



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 03:20 PM EDT

PDB ID : 5OBM
Title : Crystal structure of Gentamicin bound to the yeast 80S ribosome
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2017-06-28
Resolution : 3.40 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

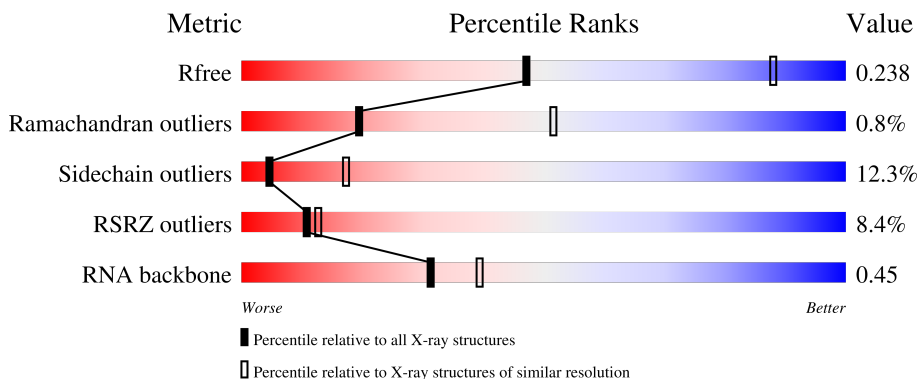
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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	1	3396	 65% 23% 9%
1	5	3396	 61% 27% 8%
2	3	121	 79% 21%
2	7	121	 74% 22%
3	4	158	 71% 25%

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Mol	Chain	Length	Quality of chain
3	8	158	69% 28% .
4	L2	252	91% 9% 3%
4	l2	252	92% 8% 2%
5	L3	386	87% 13% %
5	l3	386	88% 12%
6	L4	361	89% 11%
6	l4	361	89% 11% 2%
7	L5	296	91% 9% 7%
7	l5	296	86% 12% 2%
8	L6	176	77% 11% 11% %
8	l6	176	76% 13% . 11%
9	L7	223	91% 9% %
9	l7	223	90% 9%
10	L8	233	91% 9% 14%
10	l8	233	91% 8% . 16%
11	L9	191	85% 15% 3%
11	l9	191	90% 10% %
12	M0	221	84% 12% . 3%
12	m0	221	79% 15% . 5% 2%
13	M1	169	87% 12% . 19%
13	m1	169	85% 14% . %
14	M3	194	85% 14% .. 6%
14	m3	194	90% 10% 8%
15	M4	137	91% 9% . %
15	m4	137	91% 9% %

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Mol	Chain	Length	Quality of chain
16	M5	203	9% 88% 12%
16	m5	203	9% 88% 12%
17	M6	197	% 91% 9%
17	m6	197	90% 10%
18	M7	184	14% 84% 16%
18	m7	184	% 73% 11% 16%
19	M8	185	2% 91% 9%
19	m8	185	2% 88% 12%
20	M9	188	4% 89% 8%
20	m9	188	6% 92% 8%
21	N0	172	7% 82% 18%
21	n0	172	% 88% 12%
22	N1	159	5% 87% 12%
22	n1	159	3% 86% 14%
23	N2	100	14% 92% 8%
23	n2	100	26% 88% 10%
24	N3	136	3% 94% 6%
24	n3	136	% 93% 7%
25	N4	155	17% 59% 5% 37%
26	N5	121	10% 91% 9%
26	n5	121	7% 91% 8%
27	N6	126	12% 89% 10%
27	n6	126	9% 85% 15%
28	N7	135	52% 89% 11%
28	n7	135	27% 90% 10%

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Mol	Chain	Length	Quality of chain
29	N8	148	14% 86% 13%
29	n8	148	4% 86% 14%
30	N9	58	14% 88% 12%
30	n9	58	2% 86% 12%
31	O0	100	13% 90% 6%
31	o0	100	8% 87% 13%
32	O1	109	11% 87% 13%
32	o1	109	5% 83% 17%
33	O2	127	2% 91% 9%
33	o2	127	% 86% 14%
34	O3	106	94% 6%
34	o3	106	91% 9%
35	O4	112	13% 90% 9%
35	o4	112	7% 93% 6%
36	O5	119	4% 87% 13%
36	o5	119	4% 89% 10%
37	O6	99	7% 88% 12%
37	o6	99	15% 89% 10%
38	O7	87	2% 91% 9%
38	o7	87	2% 86% 14%
39	O8	77	12% 87% 13%
39	o8	77	29% 90% 10%
40	O9	50	4% 86% 14%
40	o9	50	2% 86% 14%
41	Q0	52	12% 90% 10%

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Mol	Chain	Length	Quality of chain
41	q0	52	79% 21%
42	Q1	25	84% 16%
42	q1	25	88% 12%
43	Q2	105	10% 91% 8%
43	q2	105	83% 16%
44	Q3	91	2% 93% 7%
44	q3	91	93% 7%
45	2	1800	66% 26% 5%
45	6	1800	65% 28% 5%
46	S0	206	28% 90% 10%
46	s0	206	5% 88% 12%
47	S1	216	22% 85% 12%
47	s1	216	8% 91% 9%
48	S2	217	14% 93% 6%
48	s2	217	6% 89% 11%
49	S3	223	22% 91% 9%
49	s3	223	13% 84% 16%
50	S4	260	32% 88% 12%
50	s4	260	15% 89% 11%
51	S5	206	27% 91% 9%
51	s5	206	6% 87% 13%
52	S6	236	13% 85% 11%
52	s6	236	8% 79% 13% 8%
53	S7	186	16% 89% 8%
53	s7	186	11% 90% 9%

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Mol	Chain	Length	Quality of chain
54	S8	200	
54	s8	200	
55	S9	185	
55	s9	185	
56	C0	105	
56	c0	105	
57	C1	156	
57	c1	156	
58	C2	143	
58	c2	143	
59	C3	150	
59	c3	150	
60	C4	128	
60	c4	128	
61	C5	141	
61	c5	141	
62	C6	142	
62	c6	142	
63	C7	136	
63	c7	136	
64	C8	145	
64	c8	145	
65	C9	143	
65	c9	143	
66	D0	110	

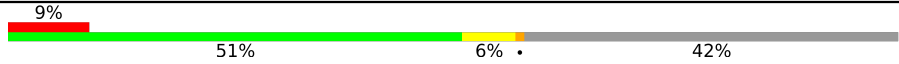

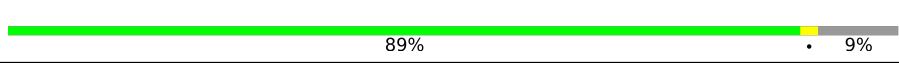
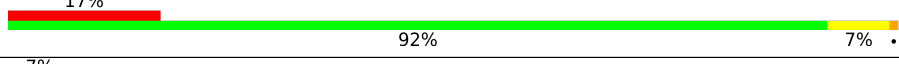

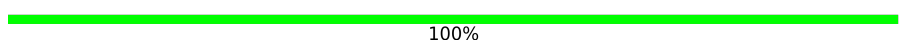
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Mol	Chain	Length	Quality of chain
66	d0	110	27% 80% 18% .
67	D1	87	30% 87% 13%
67	d1	87	8% 89% 11%
68	D2	129	22% 88% 11% .
68	d2	129	4% 88% 11% .
69	D3	144	11% 91% 9%
69	d3	144	% 92% 8%
70	D4	134	20% 90% 10%
70	d4	134	11% 89% 9% ..
71	D5	70	69% 77% 23%
71	d5	70	4% 93% . ..
72	D6	97	26% 81% 18% .
72	d6	97	2% 88% 11% .
73	D7	81	42% 89% 11%
73	d7	81	12% 90% 10%
74	D8	63	46% 90% 10%
74	d8	63	27% 75% 25%
75	D9	53	30% 81% 19%
75	d9	53	9% 79% 21%
76	E0	62	29% 85% 11% .
76	e0	62	10% 85% 13% .
77	E1	72	32% 85% 14% .
77	e1	72	29% 78% 19% .
78	SR	318	47% 93% 7%
78	sR	318	15% 92% 8%

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Mol	Chain	Length	Quality of chain
79	SM	272	
79	sM	272	
80	m2	165	
81	n4	135	
82	p0	312	
83	p1	47	

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
84	MG	1	3444	-	-	-	X
84	MG	1	3447	-	-	-	X
84	MG	1	3461	-	-	-	X
84	MG	1	3481	-	-	-	X
84	MG	1	3483	-	-	-	X
84	MG	1	3493	-	-	-	X
84	MG	1	3495	-	-	-	X
84	MG	1	3499	-	-	-	X
84	MG	1	3508	-	-	-	X
84	MG	1	3510	-	-	-	X
84	MG	1	3514	-	-	-	X
84	MG	1	3515	-	-	-	X
84	MG	1	3521	-	-	-	X
84	MG	1	3545	-	-	-	X
84	MG	1	3627	-	-	-	X
84	MG	1	3628	-	-	-	X
84	MG	1	3667	-	-	-	X
84	MG	1	3726	-	-	-	X
84	MG	1	3738	-	-	-	X
84	MG	1	3742	-	-	-	X
84	MG	1	3758	-	-	-	X
84	MG	1	3759	-	-	-	X
84	MG	1	3763	-	-	-	X
84	MG	1	3764	-	-	-	X
84	MG	1	3769	-	-	-	X
84	MG	1	3782	-	-	-	X
84	MG	1	3803	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	1	3804	-	-	-	X
84	MG	1	3815	-	-	-	X
84	MG	1	3816	-	-	-	X
84	MG	1	3818	-	-	-	X
84	MG	1	3820	-	-	-	X
84	MG	1	3823	-	-	-	X
84	MG	1	3827	-	-	-	X
84	MG	1	3829	-	-	-	X
84	MG	1	3842	-	-	-	X
84	MG	1	3847	-	-	-	X
84	MG	1	3865	-	-	-	X
84	MG	1	3873	-	-	-	X
84	MG	1	3876	-	-	-	X
84	MG	1	3879	-	-	-	X
84	MG	1	3880	-	-	-	X
84	MG	1	3932	-	-	-	X
84	MG	1	3934	-	-	-	X
84	MG	1	3948	-	-	-	X
84	MG	1	3950	-	-	-	X
84	MG	1	3952	-	-	-	X
84	MG	1	3955	-	-	-	X
84	MG	1	3985	-	-	-	X
84	MG	2	1913	-	-	-	X
84	MG	2	1929	-	-	-	X
84	MG	2	1931	-	-	-	X
84	MG	2	1940	-	-	-	X
84	MG	2	1977	-	-	-	X
84	MG	2	1978	-	-	-	X
84	MG	2	1979	-	-	-	X
84	MG	2	1980	-	-	-	X
84	MG	2	1984	-	-	-	X
84	MG	2	2001	-	-	-	X
84	MG	2	2004	-	-	-	X
84	MG	2	2015	-	-	-	X
84	MG	2	2017	-	-	-	X
84	MG	3	206	-	-	-	X
84	MG	3	208	-	-	-	X
84	MG	4	206	-	-	-	X
84	MG	4	208	-	-	-	X
84	MG	4	221	-	-	-	X
84	MG	5	3442	-	-	-	X
84	MG	5	3469	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	5	3492	-	-	-	X
84	MG	5	3524	-	-	-	X
84	MG	5	3526	-	-	-	X
84	MG	5	3542	-	-	-	X
84	MG	5	3558	-	-	-	X
84	MG	5	3563	-	-	-	X
84	MG	5	3564	-	-	-	X
84	MG	5	3574	-	-	-	X
84	MG	5	3577	-	-	-	X
84	MG	5	3583	-	-	-	X
84	MG	5	3588	-	-	-	X
84	MG	5	3591	-	-	-	X
84	MG	5	3593	-	-	-	X
84	MG	5	3594	-	-	-	X
84	MG	5	3601	-	-	-	X
84	MG	5	3624	-	-	-	X
84	MG	5	3634	-	-	-	X
84	MG	5	3645	-	-	-	X
84	MG	5	3664	-	-	-	X
84	MG	5	3697	-	-	-	X
84	MG	5	3706	-	-	-	X
84	MG	5	3751	-	-	-	X
84	MG	5	3755	-	-	-	X
84	MG	5	3766	-	-	-	X
84	MG	5	3768	-	-	-	X
84	MG	5	3775	-	-	-	X
84	MG	5	3813	-	-	-	X
84	MG	5	3855	-	-	-	X
84	MG	5	3859	-	-	-	X
84	MG	5	3863	-	-	-	X
84	MG	5	3868	-	-	-	X
84	MG	5	3869	-	-	-	X
84	MG	5	3878	-	-	-	X
84	MG	5	3896	-	-	-	X
84	MG	5	3904	-	-	-	X
84	MG	5	3915	-	-	-	X
84	MG	5	3934	-	-	-	X
84	MG	5	3936	-	-	-	X
84	MG	5	3948	-	-	-	X
84	MG	5	3954	-	-	-	X
84	MG	5	3958	-	-	-	X
84	MG	5	3965	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	5	3966	-	-	-	X
84	MG	5	3970	-	-	-	X
84	MG	5	3974	-	-	-	X
84	MG	5	3975	-	-	-	X
84	MG	5	3984	-	-	-	X
84	MG	5	4007	-	-	-	X
84	MG	5	4030	-	-	-	X
84	MG	5	4046	-	-	-	X
84	MG	5	4052	-	-	-	X
84	MG	5	4097	-	-	-	X
84	MG	5	4129	-	-	-	X
84	MG	6	1901	-	-	-	X
84	MG	6	1903	-	-	-	X
84	MG	6	1933	-	-	-	X
84	MG	6	1940	-	-	-	X
84	MG	6	1944	-	-	-	X
84	MG	6	1945	-	-	-	X
84	MG	6	1960	-	-	-	X
84	MG	6	1967	-	-	-	X
84	MG	6	1968	-	-	-	X
84	MG	6	1989	-	-	-	X
84	MG	6	1991	-	-	-	X
84	MG	6	1992	-	-	-	X
84	MG	6	1993	-	-	-	X
84	MG	6	2090	-	-	-	X
84	MG	6	2106	-	-	-	X
84	MG	6	2107	-	-	-	X
84	MG	6	2121	-	-	-	X
84	MG	8	201	-	-	-	X
84	MG	8	213	-	-	-	X
84	MG	8	216	-	-	-	X
84	MG	D3	204	-	-	-	X
84	MG	S2	301	-	-	-	X
84	MG	c1	201	-	-	-	X
84	MG	c3	201	-	-	-	X
84	MG	d1	101	-	-	-	X
84	MG	d3	201	-	-	-	X
84	MG	l3	406	-	-	-	X
84	MG	l3	408	-	-	-	X
84	MG	l8	301	-	-	-	X
84	MG	m6	208	-	-	-	X
84	MG	m7	207	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	MG	m8	202	-	-	-	X

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 404238 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1	3100	Total	C	N	O	P	0	0	0
			66304	29617	11950	21637	3100			
1	5	3134	Total	C	N	O	P	0	0	0
			67039	29943	12089	21873	3134			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
2	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	156	Total	C	N	O	P	0	0	0
			3313	1482	582	1093	156			
3	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L3	386	Total	C	N	O	S	0	0	0
			3081	1956	584	533	8			
5	l3	386	Total	C	N	O	S	0	0	0
			3081	1956	584	533	8			

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L4	361	Total	C	N	O	S	0	0	0
			2749	1730	522	494	3			
6	l4	361	Total	C	N	O	S	0	0	0
			2749	1730	522	494	3			

- Molecule 7 is a protein called 60S ribosomal protein L5.

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

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L8	233	Total	C	N	O	S	0	0	0
			1817	1159	326	329	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	l8	231	Total 1763	C 1130	N 316	O 314	S 3	0	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M0	212	Total 1707	C 1084	N 323	O 295	S 5	0	0	0
12	m0	211	Total 1716	C 1090	N 324	O 296	S 6	0	0	0

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

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

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	M7	183	Total	C	N	O	0	0	0
			1415	877	281	257			
18	m7	155	Total	C	N	O	0	0	0
			1227	764	238	225			

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	M9	182	Total	C	N	O	0	0	0
			1474	905	319	250			
20	m9	188	Total	C	N	O	0	0	0
			1521	935	326	260			

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

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

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	O1	109	Total	C	N	O	S	0	0	0
			890	565	168	156	1			
32	o1	109	Total	C	N	O	S	0	0	0
			890	565	168	156	1			

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	O4	112	Total	C	N	O	S	0	0	0
			881	546	179	152	4			
35	o4	112	Total	C	N	O	S	0	0	0
			881	546	179	152	4			

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

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

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

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				
39	O8	77	612	391	115	106		0	0	0
39	o8	77	612	391	115	106		0	0	0

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
45	2	1712	Total 36488	C 16313	N 6466	O 11997	P 1712	0	0	0
45	6	1739	Total 37060	C 16570	N 6568	O 12183	P 1739	0	0	0

- Molecule 46 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	S0	206	Total 1612	C 1034	N 285	O 291	S 2	0	0	0
46	s0	206	Total 1612	C 1034	N 285	O 291	S 2	0	0	0

- Molecule 47 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 48 is a protein called 40S ribosomal protein S2.

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

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	S3	223	Total 1734	C 1101	N 313	O 314	S 6	0	0	0
49	s3	223	Total 1728	C 1098	N 310	O 314	S 6	0	0	0

- Molecule 50 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	S6	226	Total 1813	C 1137	N 350	O 323	S 3	0	0	0
52	s6	218	Total 1755	C 1102	N 337	O 313	S 3	0	0	0

- Molecule 53 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
53	S7	184	Total 1481	C 951	N 265	O 265	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
53	s7	186	1491	957	267	267	0	0	0

- Molecule 54 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	S8	188	1489	925	298	264	2	0	0	0
54	s8	186	1471	913	294	262	2	0	0	0

- Molecule 55 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	S9	185	1494	943	289	261	1	0	0	0
55	s9	185	1494	943	289	261	1	0	0	0

- Molecule 56 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	C0	96	772	499	126	145	2	0	0	0
56	c0	96	761	490	125	144	2	0	0	0

- Molecule 57 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	C1	155	1213	774	230	206	3	0	0	0
57	c1	142	1138	729	217	189	3	0	0	0

- Molecule 58 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
58	C2	124	890	560	156	172	2	0	0	0
58	c2	124	890	560	156	172	2	0	0	0

- Molecule 59 is a protein called 40S ribosomal protein S13.

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

- Molecule 60 is a protein called 40S ribosomal protein S14-B.

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

- Molecule 61 is a protein called 40S ribosomal protein S15.

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

- Molecule 62 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 63 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
63	C7	120	Total	C	N	O	S	0	0	0
			965	603	183	177	2			
63	c7	117	Total	C	N	O	S	0	0	0
			917	569	175	171	2			

- Molecule 64 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 66 is a protein called 40S ribosomal protein S20.

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

- Molecule 67 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 69 is a protein called 40S ribosomal protein S23-A.

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

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

- Molecule 70 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
70	D4	134	1073	676	208	189	0	0	0
70	d4	133	1065	672	207	186	0	0	0

- Molecule 71 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S26-B.

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

- Molecule 73 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	D9	53	Total	C	N	O	S	0	0	0
			443	275	92	72	4			
75	d9	53	Total	C	N	O	S	0	0	0
			443	275	92	72	4			

- Molecule 76 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
76	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
77	e1	72	Total	C	N	O	S	0	0	0
			575	368	108	95	4			

- Molecule 78 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	SR	318	Total	C	N	O	S	0	0	0
			2441	1543	418	472	8			
78	sR	318	Total	C	N	O	S	0	0	0
			2441	1543	418	472	8			

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 79 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
79	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
79	sM	129	923	546	184	193	0	0	0

- Molecule 80 is a protein called 60S ribosomal protein L12.

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

- Molecule 81 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	n4	135	1044	654	209	180	1	0	0	0

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

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

- Molecule 83 is a protein called Ribosomal protein P1 alpha.

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

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	1	588	Total	Mg	0	0
			588	588		
84	3	19	Total	Mg	0	0
			19	19		
84	4	23	Total	Mg	0	0
			23	23		
84	L2	5	Total	Mg	0	0
			5	5		
84	L3	3	Total	Mg	0	0
			3	3		
84	L4	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	L5	1	Total 1	Mg 1	0	0
84	L7	1	Total 1	Mg 1	0	0
84	L8	1	Total 1	Mg 1	0	0
84	L9	1	Total 1	Mg 1	0	0
84	M0	4	Total 4	Mg 4	0	0
84	M3	5	Total 5	Mg 5	0	0
84	M5	5	Total 5	Mg 5	0	0
84	M6	1	Total 1	Mg 1	0	0
84	M7	5	Total 5	Mg 5	0	0
84	M8	1	Total 1	Mg 1	0	0
84	N0	4	Total 4	Mg 4	0	0
84	N1	2	Total 2	Mg 2	0	0
84	N3	4	Total 4	Mg 4	0	0
84	N4	1	Total 1	Mg 1	0	0
84	N5	1	Total 1	Mg 1	0	0
84	N8	3	Total 3	Mg 3	0	0
84	O2	4	Total 4	Mg 4	0	0
84	O3	1	Total 1	Mg 1	0	0
84	O4	3	Total 3	Mg 3	0	0
84	O6	1	Total 1	Mg 1	0	0
84	O7	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	Q1	1	Total 1	Mg 1	0	0
84	Q2	4	Total 4	Mg 4	0	0
84	2	142	Total 142	Mg 142	0	0
84	S1	1	Total 1	Mg 1	0	0
84	S2	1	Total 1	Mg 1	0	0
84	S3	1	Total 1	Mg 1	0	0
84	S4	1	Total 1	Mg 1	0	0
84	C1	1	Total 1	Mg 1	0	0
84	C3	1	Total 1	Mg 1	0	0
84	C8	1	Total 1	Mg 1	0	0
84	D3	5	Total 5	Mg 5	0	0
84	5	750	Total 750	Mg 750	0	0
84	7	30	Total 30	Mg 30	0	0
84	8	20	Total 20	Mg 20	0	0
84	l2	5	Total 5	Mg 5	0	0
84	l3	11	Total 11	Mg 11	0	0
84	l4	2	Total 2	Mg 2	0	0
84	l5	6	Total 6	Mg 6	0	0
84	l6	2	Total 2	Mg 2	0	0
84	l7	3	Total 3	Mg 3	0	0
84	l8	1	Total 1	Mg 1	0	0

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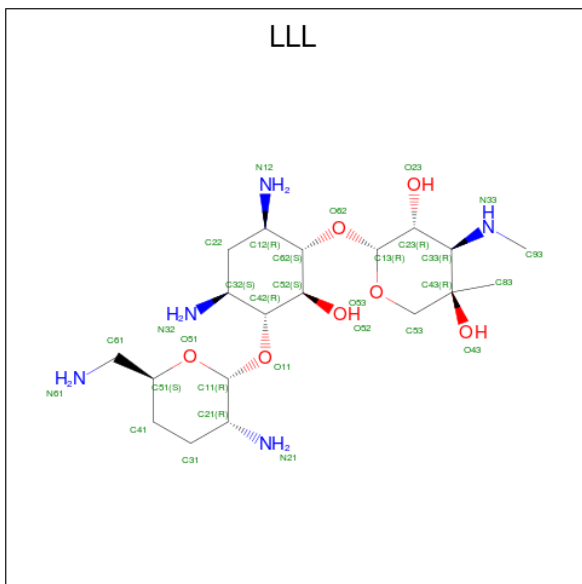
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	l9	8	Total Mg 8 8	0	0
84	m0	2	Total Mg 2 2	0	0
84	m3	4	Total Mg 4 4	0	0
84	m4	6	Total Mg 6 6	0	0
84	m5	3	Total Mg 3 3	0	0
84	m6	8	Total Mg 8 8	0	0
84	m7	7	Total Mg 7 7	0	0
84	m8	4	Total Mg 4 4	0	0
84	m9	2	Total Mg 2 2	0	0
84	n0	7	Total Mg 7 7	0	0
84	n1	2	Total Mg 2 2	0	0
84	n3	2	Total Mg 2 2	0	0
84	n5	3	Total Mg 3 3	0	0
84	n8	3	Total Mg 3 3	0	0
84	n9	1	Total Mg 1 1	0	0
84	o1	1	Total Mg 1 1	0	0
84	o2	3	Total Mg 3 3	0	0
84	o3	2	Total Mg 2 2	0	0
84	o4	2	Total Mg 2 2	0	0
84	q0	1	Total Mg 1 1	0	0
84	q1	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	q2	7	Total 7	Mg 7	0	0
84	q3	3	Total 3	Mg 3	0	0
84	6	263	Total 263	Mg 263	0	0
84	s0	1	Total 1	Mg 1	0	0
84	s2	2	Total 2	Mg 2	0	0
84	s3	1	Total 1	Mg 1	0	0
84	s4	1	Total 1	Mg 1	0	0
84	s5	3	Total 3	Mg 3	0	0
84	s6	1	Total 1	Mg 1	0	0
84	c1	1	Total 1	Mg 1	0	0
84	c3	6	Total 6	Mg 6	0	0
84	c4	1	Total 1	Mg 1	0	0
84	c8	3	Total 3	Mg 3	0	0
84	d1	2	Total 2	Mg 2	0	0
84	d2	1	Total 1	Mg 1	0	0
84	d3	5	Total 5	Mg 5	0	0
84	d5	1	Total 1	Mg 1	0	0
84	d6	3	Total 3	Mg 3	0	0
84	d7	1	Total 1	Mg 1	0	0
84	d9	1	Total 1	Mg 1	0	0
84	sR	1	Total 1	Mg 1	0	0

- Molecule 85 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-O-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		
85	1	1	Total	C	N	O	0	0
			31	19	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
85	1	1	31	19	5	7	0	0
85	1	1	31	19	5	7	0	0
85	1	1	31	19	5	7	0	0
85	1	1	31	19	5	7	0	0
85	1	1	31	19	5	7	0	0
85	3	1	31	19	5	7	0	0
85	4	1	31	19	5	7	0	0
85	L3	1	31	19	5	7	0	0
85	2	1	31	19	5	7	0	0
85	2	1	31	19	5	7	0	0
85	2	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0
85	5	1	31	19	5	7	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	5	1	Total 31	C 19	N 5	O 7	0	0
85	7	1	Total 31	C 19	N 5	O 7	0	0
85	7	1	Total 31	C 19	N 5	O 7	0	0
85	7	1	Total 31	C 19	N 5	O 7	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
85	8	1	Total 31	C 19	N 5	O 7	0	0
85	8	1	Total 31	C 19	N 5	O 7	0	0
85	13	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0
85	6	1	Total 31	C 19	N 5	O 7	0	0

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	O4	1	Total 1	Zn 1	0	0
86	O7	1	Total 1	Zn 1	0	0
86	Q0	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	Q2	1	Total 1	Zn 1	0	0
86	Q3	1	Total 1	Zn 1	0	0
86	D6	1	Total 1	Zn 1	0	0
86	D7	1	Total 1	Zn 1	0	0
86	D9	1	Total 1	Zn 1	0	0
86	E1	1	Total 1	Zn 1	0	0
86	o4	1	Total 1	Zn 1	0	0
86	o7	1	Total 1	Zn 1	0	0
86	q0	1	Total 1	Zn 1	0	0
86	q2	1	Total 1	Zn 1	0	0
86	q3	1	Total 1	Zn 1	0	0
86	d6	1	Total 1	Zn 1	0	0
86	d7	1	Total 1	Zn 1	0	0
86	d9	1	Total 1	Zn 1	0	0
86	e1	1	Total 1	Zn 1	0	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	1	473	Total 473	O 473	0	0
87	3	15	Total 15	O 15	0	0
87	4	5	Total 5	O 5	0	0
87	L2	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	L3	7	Total O 7 7	0	0
87	L4	2	Total O 2 2	0	0
87	L5	2	Total O 2 2	0	0
87	M0	1	Total O 1 1	0	0
87	M3	2	Total O 2 2	0	0
87	M5	3	Total O 3 3	0	0
87	M6	6	Total O 6 6	0	0
87	M7	5	Total O 5 5	0	0
87	N0	4	Total O 4 4	0	0
87	N1	3	Total O 3 3	0	0
87	N3	5	Total O 5 5	0	0
87	N4	2	Total O 2 2	0	0
87	N5	2	Total O 2 2	0	0
87	N8	3	Total O 3 3	0	0
87	N9	2	Total O 2 2	0	0
87	O2	2	Total O 2 2	0	0
87	O4	1	Total O 1 1	0	0
87	O7	1	Total O 1 1	0	0
87	Q1	1	Total O 1 1	0	0
87	Q2	1	Total O 1 1	0	0
87	2	111	Total O 111 111	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	S1	1	Total O 1 1	0	0
87	S3	3	Total O 3 3	0	0
87	S4	1	Total O 1 1	0	0
87	S8	1	Total O 1 1	0	0
87	C9	2	Total O 2 2	0	0
87	D0	1	Total O 1 1	0	0
87	D3	1	Total O 1 1	0	0
87	SR	2	Total O 2 2	0	0
87	5	514	Total O 514 514	0	0
87	7	33	Total O 33 33	0	0
87	8	11	Total O 11 11	0	0
87	12	7	Total O 7 7	0	0
87	13	6	Total O 6 6	0	0
87	15	5	Total O 5 5	0	0
87	19	3	Total O 3 3	0	0
87	m0	1	Total O 1 1	0	0
87	m4	1	Total O 1 1	0	0
87	m5	2	Total O 2 2	0	0
87	m6	8	Total O 8 8	0	0
87	m7	4	Total O 4 4	0	0
87	m9	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	n0	4	Total O 4 4	0	0
87	n1	2	Total O 2 2	0	0
87	n3	2	Total O 2 2	0	0
87	n4	1	Total O 1 1	0	0
87	n5	2	Total O 2 2	0	0
87	n6	1	Total O 1 1	0	0
87	n8	4	Total O 4 4	0	0
87	n9	1	Total O 1 1	0	0
87	o0	1	Total O 1 1	0	0
87	o1	2	Total O 2 2	0	0
87	o2	4	Total O 4 4	0	0
87	o4	2	Total O 2 2	0	0
87	q0	1	Total O 1 1	0	0
87	q2	2	Total O 2 2	0	0
87	q3	3	Total O 3 3	0	0
87	6	224	Total O 224 224	0	0
87	s4	1	Total O 1 1	0	0
87	s5	1	Total O 1 1	0	0
87	s7	1	Total O 1 1	0	0
87	c3	5	Total O 5 5	0	0
87	c6	1	Total O 1 1	0	0

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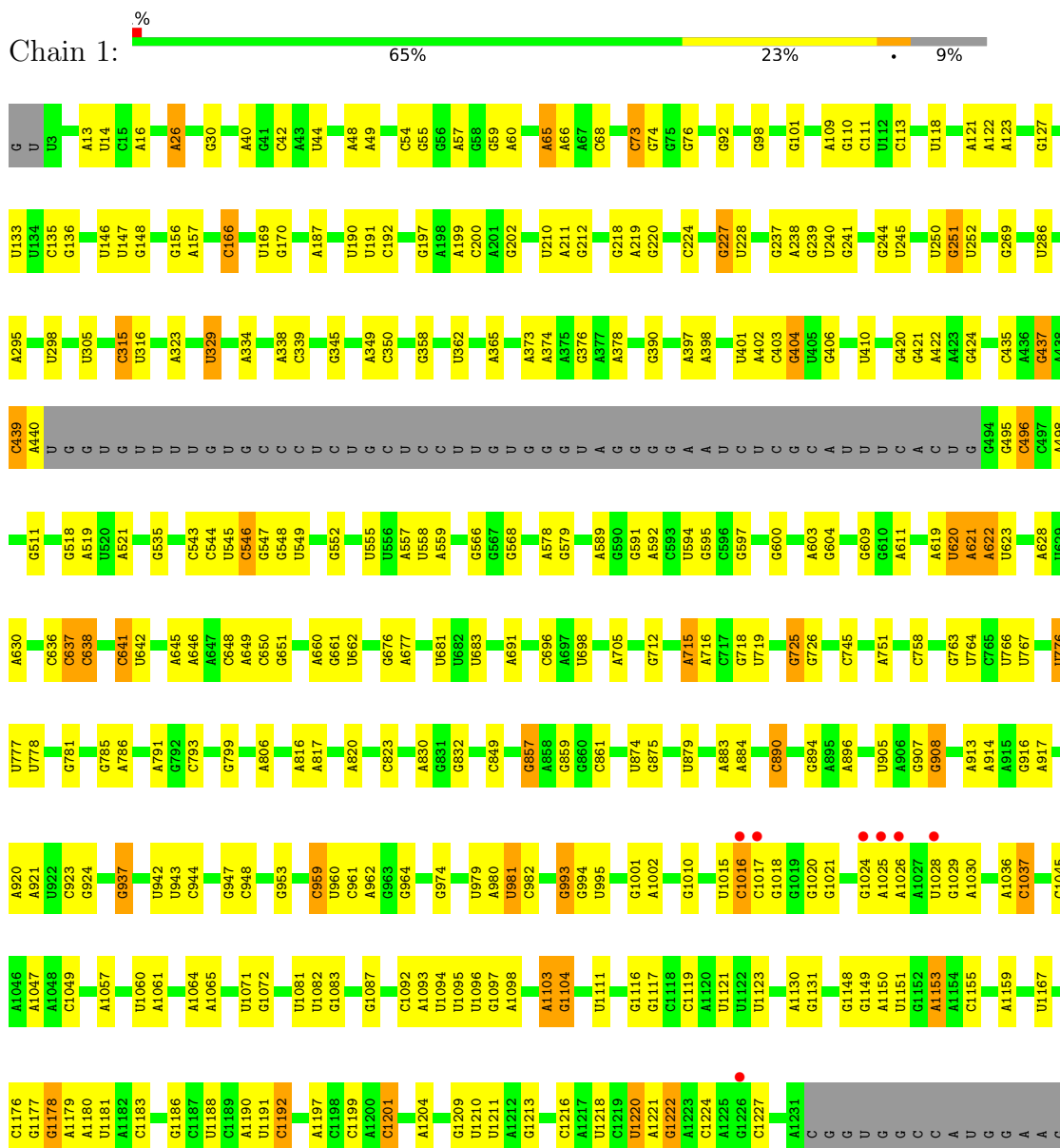
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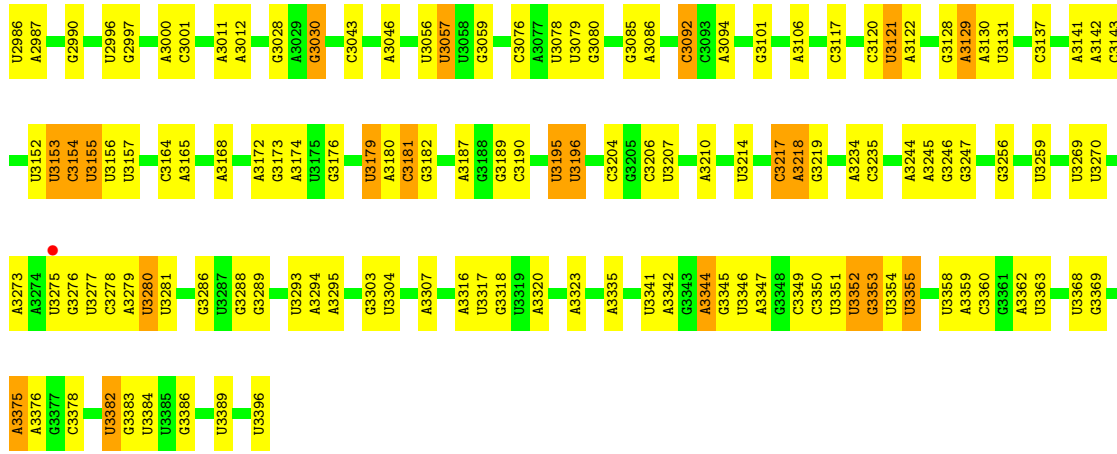
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	c8	3	Total O 3 3	0	0
87	c9	5	Total O 5 5	0	0
87	d3	5	Total O 5 5	0	0
87	d5	3	Total O 3 3	0	0
87	d6	3	Total O 3 3	0	0
87	d9	2	Total O 2 2	0	0
87	e1	1	Total O 1 1	0	0
87	sR	1	Total O 1 1	0	0

3 Residue-property plots

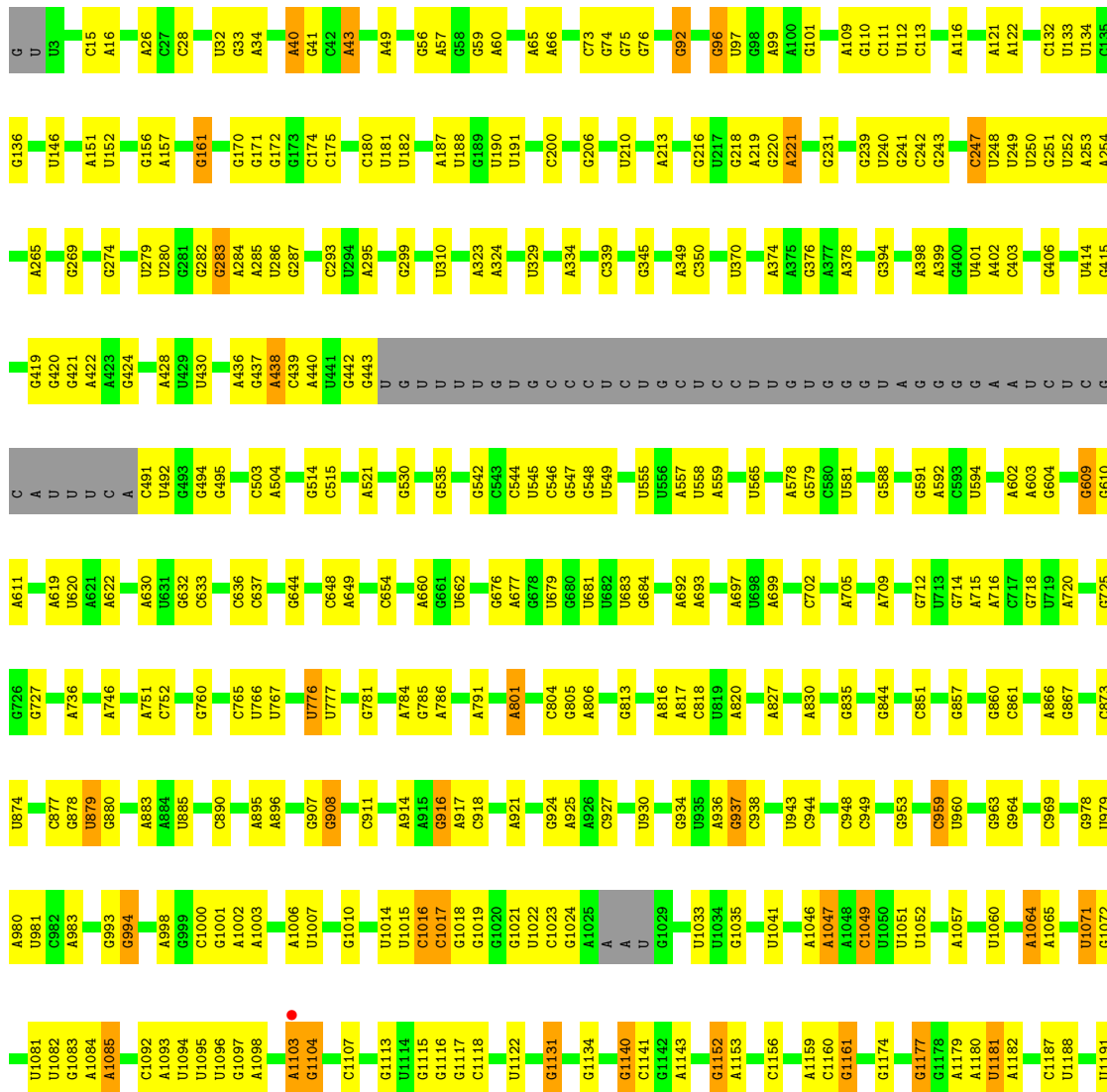
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

