G	C8-N9-C1'	-5.26	120.16	127.00
36	5	910	G	N7-C8-N9	5.26	115.73	113.10
1	2	814	A	P-O3'-C3'	5.26	126.01	119.70
36	1	2382	G	N1-C6-O6	5.26	123.06	119.90
36	1	2619	G	C4-N9-C1'	5.26	133.34	126.50
11	s9	99	LEU	CA-CB-CG	5.26	127.40	115.30
36	5	2417	U	C5-C6-N1	-5.26	120.07	122.70
36	5	2614	G	C8-N9-C1'	-5.26	120.16	127.00
1	2	783	G	C4-C5-N7	5.26	112.90	110.80
38	4	54	A	C5-N7-C8	-5.26	101.27	103.90
1	6	931	C	C6-N1-C2	5.26	122.40	120.30
36	5	922	U	O5'-P-OP1	-5.26	100.97	105.70
36	5	2266	U	C5-C6-N1	5.26	125.33	122.70
1	2	1611	A	N1-C2-N3	5.25	131.93	129.30
36	1	2142	A	C4-C5-C6	5.25	119.63	117.00
36	5	3120	C	C5-C6-N1	5.25	123.63	121.00
38	8	70	G	C8-N9-C1'	-5.25	120.17	127.00
70	o4	30	LEU	CA-CB-CG	-5.25	103.22	115.30
36	1	718	G	N7-C8-N9	5.25	115.73	113.10
36	5	197	G	N7-C8-N9	5.25	115.73	113.10
36	5	3285	C	N1-C2-O2	5.25	122.05	118.90
37	3	47	C	C5-C6-N1	5.25	123.62	121.00
53	M7	121	GLN	C-N-CA	5.25	134.82	121.70
1	6	765	G	N3-C2-N2	-5.25	116.22	119.90
36	5	347	G	C6-C5-N7	-5.25	127.25	130.40
36	5	2400	G	N3-C4-C5	5.25	131.22	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2647	A	C5-N7-C8	-5.25	101.28	103.90
37	7	89	G	N1-C6-O6	5.25	123.05	119.90
36	1	1724	U	O4'-C1'-N1	5.25	112.40	108.20
36	1	1870	C	C6-N1-C2	-5.25	118.20	120.30
36	5	1521	G	N3-C4-C5	5.25	131.22	128.60
36	5	1625	A	C8-N9-C4	5.25	107.90	105.80
1	2	543	C	C4-C5-C6	5.24	120.02	117.40
36	1	545	U	C5-C6-N1	5.24	125.32	122.70
36	1	2957	G	N9-C4-C5	-5.24	103.30	105.40
36	5	2186	U	N1-C2-O2	5.24	126.47	122.80
36	1	2967	A	C4-C5-N7	5.24	113.32	110.70
36	5	912	G	N1-C6-O6	5.24	123.05	119.90
36	5	2145	A	C6-C5-N7	-5.24	128.63	132.30
36	1	1017	C	C2-N1-C1'	5.24	124.56	118.80
36	1	1609	C	C6-N1-C2	5.24	122.40	120.30
36	1	1661	G	C4-N9-C1'	5.24	133.31	126.50
36	1	3175	U	C2-N1-C1'	5.24	123.99	117.70
1	6	1100	G	C5-C6-O6	-5.24	125.46	128.60
36	1	55	G	C4-N9-C1'	-5.24	119.69	126.50
36	1	1843	C	C2-N1-C1'	5.24	124.56	118.80
1	6	334	G	N3-C4-C5	5.24	131.22	128.60
36	5	816	A	OP1-P-OP2	5.24	127.46	119.60
36	5	1150	A	O5'-P-OP1	5.24	116.99	110.70
36	5	2591	A	C8-N9-C4	5.24	107.90	105.80
37	7	114	U	C5-C6-N1	-5.24	120.08	122.70
62	n6	111	LEU	CA-CB-CG	-5.24	103.25	115.30
38	4	39	G	N3-C4-N9	5.24	129.14	126.00
36	5	2112	U	P-O3'-C3'	5.24	125.98	119.70
36	5	2300	G	N3-C4-N9	5.24	129.14	126.00
36	5	2876	C	N1-C2-O2	5.24	122.04	118.90
1	6	1156	C	C5-C6-N1	5.24	123.62	121.00
36	5	1242	G	N3-C4-C5	-5.24	125.98	128.60
36	5	1389	G	N9-C4-C5	-5.23	103.31	105.40
36	1	2629	U	N1-C2-N3	-5.23	111.76	114.90
64	N8	66	ALA	N-CA-C	-5.23	96.87	111.00
36	1	792	G	N3-C4-N9	-5.23	122.86	126.00
36	1	906	A	N9-C4-C5	5.23	107.89	105.80
36	1	2205	U	P-O3'-C3'	5.23	125.98	119.70
36	5	2126	A	C8-N9-C4	5.23	107.89	105.80
36	1	353	G	C4-N9-C1'	-5.23	119.70	126.50
36	1	2818	U	P-O3'-C3'	5.23	125.97	119.70
36	5	283	G	N7-C8-N9	5.23	115.72	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	868	C	N3-C2-O2	5.23	125.56	121.90
38	8	82	U	P-O3'-C3'	5.23	125.97	119.70
1	2	1059	U	N1-C2-O2	5.23	126.46	122.80
40	L3	102	LEU	CA-CB-CG	5.23	127.32	115.30
1	6	25	C	P-O3'-C3'	5.23	125.97	119.70
24	d2	93	LEU	CA-CB-CG	5.23	127.32	115.30
36	1	867	G	N1-C6-O6	5.23	123.04	119.90
36	1	1284	C	P-O3'-C3'	5.23	125.97	119.70
1	6	275	C	C2-N1-C1'	5.23	124.55	118.80
1	2	571	G	N3-C4-N9	5.22	129.13	126.00
36	1	2688	U	C6-N1-C2	5.22	124.14	121.00
38	4	126	A	P-O3'-C3'	5.22	125.97	119.70
36	5	2397	A	N1-C2-N3	5.22	131.91	129.30
36	1	644	G	C8-N9-C1'	-5.22	120.21	127.00
36	1	2308	C	C6-N1-C1'	5.22	127.07	120.80
38	4	64	U	N3-C2-O2	-5.22	118.55	122.20
36	5	1697	A	O5'-P-OP2	5.22	116.97	110.70
36	1	916	G	C4-N9-C1'	5.22	133.29	126.50
36	1	2131	A	N1-C2-N3	-5.22	126.69	129.30
36	1	2606	G	C4-N9-C1'	5.22	133.29	126.50
36	5	1303	A	C8-N9-C4	5.22	107.89	105.80
36	1	2675	C	C2-N1-C1'	5.22	124.54	118.80
1	6	139	C	P-O3'-C3'	5.22	125.96	119.70
1	6	174	U	C2-N1-C1'	5.22	123.96	117.70
36	5	1392	G	N3-C4-C5	-5.22	125.99	128.60
36	5	2417	U	C2-N1-C1'	-5.22	111.44	117.70
36	1	227	G	N3-C4-C5	-5.22	125.99	128.60
36	1	1537	A	O5'-P-OP1	-5.22	101.00	105.70
36	5	2355	G	C5-C6-O6	-5.22	125.47	128.60
36	5	3057	U	C2-N1-C1'	5.22	123.96	117.70
38	8	80	A	P-O3'-C3'	5.22	125.96	119.70
1	6	1631	A	N9-C4-C5	5.21	107.89	105.80
36	5	3011	A	C8-N9-C1'	5.21	137.09	127.70
38	8	75	G	C8-N9-C1'	5.21	133.78	127.00
36	1	1889	G	N3-C2-N2	-5.21	116.25	119.90
36	1	3217	C	C6-N1-C1'	-5.21	114.55	120.80
1	2	192	U	N3-C2-O2	-5.21	118.55	122.20
1	2	1327	C	C5-C6-N1	5.21	123.61	121.00
36	5	823	C	C6-N1-C2	-5.21	118.22	120.30
36	1	569	A	N9-C4-C5	-5.21	103.72	105.80
36	1	2366	C	C4-C5-C6	-5.21	114.80	117.40
36	5	517	G	N1-C6-O6	5.21	123.03	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	417	A	C8-N9-C4	-5.21	103.72	105.80
36	5	341	G	OP2-P-O3'	5.21	116.66	105.20
36	5	2937	G	N9-C4-C5	-5.21	103.32	105.40
36	5	348	A	N1-C6-N6	5.21	121.72	118.60
36	5	2610	G	C4-N9-C1'	-5.21	119.73	126.50
36	5	339	C	N3-C4-C5	5.21	123.98	121.90
1	2	1430	U	N3-C4-C5	-5.20	111.48	114.60
36	1	2922	G	C6-C5-N7	-5.20	127.28	130.40
36	1	1635	G	C4-N9-C1'	-5.20	119.74	126.50
36	1	1713	G	C4-N9-C1'	-5.20	119.74	126.50
36	1	3060	C	C6-N1-C2	-5.20	118.22	120.30
36	5	1868	G	OP1-P-O3'	5.20	116.64	105.20
36	1	845	G	C8-N9-C4	5.20	108.48	106.40
36	1	1115	G	N9-C4-C5	-5.20	103.32	105.40
36	1	63	A	N1-C6-N6	5.20	121.72	118.60
36	1	1005	G	C8-N9-C4	5.20	108.48	106.40
36	5	2108	C	C6-N1-C2	5.20	122.38	120.30
36	1	2550	U	N3-C2-O2	-5.20	118.56	122.20
36	5	1511	U	C2-N1-C1'	-5.20	111.46	117.70
36	5	2549	G	N3-C4-C5	5.20	131.20	128.60
36	1	964	G	N3-C4-N9	5.20	129.12	126.00
36	1	3249	C	C2-N1-C1'	-5.20	113.09	118.80
36	5	43	A	O4'-C1'-N9	5.20	112.36	108.20
36	5	1495	U	C5-C4-O4	5.20	129.02	125.90
36	5	1675	G	N3-C4-C5	5.20	131.20	128.60
1	2	558	U	C2-N1-C1'	5.19	123.93	117.70
36	5	2278	C	N1-C2-O2	5.19	122.02	118.90
36	1	354	U	C2-N1-C1'	5.19	123.93	117.70
36	1	1510	G	N3-C4-C5	-5.19	126.00	128.60
1	2	1058	U	P-O3'-C3'	5.19	125.93	119.70
36	1	984	G	C6-C5-N7	-5.19	127.29	130.40
36	5	247	C	C6-N1-C2	-5.19	118.22	120.30
36	5	2966	G	OP2-P-O3'	5.19	116.61	105.20
1	2	17	C	C6-N1-C2	-5.19	118.22	120.30
36	1	700	C	C6-N1-C2	-5.19	118.22	120.30
36	1	966	U	N3-C4-O4	5.19	123.03	119.40
36	1	1556	C	C5-C6-N1	5.19	123.59	121.00
36	1	2966	G	N1-C2-N2	-5.19	111.53	116.20
36	1	695	C	C6-N1-C2	5.19	122.37	120.30
36	1	2984	C	C2-N1-C1'	-5.19	113.09	118.80
1	6	976	G	N1-C6-O6	5.19	123.01	119.90
38	8	44	A	C4-C5-N7	5.19	113.29	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1785	U	C5-C6-N1	-5.18	120.11	122.70
36	1	2913	C	C6-N1-C2	-5.18	118.23	120.30
36	5	1389	G	O5'-P-OP2	5.18	116.92	110.70
36	1	2875	U	C2-N1-C1'	5.18	123.92	117.70
1	6	1482	C	C6-N1-C2	-5.18	118.23	120.30
36	5	347	G	C4-C5-N7	5.18	112.87	110.80
36	5	422	A	N1-C2-N3	5.18	131.89	129.30
36	1	657	A	OP1-P-O3'	5.18	116.60	105.20
36	1	914	A	N1-C6-N6	-5.18	115.49	118.60
36	5	2954	U	N3-C2-O2	-5.18	118.57	122.20
36	5	3368	U	C6-N1-C2	5.18	124.11	121.00
36	1	2874	G	C8-N9-C4	-5.18	104.33	106.40
36	5	869	G	C8-N9-C4	5.18	108.47	106.40
37	7	17	A	C8-N9-C4	5.18	107.87	105.80
48	m1	112	LEU	CA-CB-CG	5.18	127.21	115.30
1	2	780	A	N1-C2-N3	5.18	131.89	129.30
38	4	54	A	C6-C5-N7	-5.18	128.68	132.30
36	5	641	C	C5-C4-N4	-5.18	116.58	120.20
36	5	1152	G	O4'-C1'-N9	5.18	112.34	108.20
36	1	336	A	O4'-C1'-N9	-5.17	104.06	108.20
36	1	867	G	C6-C5-N7	-5.17	127.30	130.40
1	6	1642	G	C4-C5-C6	5.17	121.90	118.80
1	2	145	A	N1-C2-N3	5.17	131.89	129.30
1	2	1600	A	N9-C1'-C2'	5.17	120.72	114.00
36	1	2403	G	N7-C8-N9	5.17	115.69	113.10
1	6	581	U	C5-C6-N1	-5.17	120.11	122.70
36	1	979	U	N3-C2-O2	-5.17	118.58	122.20
36	1	1726	C	C6-N1-C2	5.17	122.37	120.30
36	5	2809	C	C6-N1-C2	-5.17	118.23	120.30
36	5	2937	G	C8-N9-C4	5.17	108.47	106.40
36	5	3287	U	N1-C2-O2	5.17	126.42	122.80
1	2	1090	C	C6-N1-C2	5.17	122.37	120.30
36	1	384	A	N9-C4-C5	-5.17	103.73	105.80
1	2	794	U	C2-N1-C1'	5.17	123.90	117.70
36	1	1902	G	C8-N9-C1'	-5.17	120.28	127.00
1	6	577	G	C5-C6-O6	-5.17	125.50	128.60
36	5	227	G	C4-N9-C1'	5.17	133.22	126.50
36	5	2354	C	C6-N1-C2	-5.17	118.23	120.30
36	5	2355	G	OP1-P-O3'	5.17	116.57	105.20
36	5	2364	G	O5'-P-OP2	-5.17	101.05	105.70
36	5	2383	C	C2-N1-C1'	-5.17	113.12	118.80
36	5	3120	C	N1-C2-O2	5.17	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1858	A	C6-N1-C2	-5.17	115.50	118.60
1	2	1202	A	C2-N3-C4	5.16	113.18	110.60
1	2	1361	U	C5-C6-N1	5.16	125.28	122.70
24	D2	28	ARG	C-N-CD	-5.16	109.24	120.60
36	1	2138	A	N1-C6-N6	5.16	121.70	118.60
36	1	2315	G	O4'-C1'-N9	5.16	112.33	108.20
1	6	765	G	C4-N9-C1'	-5.16	119.79	126.50
36	5	2355	G	O5'-P-OP1	-5.16	101.05	105.70
36	5	3354	U	N1-C2-O2	5.16	126.41	122.80
36	5	2122	G	N3-C4-C5	5.16	131.18	128.60
36	1	1510	G	N3-C4-N9	5.16	129.10	126.00
1	2	272	U	C2-N1-C1'	5.16	123.89	117.70
36	1	1382	G	N3-C4-N9	-5.16	122.90	126.00
36	1	1522	U	O4'-C1'-N1	5.16	112.33	108.20
36	1	1635	G	N3-C4-C5	5.16	131.18	128.60
36	1	2248	C	OP1-P-O3'	5.16	116.55	105.20
36	5	2899	C	C2-N1-C1'	5.16	124.47	118.80
36	1	1140	G	C4-N9-C1'	5.16	133.20	126.50
36	1	1192	C	C5-C4-N4	-5.16	116.59	120.20
36	5	2943	G	C4-N9-C1'	5.16	133.20	126.50
1	2	1600	A	C8-N9-C1'	-5.16	118.42	127.70
36	5	32	U	C2-N1-C1'	5.16	123.89	117.70
36	5	2735	U	C5-C6-N1	5.16	125.28	122.70
36	1	2824	G	O5'-P-OP2	-5.15	101.06	105.70
1	2	1778	G	N3-C4-C5	-5.15	126.02	128.60
36	1	1306	G	C4-N9-C1'	5.15	133.20	126.50
36	1	2967	A	C8-N9-C4	5.15	107.86	105.80
38	4	47	C	O5'-P-OP2	5.15	116.88	110.70
36	5	315	C	C2-N1-C1'	5.15	124.47	118.80
1	2	502	U	C5-C6-N1	5.15	125.28	122.70
36	1	41	G	N1-C6-O6	-5.15	116.81	119.90
36	1	580	C	C6-N1-C2	5.15	122.36	120.30
1	6	326	G	C4-N9-C1'	-5.15	119.81	126.50
1	6	1197	C	N3-C2-O2	-5.15	118.30	121.90
36	5	102	C	C5-C6-N1	5.15	123.58	121.00
38	8	52	A	N1-C6-N6	-5.15	115.51	118.60
36	1	2290	C	C6-N1-C2	5.15	122.36	120.30
36	5	3180	A	N9-C4-C5	-5.15	103.74	105.80
36	1	2370	G	O5'-P-OP1	-5.15	101.07	105.70
36	5	860	G	C4-C5-N7	5.15	112.86	110.80
36	1	2150	G	N3-C4-C5	5.14	131.17	128.60
36	1	3382	U	C6-N1-C1'	-5.14	114.00	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	230	U	C5-C6-N1	5.14	125.27	122.70
1	2	633	U	C5-C6-N1	-5.14	120.13	122.70
36	5	2852	C	C2-N1-C1'	5.14	124.46	118.80
1	2	1644	C	C5-C6-N1	5.14	123.57	121.00
39	L2	237	LEU	CA-CB-CG	-5.14	103.48	115.30
36	5	881	C	N1-C2-O2	5.14	121.98	118.90
53	m7	95	LEU	CA-CB-CG	-5.14	103.48	115.30
36	1	1525	G	N3-C4-C5	-5.14	126.03	128.60
1	6	122	U	C5-C6-N1	5.14	125.27	122.70
36	5	1888	U	C2-N1-C1'	5.14	123.87	117.70
1	2	815	G	P-O3'-C3'	5.14	125.86	119.70
36	1	2363	A	C8-N9-C4	-5.14	103.75	105.80
1	6	742	U	C6-N1-C2	-5.14	117.92	121.00
36	5	1667	A	N7-C8-N9	5.14	116.37	113.80
36	1	2649	A	C8-N9-C4	-5.14	103.75	105.80
36	5	2608	G	N7-C8-N9	-5.14	110.53	113.10
1	2	618	U	C5-C6-N1	5.13	125.27	122.70
3	S1	219	LYS	C-N-CA	5.13	134.54	121.70
36	1	149	U	C6-N1-C2	-5.13	117.92	121.00
36	1	2988	C	C5-C6-N1	5.13	123.57	121.00
36	1	3325	G	C4-N9-C1'	-5.13	119.82	126.50
52	M6	27	LEU	CA-CB-CG	-5.13	103.49	115.30
1	6	1481	C	P-O3'-C3'	5.13	125.86	119.70
36	5	92	G	N9-C4-C5	-5.13	103.35	105.40
63	n7	5	LEU	CA-CB-CG	-5.13	103.49	115.30
1	2	1051	G	OP1-P-O3'	5.13	116.49	105.20
36	1	1915	A	N7-C8-N9	-5.13	111.23	113.80
36	5	1264	G	C8-N9-C4	-5.13	104.35	106.40
36	1	1603	A	N1-C2-N3	5.13	131.87	129.30
36	1	2171	G	O5'-P-OP1	-5.13	101.08	105.70
36	5	627	U	C6-N1-C2	-5.13	117.92	121.00
36	5	1496	C	C6-N1-C1'	-5.13	114.64	120.80
36	5	2709	C	C6-N1-C2	5.13	122.35	120.30
1	2	16	G	C8-N9-C4	-5.13	104.35	106.40
36	1	1222	G	P-O3'-C3'	5.13	125.86	119.70
36	1	1834	U	C6-N1-C2	-5.13	117.92	121.00
36	5	19	U	C6-N1-C1'	5.13	128.38	121.20
36	5	354	U	C6-N1-C1'	-5.13	114.02	121.20
37	7	91	G	N3-C4-N9	-5.13	122.92	126.00
36	1	47	C	C4-C5-C6	5.13	119.96	117.40
36	5	925	A	O5'-P-OP1	-5.13	101.09	105.70
36	5	970	A	N9-C1'-C2'	-5.13	106.36	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1027	A	OP1-P-O3'	5.13	116.48	105.20
38	4	24	G	N3-C4-N9	-5.12	122.92	126.00
36	5	1892	G	OP1-P-O3'	5.12	116.48	105.20
36	1	812	G	O5'-P-OP2	-5.12	101.09	105.70
36	5	1306	G	OP2-P-O3'	5.12	116.47	105.20
36	5	2346	C	OP1-P-O3'	5.12	116.47	105.20
36	1	2130	G	N3-C4-C5	5.12	131.16	128.60
36	1	1607	U	C2-N1-C1'	5.12	123.84	117.70
36	1	2305	G	C8-N9-C4	-5.12	104.35	106.40
36	5	3002	C	C6-N1-C2	5.12	122.35	120.30
36	5	3157	U	C5-C6-N1	5.12	125.26	122.70
36	5	3197	G	N3-C2-N2	-5.12	116.32	119.90
36	5	2837	A	N9-C4-C5	-5.12	103.75	105.80
36	1	1536	G	OP1-P-O3'	5.12	116.45	105.20
36	1	2871	G	C5-C6-O6	-5.12	125.53	128.60
36	5	838	G	N3-C4-C5	-5.12	126.04	128.60
36	5	1178	G	N1-C6-O6	-5.12	116.83	119.90
36	5	1588	A	C8-N9-C4	5.12	107.85	105.80
36	5	2348	A	N1-C6-N6	-5.12	115.53	118.60
36	1	952	A	N1-C6-N6	-5.11	115.53	118.60
38	4	62	C	O5'-P-OP1	-5.11	101.10	105.70
36	5	835	G	O4'-C1'-N9	5.11	112.29	108.20
1	6	581	U	C2-N1-C1'	-5.11	111.56	117.70
1	6	912	U	P-O3'-C3'	5.11	125.83	119.70
1	6	1156	C	C6-N1-C2	-5.11	118.26	120.30
36	5	420	G	C8-N9-C1'	-5.11	120.36	127.00
36	5	2895	G	O5'-P-OP2	-5.11	101.10	105.70
1	2	549	G	C8-N9-C1'	-5.11	120.36	127.00
36	1	535	G	N3-C4-N9	5.11	129.06	126.00
36	5	970	A	N9-C4-C5	-5.11	103.76	105.80
36	1	2763	U	O5'-P-OP2	-5.11	101.10	105.70
1	6	1	U	N1-C2-O2	5.11	126.38	122.80
1	6	1615	C	OP2-P-O3'	5.11	116.44	105.20
1	2	61	A	O4'-C1'-N9	5.11	112.28	108.20
1	2	417	A	P-O3'-C3'	5.11	125.83	119.70
36	1	870	G	N3-C4-C5	-5.11	126.05	128.60
36	1	1114	U	OP2-P-O3'	5.11	116.43	105.20
1	6	266	A	C8-N9-C4	5.11	107.84	105.80
36	5	860	G	C5-C6-O6	-5.11	125.54	128.60
36	5	1442	U	C5-C6-N1	-5.11	120.15	122.70
36	5	3317	U	P-O3'-C3'	5.11	125.83	119.70
36	5	1064	A	P-O3'-C3'	5.10	125.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1612	A	N9-C1'-C2'	-5.10	106.39	112.00
36	5	1909	A	N7-C8-N9	-5.10	111.25	113.80
38	8	46	G	N3-C4-N9	5.10	129.06	126.00
1	2	321	C	OP1-P-O3'	5.10	116.42	105.20
36	5	2521	U	C5-C6-N1	-5.10	120.15	122.70
1	2	1456	C	C2-N1-C1'	5.10	124.41	118.80
1	2	1157	A	N7-C8-N9	5.10	116.35	113.80
36	1	2335	G	N7-C8-N9	5.10	115.65	113.10
36	1	2424	A	N9-C4-C5	-5.10	103.76	105.80
1	6	337	G	C5-N7-C8	-5.10	101.75	104.30
36	5	1606	U	OP2-P-O3'	5.10	116.41	105.20
36	5	2642	A	N1-C2-N3	5.10	131.85	129.30
36	5	2813	A	C5-N7-C8	-5.10	101.35	103.90
36	1	1525	G	C8-N9-C4	-5.09	104.36	106.40
36	1	1769	G	N7-C8-N9	5.09	115.65	113.10
36	1	661	G	C4-N9-C1'	5.09	133.12	126.50
36	1	1661	G	N3-C4-N9	5.09	129.06	126.00
36	1	1762	C	C6-N1-C2	-5.09	118.26	120.30
1	6	363	G	N1-C6-O6	5.09	122.95	119.90
1	6	429	G	N1-C6-O6	5.09	122.95	119.90
36	5	360	G	C6-C5-N7	-5.09	127.34	130.40
36	5	2614	G	N3-C4-N9	5.09	129.06	126.00
80	p0	93	LEU	CA-CB-CG	5.09	127.01	115.30
36	1	395	A	C8-N9-C4	-5.09	103.76	105.80
1	6	1573	A	P-O3'-C3'	5.09	125.81	119.70
36	1	1542	G	C4-C5-N7	5.09	112.83	110.80
37	3	44	C	C6-N1-C2	5.09	122.33	120.30
1	6	275	C	N1-C2-O2	5.09	121.95	118.90
36	5	635	G	C6-C5-N7	-5.09	127.35	130.40
36	5	2719	U	N1-C2-O2	-5.09	119.24	122.80
36	1	2141	U	N1-C2-O2	-5.09	119.24	122.80
36	5	1761	C	OP1-P-O3'	5.09	116.39	105.20
36	5	2856	G	N1-C6-O6	5.09	122.95	119.90
1	2	1399	C	C6-N1-C2	-5.08	118.27	120.30
1	6	1458	G	C8-N9-C1'	-5.08	120.39	127.00
36	5	982	C	C5-C6-N1	5.08	123.54	121.00
36	5	1762	C	C5-C6-N1	5.08	123.54	121.00
36	5	2814	G	N1-C6-O6	-5.08	116.85	119.90
36	5	2842	U	C6-N1-C1'	-5.08	114.08	121.20
36	1	188	U	C6-N1-C2	-5.08	117.95	121.00
36	1	98	G	N9-C4-C5	-5.08	103.37	105.40
36	1	2922	G	C5-C6-O6	-5.08	125.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	336	G	N3-C4-N9	-5.08	122.95	126.00
36	5	3056	U	C6-N1-C2	5.08	124.05	121.00
36	1	1480	G	C4-C5-N7	5.08	112.83	110.80
36	1	2145	A	C6-C5-N7	-5.08	128.75	132.30
36	1	2675	C	C6-N1-C1'	-5.08	114.71	120.80
36	1	2683	U	C5-C6-N1	-5.08	120.16	122.70
36	5	385	A	N1-C6-N6	5.08	121.65	118.60
36	5	2947	G	N9-C4-C5	5.08	107.43	105.40
1	2	617	U	C5-C6-N1	5.07	125.24	122.70
36	1	55	G	N9-C1'-C2'	-5.07	106.42	112.00
36	1	2819	A	C8-N9-C4	-5.07	103.77	105.80
1	6	224	C	C6-N1-C2	-5.07	118.27	120.30
36	1	2358	A	OP1-P-O3'	5.07	116.35	105.20
36	5	2968	G	OP2-P-O3'	5.07	116.36	105.20
1	2	1339	C	C6-N1-C2	-5.07	118.27	120.30
1	2	1467	C	C6-N1-C2	-5.07	118.27	120.30
36	1	588	G	OP2-P-O3'	5.07	116.35	105.20
36	1	1086	C	C5-C6-N1	5.07	123.53	121.00
36	5	793	C	C5-C6-N1	5.07	123.53	121.00
36	5	1095	U	C2-N1-C1'	5.07	123.78	117.70
36	1	718	G	C2-N3-C4	-5.07	109.37	111.90
36	1	2221	G	C8-N9-C1'	5.07	133.59	127.00
1	6	155	U	N3-C2-O2	-5.07	118.65	122.20
36	5	2288	G	C4-N9-C1'	5.07	133.09	126.50
1	2	187	G	OP1-P-O3'	5.07	116.34	105.20
36	1	1124	U	N3-C2-O2	-5.06	118.66	122.20
36	1	2606	G	N3-C4-C5	-5.06	126.07	128.60
36	5	1663	C	C6-N1-C2	5.06	122.33	120.30
36	5	2424	A	C6-N1-C2	5.06	121.64	118.60
36	1	2372	A	C8-N9-C4	-5.06	103.78	105.80
36	1	2645	G	N9-C4-C5	-5.06	103.38	105.40
36	1	2762	A	N9-C4-C5	5.06	107.83	105.80
1	6	1728	A	C8-N9-C4	-5.06	103.78	105.80
36	5	813	G	C5-C6-O6	-5.06	125.56	128.60
1	2	1182	U	N3-C2-O2	-5.06	118.66	122.20
36	1	2794	G	C8-N9-C1'	5.06	133.58	127.00
36	5	3087	A	N3-C4-N9	-5.06	123.35	127.40
36	1	1599	G	C8-N9-C4	5.06	108.42	106.40
36	1	2645	G	C5-C6-O6	-5.06	125.56	128.60
38	4	58	G	N3-C4-N9	5.06	129.04	126.00
36	1	2513	U	C5-C6-N1	5.06	125.23	122.70
36	1	3228	C	N3-C4-C5	-5.06	119.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	M3	85	LEU	CA-CB-CG	5.06	126.93	115.30
36	5	1396	C	C6-N1-C2	5.06	122.32	120.30
36	5	1897	G	C4-C5-N7	5.06	112.82	110.80
36	5	2405	C	C5-C6-N1	-5.06	118.47	121.00
36	5	2726	C	C6-N1-C2	-5.06	118.28	120.30
1	2	1456	C	N1-C2-O2	5.06	121.93	118.90
36	1	2380	U	C6-N1-C2	5.06	124.03	121.00
41	L4	318	LEU	CA-CB-CG	5.06	126.93	115.30
1	6	1148	C	C6-N1-C2	-5.06	118.28	120.30
36	5	664	U	N3-C2-O2	-5.06	118.66	122.20
1	6	687	G	N3-C2-N2	-5.05	116.36	119.90
36	1	620	U	C4-C5-C6	5.05	122.73	119.70
36	5	345	G	N1-C6-O6	5.05	122.93	119.90
36	5	2837	A	N3-C4-C5	5.05	130.34	126.80
1	2	403	G	N7-C8-N9	5.05	115.63	113.10
36	5	3085	G	N3-C4-C5	5.05	131.13	128.60
36	1	3217	C	C6-N1-C2	-5.05	118.28	120.30
1	6	1	U	C6-N1-C1'	-5.05	114.13	121.20
1	2	1082	C	C2-N1-C1'	5.05	124.35	118.80
36	1	2138	A	N9-C4-C5	-5.05	103.78	105.80
36	1	2359	C	C5-C6-N1	5.05	123.52	121.00
36	5	2751	G	N3-C4-C5	5.05	131.12	128.60
1	2	966	A	C8-N9-C4	5.05	107.82	105.80
14	C2	58	LEU	CA-CB-CG	5.05	126.91	115.30
36	1	1111	U	C6-N1-C2	5.05	124.03	121.00
36	1	3143	C	C6-N1-C2	5.05	122.32	120.30
36	1	3344	A	O4'-C1'-N9	5.05	112.24	108.20
38	4	75	G	N3-C4-C5	5.05	131.12	128.60
36	5	1846	C	C6-N1-C2	5.05	122.32	120.30
1	2	1244	A	P-O3'-C3'	5.04	125.75	119.70
1	6	1646	C	C6-N1-C2	-5.04	118.28	120.30
36	1	2101	C	P-O3'-C3'	5.04	125.75	119.70
36	5	895	A	C8-N9-C4	-5.04	103.78	105.80
36	5	2689	A	O4'-C1'-N9	5.04	112.23	108.20
36	5	3286	G	N3-C4-C5	5.04	131.12	128.60
36	1	2366	C	C5-C6-N1	5.04	123.52	121.00
36	1	2955	U	C5-C6-N1	5.04	125.22	122.70
36	5	1324	U	C6-N1-C2	5.04	124.02	121.00
36	5	2163	C	C5-C6-N1	5.04	123.52	121.00
36	5	2615	G	O5'-P-OP1	-5.04	101.16	105.70
36	5	2794	G	O4'-C1'-N9	5.04	112.23	108.20
36	5	2987	A	C2-N3-C4	5.04	113.12	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	91	G	N3-C4-C5	5.04	131.12	128.60
36	1	2286	U	C2-N1-C1'	-5.04	111.65	117.70
1	6	321	C	OP1-P-O3'	5.04	116.29	105.20
1	2	387	A	O5'-P-OP2	-5.04	101.17	105.70
36	1	1190	A	C4-N9-C1'	5.04	135.37	126.30
36	1	1525	G	N7-C8-N9	5.04	115.62	113.10
36	1	2513	U	OP1-P-O3'	5.04	116.28	105.20
1	6	1456	C	O4'-C1'-N1	5.04	112.23	108.20
36	5	1188	U	N1-C2-N3	5.04	117.92	114.90
36	5	1639	C	C5-C6-N1	5.04	123.52	121.00
36	5	2834	G	C4-N9-C1'	5.04	133.05	126.50
37	7	62	U	C6-N1-C2	5.04	124.02	121.00
1	2	1000	C	C2-N1-C1'	5.03	124.34	118.80
36	5	20	A	OP2-P-O3'	5.03	116.28	105.20
36	5	2935	U	C5-C6-N1	5.03	125.22	122.70
1	2	1520	U	C6-N1-C2	5.03	124.02	121.00
36	1	120	G	N3-C4-C5	-5.03	126.08	128.60
36	1	211	A	O5'-P-OP1	-5.03	101.17	105.70
36	1	1925	U	C5-C6-N1	-5.03	120.19	122.70
36	1	2282	U	N3-C2-O2	-5.03	118.68	122.20
1	6	965	U	N1-C2-O2	5.03	126.32	122.80
36	5	927	C	C5-C6-N1	5.03	123.52	121.00
36	5	1693	C	C6-N1-C2	5.03	122.31	120.30
36	5	2924	U	C5-C6-N1	-5.03	120.19	122.70
36	5	139	G	N9-C4-C5	-5.03	103.39	105.40
36	5	1151	U	C4-C5-C6	5.03	122.72	119.70
36	5	1355	A	P-O3'-C3'	5.03	125.73	119.70
36	5	1630	U	C6-N1-C2	5.03	124.02	121.00
36	1	2125	A	N1-C2-N3	5.03	131.81	129.30
36	5	801	A	O4'-C1'-N9	-5.03	104.18	108.20
36	5	822	G	C8-N9-C4	-5.03	104.39	106.40
36	5	3143	C	C2-N1-C1'	-5.03	113.27	118.80
36	5	3244	A	C8-N9-C4	5.03	107.81	105.80
36	1	315	C	N1-C2-O2	5.02	121.91	118.90
36	1	3319	U	P-O3'-C3'	5.02	125.73	119.70
36	5	207	U	C5-C6-N1	5.02	125.21	122.70
36	1	2371	G	N9-C4-C5	-5.02	103.39	105.40
36	1	2417	U	C6-N1-C2	5.02	124.01	121.00
36	1	2420	C	C5-C6-N1	5.02	123.51	121.00
36	1	2549	G	N3-C4-C5	5.02	131.11	128.60
1	6	755	A	N9-C1'-C2'	-5.02	106.47	112.00
36	5	1201	C	C6-N1-C2	5.02	122.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3218	A	P-O3'-C3'	5.02	125.73	119.70
1	2	1600	A	C4-C5-C6	5.02	119.51	117.00
36	5	344	A	C5-N7-C8	-5.02	101.39	103.90
36	1	3048	A	C8-N9-C4	5.02	107.81	105.80
1	6	443	C	C6-N1-C2	5.02	122.31	120.30
1	6	1243	G	N3-C4-N9	5.02	129.01	126.00
36	5	518	G	C8-N9-C1'	-5.02	120.47	127.00
36	5	2136	C	C6-N1-C2	5.02	122.31	120.30
36	5	2177	G	C8-N9-C4	5.02	108.41	106.40
1	2	814	A	C3'-C2'-C1'	5.02	105.52	101.50
14	C2	125	ASN	C-N-CA	5.02	134.24	121.70
36	1	1761	C	OP1-P-O3'	5.02	116.24	105.20
45	L8	189	LEU	CA-CB-CG	5.02	126.84	115.30
1	6	308	C	C6-N1-C2	5.02	122.31	120.30
36	5	1148	G	N1-C2-N2	-5.02	111.68	116.20
26	D4	50	ALA	C-N-CA	5.02	134.24	121.70
38	8	21	C	C5-C6-N1	-5.02	118.49	121.00
36	1	1306	G	C4-C5-N7	5.01	112.81	110.80
1	6	308	C	C2-N1-C1'	-5.01	113.28	118.80
36	1	3175	U	N3-C2-O2	-5.01	118.69	122.20
15	c3	28	LEU	C-N-CA	5.01	134.23	121.70
36	1	415	G	N3-C4-C5	5.01	131.11	128.60
1	6	553	G	C6-C5-N7	-5.01	127.39	130.40
36	5	1825	G	N3-C4-C5	-5.01	126.09	128.60
36	5	2912	G	N3-C4-N9	-5.01	122.99	126.00
36	1	2704	A	OP2-P-O3'	5.01	116.22	105.20
36	1	2813	A	C8-N9-C4	-5.01	103.80	105.80
1	6	403	G	OP2-P-O3'	5.01	116.22	105.20
1	2	1514	U	N1-C2-O2	5.01	126.30	122.80
38	4	82	U	C2-N3-C4	5.01	130.00	127.00
38	4	114	G	N3-C4-N9	-5.01	123.00	126.00
1	6	1210	C	C5-C6-N1	5.01	123.50	121.00
1	2	1038	U	C2-N1-C1'	-5.00	111.69	117.70
36	1	3036	G	N3-C4-N9	-5.00	123.00	126.00
38	8	83	C	C6-N1-C1'	5.00	126.81	120.80
1	2	987	G	N9-C4-C5	-5.00	103.40	105.40
36	1	2681	U	C5-C6-N1	5.00	125.20	122.70
36	1	3210	A	N9-C4-C5	-5.00	103.80	105.80
36	5	726	G	C6-C5-N7	-5.00	127.40	130.40
1	2	1535	U	OP2-P-O3'	5.00	116.20	105.20
36	1	1094	U	C2-N1-C1'	5.00	123.70	117.70
36	5	1425	U	C5-C6-N1	-5.00	120.20	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2735	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (141) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	28	SER	Peptide
14	C2	102	GLY	Peptide
14	C2	88	LEU	Peptide
14	C2	91	VAL	Peptide
16	C4	38	THR	Peptide
17	C5	12	PHE	Peptide
17	C5	124	THR	Peptide
18	C6	113	ASP	Peptide
18	C6	40	GLU	Peptide
18	C6	58	ASP	Peptide
19	C7	22	PRO	Peptide
20	C8	27	LYS	Peptide
20	C8	83	ALA	Peptide
20	C8	90	ASN	Peptide
24	D2	83	ILE	Peptide
25	D3	44	GLY	Peptide
26	D4	46	GLU	Peptide
26	D4	50	ALA	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
28	D6	10	ARG	Peptide
28	D6	11	ASN	Peptide
29	D7	50	ALA	Peptide
33	E1	101	ALA	Peptide
33	E1	138	ARG	Peptide
33	E1	143	LYS	Peptide
33	E1	146	SER	Peptide
33	E1	147	VAL	Peptide
40	L3	2	SER	Peptide
40	L3	349	LYS	Peptide
42	L5	257	GLU	Peptide
42	L5	258	LYS	Peptide
42	L5	275	THR	Peptide
43	L6	129	GLU	Peptide
43	L6	173	MET	Peptide
45	L8	30	THR	Peptide

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Mol	Chain	Res	Type	Group
45	L8	77	GLN	Peptide
46	L9	49	ASN	Peptide
51	M5	73	ARG	Peptide
52	M6	110	PRO	Peptide
53	M7	157	VAL	Peptide
53	M7	158	ALA	Peptide
56	N0	12	ARG	Peptide
56	N0	133	ALA	Peptide
56	N0	166	LYS	Peptide
56	N0	22	PRO	Peptide
60	N4	80	ARG	Peptide
60	N4	81	PRO	Peptide
62	N6	83	ASP	Peptide
64	N8	30	GLY	Peptide
64	N8	46	ASP	Peptide
65	N9	19	ASN	Peptide
67	O1	6	ASP	Peptide
69	O3	91	ALA	Peptide
71	O5	90	ARG	Peptide
72	O6	26	ILE	Peptide
2	S0	94	GLY	Peptide
3	S1	131	ASP	Peptide
3	S1	205	PHE	Peptide
3	S1	206	PRO	Peptide
3	S1	36	SER	Peptide
4	S2	144	TRP	Peptide
6	S4	193	GLY	Peptide
7	S5	44	ASN	Peptide
7	S5	56	ALA	Peptide
7	S5	65	ARG	Peptide
9	S7	110	GLN	Peptide
9	S7	131	PHE	Peptide
9	S7	31	SER	Peptide
9	S7	64	VAL	Peptide
34	SR	96	THR	Peptide
12	c0	83	PRO	Peptide
14	c2	102	GLY	Peptide
15	c3	29	SER	Peptide
17	c5	129	GLY	Peptide
17	c5	50	THR	Peptide
17	c5	52	LYS	Peptide
17	c5	67	ALA	Peptide

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Mol	Chain	Res	Type	Group
18	c6	40	GLU	Peptide
20	c8	90	ASN	Peptide
22	d0	51	VAL	Peptide
22	d0	70	THR	Peptide
27	d5	85	LYS	Peptide
27	d5	87	GLY	Peptide
32	e0	44	PHE	Peptide
32	e0	51	ASN	Peptide
33	e1	135	HIS	Peptide
33	e1	147	VAL	Peptide
33	e1	83	LYS	Peptide
39	l2	211	HIS	Peptide
39	l2	48	ILE	Peptide
40	l3	346	THR	Peptide
41	l4	300	ARG	Peptide
42	l5	269	SER	Peptide
42	l5	270	LYS	Peptide
43	l6	67	GLY	Peptide
44	l7	226	GLY	Peptide
44	l7	228	SER	Peptide
45	l8	120	LYS	Peptide
45	l8	24	ASN	Peptide
45	l8	25	PRO	Peptide
48	m1	94	ARG	Peptide
49	m3	150	PRO	Peptide
49	m3	74	GLY	Peptide
50	m4	48	GLY	Peptide
51	m5	146	ALA	Peptide
51	m5	69	GLY	Peptide
52	m6	109	PRO	Peptide
56	n0	133	ALA	Peptide
56	n0	170	THR	Peptide
58	n2	51	GLY	Peptide
63	n7	101	PHE	Peptide
63	n7	5	LEU	Peptide
65	n9	19	ASN	Peptide
67	o1	6	ASP	Peptide
67	o1	82	GLU	Peptide
70	o4	81	CYS	Peptide
71	o5	118	ILE	Peptide
72	o6	63	ASN	Peptide
80	p0	92	PRO	Peptide

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Mol	Chain	Res	Type	Group
79	q3	49	ARG	Peptide
79	q3	51	ALA	Peptide
2	s0	94	GLY	Peptide
4	s2	106	ASP	Peptide
4	s2	144	TRP	Peptide
5	s3	221	SER	Peptide
7	s5	100	ASN	Peptide
7	s5	27	THR	Peptide
7	s5	44	ASN	Peptide
7	s5	56	ALA	Peptide
8	s6	164	LYS	Peptide
9	s7	115	SER	Peptide
9	s7	130	VAL	Peptide
9	s7	30	SER	Peptide
9	s7	31	SER	Peptide
9	s7	64	VAL	Peptide
9	s7	9	LEU	Peptide
11	s9	88	GLU	Peptide
11	s9	89	ASP	Peptide
35	sM	51	ARG	Peptide
34	sR	161	ALA	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/206 (99%)	174 (85%)	26 (13%)	4 (2%)	7	39
2	s0	204/206 (99%)	176 (86%)	23 (11%)	5 (2%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S1	212/216 (98%)	162 (76%)	45 (21%)	5 (2%)	6	35
3	s1	214/216 (99%)	195 (91%)	15 (7%)	4 (2%)	8	40
4	S2	215/217 (99%)	194 (90%)	19 (9%)	2 (1%)	17	54
4	s2	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	29	66
5	S3	221/223 (99%)	202 (91%)	15 (7%)	4 (2%)	8	41
5	s3	221/223 (99%)	195 (88%)	18 (8%)	8 (4%)	3	29
6	S4	258/260 (99%)	226 (88%)	30 (12%)	2 (1%)	19	56
6	s4	258/260 (99%)	234 (91%)	21 (8%)	3 (1%)	13	48
7	S5	204/206 (99%)	178 (87%)	21 (10%)	5 (2%)	5	35
7	s5	204/206 (99%)	183 (90%)	18 (9%)	3 (2%)	10	44
8	S6	224/236 (95%)	209 (93%)	9 (4%)	6 (3%)	5	33
8	s6	216/236 (92%)	196 (91%)	17 (8%)	3 (1%)	11	45
9	S7	182/185 (98%)	154 (85%)	20 (11%)	8 (4%)	2	24
9	s7	183/185 (99%)	157 (86%)	23 (13%)	3 (2%)	9	43
10	S8	184/200 (92%)	160 (87%)	23 (12%)	1 (0%)	29	66
10	s8	184/200 (92%)	171 (93%)	11 (6%)	2 (1%)	14	50
11	S9	183/185 (99%)	162 (88%)	20 (11%)	1 (0%)	29	66
11	s9	183/185 (99%)	169 (92%)	14 (8%)	0	100	100
12	C0	90/105 (86%)	77 (86%)	10 (11%)	3 (3%)	4	31
12	c0	90/105 (86%)	65 (72%)	19 (21%)	6 (7%)	1	16
13	C1	140/156 (90%)	128 (91%)	10 (7%)	2 (1%)	11	45
13	c1	144/156 (92%)	130 (90%)	11 (8%)	3 (2%)	7	38
14	C2	118/143 (82%)	87 (74%)	27 (23%)	4 (3%)	3	30
14	c2	122/143 (85%)	89 (73%)	25 (20%)	8 (7%)	1	16
15	C3	148/150 (99%)	134 (90%)	12 (8%)	2 (1%)	11	45
15	c3	148/150 (99%)	129 (87%)	16 (11%)	3 (2%)	7	39
16	C4	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	56
16	c4	126/128 (98%)	111 (88%)	15 (12%)	0	100	100
17	C5	120/141 (85%)	100 (83%)	18 (15%)	2 (2%)	9	42
17	c5	117/141 (83%)	99 (85%)	14 (12%)	4 (3%)	3	30
18	C6	139/141 (99%)	121 (87%)	14 (10%)	4 (3%)	4	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	c6	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	59
19	C7	113/136 (83%)	100 (88%)	12 (11%)	1 (1%)	17	54
19	c7	115/136 (85%)	104 (90%)	10 (9%)	1 (1%)	17	54
20	C8	143/145 (99%)	123 (86%)	17 (12%)	3 (2%)	7	38
20	c8	143/145 (99%)	122 (85%)	18 (13%)	3 (2%)	7	38
21	C9	141/143 (99%)	125 (89%)	16 (11%)	0	100	100
21	c9	141/143 (99%)	128 (91%)	12 (8%)	1 (1%)	22	59
22	D0	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
22	d0	99/107 (92%)	88 (89%)	9 (9%)	2 (2%)	7	39
23	D1	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	6	35
23	d1	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	56
24	d2	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	56
25	D3	142/144 (99%)	119 (84%)	19 (13%)	4 (3%)	5	33
25	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
26	D4	132/134 (98%)	121 (92%)	8 (6%)	3 (2%)	6	36
26	d4	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	10	44
27	D5	68/70 (97%)	52 (76%)	14 (21%)	2 (3%)	4	32
27	d5	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
28	D6	95/97 (98%)	68 (72%)	17 (18%)	10 (10%)	0	6
28	d6	95/97 (98%)	77 (81%)	17 (18%)	1 (1%)	14	50
29	D7	79/81 (98%)	69 (87%)	9 (11%)	1 (1%)	12	47
29	d7	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	12	47
30	D8	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
30	d8	61/63 (97%)	52 (85%)	9 (15%)	0	100	100
31	D9	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
31	d9	51/53 (96%)	45 (88%)	4 (8%)	2 (4%)	3	27
32	E0	58/60 (97%)	51 (88%)	4 (7%)	3 (5%)	2	21
32	e0	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	2	21
33	E1	69/152 (45%)	44 (64%)	19 (28%)	6 (9%)	1	10
33	e1	41/152 (27%)	31 (76%)	8 (20%)	2 (5%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	298 (94%)	18 (6%)	0	100	100
34	sR	311/318 (98%)	291 (94%)	19 (6%)	1 (0%)	41	74
35	SM	131/272 (48%)	116 (88%)	12 (9%)	3 (2%)	6	36
35	sM	113/272 (42%)	94 (83%)	13 (12%)	6 (5%)	2	21
39	L2	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
39	l2	250/252 (99%)	230 (92%)	19 (8%)	1 (0%)	34	69
40	L3	384/386 (100%)	352 (92%)	30 (8%)	2 (0%)	29	66
40	l3	384/386 (100%)	361 (94%)	19 (5%)	4 (1%)	15	51
41	L4	359/361 (99%)	321 (89%)	35 (10%)	3 (1%)	19	56
41	l4	359/361 (99%)	322 (90%)	31 (9%)	6 (2%)	9	42
42	L5	292/296 (99%)	264 (90%)	23 (8%)	5 (2%)	9	42
42	l5	292/296 (99%)	276 (94%)	16 (6%)	0	100	100
43	L6	152/176 (86%)	142 (93%)	6 (4%)	4 (3%)	5	34
43	l6	153/176 (87%)	139 (91%)	11 (7%)	3 (2%)	7	39
44	L7	220/223 (99%)	205 (93%)	15 (7%)	0	100	100
44	l7	221/223 (99%)	210 (95%)	9 (4%)	2 (1%)	17	54
45	L8	231/233 (99%)	202 (87%)	25 (11%)	4 (2%)	9	42
45	l8	229/233 (98%)	201 (88%)	23 (10%)	5 (2%)	6	37
46	L9	189/191 (99%)	173 (92%)	15 (8%)	1 (0%)	29	66
46	l9	188/191 (98%)	176 (94%)	9 (5%)	3 (2%)	9	43
47	M0	204/221 (92%)	193 (95%)	11 (5%)	0	100	100
47	m0	205/221 (93%)	186 (91%)	18 (9%)	1 (0%)	29	66
48	M1	167/169 (99%)	136 (81%)	29 (17%)	2 (1%)	13	48
48	m1	167/169 (99%)	141 (84%)	20 (12%)	6 (4%)	3	29
49	M3	191/194 (98%)	172 (90%)	14 (7%)	5 (3%)	5	34
49	m3	192/194 (99%)	162 (84%)	25 (13%)	5 (3%)	5	34
50	M4	134/137 (98%)	123 (92%)	9 (7%)	2 (2%)	10	44
50	m4	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
51	M5	201/203 (99%)	181 (90%)	18 (9%)	2 (1%)	15	51
51	m5	201/203 (99%)	185 (92%)	13 (6%)	3 (2%)	10	44
52	M6	195/197 (99%)	182 (93%)	11 (6%)	2 (1%)	15	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m6	195/197 (99%)	185 (95%)	10 (5%)	0	100	100
53	M7	181/184 (98%)	168 (93%)	11 (6%)	2 (1%)	14	50
53	m7	171/184 (93%)	159 (93%)	12 (7%)	0	100	100
54	M8	183/185 (99%)	171 (93%)	11 (6%)	1 (0%)	29	66
54	m8	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
55	M9	186/188 (99%)	174 (94%)	10 (5%)	2 (1%)	14	50
55	m9	181/188 (96%)	171 (94%)	9 (5%)	1 (1%)	25	62
56	N0	168/172 (98%)	154 (92%)	12 (7%)	2 (1%)	13	48
56	n0	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
57	N1	157/159 (99%)	143 (91%)	13 (8%)	1 (1%)	25	62
57	n1	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	62
58	N2	96/98 (98%)	86 (90%)	10 (10%)	0	100	100
58	n2	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	15	51
59	N3	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
59	n3	132/135 (98%)	128 (97%)	3 (2%)	1 (1%)	19	56
60	N4	118/155 (76%)	110 (93%)	8 (7%)	0	100	100
60	n4	114/155 (74%)	106 (93%)	8 (7%)	0	100	100
61	N5	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
61	n5	118/121 (98%)	102 (86%)	15 (13%)	1 (1%)	19	56
62	N6	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
62	n6	122/126 (97%)	116 (95%)	4 (3%)	2 (2%)	9	43
63	N7	133/135 (98%)	120 (90%)	11 (8%)	2 (2%)	10	44
63	n7	133/135 (98%)	117 (88%)	14 (10%)	2 (2%)	10	44
64	N8	146/148 (99%)	125 (86%)	16 (11%)	5 (3%)	3	30
64	n8	146/148 (99%)	128 (88%)	16 (11%)	2 (1%)	11	45
65	N9	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
65	n9	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	3	29
66	O0	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
66	o0	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
67	O1	107/109 (98%)	97 (91%)	7 (6%)	3 (3%)	5	33
67	o1	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	O2	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
68	o2	125/127 (98%)	112 (90%)	13 (10%)	0	100	100
69	O3	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
69	o3	104/106 (98%)	93 (89%)	11 (11%)	0	100	100
70	O4	110/112 (98%)	102 (93%)	6 (6%)	2 (2%)	8	41
70	o4	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	17	54
71	O5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	9	42
71	o5	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	17	54
72	O6	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	15	51
72	o6	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	15	51
73	O7	82/84 (98%)	76 (93%)	5 (6%)	1 (1%)	13	48
73	o7	80/84 (95%)	74 (92%)	5 (6%)	1 (1%)	12	47
74	O8	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
74	o8	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12	47
75	O9	47/50 (94%)	43 (92%)	4 (8%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	7	38
76	Q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7	39
76	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	39
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	89 (86%)	14 (14%)	0	100	100
78	q2	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
79	Q3	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
79	q3	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
80	p0	134/312 (43%)	121 (90%)	12 (9%)	1 (1%)	22	59
All	All	22212/23608 (94%)	19993 (90%)	1922 (9%)	297 (1%)	12	47