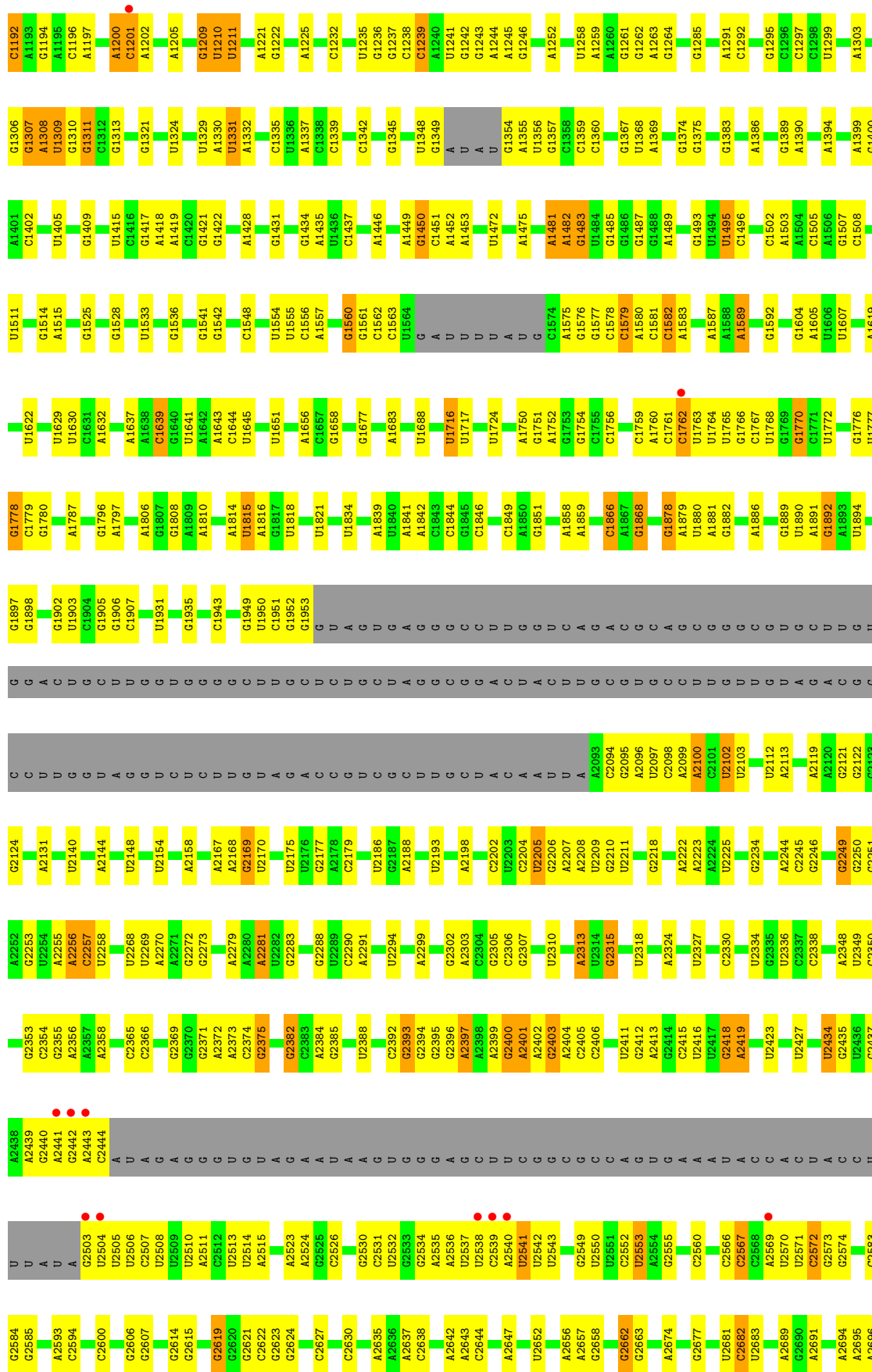
- Molecule 1: 25S ribosomal RNA

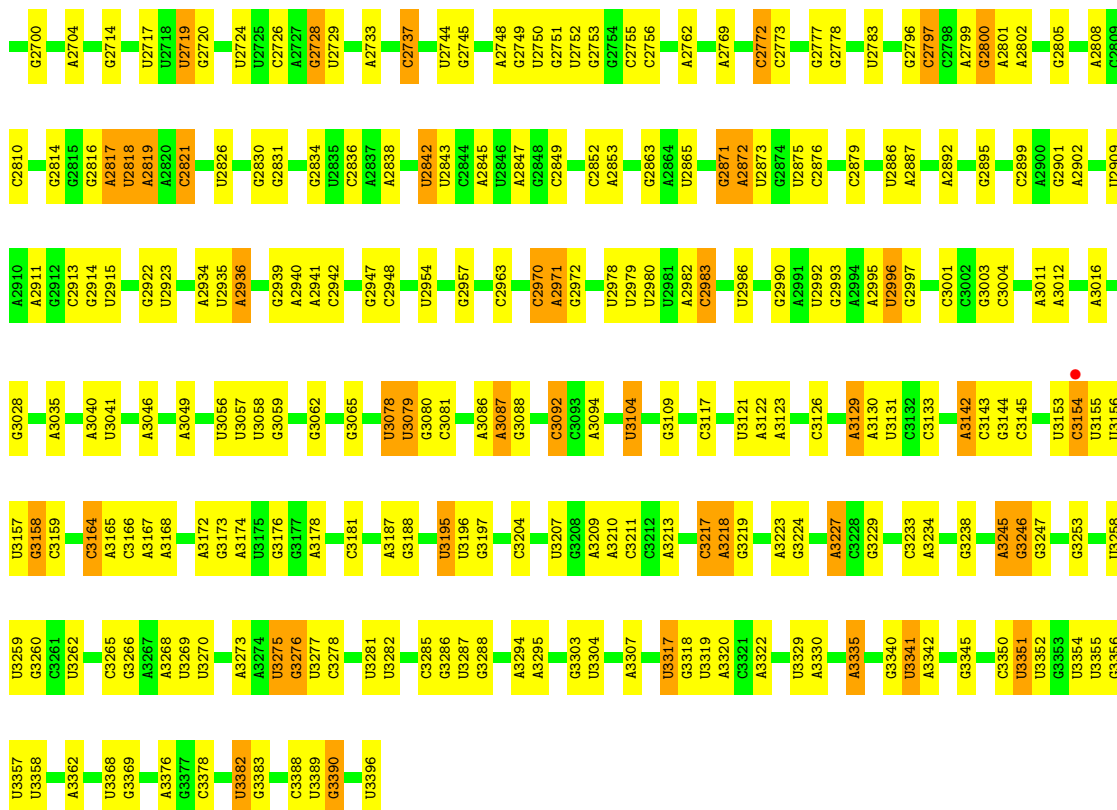




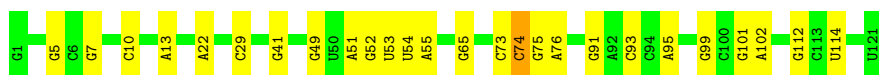
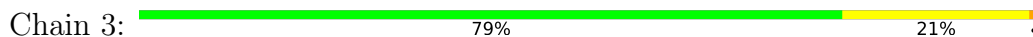
• Molecule 1: 25S ribosomal RNA



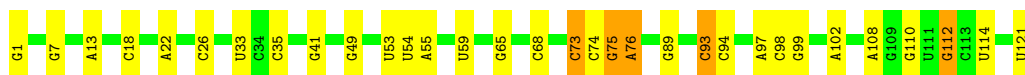




• Molecule 2: 5S Ribosomal RNA



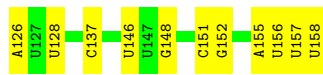
• Molecule 2: 5S Ribosomal RNA



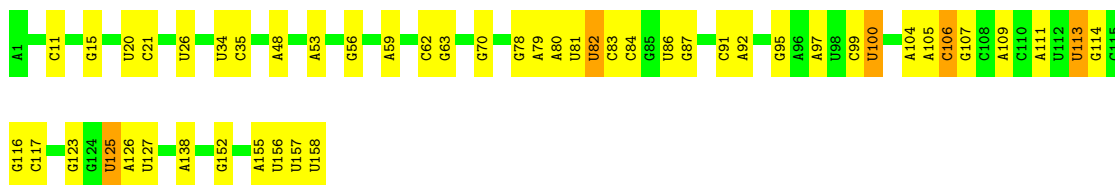
• Molecule 3: 5.8S ribosomal RNA



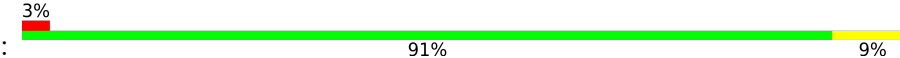
• Molecule 3: 5.8S ribosomal RNA

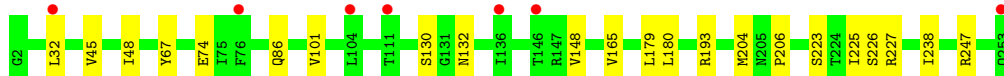


Chain 8:  69% 28%



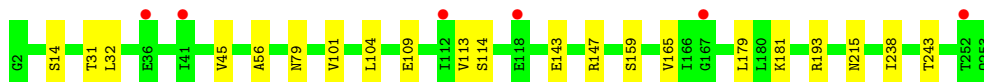
• Molecule 4: 60S ribosomal protein L2-A

Chain L2:  3% 91% 9%

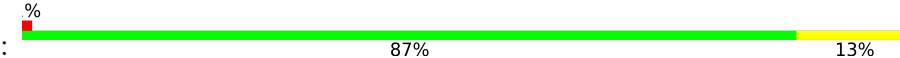


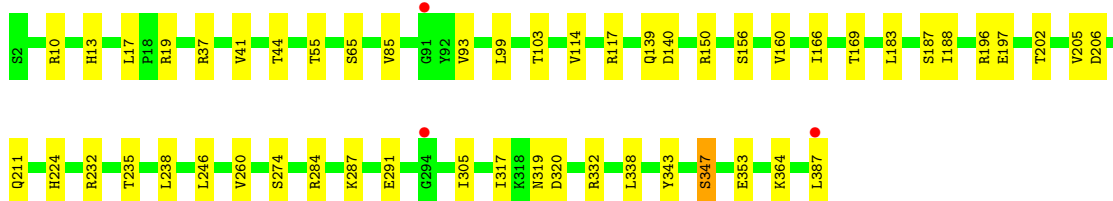
• Molecule 4: 60S ribosomal protein L2-A

Chain L2:  2% 92% 8%



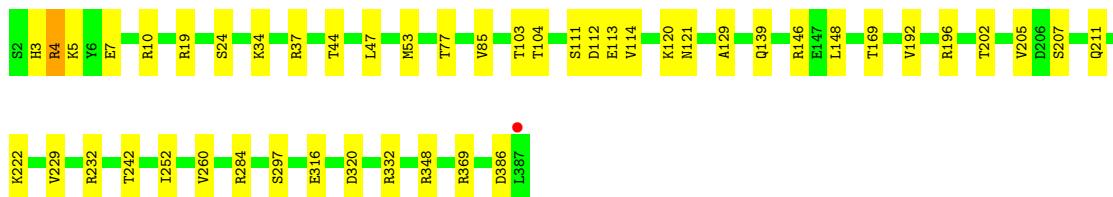
• Molecule 5: 60S ribosomal protein L3

Chain L3:  1% 87% 13%



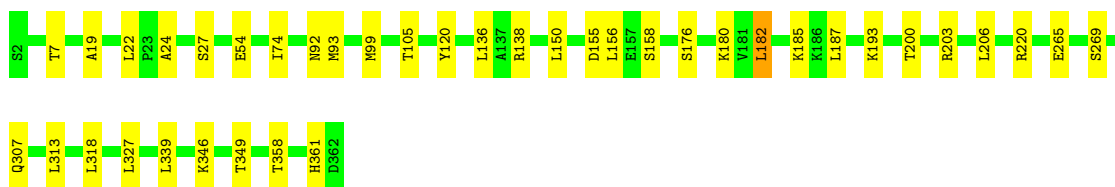
• Molecule 5: 60S ribosomal protein L3

Chain L3:  88% 12%

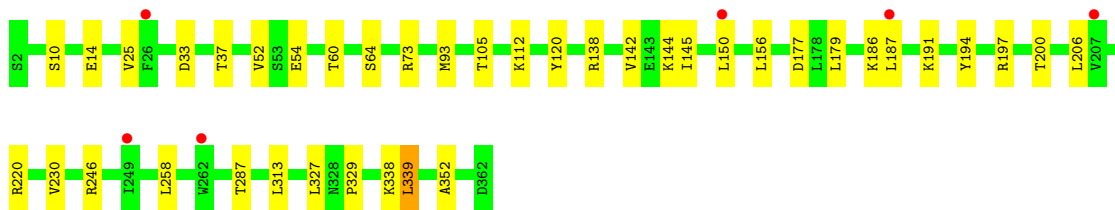
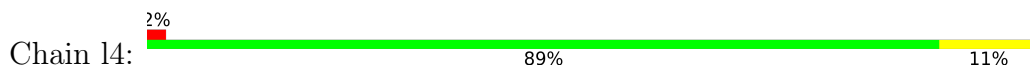


• Molecule 6: 60S ribosomal protein L4-A

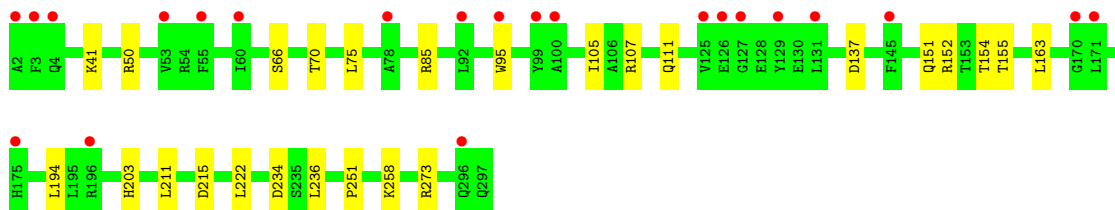
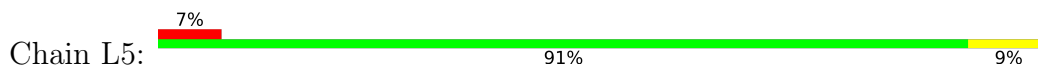
Chain L4:  89% 11%



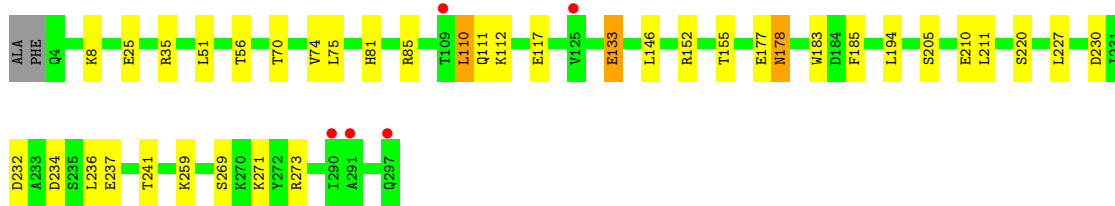
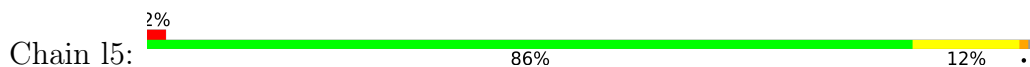
- Molecule 6: 60S ribosomal protein L4-A



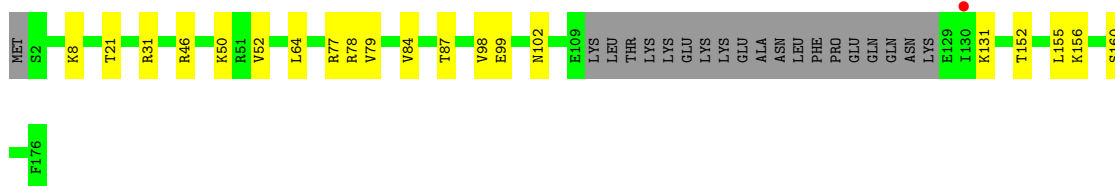
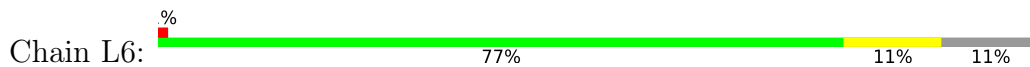
- Molecule 7: 60S ribosomal protein L5

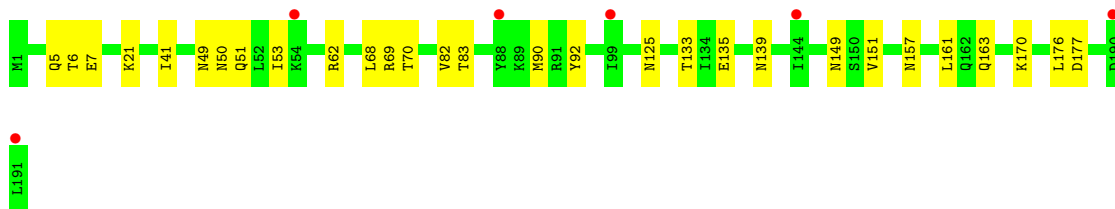


- Molecule 8: 60S ribosomal protein L6-A

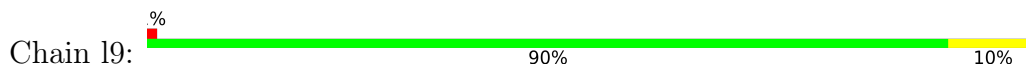


- Molecule 8: 60S ribosomal protein L6-A

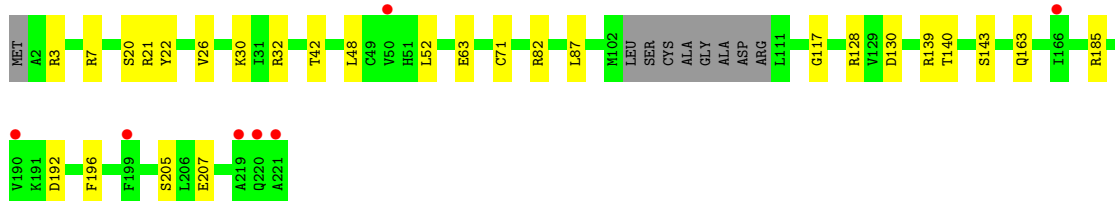
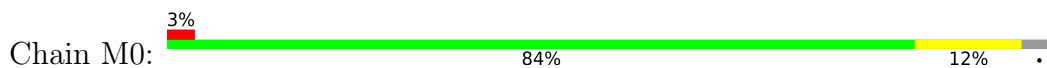




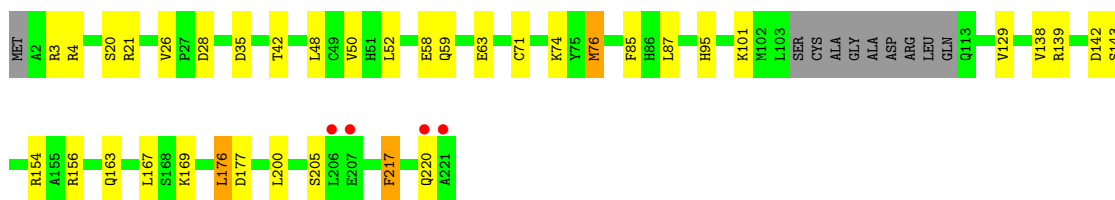
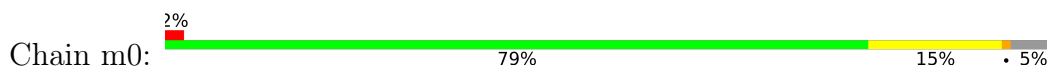
- Molecule 11: 60S ribosomal protein L9-A



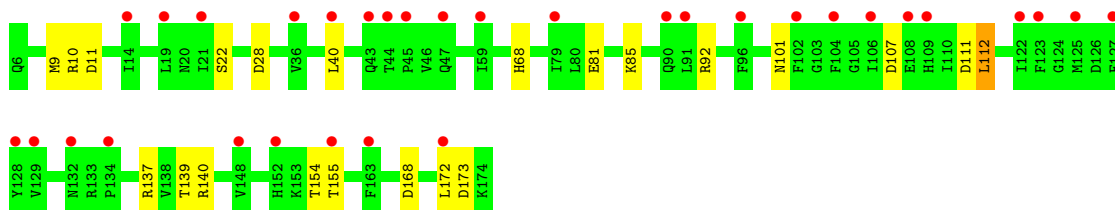
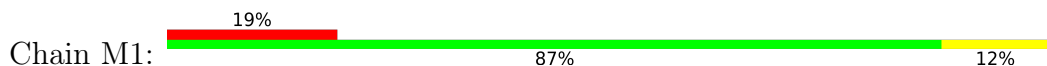
- Molecule 12: 60S ribosomal protein L10



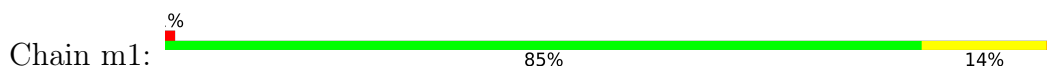
- Molecule 12: 60S ribosomal protein L10

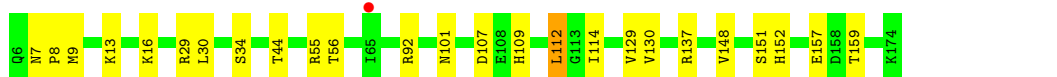


- Molecule 13: 60S ribosomal protein L11-B

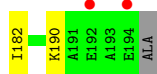
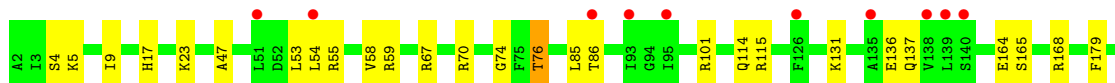
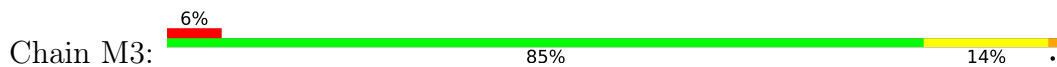


- Molecule 13: 60S ribosomal protein L11-B

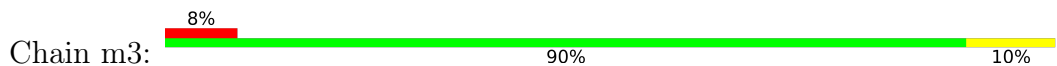




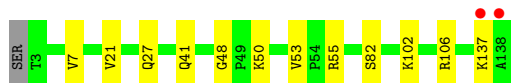
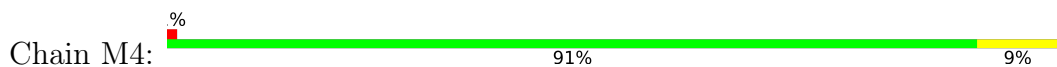
• Molecule 14: 60S ribosomal protein L13-A



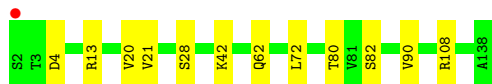
• Molecule 14: 60S ribosomal protein L13-A



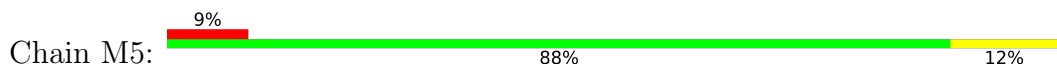
• Molecule 15: 60S ribosomal protein L14-A



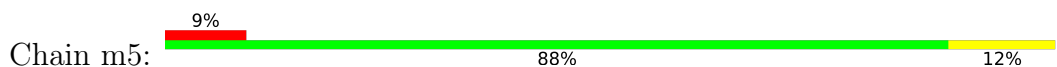
• Molecule 15: 60S ribosomal protein L14-A

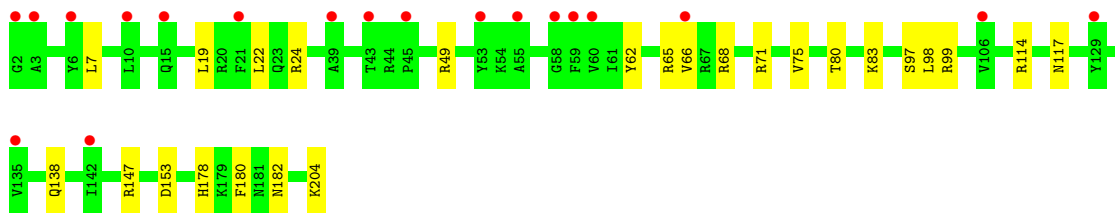


• Molecule 16: 60S ribosomal protein L15-A

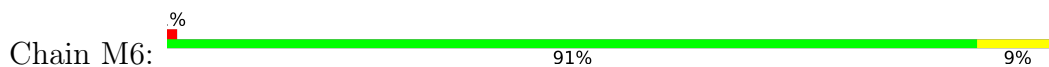


• Molecule 16: 60S ribosomal protein L15-A





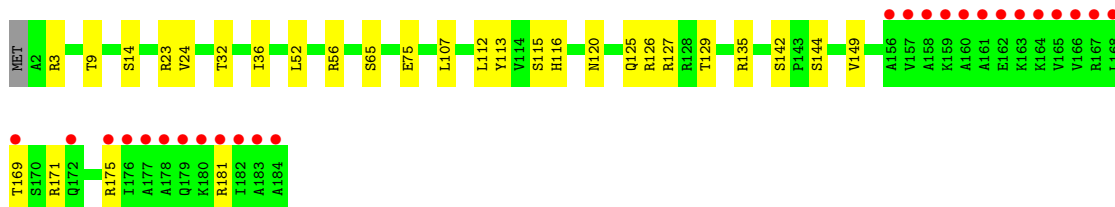
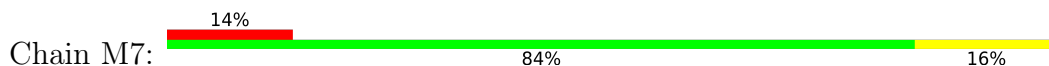
• Molecule 17: 60S ribosomal protein L16-A



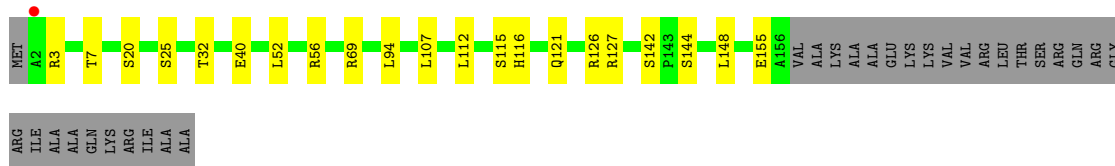
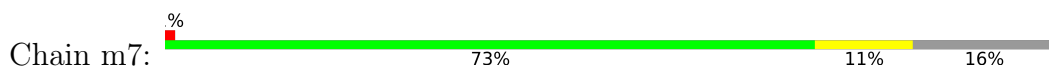
• Molecule 17: 60S ribosomal protein L16-A



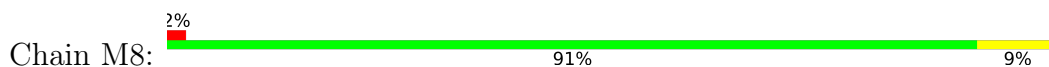
• Molecule 18: 60S ribosomal protein L17-A



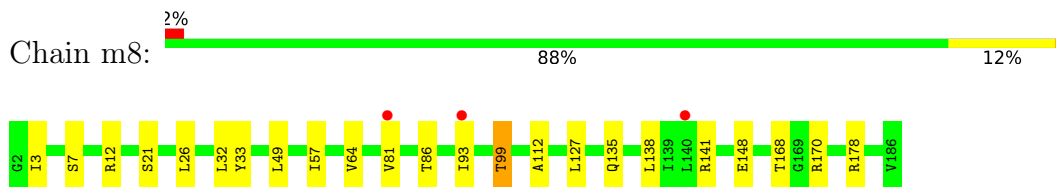
• Molecule 18: 60S ribosomal protein L17-A



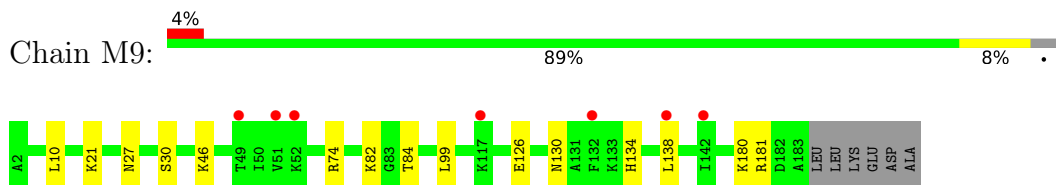
• Molecule 19: 60S ribosomal protein L18-A



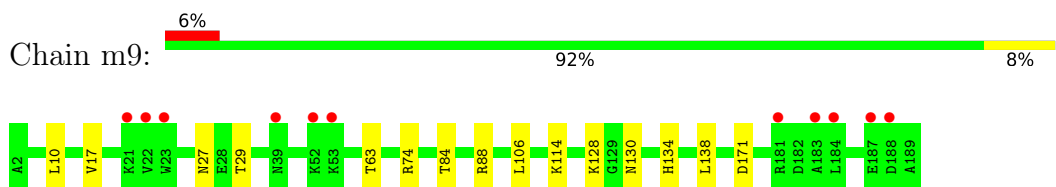
- Molecule 19: 60S ribosomal protein L18-A



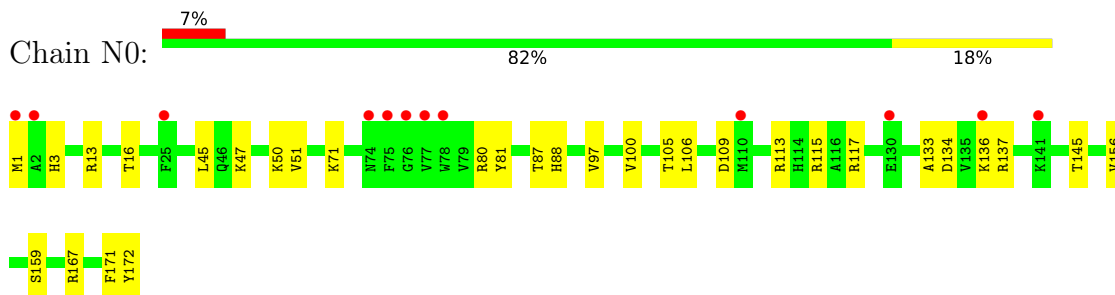
- Molecule 20: 60S ribosomal protein L19-A



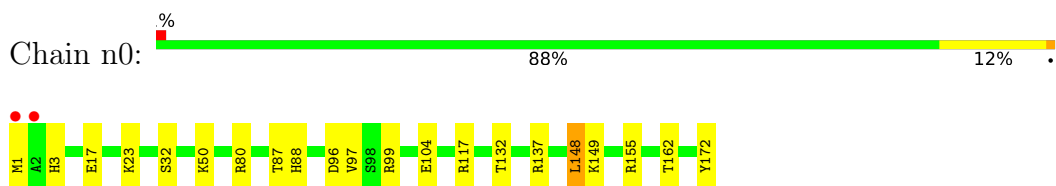
- Molecule 20: 60S ribosomal protein L19-A



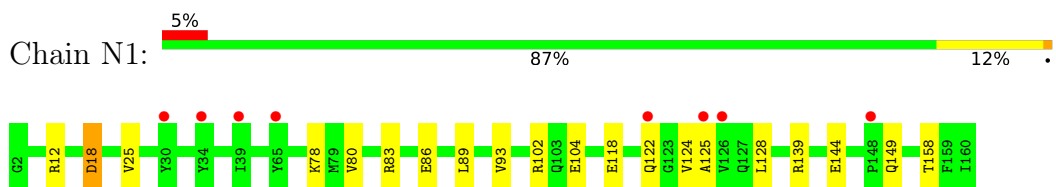
- Molecule 21: 60S ribosomal protein L20-A



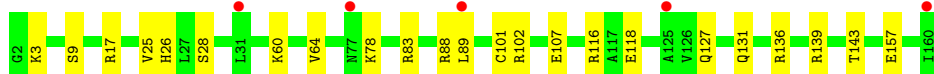
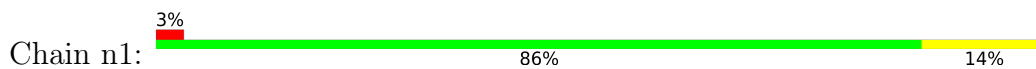
- Molecule 21: 60S ribosomal protein L20-A



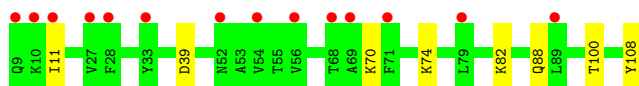
- Molecule 22: 60S ribosomal protein L21-A



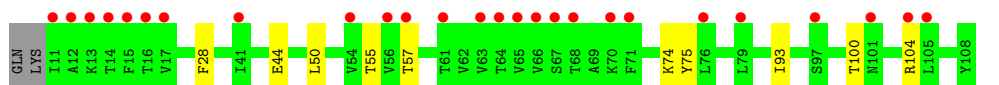
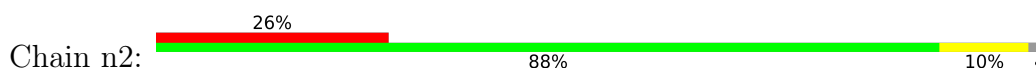
- Molecule 22: 60S ribosomal protein L21-A



- Molecule 23: 60S ribosomal protein L22-A



- Molecule 23: 60S ribosomal protein L22-A



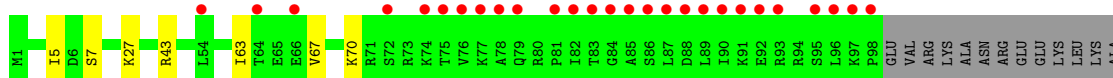
- Molecule 24: 60S ribosomal protein L23-A



- Molecule 24: 60S ribosomal protein L23-A



- Molecule 25: 60S ribosomal protein L24-A

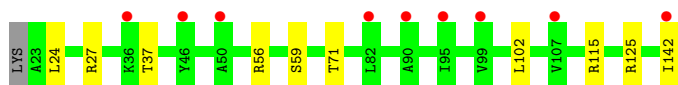


- Molecule 26: 60S ribosomal protein L25

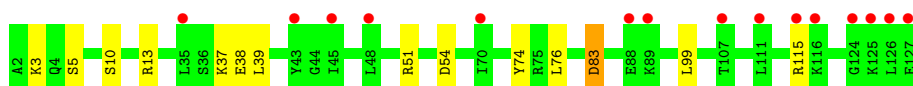
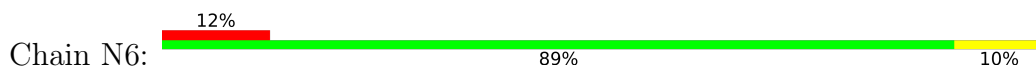




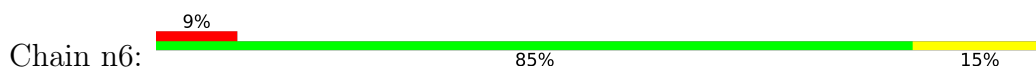
- Molecule 26: 60S ribosomal protein L25



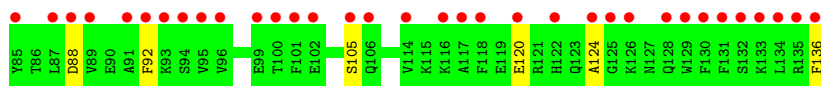
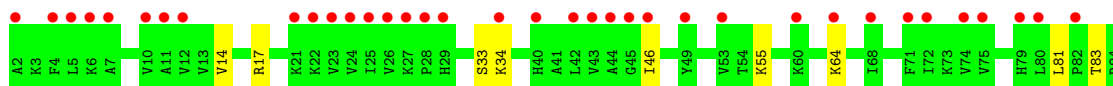
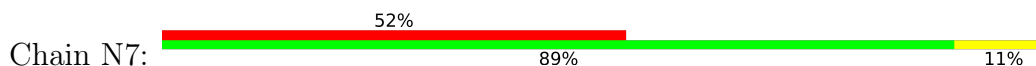
- Molecule 27: 60S ribosomal protein L26-A



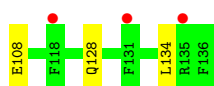
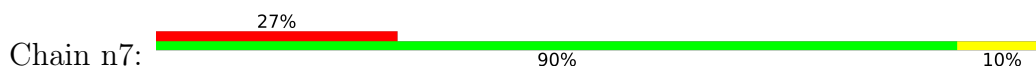
- Molecule 27: 60S ribosomal protein L26-A



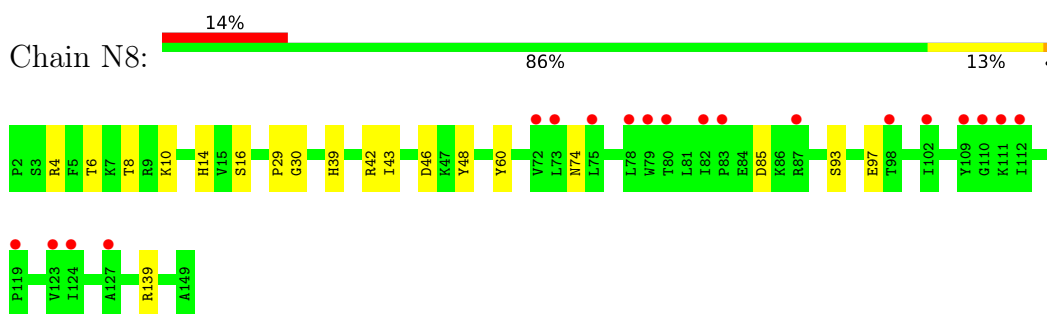
- Molecule 28: 60S ribosomal protein L27-A



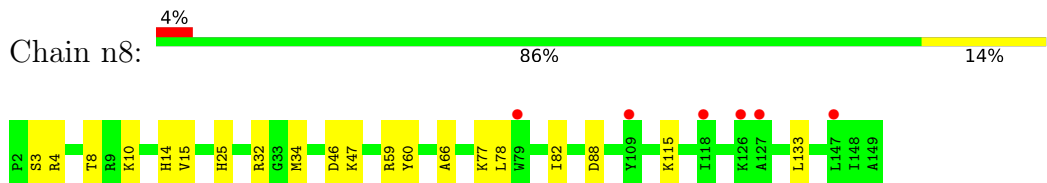
- Molecule 28: 60S ribosomal protein L27-A



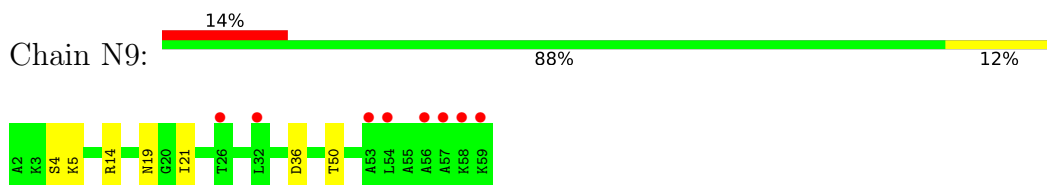
- Molecule 29: 60S ribosomal protein L28



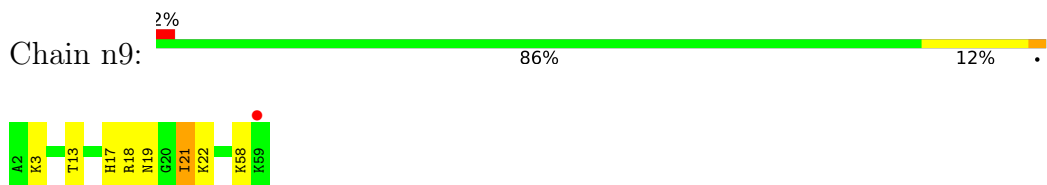
- Molecule 29: 60S ribosomal protein L28



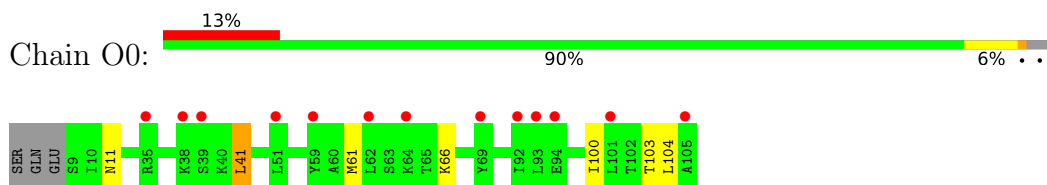
- Molecule 30: 60S ribosomal protein L29



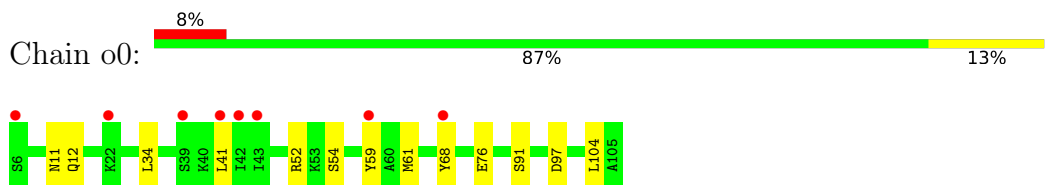
- Molecule 30: 60S ribosomal protein L29



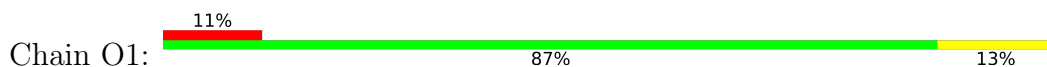
- Molecule 31: 60S ribosomal protein L30

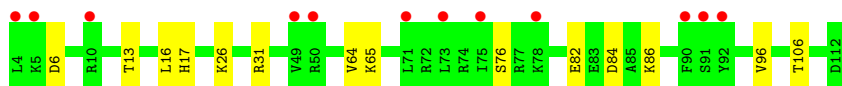


- Molecule 31: 60S ribosomal protein L30

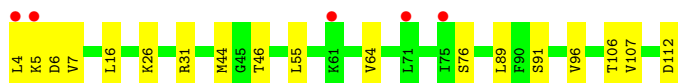
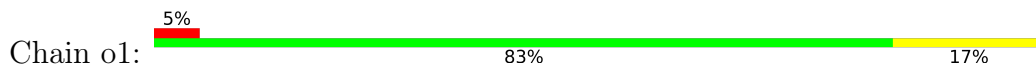