All (297) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S1	207	LEU
8	S6	153	VAL
9	S7	111	LYS

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Mol	Chain	Res	Type
12	C0	87	VAL
12	C0	88	PRO
18	C6	58	ASP
18	C6	59	LYS
20	C8	28	ILE
20	C8	92	ILE
24	D2	83	ILE
25	D3	97	ASP
33	E1	86	THR
35	SM	167	PRO
43	L6	98	VAL
46	L9	50	ASN
50	M4	8	LYS
52	M6	111	PRO
64	N8	48	TYR
5	s3	220	PRO
6	s4	196	VAL
12	c0	84	GLU
12	c0	88	PRO
13	c1	133	LYS
14	c2	91	VAL
17	c5	126	VAL
18	c6	116	LEU
20	c8	91	ASP
21	c9	34	VAL
24	d2	6	VAL
29	d7	62	ILE
32	e0	4	VAL
43	l6	98	VAL
48	m1	95	ASN
48	m1	115	LYS
51	m5	147	ARG
3	S1	63	GLY
3	S1	206	PRO
5	S3	217	ILE
8	S6	154	ARG
8	S6	173	PRO
8	S6	174	LYS
9	S7	133	THR
13	C1	6	THR
13	C1	7	VAL
14	C2	91	VAL

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Mol	Chain	Res	Type
18	C6	138	PHE
19	C7	88	VAL
28	D6	45	VAL
28	D6	65	PRO
28	D6	75	VAL
28	D6	86	VAL
29	D7	62	ILE
42	L5	261	THR
42	L5	276	LYS
43	L6	5	LYS
45	L8	36	ILE
48	M1	11	ASP
57	N1	124	VAL
67	O1	6	ASP
5	s3	216	PRO
5	s3	217	ILE
5	s3	221	SER
7	s5	58	LEU
8	s6	153	VAL
9	s7	10	SER
9	s7	11	GLN
12	c0	82	LEU
12	c0	87	VAL
13	c1	7	VAL
14	c2	63	VAL
14	c2	84	ASN
14	c2	119	SER
15	c3	66	ILE
17	c5	127	ARG
19	c7	88	VAL
26	d4	52	LYS
35	sM	66	ALA
35	sM	83	LYS
44	l7	229	PHE
59	n3	42	SER
63	n7	18	TYR
65	n9	21	ILE
67	o1	83	GLU
72	o6	63	ASN
74	o8	17	ARG
80	p0	33	VAL
4	S2	146	THR

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Mol	Chain	Res	Type
7	S5	58	LEU
9	S7	112	ARG
9	S7	132	PRO
9	S7	134	GLU
14	C2	89	ILE
14	C2	106	ILE
15	C3	28	LEU
23	D1	82	VAL
26	D4	5	VAL
27	D5	88	ILE
28	D6	46	GLU
33	E1	89	LYS
33	E1	98	VAL
33	E1	137	ASP
33	E1	148	TYR
42	L5	259	LYS
43	L6	6	ALA
56	N0	13	ARG
63	N7	17	ARG
67	O1	5	LYS
70	O4	83	ASN
71	O5	91	ALA
5	s3	45	LYS
5	s3	115	ILE
6	s4	163	ASP
7	s5	184	PHE
13	c1	61	THR
14	c2	106	ILE
14	c2	109	GLU
17	c5	51	SER
17	c5	130	ARG
31	d9	19	ARG
33	e1	136	LYS
33	e1	148	TYR
34	sR	318	ALA
47	m0	175	ASN
62	n6	77	LYS
64	n8	79	TRP
2	S0	4	PRO
2	S0	191	ARG
5	S3	211	PRO
7	S5	51	VAL

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Mol	Chain	Res	Type
7	S5	64	VAL
10	S8	152	ILE
12	C0	60	SER
14	C2	109	GLU
25	D3	96	VAL
26	D4	4	ALA
28	D6	64	LEU
35	SM	87	THR
40	L3	108	GLU
42	L5	20	PHE
49	M3	5	LYS
49	M3	77	LEU
49	M3	166	ALA
52	M6	110	PRO
64	N8	78	LEU
70	O4	82	ALA
3	s1	177	GLN
3	s1	179	SER
4	s2	106	ASP
8	s6	70	PRO
9	s7	74	GLN
22	d0	97	VAL
26	d4	32	ARG
28	d6	61	GLU
31	d9	6	VAL
35	sM	50	ASN
35	sM	65	THR
41	l4	145	ILE
44	l7	191	VAL
45	l8	120	LYS
45	l8	196	ALA
48	m1	10	ARG
49	m3	51	LEU
49	m3	140	SER
58	n2	20	SER
61	n5	77	GLU
64	n8	48	TYR
67	o1	7	VAL
3	S1	62	LYS
4	S2	150	GLN
6	S4	196	VAL
7	S5	31	GLU

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Mol	Chain	Res	Type
7	S5	37	GLN
20	C8	14	ILE
25	D3	3	LYS
32	E0	5	HIS
32	E0	10	ARG
45	L8	31	PRO
49	M3	62	THR
53	M7	156	ALA
53	M7	158	ALA
54	M8	162	ALA
55	M9	95	TRP
56	N0	167	ARG
64	N8	47	LYS
64	N8	117	ARG
2	s0	189	VAL
3	s1	223	PHE
20	c8	92	ILE
22	d0	51	VAL
40	l3	187	SER
41	l4	24	ALA
41	l4	90	PHE
41	l4	329	PRO
43	l6	97	ASN
45	l8	25	PRO
48	m1	11	ASP
48	m1	94	ARG
51	m5	146	ALA
51	m5	183	THR
55	m9	35	ALA
57	n1	136	ARG
62	n6	18	ALA
65	n9	18	ARG
71	o5	40	SER
2	S0	158	VAL
5	S3	212	LYS
6	S4	195	ILE
8	S6	69	LEU
8	S6	70	PRO
9	S7	31	SER
11	S9	134	ILE
16	C4	42	VAL
17	C5	125	PRO

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Mol	Chain	Res	Type
17	C5	126	VAL
18	C6	39	VAL
23	D1	10	GLU
33	E1	84	VAL
40	L3	174	LYS
41	L4	24	ALA
43	L6	140	VAL
45	L8	37	GLY
48	M1	114	ILE
49	M3	47	ALA
51	M5	95	GLN
55	M9	130	ASN
63	N7	103	GLN
64	N8	57	GLY
73	O7	29	VAL
76	Q0	79	GLU
2	s0	103	THR
3	s1	210	ILE
5	s3	144	ALA
12	c0	35	ILE
40	l3	129	ALA
40	l3	385	LYS
41	l4	91	GLY
45	l8	203	VAL
46	l9	144	ILE
49	m3	47	ALA
63	n7	34	LYS
75	o9	11	GLN
9	S7	131	PHE
27	D5	41	ILE
32	E0	47	VAL
41	L4	317	PRO
51	M5	75	VAL
2	s0	158	VAL
12	c0	83	PRO
15	c3	22	ALA
32	e0	60	PRO
35	sM	51	ARG
39	l2	56	ALA
43	l6	10	TYR
45	l8	237	ILE
49	m3	48	PRO

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Mol	Chain	Res	Type
3	S1	210	ILE
71	O5	4	VAL
8	s6	69	LEU
14	c2	66	VAL
32	e0	47	VAL
40	l3	188	ILE
48	m1	114	ILE
76	q0	78	ILE
2	S0	103	THR
26	D4	35	VAL
28	D6	36	ILE
28	D6	84	VAL
35	SM	53	ARG
41	L4	131	VAL
45	L8	157	VAL
67	O1	7	VAL
5	s3	91	VAL
6	s4	90	ILE
10	s8	101	ILE
5	S3	222	VAL
9	S7	98	ILE
28	D6	19	LYS
28	D6	58	VAL
50	M4	6	ILE
72	O6	3	VAL
10	s8	78	ILE
14	c2	115	VAL
15	c3	60	VAL
20	c8	14	ILE
35	sM	43	ASP
41	l4	166	VAL
49	m3	60	ALA
70	o4	89	ILE
15	C3	22	ALA
42	L5	125	VAL
2	s0	10	THR
2	s0	194	PRO
7	s5	29	ILE
46	l9	79	ILE
46	l9	167	VAL
25	D3	64	PRO
73	o7	40	PRO

5.3.2 Protein sidechains [i](#)

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	164/173 (95%)	131 (80%)	33 (20%)	1	8
2	s0	165/173 (95%)	135 (82%)	30 (18%)	1	11
3	S1	191/192 (100%)	148 (78%)	43 (22%)	1	6
3	s1	192/192 (100%)	158 (82%)	34 (18%)	2	12
4	S2	176/176 (100%)	135 (77%)	41 (23%)	1	6
4	s2	176/176 (100%)	141 (80%)	35 (20%)	1	8
5	S3	182/182 (100%)	145 (80%)	37 (20%)	1	8
5	s3	182/182 (100%)	142 (78%)	40 (22%)	1	6
6	S4	221/221 (100%)	182 (82%)	39 (18%)	2	12
6	s4	221/221 (100%)	189 (86%)	32 (14%)	3	18
7	S5	173/173 (100%)	140 (81%)	33 (19%)	1	9
7	s5	173/173 (100%)	142 (82%)	31 (18%)	2	11
8	S6	188/201 (94%)	153 (81%)	35 (19%)	1	10
8	s6	187/201 (93%)	157 (84%)	30 (16%)	2	15
9	S7	165/165 (100%)	133 (81%)	32 (19%)	1	9
9	s7	165/165 (100%)	129 (78%)	36 (22%)	1	6
10	S8	150/161 (93%)	126 (84%)	24 (16%)	2	15
10	s8	150/161 (93%)	123 (82%)	27 (18%)	1	11
11	S9	158/158 (100%)	125 (79%)	33 (21%)	1	7
11	s9	158/158 (100%)	137 (87%)	21 (13%)	4	22
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2	13
12	c0	73/98 (74%)	60 (82%)	13 (18%)	2	12
13	C1	127/137 (93%)	113 (89%)	14 (11%)	6	29
13	c1	129/137 (94%)	105 (81%)	24 (19%)	1	10
14	C2	88/119 (74%)	65 (74%)	23 (26%)	0	4
14	c2	88/119 (74%)	62 (70%)	26 (30%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	C3	127/127 (100%)	107 (84%)	20 (16%)	2	16
15	c3	127/127 (100%)	100 (79%)	27 (21%)	1	7
16	C4	81/97 (84%)	59 (73%)	22 (27%)	0	3
16	c4	97/97 (100%)	76 (78%)	21 (22%)	1	7
17	C5	101/117 (86%)	81 (80%)	20 (20%)	1	8
17	c5	98/117 (84%)	85 (87%)	13 (13%)	4	22
18	C6	117/117 (100%)	92 (79%)	25 (21%)	1	7
18	c6	117/117 (100%)	97 (83%)	20 (17%)	2	13
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	6
19	c7	92/124 (74%)	73 (79%)	19 (21%)	1	7
20	C8	128/128 (100%)	97 (76%)	31 (24%)	0	5
20	c8	128/128 (100%)	103 (80%)	25 (20%)	1	9
21	C9	115/115 (100%)	91 (79%)	24 (21%)	1	7
21	c9	115/115 (100%)	92 (80%)	23 (20%)	1	8
22	D0	98/100 (98%)	78 (80%)	20 (20%)	1	8
22	d0	94/100 (94%)	76 (81%)	18 (19%)	1	9
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	8
23	d1	74/74 (100%)	60 (81%)	14 (19%)	1	9
24	D2	110/110 (100%)	92 (84%)	18 (16%)	2	15
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3	18
25	D3	119/119 (100%)	96 (81%)	23 (19%)	1	9
25	d3	119/119 (100%)	108 (91%)	11 (9%)	9	36
26	D4	112/112 (100%)	89 (80%)	23 (20%)	1	7
26	d4	112/112 (100%)	89 (80%)	23 (20%)	1	7
27	D5	61/61 (100%)	40 (66%)	21 (34%)	0	1
27	d5	61/61 (100%)	54 (88%)	7 (12%)	5	27
28	D6	83/83 (100%)	59 (71%)	24 (29%)	0	2
28	d6	83/83 (100%)	71 (86%)	12 (14%)	3	18
29	D7	70/70 (100%)	60 (86%)	10 (14%)	3	19
29	d7	70/70 (100%)	57 (81%)	13 (19%)	1	10
30	D8	56/56 (100%)	40 (71%)	16 (29%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d8	56/56 (100%)	38 (68%)	18 (32%)	0	1
31	D9	47/47 (100%)	37 (79%)	10 (21%)	1	7
31	d9	47/47 (100%)	39 (83%)	8 (17%)	2	13
32	E0	51/51 (100%)	42 (82%)	9 (18%)	2	12
32	e0	51/51 (100%)	35 (69%)	16 (31%)	0	1
33	E1	62/135 (46%)	41 (66%)	21 (34%)	0	1
33	e1	39/135 (29%)	30 (77%)	9 (23%)	1	6
34	SR	259/260 (100%)	229 (88%)	30 (12%)	5	27
34	sR	255/260 (98%)	230 (90%)	25 (10%)	8	33
35	SM	97/227 (43%)	77 (79%)	20 (21%)	1	7
35	sM	93/227 (41%)	70 (75%)	23 (25%)	0	5
39	L2	193/194 (100%)	160 (83%)	33 (17%)	2	13
39	l2	192/194 (99%)	148 (77%)	44 (23%)	1	6
40	L3	320/322 (99%)	260 (81%)	60 (19%)	1	10
40	l3	318/322 (99%)	246 (77%)	72 (23%)	1	6
41	L4	288/288 (100%)	242 (84%)	46 (16%)	2	15
41	l4	288/288 (100%)	232 (81%)	56 (19%)	1	9
42	L5	242/244 (99%)	194 (80%)	48 (20%)	1	8
42	l5	243/244 (100%)	200 (82%)	43 (18%)	2	12
43	L6	134/153 (88%)	108 (81%)	26 (19%)	1	9
43	l6	135/153 (88%)	113 (84%)	22 (16%)	2	15
44	L7	186/187 (100%)	166 (89%)	20 (11%)	6	29
44	l7	187/187 (100%)	161 (86%)	26 (14%)	3	20
45	L8	187/191 (98%)	154 (82%)	33 (18%)	2	12
45	l8	177/191 (93%)	143 (81%)	34 (19%)	1	9
46	L9	171/171 (100%)	128 (75%)	43 (25%)	0	4
46	l9	170/171 (99%)	129 (76%)	41 (24%)	0	5
47	M0	177/187 (95%)	153 (86%)	24 (14%)	3	21
47	m0	177/187 (95%)	140 (79%)	37 (21%)	1	7
48	M1	147/147 (100%)	121 (82%)	26 (18%)	2	12
48	m1	147/147 (100%)	117 (80%)	30 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	M3	154/154 (100%)	119 (77%)	35 (23%)	1	6
49	m3	154/154 (100%)	125 (81%)	29 (19%)	1	10
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1	9
50	m4	108/108 (100%)	87 (81%)	21 (19%)	1	9
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	13
51	m5	175/175 (100%)	150 (86%)	25 (14%)	3	19
52	M6	160/160 (100%)	134 (84%)	26 (16%)	2	15
52	m6	160/160 (100%)	124 (78%)	36 (22%)	1	6
53	M7	140/146 (96%)	102 (73%)	38 (27%)	0	3
53	m7	139/146 (95%)	103 (74%)	36 (26%)	0	4
54	M8	150/150 (100%)	125 (83%)	25 (17%)	2	14
54	m8	150/150 (100%)	127 (85%)	23 (15%)	2	17
55	M9	153/153 (100%)	116 (76%)	37 (24%)	0	5
55	m9	149/153 (97%)	112 (75%)	37 (25%)	0	5
56	N0	155/156 (99%)	126 (81%)	29 (19%)	1	10
56	n0	156/156 (100%)	126 (81%)	30 (19%)	1	9
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	7
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	8
58	N2	85/85 (100%)	73 (86%)	12 (14%)	3	20
58	n2	85/85 (100%)	70 (82%)	15 (18%)	2	12
59	N3	103/103 (100%)	89 (86%)	14 (14%)	3	21
59	n3	103/103 (100%)	88 (85%)	15 (15%)	3	18
60	N4	85/129 (66%)	73 (86%)	12 (14%)	3	20
60	n4	97/129 (75%)	85 (88%)	12 (12%)	4	24
61	N5	104/105 (99%)	82 (79%)	22 (21%)	1	7
61	n5	104/105 (99%)	84 (81%)	20 (19%)	1	9
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1	8
62	n6	107/109 (98%)	85 (79%)	22 (21%)	1	7
63	N7	115/115 (100%)	93 (81%)	22 (19%)	1	9
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1	7
64	N8	118/118 (100%)	96 (81%)	22 (19%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	8
65	N9	46/46 (100%)	39 (85%)	7 (15%)	3	17
65	n9	46/46 (100%)	40 (87%)	6 (13%)	4	22
66	O0	81/84 (96%)	61 (75%)	20 (25%)	0	5
66	o0	84/84 (100%)	71 (84%)	13 (16%)	2	17
67	O1	92/96 (96%)	74 (80%)	18 (20%)	1	9
67	o1	94/96 (98%)	75 (80%)	19 (20%)	1	8
68	O2	109/109 (100%)	92 (84%)	17 (16%)	2	17
68	o2	109/109 (100%)	91 (84%)	18 (16%)	2	14
69	O3	90/90 (100%)	76 (84%)	14 (16%)	2	17
69	o3	90/90 (100%)	72 (80%)	18 (20%)	1	8
70	O4	95/95 (100%)	73 (77%)	22 (23%)	1	6
70	o4	95/95 (100%)	80 (84%)	15 (16%)	2	16
71	O5	104/104 (100%)	85 (82%)	19 (18%)	1	10
71	o5	103/104 (99%)	84 (82%)	19 (18%)	1	10
72	O6	81/81 (100%)	58 (72%)	23 (28%)	0	2
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0	3
73	O7	69/69 (100%)	51 (74%)	18 (26%)	0	4
73	o7	67/69 (97%)	55 (82%)	12 (18%)	2	11
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	6
74	o8	67/68 (98%)	54 (81%)	13 (19%)	1	9
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	8
75	o9	45/45 (100%)	38 (84%)	7 (16%)	2	17
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	7
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1	9
77	Q1	23/23 (100%)	20 (87%)	3 (13%)	4	22
77	q1	23/23 (100%)	13 (56%)	10 (44%)	0	0
78	Q2	90/90 (100%)	69 (77%)	21 (23%)	1	6
78	q2	90/90 (100%)	77 (86%)	13 (14%)	3	19
79	Q3	71/71 (100%)	58 (82%)	13 (18%)	1	10
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
80	p0	105/254 (41%)	91 (87%)	14 (13%)	4 22
All	All	18730/19834 (94%)	15159 (81%)	3571 (19%)	1 9

All (3571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	7	PHE
2	S0	8	ASP
2	S0	27	ARG
2	S0	32	HIS
2	S0	33	GLN
2	S0	37	VAL
2	S0	49	ASN
2	S0	50	VAL
2	S0	52	LYS
2	S0	62	ARG
2	S0	76	ILE
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	101	ARG
2	S0	103	THR
2	S0	111	ILE
2	S0	114	SER
2	S0	117	GLU
2	S0	119	ARG
2	S0	123	VAL
2	S0	131	GLN
2	S0	139	VAL
2	S0	154	GLU
2	S0	157	ASP
2	S0	165	ARG
2	S0	170	ILE
2	S0	172	LEU
2	S0	177	LEU
2	S0	184	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	200	ASP
3	S1	21	VAL
3	S1	22	ASP
3	S1	29	TRP

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Mol	Chain	Res	Type
3	S1	38	PHE
3	S1	42	ASN
3	S1	46	THR
3	S1	47	LEU
3	S1	55	LYS
3	S1	61	LEU
3	S1	66	VAL
3	S1	70	LEU
3	S1	74	GLN
3	S1	76	SER
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	85	LYS
3	S1	91	VAL
3	S1	96	LEU
3	S1	97	LEU
3	S1	105	PHE
3	S1	108	ASP
3	S1	111	ARG
3	S1	112	SER
3	S1	115	ARG
3	S1	117	TRP
3	S1	131	ASP
3	S1	135	LEU
3	S1	148	ASN
3	S1	149	GLN
3	S1	154	SER
3	S1	177	GLN
3	S1	180	THR
3	S1	181	LEU
3	S1	183	GLN
3	S1	184	LEU
3	S1	193	ILE
3	S1	202	LYS
3	S1	214	LYS
3	S1	218	LEU
3	S1	220	GLN
3	S1	222	LYS
3	S1	223	PHE
4	S2	41	LEU
4	S2	53	ILE

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Mol	Chain	Res	Type
4	S2	55	GLU
4	S2	58	LEU
4	S2	64	LYS
4	S2	69	ILE
4	S2	72	LEU
4	S2	73	LEU
4	S2	77	GLN
4	S2	81	MET
4	S2	91	ARG
4	S2	94	GLN
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	117	THR
4	S2	119	LYS
4	S2	130	ILE
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	148	LEU
4	S2	156	THR
4	S2	159	THR
4	S2	179	VAL
4	S2	195	ASP
4	S2	200	SER
4	S2	206	THR
4	S2	208	GLU
4	S2	218	ILE
4	S2	221	THR
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	237	VAL
4	S2	240	LEU
4	S2	245	ASP
4	S2	246	GLU
5	S3	4	LEU
5	S3	7	LYS
5	S3	23	GLU

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Mol	Chain	Res	Type
5	S3	57	ASP
5	S3	65	ARG
5	S3	66	ILE
5	S3	76	ARG
5	S3	84	ILE
5	S3	89	GLU
5	S3	92	GLN
5	S3	93	ASP
5	S3	94	ARG
5	S3	103	GLU
5	S3	104	SER
5	S3	105	MET
5	S3	113	LEU
5	S3	115	ILE
5	S3	117	ARG
5	S3	127	MET
5	S3	134	CYS
5	S3	141	LYS
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	158	ILE
5	S3	164	VAL
5	S3	170	THR
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	178	ARG
5	S3	182	LEU
5	S3	190	ARG
5	S3	195	SER
5	S3	197	THR
5	S3	212	LYS
5	S3	217	ILE
6	S4	6	LYS
6	S4	7	LYS
6	S4	9	LEU
6	S4	23	LEU
6	S4	37	LYS
6	S4	38	LEU
6	S4	39	ARG
6	S4	40	GLU

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Mol	Chain	Res	Type
6	S4	57	ASN
6	S4	77	ARG
6	S4	78	THR
6	S4	92	LEU
6	S4	116	ASP
6	S4	129	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	140	VAL
6	S4	146	THR
6	S4	160	VAL
6	S4	164	LEU
6	S4	176	ASP
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	192	ILE
6	S4	197	HIS
6	S4	206	ASP
6	S4	211	LYS
6	S4	215	ASP
6	S4	218	PHE
6	S4	222	LEU
6	S4	227	VAL
6	S4	236	ILE
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	247	SER
6	S4	256	ARG
6	S4	259	GLN
7	S5	23	VAL
7	S5	24	VAL
7	S5	25	LEU
7	S5	32	GLU
7	S5	41	LYS
7	S5	43	PHE
7	S5	46	TRP
7	S5	53	VAL
7	S5	63	GLN
7	S5	65	ARG
7	S5	76	ARG

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Mol	Chain	Res	Type
7	S5	89	ILE
7	S5	90	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	96	SER
7	S5	112	ARG
7	S5	119	ASP
7	S5	123	VAL
7	S5	127	GLN
7	S5	146	THR
7	S5	147	THR
7	S5	156	ARG
7	S5	157	ARG
7	S5	161	ASP
7	S5	186	ASN
7	S5	194	LEU
7	S5	203	LYS
7	S5	209	TYR
7	S5	216	GLU
7	S5	219	ARG
7	S5	223	SER
7	S5	225	ARG
8	S6	7	TYR
8	S6	12	SER
8	S6	13	GLN
8	S6	21	GLU
8	S6	25	ARG
8	S6	45	PHE
8	S6	58	LYS
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	81	VAL
8	S6	82	SER
8	S6	97	VAL
8	S6	98	ARG
8	S6	105	ASP
8	S6	109	LEU
8	S6	120	GLU
8	S6	124	LEU
8	S6	126	ASP
8	S6	127	THR

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Mol	Chain	Res	Type
8	S6	129	VAL
8	S6	140	ASN
8	S6	143	LYS
8	S6	151	ASP
8	S6	154	ARG
8	S6	155	ASP
8	S6	157	VAL
8	S6	158	ILE
8	S6	175	ILE
8	S6	176	GLN
8	S6	177	ARG
8	S6	178	LEU
8	S6	211	LEU
8	S6	212	LEU
8	S6	223	LYS
9	S7	9	LEU
9	S7	28	GLU
9	S7	29	ASN
9	S7	37	GLU
9	S7	38	LEU
9	S7	46	ILE
9	S7	55	LYS
9	S7	60	ILE
9	S7	64	VAL
9	S7	70	PHE
9	S7	77	LEU
9	S7	80	GLU
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	103	SER
9	S7	106	SER
9	S7	110	GLN
9	S7	114	ARG
9	S7	116	ARG
9	S7	117	THR
9	S7	126	LEU
9	S7	131	PHE
9	S7	139	ARG
9	S7	143	LEU
9	S7	144	VAL
9	S7	159	VAL

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Mol	Chain	Res	Type
9	S7	163	ASP
9	S7	168	SER
9	S7	174	ASN
9	S7	181	ILE
9	S7	185	ILE
10	S8	5	ARG
10	S8	8	ARG
10	S8	14	THR
10	S8	20	GLN
10	S8	21	PHE
10	S8	28	GLU
10	S8	29	LEU
10	S8	36	THR
10	S8	49	ARG
10	S8	56	ARG
10	S8	58	LEU
10	S8	72	ILE
10	S8	87	ASN
10	S8	123	LYS
10	S8	137	LYS
10	S8	138	ASN
10	S8	140	GLU
10	S8	151	LYS
10	S8	152	ILE
10	S8	164	ARG
10	S8	176	SER
10	S8	184	LEU
10	S8	196	LEU
10	S8	199	LYS
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	22	SER
11	S9	28	LEU
11	S9	39	LYS
11	S9	46	SER
11	S9	49	LEU
11	S9	54	ARG
11	S9	60	LEU
11	S9	79	ARG
11	S9	89	ASP

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Mol	Chain	Res	Type
11	S9	91	LYS
11	S9	92	LYS
11	S9	93	LEU
11	S9	96	VAL
11	S9	97	LEU
11	S9	99	LEU
11	S9	105	LEU
11	S9	109	LEU
11	S9	110	GLN
11	S9	118	LEU
11	S9	126	ARG
11	S9	130	THR
11	S9	133	HIS
11	S9	134	ILE
11	S9	138	LYS
11	S9	141	VAL
11	S9	149	ARG
11	S9	161	THR
11	S9	171	ARG
11	S9	182	GLU
12	C0	1	MET
12	C0	7	ASP
12	C0	22	VAL
12	C0	28	ASN
12	C0	32	HIS
12	C0	46	LEU
12	C0	47	GLN
12	C0	55	VAL
12	C0	56	LYS
12	C0	76	LEU
12	C0	78	GLU
12	C0	81	ASN
12	C0	82	LEU
13	C1	21	ASN
13	C1	29	LYS
13	C1	40	LEU
13	C1	67	ARG
13	C1	69	LYS
13	C1	72	THR
13	C1	74	THR
13	C1	83	THR
13	C1	99	ARG

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Mol	Chain	Res	Type
13	C1	123	VAL
13	C1	131	ILE
13	C1	132	SER
13	C1	138	ASN
13	C1	140	VAL
14	C2	26	ASP
14	C2	28	LEU
14	C2	33	ARG
14	C2	36	LEU
14	C2	43	ARG
14	C2	50	LYS
14	C2	58	LEU
14	C2	59	LEU
14	C2	61	VAL
14	C2	66	VAL
14	C2	71	ILE
14	C2	83	GLU
14	C2	85	LYS
14	C2	88	LEU
14	C2	89	ILE
14	C2	93	ASP
14	C2	103	LEU
14	C2	121	VAL
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	138	GLU
14	C2	139	HIS
15	C3	3	ARG
15	C3	9	LYS
15	C3	12	SER
15	C3	16	ILE
15	C3	27	LYS
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	55	ARG
15	C3	56	ASP
15	C3	58	HIS
15	C3	64	ARG
15	C3	67	THR
15	C3	76	LYS

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Mol	Chain	Res	Type
15	C3	88	LEU
15	C3	102	LEU
15	C3	115	LEU
15	C3	125	LEU
15	C3	143	SER
15	C3	150	VAL
16	C4	13	VAL
16	C4	14	PHE
16	C4	26	THR
16	C4	28	VAL
16	C4	29	HIS
16	C4	38	THR
16	C4	39	ILE
16	C4	43	THR
16	C4	51	ASP
16	C4	79	VAL
16	C4	89	THR
16	C4	92	LYS
16	C4	93	THR
16	C4	103	ARG
16	C4	105	LEU
16	C4	108	SER
16	C4	114	ARG
16	C4	124	ASP
16	C4	129	LYS
16	C4	133	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	22	LEU
17	C5	26	LEU
17	C5	27	GLU
17	C5	31	GLU
17	C5	34	VAL
17	C5	35	LYS
17	C5	36	LEU
17	C5	40	ARG
17	C5	44	ARG
17	C5	50	THR
17	C5	65	LEU
17	C5	69	GLU
17	C5	70	ASN
17	C5	78	THR

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Mol	Chain	Res	Type
17	C5	86	VAL
17	C5	89	MET
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
17	C5	128	HIS
18	C6	4	VAL
18	C6	13	LYS
18	C6	14	LYS
18	C6	15	SER
18	C6	26	LYS
18	C6	43	ILE
18	C6	44	LEU
18	C6	47	LYS
18	C6	53	LEU
18	C6	54	LEU
18	C6	58	ASP
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	74	HIS
18	C6	76	SER
18	C6	98	ASP
18	C6	101	SER
18	C6	123	ARG
18	C6	128	LYS
18	C6	136	SER
18	C6	137	ARG
18	C6	138	PHE
18	C6	141	SER
18	C6	143	ARG
19	C7	3	ARG
19	C7	5	ARG
19	C7	6	THR
19	C7	8	THR
19	C7	19	ARG
19	C7	29	GLN
19	C7	38	ILE
19	C7	46	LEU
19	C7	49	LYS
19	C7	62	GLN
19	C7	69	ILE

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Mol	Chain	Res	Type
19	C7	70	SER
19	C7	71	PHE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	12	GLN
20	C8	13	HIS
20	C8	14	ILE
20	C8	15	LEU
20	C8	16	ARG
20	C8	17	LEU
20	C8	28	ILE
20	C8	38	VAL
20	C8	54	LEU
20	C8	60	GLU
20	C8	71	GLN
20	C8	74	GLN
20	C8	85	PHE
20	C8	89	GLN
20	C8	92	ILE
20	C8	93	THR
20	C8	108	LYS
20	C8	110	ARG
20	C8	116	LEU
20	C8	119	ILE
20	C8	120	ARG
20	C8	132	ARG
20	C8	133	VAL
20	C8	136	GLN
20	C8	138	THR
20	C8	140	THR
20	C8	143	ARG
21	C9	4	VAL

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Mol	Chain	Res	Type
21	C9	13	ASP
21	C9	22	LEU
21	C9	27	LYS
21	C9	28	LEU
21	C9	33	TYR
21	C9	35	ASP
21	C9	55	TYR
21	C9	57	ARG
21	C9	63	ARG
21	C9	67	MET
21	C9	75	LYS
21	C9	84	LYS
21	C9	89	ARG
21	C9	94	ILE
21	C9	97	SER
21	C9	111	ILE
21	C9	125	SER
21	C9	126	GLU
21	C9	129	GLN
21	C9	130	ARG
21	C9	131	ASP
21	C9	140	LEU
21	C9	144	GLU
22	D0	17	GLN
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	30	LYS
22	D0	31	VAL
22	D0	34	LEU
22	D0	42	VAL
22	D0	47	GLN
22	D0	48	HIS
22	D0	51	VAL
22	D0	60	THR
22	D0	61	LYS
22	D0	66	SER
22	D0	70	THR
22	D0	74	GLU
22	D0	81	THR
22	D0	89	ARG
22	D0	103	ILE

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Mol	Chain	Res	Type
22	D0	108	ILE
23	D1	3	ASN
23	D1	5	LYS
23	D1	10	GLU
23	D1	18	SER
23	D1	32	VAL
23	D1	33	GLN
23	D1	41	GLU
23	D1	49	GLU
23	D1	52	THR
23	D1	60	ARG
23	D1	62	ARG
23	D1	69	LEU
23	D1	76	ASP
23	D1	78	LEU
23	D1	80	LYS
24	D2	7	LEU
24	D2	20	THR
24	D2	23	ARG
24	D2	24	GLN
24	D2	27	ILE
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	76	SER
24	D2	83	ILE
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	111	MET
24	D2	121	VAL
24	D2	122	SER
25	D3	7	ARG
25	D3	9	LEU
25	D3	18	HIS
25	D3	19	ARG
25	D3	28	ASN
25	D3	46	SER
25	D3	79	ASN
25	D3	82	LYS

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Mol	Chain	Res	Type
25	D3	83	VAL
25	D3	94	ASN
25	D3	100	ASP
25	D3	107	PHE
25	D3	110	LYS
25	D3	114	LYS
25	D3	117	ILE
25	D3	126	LYS
25	D3	131	SER
25	D3	132	LEU
25	D3	133	LEU
25	D3	138	GLU
25	D3	140	LYS
25	D3	144	ARG
25	D3	145	SER
26	D4	10	ARG
26	D4	17	LEU
26	D4	21	LYS
26	D4	32	ARG
26	D4	34	ASN
26	D4	35	VAL
26	D4	46	GLU
26	D4	47	VAL
26	D4	49	LYS
26	D4	51	GLU
26	D4	57	VAL
26	D4	61	ARG
26	D4	88	THR
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	121	THR
26	D4	124	ARG
26	D4	128	LYS
26	D4	129	VAL
26	D4	131	ARG
26	D4	132	ARG
26	D4	135	ASP
27	D5	38	HIS
27	D5	41	ILE
27	D5	42	LEU
27	D5	43	ASP

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Mol	Chain	Res	Type
27	D5	49	ARG
27	D5	58	ARG
27	D5	59	TYR
27	D5	67	ASP
27	D5	68	ARG
27	D5	69	LEU
27	D5	70	LYS
27	D5	71	ILE
27	D5	75	LEU
27	D5	85	LYS
27	D5	88	ILE
27	D5	92	ILE
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
27	D5	103	ARG
27	D5	105	THR
28	D6	5	ARG
28	D6	12	LYS
28	D6	36	ILE
28	D6	38	ARG
28	D6	39	MET
28	D6	41	ILE
28	D6	44	ILE
28	D6	45	VAL
28	D6	52	ASP
28	D6	58	VAL
28	D6	61	GLU
28	D6	66	LYS
28	D6	67	THR
28	D6	69	ASN
28	D6	70	LYS
28	D6	71	LEU
28	D6	74	CYS
28	D6	76	SER
28	D6	79	ILE
28	D6	82	ARG
28	D6	84	VAL
28	D6	87	ARG
28	D6	90	GLU
28	D6	91	ASP
29	D7	3	LEU

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Mol	Chain	Res	Type
29	D7	20	LYS
29	D7	30	SER
29	D7	33	LEU
29	D7	34	ASP
29	D7	57	GLU
29	D7	60	SER
29	D7	75	GLU
29	D7	77	THR
29	D7	78	SER
30	D8	14	LYS
30	D8	15	VAL
30	D8	18	ARG
30	D8	19	THR
30	D8	30	VAL
30	D8	32	PHE
30	D8	33	LEU
30	D8	36	THR
30	D8	39	THR
30	D8	44	VAL
30	D8	49	ARG
30	D8	56	LEU
30	D8	58	GLU
30	D8	62	GLU
30	D8	64	ARG
30	D8	65	ARG
31	D9	6	VAL
31	D9	8	PHE
31	D9	12	ARG
31	D9	19	ARG
31	D9	22	ARG
31	D9	25	SER
31	D9	28	THR
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
32	E0	8	LEU
32	E0	20	LYS
32	E0	26	LYS
32	E0	28	LYS
32	E0	42	ARG
32	E0	43	ARG
32	E0	45	VAL

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Mol	Chain	Res	Type
32	E0	47	VAL
32	E0	56	MET
33	E1	84	VAL
33	E1	85	TYR
33	E1	86	THR
33	E1	89	LYS
33	E1	90	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	98	VAL
33	E1	107	LYS
33	E1	111	GLU
33	E1	113	LYS
33	E1	119	ARG
33	E1	120	GLU
33	E1	130	VAL
33	E1	138	ARG
33	E1	140	TYR
33	E1	147	VAL
33	E1	148	TYR
33	E1	149	LYS
33	E1	151	ASN
34	SR	4	ASN
34	SR	6	VAL
34	SR	9	LEU
34	SR	14	GLU
34	SR	17	ASN
34	SR	29	GLN
34	SR	44	SER
34	SR	46	LYS
34	SR	52	GLN
34	SR	59	ARG
34	SR	64	HIS
34	SR	76	ASP
34	SR	106	HIS
34	SR	117	LYS
34	SR	136	ILE
34	SR	141	LEU
34	SR	149	ASP
34	SR	153	GLN
34	SR	159	ASN

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Mol	Chain	Res	Type
34	SR	165	ASP
34	SR	184	ASN
34	SR	185	GLN
34	SR	195	HIS
34	SR	202	LEU
34	SR	207	ASP
34	SR	238	ASP
34	SR	266	ASP
34	SR	268	GLN
34	SR	292	LEU
34	SR	317	THR
35	SM	33	LYS
35	SM	34	LYS
35	SM	43	ASP
35	SM	48	ARG
35	SM	51	ARG
35	SM	64	LYS
35	SM	68	ARG
35	SM	69	ARG
35	SM	72	ARG
35	SM	74	LYS
35	SM	76	VAL
35	SM	77	THR
35	SM	78	ASP
35	SM	79	SER
35	SM	83	LYS
35	SM	95	SER
35	SM	100	THR
35	SM	103	LYS
35	SM	105	LYS
35	SM	116	GLU
39	L2	14	SER
39	L2	20	THR
39	L2	23	ARG
39	L2	37	ARG
39	L2	44	ILE
39	L2	45	VAL
39	L2	50	HIS
39	L2	62	VAL
39	L2	72	ARG
39	L2	74	GLU
39	L2	101	VAL

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Mol	Chain	Res	Type
39	L2	104	LEU
39	L2	109	GLU
39	L2	113	VAL
39	L2	116	VAL
39	L2	119	LYS
39	L2	143	GLU
39	L2	152	SER
39	L2	157	VAL
39	L2	165	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	191	LEU
39	L2	193	ARG
39	L2	199	THR
39	L2	202	VAL
39	L2	204	MET
39	L2	225	ILE
39	L2	238	ILE
39	L2	241	ARG
39	L2	243	THR
39	L2	246	LEU
39	L2	252	THR
40	L3	4	ARG
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	20	LYS
40	L3	25	ILE
40	L3	37	ARG
40	L3	41	VAL
40	L3	44	THR
40	L3	47	LEU
40	L3	55	THR
40	L3	70	ARG
40	L3	81	THR
40	L3	85	VAL
40	L3	94	GLU
40	L3	95	THR
40	L3	101	SER
40	L3	102	LEU
40	L3	103	THR
40	L3	110	LEU

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Mol	Chain	Res	Type
40	L3	112	ASP
40	L3	114	VAL
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	156	SER
40	L3	167	ARG
40	L3	169	THR
40	L3	173	GLN
40	L3	187	SER
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	202	THR
40	L3	206	ASP
40	L3	210	GLU
40	L3	221	THR
40	L3	229	VAL
40	L3	232	ARG
40	L3	236	LYS
40	L3	241	LYS
40	L3	246	LEU
40	L3	252	ILE
40	L3	260	VAL
40	L3	261	MET
40	L3	277	SER
40	L3	291	GLU
40	L3	308	MET
40	L3	319	ASN
40	L3	320	ASP
40	L3	324	VAL
40	L3	328	ILE
40	L3	332	ARG
40	L3	338	LEU
40	L3	343	TYR
40	L3	344	THR
40	L3	347	SER
40	L3	367	LYS
40	L3	372	THR
40	L3	387	LEU
41	L4	33	ASP
41	L4	37	THR

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Mol	Chain	Res	Type
41	L4	47	ARG
41	L4	60	THR
41	L4	69	ARG
41	L4	73	ARG
41	L4	76	ARG
41	L4	93	MET
41	L4	112	LYS
41	L4	120	TYR
41	L4	124	SER
41	L4	133	SER
41	L4	138	ARG
41	L4	141	ARG
41	L4	148	ILE
41	L4	150	LEU
41	L4	156	LEU
41	L4	158	SER
41	L4	161	LYS
41	L4	170	LYS
41	L4	177	ASP
41	L4	179	LEU
41	L4	187	LEU
41	L4	194	TYR
41	L4	201	GLN
41	L4	203	ARG
41	L4	206	LEU
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	232	SER
41	L4	246	ARG
41	L4	258	LEU
41	L4	259	ASP
41	L4	261	VAL
41	L4	283	THR
41	L4	287	THR
41	L4	306	THR
41	L4	307	GLN
41	L4	310	THR
41	L4	313	LEU
41	L4	323	VAL
41	L4	327	LEU
41	L4	332	LYS

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Mol	Chain	Res	Type
41	L4	338	LYS
41	L4	349	THR
42	L5	8	LYS
42	L5	10	SER
42	L5	13	SER
42	L5	14	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	34	LYS
42	L5	35	ARG
42	L5	41	LYS
42	L5	62	CYS
42	L5	68	THR
42	L5	69	ILE
42	L5	70	THR
42	L5	92	LEU
42	L5	93	THR
42	L5	95	TRP
42	L5	105	ILE
42	L5	107	ARG
42	L5	109	THR
42	L5	110	LEU
42	L5	113	LEU
42	L5	118	THR
42	L5	131	LEU
42	L5	137	ASP
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	152	ARG
42	L5	154	THR
42	L5	155	THR
42	L5	159	VAL
42	L5	163	LEU
42	L5	179	ARG
42	L5	185	PHE
42	L5	188	GLU
42	L5	190	ILE
42	L5	203	HIS
42	L5	211	LEU
42	L5	218	ARG
42	L5	222	LEU

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Mol	Chain	Res	Type
42	L5	232	ASP
42	L5	234	ASP
42	L5	261	THR
42	L5	263	GLU
42	L5	264	GLN
42	L5	273	ARG
42	L5	277	LEU
42	L5	293	LEU
43	L6	5	LYS
43	L6	15	VAL
43	L6	21	THR
43	L6	28	GLN
43	L6	31	ARG
43	L6	34	LEU
43	L6	35	VAL
43	L6	38	THR
43	L6	46	ARG
43	L6	52	VAL
43	L6	58	LEU
43	L6	64	LEU
43	L6	65	ILE
43	L6	66	SER
43	L6	78	ARG
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	98	VAL
43	L6	99	GLU
43	L6	100	LYS
43	L6	108	LYS
43	L6	109	GLU
43	L6	134	ARG
43	L6	160	SER
43	L6	167	ASN
44	L7	25	GLN
44	L7	46	GLU
44	L7	60	ARG
44	L7	82	LYS
44	L7	83	LEU
44	L7	84	VAL
44	L7	88	ARG
44	L7	92	ILE

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Mol	Chain	Res	Type
44	L7	101	LYS
44	L7	109	THR
44	L7	121	LYS
44	L7	124	LEU
44	L7	140	SER
44	L7	175	LYS
44	L7	178	ILE
44	L7	179	LEU
44	L7	181	ILE
44	L7	184	LEU
44	L7	216	VAL
44	L7	239	LEU
45	L8	26	LEU
45	L8	27	THR
45	L8	36	ILE
45	L8	41	GLN
45	L8	63	LYS
45	L8	66	SER
45	L8	74	THR
45	L8	79	GLN
45	L8	83	ASP
45	L8	84	ARG
45	L8	92	LYS
45	L8	95	ASN
45	L8	118	GLU
45	L8	132	VAL
45	L8	134	TYR
45	L8	136	LEU
45	L8	150	LEU
45	L8	160	ILE
45	L8	162	LEU
45	L8	163	VAL
45	L8	169	LEU
45	L8	180	VAL
45	L8	185	ARG
45	L8	186	LEU
45	L8	189	LEU
45	L8	190	VAL
45	L8	197	VAL
45	L8	203	VAL
45	L8	214	LEU
45	L8	232	HIS

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Mol	Chain	Res	Type
45	L8	246	MET
45	L8	248	LYS
45	L8	251	LYS
46	L9	5	GLN
46	L9	9	GLN
46	L9	18	VAL
46	L9	19	SER
46	L9	20	ILE
46	L9	33	THR
46	L9	41	ILE
46	L9	44	THR
46	L9	48	VAL
46	L9	49	ASN
46	L9	50	ASN
46	L9	52	LEU
46	L9	65	VAL
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	80	THR
46	L9	82	VAL
46	L9	92	TYR
46	L9	94	TYR
46	L9	104	VAL
46	L9	107	ASP
46	L9	123	ILE
46	L9	132	VAL
46	L9	135	GLU
46	L9	137	SER
46	L9	138	THR
46	L9	139	ASN
46	L9	140	VAL
46	L9	141	LYS
46	L9	146	LEU
46	L9	150	SER
46	L9	151	VAL
46	L9	157	ASN
46	L9	162	GLN
46	L9	164	ILE
46	L9	170	LYS
46	L9	172	ILE
46	L9	175	PHE

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Mol	Chain	Res	Type
46	L9	182	SER
46	L9	188	THR
46	L9	189	GLU
46	L9	191	LEU
47	M0	3	ARG
47	M0	7	ARG
47	M0	14	ASN
47	M0	30	LYS
47	M0	32	ARG
47	M0	33	ILE
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	74	LYS
47	M0	87	LEU
47	M0	91	VAL
47	M0	116	ARG
47	M0	125	LEU
47	M0	130	ASP
47	M0	144	ASN
47	M0	145	LYS
47	M0	156	ARG
47	M0	165	ILE
47	M0	177	ASP
47	M0	185	ARG
47	M0	191	LYS
47	M0	192	ASP
47	M0	203	LYS
48	M1	7	ASN
48	M1	10	ARG
48	M1	12	LEU
48	M1	13	LYS
48	M1	17	LEU
48	M1	19	LEU
48	M1	20	ASN
48	M1	23	VAL
48	M1	25	GLU
48	M1	28	ASP
48	M1	44	THR
48	M1	56	THR
48	M1	70	THR
48	M1	80	LEU

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Mol	Chain	Res	Type
48	M1	82	ARG
48	M1	94	ARG
48	M1	95	ASN
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	137	ARG
48	M1	138	VAL
48	M1	139	THR
48	M1	140	ARG
48	M1	155	THR
48	M1	173	ASP
49	M3	4	SER
49	M3	10	LEU
49	M3	13	HIS
49	M3	14	PHE
49	M3	15	ARG
49	M3	23	LYS
49	M3	27	ASP
49	M3	42	ARG
49	M3	46	ILE
49	M3	54	LEU
49	M3	55	ARG
49	M3	58	VAL
49	M3	59	ARG
49	M3	67	ARG
49	M3	69	VAL
49	M3	77	LEU
49	M3	85	LEU
49	M3	100	ARG
49	M3	107	GLU
49	M3	108	ILE
49	M3	112	ASN
49	M3	114	GLN
49	M3	117	LYS
49	M3	120	GLN
49	M3	124	ILE
49	M3	131	LYS
49	M3	134	GLU
49	M3	136	GLU
49	M3	140	SER
49	M3	144	THR

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Mol	Chain	Res	Type
49	M3	147	ILE
49	M3	164	GLU
49	M3	165	SER
49	M3	171	ARG
49	M3	190	LYS
50	M4	10	SER
50	M4	20	VAL
50	M4	27	GLN
50	M4	28	SER
50	M4	47	ASP
50	M4	50	LYS
50	M4	55	ARG
50	M4	58	ILE
50	M4	60	LEU
50	M4	64	VAL
50	M4	69	THR
50	M4	72	LEU
50	M4	102	LYS
50	M4	108	ARG
50	M4	113	THR
50	M4	115	PHE
50	M4	129	TYR
50	M4	130	THR
50	M4	132	LYS
50	M4	133	LYS
50	M4	135	LEU
51	M5	7	LEU
51	M5	10	LEU
51	M5	17	ASP
51	M5	18	VAL
51	M5	20	ARG
51	M5	22	LEU
51	M5	38	ARG
51	M5	41	ARG
51	M5	50	ARG
51	M5	60	VAL
51	M5	62	TYR
51	M5	75	VAL
51	M5	80	THR
51	M5	83	LYS
51	M5	92	LEU
51	M5	98	LEU

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Mol	Chain	Res	Type
51	M5	104	GLU
51	M5	105	ARG
51	M5	123	GLN
51	M5	133	ILE
51	M5	134	LEU
51	M5	138	GLN
51	M5	151	ILE
51	M5	159	ARG
51	M5	178	HIS
51	M5	182	ASN
51	M5	183	THR
51	M5	189	LYS
51	M5	194	GLN
51	M5	198	SER
52	M6	34	VAL
52	M6	41	LEU
52	M6	44	SER
52	M6	58	LEU
52	M6	67	THR
52	M6	74	ARG
52	M6	78	ARG
52	M6	84	LEU
52	M6	85	ARG
52	M6	102	LEU
52	M6	106	GLU
52	M6	110	PRO
52	M6	115	LYS
52	M6	116	LYS
52	M6	117	ARG
52	M6	119	VAL
52	M6	122	GLN
52	M6	124	LEU
52	M6	128	ARG
52	M6	134	LYS
52	M6	140	LYS
52	M6	143	THR
52	M6	160	ARG
52	M6	182	ASN
52	M6	187	GLU
52	M6	190	VAL
53	M7	3	ARG
53	M7	7	THR

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Mol	Chain	Res	Type
53	M7	9	THR
53	M7	16	SER
53	M7	22	LEU
53	M7	23	ARG
53	M7	24	VAL
53	M7	34	GLN
53	M7	36	ILE
53	M7	42	THR
53	M7	52	LEU
53	M7	53	ASP
53	M7	55	GLN
53	M7	56	ARG
53	M7	61	ARG
53	M7	65	SER
53	M7	67	ILE
53	M7	69	ARG
53	M7	75	GLU
53	M7	90	PHE
53	M7	94	LEU
53	M7	111	LYS
53	M7	112	LEU
53	M7	114	VAL
53	M7	121	GLN
53	M7	126	ARG
53	M7	127	ARG
53	M7	138	LYS
53	M7	142	SER
53	M7	144	SER
53	M7	149	VAL
53	M7	153	LYS
53	M7	165	VAL
53	M7	168	LEU
53	M7	172	GLN
53	M7	173	ARG
53	M7	180	LYS
53	M7	182	ILE
54	M8	6	THR
54	M8	8	LYS
54	M8	13	SER
54	M8	17	THR
54	M8	21	SER
54	M8	24	VAL

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Mol	Chain	Res	Type
54	M8	26	LEU
54	M8	32	LEU
54	M8	39	ARG
54	M8	41	ASP
54	M8	49	LEU
54	M8	57	ILE
54	M8	69	ARG
54	M8	74	GLU
54	M8	86	THR
54	M8	93	ILE
54	M8	113	LYS
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	150	VAL
54	M8	155	MET
54	M8	161	LYS
54	M8	171	LYS
54	M8	180	ARG
55	M9	8	LYS
55	M9	10	LEU
55	M9	20	ARG
55	M9	25	ASP
55	M9	30	SER
55	M9	31	GLU
55	M9	39	ASN
55	M9	42	ARG
55	M9	47	ASN
55	M9	49	THR
55	M9	52	LYS
55	M9	59	SER
55	M9	60	LYS
55	M9	62	ARG
55	M9	72	GLU
55	M9	74	ARG
55	M9	82	LYS
55	M9	84	THR
55	M9	85	ARG
55	M9	86	GLU
55	M9	97	ARG
55	M9	98	ARG
55	M9	99	LEU

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Mol	Chain	Res	Type
55	M9	103	ARG
55	M9	108	LYS
55	M9	110	ARG
55	M9	120	TYR
55	M9	126	GLU
55	M9	128	LYS
55	M9	130	ASN
55	M9	134	HIS
55	M9	138	LEU
55	M9	143	ILE
55	M9	165	LYS
55	M9	175	GLN
55	M9	182	ASP
55	M9	185	LEU
56	N0	12	ARG
56	N0	13	ARG
56	N0	16	THR
56	N0	18	SER
56	N0	32	SER
56	N0	51	VAL
56	N0	61	ILE
56	N0	71	LYS
56	N0	80	ARG
56	N0	85	SER
56	N0	87	THR
56	N0	97	VAL
56	N0	98	SER
56	N0	113	ARG
56	N0	117	ARG
56	N0	123	ILE
56	N0	131	LYS
56	N0	132	THR
56	N0	136	LYS
56	N0	137	ARG
56	N0	138	GLN
56	N0	145	THR
56	N0	155	ARG
56	N0	160	THR
56	N0	164	SER
56	N0	166	LYS
56	N0	167	ARG
56	N0	171	PHE

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Mol	Chain	Res	Type
56	N0	172	TYR
57	N1	12	ARG
57	N1	18	ASP
57	N1	26	HIS
57	N1	27	LEU
57	N1	29	THR
57	N1	55	LYS
57	N1	64	VAL
57	N1	71	SER
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	88	ARG
57	N1	89	LEU
57	N1	102	ARG
57	N1	104	GLU
57	N1	106	LEU
57	N1	108	ARG
57	N1	120	LYS
57	N1	124	VAL
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	139	ARG
57	N1	143	THR
57	N1	149	GLN
57	N1	158	THR
58	N2	25	ASN
58	N2	29	ASP
58	N2	38	ILE
58	N2	39	ASP
58	N2	43	VAL
58	N2	49	ASN
58	N2	52	ASN
58	N2	74	LYS
58	N2	82	LYS
58	N2	93	ILE
58	N2	95	PHE
58	N2	100	THR
59	N3	13	ILE

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Mol	Chain	Res	Type
59	N3	40	LYS
59	N3	44	SER
59	N3	45	ARG
59	N3	64	LYS
59	N3	69	LEU
59	N3	72	LYS
59	N3	83	LYS
59	N3	91	VAL
59	N3	102	ILE
59	N3	115	THR
59	N3	120	LYS
59	N3	125	LEU
59	N3	135	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	7	SER
60	N4	19	THR
60	N4	39	LEU
60	N4	43	ARG
60	N4	96	LEU
60	N4	107	GLU
60	N4	113	LYS
60	N4	115	LYS
60	N4	123	ARG
60	N4	130	SER
61	N5	26	VAL
61	N5	27	ARG
61	N5	34	LEU
61	N5	38	LEU
61	N5	40	LEU
61	N5	45	LYS
61	N5	48	SER
61	N5	49	LYS
61	N5	58	ASP
61	N5	63	ILE
61	N5	68	THR
61	N5	69	SER
61	N5	86	VAL
61	N5	92	LYS
61	N5	97	LYS
61	N5	108	LEU
61	N5	111	ASN

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Mol	Chain	Res	Type
61	N5	112	THR
61	N5	115	ARG
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	7	ASP
62	N6	13	ARG
62	N6	17	LYS
62	N6	37	LYS
62	N6	39	LEU
62	N6	42	GLN
62	N6	50	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	87	LYS
62	N6	94	SER
62	N6	97	ILE
62	N6	103	LYS
62	N6	113	LYS
62	N6	115	ARG
62	N6	125	LYS
62	N6	126	LEU
63	N7	5	LEU
63	N7	14	VAL
63	N7	15	ARG
63	N7	17	ARG
63	N7	24	VAL
63	N7	34	LYS
63	N7	36	HIS
63	N7	46	ILE
63	N7	53	VAL
63	N7	54	THR
63	N7	64	LYS
63	N7	81	LEU
63	N7	83	THR
63	N7	90	GLU
63	N7	92	PHE

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Mol	Chain	Res	Type
63	N7	99	GLU
63	N7	103	GLN
63	N7	107	ARG
63	N7	109	GLU
63	N7	121	ARG
63	N7	128	GLN
63	N7	134	LEU
64	N8	10	LYS
64	N8	16	SER
64	N8	22	ILE
64	N8	26	ARG
64	N8	32	ARG
64	N8	40	HIS
64	N8	42	ARG
64	N8	43	ILE
64	N8	44	ASN
64	N8	56	VAL
64	N8	60	TYR
64	N8	65	GLN
64	N8	67	HIS
64	N8	78	LEU
64	N8	84	GLU
64	N8	85	ASP
64	N8	96	LYS
64	N8	115	LYS
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	139	ARG
65	N9	22	LYS
65	N9	23	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	33	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	10	ILE
66	O0	16	LEU
66	O0	29	SER
66	O0	32	LYS
66	O0	34	LEU
66	O0	36	GLN

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Mol	Chain	Res	Type
66	O0	40	LYS
66	O0	41	LEU
66	O0	48	THR
66	O0	52	ARG
66	O0	54	SER
66	O0	61	MET
66	O0	63	SER
66	O0	79	THR
66	O0	83	LYS
66	O0	87	VAL
66	O0	93	LEU
66	O0	97	ASP
66	O0	100	ILE
66	O0	104	LEU
67	O1	8	VAL
67	O1	13	THR
67	O1	24	SER
67	O1	26	LYS
67	O1	28	ARG
67	O1	31	ARG
67	O1	36	ILE
67	O1	46	THR
67	O1	47	ASP
67	O1	55	LEU
67	O1	61	LYS
67	O1	64	VAL
67	O1	74	ARG
67	O1	79	ARG
67	O1	86	LYS
67	O1	89	LEU
67	O1	106	THR
67	O1	110	GLU
68	O2	4	LEU
68	O2	10	VAL
68	O2	19	ARG
68	O2	27	ARG
68	O2	33	ARG
68	O2	40	SER
68	O2	44	ARG
68	O2	61	LYS
68	O2	62	LYS
68	O2	67	SER

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Mol	Chain	Res	Type
68	O2	73	THR
68	O2	75	LEU
68	O2	76	VAL
68	O2	89	THR
68	O2	106	VAL
68	O2	122	PRO
68	O2	126	LEU
69	O3	3	GLU
69	O3	4	SER
69	O3	9	VAL
69	O3	14	LEU
69	O3	15	SER
69	O3	20	LYS
69	O3	21	ARG
69	O3	33	GLU
69	O3	49	ILE
69	O3	59	VAL
69	O3	60	ARG
69	O3	81	VAL
69	O3	98	VAL
69	O3	105	SER
70	O4	3	GLN
70	O4	8	ARG
70	O4	15	THR
70	O4	18	ASN
70	O4	20	ILE
70	O4	29	ILE
70	O4	33	GLN
70	O4	51	LEU
70	O4	52	GLN
70	O4	55	SER
70	O4	58	ARG
70	O4	59	PRO
70	O4	65	VAL
70	O4	69	HIS
70	O4	72	VAL
70	O4	73	SER
70	O4	74	ARG
70	O4	81	CYS
70	O4	90	ILE
70	O4	95	ILE
70	O4	102	LYS

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Mol	Chain	Res	Type
70	O4	104	VAL
71	O5	13	SER
71	O5	15	GLU
71	O5	16	GLN
71	O5	21	LEU
71	O5	27	GLU
71	O5	28	LEU
71	O5	31	LEU
71	O5	45	LYS
71	O5	47	VAL
71	O5	49	LYS
71	O5	71	LYS
71	O5	81	ARG
71	O5	86	ARG
71	O5	89	ARG
71	O5	96	GLU
71	O5	100	VAL
71	O5	101	THR
71	O5	107	LYS
71	O5	118	ILE
72	O6	11	LEU
72	O6	13	LYS
72	O6	17	VAL
72	O6	20	MET
72	O6	26	ILE
72	O6	29	LYS
72	O6	34	SER
72	O6	36	ARG
72	O6	42	SER
72	O6	45	ARG
72	O6	53	TYR
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	62	ARG
72	O6	68	ARG
72	O6	70	ARG
72	O6	76	ARG
72	O6	79	SER
72	O6	81	THR
72	O6	88	GLU
72	O6	98	ARG

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Mol	Chain	Res	Type
72	O6	99	ARG
73	O7	11	ARG
73	O7	12	HIS
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	28	HIS
73	O7	33	THR
73	O7	34	CYS
73	O7	36	SER
73	O7	43	LYS
73	O7	45	ARG
73	O7	46	SER
73	O7	55	ARG
73	O7	61	THR
73	O7	64	MET
73	O7	67	LEU
73	O7	71	SER
73	O7	84	SER
74	O8	5	ILE
74	O8	6	THR
74	O8	8	ILE
74	O8	19	ASP
74	O8	24	THR
74	O8	31	LEU
74	O8	41	THR
74	O8	48	SER
74	O8	50	SER
74	O8	51	LEU
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	77	ARG
75	O9	4	GLN
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	27	ILE
75	O9	34	THR
75	O9	45	ARG
75	O9	49	MET

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Mol	Chain	Res	Type
75	O9	51	ILE
76	Q0	78	ILE
76	Q0	85	LEU
76	Q0	91	CYS
76	Q0	93	LYS
76	Q0	97	ARG
76	Q0	99	CYS
76	Q0	106	ARG
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
77	Q1	2	ARG
77	Q1	11	ARG
77	Q1	19	LYS
78	Q2	8	ARG
78	Q2	21	THR
78	Q2	28	TYR
78	Q2	35	LEU
78	Q2	38	GLN
78	Q2	45	ARG
78	Q2	47	GLN
78	Q2	60	LYS
78	Q2	63	LYS
78	Q2	64	THR
78	Q2	71	ARG
78	Q2	72	LEU
78	Q2	78	LYS
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	97	LYS
78	Q2	100	LYS
78	Q2	104	LEU
78	Q2	105	GLN
79	Q3	4	ARG
79	Q3	7	LYS
79	Q3	11	THR
79	Q3	24	ARG
79	Q3	25	GLN
79	Q3	40	SER
79	Q3	45	LYS

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Mol	Chain	Res	Type
79	Q3	46	THR
79	Q3	49	ARG
79	Q3	60	CYS
79	Q3	73	THR
79	Q3	78	THR
79	Q3	91	GLU
2	s0	6	THR
2	s0	9	LEU
2	s0	12	GLU
2	s0	24	LEU
2	s0	32	HIS
2	s0	41	ARG
2	s0	45	VAL
2	s0	50	VAL
2	s0	59	LEU
2	s0	62	ARG
2	s0	72	ASP
2	s0	88	LYS
2	s0	101	ARG
2	s0	103	THR
2	s0	111	ILE
2	s0	131	GLN
2	s0	139	VAL
2	s0	144	ILE
2	s0	153	SER
2	s0	157	ASP
2	s0	162	CYS
2	s0	167	LYS
2	s0	172	LEU
2	s0	180	GLU
2	s0	183	ARG
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	202	TYR
2	s0	203	PHE
3	s1	21	VAL
3	s1	36	SER
3	s1	47	LEU
3	s1	51	SER
3	s1	55	LYS
3	s1	56	SER

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Mol	Chain	Res	Type
3	s1	62	LYS
3	s1	70	LEU
3	s1	81	PHE
3	s1	83	LYS
3	s1	85	LYS
3	s1	103	MET
3	s1	105	PHE
3	s1	108	ASP
3	s1	110	LEU
3	s1	125	VAL
3	s1	127	VAL
3	s1	137	ILE
3	s1	146	GLN
3	s1	150	VAL
3	s1	158	SER
3	s1	159	SER
3	s1	177	GLN
3	s1	180	THR
3	s1	181	LEU
3	s1	185	THR
3	s1	194	ASN
3	s1	202	LYS
3	s1	203	ASP
3	s1	211	HIS
3	s1	212	VAL
3	s1	213	ARG
3	s1	219	LYS
3	s1	222	LYS
4	s2	53	ILE
4	s2	54	GLU
4	s2	65	GLU
4	s2	69	ILE
4	s2	72	LEU
4	s2	73	LEU
4	s2	77	GLN
4	s2	79	GLU
4	s2	80	VAL
4	s2	81	MET
4	s2	83	ILE
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG

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Mol	Chain	Res	Type
4	s2	94	GLN
4	s2	96	THR
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	113	LEU
4	s2	115	ILE
4	s2	117	THR
4	s2	139	ILE
4	s2	141	ARG
4	s2	148	LEU
4	s2	161	LYS
4	s2	170	ILE
4	s2	185	LYS
4	s2	195	ASP
4	s2	206	THR
4	s2	229	LEU
4	s2	233	GLN
4	s2	237	VAL
4	s2	242	ILE
4	s2	250	GLN
5	s3	4	LEU
5	s3	7	LYS
5	s3	10	LYS
5	s3	26	THR
5	s3	37	VAL
5	s3	40	ARG
5	s3	44	THR
5	s3	53	THR
5	s3	55	THR
5	s3	67	ASN
5	s3	69	LEU
5	s3	76	ARG
5	s3	83	THR
5	s3	84	ILE
5	s3	91	VAL
5	s3	92	GLN
5	s3	94	ARG
5	s3	105	MET
5	s3	115	ILE
5	s3	117	ARG
5	s3	127	MET

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Mol	Chain	Res	Type
5	s3	141	LYS
5	s3	142	LEU
5	s3	143	ARG
5	s3	146	ARG
5	s3	148	LYS
5	s3	157	LEU
5	s3	158	ILE
5	s3	159	HIS
5	s3	162	GLN
5	s3	168	ILE
5	s3	175	VAL
5	s3	178	ARG
5	s3	189	MET
5	s3	202	LEU
5	s3	209	ILE
5	s3	212	LYS
5	s3	213	GLU
5	s3	215	GLU
5	s3	218	LEU
6	s4	6	LYS
6	s4	7	LYS
6	s4	9	LEU
6	s4	23	LEU
6	s4	26	CYS
6	s4	30	ARG
6	s4	38	LEU
6	s4	42	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	67	GLN
6	s4	92	LEU
6	s4	113	ARG
6	s4	116	ASP
6	s4	120	SER
6	s4	126	VAL
6	s4	131	LEU
6	s4	139	VAL
6	s4	147	ILE
6	s4	148	ARG
6	s4	163	ASP
6	s4	180	LEU
6	s4	181	VAL

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Mol	Chain	Res	Type
6	s4	182	TYR
6	s4	194	THR
6	s4	206	ASP
6	s4	221	ARG
6	s4	222	LEU
6	s4	227	VAL
6	s4	244	ILE
6	s4	245	LYS
6	s4	246	LEU
7	s5	23	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	33	VAL
7	s5	38	THR
7	s5	51	VAL
7	s5	59	VAL
7	s5	63	GLN
7	s5	64	VAL
7	s5	68	ILE
7	s5	70	VAL
7	s5	76	ARG
7	s5	83	ARG
7	s5	84	LYS
7	s5	93	LEU
7	s5	119	ASP
7	s5	125	THR
7	s5	128	ASN
7	s5	146	THR
7	s5	149	VAL
7	s5	157	ARG
7	s5	161	ASP
7	s5	162	VAL
7	s5	167	ARG
7	s5	187	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	208	SER
7	s5	216	GLU
7	s5	223	SER
8	s6	15	THR
8	s6	21	GLU

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Mol	Chain	Res	Type
8	s6	25	ARG
8	s6	30	LYS
8	s6	31	ARG
8	s6	44	GLU
8	s6	65	GLN
8	s6	71	THR
8	s6	78	THR
8	s6	87	ARG
8	s6	93	LYS
8	s6	96	SER
8	s6	108	VAL
8	s6	109	LEU
8	s6	111	LEU
8	s6	121	LEU
8	s6	122	GLU
8	s6	124	LEU
8	s6	128	THR
8	s6	129	VAL
8	s6	143	LYS
8	s6	151	ASP
8	s6	154	ARG
8	s6	155	ASP
8	s6	169	TYR
8	s6	176	GLN
8	s6	177	ARG
8	s6	179	VAL
8	s6	193	LEU
8	s6	215	ARG
9	s7	9	LEU
9	s7	11	GLN
9	s7	24	PHE
9	s7	25	VAL
9	s7	35	LYS
9	s7	39	ARG
9	s7	41	LEU
9	s7	49	ILE
9	s7	50	ASP
9	s7	64	VAL
9	s7	67	LEU
9	s7	75	THR
9	s7	77	LEU
9	s7	79	ARG

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Mol	Chain	Res	Type
9	s7	86	GLN
9	s7	87	ASP
9	s7	97	ARG
9	s7	101	LYS
9	s7	105	THR
9	s7	108	GLN
9	s7	109	VAL
9	s7	112	ARG
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	118	LEU
9	s7	123	ASP
9	s7	126	LEU
9	s7	134	GLU
9	s7	139	ARG
9	s7	144	VAL
9	s7	159	VAL
9	s7	163	ASP
9	s7	166	LEU
9	s7	167	GLU
9	s7	185	ILE
10	s8	7	SER
10	s8	12	SER
10	s8	18	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	58	LEU
10	s8	59	ARG
10	s8	60	ILE
10	s8	61	GLU
10	s8	66	SER
10	s8	74	LYS
10	s8	77	ARG
10	s8	97	THR
10	s8	121	LEU
10	s8	123	LYS
10	s8	138	ASN
10	s8	151	LYS
10	s8	152	ILE
10	s8	154	SER

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Mol	Chain	Res	Type
10	s8	155	SER
10	s8	168	CYS
10	s8	176	SER
10	s8	183	ILE
10	s8	184	LEU
10	s8	193	LEU
10	s8	199	LYS
11	s9	7	THR
11	s9	28	LEU
11	s9	39	LYS
11	s9	46	SER
11	s9	49	LEU
11	s9	90	LYS
11	s9	93	LEU
11	s9	100	LYS
11	s9	101	VAL
11	s9	105	LEU
11	s9	109	LEU
11	s9	120	LYS
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	141	VAL
11	s9	145	SER
11	s9	149	ARG
11	s9	180	LYS
11	s9	182	GLU
11	s9	186	GLU
12	c0	5	LYS
12	c0	15	LEU
12	c0	20	VAL
12	c0	21	VAL
12	c0	26	ASP
12	c0	27	PHE
12	c0	33	GLU
12	c0	40	LEU
12	c0	49	LEU
12	c0	52	LYS
12	c0	55	VAL
12	c0	76	LEU
12	c0	77	ARG
13	c1	3	THR

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Mol	Chain	Res	Type
13	c1	5	LEU
13	c1	6	THR
13	c1	10	GLU
13	c1	21	ASN
13	c1	26	LYS
13	c1	27	THR
13	c1	28	SER
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	53	TYR
13	c1	56	LYS
13	c1	60	PHE
13	c1	61	THR
13	c1	67	ARG
13	c1	72	THR
13	c1	74	THR
13	c1	83	THR
13	c1	115	PHE
13	c1	125	VAL
13	c1	140	VAL
14	c2	28	LEU
14	c2	36	LEU
14	c2	39	ASP
14	c2	43	ARG
14	c2	45	LEU
14	c2	50	LYS
14	c2	58	LEU
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	66	VAL
14	c2	71	ILE
14	c2	74	LEU
14	c2	83	GLU
14	c2	85	LYS
14	c2	93	ASP
14	c2	97	LEU
14	c2	103	LEU
14	c2	116	VAL

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Mol	Chain	Res	Type
14	c2	120	VAL
14	c2	121	VAL
14	c2	129	GLU
14	c2	132	GLU
14	c2	136	ILE
14	c2	139	HIS
14	c2	140	PHE
15	c3	6	SER
15	c3	14	SER
15	c3	16	ILE
15	c3	18	TYR
15	c3	21	ASN
15	c3	28	LEU
15	c3	49	GLN
15	c3	58	HIS
15	c3	64	ARG
15	c3	66	ILE
15	c3	70	LYS
15	c3	72	MET
15	c3	80	LEU
15	c3	83	GLU
15	c3	84	ILE
15	c3	86	GLU
15	c3	88	LEU
15	c3	104	ARG
15	c3	115	LEU
15	c3	125	LEU
15	c3	127	ARG
15	c3	134	VAL
15	c3	138	ASN
15	c3	139	TRP
15	c3	143	SER
15	c3	149	LEU
15	c3	150	VAL
16	c4	12	GLN
16	c4	13	VAL
16	c4	28	VAL
16	c4	31	THR
16	c4	33	LEU
16	c4	34	SER
16	c4	38	THR
16	c4	42	VAL

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Mol	Chain	Res	Type
16	c4	51	ASP
16	c4	52	ARG
16	c4	61	MET
16	c4	65	GLN
16	c4	66	ASP
16	c4	81	VAL
16	c4	92	LYS
16	c4	102	LEU
16	c4	114	ARG
16	c4	118	VAL
16	c4	124	ASP
16	c4	136	ARG
16	c4	137	LEU
17	c5	21	ASP
17	c5	24	LYS
17	c5	27	GLU
17	c5	36	LEU
17	c5	40	ARG
17	c5	42	ARG
17	c5	69	GLU
17	c5	94	VAL
17	c5	107	ILE
17	c5	110	GLU
17	c5	121	ILE
17	c5	122	THR
17	c5	124	THR
18	c6	17	THR
18	c6	28	LEU
18	c6	40	GLU
18	c6	43	ILE
18	c6	45	ARG
18	c6	48	VAL
18	c6	53	LEU
18	c6	57	LEU
18	c6	58	ASP
18	c6	68	ARG
18	c6	69	VAL
18	c6	90	VAL
18	c6	94	GLN
18	c6	98	ASP
18	c6	113	ASP
18	c6	114	ARG

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Mol	Chain	Res	Type
18	c6	117	LEU
18	c6	123	ARG
18	c6	128	LYS
18	c6	137	ARG
19	c7	3	ARG
19	c7	8	THR
19	c7	19	ARG
19	c7	27	ASP
19	c7	29	GLN
19	c7	34	LEU
19	c7	38	ILE
19	c7	46	LEU
19	c7	60	ARG
19	c7	69	ILE
19	c7	78	ARG
19	c7	83	GLN
19	c7	88	VAL
19	c7	89	SER
19	c7	101	ASN
19	c7	106	THR
19	c7	108	ASP
19	c7	109	LEU
19	c7	110	VAL
20	c8	3	LEU
20	c8	4	VAL
20	c8	6	GLN
20	c8	7	GLU
20	c8	13	HIS
20	c8	15	LEU
20	c8	17	LEU
20	c8	20	THR
20	c8	25	ASN
20	c8	28	ILE
20	c8	36	LYS
20	c8	40	ARG
20	c8	55	HIS
20	c8	61	LEU
20	c8	77	THR
20	c8	81	ILE
20	c8	92	ILE
20	c8	94	ASP
20	c8	100	THR

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Mol	Chain	Res	Type
20	c8	103	ASN
20	c8	105	VAL
20	c8	119	ILE
20	c8	136	GLN
20	c8	138	THR
20	c8	144	ARG
21	c9	6	VAL
21	c9	13	ASP
21	c9	23	GLN
21	c9	27	LYS
21	c9	28	LEU
21	c9	33	TYR
21	c9	34	VAL
21	c9	35	ASP
21	c9	57	ARG
21	c9	68	ARG
21	c9	71	VAL
21	c9	75	LYS
21	c9	86	ARG
21	c9	89	ARG
21	c9	111	ILE
21	c9	123	ARG
21	c9	126	GLU
21	c9	132	LEU
21	c9	135	ILE
21	c9	139	THR
21	c9	140	LEU
21	c9	142	GLU
21	c9	144	GLU
22	d0	23	ARG
22	d0	27	THR
22	d0	30	LYS
22	d0	34	LEU
22	d0	44	ASN
22	d0	47	GLN
22	d0	51	VAL
22	d0	57	ARG
22	d0	60	THR
22	d0	70	THR
22	d0	74	GLU
22	d0	81	THR
22	d0	88	LYS

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Mol	Chain	Res	Type
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	115	GLU
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	32	VAL
23	d1	38	LYS
23	d1	49	GLU
23	d1	52	THR
23	d1	56	SER
23	d1	59	VAL
23	d1	62	ARG
23	d1	68	SER
23	d1	70	ASN
24	d2	4	SER
24	d2	5	SER
24	d2	7	LEU
24	d2	15	ASN
24	d2	23	ARG
24	d2	37	PHE
24	d2	57	ARG
24	d2	65	LEU
24	d2	79	PHE
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	121	VAL
24	d2	122	SER
24	d2	126	LEU
24	d2	129	VAL
25	d3	9	LEU
25	d3	16	ARG
25	d3	19	ARG
25	d3	41	SER
25	d3	71	CYS
25	d3	73	ARG
25	d3	79	ASN

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Mol	Chain	Res	Type
25	d3	84	THR
25	d3	103	LEU
25	d3	107	PHE
25	d3	133	LEU
26	d4	6	THR
26	d4	10	ARG
26	d4	13	ILE
26	d4	14	SER
26	d4	22	GLN
26	d4	35	VAL
26	d4	42	GLU
26	d4	43	LYS
26	d4	44	LEU
26	d4	47	VAL
26	d4	49	LYS
26	d4	57	VAL
26	d4	58	PHE
26	d4	62	THR
26	d4	77	ASN
26	d4	83	LYS
26	d4	88	THR
26	d4	100	VAL
26	d4	105	ARG
26	d4	125	LEU
26	d4	128	LYS
26	d4	131	ARG
26	d4	133	ASN
27	d5	45	GLU
27	d5	46	LYS
27	d5	51	LEU
27	d5	53	GLU
27	d5	57	TYR
27	d5	81	ARG
27	d5	102	THR
28	d6	10	ARG
28	d6	12	LYS
28	d6	15	ARG
28	d6	18	VAL
28	d6	33	ASP
28	d6	44	ILE
28	d6	53	LEU
28	d6	58	VAL

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Mol	Chain	Res	Type
28	d6	74	CYS
28	d6	82	ARG
28	d6	85	ARG
28	d6	89	ARG
29	d7	3	LEU
29	d7	4	VAL
29	d7	20	LYS
29	d7	22	LYS
29	d7	34	ASP
29	d7	37	CYS
29	d7	42	ASN
29	d7	43	ILE
29	d7	44	THR
29	d7	52	THR
29	d7	61	THR
29	d7	77	THR
29	d7	81	ARG
30	d8	5	THR
30	d8	11	LYS
30	d8	18	ARG
30	d8	19	THR
30	d8	22	ARG
30	d8	28	VAL
30	d8	30	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	36	THR
30	d8	39	THR
30	d8	40	ILE
30	d8	41	VAL
30	d8	49	ARG
30	d8	54	LEU
30	d8	62	GLU
30	d8	64	ARG
30	d8	65	ARG
31	d9	8	PHE
31	d9	10	HIS
31	d9	12	ARG
31	d9	31	ILE
31	d9	32	ARG
31	d9	36	LEU
31	d9	53	ASN

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Mol	Chain	Res	Type
31	d9	54	LYS
32	e0	3	LYS
32	e0	7	SER
32	e0	8	LEU
32	e0	10	ARG
32	e0	13	LYS
32	e0	16	SER
32	e0	22	GLU
32	e0	23	LYS
32	e0	26	LYS
32	e0	28	LYS
32	e0	29	LYS
32	e0	31	LYS
32	e0	36	LYS
32	e0	44	PHE
32	e0	53	LYS
32	e0	56	MET
33	e1	84	VAL
33	e1	85	TYR
33	e1	90	LYS
33	e1	126	CYS
33	e1	135	HIS
33	e1	140	TYR
33	e1	141	CYS
33	e1	147	VAL
33	e1	148	TYR
34	sR	25	THR
34	sR	29	GLN
34	sR	42	LEU
34	sR	48	THR
34	sR	52	GLN
34	sR	58	VAL
34	sR	59	ARG
34	sR	64	HIS
34	sR	76	ASP
34	sR	96	THR
34	sR	106	HIS
34	sR	145	LEU
34	sR	167	VAL
34	sR	176	LYS
34	sR	182	ASN
34	sR	188	ILE

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Mol	Chain	Res	Type
34	sR	207	ASP
34	sR	232	TYR
34	sR	256	THR
34	sR	266	ASP
34	sR	275	ARG
34	sR	277	GLU
34	sR	297	ASP
34	sR	308	ASN
34	sR	309	VAL
35	sM	23	LYS
35	sM	30	THR
35	sM	43	ASP
35	sM	50	ASN
35	sM	53	ARG
35	sM	61	ILE
35	sM	62	ARG
35	sM	68	ARG
35	sM	74	LYS
35	sM	75	ASP
35	sM	77	THR
35	sM	82	THR
35	sM	83	LYS
35	sM	88	ARG
35	sM	89	ARG
35	sM	91	THR
35	sM	93	ARG
35	sM	97	THR
35	sM	102	THR
35	sM	105	LYS
35	sM	116	GLU
35	sM	134	ASP
35	sM	137	GLU
39	l2	5	ILE
39	l2	15	ILE
39	l2	23	ARG
39	l2	32	LEU
39	l2	41	ILE
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	48	ILE
39	l2	64	ARG

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Mol	Chain	Res	Type
39	l2	70	ARG
39	l2	101	VAL
39	l2	107	VAL
39	l2	109	GLU
39	l2	113	VAL
39	l2	119	LYS
39	l2	128	ARG
39	l2	130	SER
39	l2	134	VAL
39	l2	137	ILE
39	l2	142	ASP
39	l2	147	ARG
39	l2	152	SER
39	l2	155	LYS
39	l2	157	VAL
39	l2	165	VAL
39	l2	179	LEU
39	l2	180	LEU
39	l2	181	LYS
39	l2	190	ARG
39	l2	191	LEU
39	l2	193	ARG
39	l2	194	ASN
39	l2	199	THR
39	l2	202	VAL
39	l2	223	SER
39	l2	224	THR
39	l2	225	ILE
39	l2	241	ARG
39	l2	243	THR
39	l2	246	LEU
39	l2	247	ARG
39	l2	249	SER
39	l2	251	LYS
40	l3	2	SER
40	l3	3	HIS
40	l3	4	ARG
40	l3	7	GLU
40	l3	10	ARG
40	l3	17	LEU
40	l3	20	LYS
40	l3	28	ARG

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Mol	Chain	Res	Type
40	l3	30	LYS
40	l3	37	ARG
40	l3	39	LYS
40	l3	41	VAL
40	l3	43	LEU
40	l3	47	LEU
40	l3	50	LYS
40	l3	55	THR
40	l3	56	ILE
40	l3	65	SER
40	l3	70	ARG
40	l3	73	VAL
40	l3	77	THR
40	l3	81	THR
40	l3	85	VAL
40	l3	95	THR
40	l3	102	LEU
40	l3	103	THR
40	l3	110	LEU
40	l3	114	VAL
40	l3	116	ARG
40	l3	120	LYS
40	l3	139	GLN
40	l3	148	LEU
40	l3	162	VAL
40	l3	169	THR
40	l3	183	LEU
40	l3	184	ASN
40	l3	188	ILE
40	l3	192	VAL
40	l3	196	ARG
40	l3	201	LYS
40	l3	202	THR
40	l3	205	VAL
40	l3	221	THR
40	l3	227	GLU
40	l3	229	VAL
40	l3	232	ARG
40	l3	235	THR
40	l3	237	LYS
40	l3	238	LEU
40	l3	244	ARG

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Mol	Chain	Res	Type
40	13	246	LEU
40	13	252	ILE
40	13	260	VAL
40	13	266	ARG
40	13	272	TYR
40	13	284	ARG
40	13	287	LYS
40	13	304	THR
40	13	308	MET
40	13	317	ILE
40	13	319	ASN
40	13	320	ASP
40	13	324	VAL
40	13	328	ILE
40	13	332	ARG
40	13	338	LEU
40	13	339	ARG
40	13	340	LYS
40	13	364	LYS
40	13	365	PHE
40	13	367	LYS
40	13	369	ARG
41	14	3	ARG
41	14	14	GLU
41	14	22	LEU
41	14	37	THR
41	14	48	GLN
41	14	52	VAL
41	14	71	VAL
41	14	76	ARG
41	14	92	ASN
41	14	93	MET
41	14	99	MET
41	14	103	THR
41	14	105	THR
41	14	120	TYR
41	14	133	SER
41	14	136	LEU
41	14	138	ARG
41	14	141	ARG
41	14	144	LYS
41	14	150	LEU

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Mol	Chain	Res	Type
41	14	156	LEU
41	14	161	LYS
41	14	170	LYS
41	14	172	VAL
41	14	177	ASP
41	14	179	LEU
41	14	184	SER
41	14	186	LYS
41	14	187	LEU
41	14	193	LYS
41	14	194	TYR
41	14	200	THR
41	14	203	ARG
41	14	217	LYS
41	14	220	ARG
41	14	230	VAL
41	14	232	SER
41	14	246	ARG
41	14	256	THR
41	14	258	LEU
41	14	259	ASP
41	14	261	VAL
41	14	267	VAL
41	14	275	THR
41	14	287	THR
41	14	295	ILE
41	14	304	GLN
41	14	307	GLN
41	14	310	THR
41	14	313	LEU
41	14	327	LEU
41	14	345	GLU
41	14	347	THR
41	14	356	THR
41	14	359	LEU
41	14	360	LYS
42	15	4	GLN
42	15	5	LYS
42	15	25	GLU
42	15	32	GLN
42	15	34	LYS
42	15	35	ARG

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Mol	Chain	Res	Type
42	15	38	THR
42	15	51	LEU
42	15	56	THR
42	15	65	ILE
42	15	69	ILE
42	15	70	THR
42	15	74	VAL
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	115	LEU
42	15	118	THR
42	15	133	GLU
42	15	137	ASP
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE
42	15	152	ARG
42	15	155	THR
42	15	177	GLU
42	15	185	PHE
42	15	186	GLU
42	15	189	GLU
42	15	190	ILE
42	15	194	LEU
42	15	203	HIS
42	15	211	LEU
42	15	213	ASP
42	15	218	ARG
42	15	227	LEU
42	15	234	ASP
42	15	258	LYS
42	15	259	LYS
42	15	268	GLU
42	15	273	ARG
42	15	275	THR
42	15	282	ARG
43	16	8	LYS
43	16	15	VAL
43	16	20	LYS
43	16	21	THR
43	16	26	ARG

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Mol	Chain	Res	Type
43	16	29	LYS
43	16	33	SER
43	16	41	ILE
43	16	46	ARG
43	16	50	LYS
43	16	52	VAL
43	16	54	TYR
43	16	64	LEU
43	16	79	VAL
43	16	88	SER
43	16	91	VAL
43	16	98	VAL
43	16	108	LYS
43	16	109	GLU
43	16	152	THR
43	16	155	LEU
43	16	166	LYS
44	17	22	THR
44	17	33	ARG
44	17	45	LEU
44	17	60	ARG
44	17	77	VAL
44	17	82	LYS
44	17	83	LEU
44	17	84	VAL
44	17	87	VAL
44	17	88	ARG
44	17	90	LYS
44	17	98	LYS
44	17	101	LYS
44	17	103	LEU
44	17	108	LEU
44	17	110	ARG
44	17	124	LEU
44	17	158	LYS
44	17	178	ILE
44	17	179	LEU
44	17	184	LEU
44	17	196	LYS
44	17	208	SER
44	17	216	VAL
44	17	229	PHE

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Mol	Chain	Res	Type
44	17	239	LEU
45	18	27	THR
45	18	50	VAL
45	18	68	ARG
45	18	70	LYS
45	18	79	GLN
45	18	81	THR
45	18	83	ASP
45	18	89	GLU
45	18	92	LYS
45	18	98	ARG
45	18	109	LEU
45	18	136	LEU
45	18	146	LYS
45	18	150	LEU
45	18	156	ASP
45	18	160	ILE
45	18	163	VAL
45	18	164	VAL
45	18	169	LEU
45	18	172	LYS
45	18	180	VAL
45	18	183	LYS
45	18	194	THR
45	18	197	VAL
45	18	200	LEU
45	18	208	GLU
45	18	214	LEU
45	18	217	THR
45	18	221	ASN
45	18	230	LYS
45	18	240	ASN
45	18	241	LYS
45	18	245	LYS
45	18	248	LYS
46	19	4	ILE
46	19	5	GLN
46	19	6	THR
46	19	17	THR
46	19	18	VAL
46	19	19	SER
46	19	21	LYS

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Mol	Chain	Res	Type
46	19	30	PRO
46	19	35	THR
46	19	43	VAL
46	19	48	VAL
46	19	52	LEU
46	19	55	VAL
46	19	65	VAL
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	80	THR
46	19	82	VAL
46	19	92	TYR
46	19	105	GLU
46	19	106	LYS
46	19	124	ARG
46	19	130	ASP
46	19	133	THR
46	19	134	ILE
46	19	138	THR
46	19	140	VAL
46	19	144	ILE
46	19	147	SER
46	19	149	ASN
46	19	150	SER
46	19	151	VAL
46	19	157	ASN
46	19	162	GLN
46	19	164	ILE
46	19	165	CYS
46	19	177	ASP
46	19	181	VAL
46	19	186	PHE
46	19	189	GLU
47	m0	20	SER
47	m0	21	ARG
47	m0	24	ARG
47	m0	26	VAL
47	m0	32	ARG
47	m0	36	LEU
47	m0	39	LYS
47	m0	42	THR

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Mol	Chain	Res	Type
47	m0	48	LEU
47	m0	52	LEU
47	m0	58	GLU
47	m0	61	SER
47	m0	62	SER
47	m0	63	GLU
47	m0	87	LEU
47	m0	113	GLN
47	m0	129	VAL
47	m0	130	ASP
47	m0	135	ILE
47	m0	139	ARG
47	m0	142	ASP
47	m0	143	SER
47	m0	144	ASN
47	m0	145	LYS
47	m0	163	GLN
47	m0	167	LEU
47	m0	169	LYS
47	m0	174	THR
47	m0	175	ASN
47	m0	177	ASP
47	m0	178	ARG
47	m0	186	GLU
47	m0	205	SER
47	m0	210	ILE
47	m0	212	GLU
47	m0	215	GLU
47	m0	217	PHE
48	m1	7	ASN
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS
48	m1	30	LEU
48	m1	31	THR
48	m1	35	LYS
48	m1	46	VAL
48	m1	48	SER
48	m1	80	LEU
48	m1	87	LYS
48	m1	92	ARG

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Mol	Chain	Res	Type
48	m1	94	ARG
48	m1	97	SER
48	m1	106	ILE
48	m1	107	ASP
48	m1	112	LEU
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	139	THR
48	m1	140	ARG
48	m1	143	ARG
48	m1	147	THR
48	m1	151	SER
48	m1	152	HIS
48	m1	158	ASP
48	m1	171	VAL
48	m1	174	LYS
49	m3	9	ILE
49	m3	13	HIS
49	m3	15	ARG
49	m3	46	ILE
49	m3	54	LEU
49	m3	55	ARG
49	m3	58	VAL
49	m3	63	VAL
49	m3	67	ARG
49	m3	68	LYS
49	m3	69	VAL
49	m3	75	PHE
49	m3	76	THR
49	m3	77	LEU
49	m3	85	LEU
49	m3	97	VAL
49	m3	100	ARG
49	m3	107	GLU
49	m3	114	GLN
49	m3	123	ILE
49	m3	124	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	153	ASP
49	m3	164	GLU

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Mol	Chain	Res	Type
49	m3	171	ARG
49	m3	176	GLU
49	m3	184	GLU
49	m3	194	GLU
50	m4	4	ASP
50	m4	10	SER
50	m4	13	ARG
50	m4	20	VAL
50	m4	23	ILE
50	m4	27	GLN
50	m4	28	SER
50	m4	42	LYS
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	69	THR
50	m4	72	LEU
50	m4	74	ARG
50	m4	90	VAL
50	m4	106	ARG
50	m4	107	GLU
50	m4	108	ARG
50	m4	131	VAL
50	m4	132	LYS
50	m4	135	LEU
51	m5	10	LEU
51	m5	18	VAL
51	m5	22	LEU
51	m5	24	ARG
51	m5	31	ARG
51	m5	41	ARG
51	m5	49	ARG
51	m5	50	ARG
51	m5	68	ARG
51	m5	71	ARG
51	m5	73	ARG
51	m5	87	GLN
51	m5	91	GLU
51	m5	92	LEU
51	m5	96	ARG
51	m5	109	ARG
51	m5	117	ASN