- Molecule 32: 60S ribosomal protein L31-A

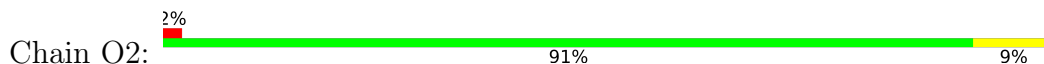




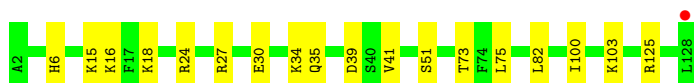
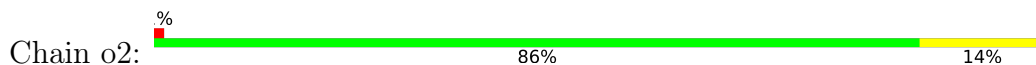
- Molecule 32: 60S ribosomal protein L31-A



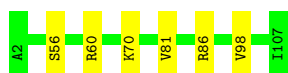
- Molecule 33: 60S ribosomal protein L32



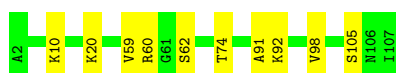
- Molecule 33: 60S ribosomal protein L32



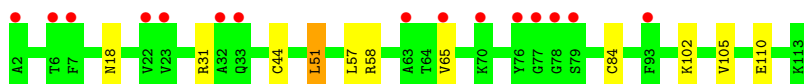
- Molecule 34: 60S ribosomal protein L33-A



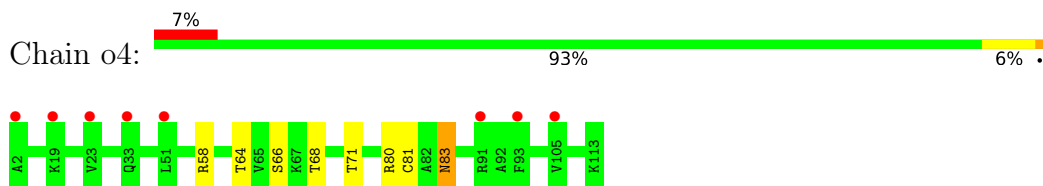
- Molecule 34: 60S ribosomal protein L33-A



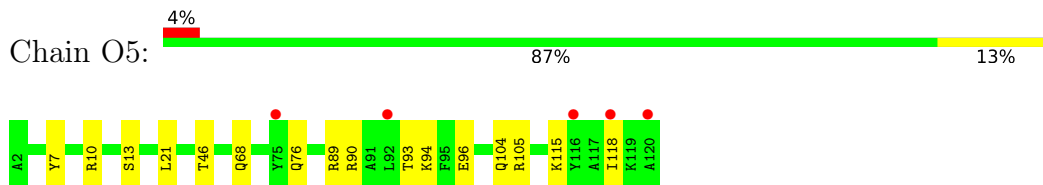
- Molecule 35: 60S ribosomal protein L34-A



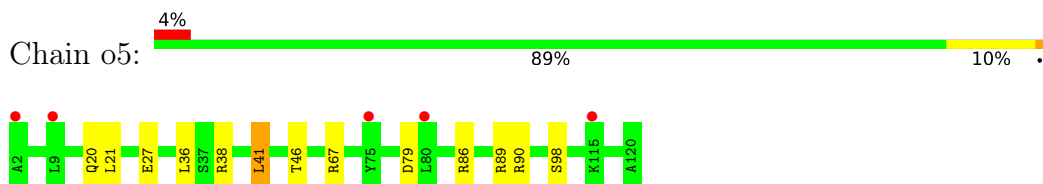
- Molecule 35: 60S ribosomal protein L34-A



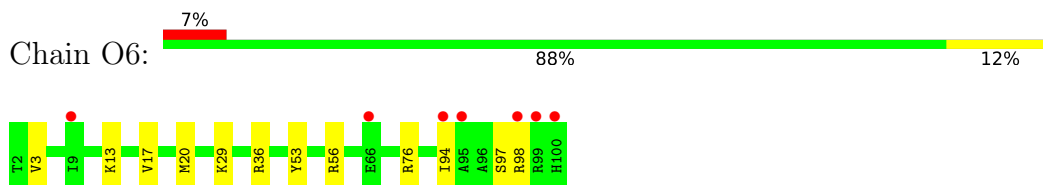
- Molecule 36: 60S ribosomal protein L35-A



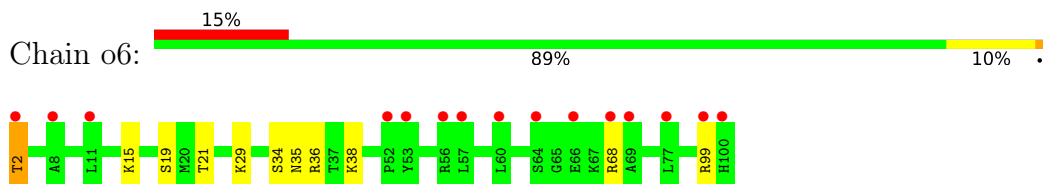
- Molecule 36: 60S ribosomal protein L35-A



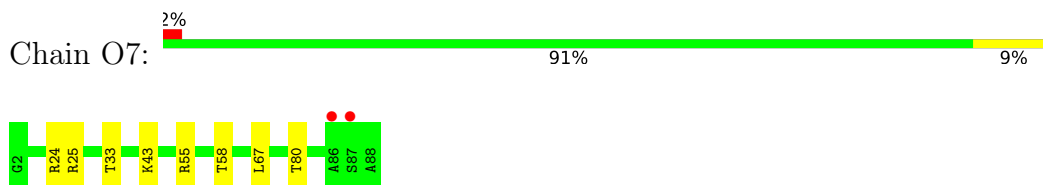
- Molecule 37: 60S ribosomal protein L36-A



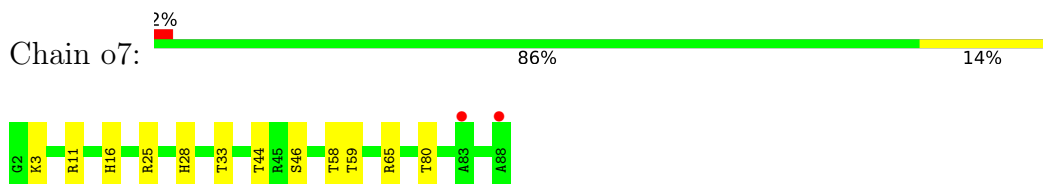
- Molecule 37: 60S ribosomal protein L36-A



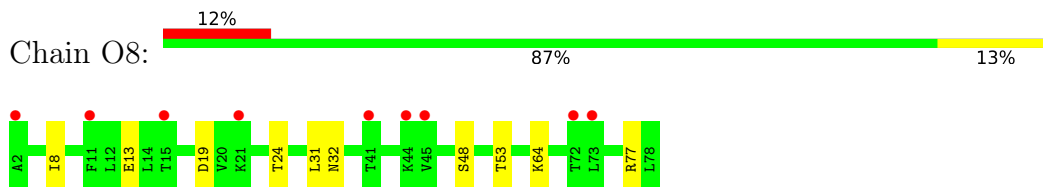
- Molecule 38: 60S ribosomal protein L37-A



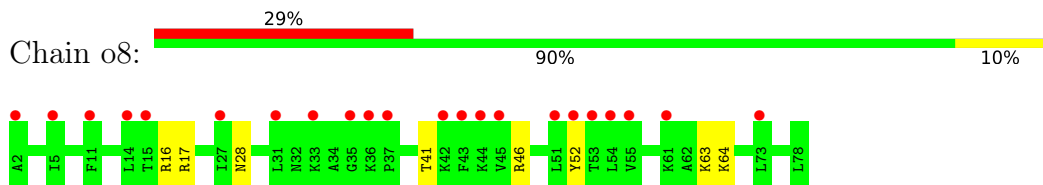
- Molecule 38: 60S ribosomal protein L37-A



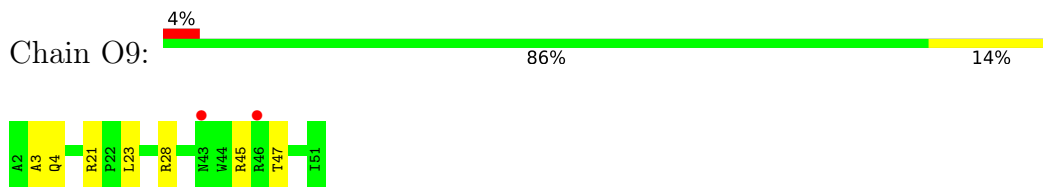
- Molecule 39: 60S ribosomal protein L38



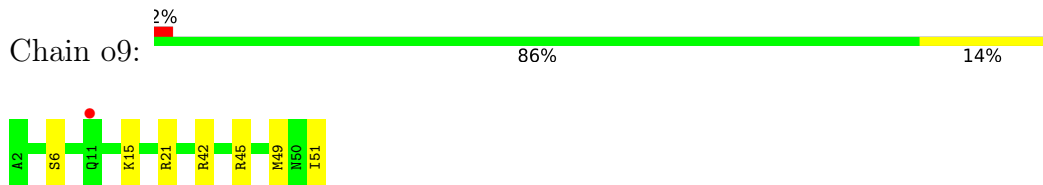
- Molecule 39: 60S ribosomal protein L38



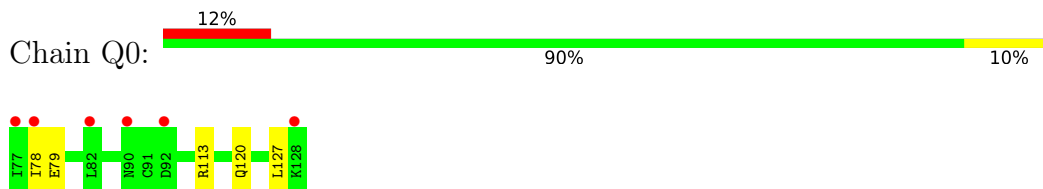
- Molecule 40: 60S ribosomal protein L39



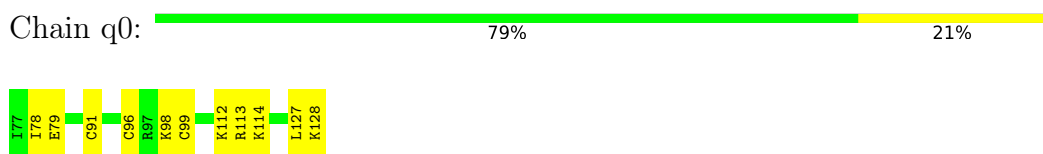
- Molecule 40: 60S ribosomal protein L39



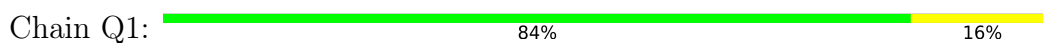
- Molecule 41: Ubiquitin-60S ribosomal protein L40



- Molecule 41: Ubiquitin-60S ribosomal protein L40

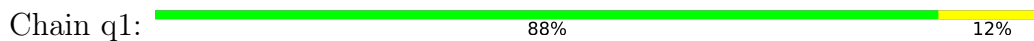


- Molecule 42: 60S ribosomal protein L41-A

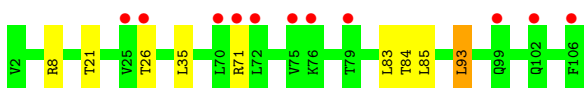
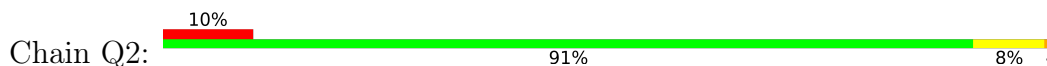




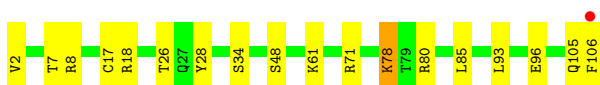
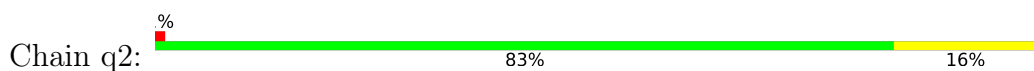
• Molecule 42: 60S ribosomal protein L41-A



• Molecule 43: 60S ribosomal protein L42-A



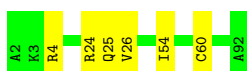
• Molecule 43: 60S ribosomal protein L42-A



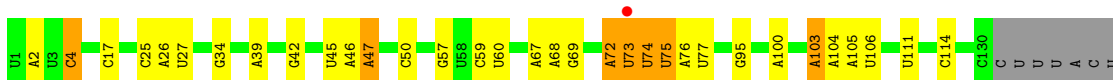
• Molecule 44: 60S ribosomal protein L43-A

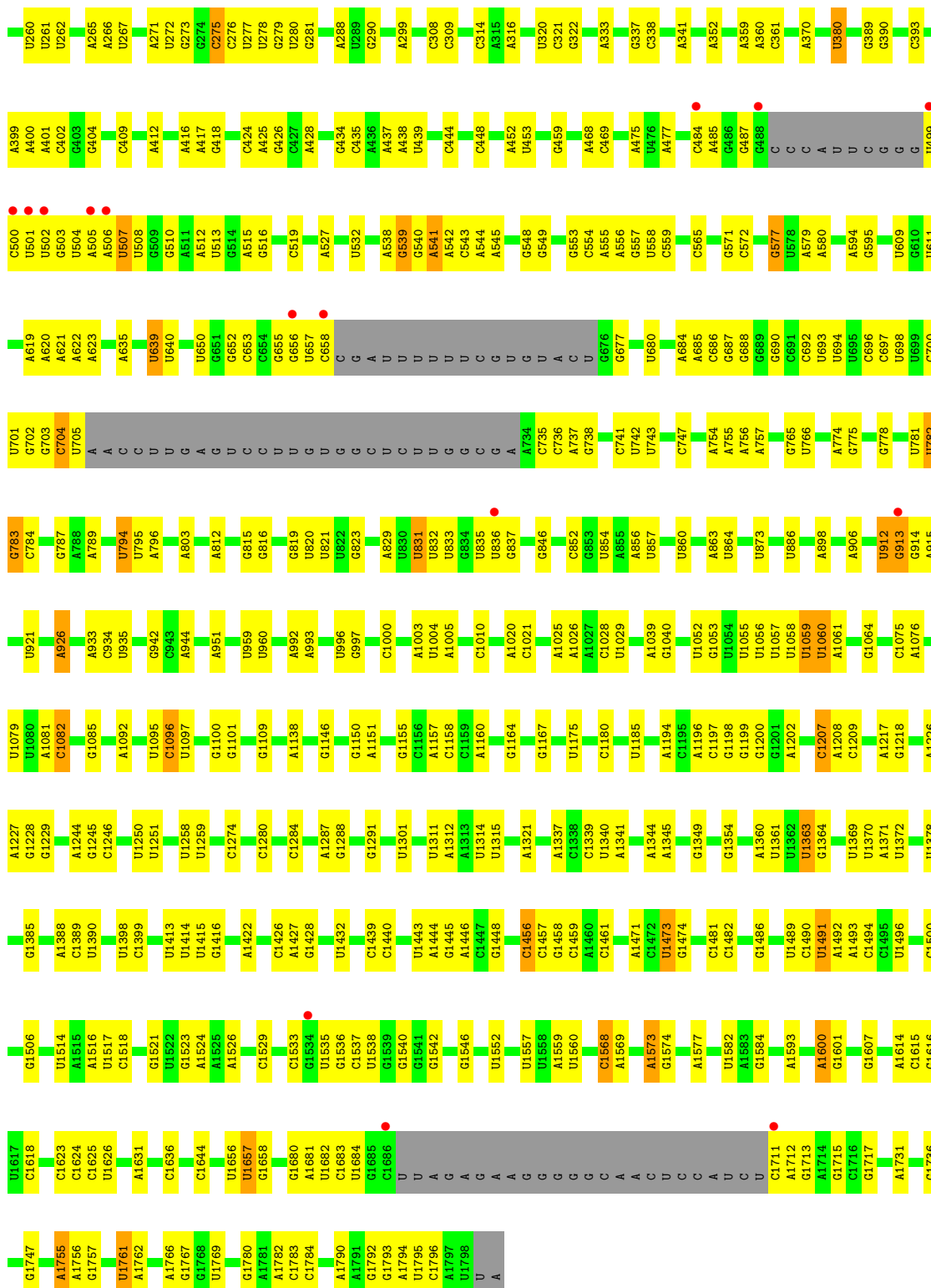


• Molecule 44: 60S ribosomal protein L43-A



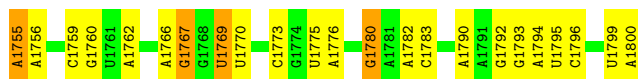
• Molecule 45: 18S ribosomal RNA



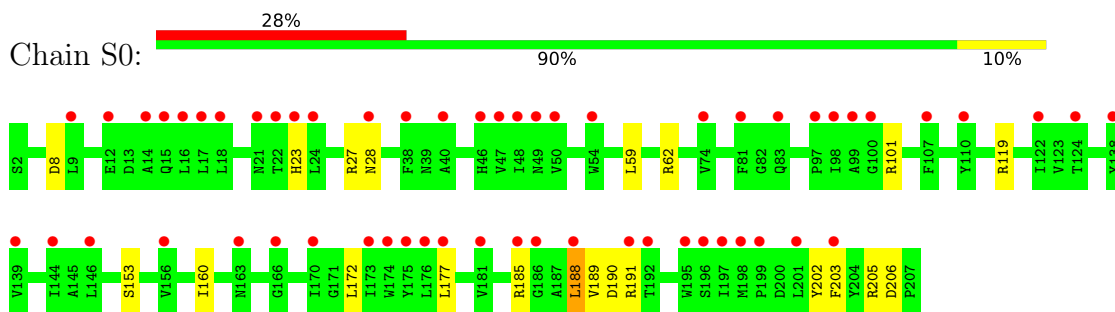


• Molecule 45: 18S ribosomal RNA

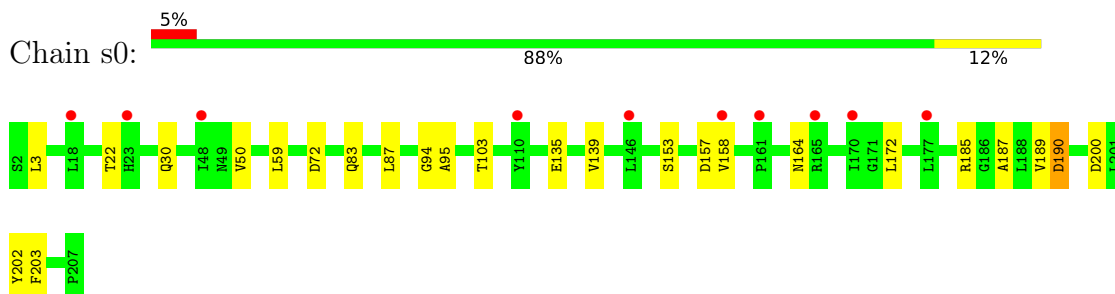




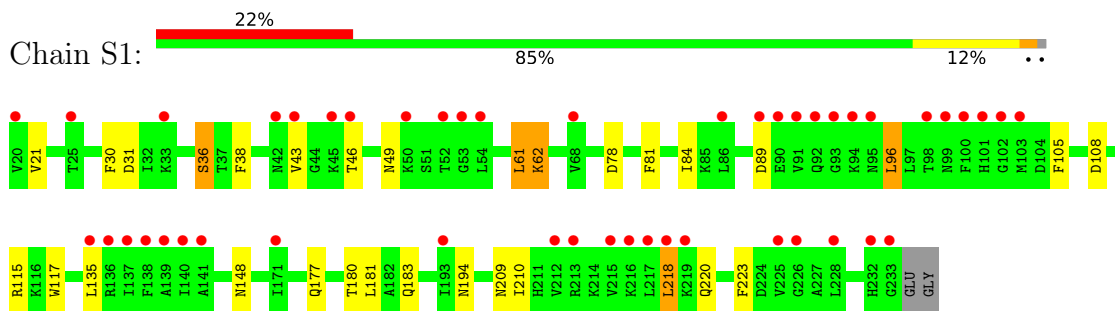
- Molecule 46: 40S ribosomal protein S0-A



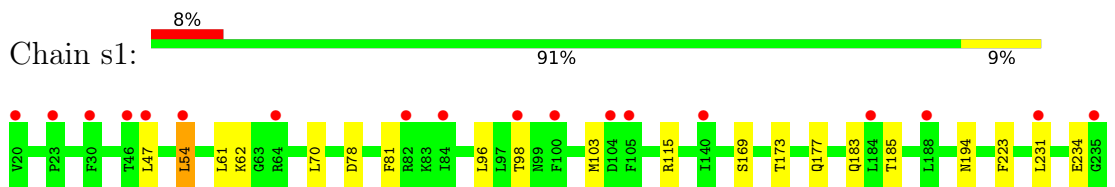
- Molecule 46: 40S ribosomal protein S0-A



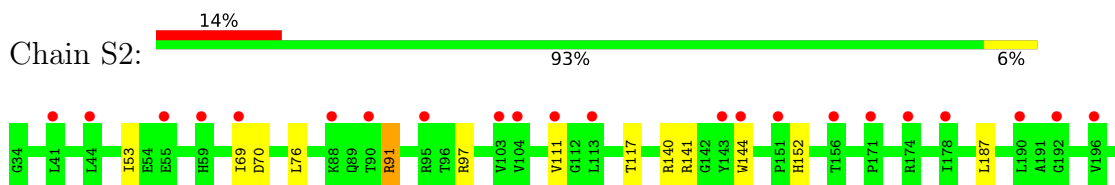
- Molecule 47: 40S ribosomal protein S1-A

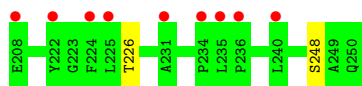


- Molecule 47: 40S ribosomal protein S1-A

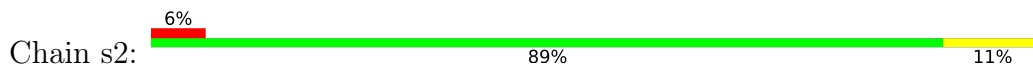


- Molecule 48: 40S ribosomal protein S2

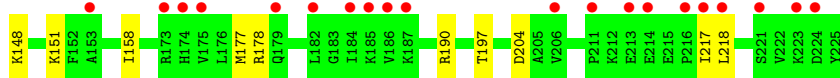
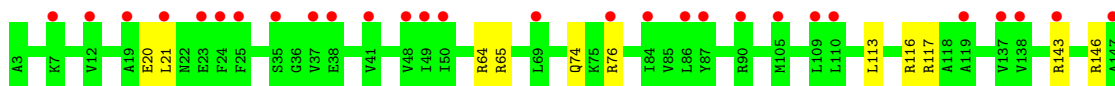
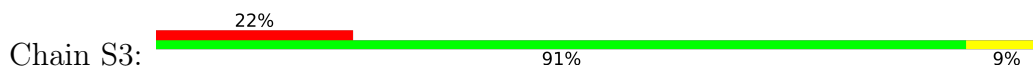




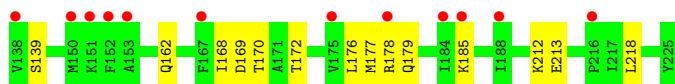
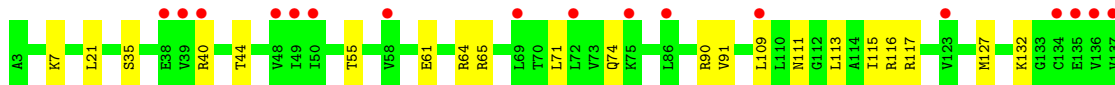
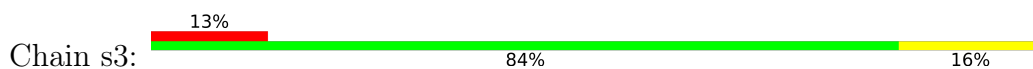
- Molecule 48: 40S ribosomal protein S2



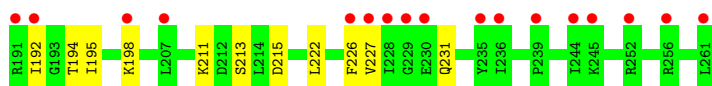
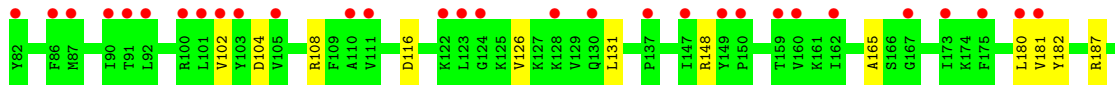
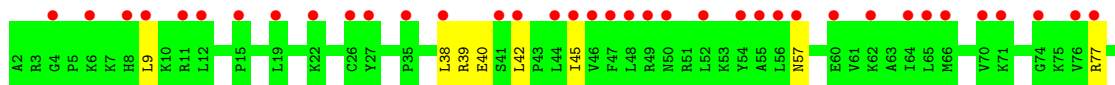
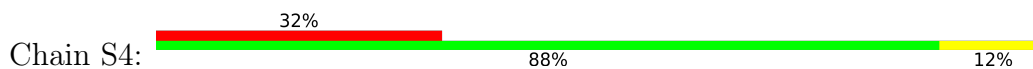
- Molecule 49: 40S ribosomal protein S3



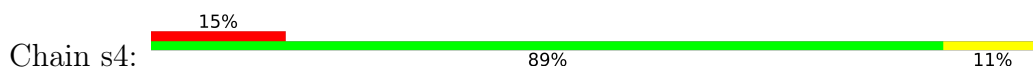
- Molecule 49: 40S ribosomal protein S3

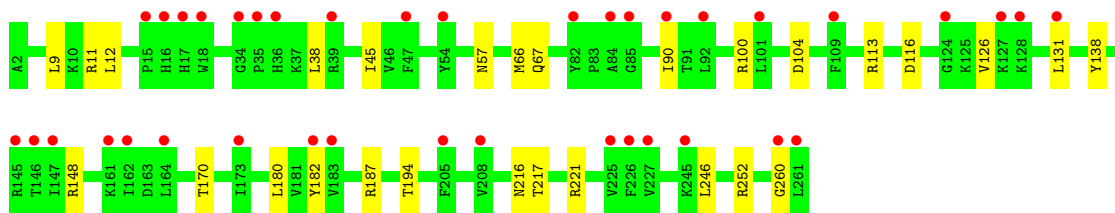


- Molecule 50: 40S ribosomal protein S4-A

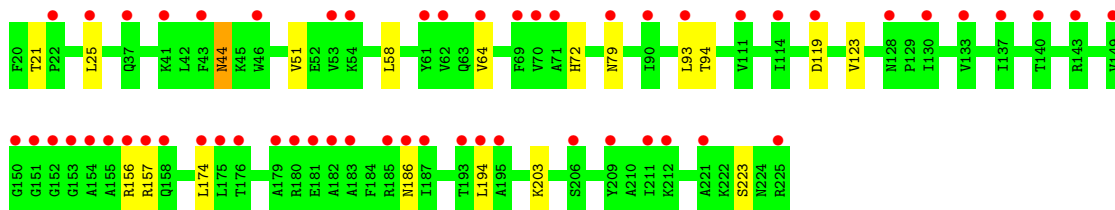


- Molecule 50: 40S ribosomal protein S4-A

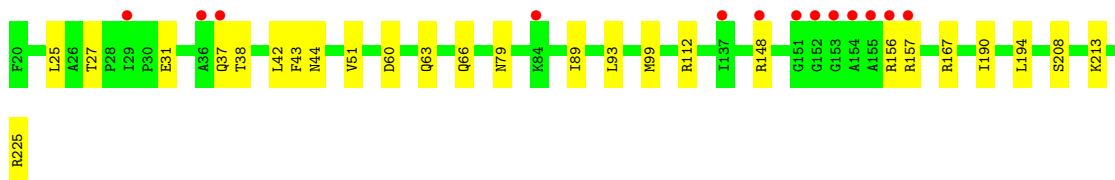
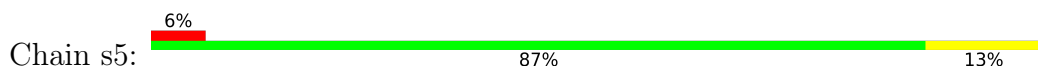




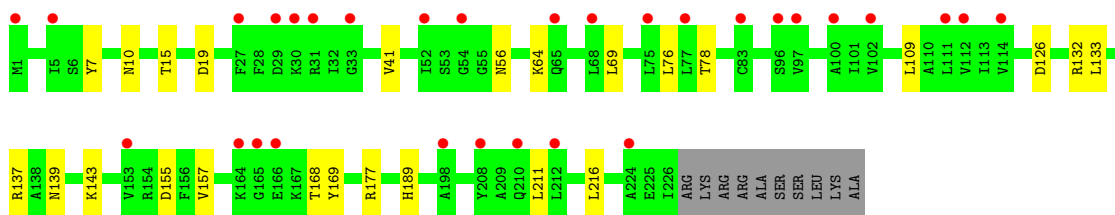
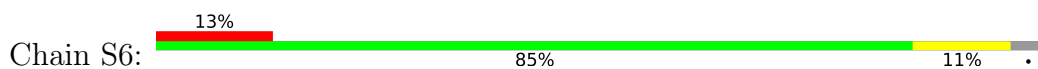
• Molecule 51: 40S ribosomal protein S5



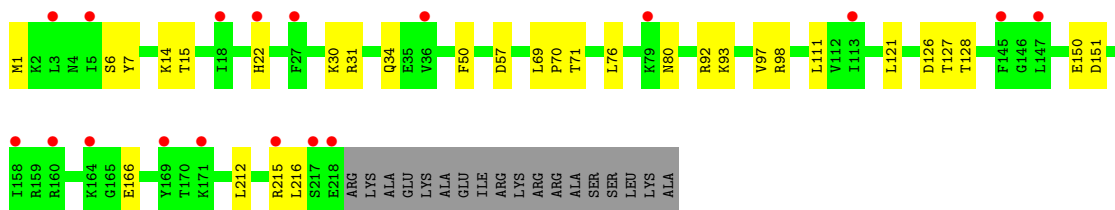
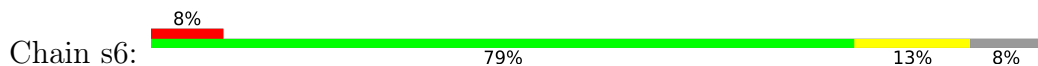
• Molecule 51: 40S ribosomal protein S5




• Molecule 52: 40S ribosomal protein S6-A

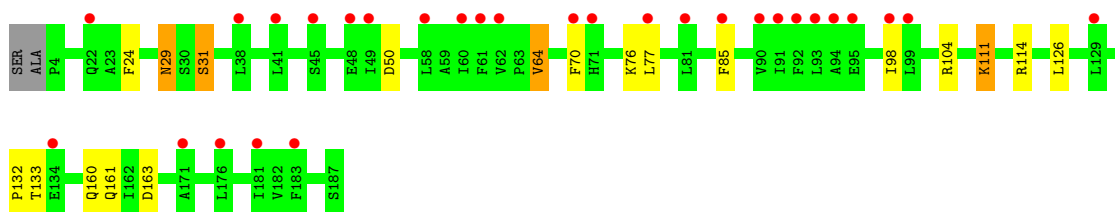


• Molecule 52: 40S ribosomal protein S6-A




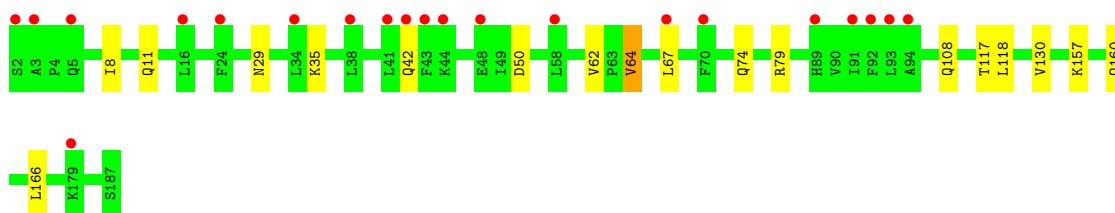
- Molecule 53: 40S ribosomal protein S7-A

Chain S7: 




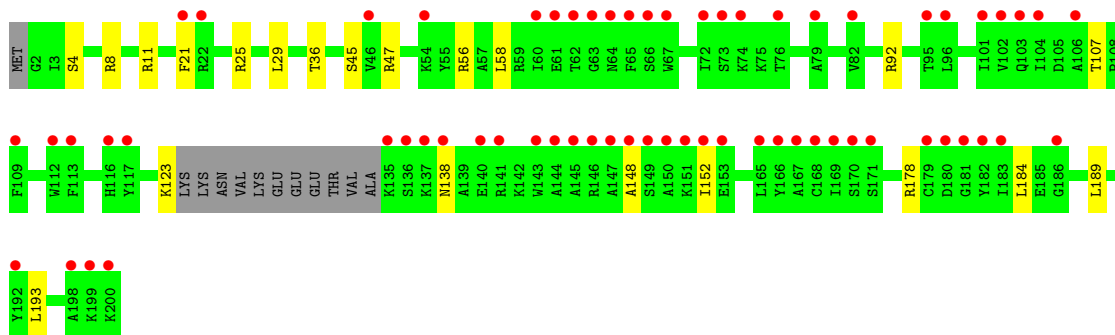
- Molecule 53: 40S ribosomal protein S7-A

Chain s7: 




- Molecule 54: 40S ribosomal protein S8-A

Chain S8: 




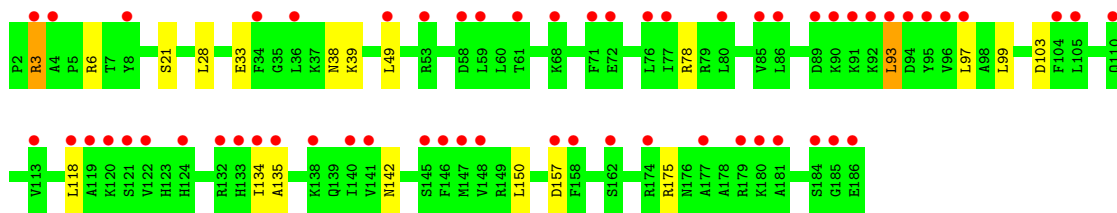
- Molecule 54: 40S ribosomal protein S8-A

Chain s8: 

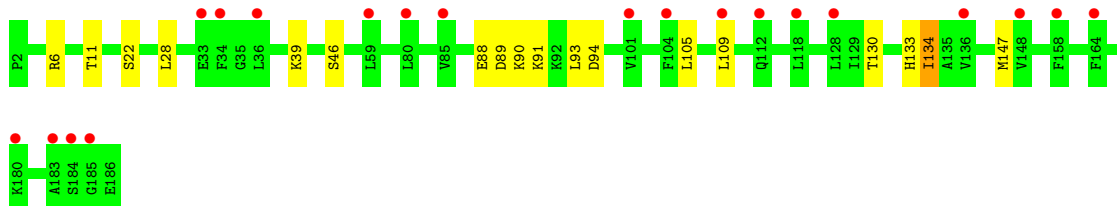
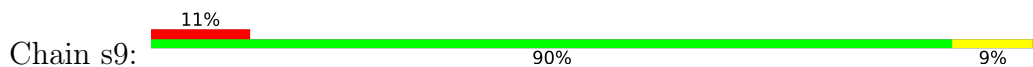


- Molecule 55: 40S ribosomal protein S9-A

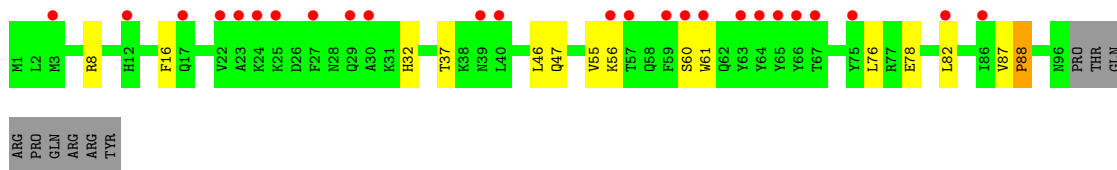
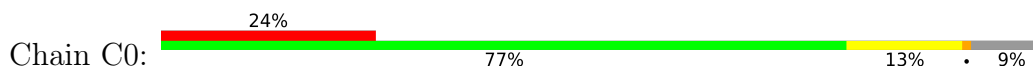
Chain S9: 



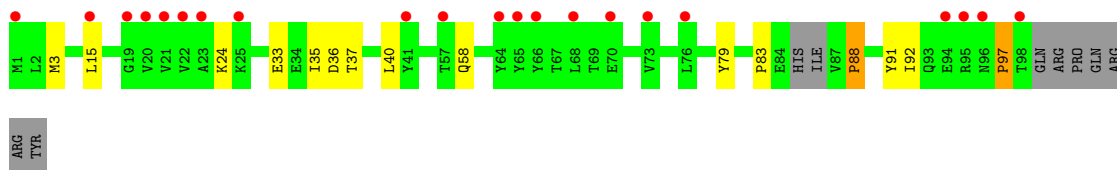
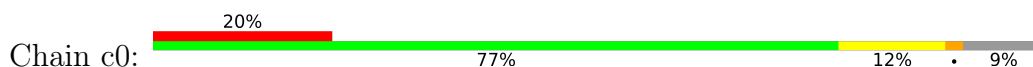
• Molecule 55: 40S ribosomal protein S9-A



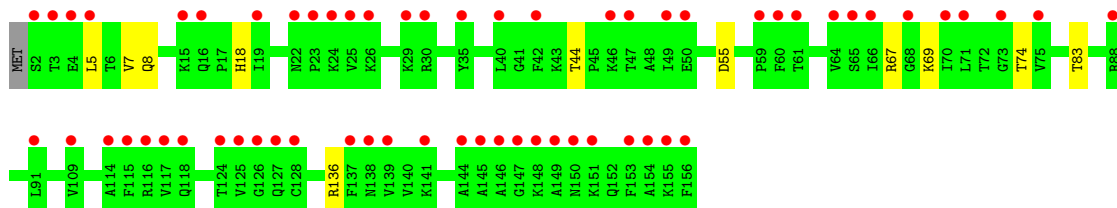
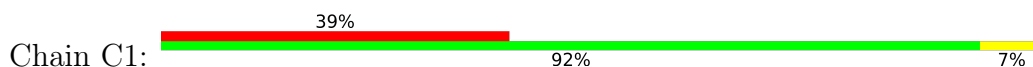
• Molecule 56: 40S ribosomal protein S10-A



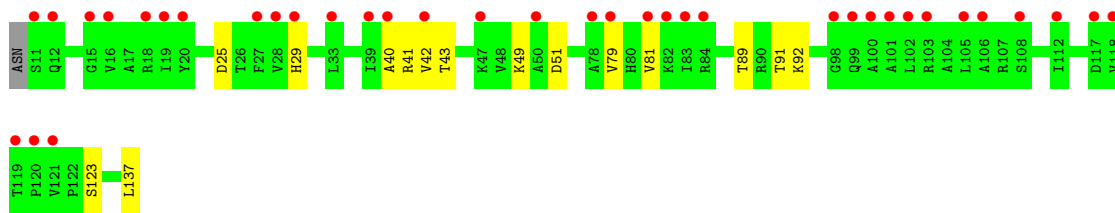
• Molecule 56: 40S ribosomal protein S10-A



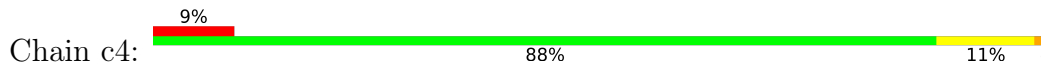
• Molecule 57: 40S ribosomal protein S11-A



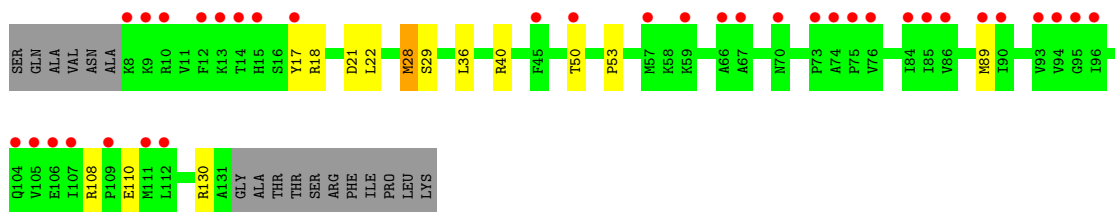
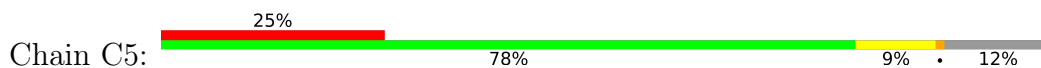
• Molecule 57: 40S ribosomal protein S11-A



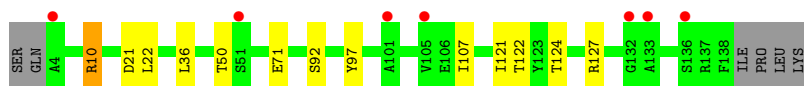
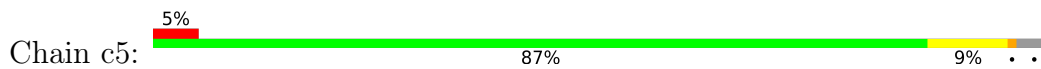
● Molecule 60: 40S ribosomal protein S14-B