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Mol	Chain	Res	Type
51	m5	137	PRO
51	m5	155	VAL
51	m5	165	THR
51	m5	176	LYS
51	m5	190	THR
51	m5	194	GLN
51	m5	201	ARG
51	m5	204	LYS
52	m6	4	GLU
52	m6	12	LYS
52	m6	34	VAL
52	m6	40	GLU
52	m6	41	LEU
52	m6	44	SER
52	m6	58	LEU
52	m6	59	ARG
52	m6	67	THR
52	m6	74	ARG
52	m6	77	SER
52	m6	78	ARG
52	m6	80	PHE
52	m6	85	ARG
52	m6	102	LEU
52	m6	106	GLU
52	m6	108	ILE
52	m6	115	LYS
52	m6	116	LYS
52	m6	117	ARG
52	m6	119	VAL
52	m6	122	GLN
52	m6	124	LEU
52	m6	126	VAL
52	m6	127	LEU
52	m6	128	ARG
52	m6	134	LYS
52	m6	143	THR
52	m6	152	VAL
52	m6	160	ARG
52	m6	167	TYR
52	m6	170	LYS
52	m6	171	LYS
52	m6	180	SER

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Mol	Chain	Res	Type
52	m6	182	ASN
52	m6	184	THR
53	m7	7	THR
53	m7	16	SER
53	m7	22	LEU
53	m7	24	VAL
53	m7	31	GLU
53	m7	32	THR
53	m7	34	GLN
53	m7	41	LEU
53	m7	49	GLU
53	m7	52	LEU
53	m7	53	ASP
53	m7	55	GLN
53	m7	56	ARG
53	m7	69	ARG
53	m7	74	LYS
53	m7	75	GLU
53	m7	80	LYS
53	m7	82	ARG
53	m7	96	GLN
53	m7	107	LEU
53	m7	114	VAL
53	m7	115	SER
53	m7	120	ASN
53	m7	126	ARG
53	m7	142	SER
53	m7	144	SER
53	m7	149	VAL
53	m7	153	LYS
53	m7	168	LEU
53	m7	169	THR
53	m7	171	ARG
53	m7	172	GLN
53	m7	175	ARG
53	m7	180	LYS
53	m7	181	ARG
53	m7	182	ILE
54	m8	17	THR
54	m8	21	SER
54	m8	26	LEU
54	m8	32	LEU

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Mol	Chain	Res	Type
54	m8	41	ASP
54	m8	49	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	80	THR
54	m8	86	THR
54	m8	99	THR
54	m8	105	ARG
54	m8	113	LYS
54	m8	135	GLN
54	m8	138	LEU
54	m8	146	SER
54	m8	161	LYS
54	m8	165	ILE
54	m8	167	SER
54	m8	168	THR
54	m8	170	ARG
54	m8	178	ARG
54	m8	180	ARG
55	m9	7	GLN
55	m9	10	LEU
55	m9	13	SER
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	30	SER
55	m9	31	GLU
55	m9	36	ASN
55	m9	37	SER
55	m9	42	ARG
55	m9	43	LYS
55	m9	46	LYS
55	m9	47	ASN
55	m9	52	LYS
55	m9	55	VAL
55	m9	56	THR
55	m9	63	THR
55	m9	69	SER
55	m9	70	LYS
55	m9	74	ARG
55	m9	84	THR
55	m9	88	ARG

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Mol	Chain	Res	Type
55	m9	98	ARG
55	m9	99	LEU
55	m9	105	LEU
55	m9	106	LEU
55	m9	114	LYS
55	m9	126	GLU
55	m9	133	LYS
55	m9	134	HIS
55	m9	138	LEU
55	m9	152	GLU
55	m9	153	LYS
55	m9	164	LEU
55	m9	173	ARG
55	m9	175	GLN
56	n0	3	HIS
56	n0	13	ARG
56	n0	17	GLU
56	n0	21	GLU
56	n0	23	LYS
56	n0	32	SER
56	n0	45	LEU
56	n0	50	LYS
56	n0	51	VAL
56	n0	53	LYS
56	n0	60	SER
56	n0	73	LYS
56	n0	80	ARG
56	n0	81	TYR
56	n0	87	THR
56	n0	97	VAL
56	n0	98	SER
56	n0	104	GLU
56	n0	109	ASP
56	n0	117	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	136	LYS
56	n0	137	ARG
56	n0	148	LEU
56	n0	155	ARG
56	n0	160	THR
56	n0	161	LYS

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Mol	Chain	Res	Type
56	n0	167	ARG
56	n0	172	TYR
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	31	LEU
57	n1	35	LYS
57	n1	60	LYS
57	n1	64	VAL
57	n1	68	THR
57	n1	71	SER
57	n1	78	LYS
57	n1	79	MET
57	n1	80	VAL
57	n1	83	ARG
57	n1	93	VAL
57	n1	102	ARG
57	n1	104	GLU
57	n1	118	GLU
57	n1	126	VAL
57	n1	128	LEU
57	n1	139	ARG
57	n1	140	ILE
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
57	n1	158	THR
57	n1	160	ILE
58	n2	19	VAL
58	n2	21	SER
58	n2	37	LEU
58	n2	43	VAL
58	n2	50	LEU
58	n2	54	VAL
58	n2	55	THR
58	n2	58	GLU
58	n2	62	VAL
58	n2	63	VAL
58	n2	68	THR
58	n2	74	LYS
58	n2	98	THR

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Mol	Chain	Res	Type
58	n2	100	THR
58	n2	105	LEU
59	n3	4	ASN
59	n3	13	ILE
59	n3	14	SER
59	n3	19	VAL
59	n3	23	MET
59	n3	42	SER
59	n3	64	LYS
59	n3	69	LEU
59	n3	84	SER
59	n3	88	ARG
59	n3	93	LEU
59	n3	94	TYR
59	n3	112	SER
59	n3	128	ARG
59	n3	135	VAL
60	n4	7	SER
60	n4	19	THR
60	n4	39	LEU
60	n4	60	LYS
60	n4	63	ILE
60	n4	79	GLN
60	n4	83	THR
60	n4	87	LEU
60	n4	90	ILE
60	n4	97	LYS
60	n4	126	GLU
60	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	45	LYS
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	68	THR
61	n5	69	SER
61	n5	71	THR
61	n5	73	MET
61	n5	74	LYS
61	n5	108	LEU

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Mol	Chain	Res	Type
61	n5	115	ARG
61	n5	125	ARG
61	n5	135	ILE
61	n5	137	ASN
61	n5	138	ARG
61	n5	139	ILE
61	n5	142	ILE
62	n6	3	LYS
62	n6	4	GLN
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	17	LYS
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	56	VAL
62	n6	57	LEU
62	n6	74	TYR
62	n6	76	LEU
62	n6	87	LYS
62	n6	95	VAL
62	n6	103	LYS
62	n6	105	VAL
62	n6	106	ILE
62	n6	112	ASP
62	n6	115	ARG
63	n7	3	LYS
63	n7	14	VAL
63	n7	28	PRO
63	n7	30	ASP
63	n7	34	LYS
63	n7	35	SER
63	n7	36	HIS
63	n7	46	ILE
63	n7	52	LYS
63	n7	55	LYS
63	n7	57	HIS
63	n7	72	ILE
63	n7	74	VAL

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Mol	Chain	Res	Type
63	n7	81	LEU
63	n7	90	GLU
63	n7	93	LYS
63	n7	95	VAL
63	n7	98	THR
63	n7	99	GLU
63	n7	100	THR
63	n7	105	SER
63	n7	121	ARG
63	n7	126	LYS
63	n7	132	SER
63	n7	134	LEU
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	14	HIS
64	n8	24	LYS
64	n8	26	ARG
64	n8	27	LYS
64	n8	42	ARG
64	n8	46	ASP
64	n8	60	TYR
64	n8	65	GLN
64	n8	67	HIS
64	n8	73	LEU
64	n8	78	LEU
64	n8	82	ILE
64	n8	85	ASP
64	n8	91	LEU
64	n8	97	GLU
64	n8	98	THR
64	n8	115	LYS
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
64	n8	139	ARG
65	n9	26	THR
65	n9	33	LYS
65	n9	47	LEU
65	n9	50	THR
65	n9	58	LYS
65	n9	59	LYS

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Mol	Chain	Res	Type
66	o0	10	ILE
66	o0	32	LYS
66	o0	34	LEU
66	o0	39	SER
66	o0	40	LYS
66	o0	41	LEU
66	o0	52	ARG
66	o0	61	MET
66	o0	68	TYR
66	o0	86	ARG
66	o0	97	ASP
66	o0	100	ILE
66	o0	103	THR
67	o1	6	ASP
67	o1	7	VAL
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	24	SER
67	o1	26	LYS
67	o1	31	ARG
67	o1	44	MET
67	o1	46	THR
67	o1	55	LEU
67	o1	64	VAL
67	o1	84	ASP
67	o1	90	PHE
67	o1	96	VAL
67	o1	102	LYS
67	o1	106	THR
67	o1	107	VAL
67	o1	110	GLU
68	o2	10	VAL
68	o2	14	THR
68	o2	24	ARG
68	o2	25	TYR
68	o2	33	ARG
68	o2	34	LYS
68	o2	45	ARG
68	o2	51	SER
68	o2	62	LYS
68	o2	67	SER

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Mol	Chain	Res	Type
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	87	MET
68	o2	89	THR
68	o2	106	VAL
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	10	LYS
69	o3	19	SER
69	o3	21	ARG
69	o3	28	SER
69	o3	31	LYS
69	o3	40	ASP
69	o3	48	ARG
69	o3	49	ILE
69	o3	57	LYS
69	o3	59	VAL
69	o3	60	ARG
69	o3	70	LYS
69	o3	80	VAL
69	o3	81	VAL
69	o3	86	ARG
69	o3	98	VAL
69	o3	106	ASN
70	o4	16	ARG
70	o4	17	SER
70	o4	44	CYS
70	o4	46	ASP
70	o4	47	CYS
70	o4	55	SER
70	o4	58	ARG
70	o4	65	VAL
70	o4	71	THR
70	o4	73	SER
70	o4	79	SER
70	o4	80	ARG
70	o4	83	ASN
70	o4	88	ARG
70	o4	102	LYS
71	o5	4	VAL

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Mol	Chain	Res	Type
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	28	LEU
71	o5	36	LEU
71	o5	38	ARG
71	o5	45	LYS
71	o5	46	THR
71	o5	57	VAL
71	o5	69	LEU
71	o5	81	ARG
71	o5	85	THR
71	o5	89	ARG
71	o5	90	ARG
71	o5	94	LYS
71	o5	107	LYS
71	o5	115	LYS
71	o5	119	LYS
72	o6	7	ILE
72	o6	9	ILE
72	o6	17	VAL
72	o6	21	THR
72	o6	26	ILE
72	o6	29	LYS
72	o6	34	SER
72	o6	36	ARG
72	o6	38	LYS
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	60	LEU
72	o6	68	ARG
72	o6	70	ARG
72	o6	76	ARG
72	o6	81	THR
72	o6	88	GLU
72	o6	90	MET
72	o6	94	ILE
72	o6	98	ARG
73	o7	17	THR
73	o7	19	CYS

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Mol	Chain	Res	Type
73	o7	25	ARG
73	o7	34	CYS
73	o7	46	SER
73	o7	52	LYS
73	o7	55	ARG
73	o7	59	THR
73	o7	64	MET
73	o7	65	ARG
73	o7	67	LEU
73	o7	68	LYS
74	o8	17	ARG
74	o8	22	THR
74	o8	24	THR
74	o8	31	LEU
74	o8	41	THR
74	o8	50	SER
74	o8	52	TYR
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	67	GLN
74	o8	68	SER
75	o9	5	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	29	LEU
75	o9	45	ARG
75	o9	48	LYS
75	o9	51	ILE
76	q0	79	GLU
76	q0	85	LEU
76	q0	89	TYR
76	q0	90	ASN
76	q0	92	ASP
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	2	ARG
77	q1	6	ARG
77	q1	9	ARG

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Mol	Chain	Res	Type
77	q1	13	LEU
77	q1	15	ARG
77	q1	16	LYS
77	q1	18	ARG
77	q1	19	LYS
77	q1	21	ARG
77	q1	23	ARG
78	q2	7	THR
78	q2	8	ARG
78	q2	22	GLN
78	q2	38	GLN
78	q2	43	TYR
78	q2	45	ARG
78	q2	48	SER
78	q2	57	VAL
78	q2	78	LYS
78	q2	85	LEU
78	q2	93	LEU
78	q2	100	LYS
78	q2	104	LEU
79	q3	8	VAL
79	q3	16	VAL
79	q3	21	SER
79	q3	24	ARG
79	q3	42	CYS
79	q3	45	LYS
79	q3	46	THR
79	q3	48	LYS
79	q3	54	ILE
79	q3	56	THR
79	q3	57	CYS
79	q3	59	CYS
79	q3	60	CYS
79	q3	62	LYS
79	q3	82	THR
80	p0	5	ARG
80	p0	10	GLU
80	p0	15	LEU
80	p0	48	ARG
80	p0	51	VAL
80	p0	52	LEU
80	p0	55	LYS

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Mol	Chain	Res	Type
80	p0	67	LEU
80	p0	72	ASP
80	p0	73	PHE
80	p0	93	LEU
80	p0	104	ARG
80	p0	105	VAL
80	p0	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	149	GLN
7	S5	104	ASN
7	S5	224	ASN
8	S6	59	GLN
8	S6	176	GLN
10	S8	32	GLN
13	C1	14	GLN
19	C7	83	GLN
20	C8	63	GLN
26	D4	110	GLN
34	SR	106	HIS
40	L3	139	GLN
41	L4	201	GLN
42	L5	17	GLN
42	L5	40	HIS
46	L9	163	GLN
47	M0	144	ASN
49	M3	25	HIS
51	M5	178	HIS
51	M5	194	GLN
59	N3	98	ASN
62	N6	110	HIS
63	N7	78	ASN
65	N9	19	ASN
70	O4	34	HIS
71	O5	16	GLN
3	s1	209	ASN
5	s3	74	GLN
12	c0	32	HIS
13	c1	14	GLN
13	c1	21	ASN

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Mol	Chain	Res	Type
20	c8	122	HIS
26	d4	22	GLN
28	d6	72	HIS
32	e0	17	GLN
39	l2	19	HIS
39	l2	140	ASN
39	l2	187	HIS
41	l4	175	HIS
42	l5	40	HIS
42	l5	264	GLN
45	l8	33	ASN
48	m1	95	ASN
48	m1	101	ASN
49	m3	99	HIS
52	m6	29	ASN
54	m8	5	HIS
54	m8	9	GLN
54	m8	73	GLN
57	n1	146	ASN
59	n3	47	ASN
60	n4	79	GLN
63	n7	57	HIS
67	o1	43	HIS
68	o2	13	HIS
68	o2	35	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1680/1800 (93%)	462 (27%)	67 (3%)
1	6	1695/1800 (94%)	427 (25%)	51 (3%)
36	1	3071/3396 (90%)	760 (24%)	101 (3%)
36	5	3120/3396 (91%)	739 (23%)	109 (3%)
37	3	120/121 (99%)	20 (16%)	1 (0%)
37	7	120/121 (99%)	15 (12%)	1 (0%)
38	4	157/158 (99%)	48 (30%)	6 (3%)
38	8	156/158 (98%)	41 (26%)	8 (5%)
All	All	10119/10950 (92%)	2512 (24%)	344 (3%)

All (2512) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	39	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	77	U
1	2	78	A
1	2	79	C
1	2	80	A
1	2	104	A
1	2	105	A
1	2	114	C
1	2	115	G
1	2	128	U
1	2	137	U
1	2	140	A
1	2	141	U
1	2	143	G
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	160	C
1	2	161	U

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Mol	Chain	Res	Type
1	2	178	U
1	2	185	U
1	2	186	C
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	220	A
1	2	249	U
1	2	250	C
1	2	257	A
1	2	260	U
1	2	261	U
1	2	265	A
1	2	266	A
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	282	C
1	2	288	A
1	2	290	G
1	2	299	A
1	2	301	A
1	2	309	C
1	2	312	A
1	2	314	C

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Mol	Chain	Res	Type
1	2	316	A
1	2	319	U
1	2	320	U
1	2	321	C
1	2	322	G
1	2	323	A
1	2	324	U
1	2	333	A
1	2	337	G
1	2	338	C
1	2	341	A
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	378	A
1	2	380	U
1	2	390	G
1	2	393	C
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	437	A
1	2	439	U
1	2	444	C
1	2	448	C
1	2	454	U
1	2	459	G
1	2	475	A
1	2	477	A
1	2	484	C
1	2	485	A

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Mol	Chain	Res	Type
1	2	486	G
1	2	488	G
1	2	501	U
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	512	A
1	2	513	U
1	2	515	A
1	2	516	G
1	2	519	C
1	2	527	A
1	2	532	U
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	545	A
1	2	548	G
1	2	554	C
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	570	A
1	2	571	G
1	2	572	C
1	2	579	A
1	2	580	A
1	2	582	U
1	2	594	A

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Mol	Chain	Res	Type
1	2	595	G
1	2	606	A
1	2	609	U
1	2	610	G
1	2	611	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	630	A
1	2	635	A
1	2	638	U
1	2	639	U
1	2	640	U
1	2	648	G
1	2	650	U
1	2	684	A
1	2	686	C
1	2	691	C
1	2	696	C
1	2	700	C
1	2	742	U
1	2	743	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	758	U
1	2	759	U
1	2	765	G
1	2	766	U
1	2	771	A
1	2	774	A
1	2	775	G
1	2	779	U
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	794	U

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Mol	Chain	Res	Type
1	2	795	U
1	2	803	A
1	2	806	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	819	G
1	2	820	U
1	2	821	U
1	2	831	U
1	2	833	U
1	2	856	A
1	2	860	U
1	2	863	A
1	2	864	U
1	2	871	G
1	2	873	U
1	2	896	U
1	2	897	C
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	916	U
1	2	921	U
1	2	926	A
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	958	U
1	2	959	U
1	2	960	U
1	2	966	A
1	2	970	A
1	2	973	A
1	2	988	A
1	2	992	A
1	2	993	A

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Mol	Chain	Res	Type
1	2	995	A
1	2	997	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1007	C
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1032	G
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1057	U
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1063	U
1	2	1074	G
1	2	1079	U
1	2	1081	A
1	2	1082	C
1	2	1083	G
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1093	A
1	2	1094	G
1	2	1095	U
1	2	1096	C
1	2	1097	U
1	2	1099	U
1	2	1100	G
1	2	1109	G
1	2	1138	A
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A

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Mol	Chain	Res	Type
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1185	U
1	2	1188	G
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1204	A
1	2	1205	C
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1241	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1257	U
1	2	1258	U
1	2	1260	U
1	2	1286	U
1	2	1288	G
1	2	1301	U
1	2	1314	U
1	2	1315	U
1	2	1321	A
1	2	1329	A
1	2	1336	A
1	2	1337	A
1	2	1339	C

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Mol	Chain	Res	Type
1	2	1340	U
1	2	1341	A
1	2	1342	C
1	2	1343	U
1	2	1344	A
1	2	1345	A
1	2	1349	G
1	2	1354	G
1	2	1360	A
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1379	C
1	2	1380	U
1	2	1383	G
1	2	1384	A
1	2	1385	G
1	2	1386	G
1	2	1388	A
1	2	1390	U
1	2	1397	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1432	U
1	2	1446	A
1	2	1448	G
1	2	1454	G
1	2	1457	C
1	2	1459	C
1	2	1460	A
1	2	1461	C

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Mol	Chain	Res	Type
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1481	C
1	2	1482	C
1	2	1486	G
1	2	1487	A
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1494	C
1	2	1499	G
1	2	1500	C
1	2	1506	G
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1542	G
1	2	1556	A
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1572	G
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1601	G
1	2	1607	G
1	2	1614	A
1	2	1616	G
1	2	1624	C

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Mol	Chain	Res	Type
1	2	1631	A
1	2	1634	C
1	2	1636	C
1	2	1643	U
1	2	1644	C
1	2	1656	U
1	2	1657	U
1	2	1658	G
1	2	1664	C
1	2	1681	A
1	2	1683	C
1	2	1684	U
1	2	1693	A
1	2	1712	A
1	2	1713	G
1	2	1716	C
1	2	1729	C
1	2	1731	A
1	2	1742	U
1	2	1750	A
1	2	1752	U
1	2	1754	A
1	2	1755	A
1	2	1757	G
1	2	1759	C
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1791	A
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
1	2	1798	U
36	1	13	A

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Mol	Chain	Res	Type
36	1	14	U
36	1	21	G
36	1	26	A
36	1	40	A
36	1	41	G
36	1	43	A
36	1	44	U
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	71	A
36	1	73	C
36	1	74	G
36	1	76	G
36	1	77	A
36	1	85	A
36	1	92	G
36	1	93	C
36	1	99	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	120	G
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	142	C
36	1	145	G
36	1	148	G
36	1	156	G
36	1	157	A
36	1	161	G
36	1	166	C
36	1	168	U
36	1	169	U
36	1	170	G
36	1	174	C
36	1	182	U

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Mol	Chain	Res	Type
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	199	A
36	1	200	C
36	1	210	U
36	1	213	A
36	1	217	U
36	1	218	G
36	1	219	A
36	1	220	G
36	1	221	A
36	1	238	A
36	1	240	U
36	1	242	C
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	265	A
36	1	269	G
36	1	279	U
36	1	282	G
36	1	283	G
36	1	284	A
36	1	286	U
36	1	288	C
36	1	295	A
36	1	296	A
36	1	298	U
36	1	301	G
36	1	303	G
36	1	304	G
36	1	305	U
36	1	315	C
36	1	316	U
36	1	323	A
36	1	329	U
36	1	335	G

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Mol	Chain	Res	Type
36	1	336	A
36	1	339	C
36	1	349	A
36	1	350	C
36	1	362	U
36	1	370	U
36	1	376	G
36	1	397	A
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	404	G
36	1	420	G
36	1	421	G
36	1	422	A
36	1	495	G
36	1	498	A
36	1	510	G
36	1	516	A
36	1	518	G
36	1	520	U
36	1	521	A
36	1	535	G
36	1	544	C
36	1	545	U
36	1	546	C
36	1	547	G
36	1	548	G
36	1	549	U
36	1	551	A
36	1	552	G
36	1	555	U
36	1	556	U
36	1	557	A
36	1	558	U
36	1	559	A
36	1	569	A
36	1	578	A
36	1	579	G
36	1	604	G

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Mol	Chain	Res	Type
36	1	609	G
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	637	C
36	1	638	C
36	1	639	G
36	1	646	A
36	1	649	A
36	1	657	A
36	1	660	A
36	1	677	A
36	1	679	U
36	1	681	U
36	1	690	A
36	1	691	A
36	1	702	C
36	1	704	U
36	1	705	A
36	1	706	A
36	1	708	G
36	1	712	G
36	1	713	U
36	1	715	A
36	1	716	A
36	1	719	U
36	1	720	A
36	1	726	G
36	1	727	G
36	1	747	A
36	1	758	C
36	1	763	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	781	G
36	1	784	A
36	1	785	G

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Mol	Chain	Res	Type
36	1	790	U
36	1	800	G
36	1	801	A
36	1	802	C
36	1	806	A
36	1	808	A
36	1	817	A
36	1	819	U
36	1	830	A
36	1	849	C
36	1	851	C
36	1	854	G
36	1	861	C
36	1	871	U
36	1	874	U
36	1	877	C
36	1	879	U
36	1	883	A
36	1	896	A
36	1	900	G
36	1	907	G
36	1	908	G
36	1	913	A
36	1	914	A
36	1	916	G
36	1	917	A
36	1	920	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	934	G
36	1	937	G
36	1	943	U
36	1	944	C
36	1	959	C
36	1	960	U
36	1	974	G
36	1	978	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C

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Mol	Chain	Res	Type
36	1	993	G
36	1	994	G
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1014	U
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1037	C
36	1	1041	U
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1063	G
36	1	1064	A
36	1	1065	A
36	1	1071	U
36	1	1072	G
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1087	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1123	U
36	1	1128	U
36	1	1129	A

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Mol	Chain	Res	Type
36	1	1131	G
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1175	C
36	1	1177	G
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1189	C
36	1	1191	U
36	1	1192	C
36	1	1193	A
36	1	1200	A
36	1	1201	C
36	1	1202	A
36	1	1206	G
36	1	1209	G
36	1	1221	A
36	1	1222	G
36	1	1223	A
36	1	1229	G
36	1	1281	G
36	1	1285	G
36	1	1292	C
36	1	1295	G
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1312	C
36	1	1313	G
36	1	1318	A
36	1	1325	U
36	1	1330	A
36	1	1345	G
36	1	1346	G
36	1	1348	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1386	A
36	1	1392	G

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Mol	Chain	Res	Type
36	1	1399	A
36	1	1400	G
36	1	1417	G
36	1	1418	A
36	1	1419	A
36	1	1429	G
36	1	1431	G
36	1	1433	A
36	1	1434	G
36	1	1437	C
36	1	1438	U
36	1	1446	A
36	1	1450	G
36	1	1455	U
36	1	1481	A
36	1	1482	A
36	1	1484	U
36	1	1485	G
36	1	1502	C
36	1	1503	A
36	1	1508	C
36	1	1510	G
36	1	1519	G
36	1	1522	U
36	1	1524	A
36	1	1526	U
36	1	1527	C
36	1	1533	U
36	1	1534	A
36	1	1536	G
36	1	1541	G
36	1	1554	U
36	1	1555	U
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1565	G
36	1	1573	G
36	1	1574	C

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Mol	Chain	Res	Type
36	1	1575	A
36	1	1576	G
36	1	1579	C
36	1	1580	A
36	1	1581	C
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1594	A
36	1	1595	U
36	1	1596	C
36	1	1605	A
36	1	1607	U
36	1	1608	C
36	1	1613	A
36	1	1614	C
36	1	1619	A
36	1	1620	U
36	1	1621	A
36	1	1625	A
36	1	1629	U
36	1	1632	A
36	1	1636	U
36	1	1638	A
36	1	1639	C
36	1	1641	U
36	1	1643	A
36	1	1645	U
36	1	1647	A
36	1	1649	U
36	1	1655	G
36	1	1656	A
36	1	1657	C
36	1	1658	G
36	1	1659	U
36	1	1683	A
36	1	1708	C
36	1	1717	U
36	1	1724	U
36	1	1725	C

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Mol	Chain	Res	Type
36	1	1729	A
36	1	1736	G
36	1	1741	A
36	1	1750	A
36	1	1751	G
36	1	1759	C
36	1	1760	A
36	1	1761	C
36	1	1762	C
36	1	1763	U
36	1	1764	U
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1769	G
36	1	1770	G
36	1	1779	C
36	1	1780	G
36	1	1781	C
36	1	1793	C
36	1	1795	U
36	1	1797	A
36	1	1801	U
36	1	1806	A
36	1	1808	G
36	1	1809	A
36	1	1810	A
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1849	C
36	1	1855	U
36	1	1858	A

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Mol	Chain	Res	Type
36	1	1866	C
36	1	1867	A
36	1	1876	U
36	1	1878	G
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1901	A
36	1	1906	G
36	1	1913	A
36	1	1926	C
36	1	1930	A
36	1	1931	U
36	1	1932	A
36	1	1937	U
36	1	1948	G
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	2094	C
36	1	2102	U
36	1	2107	A
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2117	A
36	1	2121	G
36	1	2122	G
36	1	2125	A
36	1	2130	G
36	1	2131	A
36	1	2134	G
36	1	2139	A
36	1	2140	U
36	1	2142	A
36	1	2144	A
36	1	2158	A
36	1	2169	G
36	1	2174	G
36	1	2178	A
36	1	2179	C
36	1	2184	U

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Mol	Chain	Res	Type
36	1	2193	U
36	1	2198	A
36	1	2201	G
36	1	2205	U
36	1	2206	G
36	1	2207	A
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2225	U
36	1	2228	A
36	1	2244	A
36	1	2248	C
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	A
36	1	2258	U
36	1	2259	A
36	1	2272	G
36	1	2273	G
36	1	2277	C
36	1	2281	A
36	1	2282	U
36	1	2283	G
36	1	2288	G
36	1	2298	U
36	1	2307	G
36	1	2308	C
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2319	U
36	1	2334	U
36	1	2335	G
36	1	2336	U
36	1	2361	A
36	1	2364	G
36	1	2372	A
36	1	2373	A
36	1	2374	C

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Mol	Chain	Res	Type
36	1	2375	G
36	1	2383	C
36	1	2385	G
36	1	2393	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2411	U
36	1	2418	G
36	1	2434	U
36	1	2435	G
36	1	2514	U
36	1	2515	A
36	1	2521	U
36	1	2522	G
36	1	2523	A
36	1	2525	G
36	1	2526	C
36	1	2531	C
36	1	2532	U
36	1	2533	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2550	U
36	1	2552	C
36	1	2553	U
36	1	2554	A
36	1	2555	G
36	1	2558	U
36	1	2559	U
36	1	2560	C
36	1	2561	A

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Mol	Chain	Res	Type
36	1	2567	C
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2574	G
36	1	2577	C
36	1	2580	A
36	1	2581	U
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2595	A
36	1	2606	G
36	1	2607	G
36	1	2608	G
36	1	2614	G
36	1	2619	G
36	1	2620	G
36	1	2637	A
36	1	2652	U
36	1	2656	A
36	1	2657	A
36	1	2658	G
36	1	2672	G
36	1	2674	A
36	1	2676	A
36	1	2677	G
36	1	2681	U
36	1	2684	C
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2695	A
36	1	2696	A
36	1	2700	G
36	1	2705	A
36	1	2714	G
36	1	2728	G

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Mol	Chain	Res	Type
36	1	2737	C
36	1	2738	A
36	1	2740	A
36	1	2752	U
36	1	2753	G
36	1	2754	G
36	1	2758	A
36	1	2762	A
36	1	2768	U
36	1	2772	C
36	1	2773	C
36	1	2775	U
36	1	2777	G
36	1	2778	G
36	1	2780	A
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2802	A
36	1	2808	A
36	1	2809	C
36	1	2810	C
36	1	2814	G
36	1	2817	A
36	1	2818	U
36	1	2821	C
36	1	2822	U
36	1	2827	U
36	1	2837	A
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2846	U
36	1	2847	A
36	1	2853	A
36	1	2856	G
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2873	U

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Mol	Chain	Res	Type
36	1	2875	U
36	1	2876	C
36	1	2879	C
36	1	2880	U
36	1	2887	A
36	1	2889	C
36	1	2899	C
36	1	2910	A
36	1	2912	G
36	1	2914	G
36	1	2922	G
36	1	2923	U
36	1	2927	C
36	1	2928	C
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2945	G
36	1	2946	A
36	1	2947	G
36	1	2951	G
36	1	2954	U
36	1	2955	U
36	1	2957	G
36	1	2965	U
36	1	2966	G
36	1	2971	A
36	1	2972	G
36	1	2974	U
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2997	G
36	1	3003	G
36	1	3012	A
36	1	3030	G
36	1	3056	U
36	1	3057	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3080	G

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Mol	Chain	Res	Type
36	1	3086	A
36	1	3092	C
36	1	3115	C
36	1	3122	A
36	1	3123	A
36	1	3129	A
36	1	3130	A
36	1	3131	U
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3164	C
36	1	3165	A
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3196	U
36	1	3199	G
36	1	3207	U
36	1	3209	A
36	1	3210	A
36	1	3213	A
36	1	3216	G
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3224	G
36	1	3227	A
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3242	G
36	1	3243	A
36	1	3245	A
36	1	3247	G

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Mol	Chain	Res	Type
36	1	3253	G
36	1	3259	U
36	1	3268	A
36	1	3269	U
36	1	3270	U
36	1	3271	G
36	1	3272	C
36	1	3276	G
36	1	3279	A
36	1	3281	U
36	1	3287	U
36	1	3289	G
36	1	3294	A
36	1	3295	A
36	1	3303	G
36	1	3304	U
36	1	3307	A
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3335	A
36	1	3340	G
36	1	3341	U
36	1	3342	A
36	1	3351	U
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3358	U
36	1	3359	A
36	1	3360	C
36	1	3363	U
36	1	3364	C
36	1	3368	U
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U

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Mol	Chain	Res	Type
36	1	3383	G
36	1	3386	G
36	1	3390	G
37	3	7	G
37	3	13	A
37	3	22	A
37	3	41	G
37	3	53	U
37	3	54	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	92	A
37	3	93	C
37	3	95	A
37	3	99	G
37	3	102	A
37	3	112	G
37	3	114	U
37	3	116	C
37	3	119	U
37	3	120	C
37	3	121	U
38	4	34	U
38	4	35	C
38	4	37	A
38	4	48	A
38	4	51	G
38	4	52	A
38	4	53	A
38	4	59	A
38	4	60	U
38	4	62	C
38	4	63	G
38	4	78	G
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G

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Mol	Chain	Res	Type
38	4	86	U
38	4	87	G
38	4	89	A
38	4	90	U
38	4	91	C
38	4	95	G
38	4	96	A
38	4	102	U
38	4	104	A
38	4	106	C
38	4	110	C
38	4	111	A
38	4	112	U
38	4	113	U
38	4	123	G
38	4	124	G
38	4	125	U
38	4	126	A
38	4	127	U
38	4	128	U
38	4	129	C
38	4	132	G
38	4	137	C
38	4	138	A
38	4	151	C
38	4	152	G
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	42	G
1	6	45	U
1	6	46	A
1	6	47	A
1	6	50	C
1	6	57	G

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Mol	Chain	Res	Type
1	6	60	U
1	6	63	G
1	6	67	A
1	6	68	A
1	6	69	G
1	6	71	A
1	6	77	U
1	6	103	A
1	6	104	A
1	6	114	C
1	6	115	G
1	6	126	A
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	158	U
1	6	159	U
1	6	160	C
1	6	166	C
1	6	178	U
1	6	179	A
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	196	G
1	6	197	A
1	6	199	G
1	6	200	A
1	6	215	A
1	6	218	A
1	6	220	A
1	6	224	C

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Mol	Chain	Res	Type
1	6	226	A
1	6	230	C
1	6	232	U
1	6	233	C
1	6	234	G
1	6	237	C
1	6	238	U
1	6	239	C
1	6	240	U
1	6	241	U
1	6	243	G
1	6	248	U
1	6	250	C
1	6	257	A
1	6	261	U
1	6	265	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	276	C
1	6	277	U
1	6	278	U
1	6	280	U
1	6	281	G
1	6	299	A
1	6	301	A
1	6	314	C
1	6	316	A
1	6	318	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	331	A
1	6	333	A
1	6	337	G
1	6	338	C
1	6	344	A
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	370	A

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Mol	Chain	Res	Type
1	6	387	A
1	6	390	G
1	6	391	A
1	6	399	A
1	6	400	A
1	6	401	A
1	6	402	C
1	6	403	G
1	6	404	G
1	6	411	C
1	6	416	A
1	6	417	A
1	6	418	G
1	6	423	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	437	A
1	6	439	U
1	6	444	C
1	6	448	C
1	6	452	A
1	6	454	U
1	6	460	A
1	6	468	A
1	6	475	A
1	6	480	G
1	6	484	C
1	6	485	A
1	6	486	G
1	6	487	G
1	6	488	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	507	U
1	6	508	U
1	6	510	G
1	6	511	A

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Mol	Chain	Res	Type
1	6	512	A
1	6	513	U
1	6	514	G
1	6	515	A
1	6	519	C
1	6	523	G
1	6	527	A
1	6	534	A
1	6	535	A
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	549	G
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	560	U
1	6	565	C
1	6	568	G
1	6	570	A
1	6	571	G
1	6	572	C
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	596	C
1	6	609	U
1	6	610	G
1	6	619	A
1	6	620	A
1	6	621	A

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Mol	Chain	Res	Type
1	6	622	A
1	6	623	A
1	6	625	C
1	6	630	A
1	6	635	A
1	6	639	U
1	6	640	U
1	6	645	C
1	6	648	G
1	6	688	G
1	6	691	C
1	6	696	C
1	6	698	U
1	6	742	U
1	6	743	U
1	6	751	G
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	766	U
1	6	774	A
1	6	775	G
1	6	777	C
1	6	778	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	811	A
1	6	812	A
1	6	820	U
1	6	826	U
1	6	830	U
1	6	831	U
1	6	835	U
1	6	856	A
1	6	861	U

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Mol	Chain	Res	Type
1	6	862	A
1	6	863	A
1	6	876	G
1	6	886	U
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	926	A
1	6	933	A
1	6	935	U
1	6	942	G
1	6	951	A
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	983	A
1	6	992	A
1	6	993	A
1	6	995	A
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1025	A
1	6	1026	A
1	6	1028	C
1	6	1029	U
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1062	A
1	6	1071	U

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Mol	Chain	Res	Type
1	6	1072	C
1	6	1074	G
1	6	1082	C
1	6	1092	A
1	6	1093	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1099	U
1	6	1100	G
1	6	1111	G
1	6	1113	A
1	6	1138	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1164	G
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1197	C
1	6	1198	G
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1207	C
1	6	1208	A
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1225	U
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1239	U
1	6	1241	G
1	6	1243	G
1	6	1244	A
1	6	1245	G

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Mol	Chain	Res	Type
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1285	U
1	6	1286	U
1	6	1291	G
1	6	1301	U
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1321	A
1	6	1338	C
1	6	1341	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1348	A
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1370	U
1	6	1371	A
1	6	1383	G
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1413	U
1	6	1414	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1432	U
1	6	1433	G
1	6	1445	G
1	6	1446	A
1	6	1448	G

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Mol	Chain	Res	Type
1	6	1459	C
1	6	1460	A
1	6	1461	C
1	6	1471	A
1	6	1473	U
1	6	1481	C
1	6	1482	C
1	6	1486	G
1	6	1487	A
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1531	G
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1574	G
1	6	1582	U
1	6	1584	G
1	6	1590	G
1	6	1601	G
1	6	1616	G
1	6	1621	U
1	6	1637	C
1	6	1638	G
1	6	1656	U
1	6	1657	U

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Mol	Chain	Res	Type
1	6	1658	G
1	6	1663	G
1	6	1666	U
1	6	1678	A
1	6	1681	A
1	6	1682	U
1	6	1684	U
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1719	A
1	6	1720	G
1	6	1736	G
1	6	1742	U
1	6	1750	A
1	6	1753	A
1	6	1754	A
1	6	1755	A
1	6	1756	A
1	6	1757	G
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1790	A
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	26	A
36	5	40	A
36	5	43	A
36	5	44	U
36	5	49	A

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Mol	Chain	Res	Type
36	5	57	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	76	G
36	5	85	A
36	5	92	G
36	5	94	G
36	5	96	G
36	5	99	A
36	5	101	G
36	5	109	A
36	5	110	G
36	5	111	C
36	5	115	A
36	5	116	A
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	136	G
36	5	146	U
36	5	148	G
36	5	152	U
36	5	156	G
36	5	157	A
36	5	158	G
36	5	166	C
36	5	171	G
36	5	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	210	U
36	5	211	A
36	5	213	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	228	U

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Mol	Chain	Res	Type
36	5	239	G
36	5	240	U
36	5	241	G
36	5	245	U
36	5	246	U
36	5	248	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	262	U
36	5	263	C
36	5	269	G
36	5	274	G
36	5	282	G
36	5	283	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	296	A
36	5	315	C
36	5	316	U
36	5	323	A
36	5	329	U
36	5	334	A
36	5	338	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	351	A
36	5	369	A
36	5	370	U
36	5	376	G
36	5	387	A
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	404	G
36	5	420	G

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Mol	Chain	Res	Type
36	5	421	G
36	5	422	A
36	5	424	G
36	5	440	A
36	5	495	G
36	5	507	U
36	5	510	G
36	5	515	C
36	5	518	G
36	5	520	U
36	5	521	A
36	5	535	G
36	5	542	G
36	5	546	C
36	5	548	G
36	5	549	U
36	5	555	U
36	5	556	U
36	5	557	A
36	5	559	A
36	5	578	A
36	5	579	G
36	5	594	U
36	5	600	G
36	5	604	G
36	5	609	G
36	5	611	A
36	5	620	U
36	5	621	A
36	5	622	A
36	5	625	G
36	5	633	C
36	5	636	C
36	5	638	C
36	5	649	A
36	5	653	A
36	5	660	A
36	5	661	G
36	5	677	A
36	5	681	U
36	5	682	U
36	5	683	U

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Mol	Chain	Res	Type
36	5	705	A
36	5	706	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	720	A
36	5	726	G
36	5	736	A
36	5	750	G
36	5	758	C
36	5	761	A
36	5	766	U
36	5	767	U
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G
36	5	786	A
36	5	801	A
36	5	802	C
36	5	806	A
36	5	816	A
36	5	817	A
36	5	820	A
36	5	826	G
36	5	829	U
36	5	830	A
36	5	834	U
36	5	837	A
36	5	851	C
36	5	852	U
36	5	857	G
36	5	861	C
36	5	866	A
36	5	869	G
36	5	874	U
36	5	875	G
36	5	877	C
36	5	879	U
36	5	880	G
36	5	883	A
36	5	890	C

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Mol	Chain	Res	Type
36	5	896	A
36	5	897	U
36	5	907	G
36	5	908	G
36	5	910	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	924	G
36	5	932	U
36	5	933	A
36	5	937	G
36	5	944	C
36	5	952	A
36	5	959	C
36	5	960	U
36	5	979	U
36	5	980	A
36	5	994	G
36	5	995	U
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1010	G
36	5	1014	U
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1034	U
36	5	1035	G
36	5	1047	A

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Mol	Chain	Res	Type
36	5	1049	C
36	5	1063	G
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1092	C
36	5	1093	A
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1114	U
36	5	1115	G
36	5	1116	G
36	5	1117	G
36	5	1129	A
36	5	1131	G
36	5	1143	A
36	5	1152	G
36	5	1153	A
36	5	1154	A
36	5	1155	C
36	5	1159	A
36	5	1160	C
36	5	1161	G
36	5	1169	A
36	5	1177	G
36	5	1178	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1191	U
36	5	1200	A
36	5	1201	C
36	5	1209	G
36	5	1212	A

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Mol	Chain	Res	Type
36	5	1221	A
36	5	1222	G
36	5	1223	A
36	5	1229	G
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1244	A
36	5	1245	A
36	5	1246	G
36	5	1248	C
36	5	1252	A
36	5	1258	U
36	5	1259	A
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1270	A
36	5	1281	G
36	5	1283	C
36	5	1285	G
36	5	1301	A
36	5	1305	U
36	5	1308	A
36	5	1309	U
36	5	1312	C
36	5	1313	G
36	5	1318	A
36	5	1330	A
36	5	1346	G
36	5	1348	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1385	C
36	5	1386	A
36	5	1392	G
36	5	1399	A

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Mol	Chain	Res	Type
36	5	1400	G
36	5	1417	G
36	5	1419	A
36	5	1421	G
36	5	1427	U
36	5	1428	A
36	5	1430	U
36	5	1431	G
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1472	U
36	5	1475	A
36	5	1481	A
36	5	1482	A
36	5	1483	G
36	5	1488	G
36	5	1490	A
36	5	1502	C
36	5	1503	A
36	5	1508	C
36	5	1515	A
36	5	1527	C
36	5	1528	G
36	5	1536	G
36	5	1541	G
36	5	1550	C
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1580	A

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Mol	Chain	Res	Type
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1584	U
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1596	C
36	5	1605	A
36	5	1607	U
36	5	1608	C
36	5	1620	U
36	5	1629	U
36	5	1632	A
36	5	1633	C
36	5	1639	C
36	5	1641	U
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1646	G
36	5	1655	G
36	5	1658	G
36	5	1683	A
36	5	1715	A
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1756	C
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1767	C
36	5	1770	G
36	5	1775	G
36	5	1778	G
36	5	1780	G
36	5	1793	C

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Mol	Chain	Res	Type
36	5	1795	U
36	5	1797	A
36	5	1810	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1834	U
36	5	1837	U
36	5	1838	G
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1851	G
36	5	1866	C
36	5	1876	U
36	5	1877	U
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1884	A
36	5	1885	U
36	5	1886	A
36	5	1894	U
36	5	1901	A
36	5	1906	G
36	5	1918	C
36	5	1930	A
36	5	1935	G
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2114	C
36	5	2121	G

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Mol	Chain	Res	Type
36	5	2122	G
36	5	2131	A
36	5	2134	G
36	5	2140	U
36	5	2142	A
36	5	2144	A
36	5	2158	A
36	5	2169	G
36	5	2175	U
36	5	2176	U
36	5	2179	C
36	5	2188	A
36	5	2193	U
36	5	2205	U
36	5	2207	A
36	5	2208	A
36	5	2209	U
36	5	2210	G
36	5	2222	A
36	5	2223	A
36	5	2228	A
36	5	2229	A
36	5	2244	A
36	5	2246	G
36	5	2248	C
36	5	2249	G
36	5	2250	G
36	5	2251	G
36	5	2252	A
36	5	2253	G
36	5	2254	U
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2261	G
36	5	2262	A
36	5	2263	C
36	5	2266	U
36	5	2267	C
36	5	2269	U
36	5	2270	A

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Mol	Chain	Res	Type
36	5	2272	G
36	5	2279	A
36	5	2280	A
36	5	2281	A
36	5	2282	U
36	5	2288	G
36	5	2306	C
36	5	2307	G
36	5	2309	A
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2332	A
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2361	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2379	U
36	5	2385	G
36	5	2388	U
36	5	2393	G
36	5	2394	G
36	5	2397	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2422	C
36	5	2434	U
36	5	2435	G
36	5	2437	G
36	5	2442	G
36	5	2507	C
36	5	2510	U
36	5	2511	A
36	5	2512	C

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Mol	Chain	Res	Type
36	5	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2524	A
36	5	2525	G
36	5	2526	C
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2541	U
36	5	2542	U
36	5	2543	U
36	5	2544	U
36	5	2545	C
36	5	2547	A
36	5	2549	G
36	5	2550	U
36	5	2552	C
36	5	2555	G
36	5	2556	C
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2573	G
36	5	2574	G
36	5	2581	U
36	5	2584	G
36	5	2585	G
36	5	2586	G
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2610	G
36	5	2614	G
36	5	2619	G
36	5	2637	A

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Mol	Chain	Res	Type
36	5	2649	A
36	5	2652	U
36	5	2656	A
36	5	2657	A
36	5	2662	G
36	5	2663	G
36	5	2674	A
36	5	2677	G
36	5	2683	U
36	5	2689	A
36	5	2691	A
36	5	2694	A
36	5	2695	A
36	5	2696	A
36	5	2705	A
36	5	2714	G
36	5	2719	U
36	5	2728	G
36	5	2729	U
36	5	2737	C
36	5	2752	U
36	5	2753	G
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2778	G
36	5	2779	A
36	5	2796	G
36	5	2797	C
36	5	2798	C
36	5	2800	G
36	5	2801	A
36	5	2803	A
36	5	2808	A
36	5	2810	C
36	5	2814	G
36	5	2816	G
36	5	2817	A
36	5	2818	U
36	5	2819	A
36	5	2821	C
36	5	2829	U

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Mol	Chain	Res	Type
36	5	2834	G
36	5	2845	A
36	5	2846	U
36	5	2853	A
36	5	2856	G
36	5	2871	G
36	5	2872	A
36	5	2873	U
36	5	2875	U
36	5	2876	C
36	5	2877	G
36	5	2886	U
36	5	2887	A
36	5	2888	U
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2910	A
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2943	G
36	5	2945	G
36	5	2947	G
36	5	2948	C
36	5	2950	G
36	5	2951	G
36	5	2954	U
36	5	2955	U
36	5	2957	G
36	5	2970	C
36	5	2971	A
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2995	A
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3025	C

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Mol	Chain	Res	Type
36	5	3028	G
36	5	3030	G
36	5	3034	C
36	5	3049	A
36	5	3056	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3080	G
36	5	3086	A
36	5	3087	A
36	5	3092	C
36	5	3122	A
36	5	3129	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3150	A
36	5	3151	U
36	5	3153	U
36	5	3158	G
36	5	3159	C
36	5	3164	C
36	5	3165	A
36	5	3170	A
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3175	U
36	5	3176	G
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3194	C
36	5	3195	U
36	5	3196	U
36	5	3198	U
36	5	3207	U
36	5	3210	A
36	5	3216	G
36	5	3217	C

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Mol	Chain	Res	Type
36	5	3218	A
36	5	3219	G
36	5	3224	G
36	5	3227	A
36	5	3228	C
36	5	3229	G
36	5	3238	G
36	5	3243	A
36	5	3244	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3251	U
36	5	3253	G
36	5	3259	U
36	5	3260	G
36	5	3265	C
36	5	3266	G
36	5	3269	U
36	5	3270	U
36	5	3271	G
36	5	3273	A
36	5	3276	G
36	5	3279	A
36	5	3281	U
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3335	A
36	5	3340	G
36	5	3341	U
36	5	3342	A
36	5	3343	G