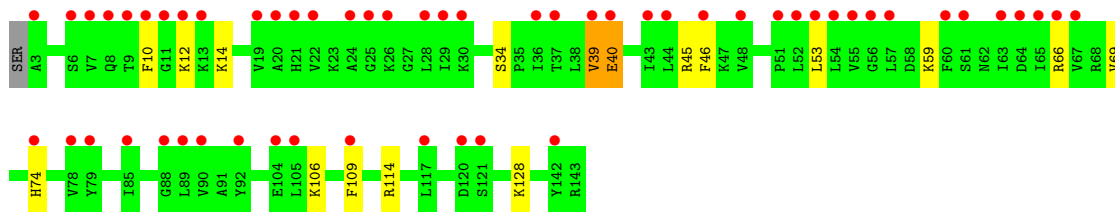
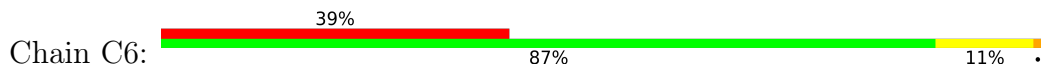
● Molecule 61: 40S ribosomal protein S15



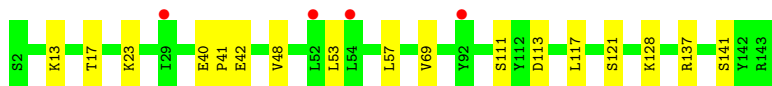
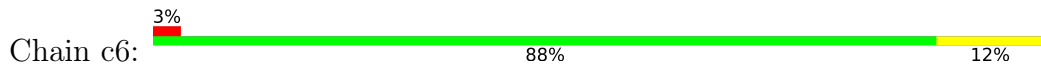
● Molecule 61: 40S ribosomal protein S15



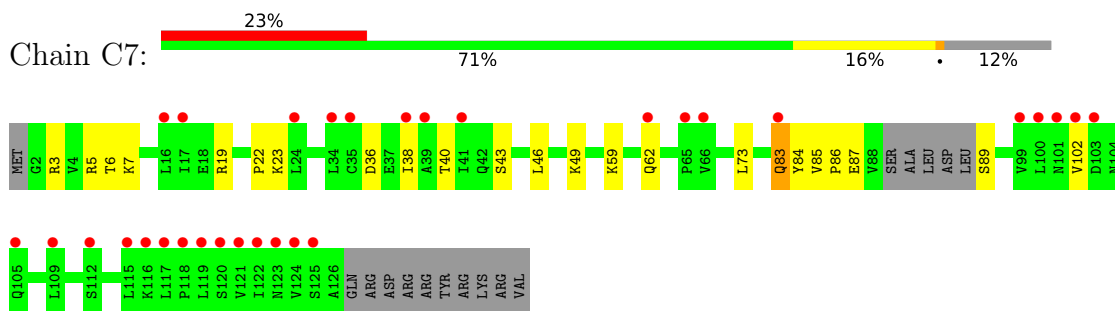
● Molecule 62: 40S ribosomal protein S16-A



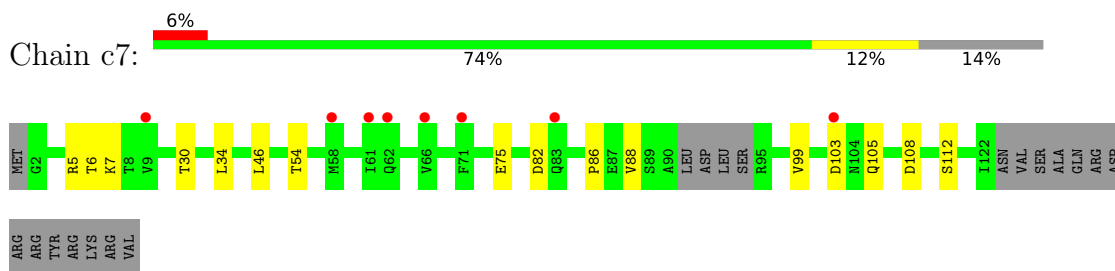
● Molecule 62: 40S ribosomal protein S16-A



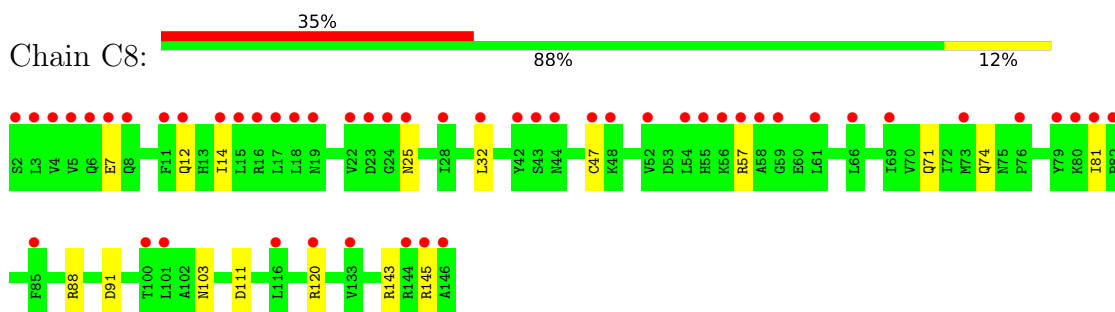
- Molecule 63: 40S ribosomal protein S17-A



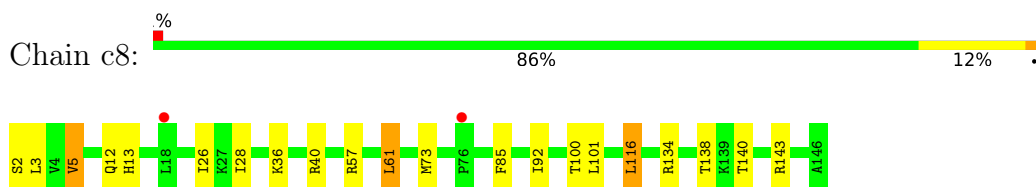
- Molecule 63: 40S ribosomal protein S17-A



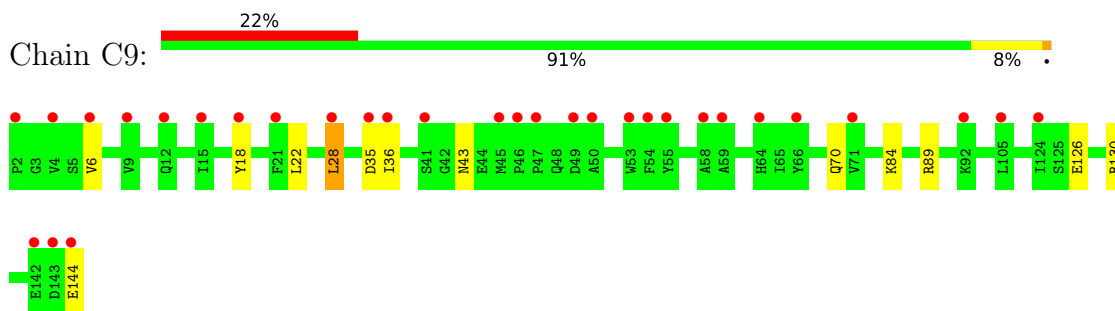
- Molecule 64: 40S ribosomal protein S18-A



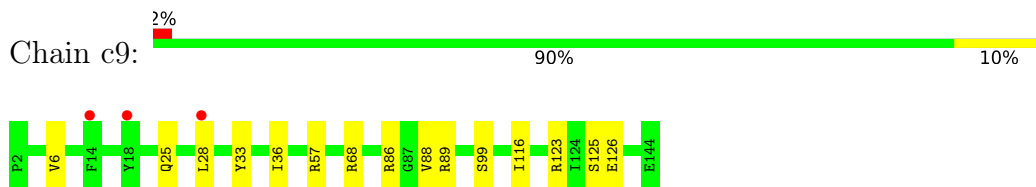
- Molecule 64: 40S ribosomal protein S18-A



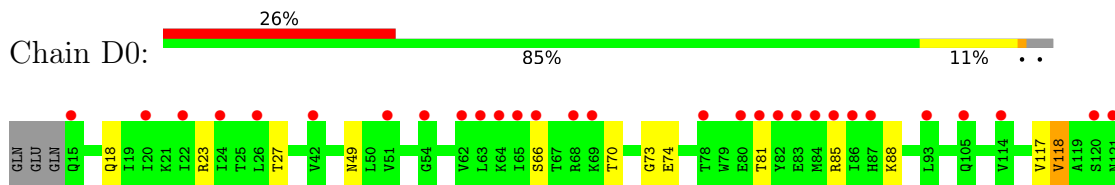
- Molecule 65: 40S ribosomal protein S19-A



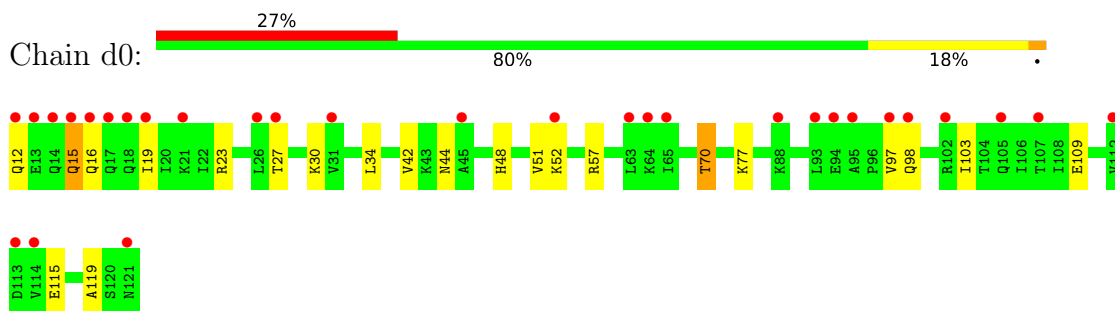
- Molecule 65: 40S ribosomal protein S19-A



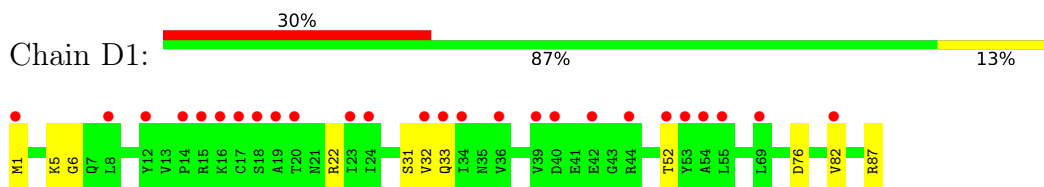
- Molecule 66: 40S ribosomal protein S20



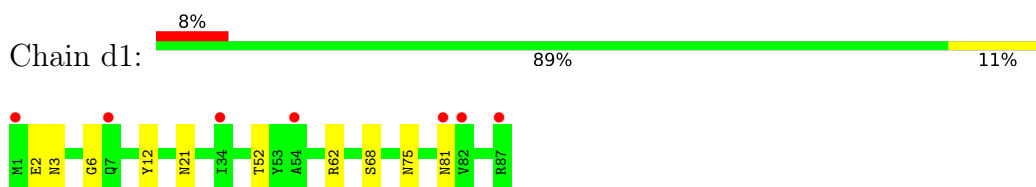
- Molecule 66: 40S ribosomal protein S20



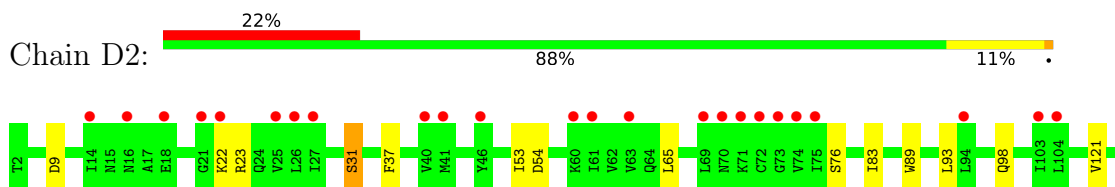
- Molecule 67: 40S ribosomal protein S21-A



- Molecule 67: 40S ribosomal protein S21-A

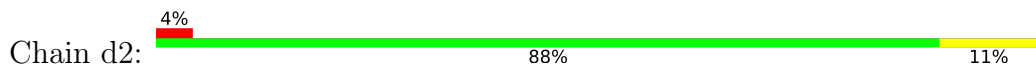


- Molecule 68: 40S ribosomal protein S22-A

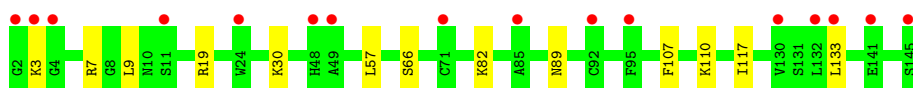




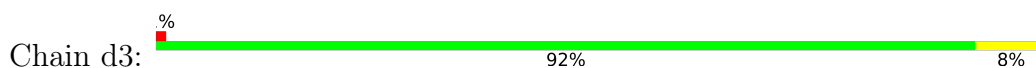
- Molecule 68: 40S ribosomal protein S22-A



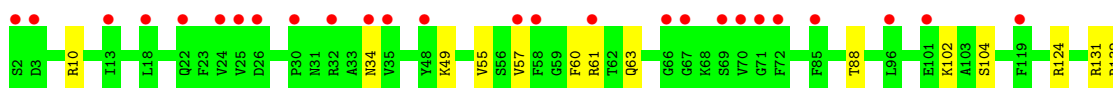
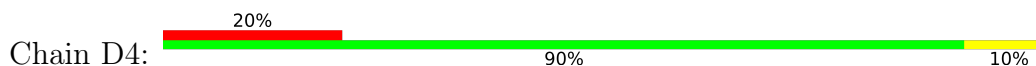
- Molecule 69: 40S ribosomal protein S23-A



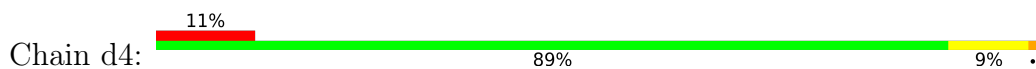
- Molecule 69: 40S ribosomal protein S23-A



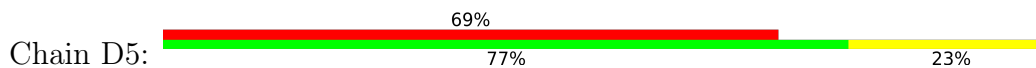
- Molecule 70: 40S ribosomal protein S24-A

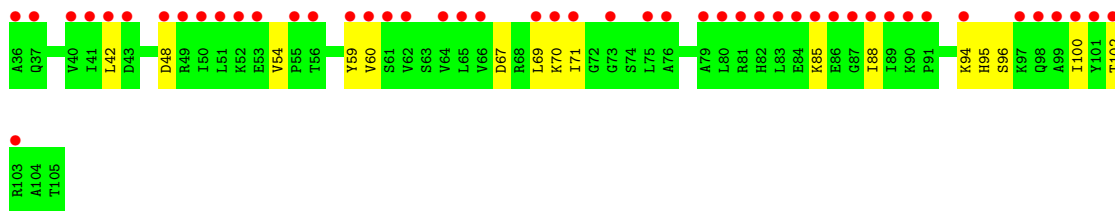


- Molecule 70: 40S ribosomal protein S24-A

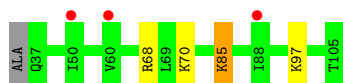


- Molecule 71: 40S ribosomal protein S25-A

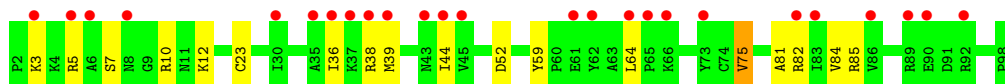
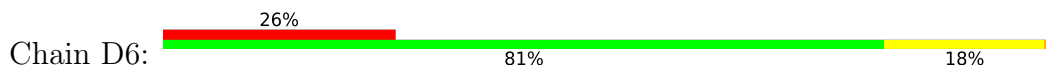




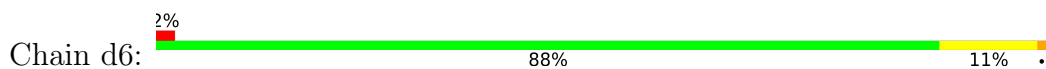
- Molecule 71: 40S ribosomal protein S25-A



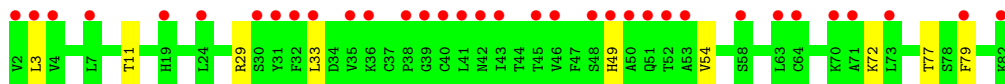
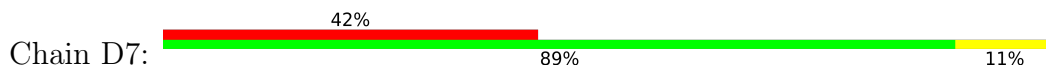
- Molecule 72: 40S ribosomal protein S26-B



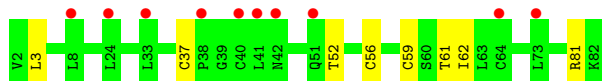
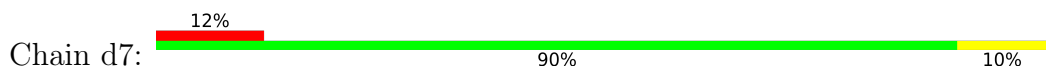
- Molecule 72: 40S ribosomal protein S26-B



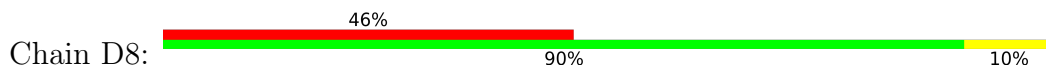
- Molecule 73: 40S ribosomal protein S27-A

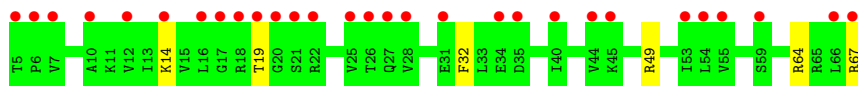


- Molecule 73: 40S ribosomal protein S27-A

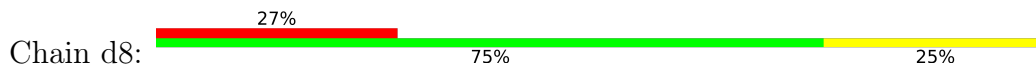


- Molecule 74: 40S ribosomal protein S28-A

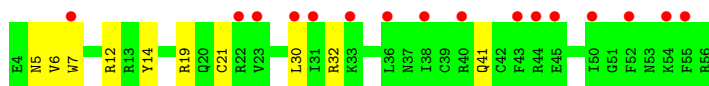
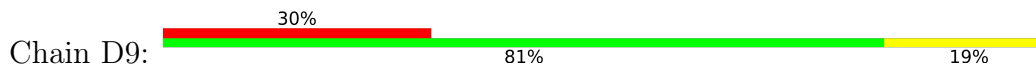




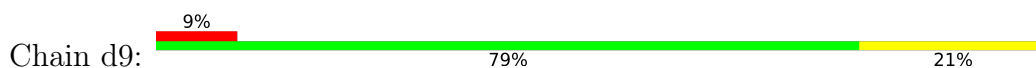
- Molecule 74: 40S ribosomal protein S28-A



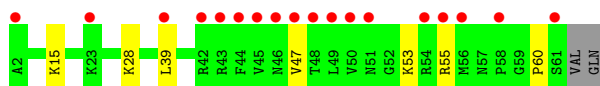
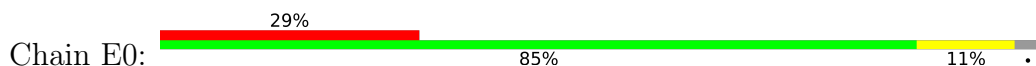
- Molecule 75: 40S ribosomal protein S29-A



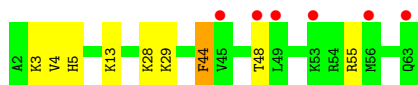
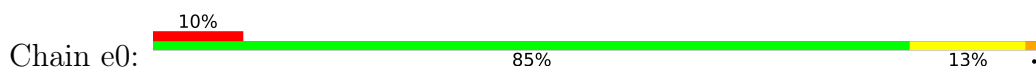
- Molecule 75: 40S ribosomal protein S29-A



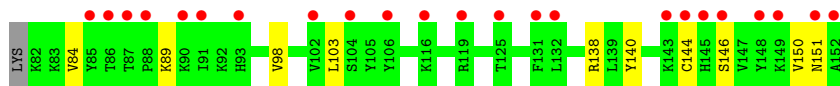
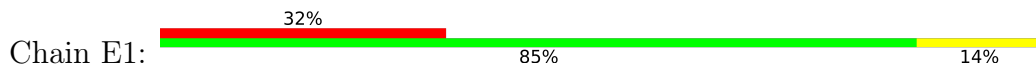
- Molecule 76: 40S ribosomal protein S30-A



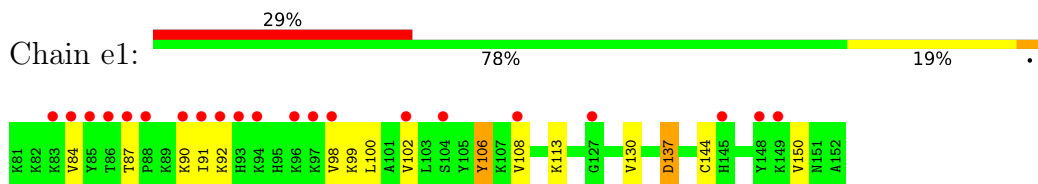
- Molecule 76: 40S ribosomal protein S30-A



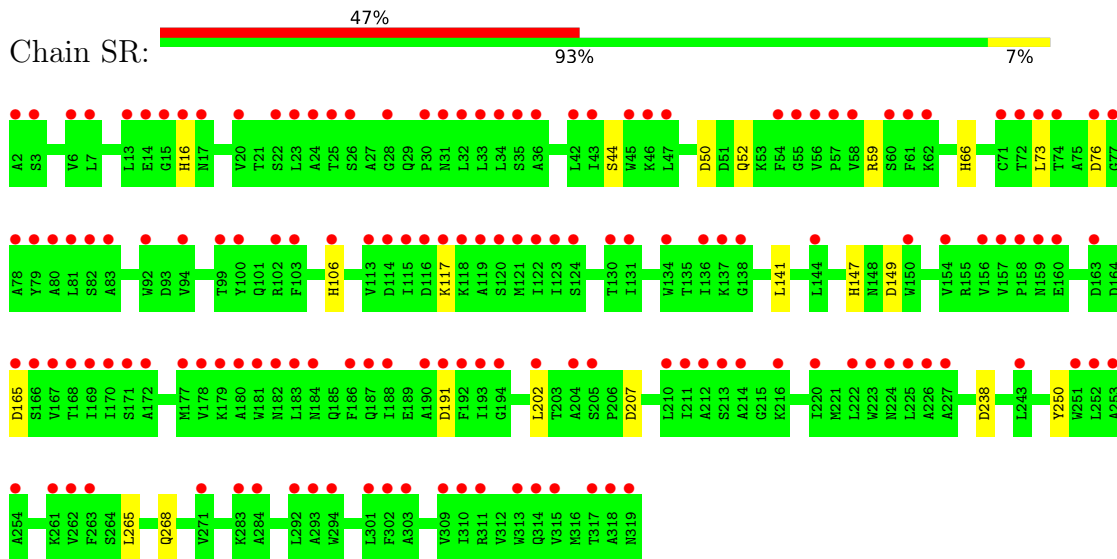
- Molecule 77: Ubiquitin-40S ribosomal protein S31



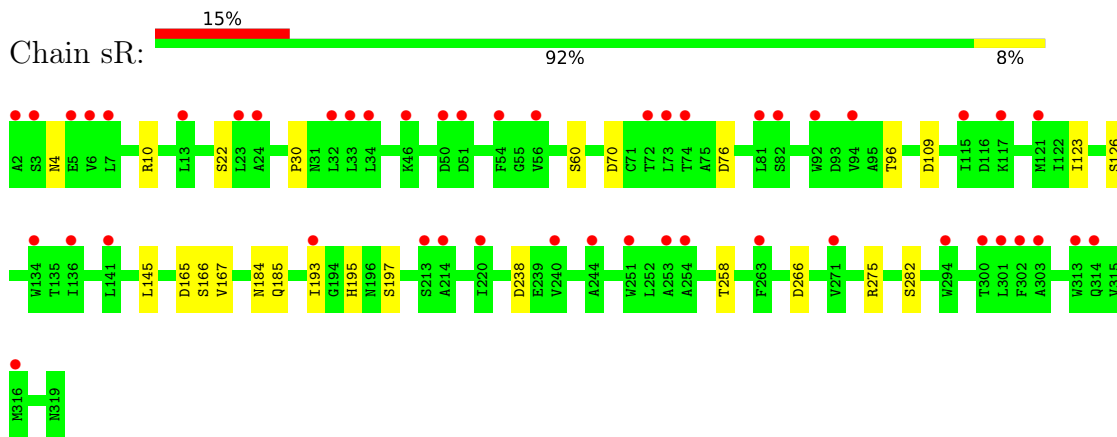
- Molecule 77: Ubiquitin-40S ribosomal protein S31



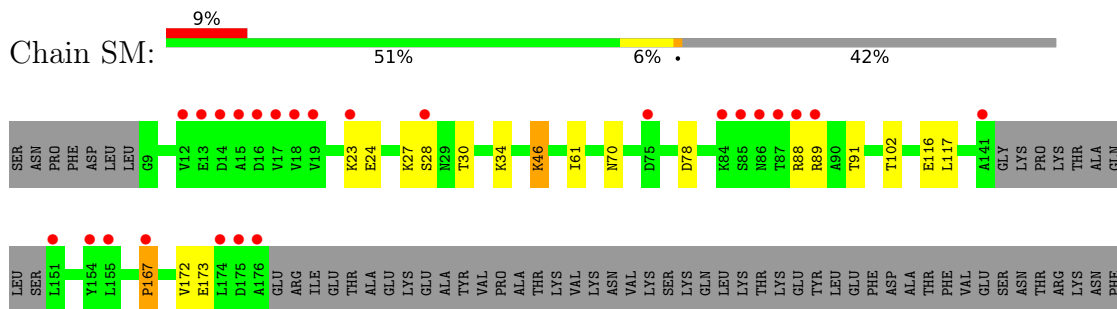
• Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 79: Suppressor protein STM1



Chain p1:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.63Å 287.00Å 304.73Å 90.00° 99.08° 90.00°	Depositor
Resolution (Å)	143.72 – 3.40 143.72 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (143.72-3.40) 92.9 (143.72-3.40)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 3.41Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.238 0.189 , 0.238	Depositor DCC
R_{free} test set	20266 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.8	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	404238	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

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

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: MG, ZN, LLL

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	1	0.73	10/74216 (0.0%)	1.29	499/115705 (0.4%)
1	5	0.83	19/75037 (0.0%)	1.37	668/116983 (0.6%)
2	3	0.62	0/2883	1.14	5/4491 (0.1%)
2	7	0.81	0/2883	1.33	18/4491 (0.4%)
3	4	0.66	0/3701	1.20	14/5760 (0.2%)
3	8	0.63	0/3746	1.18	14/5832 (0.2%)
4	L2	0.42	0/1948	0.66	0/2617
4	l2	0.44	0/1946	0.71	0/2614
5	L3	0.49	0/3152	0.67	1/4239 (0.0%)
5	l3	0.56	0/3152	0.71	1/4239 (0.0%)
6	L4	0.49	1/2801 (0.0%)	0.72	3/3792 (0.1%)
6	l4	0.47	0/2801	0.68	1/3792 (0.0%)
7	L5	0.41	0/2425	0.60	0/3271
7	l5	0.53	0/2408	0.67	1/3248 (0.0%)
8	L6	0.49	0/1260	0.63	0/1694
8	l6	0.53	0/1269	0.67	0/1705
9	L7	0.45	0/1821	0.64	0/2451
9	l7	0.54	0/1828	0.69	1/2461 (0.0%)
10	L8	0.38	0/1849	0.55	0/2495
10	l8	0.43	1/1795 (0.1%)	0.61	0/2429
11	L9	0.46	0/1539	0.64	0/2073
11	l9	0.60	0/1539	0.68	0/2073
12	M0	0.52	0/1743	0.64	0/2339
12	m0	0.63	0/1752	0.76	2/2349 (0.1%)
13	M1	0.40	0/1374	0.63	2/1842 (0.1%)
13	m1	0.54	0/1374	0.69	1/1842 (0.1%)
14	M3	0.47	0/1568	0.67	0/2106
14	m3	0.45	0/1573	0.66	0/2113
15	M4	0.48	0/1068	0.60	0/1438
15	m4	0.55	0/1074	0.67	0/1446
16	M5	0.43	0/1757	0.63	0/2354
16	m5	0.44	0/1757	0.63	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	M6	0.58	1/1585 (0.1%)	0.69	0/2128
17	m6	0.67	0/1585	0.74	3/2128 (0.1%)
18	M7	0.49	0/1438	0.65	0/1937
18	m7	0.51	0/1250	0.69	0/1683
19	M8	0.45	0/1465	0.67	0/1965
19	m8	0.49	0/1465	0.68	0/1965
20	M9	0.36	0/1491	0.57	0/1987
20	m9	0.39	0/1538	0.54	0/2050
21	N0	0.44	0/1481	0.61	0/1990
21	n0	0.58	0/1481	0.68	2/1990 (0.1%)
22	N1	0.48	0/1300	0.64	0/1743
22	n1	0.59	0/1300	0.66	0/1743
23	N2	0.34	0/812	0.53	0/1099
23	n2	0.39	0/794	0.56	0/1076
24	N3	0.51	0/1018	0.65	0/1369
24	n3	0.59	0/1018	0.74	0/1369
25	N4	0.40	0/712	0.58	0/958
26	N5	0.39	0/979	0.60	1/1321 (0.1%)
26	n5	0.41	0/974	0.64	0/1314
27	N6	0.45	0/1004	0.69	0/1341
27	n6	0.41	0/1004	0.65	0/1341
28	N7	0.37	0/1118	0.58	0/1497
28	n7	0.38	0/1118	0.55	0/1497
29	N8	0.47	0/1204	0.68	0/1612
29	n8	0.50	0/1204	0.70	0/1612
30	N9	0.50	0/473	0.68	0/629
30	n9	0.54	0/473	0.74	0/629
31	O0	0.34	0/751	0.56	1/1008 (0.1%)
31	o0	0.36	0/775	0.56	0/1040
32	O1	0.43	0/904	0.60	0/1213
32	o1	0.51	0/904	0.65	0/1213
33	O2	0.53	0/1041	0.67	0/1394
33	o2	0.49	0/1041	0.66	0/1394
34	O3	0.55	0/868	0.66	0/1168
34	o3	0.64	0/868	0.69	0/1168
35	O4	0.39	0/891	0.57	1/1191 (0.1%)
35	o4	0.39	0/891	0.61	0/1191
36	O5	0.43	0/978	0.62	0/1301
36	o5	0.39	0/978	0.58	1/1301 (0.1%)
37	O6	0.41	0/778	0.66	0/1034
37	o6	0.41	0/778	0.57	0/1034
38	O7	0.46	0/696	0.72	0/923
38	o7	0.50	0/696	0.71	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	O8	0.35	0/618	0.55	0/826
39	o8	0.36	0/618	0.60	0/826
40	O9	0.49	0/443	0.66	0/588
40	o9	0.48	0/443	0.67	0/588
41	Q0	0.55	0/423	0.74	0/562
41	q0	0.77	2/423 (0.5%)	0.80	0/562
42	Q1	0.42	0/234	0.57	0/300
42	q1	0.56	0/234	0.77	0/300
43	Q2	0.50	0/860	0.72	1/1136 (0.1%)
43	q2	0.59	0/860	0.74	0/1136
44	Q3	0.40	0/701	0.61	0/934
44	q3	0.47	0/701	0.65	0/934
45	2	0.50	0/40811	1.07	126/63585 (0.2%)
45	6	0.66	4/41451 (0.0%)	1.23	234/64581 (0.4%)
46	S0	0.35	1/1653 (0.1%)	0.56	0/2261
46	s0	0.37	0/1653	0.61	0/2261
47	S1	0.33	0/1735	0.63	3/2335 (0.1%)
47	s1	0.37	0/1748	0.63	2/2352 (0.1%)
48	S2	0.37	0/1665	0.59	0/2263
48	s2	0.41	0/1665	0.67	1/2263 (0.0%)
49	S3	0.34	0/1759	0.53	0/2368
49	s3	0.40	0/1753	0.59	0/2361
50	S4	0.36	0/2109	0.63	1/2839 (0.0%)
50	s4	0.39	0/2109	0.66	1/2839 (0.0%)
51	S5	0.59	1/1629 (0.1%)	0.52	0/2202
51	s5	0.42	0/1629	0.67	0/2202
52	S6	0.37	0/1837	0.55	0/2455
52	s6	0.40	0/1779	0.59	1/2379 (0.0%)
53	S7	0.34	0/1506	0.59	0/2028
53	s7	0.36	0/1516	0.61	1/2043 (0.0%)
54	S8	0.36	0/1514	0.58	1/2021 (0.0%)
54	s8	0.40	0/1496	0.61	0/1999
55	S9	0.34	0/1519	0.59	2/2035 (0.1%)
55	s9	0.38	0/1519	0.62	0/2035
56	C0	0.34	0/789	0.62	1/1067 (0.1%)
56	c0	0.36	0/776	0.76	4/1047 (0.4%)
57	C1	0.38	0/1239	0.54	0/1673
57	c1	0.43	0/1164	0.60	0/1569
58	C2	0.31	0/898	0.66	1/1220 (0.1%)
58	c2	0.33	0/898	0.65	2/1220 (0.2%)
59	C3	0.33	0/1215	0.52	0/1638
59	c3	0.41	0/1215	0.62	1/1638 (0.1%)
60	C4	0.30	0/901	0.60	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	c4	0.39	0/960	0.70	0/1290
61	C5	0.37	0/998	0.59	0/1341
61	c5	0.45	0/1060	0.69	1/1426 (0.1%)
62	C6	0.32	0/1125	0.57	1/1510 (0.1%)
62	c6	0.46	0/1131	0.63	0/1518
63	C7	0.35	0/975	0.61	1/1307 (0.1%)
63	c7	0.38	0/925	0.63	0/1239
64	C8	0.32	0/1211	0.54	0/1628
64	c8	0.48	0/1211	0.67	1/1628 (0.1%)
65	C9	0.33	0/1130	0.54	1/1517 (0.1%)
65	c9	0.46	0/1130	0.60	0/1517
66	D0	0.36	0/865	0.56	0/1169
66	d0	0.43	0/892	0.65	0/1205
67	D1	0.31	0/693	0.60	0/935
67	d1	0.37	0/693	0.60	0/935
68	D2	0.35	0/1038	0.61	0/1395
68	d2	0.40	0/1038	0.64	1/1395 (0.1%)
69	D3	0.43	0/1139	0.63	1/1518 (0.1%)
69	d3	0.52	1/1139 (0.1%)	0.68	0/1518
70	D4	0.38	0/1087	0.57	0/1449
70	d4	0.39	0/1079	0.60	0/1438
71	D5	0.29	0/571	0.58	0/768
71	d5	0.43	0/566	0.55	0/761
72	D6	0.48	1/782 (0.1%)	0.66	1/1047 (0.1%)
72	d6	0.52	0/782	0.72	0/1047
73	D7	0.32	0/620	0.59	0/838
73	d7	0.37	0/620	0.69	1/838 (0.1%)
74	D8	0.30	0/499	0.52	0/670
74	d8	0.40	0/499	0.60	0/670
75	D9	0.46	0/453	0.69	0/602
75	d9	0.44	0/453	0.68	0/602
76	E0	0.36	0/483	0.57	0/643
76	e0	0.40	0/499	0.67	0/665
77	E1	0.34	0/577	0.66	0/770
77	e1	0.39	0/586	0.78	0/781
78	SR	0.30	0/2494	0.55	0/3394
78	sR	0.34	0/2494	0.59	0/3394
79	SM	0.34	0/1113	0.64	1/1502 (0.1%)
79	sM	0.41	0/929	0.68	3/1246 (0.2%)
81	n4	0.42	0/1058	0.62	0/1405
82	p0	0.36	0/1092	0.56	0/1474
All	All	0.61	42/426558 (0.0%)	1.06	1636/625790 (0.3%)

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
4	L2	0	1
4	l2	0	2
5	l3	0	1
6	L4	0	1
6	l4	0	2
7	L5	0	1
7	l5	0	2
9	L7	0	1
9	l7	0	2
11	L9	0	1
12	M0	0	1
12	m0	0	1
13	M1	0	1
13	m1	0	1
14	M3	0	1
15	M4	0	1
16	m5	0	1
18	M7	0	1
19	M8	0	1
21	N0	0	2
23	n2	0	1
24	n3	0	1
25	N4	0	2
27	N6	0	1
28	N7	0	1
28	n7	0	2
29	N8	0	3
29	n8	0	1
30	N9	0	1
32	o1	0	1
33	o2	0	2
34	o3	0	1
35	o4	0	1
37	o6	0	1
40	O9	0	1
46	s0	0	3
47	S1	0	1
48	S2	0	2
49	s3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
50	S4	0	3
51	S5	0	1
51	s5	0	2
52	S6	0	1
52	s6	0	1
53	S7	0	5
53	s7	0	3
54	s8	0	2
55	s9	0	2
58	c2	0	1
59	c3	0	1
60	C4	0	2
60	c4	0	4
61	C5	0	2
61	c5	0	2
62	C6	0	1
63	C7	0	2
63	c7	0	2
64	C8	0	1
66	D0	0	2
66	d0	0	5
67	D1	0	1
68	D2	0	1
68	d2	0	1
69	d3	0	1
70	D4	0	1
70	d4	0	2
71	D5	0	3
71	d5	0	1
72	D6	0	2
72	d6	0	1
73	D7	0	1
76	e0	0	1
77	E1	0	3
77	e1	0	2
78	sR	0	4
79	SM	0	2
79	sM	0	2
80	m2	0	3
82	p0	0	1
All	All	0	130

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S5	21	THR	C-N	20.19	1.72	1.34
1	5	2971	A	N9-C4	12.79	1.45	1.37
1	5	1152	G	N9-C4	-9.61	1.30	1.38
6	L4	19	ALA	C-N	8.69	1.54	1.34
72	D6	59	TYR	C-N	8.53	1.50	1.34
1	5	1201	C	N1-C2	8.48	1.48	1.40
1	1	1201	C	N1-C2	8.02	1.48	1.40
10	l8	51	LYS	C-N	-7.65	1.16	1.34
1	5	1201	C	N1-C6	7.21	1.41	1.37
1	5	2971	A	N3-C4	6.70	1.38	1.34
46	S0	160	ILE	C-N	-6.53	1.21	1.34
1	5	2726	C	N3-C4	-6.16	1.29	1.33
1	1	1201	C	N1-C6	6.11	1.40	1.37
1	1	2093	A	N9-C4	6.02	1.41	1.37
41	q0	99	CYS	CB-SG	-5.98	1.72	1.81
69	d3	4	GLY	C-N	5.95	1.47	1.34
1	5	2971	A	C5-C4	5.78	1.42	1.38
1	5	2922	G	C5-C6	-5.74	1.36	1.42
41	q0	96	CYS	CB-SG	-5.73	1.72	1.81
1	5	2401	A	C5-C4	5.67	1.42	1.38
1	1	2983	C	N3-C4	-5.64	1.30	1.33
1	5	2100	A	N9-C4	5.43	1.41	1.37
1	5	1103	A	N3-C4	5.42	1.38	1.34
1	1	3129	A	N9-C4	-5.41	1.34	1.37
1	5	1152	G	N3-C4	-5.39	1.31	1.35
45	6	1755	A	N9-C4	5.35	1.41	1.37
1	5	1309	U	N1-C2	-5.34	1.33	1.38
45	6	1081	A	N9-C4	5.32	1.41	1.37
45	6	163	G	N9-C4	-5.31	1.33	1.38
1	1	1153	A	N3-C4	-5.28	1.31	1.34
1	1	2207	A	N9-C4	5.25	1.41	1.37
1	5	1103	A	N9-C4	5.25	1.41	1.37
45	6	1492	A	N9-C4	5.21	1.41	1.37
1	1	820	A	N9-C4	-5.18	1.34	1.37
1	5	3049	A	N9-C4	-5.17	1.34	1.37
1	1	2762	A	N3-C4	-5.14	1.31	1.34
1	5	2892	A	N9-C4	-5.09	1.34	1.37
1	1	2971	A	N9-C4	5.07	1.40	1.37
17	M6	40	GLU	CG-CD	5.07	1.59	1.51
1	5	1858	A	N9-C4	5.05	1.40	1.37
1	5	2756	C	N1-C6	-5.05	1.34	1.37
1	5	428	A	N9-C4	-5.05	1.34	1.37

All (1636) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1152	G	N3-C4-N9	-18.77	114.74	126.00
1	5	1152	G	N3-C4-C5	17.59	137.39	128.60
1	1	1201	C	C6-N1-C2	-14.35	114.56	120.30
6	L4	182	LEU	CA-CB-CG	12.68	144.47	115.30
1	5	420	G	C5-C6-O6	-12.32	121.21	128.60
1	5	2524	A	O4'-C1'-N9	11.46	117.37	108.20
1	1	1201	C	N1-C2-O2	11.31	125.69	118.90
1	5	1152	G	C2-N3-C4	-11.31	106.25	111.90
1	5	890	C	O5'-P-OP2	-11.27	95.56	105.70
1	5	1201	C	N1-C2-O2	11.16	125.59	118.90
1	5	2283	G	N1-C6-O6	10.90	126.44	119.90
1	1	1201	C	N3-C2-O2	-10.82	114.33	121.90
1	1	1104	G	O5'-P-OP1	-10.33	96.40	105.70
45	2	75	U	C2-N1-C1'	10.30	130.06	117.70
1	5	2393	G	O5'-P-OP2	-10.24	96.48	105.70
1	5	2726	C	C5-C4-N4	10.18	127.33	120.20
1	5	3245	A	C5-N7-C8	-10.11	98.85	103.90
1	1	2818	U	O5'-P-OP2	-9.95	96.75	105.70
1	5	3245	A	C2-N3-C4	-9.88	105.66	110.60
1	5	1152	G	C8-N9-C1'	9.84	139.79	127.00
1	5	3245	A	N1-C6-N6	9.70	124.42	118.60
45	6	453	U	N3-C2-O2	-9.63	115.46	122.20
1	1	2827	U	C5-C6-N1	-9.57	117.92	122.70
1	5	857	G	N1-C6-O6	9.54	125.62	119.90
1	1	2617	U	N1-C2-N3	9.51	120.60	114.90
1	1	2617	U	C5-C4-O4	9.38	131.53	125.90
1	5	934	G	N1-C6-O6	9.37	125.52	119.90
1	5	3245	A	N7-C8-N9	9.33	118.47	113.80
45	2	541	A	O4'-C1'-N9	9.24	115.59	108.20
1	5	2971	A	C8-N9-C4	-9.22	102.11	105.80
1	5	2257	C	C5-C6-N1	9.22	125.61	121.00
1	5	2560	C	N1-C2-O2	9.15	124.39	118.90
1	1	2306	C	C2-N1-C1'	9.12	128.83	118.80
45	2	572	C	O5'-P-OP1	-9.09	97.52	105.70
45	6	453	U	C2-N1-C1'	9.09	128.60	117.70
45	6	163	G	N3-C4-N9	-9.07	120.56	126.00
1	1	3154	C	C6-N1-C2	-8.96	116.72	120.30
1	1	1151	U	C6-N1-C2	-8.95	115.63	121.00
1	5	1152	G	C4-N9-C1'	-8.89	114.94	126.50
1	1	2726	C	N3-C2-O2	-8.85	115.71	121.90
1	1	439	C	C2-N1-C1'	8.80	128.48	118.80
1	5	2872	A	N1-C6-N6	8.79	123.87	118.60
1	5	934	G	C5-C6-O6	-8.77	123.34	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	6	609	U	C5-C6-N1	-8.76	118.32	122.70
1	5	2403	G	N1-C6-O6	8.74	125.15	119.90
1	5	2871	G	O5'-P-OP2	-8.69	97.88	105.70
1	1	220	G	N1-C6-O6	8.62	125.07	119.90
79	SM	167	PRO	N-CA-CB	8.62	113.64	103.30
1	5	1201	C	O4'-C1'-N1	8.60	115.08	108.20
1	1	3217	C	N1-C2-O2	8.59	124.06	118.90
1	5	1209	G	O5'-P-OP1	-8.54	98.01	105.70
1	5	2401	A	O4'-C1'-N9	8.52	115.02	108.20
45	6	1535	U	N3-C2-O2	-8.50	116.25	122.20
12	m0	176	LEU	CA-CB-CG	8.49	134.82	115.30
1	1	621	A	P-O3'-C3'	8.47	129.86	119.70
1	5	1489	A	O5'-P-OP1	-8.46	98.08	105.70
45	6	1490	C	O4'-C1'-N1	8.46	114.97	108.20
1	1	1016	C	N1-C2-O2	8.45	123.97	118.90
1	5	1201	C	N3-C2-O2	-8.45	115.98	121.90
1	1	439	C	N1-C2-O2	8.45	123.97	118.90
1	1	2957	G	N1-C6-O6	8.45	124.97	119.90
1	5	2355	G	N1-C6-O6	8.42	124.95	119.90
1	5	2726	C	N3-C4-N4	-8.36	112.15	118.00
1	1	2983	C	C5-C4-N4	8.29	126.01	120.20
45	2	74	U	O4'-C1'-N1	8.29	114.83	108.20
1	5	1897	G	N1-C6-O6	8.28	124.87	119.90
1	5	2852	C	C6-N1-C2	8.28	123.61	120.30
1	1	2355	G	N1-C6-O6	8.26	124.85	119.90
1	5	1200	A	N1-C6-N6	8.24	123.55	118.60
1	5	491	C	C2-N1-C1'	8.22	127.84	118.80
45	2	192	U	C2-N1-C1'	8.20	127.55	117.70
1	1	98	G	C8-N9-C4	8.20	109.68	106.40
1	5	2384	A	N1-C6-N6	8.17	123.50	118.60
6	14	339	LEU	CA-CB-CG	8.17	134.09	115.30
1	1	1201	C	C2-N1-C1'	8.17	127.78	118.80
1	1	3217	C	C2-N1-C1'	8.15	127.77	118.80
1	1	2827	U	C2-N1-C1'	-8.15	107.92	117.70
45	2	75	U	N1-C2-O2	8.15	128.51	122.80
45	6	1361	U	C2-N1-C1'	8.13	127.46	117.70
1	1	1016	C	N3-C2-O2	-8.10	116.23	121.90
1	5	2400	G	OP2-P-O3'	8.10	123.03	105.20
1	5	3351	U	C2-N1-C1'	8.10	127.42	117.70
45	6	1773	C	N3-C4-C5	-8.10	118.66	121.90
45	2	241	U	C2-N1-C1'	8.09	127.41	117.70
45	2	704	C	N1-C2-O2	8.08	123.75	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3278	C	N1-C2-O2	8.04	123.72	118.90
1	1	1201	C	C5-C6-N1	7.97	124.98	121.00
45	6	1490	C	C2-N1-C1'	7.96	127.56	118.80
2	7	97	A	C8-N9-C4	7.95	108.98	105.80
1	5	1402	C	C6-N1-C2	7.93	123.47	120.30
1	5	2842	U	C2-N1-C1'	7.90	127.18	117.70
45	6	781	U	C2-N1-C1'	7.89	127.17	117.70
1	5	2256	A	C2-N3-C4	7.88	114.54	110.60
45	6	609	U	C5-C4-O4	7.88	130.62	125.90
1	1	2147	A	C8-N9-C4	7.86	108.94	105.80
45	6	339	C	C6-N1-C2	-7.84	117.16	120.30
1	1	1858	A	C2-N3-C4	7.83	114.52	110.60
1	5	813	G	N1-C6-O6	7.83	124.60	119.90
1	5	3245	A	C6-C5-N7	-7.83	126.82	132.30
45	6	1560	U	N3-C2-O2	-7.82	116.72	122.20
1	1	3154	C	N1-C2-O2	7.82	123.59	118.90
1	1	2614	G	N3-C4-C5	-7.81	124.69	128.60
45	6	163	G	N3-C4-C5	7.79	132.50	128.60
1	1	545	U	C2-N1-C1'	7.79	127.05	117.70
45	6	813	U	C2-N1-C1'	7.79	127.04	117.70
45	2	934	C	C2-N1-C1'	7.78	127.36	118.80
1	1	2980	U	O5'-P-OP2	-7.76	98.71	105.70
1	1	1292	C	C6-N1-C2	7.75	123.40	120.30
45	6	609	U	N3-C4-O4	-7.75	113.98	119.40
1	1	2093	A	C2-N3-C4	7.75	114.47	110.60
45	6	1246	C	N1-C2-O2	7.74	123.55	118.90
1	5	1307	G	P-O3'-C3'	7.74	128.98	119.70
1	1	2156	C	C6-N1-C2	7.72	123.39	120.30
1	5	3104	U	O5'-P-OP2	-7.72	98.75	105.70
1	1	648	C	O5'-P-OP1	-7.70	98.77	105.70
45	6	453	U	N1-C2-O2	7.70	128.19	122.80
1	5	2257	C	C6-N1-C2	-7.68	117.23	120.30
1	1	2726	C	N3-C4-N4	-7.67	112.63	118.00
45	2	75	U	N3-C2-O2	-7.67	116.83	122.20
1	1	220	G	C5-C6-O6	-7.66	124.00	128.60
1	1	55	G	C8-N9-C4	7.65	109.46	106.40
45	6	194	U	C2-N1-C1'	7.63	126.86	117.70
1	5	2305	G	C8-N9-C4	-7.61	103.36	106.40
1	5	3245	A	C4-C5-N7	7.60	114.50	110.70
1	1	3154	C	C2-N1-C1'	7.59	127.15	118.80
45	2	1291	G	N7-C8-N9	7.55	116.88	113.10
45	6	553	G	N1-C6-O6	7.54	124.43	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	345	G	N1-C6-O6	7.54	124.42	119.90
45	6	389	G	N1-C6-O6	7.53	124.42	119.90
1	1	1556	C	C6-N1-C2	-7.52	117.29	120.30
45	6	163	G	C2-N3-C4	-7.52	108.14	111.90
1	5	1200	A	C5-C6-N6	-7.51	117.69	123.70
1	5	3382	U	N1-C2-O2	7.51	128.06	122.80
1	5	934	G	C6-C5-N7	-7.48	125.91	130.40
1	5	2355	G	C6-C5-N7	-7.48	125.91	130.40
1	1	1016	C	C6-N1-C2	-7.48	117.31	120.30
45	2	794	U	C2-N1-C1'	7.47	126.67	117.70
1	5	1003	A	N1-C6-N6	7.47	123.08	118.60
1	5	345	G	C6-C5-N7	-7.47	125.92	130.40
1	5	2119	A	N1-C6-N6	7.47	123.08	118.60
1	5	3001	C	C6-N1-C2	7.45	123.28	120.30
1	5	420	G	N9-C4-C5	-7.43	102.43	105.40
1	1	437	G	N7-C8-N9	7.43	116.81	113.10
1	5	2169	G	N3-C4-N9	-7.43	121.54	126.00
45	6	543	C	N1-C2-O2	7.42	123.35	118.90
1	1	2647	A	O5'-P-OP1	7.41	119.59	110.70
1	1	2144	A	O4'-C1'-N9	7.41	114.13	108.20
1	5	1187	C	C6-N1-C2	7.41	123.26	120.30
45	2	72	A	O5'-P-OP1	7.40	119.58	110.70
1	1	1306	G	C5-C6-O6	-7.39	124.17	128.60
45	2	1389	C	C2-N1-C1'	7.39	126.93	118.80
1	5	92	G	C4-C5-N7	7.38	113.75	110.80
1	1	406	G	O4'-C1'-N9	7.38	114.10	108.20
1	1	1351	U	N1-C2-O2	7.38	127.96	122.80
1	1	776	U	C4-C5-C6	7.37	124.12	119.70
1	1	2714	G	N3-C4-C5	7.37	132.28	128.60
1	1	2693	C	C6-N1-C2	7.36	123.25	120.30
45	2	453	U	C2-N1-C1'	7.36	126.53	117.70
1	5	880	G	O4'-C1'-N9	7.36	114.08	108.20
1	5	2553	U	C2-N1-C1'	7.34	126.51	117.70
1	5	3382	U	N3-C2-O2	-7.33	117.07	122.20
1	1	2199	G	N1-C6-O6	-7.33	115.50	119.90
1	1	3382	U	C2-N1-C1'	7.32	126.48	117.70
1	1	1016	C	C2-N1-C1'	7.30	126.83	118.80
1	1	2726	C	C5-C4-N4	7.29	125.31	120.20
45	2	1389	C	N1-C2-O2	7.28	123.27	118.90
1	1	2979	U	C2-N1-C1'	-7.27	108.97	117.70
1	5	1339	C	O5'-P-OP1	-7.27	99.16	105.70
45	6	858	G	O4'-C1'-N9	7.25	114.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2728	G	C8-N9-C4	-7.25	103.50	106.40
45	2	704	C	C2-N1-C1'	7.24	126.76	118.80
1	5	2830	G	C8-N9-C4	7.24	109.30	106.40
1	1	2842	U	C2-N1-C1'	7.24	126.38	117.70
1	1	358	G	N1-C6-O6	7.23	124.24	119.90
1	5	908	G	C8-N9-C4	-7.23	103.51	106.40
1	1	937	G	C5-C6-O6	-7.22	124.27	128.60
1	5	2630	C	C6-N1-C2	-7.22	117.41	120.30
17	m6	84	LEU	CB-CG-CD1	-7.21	98.74	111.00
1	5	92	G	C5-C6-O6	-7.21	124.28	128.60
1	1	2714	G	N3-C4-N9	-7.21	121.68	126.00
45	2	1363	U	N1-C2-O2	7.20	127.84	122.80
1	5	2399	A	C2-N3-C4	-7.20	107.00	110.60
1	1	2355	G	C5-C6-O6	-7.20	124.28	128.60
1	5	1297	C	N1-C2-O2	-7.18	114.59	118.90
1	5	1579	C	N1-C2-O2	7.17	123.20	118.90
1	5	885	U	O5'-P-OP2	-7.16	99.25	105.70
1	1	1482	A	N1-C6-N6	7.15	122.89	118.60
1	1	3137	C	C6-N1-C2	7.14	123.16	120.30
5	l3	4	ARG	NE-CZ-NH1	7.13	123.86	120.30
45	6	1490	C	N1-C2-O2	7.12	123.17	118.90
1	5	2401	A	O5'-P-OP2	-7.12	99.30	105.70
1	1	2614	G	N3-C4-N9	7.11	130.27	126.00
45	2	192	U	N1-C2-O2	7.10	127.77	122.80
1	5	1368	U	O5'-P-OP1	-7.10	99.31	105.70
1	5	420	G	N1-C6-O6	7.10	124.16	119.90
2	7	18	C	C6-N1-C2	7.10	123.14	120.30
1	5	2700	G	N3-C4-C5	-7.10	125.05	128.60
1	1	410	U	N3-C4-C5	-7.09	110.34	114.60
1	5	1342	C	C6-N1-C2	7.09	123.14	120.30
1	1	1201	C	O4'-C1'-N1	7.09	113.88	108.20
1	5	1579	C	C6-N1-C2	-7.09	117.46	120.30
45	2	794	U	N1-C2-O2	7.09	127.76	122.80
1	1	1556	C	C5-C6-N1	7.09	124.54	121.00
45	6	1585	U	O5'-P-OP2	-7.08	99.33	105.70
1	1	2617	U	C6-N1-C2	-7.08	116.75	121.00
1	5	2179	C	N3-C4-C5	-7.07	119.07	121.90
1	1	2306	C	N1-C2-O2	7.05	123.13	118.90
1	5	424	G	C5-C6-O6	-7.05	124.37	128.60
1	5	776	U	N1-C2-N3	7.03	119.12	114.90
45	6	462	G	C8-N9-C4	7.03	109.21	106.40
1	5	2644	C	N1-C2-O2	-7.03	114.68	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3154	C	N3-C2-O2	-7.02	116.98	121.90
1	5	1898	G	C4-C5-N7	-7.02	107.99	110.80
1	1	3382	U	N1-C2-O2	7.02	127.71	122.80
1	1	439	C	C6-N1-C2	-7.02	117.49	120.30
1	1	3196	U	C2-N1-C1'	7.01	126.12	117.70
1	5	2272	G	O4'-C1'-N9	7.01	113.81	108.20
1	1	424	G	C8-N9-C4	-7.01	103.60	106.40
1	5	1422	G	N1-C6-O6	6.99	124.09	119.90
1	5	2983	C	OP1-P-O3'	6.99	120.57	105.20
79	sM	167	PRO	N-CA-CB	6.98	111.68	103.30
1	5	857	G	C5-C6-O6	-6.97	124.42	128.60
1	5	1291	A	C8-N9-C4	6.97	108.59	105.80
45	6	453	U	C6-N1-C2	-6.97	116.82	121.00
1	1	2314	U	C2-N1-C1'	6.97	126.06	117.70
45	2	1180	C	C6-N1-C2	-6.97	117.51	120.30
45	6	864	U	C2-N1-C1'	6.96	126.05	117.70
1	5	644	G	C5-C6-O6	6.96	132.78	128.60
1	5	1152	G	N3-C2-N2	-6.94	115.04	119.90
1	5	3195	U	P-O3'-C3'	6.94	128.03	119.70
45	2	959	U	N1-C2-O2	6.93	127.65	122.80
1	5	3109	G	C5-C6-O6	-6.93	124.44	128.60
1	1	937	G	C4-C5-N7	6.92	113.57	110.80
1	1	1183	C	C6-N1-C2	6.92	123.07	120.30
1	5	1579	C	C2-N1-C1'	6.92	126.42	118.80
1	1	2278	C	N1-C2-O2	6.92	123.05	118.90
68	d2	93	LEU	CA-CB-CG	6.92	131.21	115.30
1	5	948	C	O5'-P-OP2	-6.91	99.48	105.70
1	5	2726	C	C6-N1-C2	-6.91	117.53	120.30
1	5	934	G	C4-C5-N7	6.91	113.56	110.80
1	1	2198	A	C8-N9-C4	6.90	108.56	105.80
1	5	1778	G	N3-C4-N9	-6.90	121.86	126.00
1	5	3195	U	N3-C2-O2	-6.90	117.37	122.20
1	1	2923	U	N3-C2-O2	6.90	127.03	122.20
1	1	2621	G	O5'-P-OP2	-6.89	99.50	105.70
45	6	103	A	C8-N9-C4	-6.89	103.04	105.80
1	1	641	C	C5-C6-N1	6.89	124.45	121.00
3	4	10	A	O5'-P-OP2	-6.89	99.50	105.70
1	5	2560	C	N3-C2-O2	-6.89	117.08	121.90
1	5	2726	C	N1-C2-N3	6.89	124.03	119.20
1	5	1104	G	N7-C8-N9	6.88	116.54	113.10
1	1	2306	C	N3-C2-O2	-6.88	117.09	121.90
1	5	2682	C	C6-N1-C2	-6.88	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	6	570	A	N1-C6-N6	6.86	122.72	118.60
1	5	2100	A	C2-N3-C4	6.86	114.03	110.60
45	6	194	U	N1-C2-O2	6.85	127.59	122.80
45	6	781	U	N1-C2-O2	6.85	127.59	122.80
1	5	2842	U	N1-C2-O2	6.84	127.59	122.80
1	1	1904	C	C6-N1-C2	-6.84	117.56	120.30
45	6	1241	G	C4-N9-C1'	6.84	135.39	126.50
1	5	3351	U	N1-C2-O2	6.83	127.58	122.80
45	6	103	A	P-O3'-C3'	6.83	127.90	119.70
1	5	1409	G	C5-C6-O6	-6.83	124.50	128.60
1	5	1903	U	N3-C4-O4	6.82	124.18	119.40
1	5	3195	U	N1-C2-O2	6.82	127.57	122.80
1	5	630	A	C8-N9-C4	6.81	108.52	105.80
1	5	2719	U	C2-N1-C1'	-6.81	109.53	117.70
1	1	1352	A	OP1-P-O3'	6.80	120.17	105.20
45	6	424	C	C6-N1-C2	6.80	123.02	120.30
1	5	936	A	N1-C6-N6	6.80	122.68	118.60
1	1	3217	C	C6-N1-C1'	-6.79	112.65	120.80
1	5	491	C	N1-C2-O2	6.79	122.98	118.90
1	5	2541	U	C2-N1-C1'	6.79	125.85	117.70
1	1	545	U	N1-C2-O2	6.78	127.55	122.80
1	5	2719	U	C5-C6-N1	-6.78	119.31	122.70
13	m1	112	LEU	CA-CB-CG	6.78	130.89	115.30
1	5	1495	U	C2-N1-C1'	6.77	125.82	117.70
1	1	959	C	C6-N1-C2	6.76	123.00	120.30
1	1	2871	G	C5-N7-C8	-6.76	100.92	104.30
1	5	2831	G	N1-C6-O6	6.76	123.96	119.90
3	8	82	U	N1-C2-N3	-6.76	110.84	114.90
1	1	859	G	C8-N9-C4	6.76	109.10	106.40
31	O0	41	LEU	CA-CB-CG	6.75	130.82	115.30
1	1	1111	U	C5-C6-N1	-6.75	119.33	122.70
1	1	591	G	N1-C6-O6	6.75	123.95	119.90
1	1	2763	U	O5'-P-OP2	-6.74	99.63	105.70
45	6	830	U	C2-N1-C1'	6.74	125.79	117.70
1	1	3129	A	C8-N9-C4	6.74	108.50	105.80
1	1	1351	U	N3-C2-O2	-6.74	117.48	122.20
45	2	959	U	N3-C2-O2	-6.74	117.48	122.20
1	5	1000	C	C6-N1-C2	6.74	123.00	120.30
1	5	2403	G	C5-C6-O6	-6.74	124.56	128.60
1	5	2643	A	C8-N9-C4	6.73	108.49	105.80
1	5	2330	C	N1-C2-O2	-6.72	114.87	118.90
45	6	321	C	P-O3'-C3'	6.72	127.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	c5	36	LEU	CA-CB-CG	6.72	130.75	115.30
1	1	3278	C	C2-N1-C1'	6.71	126.19	118.80
45	2	912	U	C2-N1-C1'	6.71	125.76	117.70
45	6	1096	C	C6-N1-C2	6.71	122.99	120.30
45	6	1052	U	O5'-P-OP2	-6.71	99.66	105.70
1	5	1716	U	P-O3'-C3'	6.71	127.75	119.70
45	6	1389	C	C2-N1-C1'	6.71	126.18	118.80
45	6	864	U	N3-C2-O2	-6.70	117.51	122.20
1	5	92	G	N1-C6-O6	6.70	123.92	119.90
45	2	539	G	C4-N9-C1'	6.69	135.20	126.50
1	5	1152	G	C5-C6-N1	-6.69	108.16	111.50
45	2	75	U	C6-N1-C1'	-6.67	111.86	121.20
47	S1	218	LEU	CA-CB-CG	6.67	130.64	115.30
1	1	1176	C	N3-C2-O2	6.67	126.57	121.90
45	6	1246	C	N3-C2-O2	-6.67	117.23	121.90
1	1	2871	G	N7-C8-N9	6.66	116.43	113.10
45	6	1614	A	N1-C6-N6	6.66	122.60	118.60
1	5	2434	U	N3-C2-O2	-6.66	117.54	122.20
1	1	1224	C	C6-N1-C2	-6.66	117.64	120.30
1	1	2550	U	N3-C2-O2	-6.64	117.55	122.20
1	1	1556	C	C2-N1-C1'	6.64	126.10	118.80
1	5	3204	C	N1-C2-O2	-6.64	114.92	118.90
1	1	2375	G	O4'-C1'-N9	6.63	113.51	108.20
1	1	2809	C	N1-C2-O2	-6.63	114.92	118.90
45	2	507	U	N1-C2-O2	6.63	127.44	122.80
1	5	1778	G	C8-N9-C1'	6.63	135.62	127.00
1	5	1303	A	N1-C6-N6	6.63	122.58	118.60
1	1	591	G	C5-C6-O6	-6.62	124.63	128.60
1	5	2817	A	C2-N3-C4	6.62	113.91	110.60
1	5	1331	U	C5-C6-N1	-6.62	119.39	122.70
1	5	1342	C	C5-C6-N1	-6.62	117.69	121.00
1	5	3092	C	C6-N1-C2	6.62	122.95	120.30
1	1	2353	G	N1-C6-O6	6.62	123.87	119.90
45	2	1363	U	N3-C2-O2	-6.62	117.57	122.20
45	2	577	G	N1-C6-O6	6.61	123.87	119.90
1	5	2871	G	C5-N7-C8	-6.61	100.99	104.30
1	5	2971	A	N3-C4-C5	-6.61	122.17	126.80
1	5	2872	A	C5-N7-C8	-6.60	100.60	103.90
65	C9	28	LEU	CA-CB-CG	6.60	130.48	115.30
1	1	2353	G	C6-C5-N7	-6.59	126.44	130.40
1	5	998	A	N1-C6-N6	-6.59	114.65	118.60
1	5	2202	C	C6-N1-C2	6.59	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2553	U	N3-C2-O2	-6.59	117.59	122.20
1	1	227	G	C8-N9-C1'	-6.59	118.44	127.00
45	6	1481	C	N1-C2-O2	6.59	122.85	118.90
1	1	545	U	N3-C2-O2	-6.58	117.59	122.20
1	1	3001	C	C6-N1-C2	6.58	122.93	120.30
1	5	1115	G	C8-N9-C4	-6.58	103.77	106.40
3	8	100	U	C2-N1-C1'	6.57	125.59	117.70
1	5	937	G	C5-C6-N1	6.57	114.79	111.50
1	5	2169	G	C8-N9-C1'	6.57	135.54	127.00
1	5	3351	U	C6-N1-C1'	-6.57	112.00	121.20
45	6	608	U	N3-C2-O2	-6.57	117.60	122.20
45	6	858	G	C4-N9-C1'	6.57	135.04	126.50
3	8	56	G	N1-C6-O6	6.56	123.84	119.90
45	6	1491	U	P-O3'-C3'	6.56	127.58	119.70
1	5	1402	C	C5-C6-N1	-6.56	117.72	121.00
1	5	2971	A	N9-C1'-C2'	6.56	122.53	114.00
45	2	1291	G	C8-N9-C4	-6.56	103.78	106.40
1	1	630	A	C8-N9-C4	6.56	108.42	105.80
45	2	934	C	C6-N1-C2	-6.56	117.68	120.30
1	5	2306	C	N1-C2-O2	6.56	122.83	118.90
1	5	784	A	N1-C6-N6	6.55	122.53	118.60
1	1	2257	C	O5'-P-OP2	-6.55	99.80	105.70
1	1	2728	G	N3-C4-C5	-6.55	125.32	128.60
45	2	864	U	N3-C2-O2	-6.55	117.62	122.20
1	5	2719	U	C6-N1-C2	6.54	124.92	121.00
2	7	1	G	C4-N9-C1'	6.54	135.00	126.50
1	1	1839	A	N1-C6-N6	-6.54	114.68	118.60
45	6	1039	A	O4'-C1'-N9	6.53	113.42	108.20
56	c0	97	PRO	N-CA-CB	6.53	111.13	103.30
45	2	158	U	P-O3'-C3'	6.52	127.52	119.70
64	c8	116	LEU	CA-CB-CG	6.50	130.26	115.30
1	1	1148	G	C4-N9-C1'	-6.50	118.05	126.50
45	6	1600	A	C5-N7-C8	-6.50	100.65	103.90
56	c0	88	PRO	N-CA-CB	6.50	111.10	103.30
1	5	1085	A	C6-C5-N7	-6.49	127.75	132.30
1	5	265	A	C8-N9-C4	6.49	108.39	105.80
1	5	1152	G	C5-N7-C8	-6.49	101.06	104.30
1	1	1367	G	N1-C6-O6	6.48	123.79	119.90
1	1	2617	U	C4-C5-C6	6.48	123.59	119.70
45	6	1214	U	N3-C2-O2	-6.48	117.67	122.20
1	1	2957	G	C5-C6-O6	-6.47	124.72	128.60
1	5	1450	G	N1-C6-O6	6.47	123.78	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	345	G	N9-C4-C5	-6.47	102.81	105.40
1	5	1450	G	C5-C6-O6	-6.47	124.72	128.60
1	1	908	G	C4-N9-C1'	6.46	134.90	126.50
1	1	212	G	C2-N3-C4	6.46	115.13	111.90
1	5	3142	A	C8-N9-C4	6.46	108.38	105.80
1	5	2745	G	C5-C6-O6	-6.46	124.72	128.60
1	5	420	G	C8-N9-C4	6.46	108.98	106.40
45	2	783	G	C5-C6-O6	-6.45	124.73	128.60
1	1	2660	G	N1-C6-O6	6.45	123.77	119.90
1	5	2978	U	C5-C6-N1	-6.44	119.48	122.70
1	5	2996	U	N1-C2-O2	6.44	127.31	122.80
45	6	1456	C	C4-C5-C6	6.44	120.62	117.40
1	1	3217	C	N3-C2-O2	-6.44	117.39	121.90
45	6	1614	A	O4'-C1'-N9	6.44	113.35	108.20
1	1	437	G	C6-C5-N7	-6.43	126.54	130.40
1	1	439	C	N3-C2-O2	-6.43	117.39	121.90
1	1	2306	C	C6-N1-C2	-6.43	117.73	120.30
45	6	934	C	C2-N1-C1'	6.43	125.88	118.80
2	3	101	G	C8-N9-C4	6.43	108.97	106.40
1	5	2553	U	N1-C2-O2	6.43	127.30	122.80
45	6	385	A	N1-C6-N6	-6.43	114.74	118.60
1	5	1103	A	C2-N3-C4	6.42	113.81	110.60
45	6	1654	G	C5-C6-O6	-6.42	124.75	128.60
1	5	1481	A	P-O3'-C3'	6.42	127.40	119.70
1	1	676	G	N3-C4-C5	-6.41	125.39	128.60
1	1	2385	G	N3-C4-C5	6.41	131.81	128.60
1	1	3355	U	N1-C2-O2	6.41	127.29	122.80
1	5	879	U	C5-C4-O4	-6.41	122.05	125.90
1	5	3087	A	C8-N9-C4	6.41	108.36	105.80
1	5	3362	A	C5-N7-C8	-6.41	100.70	103.90
45	6	1773	C	N3-C4-N4	6.41	122.49	118.00
1	5	3211	C	C6-N1-C2	6.41	122.86	120.30
1	5	2821	C	N3-C2-O2	-6.41	117.42	121.90
45	6	682	C	OP1-P-O3'	6.41	119.29	105.20
1	5	1796	G	C4-N9-C1'	-6.40	118.18	126.50
1	5	1310	G	C5-C6-N1	6.40	114.70	111.50
1	5	866	A	N1-C6-N6	-6.39	114.76	118.60
1	5	2940	A	N1-C2-N3	6.39	132.49	129.30
1	5	3276	G	OP2-P-O3'	6.39	119.25	105.20
2	7	49	G	N1-C6-O6	6.38	123.73	119.90
1	5	1778	G	C4-N9-C1'	-6.38	118.21	126.50
1	5	3016	A	N1-C6-N6	6.38	122.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1369	A	C8-N9-C4	6.37	108.35	105.80
1	5	2831	G	C5-C6-O6	-6.37	124.78	128.60
1	1	3195	U	N3-C2-O2	-6.37	117.74	122.20
1	5	969	C	C6-N1-C2	6.37	122.85	120.30
1	5	2979	U	C5-C6-N1	-6.37	119.52	122.70
1	5	2871	G	N7-C8-N9	6.37	116.28	113.10
1	5	1806	A	C8-N9-C4	6.36	108.34	105.80
1	5	1085	A	N1-C6-N6	6.36	122.42	118.60
45	2	1280	C	C6-N1-C2	-6.36	117.75	120.30
1	5	1389	G	C8-N9-C4	6.36	108.94	106.40
1	5	2418	G	OP2-P-O3'	6.36	119.19	105.20
1	1	1285	G	P-O3'-C3'	6.35	127.31	119.70
1	1	546	C	C6-N1-C2	-6.34	117.76	120.30
45	2	1274	C	C2-N1-C1'	6.34	125.78	118.80
1	1	2759	U	C5-C6-N1	6.34	125.87	122.70
45	6	400	A	N1-C6-N6	6.34	122.40	118.60
1	1	73	C	N3-C4-C5	-6.33	119.37	121.90
3	4	21	C	O5'-P-OP2	-6.33	100.00	105.70
45	6	1241	G	O4'-C1'-N9	6.33	113.27	108.20
1	5	911	C	N1-C2-O2	-6.33	115.11	118.90
1	5	2415	C	C6-N1-C2	6.33	122.83	120.30
1	5	2294	U	N1-C2-O2	6.32	127.22	122.80
1	1	3275	U	C5-C6-N1	6.32	125.86	122.70
1	1	2983	C	N3-C4-N4	-6.32	113.58	118.00
1	5	1046	A	N1-C6-N6	-6.32	114.81	118.60
47	s1	54	LEU	CA-CB-CG	6.31	129.81	115.30
1	5	948	C	C6-N1-C2	6.29	122.82	120.30
1	1	3214	U	N3-C2-O2	-6.28	117.81	122.20
1	1	2831	G	N1-C6-O6	6.28	123.67	119.90
1	5	1104	G	C8-N9-C4	-6.28	103.89	106.40
1	5	2560	C	C2-N1-C1'	6.28	125.70	118.80
45	6	74	U	C5-C6-N1	6.28	125.84	122.70
45	6	1481	C	N3-C2-O2	-6.28	117.51	121.90
56	C0	88	PRO	N-CA-CB	6.27	110.83	103.30
1	5	2179	C	N1-C2-O2	6.27	122.66	118.90
1	5	2366	C	C6-N1-C2	6.27	122.81	120.30
1	1	1581	C	N1-C2-O2	6.27	122.66	118.90
1	5	1188	U	N1-C2-N3	6.27	118.66	114.90
1	5	2971	A	C2-N3-C4	6.27	113.73	110.60
45	6	1428	G	O5'-P-OP1	-6.27	100.06	105.70
1	5	1177	G	C4-N9-C1'	6.27	134.65	126.50
45	6	1241	G	C6-C5-N7	-6.26	126.64	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	638	C	N3-C4-C5	-6.26	119.40	121.90
1	1	2846	U	N3-C2-O2	-6.26	117.82	122.20
1	5	791	A	C8-N9-C4	6.26	108.30	105.80
1	1	3085	G	N1-C6-O6	6.25	123.65	119.90
1	5	420	G	C5-C6-N1	6.25	114.62	111.50
45	6	633	U	C5-C6-N1	-6.25	119.58	122.70
1	5	2211	U	N3-C2-O2	-6.24	117.83	122.20
45	6	1097	U	N3-C2-O2	-6.24	117.83	122.20
1	1	345	G	C6-C5-N7	-6.24	126.66	130.40
1	5	2751	G	N1-C6-O6	6.24	123.64	119.90
45	6	103	A	N3-C4-C5	-6.24	122.43	126.80
1	1	1724	U	OP1-P-O3'	6.23	118.91	105.20
1	5	428	A	N1-C6-N6	6.23	122.34	118.60
45	6	1568	C	P-O3'-C3'	6.23	127.18	119.70
1	1	948	C	C6-N1-C2	6.23	122.79	120.30
1	5	1844	C	N1-C2-O2	-6.23	115.16	118.90
45	6	337	G	C4-C5-N7	6.23	113.29	110.80
1	1	1103	A	C8-N9-C4	6.22	108.29	105.80
1	5	2682	C	P-O3'-C3'	6.22	127.17	119.70
1	5	1292	C	C6-N1-C2	6.21	122.78	120.30
45	2	275	C	C5-C6-N1	6.21	124.11	121.00
1	1	2979	U	C5-C6-N1	-6.21	119.59	122.70
45	6	163	G	N3-C2-N2	-6.21	115.55	119.90
1	5	2283	G	C5-C6-N1	-6.21	108.40	111.50
1	5	438	A	P-O3'-C3'	6.21	127.15	119.70
45	6	1490	C	C6-N1-C1'	-6.21	113.35	120.80
1	1	1351	U	C2-N1-C1'	6.21	125.15	117.70
1	5	1851	G	C8-N9-C4	-6.21	103.92	106.40
45	6	577	G	C6-C5-N7	-6.20	126.68	130.40
1	5	3178	A	N1-C6-N6	6.20	122.32	118.60
1	1	1119	C	C4-C5-C6	6.20	120.50	117.40
1	5	1201	C	C6-N1-C2	-6.20	117.82	120.30
1	1	1304	A	N1-C6-N6	-6.19	114.89	118.60
1	5	2879	C	N3-C2-O2	6.19	126.23	121.90
1	5	2836	C	C5-C6-N1	-6.19	117.91	121.00
45	6	136	C	N1-C2-O2	6.19	122.61	118.90
1	1	964	G	C4-C5-N7	6.18	113.27	110.80
1	5	718	G	O4'-C1'-N9	6.18	113.15	108.20
45	6	683	C	C5-C6-N1	6.18	124.09	121.00
1	1	1329	U	P-O3'-C3'	6.18	127.12	119.70
45	6	1200	G	N1-C6-O6	6.18	123.61	119.90
1	5	1374	G	C4-C5-N7	6.18	113.27	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3130	A	O5'-P-OP1	-6.18	100.14	105.70
45	2	380	U	C2-N1-C1'	6.17	125.11	117.70
1	5	3158	G	C4-N9-C1'	6.17	134.52	126.50
45	6	781	U	C6-N1-C1'	-6.17	112.57	121.20
1	1	2821	C	O4'-C1'-N1	6.17	113.13	108.20
1	5	2541	U	N1-C2-O2	6.17	127.12	122.80
1	1	2355	G	C6-C5-N7	-6.16	126.70	130.40
45	2	1755	A	P-O3'-C3'	-6.16	112.31	119.70
1	5	857	G	C6-C5-N7	-6.16	126.71	130.40
1	5	1103	A	O4'-C1'-N9	6.16	113.12	108.20
1	5	2700	G	N3-C4-N9	6.15	129.69	126.00
1	5	415	G	C8-N9-C4	6.15	108.86	106.40
1	5	1152	G	N9-C4-C5	6.14	107.86	105.40
7	15	110	LEU	CA-CB-CG	6.14	129.43	115.30
1	1	1303	A	C8-N9-C4	6.14	108.26	105.80
1	1	2306	C	C6-N1-C1'	-6.14	113.44	120.80
1	5	280	U	O5'-P-OP2	-6.13	100.18	105.70
45	6	1413	U	C2-N1-C1'	6.13	125.06	117.70
45	6	1614	A	C5-N7-C8	-6.13	100.83	103.90
1	1	1432	C	C6-N1-C2	-6.13	117.85	120.30
45	6	75	U	P-O3'-C3'	6.13	127.06	119.70
1	1	3344	A	N7-C8-N9	6.13	116.86	113.80
45	6	1280	C	N3-C4-C5	-6.13	119.45	121.90
1	5	2621	G	C5-C6-N1	-6.12	108.44	111.50
1	5	2970	C	P-O3'-C3'	6.12	127.05	119.70
1	5	3388	C	C6-N1-C2	6.12	122.75	120.30
1	5	504	A	N1-C6-N6	6.12	122.27	118.60
1	1	1495	U	C5-C4-O4	6.12	129.57	125.90
3	4	20	U	C5-C6-N1	-6.11	119.64	122.70
45	2	380	U	N3-C2-O2	-6.11	117.92	122.20
1	5	1177	G	C8-N9-C1'	-6.11	119.05	127.00
1	1	2396	G	C4-C5-N7	-6.11	108.36	110.80
1	1	2964	G	C8-N9-C1'	6.11	134.94	127.00
1	5	994	G	O4'-C1'-N9	-6.11	103.31	108.20
1	5	2769	A	C8-N9-C4	6.10	108.24	105.80
1	5	2169	G	C6-C5-N7	6.10	134.06	130.40
6	L4	19	ALA	C-N-CA	6.10	136.94	121.70
45	2	1767	G	N3-C4-C5	6.10	131.65	128.60
1	5	949	C	C6-N1-C2	6.09	122.74	120.30
1	1	437	G	N1-C6-O6	6.09	123.56	119.90
1	5	1140	G	O5'-P-OP2	-6.09	100.22	105.70
1	5	3245	A	C8-N9-C4	-6.09	103.36	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	684	G	C8-N9-C4	6.09	108.84	106.40
45	6	337	G	C5-N7-C8	-6.09	101.26	104.30
1	5	3245	A	N1-C2-N3	6.09	132.34	129.30
45	6	1137	A	C8-N9-C4	6.09	108.23	105.80
1	1	2846	U	C2-N1-C1'	6.09	125.00	117.70
45	6	1490	C	N1-C1'-C2'	6.08	121.91	114.00
1	1	1351	U	C5-C6-N1	6.08	125.74	122.70
1	5	1367	G	N1-C6-O6	6.08	123.55	119.90
1	1	2817	A	C8-N9-C4	-6.08	103.37	105.80
1	5	654	C	C6-N1-C2	6.08	122.73	120.30
79	sM	82	THR	C-N-CA	6.08	136.91	121.70
1	1	2978	U	C5-C6-N1	-6.08	119.66	122.70
45	6	577	G	C4-C5-N7	6.08	113.23	110.80
2	7	1	G	C6-C5-N7	-6.08	126.75	130.40
45	6	108	A	C8-N9-C4	6.07	108.23	105.80
1	1	1179	A	C8-N9-C4	6.06	108.22	105.80
45	6	1518	C	N1-C2-O2	6.06	122.54	118.90
1	5	2901	G	O5'-P-OP2	-6.06	100.25	105.70
45	2	380	U	N1-C2-O2	6.06	127.04	122.80
1	5	2842	U	C5-C6-N1	6.06	125.73	122.70
2	7	98	C	N1-C2-O2	-6.06	115.27	118.90
1	5	994	G	O5'-P-OP2	-6.05	100.25	105.70
1	5	2234	G	N9-C4-C5	-6.05	102.98	105.40
45	6	1518	C	N3-C2-O2	-6.05	117.66	121.90
1	1	2617	U	N3-C4-C5	-6.05	110.97	114.60
1	1	2842	U	N1-C2-O2	6.05	127.03	122.80
1	5	2726	C	N3-C2-O2	-6.04	117.67	121.90
1	5	420	G	N3-C4-N9	6.04	129.63	126.00
45	6	337	G	N7-C8-N9	6.04	116.12	113.10
1	1	1092	C	C6-N1-C2	-6.04	117.88	120.30
1	1	2819	A	O5'-P-OP2	-6.04	100.26	105.70
1	5	644	G	N1-C6-O6	-6.04	116.28	119.90
45	2	704	C	O4'-C1'-N1	6.04	113.03	108.20
1	5	3362	A	O4'-C1'-N9	6.04	113.03	108.20
1	1	1607	U	P-O3'-C3'	6.03	126.94	119.70
1	5	345	G	C5-C6-O6	-6.03	124.98	128.60
1	5	2179	C	C2-N3-C4	6.03	122.92	119.90
45	6	1728	A	C8-N9-C4	6.03	108.21	105.80
1	1	1151	U	N1-C2-N3	6.03	118.52	114.90
1	5	3094	A	N1-C2-N3	6.03	132.31	129.30
45	6	1025	A	N1-C6-N6	6.02	122.22	118.60
1	1	2407	C	N3-C4-C5	6.02	124.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	s1	231	LEU	CA-CB-CG	6.02	129.15	115.30
1	5	2872	A	C6-C5-N7	-6.02	128.09	132.30
1	1	2870	C	C2-N1-C1'	-6.02	112.18	118.80
1	1	2996	U	C2-N1-C1'	6.02	124.92	117.70
45	6	1560	U	C2-N1-C1'	6.02	124.92	117.70
1	5	1134	G	N9-C4-C5	6.01	107.81	105.40
45	6	1580	C	N1-C2-O2	-6.01	115.29	118.90
45	2	194	U	O4'-C1'-N1	6.01	113.01	108.20
43	Q2	93	LEU	CA-CB-CG	6.01	129.12	115.30
55	S9	3	ARG	C-N-CA	-6.01	106.68	121.70
45	6	1361	U	C6-N1-C1'	-6.01	112.79	121.20
1	1	2964	G	C4-N9-C1'	-6.00	118.69	126.50
45	2	1280	C	N3-C4-C5	-6.00	119.50	121.90
1	5	1016	C	C6-N1-C2	-6.00	117.90	120.30
1	5	2750	U	C2-N3-C4	-6.00	123.40	127.00
45	6	239	C	P-O3'-C3'	6.00	126.90	119.70
56	c0	83	PRO	N-CA-CB	6.00	110.50	103.30
1	1	1130	A	C8-N9-C4	6.00	108.20	105.80
1	5	3227	A	C2-N3-C4	-6.00	107.60	110.60
1	5	2750	U	C5-C6-N1	-5.99	119.70	122.70
1	5	56	G	C8-N9-C4	5.99	108.80	106.40
1	5	2416	U	O5'-P-OP2	-5.99	100.31	105.70
1	5	1046	A	N1-C2-N3	5.99	132.30	129.30
1	1	3280	U	C2-N1-C1'	-5.99	110.51	117.70
45	2	1246	C	C2-N1-C1'	5.99	125.39	118.80
1	5	3129	A	OP1-P-OP2	5.98	128.57	119.60
45	2	507	U	C2-N1-C1'	5.97	124.87	117.70
1	5	3041	U	N3-C4-O4	-5.97	115.22	119.40
1	1	227	G	N9-C4-C5	-5.97	103.01	105.40
1	5	2948	C	N3-C2-O2	-5.97	117.72	121.90
1	1	2624	G	N7-C8-N9	5.97	116.09	113.10
3	8	113	U	C2-N1-C1'	5.97	124.86	117.70
45	6	1596	C	N3-C2-O2	-5.97	117.72	121.90
1	1	1176	C	N1-C2-O2	-5.97	115.32	118.90
1	5	2348	A	C8-N9-C4	5.97	108.19	105.80
1	1	3092	C	C6-N1-C2	5.97	122.69	120.30
69	D3	9	LEU	CA-CB-CG	5.96	129.02	115.30
45	2	1389	C	N3-C2-O2	-5.96	117.73	121.90
1	5	3362	A	C2-N3-C4	-5.96	107.62	110.60
1	5	274	G	C8-N9-C4	5.96	108.78	106.40
1	5	2733	A	N1-C6-N6	5.96	122.18	118.60
45	6	1560	U	N1-C2-O2	5.96	126.97	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2873	U	C5-C6-N1	-5.96	119.72	122.70
1	5	3362	A	N7-C8-N9	5.96	116.78	113.80
45	6	389	G	C5-C6-O6	-5.95	125.03	128.60
1	5	1851	G	N7-C8-N9	5.95	116.08	113.10
1	1	725	G	C8-N9-C4	5.95	108.78	106.40
1	5	964	G	C8-N9-C4	-5.95	104.02	106.40
1	5	1210	U	C5-C6-N1	-5.95	119.73	122.70
45	6	1480	G	C8-N9-C4	-5.95	104.02	106.40
1	5	1778	G	N3-C2-N2	-5.95	115.74	119.90
1	1	637	C	N1-C2-O2	5.94	122.47	118.90
1	1	1761	C	C2-N1-C1'	5.94	125.34	118.80
3	8	99	C	N1-C2-O2	5.94	122.47	118.90
1	1	942	U	N1-C2-N3	5.94	118.46	114.90
1	5	2567	C	C2-N1-C1'	5.94	125.33	118.80
1	1	2366	C	N3-C4-C5	5.93	124.27	121.90
45	2	1096	C	C6-N1-C2	5.93	122.67	120.30
1	5	40	A	O5'-P-OP1	-5.93	100.36	105.70
58	C2	103	LEU	CA-CB-CG	5.93	128.94	115.30
1	1	799	G	C8-N9-C4	5.93	108.77	106.40
1	5	2393	G	OP1-P-OP2	5.93	128.49	119.60
45	6	542	A	P-O3'-C3'	5.93	126.82	119.70
1	5	3245	A	C5-C6-N1	-5.93	114.74	117.70
45	6	103	A	C4-C5-C6	5.93	119.96	117.00
45	6	1535	U	P-O3'-C3'	5.93	126.81	119.70
1	5	637	C	N3-C4-C5	5.92	124.27	121.90
1	5	3078	U	OP2-P-O3'	5.92	118.23	105.20
45	6	337	G	N3-C2-N2	5.92	124.05	119.90
1	1	1103	A	N1-C6-N6	5.92	122.15	118.60
1	1	2366	C	C6-N1-C2	5.92	122.67	120.30
3	8	26	U	N3-C2-O2	-5.92	118.05	122.20
45	6	1600	A	OP1-P-O3'	5.92	118.23	105.20
1	1	1484	U	P-O3'-C3'	5.92	126.80	119.70
1	5	2384	A	C5-C6-N6	-5.92	118.97	123.70
1	5	1894	U	C5-C6-N1	-5.92	119.74	122.70
1	5	1405	U	C5-C4-O4	5.91	129.45	125.90
1	1	591	G	N9-C4-C5	-5.91	103.03	105.40
45	2	539	G	C8-N9-C1'	-5.91	119.31	127.00
45	2	831	U	P-O3'-C3'	5.91	126.79	119.70
1	5	3209	A	O4'-C1'-N9	5.91	112.93	108.20
45	6	1492	A	O4'-C1'-N9	5.91	112.93	108.20
1	5	1374	G	C5-C6-O6	-5.91	125.06	128.60
1	5	3275	U	O4'-C1'-N1	5.91	112.92	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2836	C	C4-C5-C6	5.90	120.35	117.40
1	5	1308	A	N1-C6-N6	-5.90	115.06	118.60
1	1	943	U	N1-C2-O2	-5.89	118.67	122.80
1	1	964	G	C5-N7-C8	-5.89	101.35	104.30
1	1	1639	C	C6-N1-C2	-5.89	117.94	120.30
1	1	1716	U	P-O3'-C3'	5.89	126.77	119.70
1	1	793	C	C6-N1-C2	-5.89	117.94	120.30
45	6	1361	U	N1-C2-O2	5.89	126.92	122.80
1	5	2662	G	P-O3'-C3'	5.89	126.76	119.70
1	1	637	C	C2-N1-C1'	5.88	125.27	118.80
1	5	1057	A	N9-C4-C5	-5.88	103.45	105.80
45	6	1097	U	P-O3'-C3'	5.88	126.76	119.70
1	5	2808	A	N1-C6-N6	5.87	122.12	118.60
45	2	1767	G	C4-N9-C1'	-5.87	118.87	126.50
1	5	1297	C	N3-C2-O2	5.87	126.01	121.90
45	6	17	C	C6-N1-C2	-5.87	117.95	120.30
45	6	1240	U	C5-C6-N1	5.87	125.64	122.70
45	6	1610	G	N3-C4-N9	5.87	129.52	126.00
45	2	959	U	C2-N1-C1'	5.86	124.74	117.70
45	2	192	U	C5-C6-N1	5.86	125.63	122.70
1	1	676	G	N3-C4-N9	5.86	129.51	126.00
1	1	2150	G	N1-C6-O6	5.86	123.41	119.90
17	m6	27	LEU	CA-CB-CG	-5.86	101.83	115.30
1	1	3182	G	N3-C4-N9	5.85	129.51	126.00
1	1	2863	G	C8-N9-C4	5.85	108.74	106.40
1	1	1183	C	C5-C6-N1	-5.85	118.08	121.00
45	6	1490	C	P-O3'-C3'	5.85	126.72	119.70
1	1	2726	C	C6-N1-C2	-5.84	117.96	120.30
1	1	1633	C	C5-C6-N1	5.84	123.92	121.00
1	5	2572	C	N1-C2-O2	5.84	122.41	118.90
45	6	1476	C	C6-N1-C2	-5.84	117.96	120.30
45	2	1258	U	N3-C2-O2	-5.84	118.11	122.20
45	2	577	G	C5-C6-O6	-5.84	125.10	128.60
58	c2	103	LEU	CA-CB-CG	5.84	128.72	115.30
1	5	1017	C	C2-N1-C1'	5.83	125.22	118.80
1	5	2283	G	C6-C5-N7	-5.83	126.90	130.40
1	1	48	A	C2-N3-C4	-5.83	107.69	110.60
1	5	1335	C	N1-C2-O2	-5.83	115.40	118.90
3	8	125	U	C2-N1-C1'	5.83	124.69	117.70
1	1	166	C	C6-N1-C2	-5.82	117.97	120.30
1	1	1037	C	C2-N1-C1'	5.82	125.20	118.80
1	1	637	C	P-O3'-C3'	5.82	126.69	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2614	G	C4-N9-C1'	5.82	134.07	126.50
3	8	113	U	N1-C2-O2	5.82	126.88	122.80
1	1	745	C	C6-N1-C2	5.82	122.63	120.30
1	1	1407	A	N1-C6-N6	-5.82	115.11	118.60
3	4	137	C	C6-N1-C2	5.82	122.63	120.30
1	1	1352	A	P-O3'-C3'	5.82	126.68	119.70
1	5	2572	C	C2-N1-C1'	5.82	125.20	118.80
1	1	2871	G	O5'-P-OP2	-5.81	100.47	105.70
1	1	1197	A	N1-C6-N6	5.81	122.08	118.60
3	8	113	U	N3-C2-O2	-5.81	118.14	122.20
1	5	345	G	N3-C4-N9	5.80	129.48	126.00
1	5	1200	A	C6-C5-N7	-5.80	128.24	132.30
1	1	227	G	N3-C4-N9	5.80	129.48	126.00
45	2	704	C	C6-N1-C1'	-5.80	113.84	120.80
45	2	73	U	OP1-P-O3'	5.80	117.96	105.20
1	1	546	C	C5-C6-N1	5.80	123.90	121.00
1	1	993	G	O5'-P-OP2	-5.80	100.48	105.70
1	5	32	U	N3-C2-O2	-5.80	118.14	122.20
1	5	430	U	C5-C6-N1	-5.80	119.80	122.70
1	1	55	G	N9-C4-C5	-5.79	103.08	105.40
1	5	1453	A	C8-N9-C4	5.79	108.12	105.80
1	5	1866	C	N1-C2-O2	5.79	122.38	118.90
45	6	1746	A	C8-N9-C4	5.79	108.12	105.80
1	5	3088	G	C8-N9-C4	5.79	108.72	106.40
1	5	2291	A	N1-C6-N6	5.79	122.07	118.60
45	6	1000	C	N3-C2-O2	-5.79	117.85	121.90
2	7	112	G	N1-C6-O6	-5.79	116.43	119.90
1	5	2169	G	C4-N9-C1'	-5.78	118.98	126.50
1	5	2356	A	C8-N9-C4	5.78	108.11	105.80
1	1	3153	U	N3-C2-O2	-5.78	118.16	122.20
1	1	3106	A	N1-C6-N6	-5.78	115.13	118.60
1	5	930	U	OP1-P-O3'	5.78	117.91	105.20
1	5	1481	A	C8-N9-C4	-5.78	103.49	105.80
1	5	2186	U	C5-C4-O4	5.77	129.36	125.90
1	1	3154	C	C5-C6-N1	5.77	123.89	121.00
45	2	1389	C	C6-N1-C2	-5.77	117.99	120.30
45	6	1456	C	C5-C6-N1	-5.77	118.11	121.00
1	5	96	G	N1-C6-O6	5.77	123.36	119.90
2	7	76	A	O4'-C1'-N9	5.77	112.82	108.20
1	5	1796	G	C8-N9-C4	5.76	108.70	106.40
50	S4	194	THR	N-CA-C	5.76	126.54	111.00
1	5	1174	G	C8-N9-C4	-5.76	104.10	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	938	C	C6-N1-C2	5.75	122.60	120.30
1	5	2750	U	N1-C2-N3	5.75	118.35	114.90
1	1	637	C	C5-C6-N1	5.75	123.88	121.00
1	1	995	U	N3-C2-O2	-5.75	118.17	122.20
1	5	2306	C	C2-N1-C1'	5.75	125.13	118.80
1	5	644	G	C4-C5-N7	-5.75	108.50	110.80
1	5	3011	A	N1-C6-N6	-5.75	115.15	118.60
45	6	901	G	O4'-C1'-N9	5.75	112.80	108.20
1	5	2872	A	C4-C5-N7	5.75	113.57	110.70
45	6	17	C	C5-C6-N1	5.75	123.87	121.00
1	1	2147	A	N7-C8-N9	-5.75	110.93	113.80
1	5	1866	C	C2-N1-C1'	5.75	125.12	118.80
1	1	2719	U	N1-C2-O2	-5.74	118.78	122.80
1	1	1307	G	P-O3'-C3'	5.74	126.58	119.70
1	1	1761	C	N1-C2-O2	5.74	122.34	118.90
1	1	3028	G	C6-C5-N7	-5.74	126.96	130.40
1	5	693	A	O5'-P-OP1	-5.74	100.54	105.70
45	6	864	U	C6-N1-C2	-5.74	117.56	121.00
1	1	937	G	N1-C6-O6	5.73	123.34	119.90
1	5	883	A	O5'-P-OP1	-5.73	100.54	105.70
1	5	2283	G	C5-C6-O6	-5.73	125.16	128.60
1	5	776	U	N3-C2-O2	-5.72	118.19	122.20
1	5	2169	G	N9-C4-C5	5.72	107.69	105.40
1	1	345	G	N1-C6-O6	5.72	123.33	119.90
1	1	1197	A	C5-C6-N6	-5.72	119.12	123.70
45	2	1432	U	O4'-C1'-N1	5.72	112.78	108.20
1	1	621	A	OP1-P-O3'	5.72	117.78	105.20
1	5	1131	G	N3-C4-C5	5.72	131.46	128.60
1	1	2996	U	N1-C2-O2	5.72	126.80	122.80
45	6	1675	C	C6-N1-C2	5.72	122.59	120.30
1	1	1103	A	N9-C4-C5	-5.71	103.51	105.80
1	1	2868	U	N1-C2-O2	5.71	126.80	122.80
1	5	632	G	O5'-P-OP1	5.71	117.56	110.70
1	1	439	C	C6-N1-C1'	-5.71	113.94	120.80
1	1	2281	A	O4'-C1'-N9	5.71	112.77	108.20
1	1	1292	C	C5-C6-N1	-5.71	118.15	121.00
1	5	34	A	O5'-P-OP2	-5.71	100.56	105.70
1	5	1057	A	C8-N9-C4	5.71	108.08	105.80
1	5	3195	U	C2-N1-C1'	5.71	124.55	117.70
45	6	1747	G	C5-C6-O6	-5.71	125.17	128.60
45	6	1767	G	O5'-P-OP1	-5.71	100.56	105.70
1	5	2934	A	N1-C6-N6	5.71	122.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2385	G	N3-C4-N9	-5.70	122.58	126.00
1	5	101	G	O5'-P-OP1	5.70	117.55	110.70
1	5	2371	G	C8-N9-C1'	-5.70	119.59	127.00
1	1	2602	G	C8-N9-C4	5.70	108.68	106.40
45	2	275	C	C6-N1-C2	-5.70	118.02	120.30
1	1	2941	A	O5'-P-OP2	-5.70	100.57	105.70
1	5	491	C	C6-N1-C1'	-5.70	113.96	120.80
45	6	1389	C	C6-N1-C1'	-5.70	113.96	120.80
1	5	1592	G	C5-C6-O6	-5.69	125.19	128.60
45	6	1142	A	C5-C6-N1	5.69	120.55	117.70
45	2	75	U	C5-C6-N1	5.69	125.54	122.70
45	6	194	U	N3-C2-O2	-5.69	118.22	122.20
45	6	1559	A	C2-N3-C4	-5.69	107.76	110.60
1	5	867	G	N1-C6-O6	5.68	123.31	119.90
1	5	3376	A	C8-N9-C4	-5.68	103.53	105.80
1	1	1495	U	C5-C6-N1	-5.68	119.86	122.70
1	1	3280	U	O4'-C1'-N1	5.67	112.74	108.20
1	5	1306	G	C8-N9-C4	-5.67	104.13	106.40