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Mol	Chain	Res	Type
36	5	3345	G
36	5	3348	G
36	5	3350	C
36	5	3351	U
36	5	3352	U
36	5	3353	G
36	5	3354	U
36	5	3355	U
36	5	3356	G
36	5	3357	U
36	5	3358	U
36	5	3368	U
36	5	3369	G
36	5	3378	C
36	5	3382	U
36	5	3386	G
36	5	3389	U
36	5	3390	G
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	23	A
37	7	38	U
37	7	54	U
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	93	C
37	7	95	A
37	7	101	G
37	7	102	A
37	7	103	A
37	7	112	G
38	8	16	G
38	8	18	U
38	8	21	C
38	8	34	U
38	8	35	C
38	8	48	A
38	8	49	G
38	8	52	A

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Mol	Chain	Res	Type
38	8	53	A
38	8	58	G
38	8	59	A
38	8	62	C
38	8	63	G
38	8	75	G
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	85	G
38	8	86	U
38	8	87	G
38	8	90	U
38	8	91	C
38	8	95	G
38	8	103	G
38	8	104	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	123	G
38	8	125	U
38	8	126	A
38	8	127	U
38	8	128	U
38	8	138	A
38	8	152	G
38	8	155	A
38	8	156	U
38	8	157	U

All (344) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	72	A
1	2	73	U

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Mol	Chain	Res	Type
1	2	74	U
1	2	75	U
1	2	103	A
1	2	139	C
1	2	158	U
1	2	187	G
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	321	C
1	2	322	G
1	2	417	A
1	2	484	C
1	2	501	U
1	2	503	G
1	2	512	A
1	2	541	A
1	2	542	A
1	2	555	A
1	2	571	G
1	2	582	U
1	2	622	A
1	2	755	A
1	2	779	U
1	2	782	U
1	2	794	U
1	2	811	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	913	G
1	2	1051	G
1	2	1058	U
1	2	1059	U
1	2	1081	A
1	2	1096	C
1	2	1150	G
1	2	1157	A
1	2	1196	A
1	2	1204	A
1	2	1207	C

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Mol	Chain	Res	Type
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1314	U
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1370	U
1	2	1473	U
1	2	1481	C
1	2	1489	U
1	2	1493	A
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1635	A
1	2	1656	U
1	2	1711	C
1	2	1761	U
36	1	13	A
36	1	21	G
36	1	40	A
36	1	133	U
36	1	216	G
36	1	218	G
36	1	219	A
36	1	220	G
36	1	239	G
36	1	282	G
36	1	304	G
36	1	420	G
36	1	518	G
36	1	547	G
36	1	548	G
36	1	558	U
36	1	588	G
36	1	594	U
36	1	637	C
36	1	715	A
36	1	763	G
36	1	764	U

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Mol	Chain	Res	Type
36	1	765	C
36	1	816	A
36	1	873	C
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1096	U
36	1	1097	G
36	1	1103	A
36	1	1222	G
36	1	1284	C
36	1	1307	G
36	1	1329	U
36	1	1355	A
36	1	1484	U
36	1	1514	G
36	1	1554	U
36	1	1555	U
36	1	1556	C
36	1	1562	C
36	1	1572	U
36	1	1593	A
36	1	1594	A
36	1	1607	U
36	1	1648	A
36	1	1716	U
36	1	1761	C
36	1	1763	U
36	1	1815	U
36	1	1816	A
36	1	1820	U
36	1	2101	C
36	1	2112	U
36	1	2206	G
36	1	2209	U
36	1	2227	C
36	1	2249	G
36	1	2258	U
36	1	2281	A
36	1	2282	U

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Mol	Chain	Res	Type
36	1	2360	C
36	1	2372	A
36	1	2513	U
36	1	2522	G
36	1	2525	G
36	1	2537	U
36	1	2541	U
36	1	2551	U
36	1	2554	A
36	1	2570	U
36	1	2571	U
36	1	2573	G
36	1	2585	G
36	1	2593	A
36	1	2689	A
36	1	2772	C
36	1	2801	A
36	1	2808	A
36	1	2817	A
36	1	2818	U
36	1	2913	C
36	1	2970	C
36	1	3078	U
36	1	3121	U
36	1	3169	U
36	1	3195	U
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3275	U
36	1	3303	G
36	1	3317	U
36	1	3341	U
36	1	3355	U
36	1	3375	A
36	1	3377	G
36	1	3389	U
37	3	52	G
38	4	60	U
38	4	85	G
38	4	112	U
38	4	125	U

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Mol	Chain	Res	Type
38	4	126	A
38	4	127	U
1	6	25	C
1	6	76	A
1	6	103	A
1	6	114	C
1	6	136	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	240	U
1	6	272	U
1	6	277	U
1	6	321	C
1	6	400	A
1	6	417	A
1	6	422	G
1	6	454	U
1	6	512	A
1	6	542	A
1	6	555	A
1	6	558	U
1	6	622	A
1	6	647	G
1	6	695	U
1	6	755	A
1	6	912	U
1	6	913	G
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1098	U
1	6	1196	A
1	6	1207	C
1	6	1227	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1413	U
1	6	1481	C
1	6	1489	U

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Mol	Chain	Res	Type
1	6	1491	U
1	6	1492	A
1	6	1535	U
1	6	1568	C
1	6	1573	A
1	6	1615	C
1	6	1620	C
1	6	1657	U
1	6	1681	A
1	6	1719	A
1	6	1754	A
36	5	65	A
36	5	151	A
36	5	170	G
36	5	240	U
36	5	282	G
36	5	369	A
36	5	420	G
36	5	518	G
36	5	557	A
36	5	648	C
36	5	705	A
36	5	715	A
36	5	735	A
36	5	765	C
36	5	766	U
36	5	816	A
36	5	873	C
36	5	879	U
36	5	916	G
36	5	993	G
36	5	1015	U
36	5	1016	C
36	5	1027	A
36	5	1033	U
36	5	1062	A
36	5	1064	A
36	5	1081	U
36	5	1096	U
36	5	1103	A
36	5	1152	G
36	5	1154	A

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Mol	Chain	Res	Type
36	5	1178	G
36	5	1189	C
36	5	1222	G
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1317	A
36	5	1329	U
36	5	1355	A
36	5	1481	A
36	5	1560	G
36	5	1574	C
36	5	1581	C
36	5	1582	C
36	5	1607	U
36	5	1630	U
36	5	1655	G
36	5	1716	U
36	5	1761	C
36	5	1793	C
36	5	1815	U
36	5	1816	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1878	G
36	5	1879	A
36	5	1888	U
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2206	G
36	5	2207	A
36	5	2209	U
36	5	2222	A
36	5	2249	G
36	5	2256	A
36	5	2260	U
36	5	2281	A
36	5	2282	U
36	5	2372	A

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Mol	Chain	Res	Type
36	5	2373	A
36	5	2374	C
36	5	2400	G
36	5	2418	G
36	5	2513	U
36	5	2514	U
36	5	2522	G
36	5	2537	U
36	5	2585	G
36	5	2593	A
36	5	2662	G
36	5	2677	G
36	5	2682	C
36	5	2772	C
36	5	2817	A
36	5	2818	U
36	5	2872	A
36	5	2887	A
36	5	2950	G
36	5	2970	C
36	5	3078	U
36	5	3121	U
36	5	3158	G
36	5	3172	A
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3269	U
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3341	U
36	5	3352	U
36	5	3353	G
36	5	3357	U
36	5	3382	U
37	7	86	U
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	84	C

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Mol	Chain	Res	Type
38	8	111	A
38	8	126	A
38	8	156	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1260 ligands modelled in this entry, 1239 are monoatomic - leaving 21 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	$\# Z > 2$
82	GET	1	3812	-	33,36,36	0.31	0	43,55,55	1.18	3 (6%)
82	GET	1	3810	-	33,36,36	0.32	0	43,55,55	1.57	7 (16%)
82	GET	6	2014	-	33,36,36	0.17	0	43,55,55	1.08	4 (9%)
82	GET	6	2013	-	33,36,36	0.24	0	43,55,55	0.69	1 (2%)
82	GET	1	3813	-	33,36,36	0.42	0	43,55,55	1.83	9 (20%)
82	GET	5	3849	-	33,36,36	0.42	0	43,55,55	1.25	3 (6%)
82	GET	2	2014	-	33,36,36	0.39	0	43,55,55	1.29	5 (11%)
82	GET	5	3850	-	33,36,36	0.30	0	43,55,55	1.18	4 (9%)
82	GET	1	3808	-	33,36,36	0.34	0	43,55,55	1.62	7 (16%)
82	GET	n6	201	-	33,36,36	0.22	0	43,55,55	1.11	4 (9%)
82	GET	5	3844	-	33,36,36	0.24	0	43,55,55	1.50	7 (16%)
82	GET	5	3847	-	33,36,36	0.40	0	43,55,55	1.50	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	GET	2	2012	-	33,36,36	0.30	0	43,55,55	0.98	2 (4%)
82	GET	5	3846	-	33,36,36	0.26	0	43,55,55	1.13	2 (4%)
82	GET	1	3809	-	33,36,36	0.28	0	43,55,55	1.04	5 (11%)
82	GET	2	2013	-	33,36,36	0.16	0	43,55,55	0.94	3 (6%)
82	GET	5	3851	-	33,36,36	0.21	0	43,55,55	0.66	1 (2%)
82	GET	1	3811	-	33,36,36	0.20	0	43,55,55	0.62	1 (2%)
82	GET	5	3848	-	33,36,36	0.26	0	43,55,55	1.76	3 (6%)
82	GET	5	3845	-	33,36,36	0.27	0	43,55,55	0.91	2 (4%)
82	GET	6	2015	-	33,36,36	1.93	8 (24%)	43,55,55	2.93	21 (48%)

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
82	GET	1	3812	-	-	6/13/74/74	0/3/3/3
82	GET	1	3810	-	-	2/13/74/74	0/3/3/3
82	GET	6	2014	-	-	6/13/74/74	0/3/3/3
82	GET	6	2013	-	-	1/13/74/74	0/3/3/3
82	GET	1	3813	-	-	7/13/74/74	0/3/3/3
82	GET	5	3849	-	-	4/13/74/74	0/3/3/3
82	GET	2	2014	-	-	5/13/74/74	1/3/3/3
82	GET	5	3850	-	-	6/13/74/74	0/3/3/3
82	GET	1	3808	-	-	9/13/74/74	0/3/3/3
82	GET	n6	201	-	-	6/13/74/74	0/3/3/3
82	GET	5	3844	-	-	5/13/74/74	0/3/3/3
82	GET	5	3847	-	-	8/13/74/74	0/3/3/3
82	GET	2	2012	-	-	2/13/74/74	1/3/3/3
82	GET	5	3846	-	-	6/13/74/74	0/3/3/3
82	GET	1	3809	-	-	10/13/74/74	0/3/3/3
82	GET	2	2013	-	-	6/13/74/74	0/3/3/3
82	GET	5	3851	-	-	6/13/74/74	0/3/3/3
82	GET	1	3811	-	-	1/13/74/74	0/3/3/3
82	GET	5	3848	-	-	3/13/74/74	0/3/3/3
82	GET	5	3845	-	-	1/13/74/74	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	GET	6	2015	-	-	5/13/74/74	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	6	2015	GET	C23-C33	5.14	1.64	1.53
82	6	2015	GET	C22-C12	3.63	1.61	1.53
82	6	2015	GET	C41-C31	3.54	1.61	1.52
82	6	2015	GET	C22-C32	2.91	1.60	1.53
82	6	2015	GET	C51-C61	2.68	1.56	1.52
82	6	2015	GET	O51-C11	2.40	1.48	1.41
82	6	2015	GET	C41-C51	2.17	1.58	1.52
82	6	2015	GET	C31-C21	-2.10	1.50	1.53

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	5	3848	GET	C23-C33-N33	-7.62	90.62	110.84
82	6	2015	GET	C11-C21-N21	7.35	123.45	110.20
82	6	2015	GET	O31-C31-C21	-7.02	97.61	110.22
82	1	3810	GET	O11-C11-C21	6.48	119.38	108.22
82	6	2015	GET	C31-C21-N21	-5.66	99.46	111.05
82	5	3847	GET	O11-C11-C21	5.56	117.79	108.22
82	6	2015	GET	O31-C31-C41	5.50	123.07	110.35
82	5	3848	GET	O51-C51-C41	5.40	115.46	107.87
82	6	2015	GET	C23-C33-N33	5.30	124.90	110.84
82	1	3813	GET	C23-C33-N33	-5.28	96.83	110.84
82	1	3808	GET	C23-C33-N33	-5.18	97.11	110.84
82	5	3846	GET	C23-C33-N33	-5.10	97.31	110.84
82	5	3849	GET	C23-C33-N33	-4.86	97.94	110.84
82	1	3813	GET	O11-C11-C21	4.72	116.35	108.22
82	n6	201	GET	O11-C11-C21	4.63	116.19	108.22
82	1	3813	GET	O62-C13-O53	4.62	119.36	109.08
82	6	2015	GET	O23-C23-C33	4.53	118.79	109.63
82	1	3812	GET	C23-C33-N33	-4.40	99.17	110.84
82	5	3847	GET	C11-C21-N21	4.33	118.01	110.20
82	5	3844	GET	O62-C62-C52	-4.09	96.40	107.28
82	1	3813	GET	O51-C11-C21	4.08	119.24	110.06
82	6	2014	GET	O11-C42-C32	-4.07	99.48	109.18
82	6	2015	GET	C71-C61-C51	4.05	116.77	112.02
82	2	2013	GET	O11-C42-C32	-4.03	99.57	109.18
82	6	2015	GET	O11-C42-C52	3.76	117.27	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	6	2015	GET	O51-C51-C61	3.69	116.39	107.18
82	2	2012	GET	O11-C42-C32	-3.61	100.56	109.18
82	1	3808	GET	O11-C42-C32	-3.61	100.56	109.18
82	5	3844	GET	O11-C42-C52	3.61	116.87	107.28
82	5	3844	GET	O11-C42-C32	-3.58	100.63	109.18
82	2	2014	GET	O51-C51-C41	3.57	112.88	107.87
82	5	3850	GET	C23-C33-N33	-3.56	101.41	110.84
82	5	3849	GET	C32-C22-C12	3.51	118.40	111.18
82	5	3847	GET	O62-C62-C12	-3.42	101.01	109.18
82	5	3845	GET	O11-C11-C21	3.40	114.08	108.22
82	1	3813	GET	C13-C23-C33	3.30	114.81	109.34
82	6	2015	GET	C11-O51-C51	3.30	118.38	113.06
82	1	3808	GET	O23-C23-C13	3.28	118.01	110.05
82	1	3810	GET	C32-C22-C12	3.27	117.90	111.18
82	1	3812	GET	C32-C22-C12	-3.23	104.56	111.18
82	6	2015	GET	O41-C41-C31	3.11	117.54	110.35
82	1	3813	GET	C53-O53-C13	3.08	116.50	111.53
82	1	3808	GET	C11-C21-N21	3.07	115.74	110.20
82	6	2013	GET	O62-C62-C12	-3.04	101.92	109.18
82	1	3809	GET	O62-C62-C12	-2.98	102.06	109.18
82	2	2014	GET	C71-C61-C51	2.97	115.50	112.02
82	5	3844	GET	O52-C52-C42	2.97	117.80	109.94
82	6	2015	GET	C31-C41-C51	2.95	116.41	109.68
82	1	3813	GET	C32-C22-C12	-2.93	105.16	111.18
82	6	2015	GET	O11-C11-O51	2.86	118.66	110.67
82	6	2014	GET	O11-C11-C21	-2.77	103.45	108.22
82	1	3812	GET	C13-C23-C33	2.71	113.83	109.34
82	6	2015	GET	O11-C11-C21	2.70	112.86	108.22
82	2	2013	GET	O11-C11-C21	-2.70	103.57	108.22
82	1	3810	GET	C53-O53-C13	2.68	115.86	111.53
82	2	2014	GET	O11-C42-C32	2.65	115.49	109.18
82	6	2015	GET	O62-C62-C12	-2.63	102.89	109.18
82	6	2015	GET	O61-C61-C51	2.63	113.87	108.72
82	5	3844	GET	C11-O51-C51	-2.58	108.90	113.06
82	2	2012	GET	C13-C23-C33	-2.57	105.09	109.34
82	1	3808	GET	O62-C13-C23	2.57	114.76	108.10
82	5	3847	GET	C62-C52-C42	2.54	114.23	108.96
82	n6	201	GET	C11-C21-N21	2.54	114.77	110.20
82	5	3850	GET	C71-C61-C51	2.53	114.98	112.02
82	n6	201	GET	C32-C22-C12	-2.51	106.04	111.18
82	1	3810	GET	C71-C61-C51	2.48	114.93	112.02
82	2	2013	GET	C23-C33-N33	-2.44	104.35	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	5	3850	GET	O62-C62-C52	-2.42	100.85	107.28
82	5	3849	GET	O62-C62-C52	2.41	113.69	107.28
82	6	2015	GET	O51-C11-C21	2.40	115.46	110.06
82	1	3809	GET	O51-C51-C61	2.37	113.10	107.18
82	1	3813	GET	C11-O51-C51	2.36	116.86	113.06
82	6	2015	GET	O52-C52-C62	2.36	116.19	109.94
82	2	2014	GET	C11-C21-N21	2.35	114.44	110.20
82	6	2015	GET	O52-C52-C42	2.35	116.17	109.94
82	1	3810	GET	O62-C62-C12	-2.34	103.60	109.18
82	5	3848	GET	C31-C41-C51	2.32	114.98	109.68
82	5	3846	GET	O62-C62-C12	-2.31	103.66	109.18
82	1	3810	GET	O11-C42-C32	2.29	114.64	109.18
82	5	3851	GET	C32-C22-C12	-2.28	106.50	111.18
82	2	2014	GET	O11-C11-C21	2.27	112.13	108.22
82	1	3808	GET	O52-C52-C42	2.26	115.94	109.94
82	6	2015	GET	C32-C22-C12	2.24	115.78	111.18
82	1	3810	GET	C13-C23-C33	2.22	113.01	109.34
82	n6	201	GET	C23-C33-N33	-2.19	105.04	110.84
82	5	3850	GET	O11-C42-C52	2.17	113.05	107.28
82	1	3809	GET	C62-C52-C42	2.16	113.44	108.96
82	5	3845	GET	C41-C31-C21	2.16	114.78	111.07
82	1	3808	GET	O51-C51-C41	2.15	110.89	107.87
82	1	3813	GET	O53-C13-C23	2.13	113.32	110.04
82	1	3811	GET	O11-C42-C32	-2.12	104.13	109.18
82	6	2014	GET	C71-C61-C51	2.10	114.48	112.02
82	6	2014	GET	C11-C21-N21	-2.08	106.46	110.20
82	5	3847	GET	O11-C42-C52	2.08	112.80	107.28
82	5	3844	GET	C11-C21-N21	2.07	113.94	110.20
82	1	3809	GET	O11-C42-C32	-2.07	104.23	109.18
82	5	3844	GET	O41-C41-C31	-2.07	105.55	110.35
82	6	2015	GET	C22-C12-N12	2.05	118.14	110.84
82	1	3809	GET	C32-C22-C12	2.05	115.39	111.18
82	5	3847	GET	O11-C42-C32	-2.02	104.36	109.18

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	2	2012	GET	C23-C33-N33-C93
82	2	2013	GET	C41-C51-C61-O61
82	2	2013	GET	C41-C51-C61-C71
82	2	2013	GET	O51-C51-C61-O61

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Mol	Chain	Res	Type	Atoms
82	2	2013	GET	C23-C33-N33-C93
82	2	2014	GET	C21-C11-O11-C42
82	2	2014	GET	C23-C33-N33-C93
82	1	3808	GET	C21-C11-O11-C42
82	1	3808	GET	C41-C51-C61-O61
82	1	3808	GET	C41-C51-C61-C71
82	1	3808	GET	O51-C51-C61-O61
82	1	3808	GET	O51-C51-C61-C71
82	1	3808	GET	C23-C13-O62-C62
82	1	3809	GET	C41-C51-C61-O61
82	1	3809	GET	C41-C51-C61-C71
82	1	3809	GET	O51-C51-C61-O61
82	1	3809	GET	C23-C33-N33-C93
82	1	3810	GET	C32-C42-O11-C11
82	1	3810	GET	C23-C33-N33-C93
82	1	3811	GET	C23-C33-N33-C93
82	1	3812	GET	C41-C51-C61-O61
82	1	3812	GET	C41-C51-C61-C71
82	1	3812	GET	O51-C51-C61-O61
82	1	3812	GET	O51-C51-C61-C71
82	1	3812	GET	C23-C33-N33-C93
82	1	3813	GET	C41-C51-C61-O61
82	1	3813	GET	C41-C51-C61-C71
82	1	3813	GET	O51-C51-C61-O61
82	6	2013	GET	C23-C33-N33-C93
82	6	2014	GET	C41-C51-C61-O61
82	6	2014	GET	C41-C51-C61-C71
82	6	2014	GET	O51-C51-C61-O61
82	6	2014	GET	O51-C51-C61-C71
82	6	2015	GET	C41-C51-C61-C71
82	5	3844	GET	C21-C11-O11-C42
82	5	3844	GET	C23-C33-N33-C93
82	5	3846	GET	C41-C51-C61-O61
82	5	3846	GET	C41-C51-C61-C71
82	5	3846	GET	O51-C51-C61-O61
82	5	3846	GET	O51-C51-C61-C71
82	5	3847	GET	C41-C51-C61-O61
82	5	3847	GET	C41-C51-C61-C71
82	5	3847	GET	O51-C51-C61-O61
82	5	3847	GET	O51-C51-C61-C71
82	5	3849	GET	C41-C51-C61-O61
82	5	3849	GET	C41-C51-C61-C71

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Mol	Chain	Res	Type	Atoms
82	5	3849	GET	O51-C51-C61-O61
82	5	3849	GET	O51-C51-C61-C71
82	5	3850	GET	C41-C51-C61-O61
82	5	3850	GET	C41-C51-C61-C71
82	5	3850	GET	O51-C51-C61-O61
82	5	3850	GET	O51-C51-C61-C71
82	5	3851	GET	C41-C51-C61-O61
82	5	3851	GET	C41-C51-C61-C71
82	5	3851	GET	O51-C51-C61-O61
82	5	3851	GET	C23-C33-N33-C93
82	n6	201	GET	C41-C51-C61-O61
82	n6	201	GET	C41-C51-C61-C71
82	n6	201	GET	O51-C51-C61-O61
82	n6	201	GET	C23-C33-N33-C93
82	1	3808	GET	C52-C42-O11-C11
82	5	3844	GET	C52-C42-O11-C11
82	5	3847	GET	O51-C11-O11-C42
82	2	2014	GET	O51-C11-O11-C42
82	1	3809	GET	O51-C11-O11-C42
82	1	3813	GET	O53-C13-O62-C62
82	5	3846	GET	O51-C11-O11-C42
82	1	3812	GET	O51-C11-O11-C42
82	1	3808	GET	O53-C13-O62-C62
82	6	2014	GET	O51-C11-O11-C42
82	5	3850	GET	C52-C62-O62-C13
82	5	3844	GET	O51-C11-O11-C42
82	6	2015	GET	O51-C11-O11-C42
82	2	2013	GET	O51-C51-C61-C71
82	1	3809	GET	O51-C51-C61-C71
82	1	3813	GET	O51-C51-C61-C71
82	5	3848	GET	O51-C51-C61-C71
82	n6	201	GET	O51-C51-C61-C71
82	5	3851	GET	O51-C11-O11-C42
82	5	3848	GET	C52-C42-O11-C11
82	5	3847	GET	C52-C42-O11-C11
82	6	2015	GET	O51-C51-C61-C71
82	1	3813	GET	C23-C13-O62-C62
82	2	2014	GET	C52-C42-O11-C11
82	2	2013	GET	C52-C42-O11-C11
82	6	2015	GET	O51-C51-C61-O61
82	2	2012	GET	C52-C42-O11-C11
82	1	3808	GET	O51-C11-O11-C42

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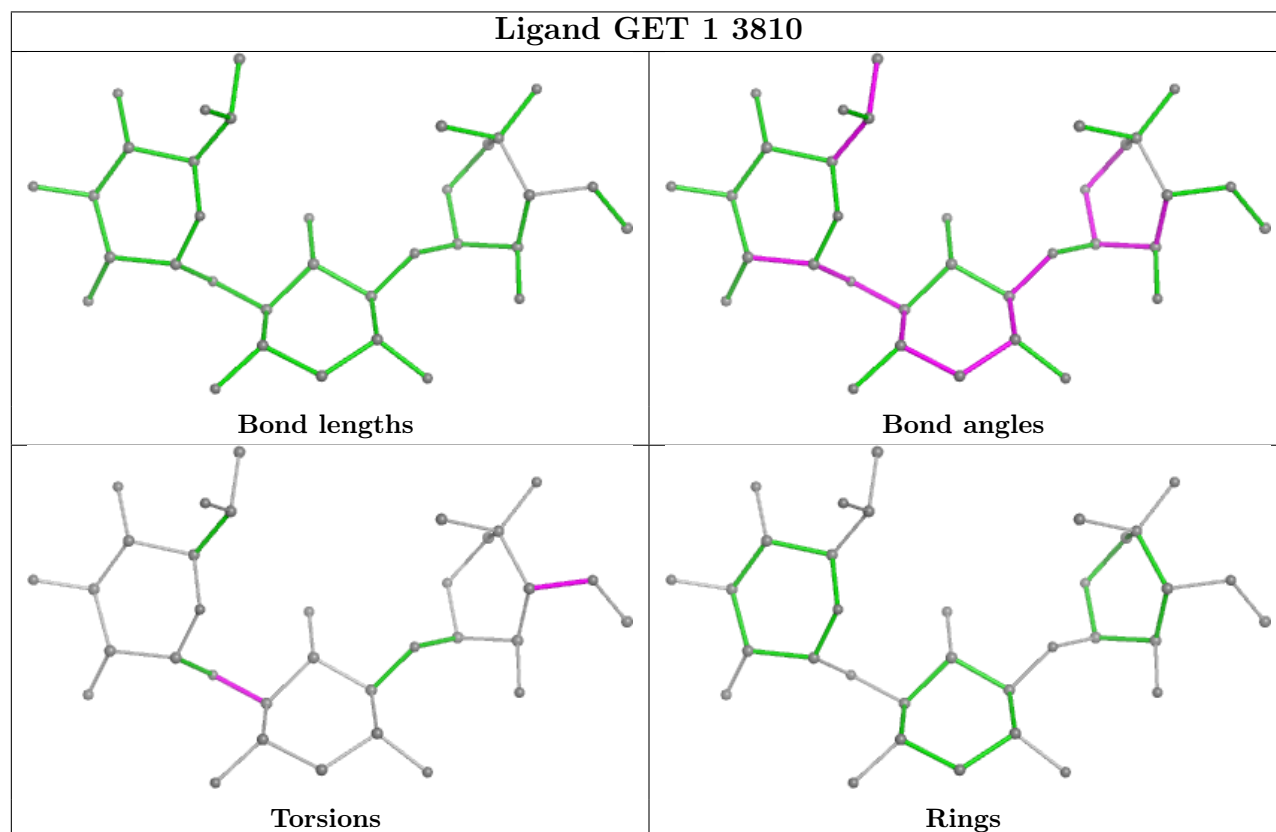
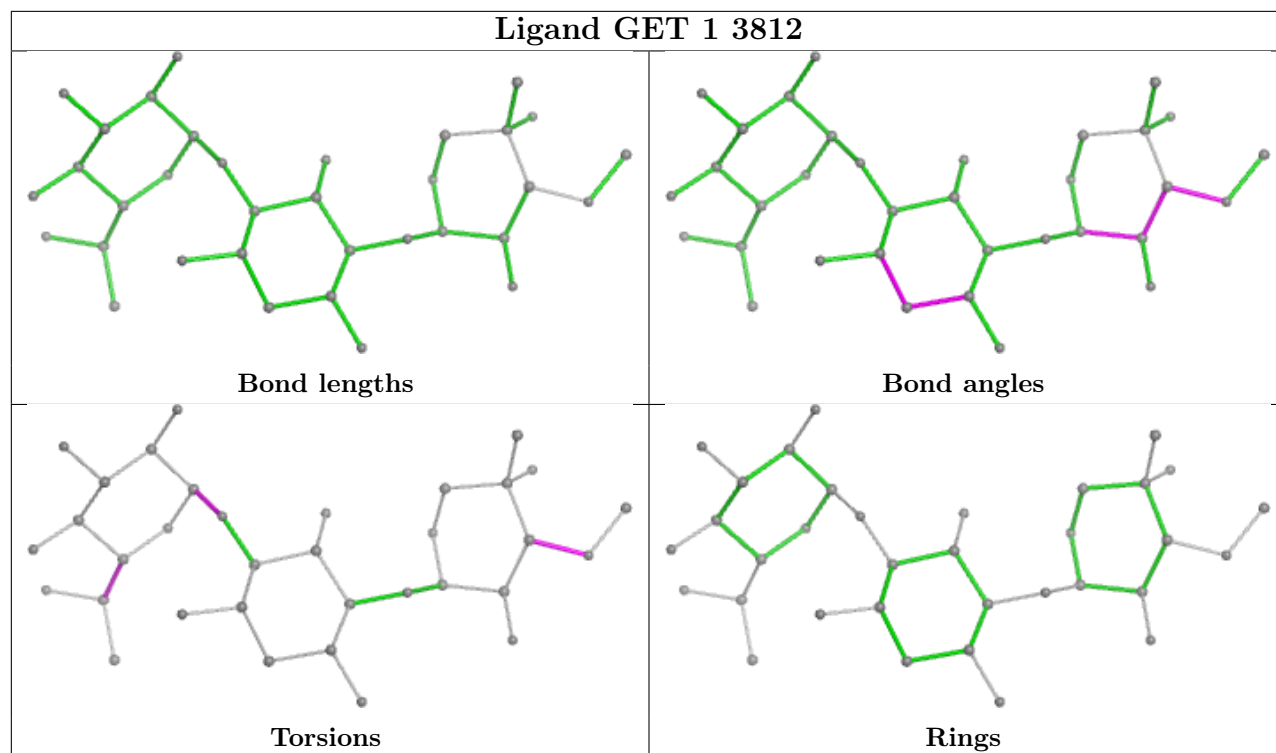
Mol	Chain	Res	Type	Atoms
82	5	3848	GET	C32-C42-O11-C11
82	5	3845	GET	C52-C42-O11-C11
82	5	3851	GET	O51-C51-C61-C71
82	1	3809	GET	C52-C62-O62-C13
82	1	3809	GET	C52-C42-O11-C11
82	1	3809	GET	O53-C13-O62-C62
82	6	2014	GET	C52-C42-O11-C11
82	5	3844	GET	O51-C51-C61-C71
82	n6	201	GET	O51-C11-O11-C42
82	1	3809	GET	C23-C13-O62-C62
82	1	3813	GET	C23-C33-N33-C93
82	5	3846	GET	C23-C33-N33-C93
82	5	3847	GET	C23-C33-N33-C93
82	5	3847	GET	C32-C42-O11-C11
82	5	3850	GET	C12-C62-O62-C13
82	2	2014	GET	C52-C62-O62-C13
82	6	2015	GET	O53-C13-O62-C62

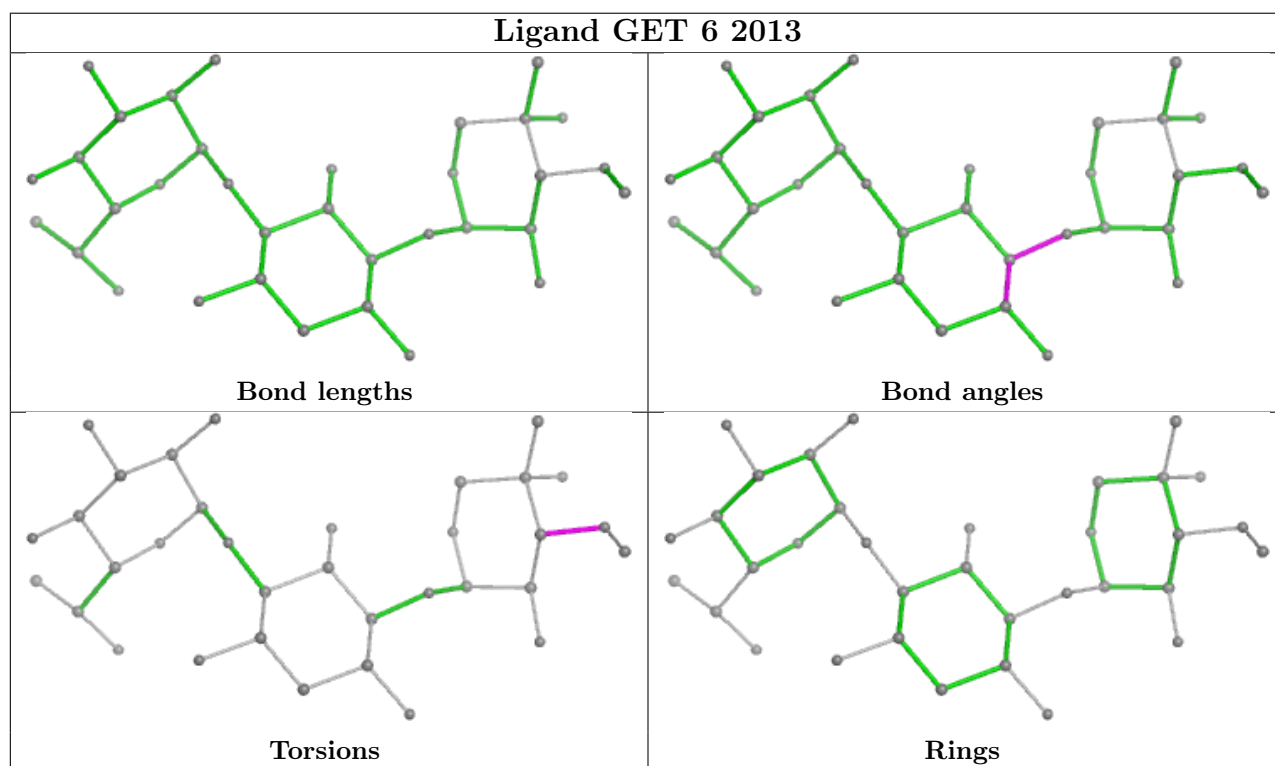
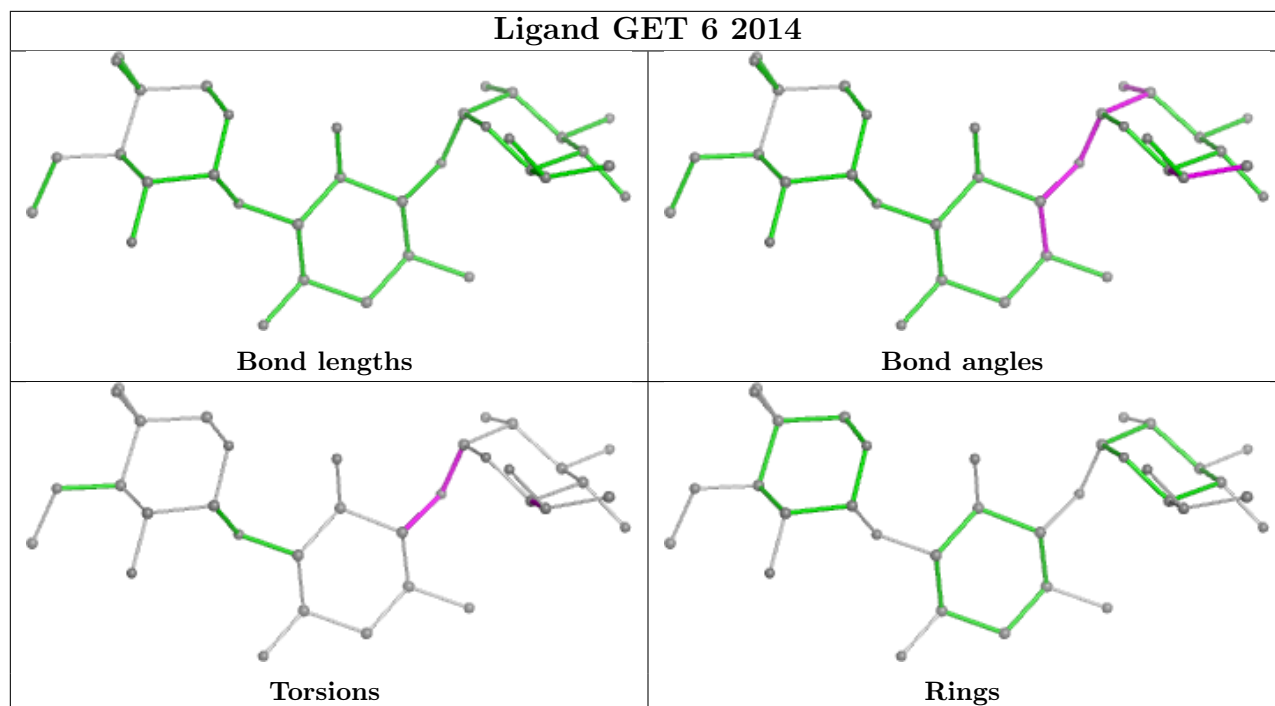
All (2) ring outliers are listed below:

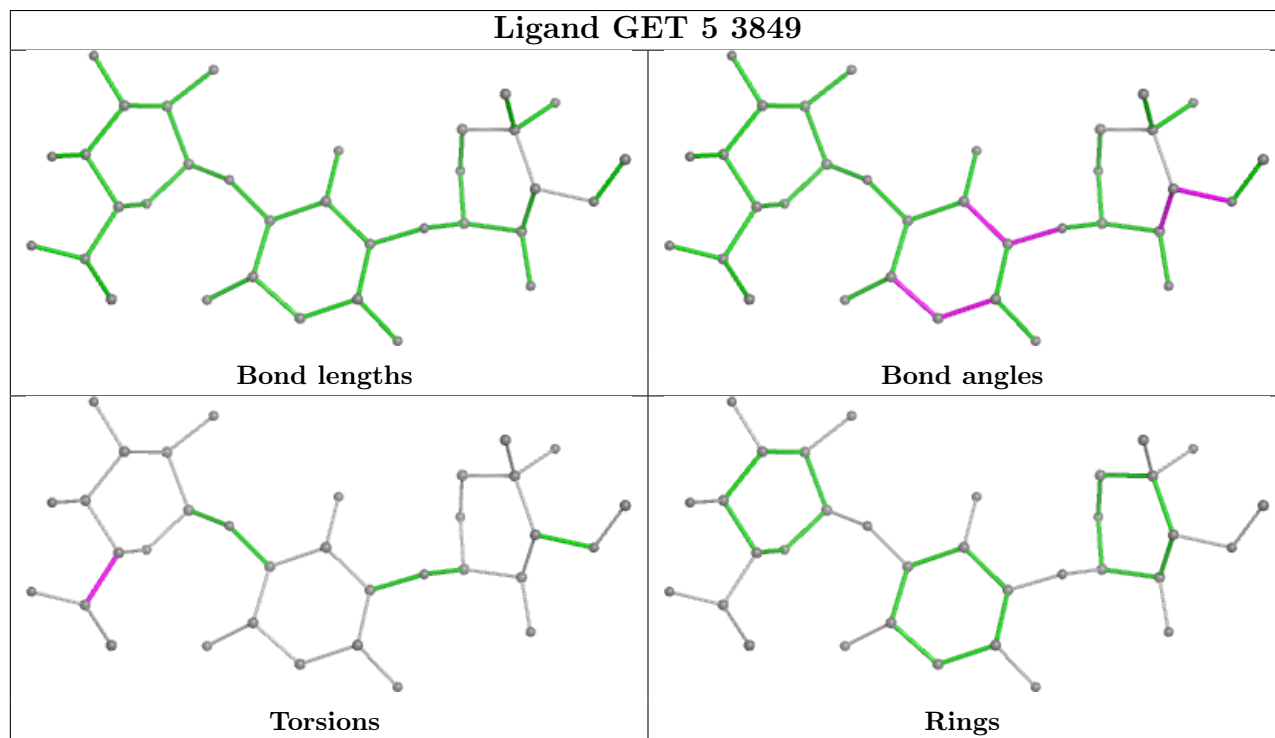
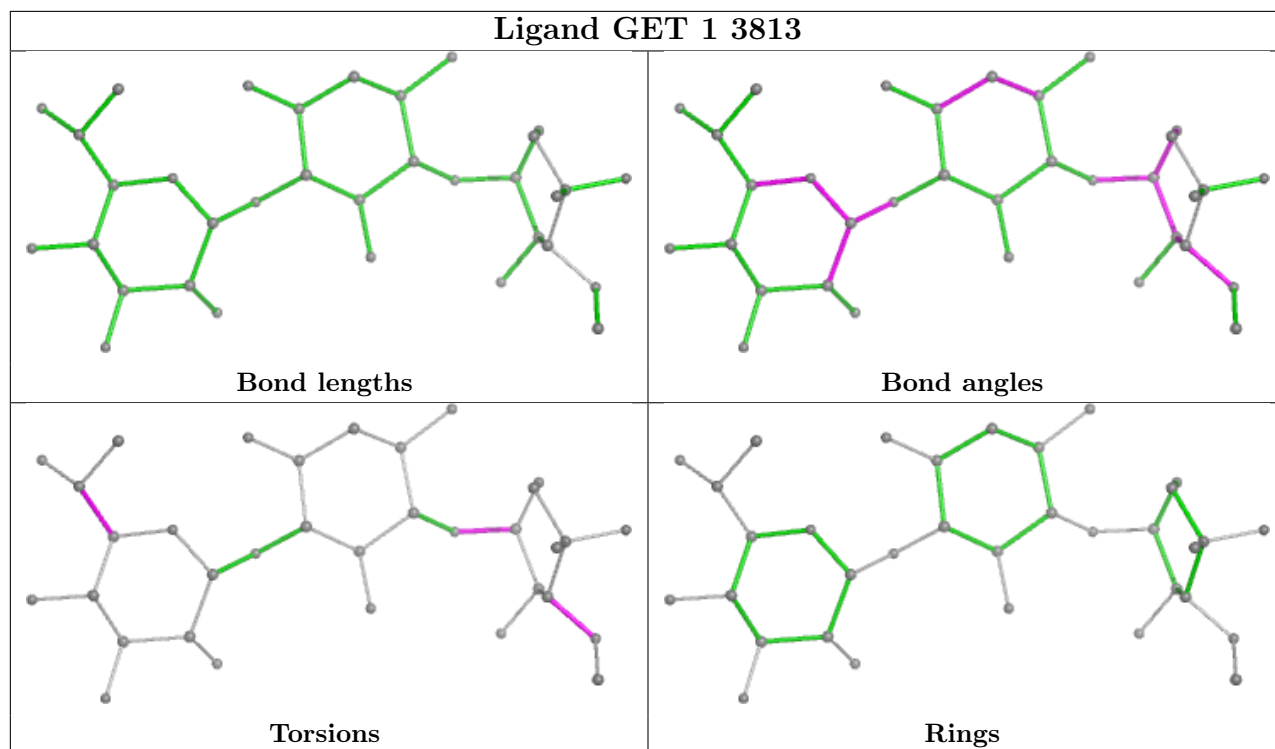
Mol	Chain	Res	Type	Atoms
82	2	2012	GET	C13-C23-C33-C43-C53-O53
82	2	2014	GET	C11-C21-C31-C41-C51-O51

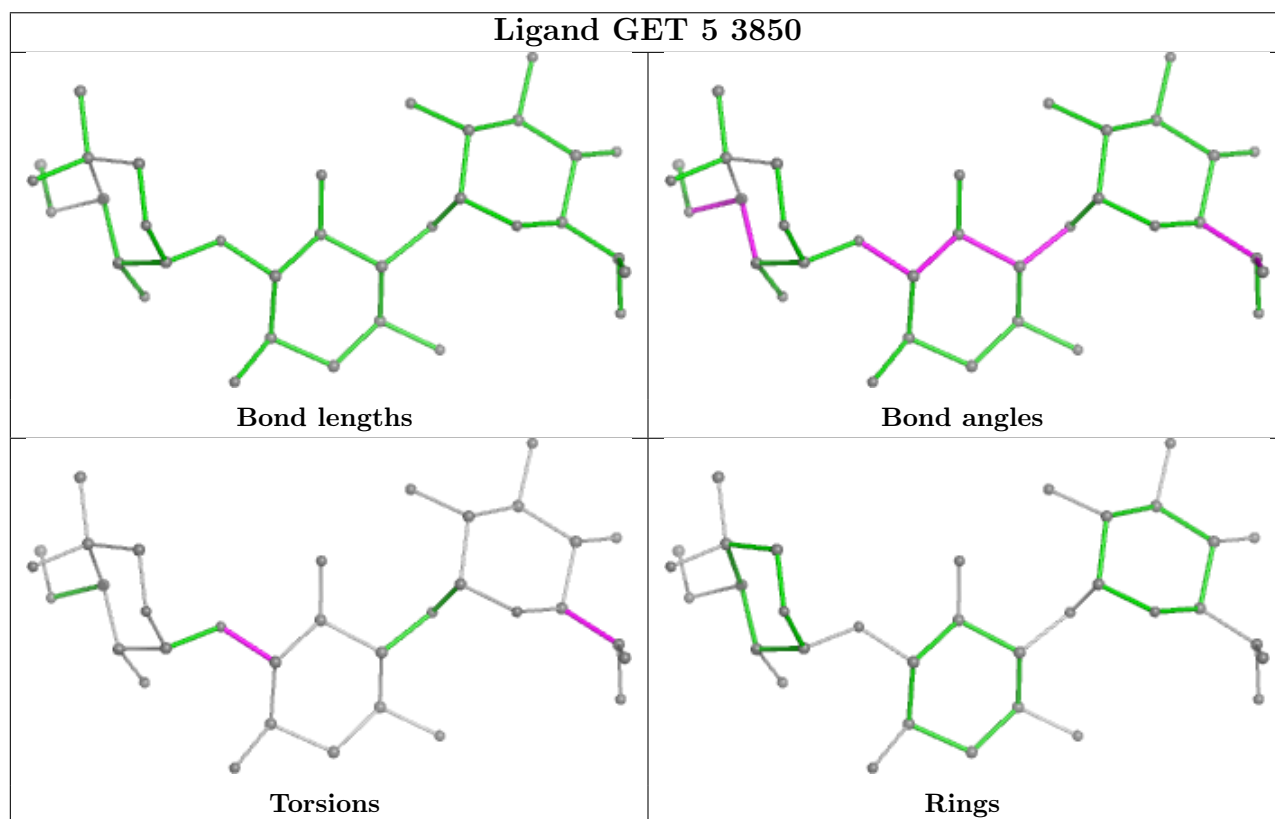
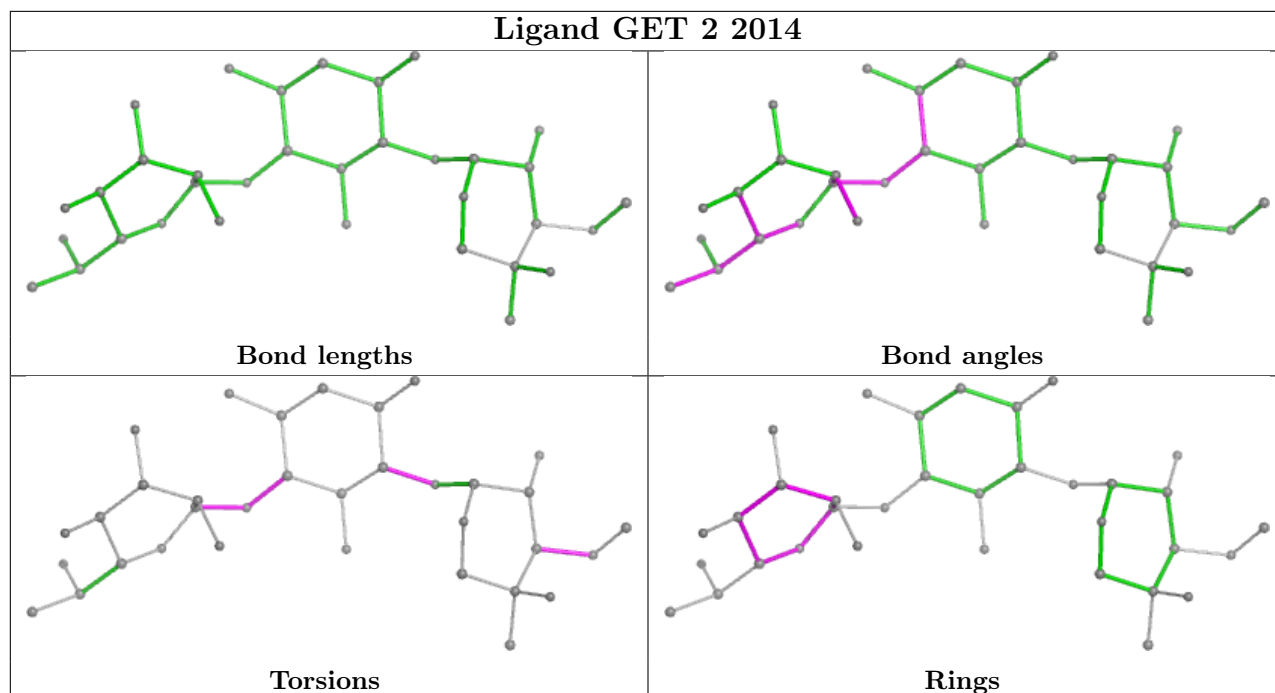
No monomer is involved in short contacts.