1	5	2553	U	C6-N1-C1'	-5.67	113.25	121.20
1	1	3000	A	C8-N9-C4	5.67	108.07	105.80
1	5	2356	A	N9-C4-C5	-5.67	103.53	105.80
1	5	1152	G	O5'-P-OP1	-5.67	100.60	105.70
1	5	1493	G	C5-C6-N1	5.67	114.33	111.50
1	5	3164	C	O4'-C1'-N1	5.67	112.73	108.20
1	1	650	C	N3-C4-N4	5.67	121.97	118.00
1	1	2541	U	P-O3'-C3'	5.67	126.50	119.70
1	5	3307	A	C8-N9-C4	5.67	108.07	105.80
1	1	650	C	N3-C2-O2	5.66	125.86	121.90
1	5	1085	A	C4-C5-C6	5.66	119.83	117.00
1	5	2124	G	N9-C4-C5	5.66	107.67	105.40
45	6	1600	A	N7-C8-N9	5.66	116.63	113.80
1	1	3043	C	C6-N1-C2	5.66	122.56	120.30
1	5	420	G	C4-C5-N7	5.66	113.06	110.80
1	1	2979	U	C5-C4-O4	5.66	129.29	125.90
1	5	420	G	C6-N1-C2	-5.66	121.71	125.10
1	5	827	A	C5-C6-N1	5.66	120.53	117.70
1	1	1188	U	N3-C2-O2	-5.65	118.24	122.20
1	1	1820	U	P-O3'-C3'	5.65	126.48	119.70
45	2	704	C	N3-C2-O2	-5.65	117.94	121.90
1	5	2541	U	N3-C2-O2	-5.65	118.24	122.20
1	5	3218	A	N1-C6-N6	5.65	121.99	118.60
45	6	609	U	N3-C2-O2	-5.64	118.25	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	641	C	O4'-C1'-N1	5.64	112.71	108.20
1	1	3344	A	C8-N9-C4	-5.64	103.54	105.80
1	5	1898	G	C6-C5-N7	5.64	133.78	130.40
1	1	2617	U	N3-C2-O2	-5.64	118.25	122.20
1	1	776	U	C5-C6-N1	-5.64	119.88	122.70
1	5	1579	C	C5-C6-N1	5.64	123.82	121.00
2	7	1	G	C8-N9-C1'	-5.64	119.67	127.00
45	6	1161	C	N1-C2-O2	-5.64	115.52	118.90
1	1	2658	G	N1-C6-O6	5.63	123.28	119.90
1	1	2808	A	O4'-C1'-N9	-5.63	103.69	108.20
1	1	2979	U	C6-N1-C1'	5.63	129.09	121.20
1	1	127	G	N1-C6-O6	5.63	123.28	119.90
1	5	827	A	C2-N3-C4	5.63	113.41	110.60
1	5	1200	A	P-O3'-C3'	5.63	126.45	119.70
1	5	1892	G	C4-N9-C1'	-5.63	119.19	126.50
1	5	3046	A	N1-C2-N3	5.63	132.11	129.30
45	6	1146	G	O5'-P-OP2	-5.63	100.64	105.70
45	2	577	G	C6-C5-N7	-5.62	127.03	130.40
45	2	794	U	C5-C6-N1	5.62	125.51	122.70
1	5	1211	U	C5-C6-N1	-5.62	119.89	122.70
1	5	2909	U	O5'-P-OP1	-5.62	100.64	105.70
45	6	793	A	P-O3'-C3'	5.62	126.45	119.70
1	5	1507	G	C4-C5-N7	5.62	113.05	110.80
1	5	1903	U	C5-C4-O4	-5.62	122.53	125.90
1	5	2830	G	N3-C4-C5	5.62	131.41	128.60
1	5	2980	U	O5'-P-OP2	-5.62	100.64	105.70
45	6	1241	G	C8-N9-C1'	-5.62	119.70	127.00
1	5	1582	C	N1-C2-O2	5.62	122.27	118.90
45	2	783	G	N9-C4-C5	-5.62	103.15	105.40
1	5	491	C	C5-C6-N1	5.62	123.81	121.00
1	1	54	C	C6-N1-C2	5.61	122.55	120.30
1	1	2260	U	C6-N1-C2	-5.61	117.63	121.00
1	5	679	U	C5-C4-O4	5.61	129.27	125.90
45	6	1599	C	N1-C2-O2	-5.61	115.53	118.90
1	1	715	A	C8-N9-C4	-5.61	103.56	105.80
1	5	2302	G	N1-C6-O6	-5.61	116.53	119.90
45	6	813	U	C6-N1-C1'	-5.61	113.34	121.20
45	6	1747	G	C8-N9-C4	5.61	108.64	106.40
1	5	827	A	N1-C6-N6	-5.61	115.23	118.60
45	2	639	U	N1-C2-O2	5.61	126.72	122.80
1	5	2330	C	N3-C2-O2	5.60	125.82	121.90
45	6	314	C	C6-N1-C2	-5.60	118.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1374	G	N1-C6-O6	5.60	123.26	119.90
1	1	1178	G	OP1-P-OP2	5.60	128.00	119.60
1	1	1555	U	C5-C6-N1	-5.60	119.90	122.70
1	1	2278	C	N1-C2-N3	-5.59	115.28	119.20
1	5	637	C	C6-N1-C2	5.59	122.54	120.30
1	5	2745	G	C4-C5-N7	5.59	113.04	110.80
1	5	1156	C	N1-C2-O2	-5.58	115.55	118.90
1	5	776	U	C5-C4-O4	5.58	129.25	125.90
1	5	2940	A	C6-N1-C2	-5.58	115.25	118.60
1	1	3196	U	O4'-C1'-N1	5.58	112.67	108.20
1	5	1637	A	N1-C6-N6	-5.58	115.25	118.60
1	5	1449	A	C8-N9-C4	-5.58	103.57	105.80
1	1	496	C	C6-N1-C2	-5.58	118.07	120.30
1	1	2873	U	N3-C4-O4	-5.58	115.50	119.40
45	6	77	U	O5'-P-OP1	-5.58	100.68	105.70
45	6	453	U	C5-C6-N1	5.58	125.49	122.70
3	4	38	U	N3-C2-O2	-5.57	118.30	122.20
1	1	1740	U	N3-C2-O2	-5.57	118.30	122.20
1	5	1118	C	N3-C4-C5	5.57	124.13	121.90
45	2	453	U	C6-N1-C2	-5.57	117.66	121.00
1	5	2627	C	N1-C2-O2	-5.57	115.56	118.90
45	2	1291	G	C5-N7-C8	-5.57	101.52	104.30
45	6	440	U	N3-C2-O2	-5.57	118.30	122.20
1	1	410	U	N1-C2-O2	-5.57	118.90	122.80
1	5	2299	A	N1-C6-N6	5.57	121.94	118.60
54	S8	29	LEU	CA-CB-CG	5.56	128.09	115.30
1	5	41	G	C4-C5-N7	5.56	113.02	110.80
1	5	1639	C	C6-N1-C2	-5.56	118.08	120.30
48	s2	113	LEU	CA-CB-CG	5.56	128.09	115.30
45	2	747	C	C6-N1-C2	-5.56	118.08	120.30
45	2	934	C	C5-C6-N1	5.56	123.78	121.00
1	1	227	G	C4-N9-C1'	5.55	133.72	126.50
1	1	435	C	C6-N1-C2	5.55	122.52	120.30
1	5	1579	C	N3-C2-O2	-5.55	118.01	121.90
45	2	782	U	OP2-P-O3'	5.55	117.41	105.20
1	5	1103	A	N1-C2-N3	-5.55	126.52	129.30
1	5	2744	U	O5'-P-OP2	-5.55	100.70	105.70
1	5	1882	G	N1-C6-O6	5.54	123.23	119.90
1	1	3355	U	C2-N1-C1'	5.54	124.35	117.70
1	5	2382	G	C6-N1-C2	-5.54	121.78	125.10
45	6	1414	U	C2-N1-C1'	5.54	124.35	117.70
35	O4	51	LEU	CA-CB-CG	5.54	128.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	912	U	N1-C2-O2	5.54	126.68	122.80
1	1	1878	G	C4-N9-C1'	5.54	133.70	126.50
1	5	718	G	C4-N9-C1'	5.54	133.70	126.50
1	1	1150	A	N1-C6-N6	-5.54	115.28	118.60
45	2	926	A	N1-C2-N3	5.53	132.07	129.30
1	5	1889	G	N7-C8-N9	5.53	115.87	113.10
1	5	2169	G	N1-C2-N2	5.53	121.18	116.20
1	5	1047	A	C8-N9-C4	-5.53	103.59	105.80
1	1	637	C	C6-N1-C1'	-5.53	114.17	120.80
1	5	345	G	C8-N9-C1'	-5.53	119.81	127.00
1	5	1892	G	N3-C4-N9	-5.53	122.68	126.00
1	1	42	C	C5-C6-N1	-5.53	118.24	121.00
1	1	1016	C	O4'-C1'-N1	5.53	112.62	108.20
2	3	99	G	N1-C6-O6	5.53	123.22	119.90
1	5	1589	A	N1-C6-N6	5.53	121.92	118.60
45	6	895	G	C5-C6-N1	-5.53	108.74	111.50
45	6	1490	C	C5-C6-N1	5.52	123.76	121.00
1	1	2218	G	C8-N9-C4	5.52	108.61	106.40
1	5	2281	A	O5'-P-OP2	-5.52	100.73	105.70
1	5	1902	G	C2-N3-C4	-5.52	109.14	111.90
45	6	320	U	C2-N1-C1'	5.52	124.32	117.70
1	1	2154	U	O5'-P-OP1	-5.51	100.74	105.70
1	5	714	G	OP1-P-OP2	5.51	127.87	119.60
1	5	2624	G	C5-C6-O6	-5.51	125.29	128.60
1	5	2852	C	C5-C6-N1	-5.51	118.24	121.00
1	1	2818	U	OP2-P-O3'	5.51	117.33	105.20
45	2	240	U	O5'-P-OP1	-5.51	100.74	105.70
45	2	1363	U	C2-N1-C1'	5.51	124.31	117.70
1	5	1866	C	C6-N1-C1'	-5.51	114.19	120.80
45	2	192	U	C6-N1-C1'	-5.51	113.49	121.20
45	2	1568	C	P-O3'-C3'	5.51	126.31	119.70
1	5	216	G	O5'-P-OP1	-5.51	100.74	105.70
1	1	65	A	O5'-P-OP2	-5.51	100.74	105.70
1	1	628	A	N1-C2-N3	5.51	132.05	129.30
45	2	1082	C	C2-N1-C1'	5.51	124.86	118.80
1	5	438	A	OP2-P-O3'	5.51	117.31	105.20
1	1	1633	C	C2-N1-C1'	5.50	124.85	118.80
1	5	2167	A	C8-N9-C4	-5.50	103.60	105.80
1	1	1385	C	C6-N1-C2	5.50	122.50	120.30
1	1	1724	U	P-O3'-C3'	5.50	126.30	119.70
1	5	2102	U	C6-N1-C2	-5.50	117.70	121.00
1	1	3141	A	C6-N1-C2	-5.50	115.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1868	G	N1-C6-O6	5.50	123.20	119.90
45	6	151	G	N3-C2-N2	-5.50	116.05	119.90
45	6	858	G	C8-N9-C1'	-5.50	119.85	127.00
45	2	191	C	C6-N1-C2	-5.50	118.10	120.30
45	2	507	U	N3-C2-O2	-5.50	118.35	122.20
1	5	2392	C	C2-N1-C1'	-5.50	112.75	118.80
45	2	192	U	N3-C2-O2	-5.49	118.36	122.20
1	1	1408	G	N1-C6-O6	-5.49	116.61	119.90
1	5	877	C	N1-C2-O2	5.49	122.19	118.90
1	5	1161	G	O5'-P-OP2	-5.49	100.76	105.70
1	5	2315	G	O5'-P-OP1	-5.49	100.76	105.70
1	5	2772	C	P-O3'-C3'	5.49	126.29	119.70
1	1	224	C	C5-C6-N1	5.49	123.74	121.00
1	5	1177	G	N3-C4-N9	5.49	129.29	126.00
45	6	308	C	C2-N1-C1'	-5.49	112.77	118.80
56	c0	91	TYR	C-N-CA	5.49	135.41	121.70
45	2	913	G	P-O3'-C3'	5.48	126.28	119.70
1	1	645	A	N1-C6-N6	-5.48	115.31	118.60
1	5	1487	G	C8-N9-C4	-5.48	104.21	106.40
1	5	2400	G	P-O3'-C3'	5.48	126.28	119.70
1	5	1049	C	C6-N1-C2	-5.48	118.11	120.30
1	5	2728	G	C6-C5-N7	-5.48	127.11	130.40
1	5	1903	U	C5-C6-N1	5.48	125.44	122.70
45	6	1058	U	P-O3'-C3'	5.48	126.27	119.70
1	1	2838	A	C8-N9-C4	5.48	107.99	105.80
45	6	426	G	C4-N9-C1'	5.48	133.62	126.50
1	5	2355	G	C5-C6-O6	-5.47	125.31	128.60
45	6	308	C	C2-N3-C4	-5.47	117.16	119.90
1	5	2895	G	N1-C6-O6	-5.47	116.62	119.90
1	1	2624	G	C8-N9-C4	-5.47	104.21	106.40
1	5	424	G	N1-C6-O6	5.47	123.18	119.90
1	5	1868	G	C6-C5-N7	-5.47	127.12	130.40
45	6	610	G	C4-N9-C1'	5.47	133.61	126.50
1	1	3181	C	N3-C2-O2	-5.47	118.07	121.90
1	5	3046	A	C2-N3-C4	-5.47	107.87	110.60
45	6	1588	G	N1-C6-O6	-5.47	116.62	119.90
1	1	1303	A	N1-C6-N6	5.46	121.88	118.60
1	5	2395	G	O5'-P-OP2	-5.46	100.78	105.70
45	6	25	C	C5-C6-N1	5.46	123.73	121.00
1	5	3330	A	C8-N9-C4	5.46	107.98	105.80
45	6	158	U	P-O3'-C3'	5.46	126.25	119.70
1	5	1762	C	C6-N1-C2	-5.46	118.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2156	C	C5-C6-N1	-5.46	118.27	121.00
1	5	959	C	P-O3'-C3'	5.46	126.25	119.70
1	5	2936	A	O5'-P-OP2	-5.46	100.79	105.70
1	1	1581	C	N3-C2-O2	-5.46	118.08	121.90
1	5	916	G	N3-C2-N2	5.46	123.72	119.90
1	5	3144	G	O5'-P-OP1	-5.46	100.79	105.70
1	5	1209	G	OP1-P-OP2	5.45	127.78	119.60
1	5	3109	G	N1-C6-O6	5.45	123.17	119.90
45	6	1257	U	N1-C2-O2	5.45	126.62	122.80
1	5	3213	A	O5'-P-OP2	-5.45	100.79	105.70
1	1	2950	G	N1-C6-O6	-5.45	116.63	119.90
1	5	805	G	C8-N9-C4	5.45	108.58	106.40
1	5	2619	G	C5-C6-O6	-5.45	125.33	128.60
1	1	2639	G	C8-N9-C4	-5.45	104.22	106.40
1	5	43	A	C6-N1-C2	5.45	121.87	118.60
1	5	92	G	C5-N7-C8	-5.45	101.58	104.30
1	5	283	G	C4-N9-C1'	5.45	133.58	126.50
3	4	120	C	C6-N1-C2	-5.44	118.12	120.30
47	S1	61	LEU	CA-CB-CG	5.44	127.82	115.30
45	6	747	C	C6-N1-C2	-5.44	118.12	120.30
1	5	43	A	N1-C2-N3	-5.44	126.58	129.30
1	5	2353	G	OP1-P-O3'	5.44	117.17	105.20
1	1	1123	U	C5-C6-N1	-5.43	119.98	122.70
1	5	1851	G	C5-N7-C8	-5.43	101.58	104.30
1	1	1349	G	C8-N9-C4	-5.43	104.23	106.40
1	1	1351	U	C6-N1-C2	-5.43	117.74	121.00
1	5	2354	C	N1-C2-O2	-5.43	115.64	118.90
1	5	3058	U	C2-N1-C1'	5.43	124.22	117.70
45	6	36	C	C6-N1-C2	5.43	122.47	120.30
1	1	2777	G	N3-C4-N9	-5.43	122.74	126.00
1	5	1716	U	OP1-P-O3'	5.43	117.14	105.20
1	5	2624	G	C6-C5-N7	-5.43	127.14	130.40
1	5	2902	A	C2-N3-C4	-5.43	107.89	110.60
1	5	1085	A	N7-C8-N9	5.43	116.51	113.80
1	5	1496	C	C2-N1-C1'	5.43	124.77	118.80
1	5	2607	G	N3-C4-N9	5.43	129.26	126.00
1	5	2205	U	C2-N1-C1'	5.42	124.21	117.70
1	5	2234	G	N1-C6-O6	5.42	123.16	119.90
1	5	2401	A	N7-C8-N9	5.42	116.51	113.80
1	1	2863	G	N3-C4-C5	5.42	131.31	128.60
1	1	1878	G	N3-C4-N9	5.42	129.25	126.00
1	5	654	C	C5-C6-N1	-5.42	118.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1415	U	C5-C6-N1	-5.42	119.99	122.70
1	5	3094	A	C2-N3-C4	-5.42	107.89	110.60
45	6	941	A	N1-C6-N6	-5.42	115.35	118.60
1	1	251	G	C4-N9-C1'	5.41	133.54	126.50
45	2	1767	G	N3-C4-N9	-5.41	122.75	126.00
1	5	1796	G	N3-C4-C5	5.41	131.31	128.60
1	5	324	A	N1-C6-N6	5.41	121.85	118.60
1	1	1220	U	N1-C2-O2	5.41	126.59	122.80
45	6	103	A	C6-N1-C2	-5.41	115.36	118.60
45	6	830	U	C6-N1-C1'	-5.41	113.63	121.20
1	1	437	G	C8-N9-C4	-5.41	104.24	106.40
1	5	2826	U	N3-C2-O2	-5.41	118.42	122.20
1	5	760	G	O4'-C1'-N9	5.40	112.52	108.20
1	1	1432	C	N3-C4-C5	-5.40	119.74	121.90
1	1	2627	C	N1-C2-O2	-5.40	115.66	118.90
1	5	2939	G	C8-N9-C4	5.40	108.56	106.40
1	5	1057	A	N1-C6-N6	5.40	121.84	118.60
1	1	1864	A	N1-C6-N6	5.40	121.84	118.60
45	2	783	G	C4-C5-N7	5.40	112.96	110.80
1	5	1122	U	C6-N1-C2	-5.40	117.76	121.00
1	1	2145	A	N1-C6-N6	5.39	121.84	118.60
1	1	2827	U	C5-C4-O4	5.39	129.14	125.90
3	4	20	U	C2-N3-C4	-5.39	123.76	127.00
1	5	2842	U	C6-N1-C1'	-5.39	113.65	121.20
1	5	2963	C	N1-C2-O2	-5.39	115.66	118.90
1	1	2175	U	N3-C2-O2	-5.39	118.42	122.20
1	1	2831	G	C5-C6-O6	-5.39	125.36	128.60
45	6	1052	U	C6-N1-C2	-5.39	117.76	121.00
1	5	998	A	N9-C4-C5	5.39	107.96	105.80
1	5	1310	G	N1-C6-O6	-5.39	116.67	119.90
1	1	1111	U	C2-N3-C4	-5.39	123.77	127.00
1	1	3375	A	C8-N9-C4	-5.39	103.64	105.80
45	6	426	G	N3-C4-C5	-5.39	125.91	128.60
1	5	3217	C	C6-N1-C2	5.38	122.45	120.30
1	5	2338	C	C6-N1-C2	-5.38	118.15	120.30
1	5	3178	A	C5-C6-N6	-5.38	119.39	123.70
3	8	106	C	O5'-P-OP2	-5.38	100.86	105.70
45	6	1118	G	N3-C4-C5	5.38	131.29	128.60
1	1	2550	U	N1-C2-O2	5.38	126.57	122.80
1	5	491	C	C6-N1-C2	-5.38	118.15	120.30
1	5	1383	G	C5-C6-N1	-5.38	108.81	111.50
45	6	1572	G	C4-C5-N7	5.38	112.95	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	6	813	U	N1-C2-O2	5.38	126.57	122.80
45	6	1663	G	C8-N9-C4	5.38	108.55	106.40
1	1	3153	U	N1-C2-O2	5.38	126.56	122.80
1	1	1092	C	N1-C2-O2	5.38	122.13	118.90
1	5	927	C	C6-N1-C2	-5.38	118.15	120.30
2	7	75	G	C8-N9-C4	5.38	108.55	106.40
45	6	194	U	C5-C6-N1	5.37	125.39	122.70
1	5	1604	G	C4-N9-C1'	5.37	133.48	126.50
21	n0	99	ARG	NE-CZ-NH1	-5.37	117.61	120.30
45	6	1000	C	C2-N1-C1'	5.37	124.71	118.80
1	1	2609	A	O5'-P-OP1	5.37	117.14	110.70
1	5	916	G	N3-C4-N9	5.37	129.22	126.00
1	1	2726	C	N1-C2-O2	5.37	122.12	118.90
45	2	1518	C	C6-N1-C2	-5.37	118.15	120.30
1	5	1311	G	O5'-P-OP2	-5.37	100.87	105.70
1	5	2148	U	C2-N1-C1'	-5.37	111.26	117.70
1	5	3262	U	N3-C2-O2	-5.37	118.44	122.20
1	5	75	G	N1-C6-O6	5.37	123.12	119.90
1	5	2313	A	C6-N1-C2	-5.37	115.38	118.60
45	6	1004	U	N1-C2-N3	5.37	118.12	114.90
1	1	199	A	O4'-C1'-N9	5.36	112.49	108.20
1	5	1192	C	OP1-P-OP2	5.36	127.65	119.60
1	5	2318	U	C5-C6-N1	-5.36	120.02	122.70
3	8	100	U	C6-N1-C1'	-5.36	113.69	121.20
1	5	2365	C	C2-N3-C4	-5.36	117.22	119.90
1	1	3028	G	N1-C6-O6	5.36	123.11	119.90
3	4	125	U	C2-N1-C1'	5.36	124.13	117.70
45	6	321	C	OP1-P-O3'	5.36	116.98	105.20
1	1	2093	A	N3-C4-C5	-5.36	123.05	126.80
1	5	1064	A	O4'-C1'-N9	-5.35	103.92	108.20
45	6	1759	C	C6-N1-C2	5.35	122.44	120.30
1	1	947	G	C8-N9-C4	5.35	108.54	106.40
1	1	2191	U	C5-C6-N1	5.35	125.38	122.70
1	1	1279	C	C5-C6-N1	5.35	123.68	121.00
1	1	1388	U	C5-C6-N1	-5.35	120.03	122.70
1	1	3195	U	N1-C2-O2	5.35	126.55	122.80
1	1	1308	A	N7-C8-N9	5.35	116.47	113.80
45	2	1560	U	N3-C2-O2	-5.35	118.46	122.20
1	5	3317	U	P-O3'-C3'	5.35	126.12	119.70
1	1	2827	U	N1-C2-O2	-5.34	119.06	122.80
1	1	2831	G	C4-C5-N7	5.34	112.94	110.80
13	M1	112	LEU	CA-CB-CG	5.34	127.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1770	G	C8-N9-C4	-5.34	104.26	106.40
1	5	2371	G	C8-N9-C4	5.34	108.54	106.40
1	5	2607	G	C5-C6-O6	-5.34	125.39	128.60
1	1	890	C	N1-C2-O2	5.34	122.10	118.90
1	1	1092	C	N3-C2-O2	-5.34	118.16	121.90
1	1	1932	A	N1-C6-N6	5.34	121.80	118.60
1	1	2983	C	N1-C2-N3	5.34	122.94	119.20
1	5	2619	G	N1-C6-O6	5.34	123.10	119.90
1	5	3094	A	C5-C6-N6	5.34	127.97	123.70
3	8	15	G	C4-C5-N7	5.34	112.94	110.80
1	1	1149	G	O5'-P-OP2	-5.34	100.90	105.70
1	1	2300	G	C2-N3-C4	-5.34	109.23	111.90
45	6	1573	A	P-O3'-C3'	5.34	126.11	119.70
1	1	1430	U	N3-C2-O2	5.34	125.94	122.20
45	2	232	U	N3-C2-O2	-5.34	118.46	122.20
1	5	2393	G	C4-C5-N7	5.34	112.93	110.80
1	1	1192	C	N3-C2-O2	-5.33	118.17	121.90
1	1	1308	A	C8-N9-C4	-5.33	103.67	105.80
1	5	804	C	C6-N1-C2	5.33	122.43	120.30
45	6	322	G	O4'-C1'-N9	-5.33	103.94	108.20
1	1	1395	G	O5'-P-OP2	-5.33	100.90	105.70
1	1	1482	A	C4-C5-N7	5.33	113.36	110.70
1	5	609	G	C5-C6-O6	-5.33	125.40	128.60
1	5	279	U	OP1-P-O3'	5.33	116.92	105.20
1	5	969	C	N3-C2-O2	5.33	125.63	121.90
1	5	3276	G	P-O3'-C3'	5.33	126.09	119.70
45	6	1052	U	N3-C2-O2	-5.33	118.47	122.20
1	1	1061	A	N1-C6-N6	5.32	121.79	118.60
1	5	2169	G	N3-C2-N2	-5.32	116.17	119.90
1	5	3382	U	C2-N1-C1'	5.32	124.09	117.70
45	6	1304	G	C8-N9-C4	5.32	108.53	106.40
1	5	963	G	C4-C5-N7	5.32	112.93	110.80
1	5	2800	G	N3-C4-N9	5.32	129.19	126.00
1	5	1907	C	C4-C5-C6	5.32	120.06	117.40
1	1	3180	A	C2-N3-C4	-5.32	107.94	110.60
1	1	3355	U	N3-C2-O2	-5.32	118.48	122.20
1	5	709	A	N1-C6-N6	5.32	121.79	118.60
45	6	187	G	OP1-P-O3'	5.32	116.89	105.20
45	2	577	G	C4-C5-N7	5.31	112.92	110.80
1	5	293	C	C6-N1-C2	5.31	122.42	120.30
1	5	2358	A	C8-N9-C4	5.31	107.92	105.80
1	5	3087	A	N7-C8-N9	-5.31	111.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1016	C	C5-C6-N1	5.31	123.65	121.00
1	1	1904	C	C2-N1-C1'	5.31	124.64	118.80
1	5	247	C	N1-C2-O2	5.31	122.08	118.90
1	5	2350	C	N3-C2-O2	-5.31	118.19	121.90
45	6	1214	U	N1-C2-O2	5.31	126.52	122.80
1	1	315	C	C6-N1-C2	-5.31	118.18	120.30
1	1	2899	C	C6-N1-C2	-5.31	118.18	120.30
1	5	1560	G	P-O3'-C3'	5.31	126.07	119.70
1	1	1177	G	N1-C6-O6	5.30	123.08	119.90
1	1	1349	G	P-O3'-C3'	5.30	126.06	119.70
45	6	1413	U	N1-C2-O2	5.30	126.51	122.80
1	1	3204	C	C6-N1-C2	-5.30	118.18	120.30
1	5	2624	G	N1-C6-O6	5.30	123.08	119.90
3	8	82	U	N1-C2-O2	5.30	126.51	122.80
1	1	1501	U	N3-C2-O2	5.30	125.91	122.20
1	1	2404	A	N1-C2-N3	5.30	131.95	129.30
45	6	1246	C	C2-N1-C1'	5.30	124.63	118.80
1	1	2353	G	C4-C5-N7	5.29	112.92	110.80
55	S9	93	LEU	CA-CB-CG	5.29	127.48	115.30
1	1	1366	A	C8-N9-C4	-5.29	103.68	105.80
1	1	2624	G	N1-C6-O6	5.29	123.08	119.90
1	1	2647	A	O5'-P-OP2	-5.29	100.94	105.70
1	5	406	G	N1-C6-O6	-5.29	116.72	119.90
1	5	1071	U	O4'-C1'-N1	5.29	112.43	108.20
45	6	934	C	C6-N1-C2	-5.29	118.18	120.30
1	1	2607	G	N1-C6-O6	5.29	123.07	119.90
1	5	1542	G	C4-N9-C1'	5.29	133.38	126.50
1	5	2353	G	C5-C6-O6	-5.29	125.43	128.60
45	6	991	G	N1-C6-O6	5.29	123.07	119.90
45	6	1199	G	C6-C5-N7	-5.29	127.23	130.40
1	1	2614	G	C8-N9-C1'	-5.29	120.13	127.00
1	5	2234	G	C8-N9-C4	5.29	108.51	106.40
1	5	2400	G	C6-C5-N7	-5.29	127.23	130.40
45	2	145	A	C8-N9-C4	-5.28	103.69	105.80
1	5	2186	U	N3-C2-O2	-5.28	118.50	122.20
1	1	776	U	N1-C2-N3	5.28	118.07	114.90
1	1	791	A	C8-N9-C4	5.28	107.91	105.80
1	1	2715	A	O5'-P-OP1	-5.28	100.95	105.70
45	6	217	A	P-O3'-C3'	5.28	126.04	119.70
59	c3	139	TRP	CA-CB-CG	-5.28	103.66	113.70
45	2	747	C	C2-N1-C1'	5.28	124.61	118.80
45	2	1644	C	C6-N1-C2	-5.28	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1007	U	C5-C6-N1	-5.28	120.06	122.70
1	5	1196	C	N1-C2-O2	5.28	122.07	118.90
1	5	1759	C	C6-N1-C1'	-5.28	114.46	120.80
45	6	19	A	N1-C6-N6	5.28	121.77	118.60
45	6	272	U	P-O3'-C3'	5.28	126.04	119.70
45	6	639	U	N1-C2-O2	5.28	126.50	122.80
1	1	227	G	C6-C5-N7	-5.28	127.23	130.40
1	1	1155	C	N1-C2-O2	5.28	122.07	118.90
1	1	2278	C	C2-N3-C4	5.28	122.54	119.90
1	1	622	A	O5'-P-OP2	-5.28	100.95	105.70
2	3	93	C	C5-C4-N4	-5.28	116.51	120.20
1	5	2622	C	C6-N1-C2	5.28	122.41	120.30
1	1	1395	G	O5'-P-OP1	5.28	117.03	110.70
45	2	241	U	N3-C2-O2	-5.28	118.51	122.20
1	5	2211	U	C4-C5-C6	5.28	122.87	119.70
1	5	3004	C	C6-N1-C2	5.28	122.41	120.30
1	5	3154	C	C2-N1-C1'	5.28	124.60	118.80
1	5	1943	C	C6-N1-C2	-5.27	118.19	120.30
1	5	1210	U	C5-C4-O4	5.27	129.06	125.90
1	1	365	A	C8-N9-C4	-5.27	103.69	105.80
1	1	1303	A	N9-C4-C5	-5.27	103.69	105.80
1	1	3214	U	N1-C2-O2	5.27	126.49	122.80
1	5	1046	A	N9-C4-C5	5.27	107.91	105.80
1	5	1177	G	C6-C5-N7	-5.27	127.24	130.40
1	5	2349	U	C5-C4-O4	-5.27	122.74	125.90
1	5	2353	G	C6-C5-N7	-5.27	127.24	130.40
45	6	1653	C	C5-C4-N4	-5.27	116.51	120.20
1	1	981	U	C5-C6-N1	5.27	125.33	122.70
1	5	414	U	O5'-P-OP2	-5.27	100.96	105.70
45	6	1614	A	C4-C5-N7	5.27	113.33	110.70
45	6	1770	U	C5-C4-O4	-5.27	122.74	125.90
1	1	645	A	C5-C6-N1	5.27	120.33	117.70
45	2	1274	C	O4'-C1'-N1	5.27	112.41	108.20
1	5	916	G	N1-C2-N2	-5.27	111.46	116.20
1	5	2306	C	C2-N3-C4	5.27	122.53	119.90
1	5	3088	G	N1-C6-O6	5.27	123.06	119.90
1	5	2818	U	O5'-P-OP1	-5.26	100.96	105.70
1	5	2886	U	O5'-P-OP2	-5.26	100.96	105.70
45	6	1081	A	C2-N3-C4	5.26	113.23	110.60
1	5	3307	A	OP1-P-OP2	5.26	127.49	119.60
1	1	1199	C	C6-N1-C2	5.26	122.41	120.30
1	1	2404	A	O4'-C1'-N9	5.26	112.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L4	313	LEU	CA-CB-CG	5.26	127.40	115.30
1	5	2834	G	C5-C6-O6	5.26	131.76	128.60
3	8	20	U	O5'-P-OP2	-5.26	100.96	105.70
1	1	2145	A	C5-C6-N6	-5.26	119.49	123.70
1	5	2290	C	C6-N1-C2	5.26	122.40	120.30
1	1	1482	A	C5-N7-C8	-5.26	101.27	103.90
1	5	718	G	C8-N9-C1'	-5.26	120.17	127.00
1	5	3335	A	C2-N3-C4	-5.26	107.97	110.60
1	1	2169	G	C4-N9-C1'	-5.25	119.67	126.50
1	5	33	G	N3-C4-N9	-5.25	122.85	126.00
1	1	2624	G	C6-C5-N7	-5.25	127.25	130.40
1	5	3079	U	OP1-P-OP2	-5.25	111.72	119.60
1	1	1148	G	C8-N9-C1'	5.25	133.83	127.00
1	5	1496	C	C6-N1-C1'	-5.25	114.50	120.80
45	6	610	G	O4'-C1'-N9	5.25	112.40	108.20
1	1	923	C	C6-N1-C2	5.25	122.40	120.30
1	5	718	G	N3-C4-N9	5.25	129.15	126.00
1	5	3133	C	C2-N3-C4	-5.25	117.28	119.90
1	1	1445	U	N1-C2-O2	-5.25	119.13	122.80
1	1	2957	G	C2-N3-C4	-5.25	109.28	111.90
3	4	17	A	N1-C6-N6	5.25	121.75	118.60
45	2	241	U	C5-C6-N1	5.25	125.32	122.70
1	5	2939	G	N7-C8-N9	-5.25	110.48	113.10
45	6	1027	A	C8-N9-C4	-5.25	103.70	105.80
1	1	2964	G	N1-C6-O6	-5.24	116.75	119.90
1	5	994	G	C8-N9-C4	5.24	108.50	106.40
1	5	2392	C	C5-C6-N1	-5.24	118.38	121.00
45	6	553	G	C6-C5-N7	-5.24	127.25	130.40
45	6	1776	A	N1-C6-N6	5.24	121.75	118.60
1	1	2377	G	N1-C6-O6	-5.24	116.75	119.90
1	5	648	C	N3-C4-C5	-5.24	119.80	121.90
1	5	801	A	N1-C6-N6	5.24	121.75	118.60
1	5	2396	G	N1-C6-O6	-5.24	116.75	119.90
1	5	2397	A	C6-N1-C2	-5.24	115.45	118.60
1	1	1382	G	N3-C4-C5	5.24	131.22	128.60
1	5	2643	A	C2-N3-C4	-5.24	107.98	110.60
1	1	3353	G	C4-N9-C1'	5.24	133.31	126.50
1	5	216	G	C8-N9-C4	-5.24	104.31	106.40
1	5	1197	A	C6-N1-C2	-5.24	115.46	118.60
1	5	2623	G	C5-C6-O6	-5.24	125.46	128.60
1	5	3117	C	C6-N1-C2	5.24	122.40	120.30
5	L3	224	HIS	C-N-CA	-5.24	111.30	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1374	G	N9-C4-C5	-5.24	103.31	105.40
73	d7	61	THR	C-N-CA	5.24	134.79	121.70
1	5	2623	G	C8-N9-C4	5.23	108.49	106.40
1	1	345	G	C5-C6-O6	-5.23	125.46	128.60
1	5	2939	G	C5-N7-C8	5.23	106.92	104.30
2	7	112	G	N3-C4-C5	-5.23	125.98	128.60
1	1	2541	U	C2-N1-C1'	5.23	123.97	117.70
1	5	963	G	N1-C6-O6	5.23	123.04	119.90
1	5	1481	A	N7-C8-N9	5.23	116.41	113.80
1	5	3154	C	P-O3'-C3'	5.23	125.97	119.70
1	5	2154	U	N3-C2-O2	5.23	125.86	122.20
1	5	2324	A	C5-N7-C8	-5.23	101.29	103.90
1	1	3376	A	C8-N9-C4	-5.23	103.71	105.80
45	6	1390	U	N3-C2-O2	-5.23	118.54	122.20
1	1	315	C	C5-C6-N1	5.22	123.61	121.00
1	1	937	G	C5-N7-C8	-5.22	101.69	104.30
1	5	998	A	C8-N9-C4	-5.22	103.71	105.80
1	5	1181	U	N1-C2-N3	5.22	118.03	114.90
1	5	1495	U	N3-C2-O2	-5.22	118.54	122.20
45	6	1016	C	C6-N1-C2	5.22	122.39	120.30
1	1	3278	C	C6-N1-C1'	-5.22	114.53	120.80
1	5	33	G	C4-C5-N7	-5.22	108.71	110.80
1	5	878	G	C8-N9-C4	-5.22	104.31	106.40
1	1	2704	A	N1-C2-N3	5.22	131.91	129.30
1	5	2635	A	O5'-P-OP2	-5.22	101.00	105.70
1	5	2642	A	C8-N9-C4	-5.22	103.71	105.80
45	2	453	U	C5-C6-N1	5.22	125.31	122.70
1	5	221	A	O5'-P-OP2	5.22	116.96	110.70
1	5	2249	G	C3'-C2'-C1'	-5.22	97.33	101.50
36	o5	41	LEU	CA-CB-CG	5.22	127.30	115.30
1	1	44	U	C5-C6-N1	-5.21	120.09	122.70
45	2	241	U	C6-N1-C2	-5.21	117.87	121.00
1	1	1345	G	C2-N3-C4	-5.21	109.29	111.90
1	1	220	G	C4-C5-N7	5.21	112.89	110.80
1	1	1878	G	C8-N9-C1'	-5.21	120.22	127.00
1	5	345	G	C4-C5-N7	5.21	112.89	110.80
1	1	857	G	N1-C6-O6	5.21	123.03	119.90
45	2	1060	U	O5'-P-OP2	-5.21	101.01	105.70
1	1	589	A	N1-C6-N6	-5.21	115.48	118.60
1	1	2897	A	O4'-C1'-N9	5.21	112.37	108.20
45	6	1614	A	C2-N3-C4	-5.21	108.00	110.60
1	5	918	C	N1-C2-O2	-5.21	115.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	424	G	N9-C4-C5	5.20	107.48	105.40
1	1	1815	U	P-O3'-C3'	5.20	125.94	119.70
47	S1	96	LEU	CA-CB-CG	5.20	127.27	115.30
1	5	2818	U	O4'-C1'-N1	-5.20	104.04	108.20
45	2	47	A	C8-N9-C4	-5.20	103.72	105.80
45	2	103	A	P-O3'-C3'	5.20	125.94	119.70
45	2	1573	A	OP2-P-O3'	5.20	116.64	105.20
45	6	1207	C	C6-N1-C2	5.20	122.38	120.30
45	6	103	A	C4-N9-C1'	5.20	135.66	126.30
45	6	1614	A	C6-C5-N7	-5.20	128.66	132.30
1	1	1197	A	C4-C5-N7	5.20	113.30	110.70
1	5	746	A	O5'-P-OP2	-5.19	101.03	105.70
1	5	2607	G	N1-C6-O6	5.19	123.02	119.90
1	1	2857	C	OP2-P-O3'	5.19	116.62	105.20
1	1	3137	C	C2-N1-C1'	-5.19	113.09	118.80
1	5	2879	C	N1-C2-O2	-5.19	115.79	118.90
1	1	650	C	N1-C2-O2	-5.19	115.79	118.90
1	1	1316	C	N3-C4-C5	-5.19	119.83	121.90
1	5	1394	A	C8-N9-C4	5.19	107.88	105.80
45	6	66	U	P-O3'-C3'	5.19	125.93	119.70
45	6	336	G	O5'-P-OP1	-5.19	101.03	105.70
45	6	1025	A	C6-C5-N7	-5.19	128.67	132.30
1	1	2772	C	P-O3'-C3'	5.19	125.92	119.70
45	2	1600	A	OP1-P-O3'	5.18	116.61	105.20
1	5	2119	A	C5-C6-N6	-5.18	119.55	123.70
1	1	1495	U	C2-N1-C1'	-5.18	111.48	117.70
1	5	374	A	P-O3'-C3'	5.18	125.92	119.70
1	5	1116	G	N9-C4-C5	5.18	107.47	105.40
45	6	1754	A	C8-N9-C4	-5.18	103.73	105.80
1	1	1061	A	C8-N9-C4	5.18	107.87	105.80
1	5	428	A	C2-N3-C4	-5.18	108.01	110.60
1	1	2772	C	C2-N1-C1'	5.18	124.50	118.80
3	4	117	C	C6-N1-C2	5.18	122.37	120.30
1	5	2737	C	N1-C2-O2	-5.18	115.79	118.90
1	5	3104	U	C5-C6-N1	-5.18	120.11	122.70
1	1	329	U	C2-N1-C1'	5.18	123.91	117.70
1	1	1220	U	N3-C2-O2	-5.18	118.58	122.20
1	1	1167	U	C5-C6-N1	-5.17	120.11	122.70
45	6	339	C	C5-C6-N1	5.17	123.59	121.00
1	1	404	G	C4-C5-N7	5.17	112.87	110.80
1	5	2375	G	O4'-C1'-N9	5.17	112.34	108.20
45	6	1258	U	C2-N1-C1'	5.17	123.91	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1037	C	N1-C2-O2	5.17	122.00	118.90
45	6	1780	G	C4-C5-N7	5.17	112.87	110.80
1	1	2323	G	N1-C6-O6	5.17	123.00	119.90
1	5	1107	C	C5-C6-N1	-5.17	118.42	121.00
1	1	437	G	C5-C6-O6	-5.17	125.50	128.60
45	2	1473	U	N3-C2-O2	-5.17	118.58	122.20
53	s7	118	LEU	CA-CB-CG	5.17	127.19	115.30
45	2	1059	U	N3-C2-O2	-5.17	118.58	122.20
1	5	2283	G	N9-C4-C5	-5.17	103.33	105.40
17	m6	84	LEU	CA-CB-CG	-5.17	103.42	115.30
1	1	1847	A	N1-C6-N6	-5.17	115.50	118.60
1	5	2800	G	N3-C4-C5	-5.17	126.02	128.60
1	5	3133	C	C5-C6-N1	-5.17	118.42	121.00
1	1	1116	G	N7-C8-N9	5.16	115.68	113.10
1	1	1407	A	N9-C4-C5	5.16	107.86	105.80
45	2	553	G	C6-C5-N7	-5.16	127.30	130.40
2	7	18	C	C5-C6-N1	-5.16	118.42	121.00
1	1	1411	C	O5'-P-OP1	5.16	116.89	110.70
1	5	3035	A	N1-C6-N6	5.16	121.70	118.60
1	1	2983	C	N1-C2-O2	-5.16	115.80	118.90
26	N5	34	LEU	CA-CB-CG	5.16	127.17	115.30
1	5	1542	G	C8-N9-C4	-5.16	104.34	106.40
1	1	362	U	OP1-P-O3'	5.16	116.55	105.20
1	1	1323	G	C5-C6-O6	-5.16	125.50	128.60
1	5	1878	G	C4-N9-C1'	5.16	133.21	126.50
1	1	884	A	N1-C6-N6	5.16	121.69	118.60
1	5	633	C	N1-C2-O2	-5.16	115.81	118.90
1	5	2330	C	C6-N1-C2	5.16	122.36	120.30
45	6	1492	A	C8-N9-C4	-5.16	103.74	105.80
1	1	345	G	N3-C4-N9	5.16	129.09	126.00
1	1	439	C	C5-C6-N1	5.16	123.58	121.00
1	1	2839	G	O5'-P-OP2	-5.16	101.06	105.70
1	1	3057	U	C5-C4-O4	5.16	128.99	125.90
1	5	1205	A	N1-C6-N6	-5.16	115.51	118.60
2	7	26	C	C6-N1-C2	-5.16	118.24	120.30
45	6	1559	A	N1-C6-N6	5.16	121.69	118.60
1	1	718	G	C5-N7-C8	-5.15	101.72	104.30
1	1	1839	A	C4-C5-N7	-5.15	108.12	110.70
45	2	783	G	N1-C6-O6	5.15	122.99	119.90
1	5	2762	A	C8-N9-C4	5.15	107.86	105.80
2	7	35	C	C6-N1-C2	5.15	122.36	120.30
45	2	238	U	C2-N1-C1'	5.15	123.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	639	U	N3-C2-O2	-5.15	118.59	122.20
1	5	943	U	N1-C2-N3	5.15	117.99	114.90
1	5	161	G	N7-C8-N9	5.15	115.67	113.10
45	6	1795	U	N1-C2-O2	-5.15	119.19	122.80
1	1	3030	G	C4-N9-C1'	5.15	133.19	126.50
45	6	109	G	C8-N9-C4	5.15	108.46	106.40
45	2	1456	C	C2-N1-C1'	5.15	124.46	118.80
1	5	1525	G	C4-N9-C1'	5.15	133.19	126.50
45	6	1775	U	C5-C6-N1	-5.15	120.13	122.70
1	5	3081	C	C6-N1-C2	5.14	122.36	120.30
1	5	2393	G	C5-N7-C8	-5.14	101.73	104.30
1	5	3390	G	N1-C6-O6	5.14	122.98	119.90
1	1	2821	C	N3-C2-O2	-5.14	118.30	121.90
1	5	844	G	C8-N9-C4	5.14	108.45	106.40
1	5	969	C	N1-C2-O2	-5.14	115.82	118.90
1	5	1307	G	OP2-P-O3'	5.14	116.50	105.20
45	6	1596	C	C5-C4-N4	5.14	123.80	120.20
45	2	912	U	C5-C6-N1	5.14	125.27	122.70
1	5	998	A	N1-C2-N3	5.13	131.87	129.30
1	5	2607	G	C6-C5-N7	-5.13	127.32	130.40
1	1	3382	U	C5-C6-N1	5.13	125.27	122.70
45	2	539	G	N3-C4-N9	5.13	129.08	126.00
1	5	1239	C	C2-N1-C1'	5.13	124.45	118.80
1	1	650	C	C5-C4-N4	-5.13	116.61	120.20
45	2	553	G	N1-C6-O6	5.13	122.98	119.90
1	5	3195	U	O4'-C1'-N1	-5.13	104.09	108.20
45	6	1769	U	O5'-P-OP2	-5.13	101.08	105.70
1	1	2847	A	C8-N9-C4	5.13	107.85	105.80
45	2	1784	C	C6-N1-C2	-5.13	118.25	120.30
1	5	1375	G	C8-N9-C4	-5.13	104.35	106.40
1	5	1815	U	P-O3'-C3'	5.13	125.86	119.70
1	5	1892	G	N3-C4-C5	5.13	131.16	128.60
1	5	2418	G	N3-C4-N9	5.13	129.08	126.00
1	1	1796	G	C4-C5-N7	-5.13	108.75	110.80
1	5	1321	G	C8-N9-C4	5.13	108.45	106.40
1	5	2348	A	N7-C8-N9	-5.13	111.24	113.80
1	5	2349	U	C5-C6-N1	5.13	125.26	122.70
1	5	2996	U	C2-N1-C1'	5.13	123.85	117.70
1	1	2862	U	C6-N1-C2	5.12	124.08	121.00
1	5	1152	G	N1-C2-N2	5.12	120.81	116.20
1	1	1204	A	N1-C6-N6	5.12	121.67	118.60
1	5	630	A	N7-C8-N9	-5.12	111.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2369	G	C5-C6-O6	-5.12	125.53	128.60
1	5	2797	C	N3-C4-C5	-5.12	119.85	121.90
45	6	1780	G	N1-C6-O6	5.12	122.97	119.90
1	5	1905	G	C8-N9-C4	5.12	108.45	106.40
1	5	2621	G	C2-N3-C4	-5.12	109.34	111.90
45	6	1390	U	O4'-C1'-N1	5.12	112.30	108.20
1	1	2607	G	OP2-P-O3'	5.12	116.46	105.20
45	2	389	G	N1-C6-O6	5.12	122.97	119.90
1	5	1306	G	C4-C5-N7	5.12	112.85	110.80
45	6	577	G	N3-C2-N2	5.12	123.48	119.90
1	1	2362	C	N1-C2-O2	5.11	121.97	118.90
1	1	2658	G	N9-C4-C5	-5.11	103.35	105.40
1	1	3155	U	N1-C2-O2	5.11	126.38	122.80
1	5	1134	G	C8-N9-C4	-5.11	104.36	106.40
1	5	2382	G	N1-C6-O6	-5.11	116.83	119.90
1	5	2635	A	C8-N9-C4	-5.11	103.75	105.80
12	m0	76	MET	CA-CB-CG	5.11	121.99	113.30
45	6	1241	G	N7-C8-N9	5.11	115.66	113.10
3	4	63	G	N7-C8-N9	5.11	115.66	113.10
45	2	1456	C	O4'-C1'-N1	5.11	112.29	108.20
21	n0	148	LEU	CA-CB-CG	5.11	127.06	115.30
1	1	2277	C	C6-N1-C2	5.11	122.34	120.30
1	1	3121	U	OP1-P-O3'	5.11	116.44	105.20
1	1	3362	A	C5-N7-C8	-5.11	101.35	103.90
45	2	794	U	N3-C2-O2	-5.11	118.62	122.20
1	1	3028	G	N3-C4-N9	5.11	129.06	126.00
2	3	101	G	C5-C6-O6	-5.11	125.54	128.60
1	5	813	G	C5-C6-N1	-5.10	108.95	111.50
1	5	835	G	O4'-C1'-N9	5.10	112.28	108.20
1	1	3179	U	C5-C6-N1	-5.10	120.15	122.70
45	2	1207	C	C6-N1-C2	5.10	122.34	120.30
1	5	2419	A	O5'-P-OP2	-5.10	101.11	105.70
1	5	1787	A	N1-C6-N6	5.10	121.66	118.60
45	2	4	C	C5-C6-N1	5.10	123.55	121.00
63	C7	73	LEU	CA-CB-CG	5.10	127.03	115.30
13	M1	172	LEU	CA-CB-CG	5.10	127.03	115.30
1	5	3341	U	C5-C4-O4	-5.10	122.84	125.90
1	5	1060	U	O5'-P-OP2	-5.10	101.11	105.70
1	1	1222	G	N3-C4-C5	-5.09	126.05	128.60
1	1	2205	U	C5-C6-N1	5.09	125.25	122.70
1	1	2396	G	C5-C6-O6	5.09	131.66	128.60
1	5	3329	U	N1-C2-N3	5.09	117.96	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	73	C	C6-N1-C2	-5.09	118.26	120.30
1	1	2401	A	C5-C6-N1	-5.09	115.16	117.70
2	7	1	G	N3-C4-N9	5.09	129.05	126.00
45	2	1573	A	P-O3'-C3'	5.09	125.81	119.70
1	5	2615	G	C5-C6-O6	-5.09	125.55	128.60
1	1	2278	C	C4-C5-C6	-5.09	114.86	117.40
45	6	639	U	N3-C2-O2	-5.09	118.64	122.20
45	6	1354	G	C8-N9-C4	-5.09	104.37	106.40
1	5	2830	G	C2-N3-C4	-5.08	109.36	111.90
1	5	2971	A	N7-C8-N9	5.08	116.34	113.80
1	1	1854	C	C6-N1-C2	-5.08	118.27	120.30
1	5	938	C	N3-C4-C5	5.08	123.93	121.90
1	5	1197	A	N1-C2-N3	5.08	131.84	129.30
45	6	389	G	N3-C4-C5	5.08	131.14	128.60
1	5	2819	A	C8-N9-C4	5.08	107.83	105.80
45	6	1654	G	C6-C5-N7	-5.08	127.35	130.40
1	1	2649	A	C8-N9-C4	-5.08	103.77	105.80
1	5	1052	U	C5-C6-N1	5.08	125.24	122.70
1	1	648	C	N3-C2-O2	-5.08	118.35	121.90
1	1	3218	A	P-O3'-C3'	5.08	125.80	119.70
45	2	1747	G	C5-C6-N1	-5.08	108.96	111.50
45	6	901	G	C4-N9-C1'	5.08	133.10	126.50
1	5	1311	G	C8-N9-C4	5.08	108.43	106.40
1	5	1902	G	C4-C5-N7	5.08	112.83	110.80
1	5	3016	A	C5-C6-N6	-5.08	119.64	123.70
1	1	1201	C	C2-N3-C4	5.07	122.44	119.90
3	4	125	U	N1-C2-O2	5.07	126.35	122.80
1	5	2423	U	N1-C2-O2	5.07	126.35	122.80
45	6	1207	C	C6-N1-C1'	-5.07	114.71	120.80
1	1	1176	C	C6-N1-C2	5.07	122.33	120.30
1	5	1806	A	N7-C8-N9	-5.07	111.27	113.80
45	6	1418	G	N1-C6-O6	5.07	122.94	119.90
1	1	1060	U	N3-C2-O2	-5.07	118.65	122.20
1	1	3076	C	C6-N1-C2	-5.07	118.27	120.30
1	5	2624	G	C4-C5-N7	5.07	112.83	110.80
1	1	751	A	C8-N9-C4	-5.07	103.77	105.80
1	5	692	A	N1-C6-N6	5.07	121.64	118.60
1	5	1194	G	C5-C6-O6	-5.07	125.56	128.60
62	C6	39	VAL	C-N-CA	5.07	134.36	121.70
2	7	73	C	N1-C2-O2	5.07	121.94	118.90
1	1	3352	U	N1-C2-O2	5.06	126.34	122.80
45	2	1761	U	P-O3'-C3'	5.06	125.77	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	410	U	C6-N1-C2	-5.06	117.96	121.00
1	5	1778	G	N3-C4-C5	5.06	131.13	128.60
58	c2	58	LEU	CA-CB-CG	5.06	126.94	115.30
1	5	644	G	C5-N7-C8	5.06	106.83	104.30
1	1	1151	U	C5-C6-N1	5.06	125.23	122.70
1	1	3028	G	C4-N9-C1'	5.06	133.07	126.50
1	1	2169	G	C8-N9-C1'	5.05	133.57	127.00
1	1	2817	A	N3-C4-C5	-5.05	123.26	126.80
1	5	112	U	O4'-C1'-N1	5.05	112.24	108.20
2	7	68	C	N3-C2-O2	-5.05	118.36	121.90
1	1	202	G	C4-C5-N7	5.05	112.82	110.80
1	5	2911	A	O5'-P-OP2	-5.05	101.15	105.70
1	1	620	U	C6-N1-C2	-5.05	117.97	121.00
1	1	98	G	N7-C8-N9	-5.05	110.58	113.10
3	4	31	G	C8-N9-C4	5.05	108.42	106.40
1	5	684	G	N7-C8-N9	-5.04	110.58	113.10
1	5	1394	A	N7-C8-N9	-5.04	111.28	113.80
1	1	26	A	N1-C6-N6	5.04	121.63	118.60
1	1	1482	A	N7-C8-N9	5.04	116.32	113.80
1	1	2842	U	N3-C2-O2	-5.04	118.67	122.20
45	2	75	U	C6-N1-C2	-5.04	117.97	121.00
1	5	1483	G	O4'-C1'-N9	5.04	112.23	108.20
1	1	437	G	C5-N7-C8	-5.04	101.78	104.30
1	5	206	G	C2-N3-C4	5.04	114.42	111.90
1	5	2915	U	N1-C2-O2	-5.04	119.27	122.80
1	5	3217	C	C2-N1-C1'	-5.04	113.25	118.80
45	6	1029	U	N3-C2-O2	-5.04	118.67	122.20
45	2	794	U	C6-N1-C1'	-5.04	114.15	121.20
45	2	1000	C	C2-N1-C1'	5.04	124.34	118.80
45	6	1414	U	N1-C2-O2	5.04	126.33	122.80
45	2	75	U	O4'-C1'-N1	-5.04	104.17	108.20
72	D6	64	LEU	CA-CB-CG	5.04	126.88	115.30
1	5	394	G	O5'-P-OP1	-5.04	101.17	105.70
1	1	1210	U	C5-C4-O4	5.03	128.92	125.90
1	1	2759	U	N3-C4-O4	5.03	122.92	119.40
1	1	2827	U	C6-N1-C1'	5.03	128.25	121.20
1	5	776	U	N3-C4-O4	-5.03	115.88	119.40
1	5	2427	U	C5-C6-N1	-5.03	120.18	122.70
45	6	1258	U	N3-C2-O2	-5.03	118.68	122.20
52	s6	212	LEU	CA-CB-CG	5.03	126.88	115.30
1	1	2186	U	C5-C4-O4	5.03	128.92	125.90
1	1	3278	C	N3-C2-O2	-5.03	118.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	85	G	N1-C6-O6	5.03	122.92	119.90
1	1	908	G	C8-N9-C1'	-5.03	120.46	127.00
1	1	3190	C	N3-C2-O2	-5.03	118.38	121.90
1	1	3195	U	P-O3'-C3'	5.03	125.74	119.70
1	5	1482	A	O5'-P-OP2	-5.03	101.17	105.70
1	5	3246	G	C5-C6-N1	-5.03	108.98	111.50
1	1	908	G	O4'-C1'-N9	-5.03	104.18	108.20
1	1	1121	U	C5-C6-N1	-5.03	120.19	122.70
45	6	136	C	C2-N1-C1'	5.03	124.33	118.80
1	1	1037	C	C6-N1-C2	-5.03	118.29	120.30
1	5	1889	G	C5-N7-C8	-5.03	101.79	104.30
2	3	74	C	N1-C2-O2	5.02	121.91	118.90
45	2	1657	U	C5-C6-N1	5.02	125.21	122.70
79	sM	43	ASP	CB-CG-OD2	5.02	122.82	118.30
1	5	1525	G	N3-C4-C5	-5.02	126.09	128.60
1	5	3040	A	O5'-P-OP1	-5.02	101.18	105.70
2	7	93	C	O5'-P-OP1	5.02	116.73	110.70
45	6	1122	G	N1-C6-O6	5.02	122.91	119.90
45	6	1187	U	C6-N1-C2	-5.02	117.99	121.00
1	1	197	G	C8-N9-C4	-5.02	104.39	106.40
1	5	591	G	C5-C6-N1	-5.02	108.99	111.50
9	17	229	PHE	CB-CG-CD1	5.02	124.31	120.80
45	6	1354	G	N7-C8-N9	5.02	115.61	113.10
1	5	2186	U	N3-C4-O4	-5.02	115.89	119.40
50	s4	260	GLY	N-CA-C	5.02	125.64	113.10
1	5	2405	C	C5-C6-N1	-5.01	118.49	121.00
45	6	295	A	C8-N9-C4	5.01	107.81	105.80
45	6	1103	U	C5-C4-O4	5.01	128.91	125.90
1	1	2201	G	OP1-P-OP2	-5.01	112.09	119.60
1	1	3189	G	C6-C5-N7	-5.01	127.39	130.40
45	6	543	C	N3-C2-O2	-5.01	118.39	121.90
1	1	2842	U	C6-N1-C1'	-5.01	114.19	121.20
1	1	2895	G	C8-N9-C4	5.01	108.40	106.40
1	5	1113	G	OP2-P-O3'	5.01	116.21	105.20
45	6	1118	G	N3-C4-N9	-5.01	123.00	126.00
1	5	2406	C	N3-C2-O2	5.00	125.40	121.90
45	6	1096	C	C5-C6-N1	-5.00	118.50	121.00
1	1	3382	U	N3-C2-O2	-5.00	118.70	122.20
1	5	2724	U	C5-C6-N1	-5.00	120.20	122.70

There are no chirality outliers.

All (130) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
60	C4	123	SER	Peptide
60	C4	49	LYS	Peptide
61	C5	17	TYR	Peptide
61	C5	28	MET	Peptide
62	C6	40	GLU	Peptide
63	C7	22	PRO	Peptide
63	C7	89	SER	Peptide
64	C8	81	ILE	Peptide
66	D0	118	VAL	Peptide
66	D0	73	GLY	Peptide
67	D1	6	GLY	Peptide
68	D2	54	ASP	Peptide
70	D4	60	PHE	Peptide
71	D5	54	VAL	Peptide
71	D5	94	LYS	Peptide
71	D5	96	SER	Peptide
72	D6	10	ARG	Peptide
72	D6	81	ALA	Peptide
73	D7	49	HIS	Peptide
77	E1	103	LEU	Peptide
77	E1	146	SER	Peptide
77	E1	84	VAL	Peptide
4	L2	48	ILE	Peptide
6	L4	318	LEU	Peptide
7	L5	251	PRO	Peptide
9	L7	29	GLU	Peptide
11	L9	21	LYS	Peptide
12	M0	117	GLY	Peptide
13	M1	11	ASP	Peptide
14	M3	74	GLY	Peptide
15	M4	48	GLY	Peptide
18	M7	120	ASN	Peptide
19	M8	161	LYS	Peptide
21	N0	133	ALA	Peptide
21	N0	3	HIS	Peptide
25	N4	67	VAL	Peptide
25	N4	70	LYS	Peptide
27	N6	83	ASP	Peptide
28	N7	124	ALA	Peptide
29	N8	115	LYS	Peptide
29	N8	30	GLY	Peptide
29	N8	46	ASP	Peptide
30	N9	19	ASN	Peptide

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Mol	Chain	Res	Type	Group
40	O9	3	ALA	Peptide
47	S1	36	SER	Peptide
48	S2	248	SER	Peptide
48	S2	91	ARG	Peptide
50	S4	165	ALA	Peptide
50	S4	192	ILE	Peptide
50	S4	213	SER	Peptide
51	S5	44	ASN	Peptide
52	S6	19	ASP	Peptide
53	S7	111	LYS	Peptide
53	S7	132	PRO	Peptide
53	S7	29	ASN	Peptide
53	S7	31	SER	Peptide
53	S7	64	VAL	Peptide
79	SM	173	GLU	Peptide
79	SM	46	LYS	Peptide
58	c2	82	PRO	Peptide
59	c3	132	VAL	Peptide
60	c4	123	SER	Peptide
60	c4	124	ASP	Peptide
60	c4	131	GLY	Peptide
60	c4	90	ARG	Peptide
61	c5	10	ARG	Peptide
61	c5	50	THR	Peptide
63	c7	112	SER	Peptide
63	c7	82	ASP	Peptide
66	d0	119	ALA	Peptide
66	d0	15	GLN	Peptide
66	d0	48	HIS	Peptide
66	d0	51	VAL	Peptide
66	d0	70	THR	Peptide
68	d2	54	ASP	Peptide
69	d3	44	GLY	Peptide
70	d4	29	HIS	Peptide
70	d4	35	VAL	Peptide
71	d5	85	LYS	Peptide
72	d6	57	SER	Peptide
76	e0	44	PHE	Peptide
77	e1	106	TYR	Peptide
77	e1	87	THR	Peptide
4	l2	143	GLU	Peptide
4	l2	215	ASN	Peptide

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Mol	Chain	Res	Type	Group
5	l3	348	ARG	Peptide
6	l4	339	LEU	Peptide
6	l4	352	ALA	Peptide
7	l5	133	GLU	Peptide
7	l5	177	GLU	Peptide
9	l7	192	GLY	Peptide
9	l7	226	GLY	Peptide
12	m0	217	PHE	Peptide
13	m1	151	SER	Peptide
80	m2	10	UNK	Peptide
80	m2	117	UNK	Peptide
80	m2	153	UNK	Peptide
16	m5	66	VAL	Peptide
23	n2	44	GLU	Peptide
24	n3	41	GLY	Peptide
28	n7	101	PHE	Peptide
28	n7	3	LYS	Peptide
29	n8	66	ALA	Peptide
32	o1	6	ASP	Peptide
33	o2	15	LYS	Peptide
33	o2	39	ASP	Peptide
34	o3	91	ALA	Peptide
35	o4	80	ARG	Peptide
37	o6	2	THR	Peptide
82	p0	92	PRO	Peptide
46	s0	187	ALA	Peptide
46	s0	72	ASP	Peptide
46	s0	94	GLY	Peptide
49	s3	90	ARG	Peptide
51	s5	44	ASN	Peptide
51	s5	99	MET	Peptide
52	s6	150	GLU	Peptide
53	s7	130	VAL	Peptide
53	s7	29	ASN	Peptide
53	s7	64	VAL	Peptide
54	s8	148	ALA	Peptide
54	s8	60	ILE	Peptide
55	s9	88	GLU	Peptide
55	s9	89	ASP	Peptide
79	sM	45	SER	Peptide
79	sM	84	LYS	Peptide
78	sR	184	ASN	Peptide