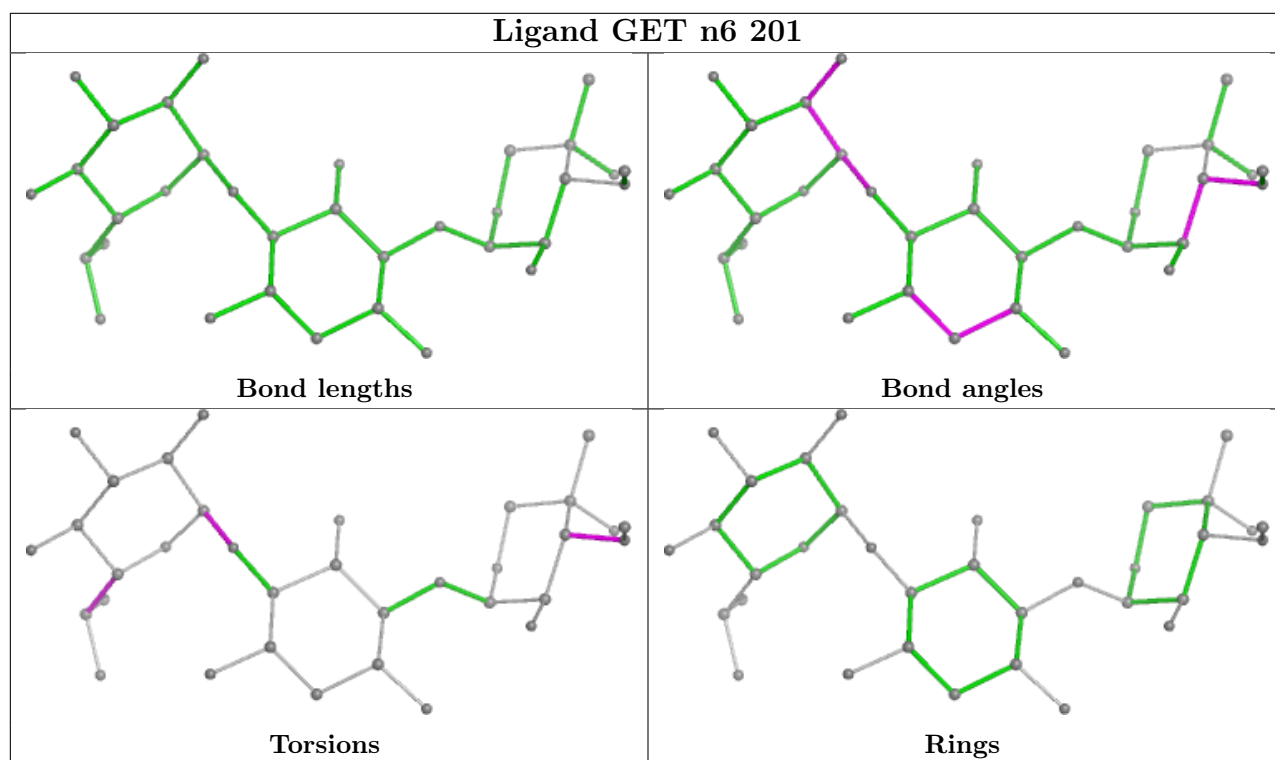
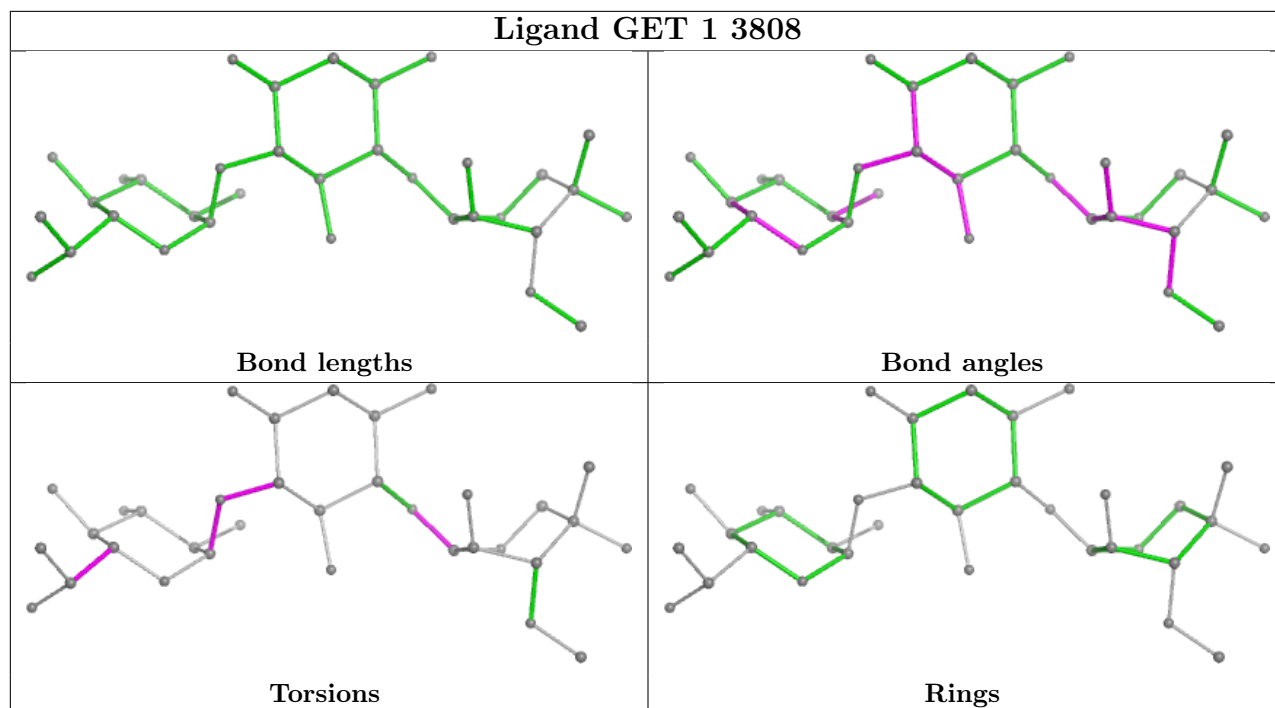
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

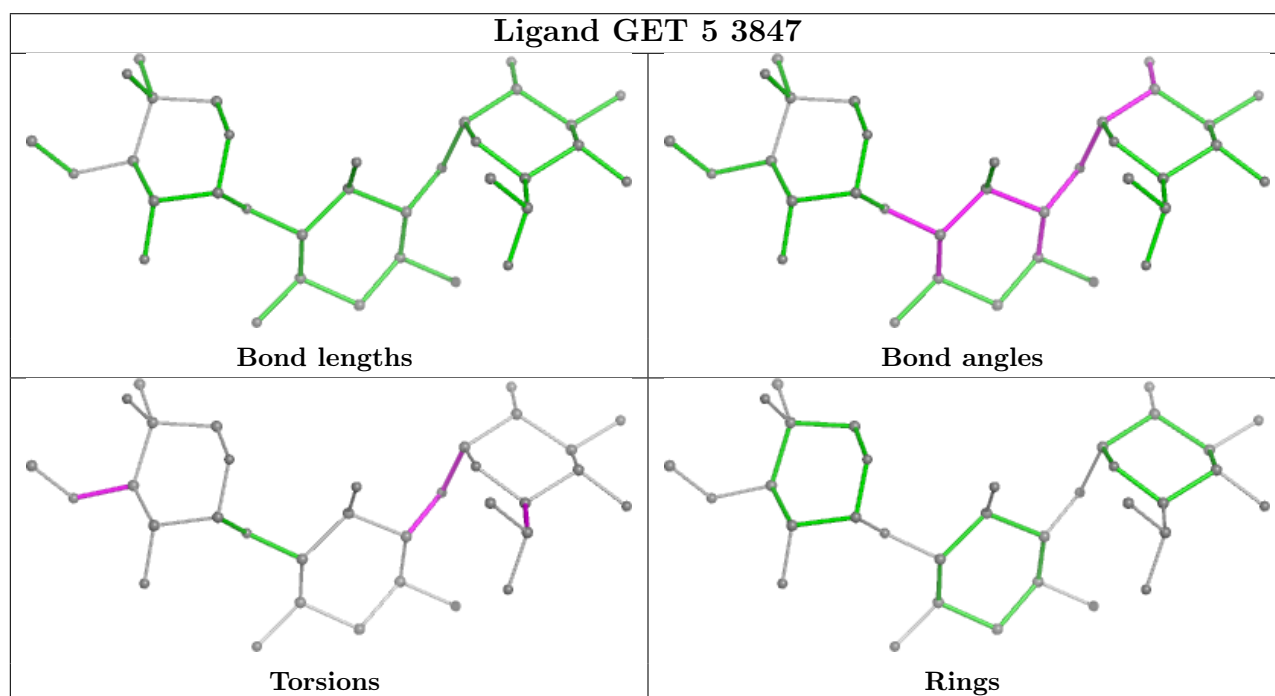
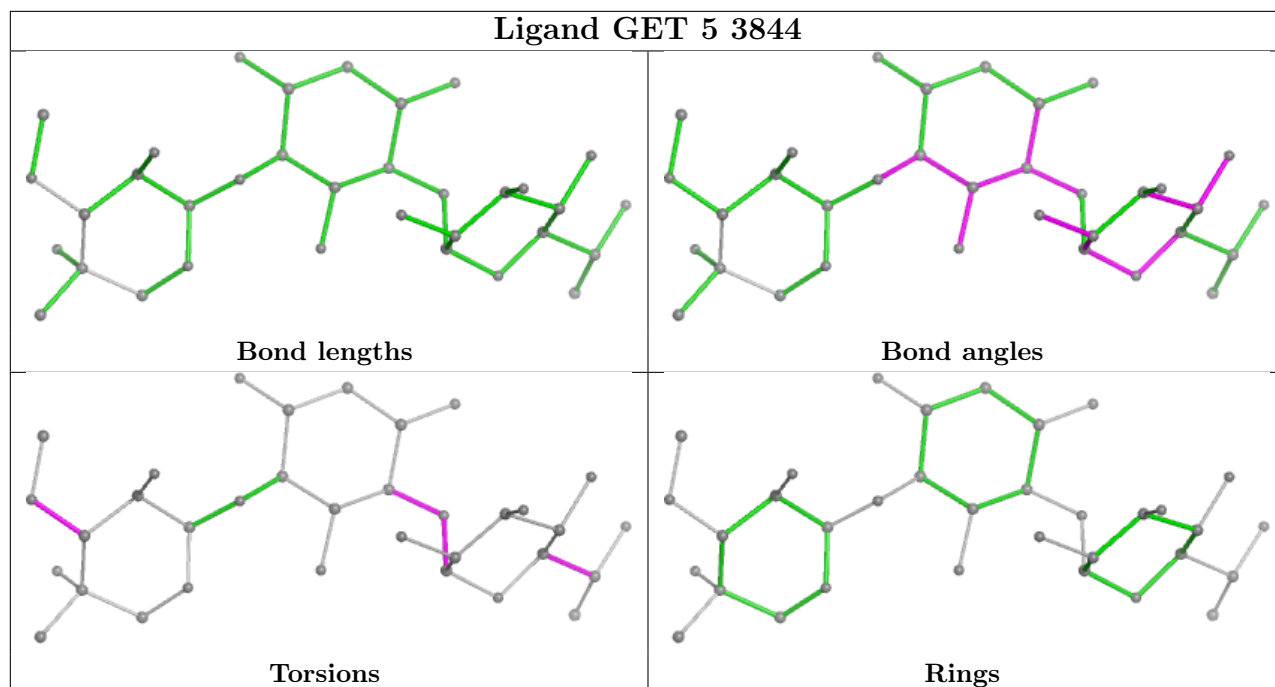


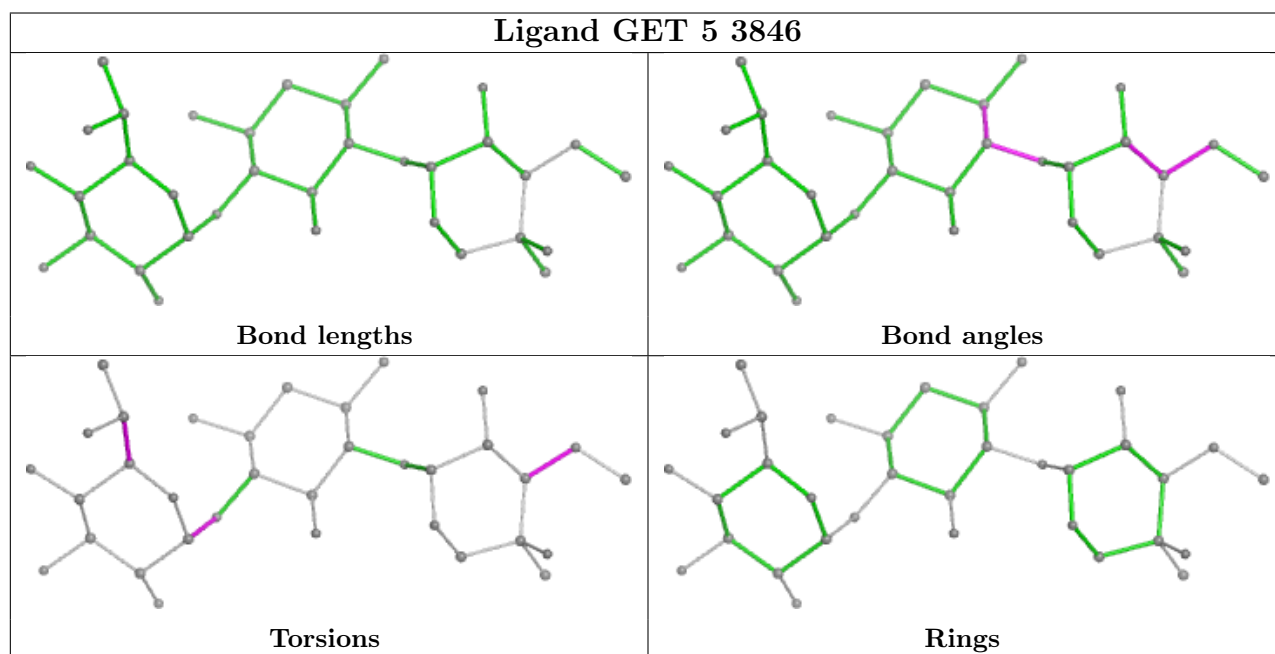
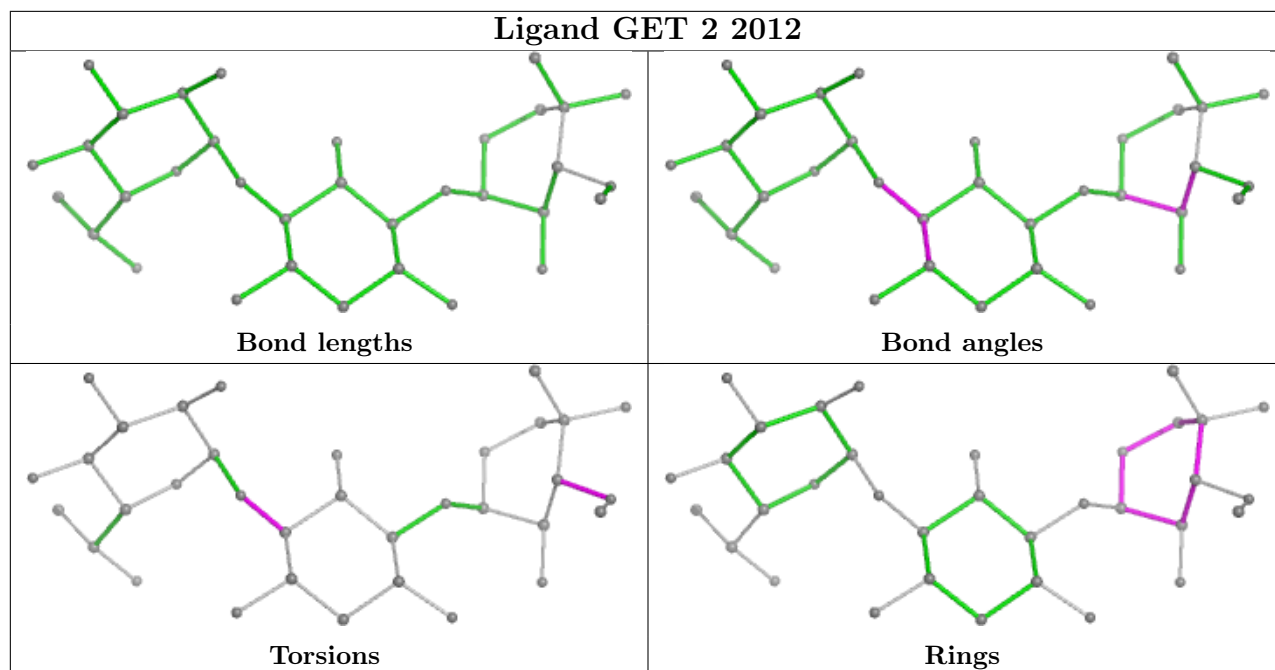


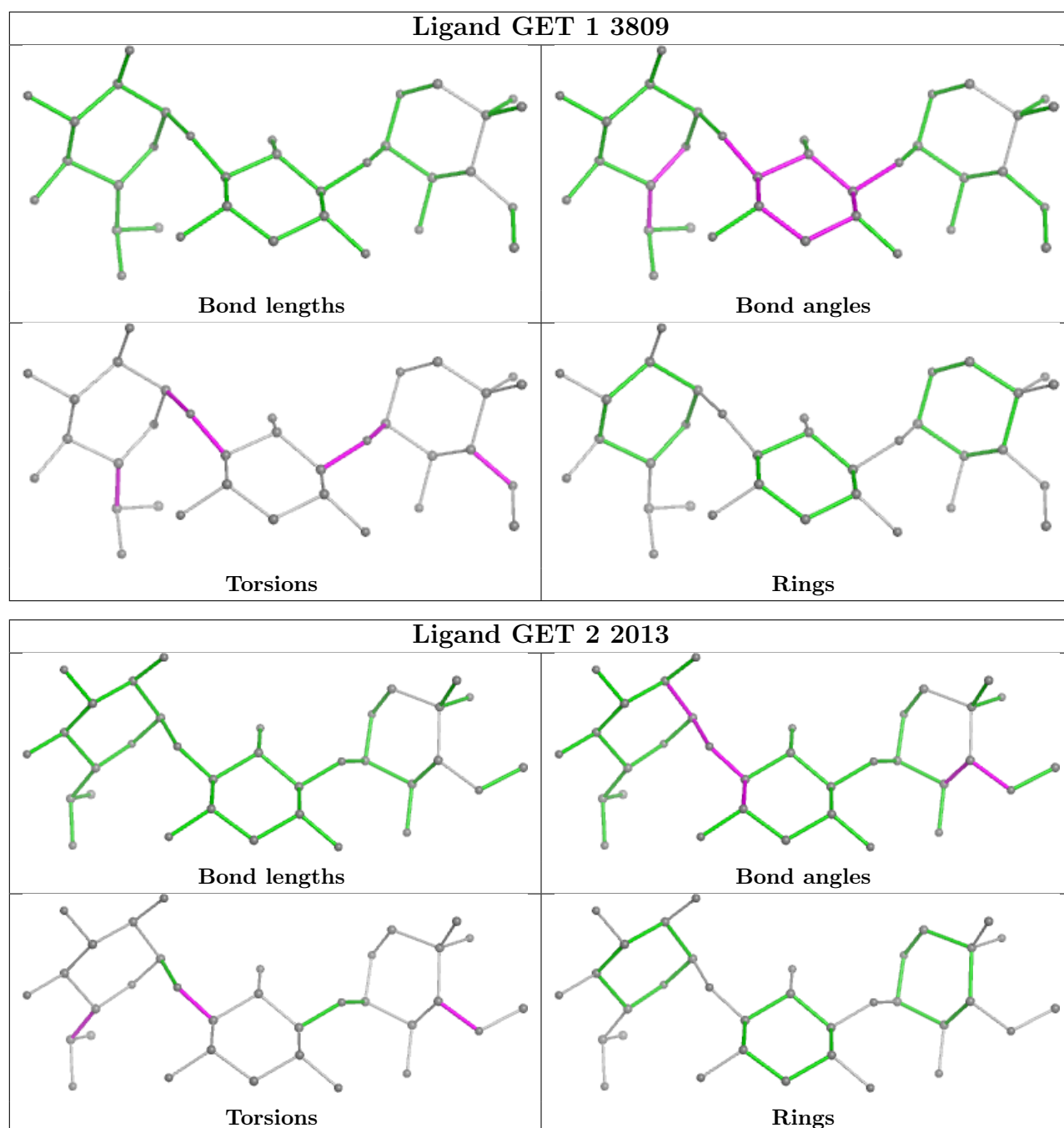


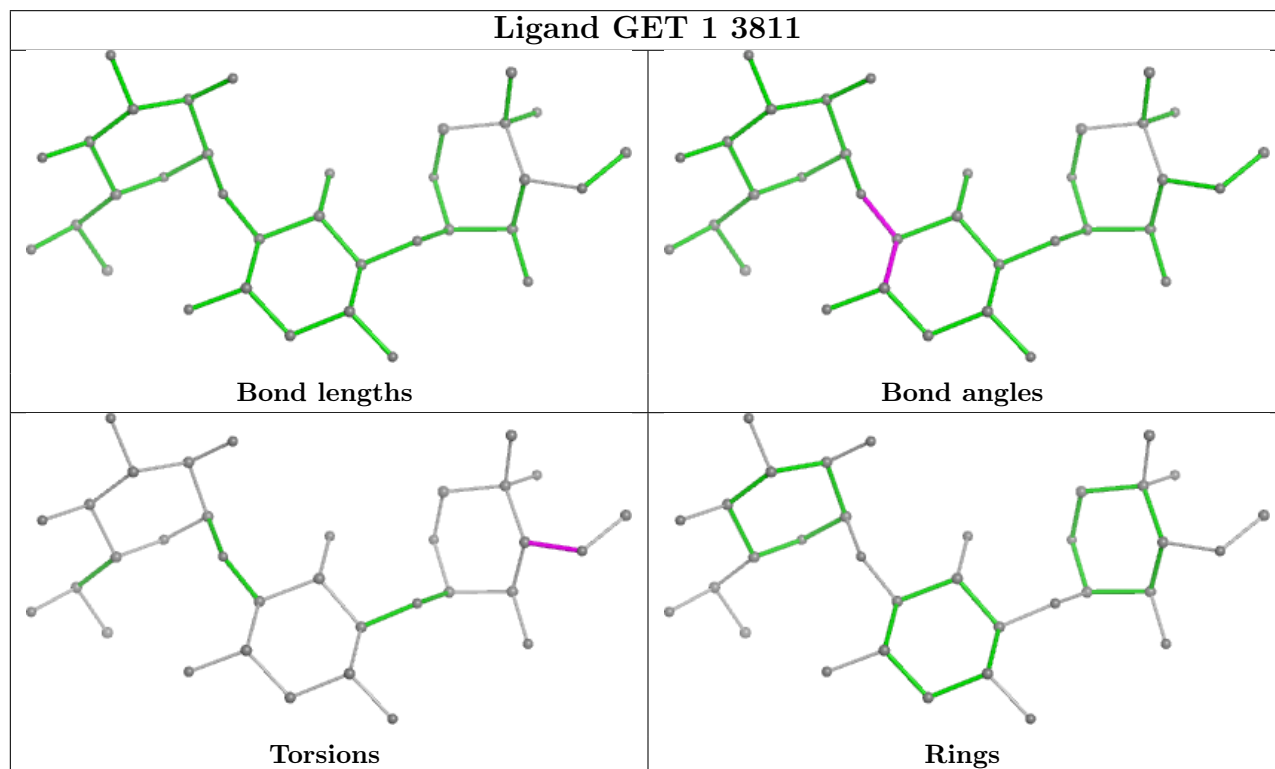
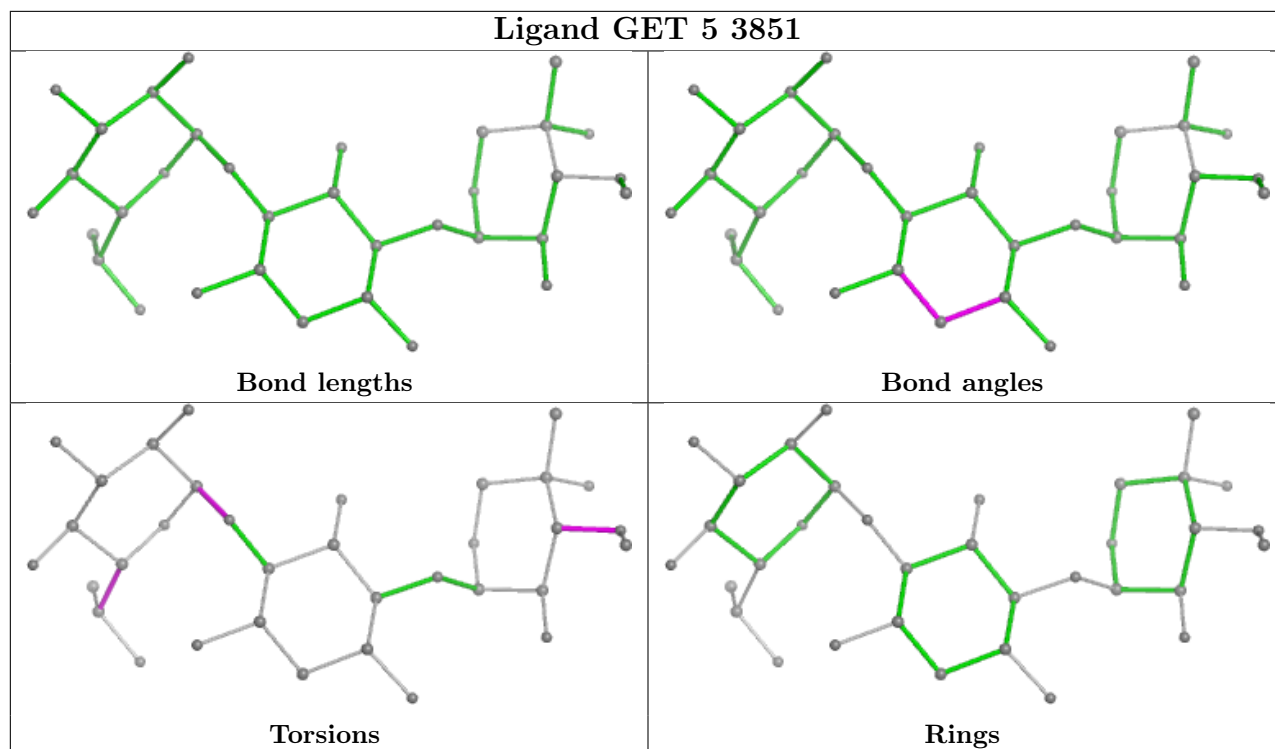


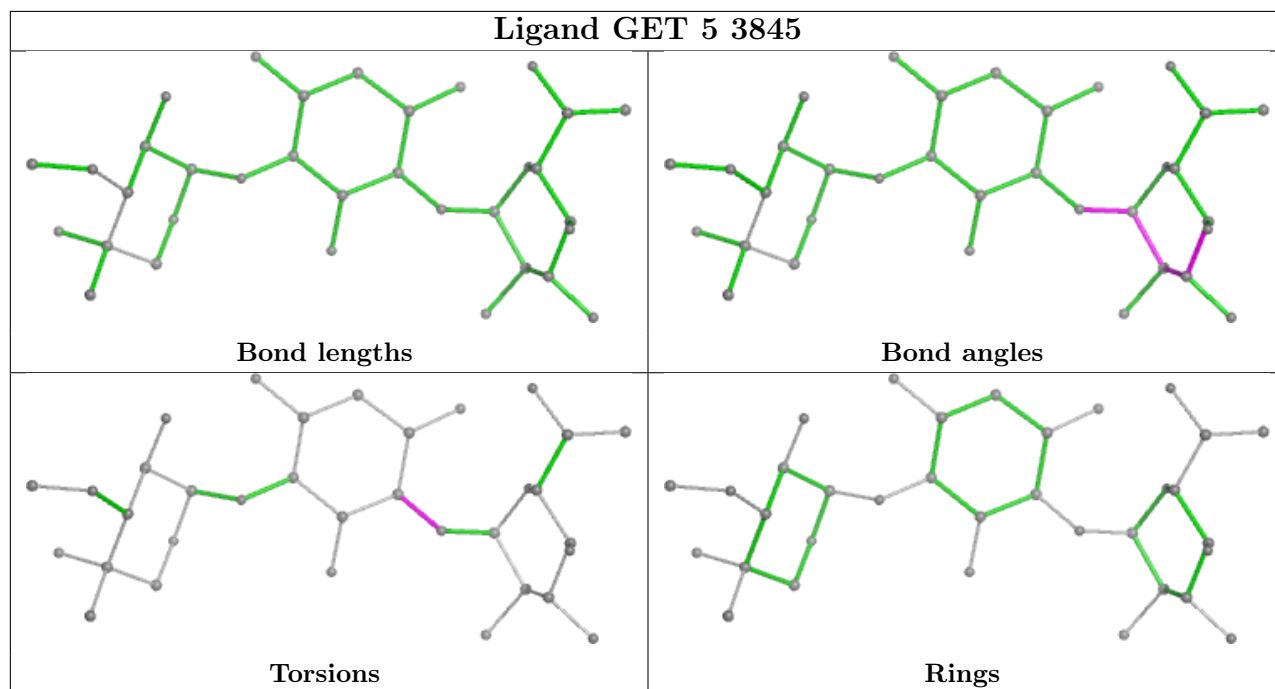
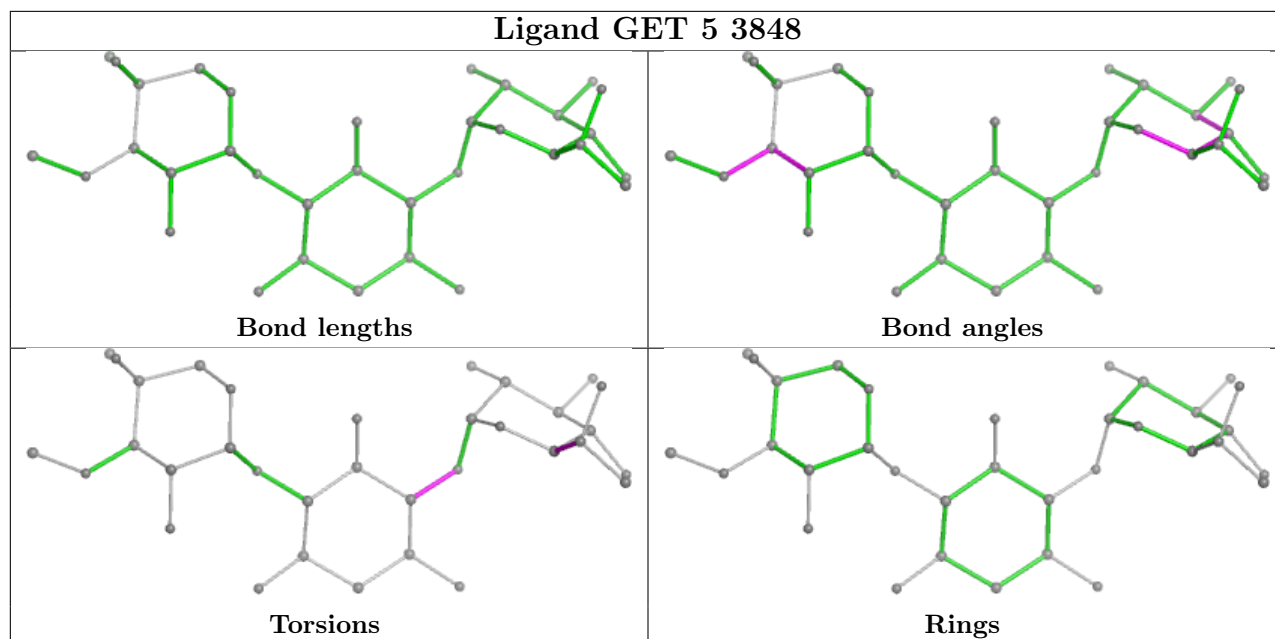


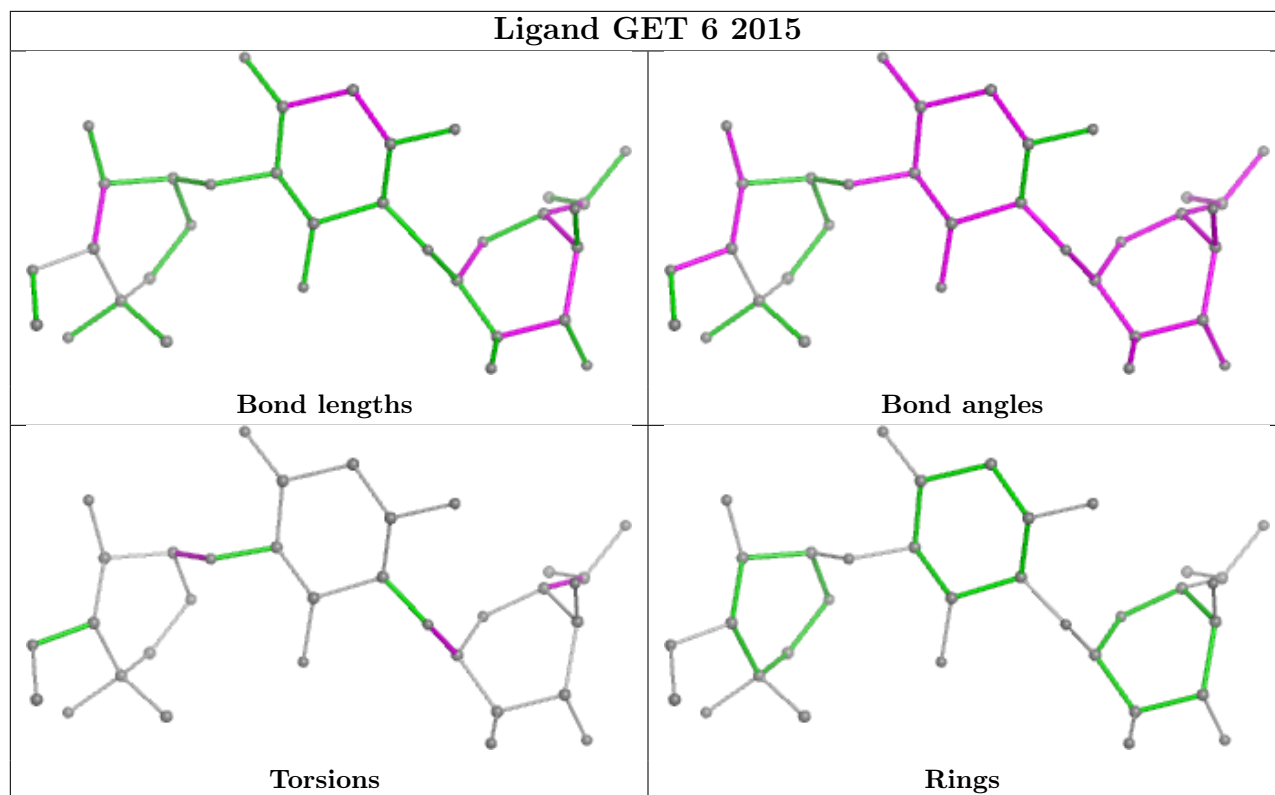












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	1
30	D8	1
18	c6	1
30	d8	1
28	D6	1
39	l2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	3.84
1	D8	5:THR	C	6:PRO	N	1.82
1	c6	4:VAL	C	5:PRO	N	1.69

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d8	5:THR	C	6:PRO	N	1.67
1	D6	59:TYR	C	60:PRO	N	1.65
1	l2	204:MET	C	205:ASN	N	1.16

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1688/1800 (93%)	0.09	34 (2%) 65 53	109, 170, 289, 329	0
1	6	1700/1800 (94%)	0.11	33 (1%) 66 55	101, 171, 254, 295	0
2	S0	206/206 (100%)	0.43	15 (7%) 15 11	173, 208, 229, 240	0
2	s0	206/206 (100%)	0.56	21 (10%) 6 5	171, 192, 212, 220	0
3	S1	214/216 (99%)	0.80	39 (18%) 1 1	194, 239, 265, 270	0
3	s1	216/216 (100%)	0.75	40 (18%) 1 1	171, 207, 229, 241	0
4	S2	217/217 (100%)	0.15	3 (1%) 75 64	147, 178, 199, 213	0
4	s2	217/217 (100%)	0.37	9 (4%) 37 27	144, 169, 192, 211	0
5	S3	223/223 (100%)	0.18	6 (2%) 54 42	133, 156, 222, 235	0
5	s3	223/223 (100%)	0.37	14 (6%) 20 13	168, 198, 240, 247	0
6	S4	260/260 (100%)	1.02	55 (21%) 0 0	175, 227, 242, 258	0
6	s4	260/260 (100%)	0.50	23 (8%) 10 7	126, 174, 193, 231	0
7	S5	206/206 (100%)	0.59	22 (10%) 6 5	153, 185, 199, 206	0
7	s5	206/206 (100%)	1.24	58 (28%) 0 0	199, 217, 245, 248	0
8	S6	226/236 (95%)	0.71	37 (16%) 1 1	166, 211, 269, 303	0
8	s6	218/236 (92%)	0.57	25 (11%) 4 4	128, 177, 205, 214	0
9	S7	184/185 (99%)	1.00	34 (18%) 1 1	209, 268, 310, 313	0
9	s7	185/185 (100%)	0.74	26 (14%) 2 2	166, 204, 230, 235	0
10	S8	188/200 (94%)	1.42	53 (28%) 0 0	160, 200, 261, 281	0
10	s8	188/200 (94%)	0.85	19 (10%) 7 5	124, 153, 209, 238	0
11	S9	185/185 (100%)	1.80	67 (36%) 0 0	162, 210, 238, 253	0
11	s9	185/185 (100%)	1.84	77 (41%) 0 0	151, 188, 220, 261	0
12	C0	92/105 (87%)	1.14	21 (22%) 0 0	141, 170, 190, 194	0
12	c0	92/105 (87%)	2.00	41 (44%) 0 0	197, 228, 244, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	142/156 (91%)	0.94	17 (11%) 4 4	161, 194, 232, 265	0
13	c1	146/156 (93%)	0.30	7 (4%) 30 22	128, 142, 181, 197	0
14	C2	120/143 (83%)	1.64	44 (36%) 0 0	212, 235, 252, 258	0
14	c2	124/143 (86%)	2.76	79 (63%) 0 0	275, 290, 306, 315	0
15	C3	150/150 (100%)	0.29	4 (2%) 54 42	167, 208, 244, 247	0
15	c3	150/150 (100%)	0.20	3 (2%) 65 53	138, 161, 184, 191	0
16	C4	127/128 (99%)	0.20	5 (3%) 39 28	147, 201, 230, 236	0
16	c4	128/128 (100%)	0.25	6 (4%) 31 23	136, 198, 216, 223	0
17	C5	122/141 (86%)	0.39	7 (5%) 23 16	134, 163, 182, 196	0
17	c5	119/141 (84%)	0.81	20 (16%) 1 1	179, 214, 233, 237	0
18	C6	141/141 (100%)	0.94	22 (15%) 2 1	133, 170, 188, 197	0
18	c6	141/141 (100%)	2.59	79 (56%) 0 0	177, 226, 241, 246	0
19	C7	117/136 (86%)	0.71	16 (13%) 3 3	162, 195, 242, 247	0
19	c7	117/136 (86%)	0.33	8 (6%) 17 12	190, 206, 225, 229	0
20	C8	145/145 (100%)	0.28	9 (6%) 20 14	133, 172, 206, 215	0
20	c8	145/145 (100%)	0.74	28 (19%) 1 1	175, 221, 248, 254	0
21	C9	143/143 (100%)	0.80	16 (11%) 5 4	138, 163, 181, 198	0
21	c9	143/143 (100%)	2.11	62 (43%) 0 0	197, 234, 253, 259	0
22	D0	105/107 (98%)	0.84	20 (19%) 1 1	125, 164, 196, 202	0
22	d0	101/107 (94%)	1.29	27 (26%) 0 0	171, 227, 255, 261	0
23	D1	87/87 (100%)	0.33	4 (4%) 32 24	182, 200, 226, 237	0
23	d1	87/87 (100%)	0.33	3 (3%) 45 34	170, 179, 208, 215	0
24	D2	129/129 (100%)	0.48	11 (8%) 10 8	176, 195, 212, 224	0
24	d2	129/129 (100%)	0.40	7 (5%) 25 19	142, 159, 172, 186	0
25	D3	144/144 (100%)	0.12	3 (2%) 63 52	130, 139, 163, 169	0
25	d3	144/144 (100%)	0.13	0 100 100	122, 131, 147, 164	0
26	D4	134/134 (100%)	1.01	30 (22%) 0 0	186, 230, 242, 250	0
26	d4	134/134 (100%)	0.42	15 (11%) 5 4	146, 190, 211, 227	0
27	D5	70/70 (100%)	1.24	14 (20%) 1 0	175, 202, 214, 217	0
27	d5	69/70 (98%)	1.58	25 (36%) 0 0	223, 244, 254, 258	0
28	D6	97/97 (100%)	0.26	5 (5%) 27 20	145, 167, 227, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.41	8 (8%) 11 9	140, 154, 218, 222	0
29	D7	81/81 (100%)	0.34	6 (7%) 14 10	196, 233, 277, 288	0
29	d7	81/81 (100%)	0.44	2 (2%) 57 45	161, 181, 221, 225	0
30	D8	63/63 (100%)	0.52	8 (12%) 3 4	169, 197, 216, 226	0
30	d8	63/63 (100%)	-0.16	1 (1%) 72 61	187, 211, 225, 229	0
31	D9	53/53 (100%)	0.72	9 (16%) 1 1	125, 132, 160, 170	0
31	d9	53/53 (100%)	1.45	15 (28%) 0 0	180, 191, 224, 249	0
32	E0	60/60 (100%)	0.80	11 (18%) 1 1	137, 178, 205, 210	0
32	e0	60/60 (100%)	0.82	10 (16%) 1 1	141, 182, 208, 215	0
33	E1	71/152 (46%)	2.02	32 (45%) 0 0	157, 207, 238, 244	0
33	e1	45/152 (29%)	2.04	24 (53%) 0 0	198, 263, 280, 283	0
34	SR	318/318 (100%)	0.99	59 (18%) 1 1	189, 218, 242, 262	0
34	sR	313/318 (98%)	0.65	42 (13%) 3 3	221, 240, 258, 318	0
35	SM	135/272 (49%)	0.07	5 (3%) 41 30	133, 155, 230, 255	0
35	sM	115/272 (42%)	0.67	25 (21%) 0 0	154, 179, 231, 293	0
36	1	3078/3396 (90%)	0.05	27 (0%) 84 76	82, 131, 236, 350	0
36	5	3127/3396 (92%)	0.09	47 (1%) 73 63	83, 121, 213, 304	0
37	3	121/121 (100%)	-0.21	0 100 100	92, 159, 191, 204	0
37	7	121/121 (100%)	-0.16	0 100 100	95, 170, 205, 211	0
38	4	158/158 (100%)	0.17	5 (3%) 47 35	100, 159, 221, 285	0
38	8	157/158 (99%)	0.23	1 (0%) 89 83	96, 132, 183, 217	0
39	L2	252/252 (100%)	0.31	13 (5%) 27 20	104, 154, 189, 209	0
39	l2	252/252 (100%)	0.20	10 (3%) 38 28	97, 127, 152, 170	0
40	L3	386/386 (100%)	0.09	10 (2%) 56 43	84, 121, 147, 180	0
40	l3	386/386 (100%)	-0.01	1 (0%) 94 90	83, 111, 131, 164	0
41	L4	361/361 (100%)	0.01	2 (0%) 89 83	94, 144, 170, 183	0
41	l4	361/361 (100%)	0.19	9 (2%) 57 45	91, 125, 147, 160	0
42	L5	294/296 (99%)	0.97	71 (24%) 0 0	127, 188, 205, 210	0
42	l5	294/296 (99%)	0.83	50 (17%) 1 1	141, 197, 221, 235	0
43	L6	156/176 (88%)	0.12	3 (1%) 66 55	109, 127, 147, 163	0
43	l6	157/176 (89%)	0.20	4 (2%) 57 45	105, 118, 143, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	L7	222/223 (99%)	0.05	2 (0%) 84 76	95, 123, 164, 193	0
44	l7	223/223 (100%)	-0.06	1 (0%) 92 88	96, 114, 149, 189	0
45	L8	233/233 (100%)	1.02	48 (20%) 1 0	188, 228, 265, 283	0
45	l8	231/233 (99%)	0.63	26 (11%) 5 4	152, 178, 213, 223	0
46	L9	191/191 (100%)	0.20	4 (2%) 63 52	113, 131, 146, 172	0
46	l9	190/191 (99%)	0.04	0 100 100	110, 125, 145, 154	0
47	M0	208/221 (94%)	-0.12	2 (0%) 82 73	97, 115, 162, 181	0
47	m0	209/221 (94%)	0.24	8 (3%) 40 30	102, 125, 180, 194	0
48	M1	169/169 (100%)	0.60	16 (9%) 8 6	151, 165, 173, 175	0
48	m1	169/169 (100%)	0.78	23 (13%) 3 3	171, 191, 201, 204	0
49	M3	193/194 (99%)	0.16	6 (3%) 49 36	109, 185, 219, 232	0
49	m3	194/194 (100%)	0.16	5 (2%) 56 43	102, 156, 197, 209	0
50	M4	136/137 (99%)	-0.21	0 100 100	118, 129, 144, 153	0
50	m4	137/137 (100%)	-0.13	0 100 100	113, 121, 146, 176	0
51	M5	203/203 (100%)	0.92	27 (13%) 3 3	117, 163, 193, 205	0
51	m5	203/203 (100%)	0.59	17 (8%) 11 8	106, 133, 154, 163	0
52	M6	197/197 (100%)	-0.09	0 100 100	83, 97, 140, 150	0
52	m6	197/197 (100%)	-0.13	1 (0%) 91 85	85, 97, 139, 147	0
53	M7	183/184 (99%)	0.14	2 (1%) 80 71	92, 108, 159, 196	0
53	m7	175/184 (95%)	0.15	3 (1%) 70 59	91, 104, 140, 157	0
54	M8	185/185 (100%)	0.22	7 (3%) 40 30	103, 149, 173, 180	0
54	m8	185/185 (100%)	0.20	1 (0%) 91 85	102, 131, 147, 155	0
55	M9	188/188 (100%)	0.43	20 (10%) 6 5	137, 167, 298, 318	0
55	m9	183/188 (97%)	0.47	18 (9%) 7 6	114, 135, 212, 223	0
56	N0	170/172 (98%)	0.07	0 100 100	104, 121, 143, 156	0
56	n0	172/172 (100%)	-0.07	0 100 100	100, 116, 137, 154	0
57	N1	159/159 (100%)	0.75	25 (15%) 2 1	100, 136, 196, 205	0
57	n1	159/159 (100%)	0.35	8 (5%) 28 21	110, 134, 182, 186	0
58	N2	98/98 (100%)	1.41	23 (23%) 0 0	186, 205, 216, 219	0
58	n2	98/98 (100%)	0.34	9 (9%) 9 6	159, 174, 187, 190	0
59	N3	135/135 (100%)	0.69	16 (11%) 4 4	95, 117, 129, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	n3	134/135 (99%)	0.35	3 (2%) 62 50	89, 104, 116, 128	0
60	N4	122/155 (78%)	0.82	17 (13%) 2 3	123, 163, 280, 283	0
60	n4	118/155 (76%)	0.66	18 (15%) 2 1	103, 136, 235, 242	0
61	N5	121/121 (100%)	0.53	13 (10%) 6 5	143, 176, 210, 245	0
61	n5	120/121 (99%)	0.26	3 (2%) 57 45	119, 143, 165, 189	0
62	N6	126/126 (100%)	1.33	30 (23%) 0 0	130, 150, 177, 192	0
62	n6	124/126 (98%)	0.98	15 (12%) 4 4	113, 138, 166, 177	0
63	N7	135/135 (100%)	1.53	47 (34%) 0 0	209, 238, 257, 269	0
63	n7	135/135 (100%)	1.14	24 (17%) 1 1	155, 177, 193, 203	0
64	N8	148/148 (100%)	0.59	17 (11%) 4 4	92, 165, 197, 210	0
64	n8	148/148 (100%)	0.24	1 (0%) 87 81	92, 144, 169, 173	0
65	N9	58/58 (100%)	0.75	10 (17%) 1 1	93, 154, 197, 203	0
65	n9	58/58 (100%)	0.68	8 (13%) 2 3	96, 150, 197, 206	0
66	O0	97/100 (97%)	0.92	18 (18%) 1 1	197, 217, 237, 241	0
66	o0	100/100 (100%)	0.20	5 (5%) 28 21	151, 166, 186, 197	0
67	O1	109/109 (100%)	0.77	16 (14%) 2 2	116, 141, 173, 183	0
67	o1	109/109 (100%)	0.78	9 (8%) 11 9	105, 132, 166, 186	0
68	O2	127/127 (100%)	0.49	6 (4%) 31 23	89, 118, 134, 153	0
68	o2	127/127 (100%)	0.15	0 100 100	88, 111, 124, 154	0
69	O3	106/106 (100%)	0.17	2 (1%) 66 55	88, 103, 119, 122	0
69	o3	106/106 (100%)	0.33	2 (1%) 66 55	89, 101, 116, 123	0
70	O4	112/112 (100%)	0.86	12 (10%) 6 5	138, 186, 249, 258	0
70	o4	112/112 (100%)	0.25	7 (6%) 20 13	113, 144, 201, 211	0
71	O5	119/119 (100%)	0.25	5 (4%) 36 27	162, 182, 210, 218	0
71	o5	119/119 (100%)	0.34	4 (3%) 45 34	129, 152, 174, 182	0
72	O6	99/99 (100%)	0.76	14 (14%) 2 2	170, 194, 221, 241	0
72	o6	99/99 (100%)	0.70	7 (7%) 16 11	150, 162, 186, 207	0
73	O7	84/84 (100%)	-0.04	0 100 100	103, 129, 178, 189	0
73	o7	82/84 (97%)	0.21	0 100 100	94, 111, 140, 153	0
74	O8	77/77 (100%)	1.02	15 (19%) 1 1	194, 216, 228, 229	0
74	o8	77/77 (100%)	1.14	16 (20%) 1 0	154, 174, 185, 187	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	O9	49/50 (98%)	0.30	0 100 100	122, 135, 142, 146	0
75	o9	50/50 (100%)	0.09	0 100 100	106, 117, 127, 129	0
76	Q0	52/52 (100%)	0.60	2 (3%) 40 30	100, 107, 147, 156	0
76	q0	52/52 (100%)	0.42	2 (3%) 40 30	101, 111, 138, 145	0
77	Q1	25/25 (100%)	1.16	3 (12%) 4 4	113, 125, 130, 132	0
77	q1	25/25 (100%)	0.62	1 (4%) 38 28	113, 121, 125, 126	0
78	Q2	105/105 (100%)	0.99	24 (22%) 0 0	113, 143, 167, 178	0
78	q2	105/105 (100%)	0.51	13 (12%) 4 4	109, 144, 170, 189	0
79	Q3	91/91 (100%)	-0.14	2 (2%) 62 50	118, 158, 189, 203	0
79	q3	91/91 (100%)	-0.04	0 100 100	102, 129, 153, 167	0
80	p0	138/312 (44%)	2.34	74 (53%) 0 0	202, 229, 270, 271	0
All	All	32690/34558 (94%)	0.42	2661 (8%) 12 9	82, 159, 244, 350	0

All (2661) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	c6	20	ALA	12.2
45	L8	199	ALA	11.8
31	d9	4	GLU	10.9
60	n4	132	GLY	9.5
6	s4	261	LEU	9.4
12	c0	23	ALA	8.9
11	S9	141	VAL	8.7
33	E1	93	HIS	8.4
51	M5	6	TYR	8.3
33	e1	87	THR	8.3
31	D9	4	GLU	8.2
6	S4	149	TYR	8.1
20	C8	2	SER	8.1
11	s9	141	VAL	8.0
42	l5	181	PRO	8.0
11	s9	134	ILE	7.9
14	c2	41	LEU	7.8
18	c6	11	GLY	7.8
14	c2	90	LYS	7.8
21	c9	84	LYS	7.7
32	E0	45	VAL	7.7
18	c6	88	GLY	7.6

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Mol	Chain	Res	Type	RSRZ
60	N4	75	THR	7.6
45	L8	198	ALA	7.6
21	c9	120	GLY	7.4
18	c6	22	VAL	7.4
18	c6	70	THR	7.3
1	2	226	A	7.3
1	6	1228	G	7.2
21	c9	55	TYR	7.2
33	E1	145	HIS	7.0
10	S8	167	ALA	7.0
47	m0	221	ALA	6.9
11	S9	142	ASN	6.9
47	m0	220	GLN	6.8
72	O6	8	ALA	6.8
7	s5	71	ALA	6.8
34	SR	212	ALA	6.7
45	l8	199	ALA	6.6
3	s1	122	GLU	6.6
36	1	2539	C	6.6
34	SR	253	ALA	6.6
60	n4	131	ALA	6.5
14	c2	62	LEU	6.5
12	c0	64	TYR	6.5
34	SR	302	PHE	6.5
18	c6	19	VAL	6.5
11	S9	95	TYR	6.5
1	2	913	G	6.4
21	c9	28	LEU	6.4
14	c2	67	THR	6.4
58	N2	95	PHE	6.4
31	d9	5	ASN	6.4
9	S7	5	GLN	6.3
13	C1	36	LYS	6.3
80	p0	88	PHE	6.3
7	s5	72	HIS	6.3
21	c9	119	LYS	6.3
18	c6	18	ALA	6.3
18	c6	114	ARG	6.2
45	l8	198	ALA	6.2
12	c0	20	VAL	6.2
8	S6	156	PHE	6.2
14	c2	111	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
21	c9	92	LYS	6.2
58	N2	71	PHE	6.2
11	S9	134	ILE	6.2
42	L5	38	THR	6.1
62	N6	45	ILE	6.1
11	s9	142	ASN	6.1
7	s5	37	GLN	6.1
11	S9	164	PHE	6.1
33	e1	86	THR	6.1
11	S9	85	VAL	6.1
80	p0	84	VAL	6.0
33	E1	90	LYS	6.0
10	S8	123	LYS	6.0
14	c2	91	VAL	6.0
6	S4	47	PHE	6.0
80	p0	26	PHE	6.0
11	S9	86	LEU	6.0
42	L5	49	TYR	5.9
11	S9	92	LYS	5.9
33	E1	89	LYS	5.9
14	c2	119	SER	5.8
36	1	2540	A	5.8
7	s5	102	ARG	5.8
11	s9	135	ALA	5.8
36	5	1025	A	5.7
21	c9	71	VAL	5.7
18	c6	55	VAL	5.7
34	SR	254	ALA	5.7
63	N7	2	ALA	5.6
10	S8	74	LYS	5.6
18	c6	49	TYR	5.6
18	c6	21	HIS	5.6
10	S8	168	CYS	5.6
21	c9	54	PHE	5.6
34	sR	314	GLN	5.6
12	c0	21	VAL	5.6
1	6	132	U	5.6
20	c8	40	ARG	5.5
74	o8	2	ALA	5.5
14	c2	126	TRP	5.5
18	c6	69	VAL	5.5
58	N2	105	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
18	c6	51	PRO	5.5
11	s9	99	LEU	5.4
18	c6	89	LEU	5.4
58	N2	27	VAL	5.4
35	sM	28	SER	5.4
80	p0	100	ILE	5.4
21	c9	58	ALA	5.4
42	L5	55	PHE	5.4
39	l2	252	THR	5.4
21	c9	101	ASN	5.4
80	p0	54	GLY	5.4
11	s9	37	LYS	5.4
14	c2	89	ILE	5.4
33	e1	85	TYR	5.4
33	E1	92	LYS	5.3
34	SR	211	ILE	5.3
26	D4	70	VAL	5.3
14	c2	43	ARG	5.3
18	c6	7	VAL	5.3
9	S7	93	LEU	5.3
14	c2	52	LEU	5.3
34	sR	32	LEU	5.3
34	sR	136	ILE	5.3
9	S7	47	ARG	5.3
58	N2	93	ILE	5.3
12	c0	62	GLN	5.3
14	C2	61	VAL	5.3
60	N4	98	PRO	5.3
42	L5	63	GLN	5.3
26	D4	25	VAL	5.3
80	p0	80	VAL	5.2
14	C2	104	GLY	5.2
71	O5	75	TYR	5.2
33	E1	91	ILE	5.2
27	d5	50	ILE	5.2
14	c2	117	GLY	5.2
14	c2	71	ILE	5.2
18	c6	117	LEU	5.2
34	SR	235	SER	5.2
58	N2	94	ARG	5.2
7	s5	44	ASN	5.1
9	s7	91	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
11	S9	5	PRO	5.1
36	5	1815	U	5.1
22	d0	66	SER	5.1
51	M5	14	LYS	5.1
7	s5	133	VAL	5.1
55	M9	184	LEU	5.1
80	p0	192	ASP	5.1
34	SR	213	SER	5.1
18	c6	133	GLY	5.1
27	D5	36	ALA	5.1
21	c9	61	VAL	5.1
18	c6	44	LEU	5.1
34	SR	252	LEU	5.1
12	c0	28	ASN	5.0
14	C2	36	LEU	5.0
14	c2	100	TRP	5.0
63	N7	14	VAL	5.0
7	s5	130	ILE	5.0
66	O0	59	TYR	5.0
22	d0	65	ILE	5.0
18	c6	90	VAL	5.0
5	s3	134	CYS	5.0
62	N6	127	GLU	5.0
80	p0	50	VAL	5.0
80	p0	194	GLY	5.0
11	S9	139	GLN	5.0
18	c6	68	ARG	4.9
80	p0	16	ARG	4.9
14	c2	28	LEU	4.9
2	S0	44	GLY	4.9
57	N1	95	HIS	4.9
33	E1	94	LYS	4.9
8	S6	146	GLY	4.9
80	p0	89	THR	4.9
14	c2	49	THR	4.9
21	c9	18	TYR	4.9
10	S8	200	LYS	4.9
14	c2	120	VAL	4.9
22	d0	86	ILE	4.9
12	c0	22	VAL	4.9
11	s9	6	ARG	4.9
18	c6	48	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
10	S8	102	VAL	4.9
11	s9	184	SER	4.9
12	c0	40	LEU	4.8
23	D1	39	VAL	4.8
12	c0	29	GLN	4.8
80	p0	86	PHE	4.8
11	S9	93	LEU	4.8
11	S9	118	LEU	4.8
45	L8	177	TYR	4.8
3	S1	26	ARG	4.8
23	d1	87	ARG	4.8
6	S4	175	PHE	4.8
9	S7	175	LYS	4.8
18	c6	92	TYR	4.8
11	s9	136	VAL	4.8
58	N2	70	LYS	4.8
18	c6	9	THR	4.8
80	p0	79	PHE	4.8
18	c6	82	ARG	4.8
8	S6	157	VAL	4.8
63	N7	75	VAL	4.8
11	s9	93	LEU	4.8
18	c6	47	LYS	4.8
32	e0	54	ARG	4.7
11	s9	7	THR	4.7
12	c0	25	LYS	4.7
74	o8	6	THR	4.7
21	c9	93	HIS	4.7
7	s5	70	VAL	4.7
14	c2	25	GLU	4.7
19	C7	74	GLN	4.7
6	S4	261	LEU	4.7
14	C2	41	LEU	4.7
42	L5	27	LYS	4.7
14	c2	70	ASN	4.7
20	c8	2	SER	4.7
22	d0	88	LYS	4.7
48	m1	49	LYS	4.7
9	s7	92	PHE	4.7
80	p0	28	VAL	4.7
63	N7	11	ALA	4.7
1	2	1710	U	4.7

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Mol	Chain	Res	Type	RSRZ
33	E1	87	THR	4.7
14	c2	61	VAL	4.7
18	c6	17	THR	4.7
9	S7	49	ILE	4.7
21	c9	83	ALA	4.7
33	E1	88	PRO	4.7
74	O8	43	PHE	4.7
14	c2	123	VAL	4.7
42	L5	77	ALA	4.6
21	c9	121	GLY	4.6
21	c9	118	PRO	4.6
58	N2	107	PHE	4.6
10	s8	200	LYS	4.6
76	Q0	128	LYS	4.6
14	c2	102	GLY	4.6
63	N7	77	TYR	4.6
12	c0	32	HIS	4.6
14	c2	32	LEU	4.6
34	sR	33	LEU	4.6
42	L5	62	CYS	4.6
48	m1	91	LEU	4.6
80	p0	15	LEU	4.6
65	N9	42	ASN	4.6
67	O1	71	LEU	4.6
26	D4	69	SER	4.5
7	s5	41	LYS	4.5
21	c9	27	LYS	4.5
1	6	1601	G	4.5
11	S9	34	PHE	4.5
9	s7	93	LEU	4.5
72	O6	50	LEU	4.5
80	p0	85	GLY	4.5
6	S4	138	TYR	4.5
33	e1	145	HIS	4.5
13	C1	35	TYR	4.5
14	c2	45	LEU	4.5
21	c9	60	SER	4.5
65	N9	41	ARG	4.5
14	c2	122	VAL	4.5
11	S9	6	ARG	4.5
3	S1	138	PHE	4.5
4	S2	90	THR	4.5

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Mol	Chain	Res	Type	RSRZ
7	s5	129	PRO	4.4
14	c2	63	VAL	4.4
51	M5	123	GLN	4.4
12	c0	45	ALA	4.4
18	c6	52	LEU	4.4
8	S6	158	ILE	4.4
60	N4	99	GLU	4.4
11	S9	104	PHE	4.4
24	D2	61	ILE	4.4
32	E0	44	PHE	4.4
21	c9	62	ALA	4.4
42	l5	146	LEU	4.4
62	N6	79	ALA	4.4
5	s3	150	MET	4.4
3	s1	156	ALA	4.4
39	L2	250	GLN	4.4
22	d0	64	LYS	4.4
11	S9	147	MET	4.4
14	c2	33	ARG	4.4
18	c6	56	GLY	4.4
18	c6	28	LEU	4.4
58	N2	108	TYR	4.4
58	N2	28	PHE	4.4
12	C0	45	ALA	4.4
63	n7	11	ALA	4.4
21	c9	91	TYR	4.4
14	c2	27	ALA	4.4
12	c0	38	LYS	4.4
14	c2	59	LEU	4.4
7	s5	132	VAL	4.4
42	L5	53	VAL	4.4
55	M9	173	ARG	4.4
3	S1	151	LYS	4.3
42	l5	27	LYS	4.3
63	N7	37	PRO	4.3
64	N8	109	TYR	4.3
27	D5	98	GLN	4.3
11	S9	136	VAL	4.3
2	S0	23	HIS	4.3
18	c6	79	TYR	4.3
63	N7	21	LYS	4.3
13	C1	60	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
19	C7	71	PHE	4.3
27	d5	51	LEU	4.3
21	c9	64	HIS	4.3
33	e1	88	PRO	4.3
17	c5	85	ILE	4.3
39	L2	247	ARG	4.3
10	S8	97	THR	4.3
10	S8	109	PHE	4.3
26	d4	7	ILE	4.3
42	l5	55	PHE	4.3
11	S9	13	SER	4.3
80	p0	61	ARG	4.2
11	S9	148	VAL	4.2
71	o5	120	ALA	4.2
12	c0	27	PHE	4.2
18	c6	12	LYS	4.2
33	e1	84	VAL	4.2
21	c9	90	PRO	4.2
71	O5	2	ALA	4.2
10	S8	67	TRP	4.2
18	c6	64	ASP	4.2
27	d5	39	ALA	4.2
36	1	2205	U	4.2
6	S4	32	SER	4.2
42	l5	127	GLY	4.2
14	c2	26	ASP	4.2
70	O4	79	SER	4.2
80	p0	77	LEU	4.2
60	n4	124	LYS	4.2
14	C2	128	ALA	4.2
59	N3	16	GLY	4.2
30	D8	40	ILE	4.2
74	o8	3	ARG	4.2
20	C8	4	VAL	4.2
9	S7	53	GLY	4.1
36	5	2539	C	4.1
12	c0	75	TYR	4.1
3	S1	25	THR	4.1
14	C2	121	VAL	4.1
17	c5	101	ALA	4.1
26	d4	30	PRO	4.1
60	N4	95	SER	4.1

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Mol	Chain	Res	Type	RSRZ
12	c0	26	ASP	4.1
35	SM	21	PRO	4.1
27	D5	99	ALA	4.1
27	D5	100	ILE	4.1
9	S7	48	GLU	4.1
8	S6	179	VAL	4.1
1	6	1059	U	4.1
70	O4	78	GLY	4.1
6	S4	137	PRO	4.1
14	C2	123	VAL	4.1
10	S8	61	GLU	4.1
11	s9	180	LYS	4.1
11	s9	156	ILE	4.1
33	e1	129	GLY	4.1
80	p0	53	MET	4.1
55	M9	183	ALA	4.1
55	m9	181	ARG	4.1
11	s9	186	GLU	4.1
58	N2	69	ALA	4.1
58	N2	106	ALA	4.1
14	c2	103	LEU	4.1
21	c9	104	VAL	4.1
26	D4	27	VAL	4.1
62	n6	109	LEU	4.1
21	c9	117	SER	4.1
6	S4	44	LEU	4.1
1	6	1052	U	4.1
7	s5	69	PHE	4.1
1	6	506	A	4.1
17	c5	82	ASN	4.1
45	l8	132	VAL	4.0
80	p0	25	LEU	4.0
39	L2	253	GLN	4.0
42	l5	180	PHE	4.0
6	S4	154	ILE	4.0
11	s9	148	VAL	4.0
20	c8	3	LEU	4.0
64	N8	110	GLY	4.0
11	s9	109	LEU	4.0
22	d0	63	LEU	4.0
11	s9	139	GLN	4.0
46	L9	191	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
72	O6	100	HIS	4.0
66	O0	35	ARG	4.0
6	S4	35	PRO	4.0
14	c2	42	ALA	4.0
34	SR	7	LEU	4.0
26	D4	67	GLY	4.0
34	SR	314	GLN	4.0
11	s9	36	LEU	4.0
11	s9	132	ARG	4.0
48	m1	51	ARG	4.0
80	p0	213	PHE	4.0
11	s9	118	LEU	4.0
34	SR	192	PHE	4.0
11	S9	3	ARG	4.0
14	C2	119	SER	4.0
57	N1	72	VAL	4.0
64	N8	60	TYR	4.0
27	D5	71	ILE	4.0
34	SR	234	LEU	4.0
80	p0	59	VAL	4.0
80	p0	214	VAL	4.0
3	s1	140	ILE	4.0
72	O6	26	ILE	4.0
21	c9	66	TYR	4.0
80	p0	66	PHE	4.0
45	L8	202	GLU	3.9
10	S8	183	ILE	3.9
34	SR	169	ILE	3.9
66	O0	90	VAL	3.9
80	p0	29	GLY	3.9
14	c2	101	ALA	3.9
80	p0	20	GLU	3.9
10	s8	54	LYS	3.9
7	s5	94	THR	3.9
21	c9	57	ARG	3.9
12	C0	12	HIS	3.9
42	l5	170	GLY	3.9
33	E1	111	GLU	3.9
34	SR	236	ALA	3.9
63	N7	74	VAL	3.9
42	L5	39	GLN	3.9
63	N7	22	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
6	S4	33	ALA	3.9
63	N7	31	GLU	3.9
70	O4	39	ALA	3.9
6	S4	148	ARG	3.9
21	c9	22	LEU	3.9
69	o3	2	ALA	3.9
27	d5	101	TYR	3.9
15	C3	42	ARG	3.9
45	L8	162	LEU	3.9
3	S1	218	LEU	3.9
8	s6	162	VAL	3.9
63	n7	126	LYS	3.9
13	C1	33	ARG	3.9
33	E1	82	LYS	3.9
1	2	225	A	3.9
3	S1	53	GLY	3.9
3	S1	156	ALA	3.9
34	SR	178	VAL	3.9
72	o6	9	ILE	3.9
78	Q2	27	GLN	3.9
21	c9	112	GLY	3.9
45	L8	132	VAL	3.9
14	c2	68	GLU	3.9
35	sM	51	ARG	3.9
74	o8	43	PHE	3.9
42	L5	31	TYR	3.8
22	d0	113	ASP	3.8
11	s9	158	PHE	3.8
33	E1	96	LYS	3.8
80	p0	76	LEU	3.8
12	c0	24	LYS	3.8
62	N6	33	ALA	3.8
5	s3	50	ILE	3.8
48	m1	59	ILE	3.8
11	s9	185	GLY	3.8
12	c0	66	TYR	3.8
18	c6	10	PHE	3.8
18	c6	135	ARG	3.8
55	m9	184	LEU	3.8
62	N6	73	VAL	3.8
1	2	1711	C	3.8
57	N1	34	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
19	C7	62	GLN	3.8
51	M5	3	ALA	3.8
57	N1	24	ALA	3.8
3	S1	20	VAL	3.8
9	S7	176	LEU	3.8
80	p0	87	VAL	3.8
2	S0	36	TYR	3.8
34	SR	241	PHE	3.8
80	p0	18	TYR	3.8
36	5	1814	A	3.8
8	S6	145	PHE	3.8
22	d0	67	THR	3.8
21	c9	70	GLN	3.8
22	D0	18	GLN	3.8
36	1	1028	U	3.8
7	s5	76	ARG	3.8
31	d9	13	ARG	3.8
7	s5	79	ASN	3.8
14	c2	88	LEU	3.8
60	N4	64	THR	3.8
60	N4	77	LYS	3.8
8	S6	96	SER	3.8
74	O8	57	ASN	3.8
45	L8	150	LEU	3.8
45	L8	161	GLU	3.8
7	s5	53	VAL	3.8
11	S9	146	PHE	3.8
12	c0	19	GLY	3.7
14	C2	62	LEU	3.7
7	s5	74	ALA	3.7
42	L5	61	ILE	3.7
60	n4	130	SER	3.7
33	E1	86	THR	3.7
78	Q2	13	LYS	3.7
33	e1	80	ARG	3.7
39	L2	242	ARG	3.7
58	N2	76	LEU	3.7
14	c2	60	VAL	3.7
21	C9	80	TYR	3.7
8	s6	135	PRO	3.7
42	L5	162	ALA	3.7
11	S9	145	SER	3.7

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Mol	Chain	Res	Type	RSRZ
34	SR	33	LEU	3.7
9	S7	126	LEU	3.7
26	D4	28	LEU	3.7
34	SR	156	VAL	3.7
41	l4	187	LEU	3.7
27	d5	42	LEU	3.7
60	n4	81	PRO	3.7
8	s6	199	GLN	3.7
1	2	1693	A	3.7
12	c0	42	VAL	3.7
14	C2	28	LEU	3.7
7	s5	90	ILE	3.7
11	s9	140	ILE	3.7
3	S1	92	GLN	3.7
60	N4	86	SER	3.7
14	c2	116	VAL	3.7
63	N7	13	VAL	3.7
18	c6	91	ALA	3.7
45	L8	249	ARG	3.7
1	2	136	C	3.7
1	6	1227	A	3.7
26	D4	65	GLY	3.7
10	S8	165	LEU	3.7
14	c2	97	LEU	3.6
34	sR	7	LEU	3.6
63	n7	92	PHE	3.6
67	O1	14	ILE	3.6
42	L5	146	LEU	3.6
55	m9	177	VAL	3.6
4	s2	92	ALA	3.6
11	S9	132	ARG	3.6
3	s1	135	LEU	3.6
26	D4	17	LEU	3.6
26	D4	26	ASP	3.6
10	s8	72	ILE	3.6
18	c6	138	PHE	3.6
42	L5	67	SER	3.6
3	s1	121	ILE	3.6
57	N1	33	VAL	3.6
2	s0	75	ALA	3.6
18	c6	119	ALA	3.6
21	c9	23	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
7	S5	94	THR	3.6
10	S8	70	GLU	3.6
18	C6	41	PRO	3.6
20	c8	132	ARG	3.6
35	sM	29	ASN	3.6
9	s7	77	LEU	3.6
14	c2	78	LEU	3.6
34	SR	32	LEU	3.6
62	n6	79	ALA	3.6
26	d4	26	ASP	3.6
51	M5	135	VAL	3.6
62	N6	103	LYS	3.6
78	Q2	32	LYS	3.6
11	s9	110	GLN	3.6
42	l5	216	GLU	3.6
36	1	1025	A	3.6
34	sR	79	TYR	3.6
42	L5	159	VAL	3.6
12	C0	3	MET	3.6
48	m1	47	GLN	3.6
62	N6	74	TYR	3.6
6	S4	31	PRO	3.6
1	2	192	U	3.6
42	L5	144	VAL	3.6
51	m5	6	TYR	3.6
66	O0	89	VAL	3.6
34	sR	145	LEU	3.6
8	S6	136	LYS	3.6
80	p0	188	VAL	3.6
12	C0	64	TYR	3.6
12	c0	39	ASN	3.6
51	m5	58	GLY	3.6
21	c9	65	ILE	3.5
33	e1	122	SER	3.5
42	L5	64	ILE	3.5
2	s0	107	PHE	3.5
45	L8	197	VAL	3.5
42	l5	92	LEU	3.5
48	m1	147	THR	3.5
11	s9	38	ASN	3.5
7	s5	43	PHE	3.5
11	S9	96	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
14	c2	79	ALA	3.5
14	c2	128	ALA	3.5
18	c6	65	ILE	3.5
21	C9	12	GLN	3.5
26	D4	6	THR	3.5
33	E1	85	TYR	3.5
14	c2	105	LYS	3.5
18	c6	66	ARG	3.5
45	L8	163	VAL	3.5
45	l8	197	VAL	3.5
18	c6	57	LEU	3.5
62	n6	104	LEU	3.5
63	N7	81	LEU	3.5
11	S9	36	LEU	3.5
42	l5	171	LEU	3.5
54	M8	96	PHE	3.5
58	N2	15	PHE	3.5
78	Q2	36	PHE	3.5
78	Q2	106	PHE	3.5
42	L5	143	LYS	3.5
71	O5	74	LYS	3.5
42	l5	63	GLN	3.5
34	SR	25	THR	3.5
66	O0	62	LEU	3.5
3	s1	165	ARG	3.5
42	L5	177	GLU	3.5
13	C1	30	ARG	3.5
32	E0	32	GLY	3.5
14	c2	115	VAL	3.5
17	c5	56	PHE	3.5
33	E1	95	HIS	3.5
18	c6	131	GLY	3.5
48	m1	134	PRO	3.5
31	D9	5	ASN	3.5
12	c0	44	LYS	3.5
63	N7	134	LEU	3.5
80	p0	19	LEU	3.5
60	n4	85	ALA	3.5
3	s1	119	THR	3.5
13	C1	61	THR	3.5
18	C6	11	GLY	3.5
6	S4	128	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
11	S9	140	ILE	3.5
12	C0	2	LEU	3.5
14	C2	59	LEU	3.5
45	L8	152	LEU	3.5
63	N7	131	PHE	3.5
13	c1	2	SER	3.5
67	O1	12	TYR	3.5
7	s5	92	ARG	3.5
14	c2	136	ILE	3.5
21	c9	124	ILE	3.5
34	SR	301	LEU	3.5
1	2	194	U	3.5
10	S8	83	TYR	3.5
14	c2	40	GLY	3.5
51	M5	148	TYR	3.5
34	sR	157	VAL	3.5
80	p0	187	VAL	3.5
5	s3	188	ILE	3.5
36	5	1816	A	3.5
9	s7	61	PHE	3.5
27	d5	38	HIS	3.5
10	S8	96	LEU	3.5
18	c6	85	ILE	3.5
18	c6	116	LEU	3.5
42	L5	60	ILE	3.5
2	s0	147	THR	3.5
6	s4	26	CYS	3.5
42	L5	48	LYS	3.5
2	s0	144	ILE	3.4
5	s3	186	VAL	3.4
2	s0	146	LEU	3.4
78	Q2	72	LEU	3.4
11	S9	144	PRO	3.4
24	D2	46	TYR	3.4
28	D6	73	TYR	3.4
42	l5	154	THR	3.4
60	N4	97	LYS	3.4
61	N5	124	VAL	3.4
27	d5	75	LEU	3.4
80	p0	63	ILE	3.4
10	s8	67	TRP	3.4
39	L2	248	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
57	N1	94	GLU	3.4
27	d5	100	ILE	3.4
8	s6	217	SER	3.4
36	5	1271	A	3.4
10	S8	8	ARG	3.4
20	c8	85	PHE	3.4
80	p0	38	MET	3.4
23	d1	33	GLN	3.4
42	l5	182	GLY	3.4
6	S4	139	VAL	3.4
11	s9	133	HIS	3.4
45	L8	165	PHE	3.4
26	D4	40	LEU	3.4
42	L5	47	PRO	3.4
42	L5	190	ILE	3.4
43	L6	109	GLU	3.4
9	s7	96	ARG	3.4
24	D2	122	SER	3.4
6	S4	13	ALA	3.4
34	sR	121	MET	3.4
6	S4	12	LEU	3.4
64	N8	79	TRP	3.4
8	s6	149	LYS	3.4
21	C9	71	VAL	3.4
1	2	820	U	3.4
57	N1	90	ASN	3.4
78	Q2	15	LYS	3.4
11	s9	17	ARG	3.4
57	N1	67	VAL	3.4
12	c0	15	LEU	3.4
11	S9	158	PHE	3.4
80	p0	199	SER	3.4
42	L5	59	ASP	3.4
36	5	1028	U	3.4
41	l4	185	LYS	3.4
60	n4	128	ALA	3.4
63	n7	41	ALA	3.4
11	s9	153	GLU	3.4
20	c8	42	TYR	3.4
18	c6	124	PRO	3.4
31	d9	11	PRO	3.4
13	C1	34	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
34	sR	163	ASP	3.4
39	L2	252	THR	3.3
14	c2	64	SER	3.3
1	6	1	U	3.3
12	C0	20	VAL	3.3
31	D9	52	PHE	3.3
45	l8	34	PHE	3.3
36	5	1352	A	3.3
42	L5	163	LEU	3.3
22	d0	107	THR	3.3
79	Q3	92	ALA	3.3
3	s1	136	ARG	3.3
12	c0	1	MET	3.3
9	s7	70	PHE	3.3
10	s8	146	ARG	3.3
39	l2	253	GLN	3.3
48	m1	60	ARG	3.3
64	N8	59	ARG	3.3
64	n8	64	GLN	3.3
11	S9	97	LEU	3.3
78	Q2	24	LYS	3.3
6	s4	188	ASN	3.3
8	S6	78	THR	3.3
8	s6	134	GLY	3.3
10	S8	192	TYR	3.3
8	s6	218	GLU	3.3
42	L5	37	VAL	3.3
42	l5	203	HIS	3.3
3	S1	137	ILE	3.3
51	M5	119	TYR	3.3
48	m1	132	ASN	3.3
34	SR	115	ILE	3.3
55	m9	174	ALA	3.3
10	S8	63	GLY	3.3
33	E1	99	LYS	3.3
80	p0	27	VAL	3.3
6	S4	246	LEU	3.3
13	c1	3	THR	3.3
14	C2	142	GLN	3.3
17	C5	125	PRO	3.3
17	c5	103	ASN	3.3
17	c5	116	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
5	s3	25	PHE	3.3
6	s4	149	TYR	3.3
63	n7	74	VAL	3.3
11	s9	2	PRO	3.3
36	5	360	G	3.3
34	sR	36	ALA	3.3
3	s1	143	THR	3.3
28	d6	17	HIS	3.3
42	L5	41	LYS	3.3
57	N1	91	LEU	3.3
51	M5	15	GLN	3.3
6	S4	225	VAL	3.3
11	S9	99	LEU	3.3
53	M7	162	GLU	3.3
22	d0	27	THR	3.3
70	O4	73	SER	3.3
11	s9	20	GLU	3.3
14	c2	104	GLY	3.3
27	d5	65	LEU	3.3
20	c8	24	GLY	3.3
35	sM	34	LYS	3.3
74	o8	5	ILE	3.3
36	1	252	U	3.3
10	S8	177	GLY	3.3
45	L8	119	GLY	3.3
45	L8	134	TYR	3.3
21	c9	53	TRP	3.3
65	n9	39	PHE	3.3
21	c9	86	ARG	3.3
48	M1	141	ARG	3.3
11	s9	143	ILE	3.3
8	S6	208	TYR	3.3
12	C0	41	TYR	3.3
11	s9	3	ARG	3.3
18	C6	132	LYS	3.3
19	c7	2	GLY	3.3
9	S7	46	ILE	3.3
10	S8	62	THR	3.3
14	c2	75	VAL	3.3
33	E1	130	VAL	3.3
48	M1	147	THR	3.3
11	s9	97	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
80	p0	212	HIS	3.2
78	Q2	81	ALA	3.2
14	C2	60	VAL	3.2
11	S9	14	THR	3.2
14	C2	95	LYS	3.2
35	sM	66	ALA	3.2
33	e1	131	PHE	3.2
45	L8	254	ASP	3.2
63	N7	20	GLY	3.2
34	SR	170	ILE	3.2
38	4	158	U	3.2
7	s5	77	TYR	3.2
35	sM	35	ALA	3.2
35	sM	53	ARG	3.2
17	c5	119	PHE	3.2
19	C7	28	PHE	3.2
21	c9	45	MET	3.2
63	N7	47	GLU	3.2
1	6	136	C	3.2
10	S8	148	ALA	3.2
18	c6	3	ALA	3.2
68	O2	2	ALA	3.2
80	p0	49	ALA	3.2
6	S4	260	GLY	3.2
11	S9	94	ASP	3.2
14	C2	32	LEU	3.2
26	D4	61	ARG	3.2
57	N1	69	LYS	3.2
13	C1	27	THR	3.2
11	S9	15	PRO	3.2
2	s0	174	TRP	3.2
36	5	358	G	3.2
59	N3	4	ASN	3.2
63	N7	30	ASP	3.2
20	C8	6	GLN	3.2
27	d5	60	VAL	3.2
34	SR	203	THR	3.2
8	S6	177	ARG	3.2
21	c9	132	LEU	3.2
14	c2	121	VAL	3.2
18	C6	133	GLY	3.2
26	D4	14	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	s0	122	ILE	3.2
27	d5	41	ILE	3.2
31	d9	16	LYS	3.2
32	e0	43	ARG	3.2
74	O8	73	LEU	3.2
78	Q2	18	ARG	3.2
22	d0	82	TYR	3.2
11	s9	128	LEU	3.2
12	c0	37	THR	3.2
3	S1	49	ASN	3.2
11	S9	138	LYS	3.2
14	C2	111	ASN	3.2
20	C8	25	ASN	3.2
32	E0	3	LYS	3.2
20	c8	131	LEU	3.2
78	q2	101	GLY	3.2
33	e1	132	LEU	3.2
80	p0	52	LEU	3.2
42	l5	62	CYS	3.2
45	L8	99	PRO	3.2
14	C2	27	ALA	3.2
33	E1	84	VAL	3.2
61	N5	41	ALA	3.2
2	S0	43	ASP	3.2
2	S0	30	GLN	3.2
2	s0	97	PRO	3.2
9	S7	52	ALA	3.2
14	C2	31	VAL	3.2
11	S9	143	ILE	3.2
42	l5	150	LEU	3.2
11	s9	145	SER	3.2
40	L3	386	ASP	3.2
11	S9	2	PRO	3.2
30	D8	45	LYS	3.2
34	SR	261	LYS	3.2
3	S1	51	SER	3.2
80	p0	11	TYR	3.2
9	s7	43	PHE	3.2
20	c8	5	VAL	3.2
1	6	1337	A	3.1
10	S8	184	LEU	3.1
11	S9	169	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
22	D0	63	LEU	3.1
45	l8	99	PRO	3.1
59	N3	77	ILE	3.1
6	S4	14	ALA	3.1
7	s5	97	LEU	3.1
18	c6	36	ILE	3.1
21	c9	113	ILE	3.1
22	d0	58	LEU	3.1
26	d4	69	SER	3.1
31	d9	31	ILE	3.1
59	N3	100	GLY	3.1
47	m0	56	GLU	3.1
72	o6	66	GLU	3.1
36	5	1820	U	3.1
80	p0	14	LYS	3.1
16	c4	126	THR	3.1
63	N7	23	VAL	3.1
4	S2	92	ALA	3.1
10	S8	30	GLY	3.1
26	D4	66	GLY	3.1
12	C0	21	VAL	3.1
8	s6	88	ARG	3.1
11	s9	129	ILE	3.1
66	O0	56	LEU	3.1
80	p0	65	GLY	3.1
5	s3	17	PHE	3.1
6	S4	15	PRO	3.1
18	c6	50	GLU	3.1
10	S8	179	CYS	3.1
17	c5	112	LEU	3.1
14	C2	102	GLY	3.1
22	d0	24	ILE	3.1
42	L5	28	THR	3.1
72	O6	2	THR	3.1
3	s1	100	PHE	3.1
7	s5	184	PHE	3.1
8	S6	190	GLN	3.1
27	d5	67	ASP	3.1
45	l8	131	ALA	3.1
31	d9	29	GLY	3.1
63	N7	3	LYS	3.1
8	S6	178	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
55	m9	182	ASP	3.1
51	M5	122	ASN	3.1
9	S7	58	LEU	3.1
10	S8	182	TYR	3.1
20	c8	48	LYS	3.1
30	D8	66	LEU	3.1
42	L5	171	LEU	3.1
8	S6	50	PHE	3.1
26	D4	35	VAL	3.1
21	c9	108	LEU	3.1
21	c9	85	SER	3.1
21	c9	116	ILE	3.1
48	m1	64	LYS	3.1
74	o8	29	LYS	3.1
51	m5	131	GLU	3.1
20	c8	44	ASN	3.1
55	M9	21	LYS	3.1
5	s3	152	PHE	3.1
55	m9	183	ALA	3.1
63	N7	4	PHE	3.1
36	1	2507	C	3.1
21	c9	123	ARG	3.1
78	q2	25	VAL	3.1
3	S1	205	PHE	3.1
10	S8	117	TYR	3.1
13	C1	137	PHE	3.1
42	l5	185	PHE	3.1
7	s5	75	GLY	3.1
11	s9	96	VAL	3.1
6	S4	131	LEU	3.1
35	SM	88	ARG	3.1
42	l5	175	HIS	3.1
45	l8	94	PHE	3.1
59	n3	81	GLN	3.1
18	c6	112	TYR	3.1
42	l5	144	VAL	3.1
35	sM	55	SER	3.1
42	l5	8	LYS	3.1
64	N8	78	LEU	3.1
72	o6	80	PHE	3.1
6	S4	157	ASN	3.1
11	S9	120	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
35	sM	38	PRO	3.1
15	C3	45	LEU	3.1
21	c9	44	GLU	3.1
36	1	358	G	3.1
60	n4	86	SER	3.1
18	C6	143	ARG	3.0
33	E1	131	PHE	3.1
51	M5	139	HIS	3.0
33	e1	83	LYS	3.0
34	sR	156	VAL	3.0
14	c2	127	GLY	3.0
33	e1	128	ALA	3.0
55	m9	7	GLN	3.0
8	S6	75	LEU	3.0
11	s9	5	PRO	3.0
14	C2	103	LEU	3.0
22	D0	84	MET	3.0
63	n7	87	LEU	3.0
10	S8	152	ILE	3.0
34	sR	61	PHE	3.0
67	O1	72	ARG	3.0
78	Q2	10	THR	3.0
6	s4	25	GLY	3.0
70	O4	32	ALA	3.0
12	C0	35	ILE	3.0
18	c6	130	GLY	3.0
17	c5	83	MET	3.0
19	c7	71	PHE	3.0
12	C0	25	LYS	3.0
65	n9	43	HIS	3.0
42	L5	76	ALA	3.0
57	n1	34	TYR	3.0
80	p0	211	SER	3.0
4	s2	178	ILE	3.0
9	s7	62	VAL	3.0
27	d5	55	PRO	3.0
58	n2	11	ILE	3.0
1	2	137	U	3.0
21	C9	59	ALA	3.0
59	N3	34	LEU	3.0
3	s1	154	SER	3.0
14	C2	120	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
21	c9	115	GLU	3.0
14	c2	69	ALA	3.0
1	2	224	C	3.0
18	C6	82	ARG	3.0
63	N7	65	ARG	3.0
18	c6	67	VAL	3.0
80	p0	101	VAL	3.0
80	p0	193	ASN	3.0
21	c9	31	PRO	3.0
60	N4	96	LEU	3.0
63	N7	41	ALA	3.0
74	o8	31	LEU	3.0
13	c1	20	PHE	3.0
78	Q2	71	ARG	3.0
22	d0	83	GLU	3.0
42	L5	46	THR	3.0
59	N3	78	VAL	3.0
80	p0	41	VAL	3.0
11	S9	177	ALA	3.0
11	s9	8	TYR	3.0
32	E0	46	ASN	3.0
6	s4	47	PHE	3.0
22	D0	61	LYS	3.0
32	E0	36	LYS	3.0
41	l4	186	LYS	3.0
9	s7	90	VAL	3.0
6	s4	48	LEU	3.0
63	n7	42	LEU	3.0
72	O6	28	TYR	3.0
34	SR	137	LYS	3.0
78	Q2	19	LYS	3.0
9	s7	134	GLU	3.0
14	c2	107	ASP	3.0
22	D0	120	SER	3.0
78	q2	72	LEU	3.0
42	L5	170	GLY	3.0
47	m0	219	ALA	3.0
57	n1	46	GLY	3.0
74	O8	34	ALA	3.0
4	s2	63	VAL	3.0
7	S5	162	VAL	3.0
9	S7	181	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
63	n7	75	VAL	3.0
20	c8	55	HIS	3.0
11	S9	80	LEU	3.0
12	C0	40	LEU	3.0
70	O4	77	GLY	3.0
2	s0	185	ARG	3.0
31	d9	12	ARG	3.0
70	O4	33	GLN	3.0
72	O6	98	ARG	3.0
74	o8	33	LYS	3.0
9	S7	70	PHE	3.0
14	c2	118	ALA	3.0
45	L8	164	VAL	3.0
63	n7	96	VAL	3.0
65	n9	37	PRO	3.0
9	s7	126	LEU	3.0
22	d0	85	ARG	3.0
28	d6	15	ARG	3.0
29	D7	73	LEU	3.0
6	S4	208	VAL	2.9
12	c0	30	ALA	2.9
62	n6	42	GLN	3.0
20	c8	129	TRP	2.9
78	q2	81	ALA	2.9
34	SR	300	THR	2.9
1	2	1445	G	2.9
18	C6	57	LEU	2.9
2	s0	46	HIS	2.9
10	S8	166	TYR	2.9
51	m5	177	GLY	2.9
33	e1	125	THR	2.9
21	C9	55	TYR	2.9
35	sM	37	VAL	2.9
57	N1	30	TYR	2.9
14	c2	93	ASP	2.9
21	c9	29	GLU	2.9
34	sR	34	LEU	2.9
62	N6	125	LYS	2.9
36	5	330	G	2.9
63	N7	82	PRO	2.9
24	D2	121	VAL	2.9
8	s6	190	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
9	S7	137	GLY	2.9
18	c6	29	ILE	2.9
9	S7	81	LEU	2.9
27	D5	41	ILE	2.9
42	L5	78	ALA	2.9
80	p0	9	ALA	2.9
54	M8	79	LYS	2.9
27	d5	40	VAL	2.9
18	c6	105	LEU	2.9
42	L5	50	ARG	2.9
57	N1	93	VAL	2.9
18	c6	132	LYS	2.9
63	n7	22	LYS	2.9
78	Q2	73	GLU	2.9
80	p0	196	VAL	2.9
3	S1	140	ILE	2.9
42	l5	61	ILE	2.9
55	M9	185	LEU	2.9
18	C6	40	GLU	2.9
42	L5	151	GLN	2.9
42	L5	188	GLU	2.9
80	p0	10	GLU	2.9
11	s9	144	PRO	2.9
26	D4	68	LYS	2.9
42	L5	40	HIS	2.9
17	C5	113	GLY	2.9
20	c8	125	ILE	2.9
26	d4	2	SER	2.9
74	o8	32	ASN	2.9
64	N8	127	ALA	2.9
42	L5	95	TRP	2.9
14	c2	95	LYS	2.9
18	C6	79	TYR	2.9
7	s5	62	VAL	2.9
51	M5	140	LYS	2.9
78	Q2	26	THR	2.9
78	q2	8	ARG	2.9
7	s5	198	LEU	2.9
48	M1	172	LEU	2.9
11	S9	91	LYS	2.9
78	q2	9	LYS	2.9
3	S1	105	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
34	SR	202	LEU	2.9
35	sM	40	PRO	2.9
5	S3	206	VAL	2.9
18	c6	60	PHE	2.9
26	d4	44	LEU	2.9
27	d5	92	ILE	2.9
45	L8	153	ILE	2.9
14	c2	66	VAL	2.9
65	N9	38	LYS	2.9
11	s9	157	ASP	2.9
19	C7	123	ASN	2.9
66	O0	55	GLU	2.9
32	E0	35	TYR	2.9
45	L8	189	LEU	2.9
62	N6	44	GLY	2.9
80	p0	190	VAL	2.9
42	l5	128	GLU	2.9
55	M9	170	ARG	2.9
1	2	651	G	2.9
42	l5	129	TYR	2.9
3	s1	141	ALA	2.9
18	c6	109	PHE	2.9
43	L6	3	ALA	2.9
45	L8	256	ALA	2.9
45	l8	165	PHE	2.9
22	d0	61	LYS	2.8
11	S9	102	GLU	2.8
35	sM	48	ARG	2.8
2	S0	146	LEU	2.8
80	p0	68	SER	2.8
7	S5	37	GLN	2.8
9	S7	90	VAL	2.8
33	E1	129	GLY	2.8
14	C2	34	THR	2.8
1	6	1588	G	2.8
3	s1	61	LEU	2.8
10	S8	69	SER	2.8
11	s9	164	PHE	2.8
35	sM	27	LYS	2.8
4	s2	196	VAL	2.8
9	S7	50	ASP	2.8
20	C8	5	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
48	m1	62	ASN	2.8
55	M9	49	THR	2.8
45	L8	226	TYR	2.8
57	N1	31	LEU	2.8
61	N5	40	LEU	2.8
7	S5	71	ALA	2.8
55	M9	181	ARG	2.8
11	s9	91	LYS	2.8
12	c0	49	LEU	2.8
27	d5	91	PRO	2.8
34	sR	144	LEU	2.8
60	N4	110	LYS	2.8
62	N6	104	LEU	2.8
10	S8	68	ALA	2.8
12	C0	23	ALA	2.8
16	C4	15	GLY	2.8
55	M9	64	ARG	2.8
66	o0	35	ARG	2.8
1	2	836	U	2.8
1	6	767	U	2.8
8	s6	93	LYS	2.8
12	C0	1	MET	2.8
31	d9	33	LYS	2.8
51	m5	148	TYR	2.8
6	S4	8	HIS	2.8
7	s5	36	ALA	2.8
14	c2	92	ALA	2.8
6	S4	9	LEU	2.8
12	c0	31	LYS	2.8
17	C5	116	LEU	2.8
6	s4	27	TYR	2.8
7	s5	137	ILE	2.8
31	D9	33	LYS	2.8
36	1	2598	G	2.8
42	L5	30	TYR	2.8
53	M7	182	ILE	2.8
58	N2	33	TYR	2.8
80	p0	201	ILE	2.8
18	c6	134	ALA	2.8
26	D4	57	VAL	2.8
9	S7	151	LYS	2.8
35	sM	52	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
80	p0	22	TYR	2.8
8	s6	177	ARG	2.8
8	S6	82	SER	2.8
14	c2	58	LEU	2.8
34	SR	225	LEU	2.8
58	n2	44	GLU	2.8
22	D0	121	ASN	2.8
20	c8	45	LEU	2.8
51	M5	10	LEU	2.8
7	s5	96	SER	2.8
62	N6	81	GLN	2.8
65	N9	43	HIS	2.8
11	S9	12	TYR	2.8
11	s9	113	VAL	2.8
57	N1	92	ARG	2.8
62	N6	80	VAL	2.8
17	C5	98	ASN	2.8
22	D0	64	LYS	2.8
33	e1	134	ASN	2.8
34	sR	62	LYS	2.8
66	O0	97	ASP	2.8
6	S4	173	ILE	2.8
11	S9	77	ILE	2.8
34	sR	315	VAL	2.8
26	D4	71	GLY	2.8
48	M1	146	GLY	2.8
63	n7	21	LYS	2.8
1	6	131	C	2.8
3	s1	142	PHE	2.8
10	S8	52	ASN	2.8
14	c2	48	SER	2.8
45	L8	253	SER	2.8
3	s1	123	ALA	2.8
14	C2	50	LYS	2.8
20	c8	61	LEU	2.8
11	S9	8	TYR	2.8
60	N4	74	LYS	2.8
62	N6	72	SER	2.8
63	N7	34	LYS	2.8
74	O8	30	LYS	2.8
5	S3	88	ALA	2.8
22	d0	93	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
40	L3	387	LEU	2.8
41	l4	223	PRO	2.8
51	M5	137	PRO	2.8
67	O1	73	LEU	2.8
18	c6	40	GLU	2.8
19	c7	103	ASP	2.8
11	S9	37	LYS	2.8
31	D9	34	TYR	2.8
22	d0	87	HIS	2.8
41	l4	79	GLY	2.8
14	C2	37	VAL	2.8
14	c2	37	VAL	2.8
23	D1	47	PRO	2.8
26	D4	41	ARG	2.8
63	N7	48	ARG	2.8
33	E1	107	LYS	2.8
7	s5	194	LEU	2.8
11	s9	181	ALA	2.8
29	D7	24	LEU	2.8
45	l8	252	ASN	2.8
49	m3	54	LEU	2.8
58	n2	69	ALA	2.8
72	o6	8	ALA	2.8
72	o6	50	LEU	2.8
10	S8	156	VAL	2.7
57	N1	32	LYS	2.7
64	N8	55	LYS	2.7
7	s5	34	GLN	2.7
45	L8	121	SER	2.7
7	s5	80	LYS	2.7
58	N2	17	VAL	2.7
7	S5	152	GLY	2.7
13	c1	147	GLY	2.7
20	C8	3	LEU	2.7
47	m0	52	LEU	2.7
60	n4	84	GLY	2.7
72	o6	77	LEU	2.7
80	p0	195	GLN	2.7
9	S7	138	LYS	2.7
11	S9	52	ILE	2.7
17	c5	100	LYS	2.7
18	c6	45	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
28	d6	44	ILE	2.7
55	m9	50	ILE	2.7
74	O8	33	LYS	2.7
7	s5	181	GLU	2.7
31	d9	34	TYR	2.7
67	O1	69	TYR	2.7
42	L5	26	GLY	2.7
3	S1	45	LYS	2.7
16	c4	127	ARG	2.7
48	m1	54	VAL	2.7
58	n2	13	LYS	2.7
80	p0	30	VAL	2.7
11	s9	152	SER	2.7
48	m1	131	MET	2.7
63	n7	82	PRO	2.7
6	S4	245	LYS	2.7
8	S6	187	LYS	2.7
11	S9	4	ALA	2.7
19	C7	3	ARG	2.7
34	SR	214	ALA	2.7
35	sM	62	ARG	2.7
71	O5	106	LYS	2.7
11	s9	130	THR	2.7
34	sR	44	SER	2.7
54	m8	99	THR	2.7
39	L2	246	LEU	2.7
15	C3	24	ALA	2.7
51	M5	68	ARG	2.7
48	m1	65	ILE	2.7
55	M9	50	ILE	2.7
55	m9	51	VAL	2.7
58	N2	56	VAL	2.7
80	p0	191	TYR	2.7
80	p0	197	PHE	2.7
9	S7	73	VAL	2.7
11	S9	135	ALA	2.7
14	c2	30	VAL	2.7
14	c2	31	VAL	2.7
18	c6	26	LYS	2.7
57	N1	23	GLY	2.7
22	D0	65	ILE	2.7
62	n6	73	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
63	n7	95	VAL	2.7
80	p0	17	GLU	2.7
19	C7	26	LEU	2.7
22	d0	26	LEU	2.7
1	2	217	A	2.7
9	S7	6	ALA	2.7
20	c8	22	VAL	2.7
27	d5	54	VAL	2.7
34	SR	157	VAL	2.7
34	sR	312	VAL	2.7
11	S9	90	LYS	2.7
13	c1	24	LYS	2.7
64	N8	126	LYS	2.7
11	S9	7	THR	2.7
16	C4	88	GLY	2.7
34	SR	220	ILE	2.7
9	s7	44	LYS	2.7
20	c8	54	LEU	2.7
33	E1	103	LEU	2.7
36	5	363	G	2.7
40	L3	4	ARG	2.7
64	N8	63	LYS	2.7
42	l5	159	VAL	2.7
16	c4	125	SER	2.7
63	n7	124	ALA	2.7
20	c8	46	VAL	2.7
14	c2	131	ASP	2.7
36	5	27	C	2.7
34	SR	233	THR	2.7
34	SR	313	TRP	2.7
14	c2	29	LYS	2.7
36	5	547	G	2.7
38	4	80	A	2.7
42	l5	163	LEU	2.7
63	N7	136	PHE	2.7
70	O4	51	LEU	2.7
14	C2	63	VAL	2.7
28	d6	73	TYR	2.7
55	M9	17	VAL	2.7
61	N5	107	VAL	2.7
65	N9	34	GLY	2.7
13	C1	24	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
14	C2	100	TRP	2.7
48	M1	118	PRO	2.7
12	C0	13	GLN	2.7
22	d0	104	THR	2.7
14	C2	122	VAL	2.7
48	M1	171	VAL	2.7
1	2	265	A	2.7
18	C6	131	GLY	2.7
20	c8	58	ALA	2.7
36	5	1269	U	2.7
3	S1	54	LEU	2.7
6	S4	52	LEU	2.7
36	5	347	G	2.7
48	m1	61	ARG	2.7
74	o8	37	PRO	2.7
22	d0	80	GLU	2.7
72	O6	97	SER	2.7
78	Q2	70	LEU	2.7
6	S4	27	TYR	2.7
6	s4	70	VAL	2.7
63	N7	12	VAL	2.7
35	sM	57	ASN	2.7
51	M5	176	LYS	2.7
2	S0	18	LEU	2.7
77	Q1	11	ARG	2.7
18	c6	125	GLU	2.7
11	s9	12	TYR	2.7
26	D4	24	VAL	2.7
51	M5	138	GLN	2.7
61	N5	123	TYR	2.7
65	n9	36	ASP	2.7
65	N9	45	HIS	2.7
78	Q2	23	HIS	2.7
32	E0	2	ALA	2.7
8	S6	77	LEU	2.6
11	s9	116	LEU	2.6
66	O0	25	LEU	2.6
6	S4	28	ALA	2.6
10	s8	199	LYS	2.6
22	D0	27	THR	2.6
24	D2	128	PHE	2.6
39	l2	155	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
64	N8	149	ALA	2.6
42	l5	22	ARG	2.6
58	N2	104	ARG	2.6
1	6	1371	A	2.6
32	e0	22	GLU	2.6
63	N7	26	VAL	2.6
10	s8	117	TYR	2.6
63	N7	18	TYR	2.6
9	S7	60	ILE	2.6
11	s9	177	ALA	2.6
14	c2	96	GLN	2.6
59	N3	17	LEU	2.6
10	S8	199	LYS	2.6
36	5	1353	U	2.6
10	s8	198	ALA	2.6
22	d0	54	GLY	2.6
36	1	1016	C	2.6
60	n4	93	ARG	2.6
74	O8	40	GLN	2.6
11	s9	105	LEU	2.6
34	sR	66	HIS	2.6
45	L8	166	LEU	2.6
7	S5	70	VAL	2.6
22	d0	114	VAL	2.6
41	L4	199	TRP	2.6
7	S5	209	TYR	2.6
11	S9	180	LYS	2.6
13	C1	23	PRO	2.6
35	SM	22	PRO	2.6
51	M5	181	ASN	2.6
65	n9	29	TYR	2.6
1	6	1338	C	2.6
36	5	1581	C	2.6
6	S4	169	ILE	2.6
17	c5	81	ARG	2.6
17	c5	84	ILE	2.6
31	d9	38	ILE	2.6
34	SR	79	TYR	2.6
20	c8	25	ASN	2.6
80	p0	104	ARG	2.6
24	D2	104	LEU	2.6
51	m5	176	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	2	249	U	2.6
20	C8	125	ILE	2.6
24	D2	41	MET	2.6
24	d2	3	ARG	2.6
9	S7	38	LEU	2.6
11	S9	128	LEU	2.6
2	S0	28	ASN	2.6
9	S7	180	GLN	2.6
18	c6	32	ASN	2.6
66	O0	95	ALA	2.6
7	S5	188	LYS	2.6
7	s5	209	TYR	2.6
10	s8	113	PHE	2.6
39	L2	241	ARG	2.6
45	L8	130	TYR	2.6
51	M5	178	HIS	2.6
14	C2	127	GLY	2.6
60	N4	109	LEU	2.6
11	s9	172	VAL	2.6
10	S8	86	SER	2.6
17	c5	98	ASN	2.6
18	C6	83	GLN	2.6
8	s6	175	ILE	2.6
8	s6	196	ARG	2.6
10	s8	55	TYR	2.6
12	c0	79	TYR	2.6
36	5	53	G	2.6
74	o8	52	TYR	2.6
18	c6	126	PRO	2.6
18	c6	127	LYS	2.6
26	D4	55	VAL	2.6
7	s5	91	GLU	2.6
42	l5	179	ARG	2.6
59	N3	36	ILE	2.6
65	n9	42	ASN	2.6
78	Q2	34	SER	2.6
1	2	1370	U	2.6
35	sM	30	THR	2.6
55	M9	52	LYS	2.6
6	S4	130	GLN	2.6
9	S7	91	ILE	2.6
22	D0	85	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
51	m5	175	ASN	2.6
80	p0	12	PHE	2.6
80	p0	185	LEU	2.6
3	S1	50	LYS	2.6
14	c2	73	LYS	2.6
18	c6	86	ALA	2.6
36	1	1580	A	2.6
3	S1	24	PHE	2.6
3	S1	100	PHE	2.6
19	c7	74	GLN	2.6
6	s4	9	LEU	2.6
19	c7	73	LEU	2.6
24	D2	83	ILE	2.6
42	L5	129	TYR	2.6
67	O1	36	ILE	2.6
70	O4	30	LEU	2.6
11	S9	119	ALA	2.6
11	s9	137	GLY	2.6
23	d1	54	ALA	2.6
55	M9	18	GLY	2.6
27	D5	91	PRO	2.6
1	2	697	C	2.6
10	S8	113	PHE	2.6
18	c6	46	PHE	2.6
6	s4	22	LYS	2.6
12	c0	61	TRP	2.6
18	c6	71	GLY	2.6
21	c9	9	VAL	2.6
39	l2	251	LYS	2.6
46	L9	85	GLY	2.6
60	n4	125	ALA	2.6
10	s8	179	CYS	2.6
3	s1	138	PHE	2.6
6	S4	69	HIS	2.6
26	D4	85	PHE	2.6
9	s7	48	GLU	2.6
12	c0	17	GLN	2.6
22	D0	94	GLU	2.6
3	S1	21	VAL	2.6
8	S6	97	VAL	2.6
78	Q2	25	VAL	2.6
42	L5	233	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
66	o0	6	SER	2.6
2	s0	184	LEU	2.6
12	c0	46	LEU	2.6
14	C2	38	HIS	2.6
14	C2	52	LEU	2.6
21	c9	95	ASP	2.6
35	sM	33	LYS	2.6
42	L5	4	GLN	2.6
42	l5	297	GLN	2.6
71	o5	106	LYS	2.6
62	n6	12	ARG	2.6
9	S7	24	PHE	2.6
6	s4	69	HIS	2.5
7	s5	104	ASN	2.5
13	C1	4	GLU	2.5
21	C9	13	ASP	2.5
42	L5	126	GLU	2.5
51	m5	93	LYS	2.5
1	2	474	A	2.5
1	2	1245	G	2.5
63	N7	101	PHE	2.5
10	s8	96	LEU	2.5
55	m9	106	LEU	2.5
6	S4	26	CYS	2.5
34	SR	232	TYR	2.5
42	L5	44	TYR	2.5
46	L9	190	ASP	2.5
48	M1	72	ARG	2.5
51	m5	123	GLN	2.5
3	s1	139	ALA	2.5
26	d4	72	PHE	2.5
9	s7	153	LEU	2.5
15	c3	27	LYS	2.5
28	d6	29	SER	2.5
39	L2	112	ILE	2.5
55	M9	24	LEU	2.5
36	5	814	U	2.5
43	l6	129	GLU	2.5
45	l8	97	TYR	2.5
80	p0	51	VAL	2.5
8	S6	83	CYS	2.5
57	n1	45	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
34	sR	180	ALA	2.5
18	C6	47	LYS	2.5
21	C9	92	LYS	2.5
22	D0	86	ILE	2.5
49	M3	95	ILE	2.5
57	N1	96	ILE	2.5
67	o1	16	LEU	2.5
4	s2	176	SER	2.5
29	D7	29	ARG	2.5
27	d5	43	ASP	2.5
55	M9	188	ASP	2.5
7	S5	193	THR	2.5
9	S7	154	LEU	2.5
67	O1	75	ILE	2.5
7	s5	61	TYR	2.5
18	C6	15	SER	2.5
20	C8	7	GLU	2.5
11	s9	104	PHE	2.5
11	s9	155	HIS	2.5
12	c0	12	HIS	2.5
18	c6	8	GLN	2.5
18	c6	13	LYS	2.5
45	L8	142	LEU	2.5
48	m1	30	LEU	2.5
62	N6	126	LEU	2.5
6	s4	78	THR	2.5
11	s9	33	GLU	2.5
11	S9	121	SER	2.5
35	SM	85	SER	2.5
42	L5	35	ARG	2.5
21	c9	10	ALA	2.5
48	m1	102	PHE	2.5
62	N6	34	PRO	2.5
77	Q1	4	LYS	2.5
3	S1	120	LEU	2.5
12	c0	43	ILE	2.5
26	D4	7	ILE	2.5
27	d5	37	GLN	2.5
28	d6	45	VAL	2.5
62	n6	80	VAL	2.5
33	E1	106	TYR	2.5
60	n4	83	THR	2.5

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Mol	Chain	Res	Type	RSRZ
6	S4	129	VAL	2.5
9	s7	42	GLN	2.5
45	l8	189	LEU	2.5
10	S8	116	HIS	2.5
28	D6	22	ARG	2.5
59	n3	4	ASN	2.5
14	C2	117	GLY	2.5
36	1	361	A	2.5
60	N4	62	GLY	2.5
8	S6	147	LEU	2.5
54	M8	97	PRO	2.5
57	N1	27	LEU	2.5
6	S4	70	VAL	2.5
11	S9	186	GLU	2.5
13	c1	4	GLU	2.5
28	D6	10	ARG	2.5
43	l6	109	GLU	2.5
1	6	1229	G	2.5
4	s2	215	PHE	2.5
7	S5	69	PHE	2.5
60	n4	88	ASP	2.5
14	C2	49	THR	2.5
19	C7	25	THR	2.5
21	C9	58	ALA	2.5
34	sR	204	ALA	2.5
63	N7	19	ALA	2.5
10	s8	41	LYS	2.5
11	s9	92	LYS	2.5
14	c2	99	GLU	2.5
17	c5	123	TYR	2.5
43	l6	8	LYS	2.5
10	s8	58	LEU	2.5
34	sR	73	LEU	2.5
34	sR	141	LEU	2.5
42	l5	195	LEU	2.5
22	d0	41	ILE	2.5
30	D8	30	VAL	2.5
58	n2	12	ALA	2.5
57	N1	70	SER	2.5
62	N6	77	LYS	2.5
72	O6	29	LYS	2.5
1	2	772	G	2.5

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Mol	Chain	Res	Type	RSRZ
12	C0	16	PHE	2.5
62	N6	78	PHE	2.5
7	s5	81	ARG	2.5
10	S8	5	ARG	2.5
33	e1	91	ILE	2.5
9	s7	63	PRO	2.5
16	C4	129	LYS	2.5
21	C9	2	PRO	2.5
45	L8	123	GLN	2.5
11	S9	76	LEU	2.5
2	s0	76	ILE	2.5
3	S1	145	LYS	2.5
6	s4	134	LYS	2.5
11	s9	18	PRO	2.5
27	D5	102	THR	2.5
51	m5	5	LYS	2.5
62	n6	108	LYS	2.5
78	q2	13	LYS	2.5
67	o1	94	GLU	2.5
6	S4	101	LEU	2.5
22	d0	84	MET	2.5
12	C0	24	LYS	2.5
48	m1	66	ALA	2.5
70	o4	2	ALA	2.5
80	p0	75	LYS	2.5
2	S0	124	THR	2.5
3	S1	143	THR	2.5
8	s6	156	PHE	2.5
22	D0	107	THR	2.5
45	L8	255	SER	2.5
48	M1	134	PRO	2.5
54	M8	100	THR	2.5
7	s5	58	LEU	2.5
20	c8	15	LEU	2.5
70	o4	51	LEU	2.5
10	S8	101	ILE	2.5
14	C2	124	LYS	2.5
32	e0	28	LYS	2.5
51	m5	135	VAL	2.5
63	N7	84	ARG	2.5
74	O8	27	ILE	2.5
14	C2	126	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
7	s5	170	GLN	2.4
18	C6	42	GLU	2.4
7	S5	157	ARG	2.4
42	l5	67	SER	2.4
13	C1	26	LYS	2.4
16	C4	112	ILE	2.4
63	N7	27	LYS	2.4
26	d4	64	PHE	2.4
29	D7	64	CYS	2.4
34	sR	263	PHE	2.4
42	l5	142	PHE	2.4
79	Q3	91	GLU	2.4
80	p0	21	GLU	2.4
2	s0	166	GLY	2.4
8	s6	136	LYS	2.4
32	e0	36	LYS	2.4
40	L3	309	GLY	2.4
57	N1	25	VAL	2.4
59	N3	39	VAL	2.4
63	N7	10	VAL	2.4
3	S1	123	ALA	2.4
36	1	24	G	2.4
8	s6	131	LYS	2.4
11	S9	89	ASP	2.4
18	c6	123	ARG	2.4
60	n4	96	LEU	2.4
24	d2	122	SER	2.4
45	L8	137	ASN	2.4
2	s0	54	TRP	2.4
42	L5	145	PHE	2.4
12	c0	41	TYR	2.4
5	s3	136	VAL	2.4
60	N4	76	VAL	2.4
66	o0	8	GLU	2.4
21	c9	46	PRO	2.4
7	s5	47	SER	2.4
14	C2	64	SER	2.4
48	M1	132	ASN	2.4
2	s0	120	LEU	2.4
11	s9	30	LEU	2.4
18	C6	13	LYS	2.4
2	S0	46	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
7	S5	148	ARG	2.4
33	E1	132	LEU	2.4
11	S9	113	VAL	2.4
34	sR	10	ARG	2.4
3	S1	121	ILE	2.4
7	s5	152	GLY	2.4
10	S8	65	PHE	2.4
11	s9	98	ALA	2.4
12	C0	30	ALA	2.4
39	l2	250	GLN	2.4
63	N7	32	GLY	2.4
70	o4	28	GLY	2.4
1	6	1491	U	2.4
11	s9	138	LYS	2.4
21	c9	77	ASN	2.4
40	L3	263	SER	2.4
33	E1	119	ARG	2.4
55	m9	24	LEU	2.4
61	n5	123	TYR	2.4
80	p0	90	ASN	2.4
6	S4	4	GLY	2.4
45	l8	143	ILE	2.4
18	c6	83	GLN	2.4
21	c9	14	PHE	2.4
9	s7	129	LEU	2.4
10	S8	6	ASP	2.4
27	d5	46	LYS	2.4
34	SR	283	LYS	2.4
45	L8	65	LEU	2.4
80	p0	72	ASP	2.4
13	c1	30	ARG	2.4
17	c5	106	GLU	2.4
69	O3	52	VAL	2.4
9	s7	162	ILE	2.4
9	S7	92	PHE	2.4
42	L5	127	GLY	2.4
45	L8	173	MET	2.4
22	D0	95	ALA	2.4
58	n2	95	PHE	2.4
14	C2	33	ARG	2.4
1	6	1686	C	2.4
8	S6	84	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
10	s8	188	GLU	2.4
17	c5	14	THR	2.4
18	C6	39	VAL	2.4
33	E1	100	LEU	2.4
35	sM	36	ASP	2.4
51	M5	143	ARG	2.4
51	m5	63	ARG	2.4
77	Q1	5	TRP	2.4
78	Q2	11	TYR	2.4
21	c9	89	ARG	2.4
29	D7	7	LEU	2.4
42	L5	131	LEU	2.4
3	s1	137	ILE	2.4
8	S6	166	GLU	2.4
34	SR	263	PHE	2.4
78	q2	100	LYS	2.4
6	S4	48	LEU	2.4
9	S7	150	GLN	2.4
19	c7	3	ARG	2.4
63	N7	50	PRO	2.4
70	o4	33	GLN	2.4
6	S4	45	ILE	2.4
7	S5	119	ASP	2.4
5	S3	8	LYS	2.4
11	S9	137	GLY	2.4
34	sR	46	LYS	2.4
55	m9	21	LYS	2.4
3	s1	217	LEU	2.4
34	SR	196	ASN	2.4
48	m1	55	ARG	2.4
24	D2	27	ILE	2.4
1	2	754	A	2.4
3	s1	97	LEU	2.4
3	s1	228	LEU	2.4
6	S4	256	ARG	2.4
8	s6	163	THR	2.4
45	L8	168	ALA	2.4
33	E1	98	VAL	2.4
42	l5	173	VAL	2.4
65	N9	35	VAL	2.4
48	m1	52	TYR	2.4
42	l5	16	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
54	M8	77	ALA	2.4
62	N6	111	LEU	2.4
65	N9	46	ALA	2.4
8	s6	153	VAL	2.4
39	L2	224	THR	2.4
8	s6	189	HIS	2.4
11	s9	182	GLU	2.4
36	1	928	C	2.4
58	N2	92	TRP	2.4
3	S1	64	ARG	2.4
12	c0	80	LEU	2.4
55	M9	81	ARG	2.4
61	N5	27	ARG	2.4
30	D8	44	VAL	2.4
40	L3	382	THR	2.4
67	o1	13	THR	2.4
3	s1	84	ILE	2.4
35	SM	23	LYS	2.4
36	5	364	G	2.4
45	L8	252	ASN	2.4
41	l4	198	ARG	2.4
19	C7	24	LEU	2.4
41	l4	219	LEU	2.4
51	M5	2	GLY	2.4
65	n9	47	LEU	2.4
70	o4	30	LEU	2.4
14	c2	65	SER	2.4
36	5	2569	A	2.4
66	O0	20	SER	2.4
67	o1	92	TYR	2.4
78	q2	106	PHE	2.4
3	s1	144	ARG	2.3
11	s9	126	ARG	2.3
3	S1	153	HIS	2.3
18	C6	78	VAL	2.3
44	l7	27	ALA	2.3
62	N6	76	LEU	2.3
62	n6	48	LEU	2.3
28	d6	67	THR	2.3
36	5	799	G	2.3
51	m5	62	TYR	2.3
42	L5	130	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
61	n5	142	ILE	2.3
62	n6	115	ARG	2.3
3	S1	135	LEU	2.3
3	s1	54	LEU	2.3
19	C7	2	GLY	2.3
26	D4	44	LEU	2.3
36	5	1764	U	2.3
8	s6	89	ASP	2.3
33	e1	124	PRO	2.3
34	sR	11	GLY	2.3
45	L8	200	LEU	2.3
53	m7	79	THR	2.3
14	c2	94	ALA	2.3
26	d4	4	ALA	2.3
59	N3	52	ALA	2.3
17	C5	119	PHE	2.3
32	e0	53	LYS	2.3
33	E1	116	LYS	2.3
62	N6	87	LYS	2.3
3	S1	152	ARG	2.3
36	5	331	G	2.3
36	5	815	G	2.3
1	6	696	C	2.3
7	s5	64	VAL	2.3
7	s5	150	GLY	2.3
8	S6	65	GLN	2.3
62	N6	35	LEU	2.3
45	L8	129	PRO	2.3
60	N4	12	LYS	2.3
7	s5	180	ARG	2.3
42	l5	60	ILE	2.3
57	N1	42	ILE	2.3
62	N6	100	HIS	2.3
22	D0	93	LEU	2.3
26	D4	74	LEU	2.3
57	n1	70	SER	2.3
21	c9	78	LYS	2.3
57	N1	58	GLN	2.3
45	L8	94	PHE	2.3
58	N2	14	THR	2.3
1	2	261	U	2.3
1	6	369	A	2.3

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Mol	Chain	Res	Type	RSRZ
4	s2	38	VAL	2.3
9	s7	38	LEU	2.3
11	s9	86	LEU	2.3
10	s8	181	GLY	2.3
27	D5	62	VAL	2.3
28	D6	34	LYS	2.3
39	L2	249	SER	2.3
8	S6	173	PRO	2.3
12	c0	13	GLN	2.3
26	d4	61	ARG	2.3
64	N8	128	ARG	2.3
67	o1	12	TYR	2.3
14	c2	44	GLY	2.3
32	E0	29	LYS	2.3
4	s2	224	PHE	2.3
8	S6	172	ALA	2.3
11	s9	34	PHE	2.3
32	e0	44	PHE	2.3
48	M1	102	PHE	2.3
62	N6	120	GLN	2.3
1	6	233	C	2.3
7	s5	115	LYS	2.3
20	c8	4	VAL	2.3
21	c9	56	LYS	2.3
42	L5	150	LEU	2.3
42	L5	173	VAL	2.3
58	n2	50	LEU	2.3
64	N8	58	MET	2.3
74	o8	34	ALA	2.3
49	m3	93	ILE	2.3
62	n6	101	PRO	2.3
12	C0	65	TYR	2.3
12	c0	36	ASP	2.3
20	c8	53	ASP	2.3
26	d4	6	THR	2.3
34	SR	265	LEU	2.3
42	l5	222	LEU	2.3
61	N5	110	VAL	2.3
78	q2	93	LEU	2.3
18	C6	46	PHE	2.3
42	L5	160	PHE	2.3
31	d9	40	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
36	1	1024	G	2.3
57	N1	44	ALA	2.3
14	C2	71	ILE	2.3
6	s4	10	LYS	2.3
7	S5	198	LEU	2.3
51	M5	134	LEU	2.3
55	m9	52	LYS	2.3
63	n7	77	TYR	2.3
74	O8	36	LYS	2.3
7	S5	161	ASP	2.3
53	m7	81	ALA	2.3
63	N7	129	TRP	2.3
63	n7	118	PHE	2.3
17	c5	37	ALA	2.3
18	c6	41	PRO	2.3
21	c9	33	TYR	2.3
48	M1	41	SER	2.3
55	M9	186	LYS	2.3
36	5	2572	C	2.3
7	S5	112	ARG	2.3
14	C2	43	ARG	2.3
42	l5	145	PHE	2.3
58	N2	80	THR	2.3
59	N3	23	MET	2.3
78	Q2	80	ARG	2.3
26	d4	25	VAL	2.3
62	n6	35	LEU	2.3
78	Q2	8	ARG	2.3
34	SR	136	ILE	2.3
34	SR	204	ALA	2.3
55	m9	178	ALA	2.3
36	5	1537	A	2.3
67	O1	59	ILE	2.3
6	s4	56	LEU	2.3
8	s6	195	VAL	2.3
11	S9	101	VAL	2.3
14	C2	116	VAL	2.3
18	c6	78	VAL	2.3
21	C9	132	LEU	2.3
69	o3	7	LEU	2.3
71	O5	73	LYS	2.3
22	d0	62	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	S1	122	GLU	2.3
17	C5	109	PRO	2.3
36	5	1631	C	2.3
38	8	110	C	2.3
78	q2	22	GLN	2.3
2	S0	25	GLY	2.3
4	S2	91	ARG	2.3
67	O1	39	PHE	2.3
10	S8	143	TRP	2.3
6	S4	56	LEU	2.3
26	D4	96	LEU	2.3
33	E1	115	THR	2.3
39	l2	156	LYS	2.3
42	L5	43	LYS	2.3
45	l8	96	LYS	2.3
32	E0	40	TYR	2.3
68	O2	76	VAL	2.3
11	S9	48	GLN	2.3
35	sM	41	SER	2.3
42	l5	133	GLU	2.3
45	L8	167	PRO	2.3
64	N8	64	GLN	2.3
13	C1	11	ARG	2.3
25	D3	4	GLY	2.3
66	O0	26	GLY	2.3
21	c9	59	ALA	2.3
1	6	237	C	2.3
9	s7	41	LEU	2.3
70	o4	29	ILE	2.3
21	c9	34	VAL	2.3
13	C1	53	TYR	2.3
42	L5	79	TYR	2.3
49	M3	89	TYR	2.3
8	s6	186	ARG	2.2
9	s7	5	GLN	2.2
36	5	813	G	2.2
2	S0	159	ALA	2.2
11	s9	40	LYS	2.2
7	s5	199	ILE	2.2
14	c2	112	ALA	2.2
24	d2	60	LYS	2.2
34	SR	62	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
61	N5	121	LYS	2.2
66	o0	100	ILE	2.2
67	o1	71	LEU	2.2
68	O2	75	LEU	2.2
76	Q0	90	ASN	2.2
77	q1	5	TRP	2.2
7	s5	185	ARG	2.2
63	N7	92	PHE	2.2
65	n9	40	ARG	2.2
32	E0	30	PRO	2.2
45	L8	133	LYS	2.2
45	l8	231	LYS	2.2
8	s6	76	LEU	2.2
9	S7	77	LEU	2.2
14	c2	36	LEU	2.2
51	M5	142	ILE	2.2
61	N5	122	ALA	2.2
62	N6	59	VAL	2.2
63	N7	96	VAL	2.2
1	2	193	U	2.2
3	s1	205	PHE	2.2
3	s1	213	ARG	2.2
16	c4	135	ARG	2.2
42	L5	172	TYR	2.2
42	l5	226	TYR	2.2
40	L3	5	LYS	2.2
65	N9	36	ASP	2.2
74	o8	36	LYS	2.2
3	S1	139	ALA	2.2
3	s1	188	LEU	2.2
18	c6	118	ILE	2.2
19	C7	17	ILE	2.2
30	D8	28	VAL	2.2
34	SR	34	LEU	2.2
42	L5	75	LEU	2.2
43	L6	11	PRO	2.2
68	O2	128	LEU	2.2
11	s9	146	PHE	2.2
24	D2	37	PHE	2.2
51	m5	4	TYR	2.2
58	n2	52	ASN	2.2
42	l5	34	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
48	M1	145	LYS	2.2
63	n7	60	LYS	2.2
67	O1	102	LYS	2.2
7	s5	29	ILE	2.2
11	s9	131	GLN	2.2
34	SR	130	THR	2.2
27	d5	76	ALA	2.2
35	sM	26	VAL	2.2
45	l8	203	VAL	2.2
58	N2	11	ILE	2.2
59	N3	101	VAL	2.2
63	N7	42	LEU	2.2
40	L3	46	PHE	2.2
42	L5	54	ARG	2.2
36	5	800	G	2.2
3	s1	120	LEU	2.2
7	s5	68	ILE	2.2
14	C2	69	ALA	2.2
22	D0	17	GLN	2.2
27	d5	88	ILE	2.2
35	sM	54	PRO	2.2
45	l8	167	PRO	2.2
47	M0	219	ALA	2.2
1	6	1379	C	2.2
40	L3	6	TYR	2.2
62	N6	115	ARG	2.2
55	M9	53	LYS	2.2
60	n4	129	LYS	2.2
67	o1	76	SER	2.2
24	d2	27	ILE	2.2
28	d6	14	GLY	2.2
64	N8	73	LEU	2.2
74	O8	32	ASN	2.2
74	O8	45	VAL	2.2
76	q0	90	ASN	2.2
59	N3	76	ALA	2.2
74	o8	10	GLN	2.2
10	S8	21	PHE	2.2
55	m9	81	ARG	2.2
1	2	1011	G	2.2
27	D5	101	TYR	2.2
45	L8	122	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
76	q0	128	LYS	2.2
22	D0	83	GLU	2.2
7	s5	134	VAL	2.2
8	S6	49	VAL	2.2
36	5	362	U	2.2
67	O1	16	LEU	2.2
80	p0	210	VAL	2.2
30	d8	45	LYS	2.2
45	l8	98	ARG	2.2
66	o0	105	ALA	2.2
11	s9	154	LYS	2.2
12	C0	66	TYR	2.2
64	N8	111	LYS	2.2
8	S6	109	LEU	2.2
42	L5	65	ILE	2.2
74	O8	5	ILE	2.2
20	c8	56	LYS	2.2
42	l5	296	GLN	2.2
44	L7	135	ALA	2.2
1	2	837	G	2.2
7	s5	140	THR	2.2
34	sR	165	ASP	2.2
36	1	1026	A	2.2
36	5	906	A	2.2
36	5	1564	U	2.2
12	c0	76	LEU	2.2
20	C8	119	ILE	2.2
21	c9	42	GLY	2.2
34	sR	210	LEU	2.2
45	L8	190	VAL	2.2
6	S4	155	LYS	2.2
51	m5	59	PHE	2.2
6	S4	29	PRO	2.2
15	c3	23	PRO	2.2
3	s1	160	HIS	2.2
18	c6	39	VAL	2.2
34	sR	211	ILE	2.2
42	l5	52	VAL	2.2
42	l5	169	GLY	2.2
48	M1	91	LEU	2.2
63	N7	57	HIS	2.2
8	S6	186	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	6	194	U	2.2
14	C2	90	LYS	2.2
33	E1	152	ALA	2.2
36	1	318	A	2.2
36	5	329	U	2.2
46	L9	90	MET	2.2
48	m1	142	LYS	2.2
51	M5	118	SER	2.2
72	O6	78	GLY	2.2
13	C1	16	GLN	2.2
34	sR	313	TRP	2.2
2	s0	98	ILE	2.2
9	S7	167	GLU	2.2
30	D8	67	ARG	2.2
33	e1	120	GLU	2.2
33	e1	90	LYS	2.2
42	L5	147	ASP	2.2
49	M3	51	LEU	2.2
51	m5	178	HIS	2.2
63	n7	89	VAL	2.2
9	s7	47	ARG	2.2
10	S8	141	ARG	2.2
18	c6	128	LYS	2.2
23	D1	54	ALA	2.2
26	D4	119	PHE	2.2
42	L5	180	PHE	2.2
70	O4	37	LYS	2.2
55	M9	7	GLN	2.2
3	s1	124	ASN	2.2
5	S3	223	LYS	2.2
6	S4	25	GLY	2.2
6	S4	146	THR	2.2
7	S5	190	ILE	2.2
10	s8	104	ILE	2.2
14	c2	46	ARG	2.2
18	c6	5	PRO	2.2
26	d4	27	VAL	2.2
34	SR	90	ARG	2.2
26	d4	3	ASP	2.2
31	D9	55	PHE	2.2
34	SR	61	PHE	2.2
67	O1	15	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
34	SR	171	SER	2.2
3	s1	155	TYR	2.2
38	4	110	C	2.2
2	S0	54	TRP	2.2
6	S4	136	VAL	2.2
8	S6	74	LYS	2.2
19	c7	24	LEU	2.2
49	M3	58	VAL	2.2
9	s7	60	ILE	2.2
16	c4	27	PHE	2.2
24	d2	125	ILE	2.2
61	N5	109	LYS	2.2
62	N6	50	ILE	2.2
63	N7	15	ARG	2.2
24	d2	128	PHE	2.2
63	n7	131	PHE	2.2
9	S7	59	ALA	2.2
19	C7	55	THR	2.2
21	C9	131	ASP	2.2
28	D6	72	HIS	2.2
34	SR	319	ASN	2.2
63	N7	79	HIS	2.2
72	o6	69	ALA	2.2
14	C2	88	LEU	2.2
21	c9	114	VAL	2.2
24	d2	126	LEU	2.2
32	e0	45	VAL	2.2
45	l8	200	LEU	2.2
55	m9	173	ARG	2.2
57	N1	151	LEU	2.2
6	s4	251	GLU	2.2
62	N6	3	LYS	2.2
64	N8	54	GLY	2.2
11	S9	130	THR	2.2
51	m5	3	ALA	2.2
66	O0	30	THR	2.2
3	s1	218	LEU	2.2
1	6	238	U	2.2
6	s4	18	TRP	2.2
6	s4	191	ARG	2.2
33	E1	139	LEU	2.2
48	m1	133	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
61	N5	22	LYS	2.2
62	n6	57	LEU	2.2
14	c2	76	GLU	2.2
34	SR	54	PHE	2.2
63	n7	108	GLU	2.2
63	N7	70	PRO	2.1
3	S1	141	ALA	2.1
34	SR	284	ALA	2.1
47	m0	218	ALA	2.1
59	n3	60	ALA	2.1
3	s1	26	ARG	2.1
11	S9	133	HIS	2.1
11	s9	85	VAL	2.1
31	D9	36	LEU	2.1
51	M5	65	ARG	2.1
51	M5	126	THR	2.1
62	N6	109	LEU	2.1
20	c8	136	GLN	2.1
24	D2	51	GLU	2.1
34	SR	251	TRP	2.1
38	4	142	C	2.1
71	o5	118	ILE	2.1
14	c2	51	ALA	2.1
42	L5	181	PRO	2.1
3	s1	231	LEU	2.1
11	s9	68	LYS	2.1
12	c0	56	LYS	2.1
5	s3	174	HIS	2.1
6	s4	254	ARG	2.1
42	l5	5	LYS	2.1
45	l8	69	LEU	2.1
57	N1	20	ARG	2.1
59	N3	93	LEU	2.1
34	SR	188	ILE	2.1
34	sR	54	PHE	2.1
42	L5	142	PHE	2.1
60	n4	90	ILE	2.1
10	S8	51	GLY	2.1
33	E1	112	GLY	2.1
42	L5	295	GLY	2.1
80	p0	40	GLU	2.1
1	6	511	A	2.1

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Mol	Chain	Res	Type	RSRZ
34	SR	158	PRO	2.1
36	5	52	A	2.1
59	N3	51	ALA	2.1
2	s0	74	VAL	2.1
8	S6	159	ARG	2.1
10	s8	192	TYR	2.1
11	s9	62	ARG	2.1
27	D5	60	VAL	2.1
32	e0	40	TYR	2.1
39	l2	247	ARG	2.1
48	M1	19	LEU	2.1
49	M3	139	LEU	2.1
57	n1	89	LEU	2.1
63	N7	95	VAL	2.1
16	c4	112	ILE	2.1
29	d7	32	PHE	2.1
48	M1	127	PHE	2.1
33	e1	127	GLY	2.1
34	sR	181	TRP	2.1
59	N3	22	ILE	2.1
36	1	3059	G	2.1
36	5	1586	G	2.1
38	4	102	U	2.1
45	L8	228	GLU	2.1
80	p0	189	GLN	2.1
11	s9	108	ARG	2.1
45	L8	149	LYS	2.1
16	C4	14	PHE	2.1
21	C9	18	TYR	2.1
26	D4	18	LEU	2.1
67	O1	33	VAL	2.1
72	O6	77	LEU	2.1
2	s0	157	ASP	2.1
18	c6	6	SER	2.1
19	C7	70	SER	2.1
34	sR	65	SER	2.1
42	l5	151	GLN	2.1
45	l8	90	THR	2.1
60	n4	92	GLU	2.1
41	L4	185	LYS	2.1
42	L5	34	LYS	2.1
78	Q2	22	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	6	25	C	2.1
5	s3	3	ALA	2.1
11	S9	174	ARG	2.1
34	SR	154	VAL	2.1
45	l8	127	PRO	2.1
57	n1	33	VAL	2.1
61	N5	38	LEU	2.1
72	O6	48	ALA	2.1
78	q2	104	LEU	2.1
61	n5	60	TYR	2.1
66	O0	58	TYR	2.1
67	o1	75	ILE	2.1
11	S9	20	GLU	2.1
36	1	902	G	2.1
36	5	353	G	2.1
39	l2	143	GLU	2.1
5	S3	12	VAL	2.1
5	S3	86	LEU	2.1
6	s4	12	LEU	2.1
15	c3	60	VAL	2.1
20	c8	133	VAL	2.1
21	c9	131	ASP	2.1
32	e0	20	LYS	2.1
34	sR	246	SER	2.1
29	d7	8	LEU	2.1
30	D8	49	ARG	2.1
48	m1	50	ALA	2.1
61	N5	24	LEU	2.1
3	S1	23	PRO	2.1
14	c2	72	ILE	2.1
22	D0	82	TYR	2.1
25	D3	29	TYR	2.1
42	L5	174	PRO	2.1
11	s9	10	LYS	2.1
36	1	2541	U	2.1
41	l4	192	GLY	2.1
5	s3	149	ALA	2.1
6	S4	36	HIS	2.1
6	S4	220	THR	2.1
39	l2	157	VAL	2.1
42	L5	22	ARG	2.1
42	L5	42	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
42	l5	37	VAL	2.1
45	L8	196	ALA	2.1
49	m3	186	ARG	2.1
70	O4	23	VAL	2.1
70	o4	32	ALA	2.1
15	C3	78	ASN	2.1
1	2	1778	G	2.1
12	C0	11	ILE	2.1
22	D0	90	TYR	2.1
36	5	1113	G	2.1
7	s5	196	GLU	2.1
8	S6	93	LYS	2.1
11	s9	41	GLU	2.1
1	6	1226	A	2.1
1	6	1411	A	2.1
5	s3	189	MET	2.1
6	S4	84	ALA	2.1
20	c8	52	VAL	2.1
31	D9	56	ARG	2.1
31	d9	56	ARG	2.1
54	M8	76	ALA	2.1
80	p0	202	LEU	2.1
72	O6	27	SER	2.1
2	s0	162	CYS	2.1
42	l5	172	TYR	2.1
55	M9	78	TYR	2.1
26	D4	31	ASN	2.1
45	L8	230	LYS	2.1
3	s1	215	VAL	2.1
10	S8	77	ARG	2.1
10	S8	178	ARG	2.1
21	C9	6	VAL	2.1
21	c9	19	ALA	2.1
40	l3	387	LEU	2.1
42	l5	4	GLN	2.1
66	O0	91	SER	2.1
74	o8	11	PHE	2.1
11	S9	43	TYR	2.1
7	s5	84	LYS	2.1
7	s5	106	LYS	2.1
12	c0	35	ILE	2.1
27	d5	102	THR	2.1

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Mol	Chain	Res	Type	RSRZ
31	D9	50	ILE	2.1
36	5	1354	G	2.1
52	m6	184	THR	2.1
14	C2	125	ASN	2.1
2	S0	50	VAL	2.1
40	L3	369	ARG	2.1
45	L8	118	GLU	2.1
60	N4	106	GLU	2.1
62	N6	57	LEU	2.1
67	O1	60	TRP	2.1
9	s7	94	ALA	2.1
80	p0	73	PHE	2.1
10	S8	103	GLN	2.1
35	sM	39	PRO	2.1
42	l5	38	THR	2.1
34	SR	290	VAL	2.1
34	sR	311	ARG	2.1
80	p0	186	THR	2.1
18	C6	44	LEU	2.1
19	C7	57	LEU	2.1
27	D5	42	LEU	2.1
42	L5	125	VAL	2.1
42	L5	169	GLY	2.1
47	m0	152	LEU	2.1
66	O0	88	GLY	2.1
74	O8	31	LEU	2.1
80	p0	44	GLU	2.1
80	p0	74	GLU	2.1
6	S4	54	TYR	2.1
14	C2	89	ILE	2.1
21	C9	75	LYS	2.1
36	1	2522	G	2.1
62	n6	45	ILE	2.1
68	O2	90	LYS	2.1
3	S1	144	ARG	2.1
3	s1	101	HIS	2.1
27	D5	93	SER	2.1
36	1	3077	A	2.1
2	s0	87	LEU	2.1
7	S5	153	GLY	2.1
8	S6	36	VAL	2.1
10	S8	114	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
10	S8	181	GLY	2.1
17	c5	125	PRO	2.1
31	d9	17	GLY	2.1
39	L2	73	GLU	2.1
39	l2	241	ARG	2.1
45	l8	185	ARG	2.1
42	L5	29	ASP	2.1
49	m3	98	ASP	2.1
55	m9	22	VAL	2.1
8	S6	171	LYS	2.1
11	s9	147	MET	2.1
35	sM	60	ALA	2.1
18	c6	106	LYS	2.1
33	e1	81	LYS	2.1
60	N4	127	LYS	2.1
6	s4	49	ARG	2.1
12	C0	58	GLN	2.1
8	S6	135	PRO	2.1
10	s8	165	LEU	2.1
19	C7	120	SER	2.1
25	D3	42	PRO	2.1
27	d5	63	SER	2.1
34	sR	25	THR	2.1
45	l8	238	LEU	2.1
1	2	214	G	2.1
1	6	1225	U	2.1
3	S1	94	LYS	2.1
3	s1	50	LYS	2.1
36	1	2538	U	2.1
21	C9	15	ILE	2.1
63	N7	68	ILE	2.1
69	O3	51	TYR	2.1
18	C6	114	ARG	2.1
5	s3	138	VAL	2.1
27	D5	65	LEU	2.1
31	d9	25	SER	2.1
41	l4	190	GLY	2.1
45	l8	93	LEU	2.1
21	C9	14	PHE	2.1
10	S8	53	LYS	2.1
45	L8	70	LYS	2.1
51	M5	136	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
55	m9	49	THR	2.1
10	S8	104	ILE	2.1
74	O8	66	ILE	2.1
10	S8	35	ASN	2.1
23	D1	87	ARG	2.1
34	SR	102	ARG	2.1
49	m3	91	ARG	2.1
2	s0	158	VAL	2.1
7	S5	133	VAL	2.1
3	S1	154	SER	2.0
17	C5	72	LYS	2.0
18	C6	130	GLY	2.1
63	n7	81	LEU	2.1
34	sR	158	PRO	2.0
36	5	361	A	2.0
58	n2	71	PHE	2.1
63	N7	94	SER	2.0
1	2	1486	G	2.0
6	s4	249	ALA	2.0
36	1	330	G	2.0
67	O1	17	HIS	2.0
34	sR	102	ARG	2.0
8	s6	133	LEU	2.0
34	SR	315	VAL	2.0
3	s1	235	GLY	2.0
45	L8	111	LYS	2.0
72	O6	46	GLU	2.0
8	S6	86	PRO	2.0
14	c2	87	PRO	2.0
17	c5	53	PRO	2.0
19	c7	120	SER	2.0
63	n7	83	THR	2.0
36	5	357	A	2.0
48	M1	148	VAL	2.0
67	o1	109	VAL	2.0
7	S5	204	GLY	2.0
7	s5	48	PHE	2.0
45	l8	91	PHE	2.0
51	M5	130	PHE	2.0
53	m7	80	LYS	2.0
1	6	648	G	2.0
1	6	1534	G	2.0

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Mol	Chain	Res	Type	RSRZ
33	e1	152	ALA	2.0
36	1	1538	G	2.0
36	5	1538	G	2.0
9	s7	49	ILE	2.0
22	D0	20	ILE	2.0
39	L2	239	ALA	2.0
11	s9	43	TYR	2.0
43	l6	2	SER	2.0
57	n1	65	TYR	2.0
62	N6	16	ARG	2.0
17	c5	124	THR	2.0
3	s1	151	LYS	2.0
8	s6	77	LEU	2.0
47	M0	217	PHE	2.0
62	n6	78	PHE	2.0
65	N9	44	LYS	2.0
18	c6	27	GLY	2.0
3	S1	103	MET	2.0
6	S4	145	ARG	2.0
7	S5	29	ILE	2.0
7	S5	102	ARG	2.0
22	d0	22	ILE	2.0
33	e1	146	SER	2.0
34	sR	294	TRP	2.0
49	M3	50	PRO	2.0
57	n1	88	ARG	2.0
7	s5	42	LEU	2.0
9	S7	16	LEU	2.0
33	e1	139	LEU	2.0
34	SR	210	LEU	2.0
35	sM	87	THR	2.0
47	m0	217	PHE	2.0
63	n7	64	LYS	2.0
36	1	224	C	2.0
36	1	1541	G	2.0
36	5	2442	G	2.0
21	c9	94	ILE	2.0
44	L7	112	ASN	2.0
60	n4	51	TRP	2.0
63	n7	68	ILE	2.0
78	Q2	33	ALA	2.0
3	S1	160	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
42	l5	75	LEU	2.0
66	O0	41	LEU	2.0
66	O0	66	LYS	2.0
1	2	119	A	2.0
4	s2	250	GLN	2.0
70	O4	89	ILE	2.0
2	S0	47	VAL	2.0
6	S4	38	LEU	2.0
18	C6	52	LEU	2.0
27	d5	66	VAL	2.0
74	O8	54	LEU	2.0
74	o8	30	LYS	2.0
13	C1	143	SER	2.0
19	C7	13	SER	2.0
1	2	1100	G	2.0
1	6	261	U	2.0
8	S6	35	GLU	2.0
26	D4	39	GLU	2.0
36	5	1536	G	2.0
42	l5	177	GLU	2.0
7	s5	138	THR	2.0
29	D7	52	THR	2.0
54	M8	99	THR	2.0
68	O2	63	THR	2.0
14	c2	22	VAL	2.0
14	c2	124	LYS	2.0
58	N2	99	LYS	2.0
3	s1	24	PHE	2.0
71	o5	41	LEU	2.0
78	q2	70	LEU	2.0
26	d4	34	ASN	2.0
1	2	993	A	2.0
10	S8	146	ARG	2.0
34	sR	35	SER	2.0
36	5	817	A	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.