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Mol	Chain	Res	Type	Group
78	sR	185	GLN	Peptide
78	sR	193	ILE	Peptide
78	sR	30	PRO	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	
4	L2	250/252 (99%)	233 (93%)	17 (7%)	0	100	100
4	l2	250/252 (99%)	227 (91%)	21 (8%)	2 (1%)	19	51
5	L3	384/386 (100%)	349 (91%)	32 (8%)	3 (1%)	19	51
5	l3	384/386 (100%)	354 (92%)	29 (8%)	1 (0%)	41	72
6	L4	359/361 (99%)	323 (90%)	34 (10%)	2 (1%)	25	57
6	l4	359/361 (99%)	313 (87%)	43 (12%)	3 (1%)	19	51
7	L5	294/296 (99%)	266 (90%)	28 (10%)	0	100	100
7	l5	292/296 (99%)	266 (91%)	24 (8%)	2 (1%)	22	55
8	L6	152/176 (86%)	141 (93%)	10 (7%)	1 (1%)	22	55
8	l6	153/176 (87%)	139 (91%)	12 (8%)	2 (1%)	12	39
9	L7	220/223 (99%)	204 (93%)	16 (7%)	0	100	100
9	l7	221/223 (99%)	206 (93%)	13 (6%)	2 (1%)	17	49
10	L8	231/233 (99%)	199 (86%)	30 (13%)	2 (1%)	17	49
10	l8	229/233 (98%)	194 (85%)	33 (14%)	2 (1%)	17	49
11	L9	189/191 (99%)	169 (89%)	20 (11%)	0	100	100
11	l9	189/191 (99%)	176 (93%)	11 (6%)	2 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M0	208/221 (94%)	188 (90%)	19 (9%)	1 (0%)	29	61
12	m0	207/221 (94%)	184 (89%)	23 (11%)	0	100	100
13	M1	167/169 (99%)	142 (85%)	25 (15%)	0	100	100
13	m1	167/169 (99%)	146 (87%)	19 (11%)	2 (1%)	13	41
14	M3	191/194 (98%)	170 (89%)	19 (10%)	2 (1%)	15	46
14	m3	192/194 (99%)	164 (85%)	26 (14%)	2 (1%)	15	46
15	M4	134/137 (98%)	120 (90%)	14 (10%)	0	100	100
15	m4	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
16	M5	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
16	m5	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
17	M6	195/197 (99%)	187 (96%)	7 (4%)	1 (0%)	29	61
17	m6	195/197 (99%)	190 (97%)	5 (3%)	0	100	100
18	M7	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
18	m7	153/184 (83%)	140 (92%)	13 (8%)	0	100	100
19	M8	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
19	m8	183/185 (99%)	167 (91%)	14 (8%)	2 (1%)	14	44
20	M9	180/188 (96%)	169 (94%)	11 (6%)	0	100	100
20	m9	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
21	N0	170/172 (99%)	157 (92%)	13 (8%)	0	100	100
21	n0	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
22	N1	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	8	31
22	n1	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
23	N2	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	15	46
23	n2	96/100 (96%)	84 (88%)	12 (12%)	0	100	100
24	N3	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
24	n3	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
25	N4	96/155 (62%)	83 (86%)	12 (12%)	1 (1%)	15	46
26	N5	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
26	n5	118/121 (98%)	108 (92%)	10 (8%)	0	100	100
27	N6	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
27	n6	124/126 (98%)	117 (94%)	5 (4%)	2 (2%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	N7	133/135 (98%)	114 (86%)	19 (14%)	0	100	100
28	n7	133/135 (98%)	116 (87%)	16 (12%)	1 (1%)	19	51
29	N8	146/148 (99%)	126 (86%)	19 (13%)	1 (1%)	22	55
29	n8	146/148 (99%)	132 (90%)	13 (9%)	1 (1%)	22	55
30	N9	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	8	32
30	n9	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	3	21
31	O0	95/100 (95%)	89 (94%)	5 (5%)	1 (1%)	14	44
31	o0	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
32	O1	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
32	o1	107/109 (98%)	96 (90%)	10 (9%)	1 (1%)	17	49
33	O2	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
33	o2	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
34	O3	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
34	o3	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
35	O4	110/112 (98%)	100 (91%)	10 (9%)	0	100	100
35	o4	110/112 (98%)	99 (90%)	10 (9%)	1 (1%)	17	49
36	O5	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
36	o5	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
37	O6	97/99 (98%)	80 (82%)	15 (16%)	2 (2%)	7	30
37	o6	97/99 (98%)	86 (89%)	11 (11%)	0	100	100
38	O7	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
38	o7	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
39	O8	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
39	o8	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
40	O9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
40	o9	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	Q0	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
41	q0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	7	30
42	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	q1	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
43	Q2	103/105 (98%)	91 (88%)	12 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	q2	103/105 (98%)	94 (91%)	8 (8%)	1 (1%)	15	46
44	Q3	89/91 (98%)	77 (86%)	12 (14%)	0	100	100
44	q3	89/91 (98%)	81 (91%)	8 (9%)	0	100	100
46	S0	204/206 (99%)	176 (86%)	27 (13%)	1 (0%)	29	61
46	s0	204/206 (99%)	170 (83%)	30 (15%)	4 (2%)	7	30
47	S1	212/216 (98%)	175 (82%)	35 (16%)	2 (1%)	17	49
47	s1	214/216 (99%)	188 (88%)	25 (12%)	1 (0%)	29	61
48	S2	215/217 (99%)	189 (88%)	25 (12%)	1 (0%)	29	61
48	s2	215/217 (99%)	196 (91%)	18 (8%)	1 (0%)	29	61
49	S3	221/223 (99%)	201 (91%)	19 (9%)	1 (0%)	29	61
49	s3	221/223 (99%)	194 (88%)	25 (11%)	2 (1%)	17	49
50	S4	258/260 (99%)	230 (89%)	27 (10%)	1 (0%)	34	67
50	s4	258/260 (99%)	225 (87%)	32 (12%)	1 (0%)	34	67
51	S5	204/206 (99%)	175 (86%)	26 (13%)	3 (2%)	10	36
51	s5	204/206 (99%)	182 (89%)	21 (10%)	1 (0%)	29	61
52	S6	224/236 (95%)	207 (92%)	17 (8%)	0	100	100
52	s6	216/236 (92%)	198 (92%)	16 (7%)	2 (1%)	17	49
53	S7	182/186 (98%)	156 (86%)	22 (12%)	4 (2%)	6	29
53	s7	184/186 (99%)	159 (86%)	23 (12%)	2 (1%)	14	44
54	S8	184/200 (92%)	158 (86%)	24 (13%)	2 (1%)	14	44
54	s8	182/200 (91%)	164 (90%)	16 (9%)	2 (1%)	14	44
55	S9	183/185 (99%)	153 (84%)	28 (15%)	2 (1%)	14	44
55	s9	183/185 (99%)	158 (86%)	23 (13%)	2 (1%)	14	44
56	C0	94/105 (90%)	73 (78%)	17 (18%)	4 (4%)	2	17
56	c0	92/105 (88%)	74 (80%)	13 (14%)	5 (5%)	2	13
57	C1	153/156 (98%)	138 (90%)	14 (9%)	1 (1%)	22	55
57	c1	140/156 (90%)	124 (89%)	15 (11%)	1 (1%)	22	55
58	C2	122/143 (85%)	91 (75%)	26 (21%)	5 (4%)	3	18
58	c2	122/143 (85%)	88 (72%)	32 (26%)	2 (2%)	9	34
59	C3	148/150 (99%)	136 (92%)	12 (8%)	0	100	100
59	c3	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	C4	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	9	34
60	c4	126/128 (98%)	107 (85%)	18 (14%)	1 (1%)	19	51
61	C5	122/141 (86%)	104 (85%)	15 (12%)	3 (2%)	5	26
61	c5	133/141 (94%)	109 (82%)	23 (17%)	1 (1%)	19	51
62	C6	139/142 (98%)	123 (88%)	15 (11%)	1 (1%)	22	55
62	c6	140/142 (99%)	124 (89%)	14 (10%)	2 (1%)	11	37
63	C7	118/136 (87%)	100 (85%)	15 (13%)	3 (2%)	5	26
63	c7	113/136 (83%)	97 (86%)	12 (11%)	4 (4%)	3	21
64	C8	143/145 (99%)	120 (84%)	21 (15%)	2 (1%)	11	37
64	c8	143/145 (99%)	125 (87%)	15 (10%)	3 (2%)	7	30
65	C9	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
65	c9	141/143 (99%)	132 (94%)	9 (6%)	0	100	100
66	D0	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	15	46
66	d0	108/110 (98%)	87 (81%)	17 (16%)	4 (4%)	3	20
67	D1	85/87 (98%)	73 (86%)	11 (13%)	1 (1%)	13	41
67	d1	85/87 (98%)	72 (85%)	12 (14%)	1 (1%)	13	41
68	D2	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	9	34
68	d2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	51
69	D3	142/144 (99%)	119 (84%)	23 (16%)	0	100	100
69	d3	142/144 (99%)	128 (90%)	14 (10%)	0	100	100
70	D4	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
70	d4	131/134 (98%)	110 (84%)	18 (14%)	3 (2%)	6	28
71	D5	68/70 (97%)	53 (78%)	12 (18%)	3 (4%)	2	16
71	d5	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
72	D6	95/97 (98%)	75 (79%)	17 (18%)	3 (3%)	4	22
72	d6	95/97 (98%)	77 (81%)	17 (18%)	1 (1%)	14	44
73	D7	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
73	d7	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	5	26
74	D8	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
74	d8	61/63 (97%)	51 (84%)	9 (15%)	1 (2%)	9	34
75	D9	51/53 (96%)	44 (86%)	5 (10%)	2 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	d9	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
76	E0	58/62 (94%)	46 (79%)	10 (17%)	2 (3%)	3	21
76	e0	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
77	E1	69/72 (96%)	53 (77%)	15 (22%)	1 (1%)	11	37
77	e1	70/72 (97%)	44 (63%)	22 (31%)	4 (6%)	1	12
78	SR	316/318 (99%)	283 (90%)	33 (10%)	0	100	100
78	sR	316/318 (99%)	293 (93%)	21 (7%)	2 (1%)	25	57
79	SM	155/272 (57%)	127 (82%)	26 (17%)	2 (1%)	12	39
79	sM	123/272 (45%)	105 (85%)	15 (12%)	3 (2%)	6	28
81	n4	133/135 (98%)	116 (87%)	14 (10%)	3 (2%)	6	28
82	p0	139/312 (45%)	124 (89%)	13 (9%)	2 (1%)	11	37
All	All	22342/23454 (95%)	19892 (89%)	2273 (10%)	177 (1%)	19	51

All (177) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L4	339	LEU
8	L6	98	VAL
25	N4	63	ILE
51	S5	64	VAL
56	C0	88	PRO
57	C1	7	VAL
72	D6	75	VAL
72	D6	84	VAL
76	E0	47	VAL
77	E1	98	VAL
79	SM	167	PRO
79	SM	172	VAL
8	l6	98	VAL
10	l8	203	VAL
13	m1	8	PRO
81	n4	67	VAL
30	n9	21	ILE
46	s0	189	VAL
54	s8	101	ILE
56	c0	88	PRO
56	c0	97	PRO
63	c7	88	VAL

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Mol	Chain	Res	Type
64	c8	92	ILE
73	d7	62	ILE
79	sM	84	LYS
79	sM	167	PRO
10	L8	36	ILE
17	M6	90	HIS
23	N2	11	ILE
29	N8	48	TYR
47	S1	62	LYS
54	S8	148	ALA
55	S9	134	ILE
56	C0	87	VAL
58	C2	22	VAL
58	C2	91	VAL
58	C2	106	ILE
62	C6	39	VAL
63	C7	83	GLN
68	D2	83	ILE
71	D5	69	LEU
75	D9	7	TRP
81	n4	76	VAL
82	p0	33	VAL
49	s3	91	VAL
53	s7	74	GLN
55	s9	91	LYS
56	c0	35	ILE
56	c0	92	ILE
58	c2	91	VAL
59	c3	66	ILE
63	c7	99	VAL
63	c7	105	GLN
66	d0	15	GLN
68	d2	6	VAL
74	d8	61	ARG
77	e1	98	VAL
22	N1	18	ASP
63	C7	84	TYR
64	C8	91	ASP
76	E0	60	PRO
81	n4	25	ASP
32	o1	7	VAL
35	o4	83	ASN

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Mol	Chain	Res	Type
51	s5	43	PHE
52	s6	70	PRO
55	s9	134	ILE
56	c0	24	LYS
59	c3	133	ALA
62	c6	42	GLU
66	d0	16	GLN
66	d0	52	LYS
67	d1	6	GLY
72	d6	46	GLU
73	d7	59	CYS
77	e1	137	ASP
78	sR	166	SER
10	L8	157	VAL
14	M3	47	ALA
31	O0	100	ILE
37	O6	97	SER
46	S0	188	LEU
49	S3	217	ILE
54	S8	152	ILE
55	S9	135	ALA
56	C0	61	TRP
60	C4	40	ALA
61	C5	28	MET
61	C5	29	SER
61	C5	53	PRO
67	D1	82	VAL
71	D5	88	ILE
5	l3	129	ALA
7	l5	269	SER
9	l7	191	VAL
9	l7	229	PHE
19	m8	99	THR
27	n6	126	LEU
28	n7	5	LEU
49	s3	115	ILE
57	c1	7	VAL
62	c6	41	PRO
66	d0	97	VAL
77	e1	92	LYS
78	sR	165	ASP
5	L3	347	SER

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Mol	Chain	Res	Type
14	M3	76	THR
48	S2	144	TRP
51	S5	58	LEU
53	S7	111	LYS
56	C0	60	SER
58	C2	89	ILE
6	l4	329	PRO
11	l9	144	ILE
14	m3	47	ALA
27	n6	125	LYS
29	n8	78	LEU
30	n9	18	ARG
53	s7	64	VAL
61	c5	10	ARG
64	c8	5	VAL
64	c8	61	LEU
70	d4	33	ALA
70	d4	53	ASP
79	sM	43	ASP
5	L3	187	SER
6	L4	24	ALA
12	M0	207	GLU
22	N1	125	ALA
47	S1	210	ILE
58	C2	66	VAL
63	C7	86	PRO
68	D2	31	SER
4	l2	238	ILE
6	l4	142	VAL
7	l5	178	ASN
13	m1	114	ILE
19	m8	112	ALA
82	p0	13	ALA
43	q2	78	LYS
46	s0	95	ALA
46	s0	190	ASP
47	s1	177	GLN
52	s6	69	LEU
59	c3	87	ASP
60	c4	132	ARG
22	N1	124	VAL
50	S4	195	ILE

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Mol	Chain	Res	Type
51	S5	51	VAL
60	C4	42	VAL
75	D9	6	VAL
4	l2	56	ALA
8	l6	130	ILE
10	l8	237	ILE
46	s0	158	VAL
54	s8	78	ILE
37	O6	3	VAL
64	C8	14	ILE
66	D0	117	VAL
72	D6	36	ILE
58	c2	115	VAL
5	L3	317	ILE
30	N9	21	ILE
53	S7	64	VAL
53	S7	98	ILE
71	D5	71	ILE
41	q0	78	ILE
53	S7	31	SER
6	l4	145	ILE
11	l9	167	VAL
14	m3	93	ILE
48	s2	238	SER
50	s4	90	ILE
59	c3	22	ALA
63	c7	86	PRO
77	e1	102	VAL
70	d4	30	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
4	L2	193/194 (100%)	172 (89%)	21 (11%)	6 23
4	l2	192/194 (99%)	175 (91%)	17 (9%)	9 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	L3	322/322 (100%)	273 (85%)	49 (15%)	3	11
5	l3	322/322 (100%)	277 (86%)	45 (14%)	3	13
6	L4	288/288 (100%)	254 (88%)	34 (12%)	5	19
6	l4	288/288 (100%)	253 (88%)	35 (12%)	5	18
7	L5	244/244 (100%)	219 (90%)	25 (10%)	7	26
7	l5	243/244 (100%)	207 (85%)	36 (15%)	3	12
8	L6	134/153 (88%)	115 (86%)	19 (14%)	3	13
8	l6	135/153 (88%)	112 (83%)	23 (17%)	2	8
9	L7	186/187 (100%)	168 (90%)	18 (10%)	8	28
9	l7	187/187 (100%)	168 (90%)	19 (10%)	7	26
10	L8	191/191 (100%)	171 (90%)	20 (10%)	7	25
10	l8	177/191 (93%)	159 (90%)	18 (10%)	7	26
11	L9	171/171 (100%)	143 (84%)	28 (16%)	2	9
11	l9	171/171 (100%)	153 (90%)	18 (10%)	7	25
12	M0	176/187 (94%)	151 (86%)	25 (14%)	3	13
12	m0	180/187 (96%)	143 (79%)	37 (21%)	1	3
13	M1	147/147 (100%)	127 (86%)	20 (14%)	3	14
13	m1	147/147 (100%)	125 (85%)	22 (15%)	3	12
14	M3	154/154 (100%)	127 (82%)	27 (18%)	2	7
14	m3	154/154 (100%)	137 (89%)	17 (11%)	6	23
15	M4	107/108 (99%)	96 (90%)	11 (10%)	7	26
15	m4	108/108 (100%)	96 (89%)	12 (11%)	6	22
16	M5	175/175 (100%)	151 (86%)	24 (14%)	3	14
16	m5	175/175 (100%)	151 (86%)	24 (14%)	3	14
17	M6	160/160 (100%)	144 (90%)	16 (10%)	7	27
17	m6	160/160 (100%)	141 (88%)	19 (12%)	5	19
18	M7	138/146 (94%)	110 (80%)	28 (20%)	1	3
18	m7	125/146 (86%)	104 (83%)	21 (17%)	2	8
19	M8	150/150 (100%)	134 (89%)	16 (11%)	6	24
19	m8	150/150 (100%)	128 (85%)	22 (15%)	3	12
20	M9	148/153 (97%)	133 (90%)	15 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	m9	153/153 (100%)	138 (90%)	15 (10%)	8	28
21	N0	156/156 (100%)	127 (81%)	29 (19%)	1	5
21	n0	156/156 (100%)	136 (87%)	20 (13%)	4	16
22	N1	136/136 (100%)	118 (87%)	18 (13%)	4	15
22	n1	136/136 (100%)	113 (83%)	23 (17%)	2	8
23	N2	87/87 (100%)	80 (92%)	7 (8%)	12	38
23	n2	85/87 (98%)	76 (89%)	9 (11%)	6	24
24	N3	104/104 (100%)	96 (92%)	8 (8%)	13	40
24	n3	104/104 (100%)	95 (91%)	9 (9%)	10	34
25	N4	57/129 (44%)	53 (93%)	4 (7%)	15	44
26	N5	104/105 (99%)	94 (90%)	10 (10%)	8	29
26	n5	104/105 (99%)	94 (90%)	10 (10%)	8	29
27	N6	109/109 (100%)	95 (87%)	14 (13%)	4	16
27	n6	109/109 (100%)	92 (84%)	17 (16%)	2	11
28	N7	115/115 (100%)	101 (88%)	14 (12%)	5	18
28	n7	115/115 (100%)	103 (90%)	12 (10%)	7	25
29	N8	118/118 (100%)	101 (86%)	17 (14%)	3	13
29	n8	118/118 (100%)	100 (85%)	18 (15%)	2	11
30	N9	46/46 (100%)	41 (89%)	5 (11%)	6	23
30	n9	46/46 (100%)	39 (85%)	7 (15%)	3	11
31	O0	81/84 (96%)	75 (93%)	6 (7%)	13	42
31	o0	84/84 (100%)	71 (84%)	13 (16%)	2	11
32	O1	96/96 (100%)	82 (85%)	14 (15%)	3	12
32	o1	96/96 (100%)	80 (83%)	16 (17%)	2	8
33	O2	109/109 (100%)	97 (89%)	12 (11%)	6	23
33	o2	109/109 (100%)	93 (85%)	16 (15%)	3	12
34	O3	90/90 (100%)	84 (93%)	6 (7%)	16	46
34	o3	90/90 (100%)	81 (90%)	9 (10%)	7	27
35	O4	95/95 (100%)	84 (88%)	11 (12%)	5	20
35	o4	95/95 (100%)	88 (93%)	7 (7%)	13	42
36	O5	104/104 (100%)	88 (85%)	16 (15%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	o5	104/104 (100%)	91 (88%)	13 (12%)	4	17
37	O6	81/81 (100%)	71 (88%)	10 (12%)	4	17
37	o6	81/81 (100%)	70 (86%)	11 (14%)	3	14
38	O7	70/70 (100%)	62 (89%)	8 (11%)	5	21
38	o7	70/70 (100%)	58 (83%)	12 (17%)	2	8
39	O8	68/68 (100%)	58 (85%)	10 (15%)	3	12
39	o8	68/68 (100%)	60 (88%)	8 (12%)	5	19
40	O9	45/45 (100%)	39 (87%)	6 (13%)	4	15
40	o9	45/45 (100%)	38 (84%)	7 (16%)	2	11
41	Q0	47/47 (100%)	42 (89%)	5 (11%)	6	24
41	q0	47/47 (100%)	39 (83%)	8 (17%)	2	8
42	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	7
42	q1	23/23 (100%)	20 (87%)	3 (13%)	4	16
43	Q2	90/90 (100%)	81 (90%)	9 (10%)	7	27
43	q2	90/90 (100%)	72 (80%)	18 (20%)	1	3
44	Q3	71/71 (100%)	65 (92%)	6 (8%)	10	35
44	q3	71/71 (100%)	65 (92%)	6 (8%)	10	35
46	S0	173/173 (100%)	153 (88%)	20 (12%)	5	20
46	s0	173/173 (100%)	154 (89%)	19 (11%)	6	23
47	S1	191/192 (100%)	161 (84%)	30 (16%)	2	10
47	s1	192/192 (100%)	174 (91%)	18 (9%)	8	30
48	S2	176/176 (100%)	163 (93%)	13 (7%)	13	42
48	s2	176/176 (100%)	154 (88%)	22 (12%)	4	17
49	S3	182/182 (100%)	162 (89%)	20 (11%)	6	23
49	s3	181/182 (100%)	149 (82%)	32 (18%)	2	6
50	S4	221/221 (100%)	195 (88%)	26 (12%)	5	19
50	s4	221/221 (100%)	195 (88%)	26 (12%)	5	19
51	S5	173/173 (100%)	158 (91%)	15 (9%)	10	34
51	s5	173/173 (100%)	150 (87%)	23 (13%)	4	15
52	S6	191/201 (95%)	167 (87%)	24 (13%)	4	17
52	s6	187/201 (93%)	160 (86%)	27 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	S7	165/166 (99%)	151 (92%)	14 (8%)	10	35
53	s7	165/166 (99%)	152 (92%)	13 (8%)	12	39
54	S8	150/161 (93%)	132 (88%)	18 (12%)	5	19
54	s8	148/161 (92%)	137 (93%)	11 (7%)	13	42
55	S9	158/158 (100%)	140 (89%)	18 (11%)	5	21
55	s9	158/158 (100%)	143 (90%)	15 (10%)	8	29
56	C0	77/98 (79%)	66 (86%)	11 (14%)	3	13
56	c0	73/98 (74%)	65 (89%)	8 (11%)	6	23
57	C1	129/137 (94%)	119 (92%)	10 (8%)	12	39
57	c1	125/137 (91%)	108 (86%)	17 (14%)	3	14
58	C2	88/119 (74%)	80 (91%)	8 (9%)	9	32
58	c2	88/119 (74%)	76 (86%)	12 (14%)	3	14
59	C3	127/127 (100%)	117 (92%)	10 (8%)	12	39
59	c3	127/127 (100%)	110 (87%)	17 (13%)	4	15
60	C4	81/97 (84%)	70 (86%)	11 (14%)	3	14
60	c4	97/97 (100%)	84 (87%)	13 (13%)	4	15
61	C5	101/117 (86%)	91 (90%)	10 (10%)	8	27
61	c5	103/117 (88%)	93 (90%)	10 (10%)	8	28
62	C6	117/118 (99%)	101 (86%)	16 (14%)	3	14
62	c6	118/118 (100%)	103 (87%)	15 (13%)	4	16
63	C7	109/124 (88%)	91 (84%)	18 (16%)	2	9
63	c7	97/124 (78%)	87 (90%)	10 (10%)	7	26
64	C8	128/128 (100%)	114 (89%)	14 (11%)	6	23
64	c8	128/128 (100%)	108 (84%)	20 (16%)	2	11
65	C9	115/115 (100%)	102 (89%)	13 (11%)	6	21
65	c9	115/115 (100%)	100 (87%)	15 (13%)	4	16
66	D0	100/103 (97%)	89 (89%)	11 (11%)	6	23
66	d0	103/103 (100%)	89 (86%)	14 (14%)	3	14
67	D1	74/74 (100%)	65 (88%)	9 (12%)	5	18
67	d1	74/74 (100%)	65 (88%)	9 (12%)	5	18
68	D2	110/110 (100%)	97 (88%)	13 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	d2	110/110 (100%)	97 (88%)	13 (12%)	5	19
69	D3	119/119 (100%)	107 (90%)	12 (10%)	7	27
69	d3	119/119 (100%)	109 (92%)	10 (8%)	11	36
70	D4	112/112 (100%)	99 (88%)	13 (12%)	5	20
70	d4	111/112 (99%)	100 (90%)	11 (10%)	8	27
71	D5	61/61 (100%)	51 (84%)	10 (16%)	2	9
71	d5	61/61 (100%)	57 (93%)	4 (7%)	16	46
72	D6	83/83 (100%)	71 (86%)	12 (14%)	3	12
72	d6	83/83 (100%)	72 (87%)	11 (13%)	4	15
73	D7	70/70 (100%)	62 (89%)	8 (11%)	5	21
73	d7	70/70 (100%)	65 (93%)	5 (7%)	14	44
74	D8	56/56 (100%)	50 (89%)	6 (11%)	6	24
74	d8	56/56 (100%)	41 (73%)	15 (27%)	0	1
75	D9	47/47 (100%)	39 (83%)	8 (17%)	2	8
75	d9	47/47 (100%)	36 (77%)	11 (23%)	1	2
76	E0	51/53 (96%)	46 (90%)	5 (10%)	8	28
76	e0	53/53 (100%)	44 (83%)	9 (17%)	2	8
77	E1	62/63 (98%)	56 (90%)	6 (10%)	8	28
77	e1	63/63 (100%)	51 (81%)	12 (19%)	1	4
78	SR	260/260 (100%)	239 (92%)	21 (8%)	11	38
78	sR	260/260 (100%)	241 (93%)	19 (7%)	14	43
79	SM	97/227 (43%)	81 (84%)	16 (16%)	2	9
79	sM	88/227 (39%)	77 (88%)	11 (12%)	4	17
81	n4	101/114 (89%)	92 (91%)	9 (9%)	9	33
82	p0	105/254 (41%)	90 (86%)	15 (14%)	3	13
All	All	18802/19697 (96%)	16495 (88%)	2307 (12%)	4	17

All (2307) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L2	32	LEU
4	L2	45	VAL
4	L2	67	TYR

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Mol	Chain	Res	Type
4	L2	74	GLU
4	L2	86	GLN
4	L2	101	VAL
4	L2	130	SER
4	L2	132	ASN
4	L2	148	VAL
4	L2	165	VAL
4	L2	179	LEU
4	L2	180	LEU
4	L2	193	ARG
4	L2	204	MET
4	L2	206	PRO
4	L2	223	SER
4	L2	225	ILE
4	L2	226	SER
4	L2	227	ARG
4	L2	238	ILE
4	L2	247	ARG
5	L3	10	ARG
5	L3	13	HIS
5	L3	17	LEU
5	L3	19	ARG
5	L3	37	ARG
5	L3	41	VAL
5	L3	44	THR
5	L3	55	THR
5	L3	65	SER
5	L3	85	VAL
5	L3	93	VAL
5	L3	99	LEU
5	L3	103	THR
5	L3	114	VAL
5	L3	117	ARG
5	L3	139	GLN
5	L3	140	ASP
5	L3	150	ARG
5	L3	156	SER
5	L3	160	VAL
5	L3	166	ILE
5	L3	169	THR
5	L3	183	LEU
5	L3	188	ILE

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Mol	Chain	Res	Type
5	L3	196	ARG
5	L3	197	GLU
5	L3	202	THR
5	L3	205	VAL
5	L3	206	ASP
5	L3	211	GLN
5	L3	232	ARG
5	L3	235	THR
5	L3	238	LEU
5	L3	246	LEU
5	L3	260	VAL
5	L3	274	SER
5	L3	284	ARG
5	L3	287	LYS
5	L3	291	GLU
5	L3	305	ILE
5	L3	319	ASN
5	L3	320	ASP
5	L3	332	ARG
5	L3	338	LEU
5	L3	343	TYR
5	L3	347	SER
5	L3	353	GLU
5	L3	364	LYS
5	L3	387	LEU
6	L4	7	THR
6	L4	22	LEU
6	L4	27	SER
6	L4	54	GLU
6	L4	74	ILE
6	L4	92	ASN
6	L4	93	MET
6	L4	99	MET
6	L4	105	THR
6	L4	120	TYR
6	L4	136	LEU
6	L4	138	ARG
6	L4	150	LEU
6	L4	155	ASP
6	L4	156	LEU
6	L4	158	SER
6	L4	176	SER

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Mol	Chain	Res	Type
6	L4	180	LYS
6	L4	182	LEU
6	L4	185	LYS
6	L4	187	LEU
6	L4	193	LYS
6	L4	200	THR
6	L4	203	ARG
6	L4	206	LEU
6	L4	220	ARG
6	L4	265	GLU
6	L4	269	SER
6	L4	307	GLN
6	L4	327	LEU
6	L4	346	LYS
6	L4	349	THR
6	L4	358	THR
6	L4	361	HIS
7	L5	41	LYS
7	L5	50	ARG
7	L5	66	SER
7	L5	70	THR
7	L5	75	LEU
7	L5	85	ARG
7	L5	95	TRP
7	L5	105	ILE
7	L5	107	ARG
7	L5	111	GLN
7	L5	137	ASP
7	L5	151	GLN
7	L5	152	ARG
7	L5	154	THR
7	L5	155	THR
7	L5	163	LEU
7	L5	194	LEU
7	L5	203	HIS
7	L5	211	LEU
7	L5	215	ASP
7	L5	222	LEU
7	L5	234	ASP
7	L5	236	LEU
7	L5	258	LYS
7	L5	273	ARG

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Mol	Chain	Res	Type
8	L6	8	LYS
8	L6	21	THR
8	L6	31	ARG
8	L6	46	ARG
8	L6	50	LYS
8	L6	52	VAL
8	L6	64	LEU
8	L6	77	ARG
8	L6	78	ARG
8	L6	79	VAL
8	L6	84	VAL
8	L6	87	THR
8	L6	99	GLU
8	L6	102	ASN
8	L6	131	LYS
8	L6	152	THR
8	L6	155	LEU
8	L6	156	LYS
8	L6	160	SER
9	L7	24	GLU
9	L7	60	ARG
9	L7	83	LEU
9	L7	92	ILE
9	L7	93	ASN
9	L7	98	LYS
9	L7	110	ARG
9	L7	111	ILE
9	L7	120	THR
9	L7	124	LEU
9	L7	175	LYS
9	L7	179	LEU
9	L7	180	SER
9	L7	182	ASP
9	L7	184	LEU
9	L7	211	SER
9	L7	229	PHE
9	L7	239	LEU
10	L8	26	LEU
10	L8	27	THR
10	L8	63	LYS
10	L8	74	THR
10	L8	79	GLN

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Mol	Chain	Res	Type
10	L8	84	ARG
10	L8	95	ASN
10	L8	99	PRO
10	L8	118	GLU
10	L8	136	LEU
10	L8	156	ASP
10	L8	164	VAL
10	L8	169	LEU
10	L8	181	LYS
10	L8	185	ARG
10	L8	190	VAL
10	L8	221	ASN
10	L8	240	ASN
10	L8	246	MET
10	L8	248	LYS
11	L9	5	GLN
11	L9	6	THR
11	L9	7	GLU
11	L9	41	ILE
11	L9	49	ASN
11	L9	50	ASN
11	L9	51	GLN
11	L9	53	ILE
11	L9	62	ARG
11	L9	68	LEU
11	L9	69	ARG
11	L9	70	THR
11	L9	82	VAL
11	L9	83	THR
11	L9	90	MET
11	L9	92	TYR
11	L9	125	ASN
11	L9	133	THR
11	L9	135	GLU
11	L9	139	ASN
11	L9	149	ASN
11	L9	151	VAL
11	L9	157	ASN
11	L9	161	LEU
11	L9	163	GLN
11	L9	170	LYS
11	L9	176	LEU

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Mol	Chain	Res	Type
11	L9	177	ASP
12	M0	3	ARG
12	M0	7	ARG
12	M0	20	SER
12	M0	21	ARG
12	M0	22	TYR
12	M0	26	VAL
12	M0	30	LYS
12	M0	32	ARG
12	M0	42	THR
12	M0	48	LEU
12	M0	52	LEU
12	M0	63	GLU
12	M0	71	CYS
12	M0	82	ARG
12	M0	87	LEU
12	M0	128	ARG
12	M0	130	ASP
12	M0	139	ARG
12	M0	140	THR
12	M0	143	SER
12	M0	163	GLN
12	M0	185	ARG
12	M0	192	ASP
12	M0	196	PHE
12	M0	205	SER
13	M1	9	MET
13	M1	10	ARG
13	M1	22	SER
13	M1	28	ASP
13	M1	40	LEU
13	M1	68	HIS
13	M1	81	GLU
13	M1	85	LYS
13	M1	92	ARG
13	M1	101	ASN
13	M1	107	ASP
13	M1	111	ASP
13	M1	112	LEU
13	M1	137	ARG
13	M1	139	THR
13	M1	140	ARG

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Mol	Chain	Res	Type
13	M1	154	THR
13	M1	155	THR
13	M1	168	ASP
13	M1	173	ASP
14	M3	4	SER
14	M3	5	LYS
14	M3	9	ILE
14	M3	17	HIS
14	M3	23	LYS
14	M3	53	LEU
14	M3	54	LEU
14	M3	55	ARG
14	M3	58	VAL
14	M3	59	ARG
14	M3	67	ARG
14	M3	70	ARG
14	M3	76	THR
14	M3	85	LEU
14	M3	86	THR
14	M3	101	ARG
14	M3	114	GLN
14	M3	115	ARG
14	M3	131	LYS
14	M3	136	GLU
14	M3	137	GLN
14	M3	164	GLU
14	M3	165	SER
14	M3	168	ARG
14	M3	179	PHE
14	M3	182	ILE
14	M3	190	LYS
15	M4	7	VAL
15	M4	21	VAL
15	M4	27	GLN
15	M4	41	GLN
15	M4	50	LYS
15	M4	53	VAL
15	M4	55	ARG
15	M4	82	SER
15	M4	102	LYS
15	M4	106	ARG
15	M4	137	LYS

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Mol	Chain	Res	Type
16	M5	17	ASP
16	M5	22	LEU
16	M5	38	ARG
16	M5	46	ASP
16	M5	50	ARG
16	M5	56	LYS
16	M5	62	TYR
16	M5	68	ARG
16	M5	71	ARG
16	M5	80	THR
16	M5	90	ASN
16	M5	96	ARG
16	M5	109	ARG
16	M5	117	ASN
16	M5	123	GLN
16	M5	124	ASP
16	M5	133	ILE
16	M5	138	GLN
16	M5	151	ILE
16	M5	152	CYS
16	M5	159	ARG
16	M5	175	ASN
16	M5	183	THR
16	M5	190	THR
17	M6	41	LEU
17	M6	58	LEU
17	M6	68	ARG
17	M6	74	ARG
17	M6	106	GLU
17	M6	119	VAL
17	M6	124	LEU
17	M6	128	ARG
17	M6	129	LEU
17	M6	143	THR
17	M6	159	LYS
17	M6	160	ARG
17	M6	166	GLU
17	M6	180	SER
17	M6	184	THR
17	M6	188	SER
18	M7	3	ARG
18	M7	9	THR

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Mol	Chain	Res	Type
18	M7	14	SER
18	M7	23	ARG
18	M7	24	VAL
18	M7	32	THR
18	M7	36	ILE
18	M7	52	LEU
18	M7	56	ARG
18	M7	65	SER
18	M7	75	GLU
18	M7	107	LEU
18	M7	112	LEU
18	M7	113	TYR
18	M7	115	SER
18	M7	116	HIS
18	M7	125	GLN
18	M7	126	ARG
18	M7	127	ARG
18	M7	129	THR
18	M7	135	ARG
18	M7	142	SER
18	M7	144	SER
18	M7	149	VAL
18	M7	169	THR
18	M7	171	ARG
18	M7	175	ARG
18	M7	181	ARG
19	M8	3	ILE
19	M8	11	LYS
19	M8	26	LEU
19	M8	32	LEU
19	M8	41	ASP
19	M8	49	LEU
19	M8	86	THR
19	M8	99	THR
19	M8	111	ARG
19	M8	135	GLN
19	M8	146	SER
19	M8	168	THR
19	M8	171	LYS
19	M8	174	ARG
19	M8	180	ARG
19	M8	185	LYS

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Mol	Chain	Res	Type
20	M9	10	LEU
20	M9	21	LYS
20	M9	27	ASN
20	M9	30	SER
20	M9	46	LYS
20	M9	74	ARG
20	M9	82	LYS
20	M9	84	THR
20	M9	99	LEU
20	M9	126	GLU
20	M9	130	ASN
20	M9	134	HIS
20	M9	138	LEU
20	M9	180	LYS
20	M9	181	ARG
21	N0	1	MET
21	N0	13	ARG
21	N0	16	THR
21	N0	45	LEU
21	N0	47	LYS
21	N0	50	LYS
21	N0	51	VAL
21	N0	71	LYS
21	N0	80	ARG
21	N0	81	TYR
21	N0	87	THR
21	N0	88	HIS
21	N0	97	VAL
21	N0	100	VAL
21	N0	105	THR
21	N0	106	LEU
21	N0	109	ASP
21	N0	113	ARG
21	N0	115	ARG
21	N0	117	ARG
21	N0	134	ASP
21	N0	136	LYS
21	N0	137	ARG
21	N0	145	THR
21	N0	156	VAL
21	N0	159	SER
21	N0	167	ARG

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Mol	Chain	Res	Type
21	N0	171	PHE
21	N0	172	TYR
22	N1	12	ARG
22	N1	18	ASP
22	N1	25	VAL
22	N1	78	LYS
22	N1	80	VAL
22	N1	83	ARG
22	N1	86	GLU
22	N1	89	LEU
22	N1	93	VAL
22	N1	102	ARG
22	N1	104	GLU
22	N1	118	GLU
22	N1	122	GLN
22	N1	128	LEU
22	N1	139	ARG
22	N1	144	GLU
22	N1	149	GLN
22	N1	158	THR
23	N2	39	ASP
23	N2	70	LYS
23	N2	74	LYS
23	N2	82	LYS
23	N2	88	GLN
23	N2	100	THR
23	N2	108	TYR
24	N3	12	ARG
24	N3	13	ILE
24	N3	45	ARG
24	N3	46	LEU
24	N3	64	LYS
24	N3	86	ARG
24	N3	102	ILE
24	N3	104	ASN
25	N4	5	ILE
25	N4	7	SER
25	N4	27	LYS
25	N4	43	ARG
26	N5	25	LYS
26	N5	27	ARG
26	N5	37	THR

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Mol	Chain	Res	Type
26	N5	45	LYS
26	N5	87	SER
26	N5	112	THR
26	N5	115	ARG
26	N5	125	ARG
26	N5	137	ASN
26	N5	142	ILE
27	N6	3	LYS
27	N6	5	SER
27	N6	10	SER
27	N6	13	ARG
27	N6	37	LYS
27	N6	38	GLU
27	N6	39	LEU
27	N6	51	ARG
27	N6	54	ASP
27	N6	74	TYR
27	N6	76	LEU
27	N6	83	ASP
27	N6	99	LEU
27	N6	115	ARG
28	N7	14	VAL
28	N7	17	ARG
28	N7	33	SER
28	N7	34	LYS
28	N7	46	ILE
28	N7	55	LYS
28	N7	64	LYS
28	N7	81	LEU
28	N7	83	THR
28	N7	88	ASP
28	N7	92	PHE
28	N7	105	SER
28	N7	120	GLU
28	N7	136	PHE
29	N8	4	ARG
29	N8	6	THR
29	N8	8	THR
29	N8	10	LYS
29	N8	14	HIS
29	N8	16	SER
29	N8	29	PRO

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Mol	Chain	Res	Type
29	N8	39	HIS
29	N8	42	ARG
29	N8	43	ILE
29	N8	60	TYR
29	N8	74	ASN
29	N8	85	ASP
29	N8	93	SER
29	N8	97	GLU
29	N8	115	LYS
29	N8	139	ARG
30	N9	4	SER
30	N9	5	LYS
30	N9	14	ARG
30	N9	36	ASP
30	N9	50	THR
31	O0	11	ASN
31	O0	41	LEU
31	O0	61	MET
31	O0	66	LYS
31	O0	103	THR
31	O0	104	LEU
32	O1	6	ASP
32	O1	13	THR
32	O1	16	LEU
32	O1	17	HIS
32	O1	26	LYS
32	O1	31	ARG
32	O1	64	VAL
32	O1	65	LYS
32	O1	76	SER
32	O1	82	GLU
32	O1	84	ASP
32	O1	86	LYS
32	O1	96	VAL
32	O1	106	THR
33	O2	14	THR
33	O2	19	ARG
33	O2	44	ARG
33	O2	54	LYS
33	O2	62	LYS
33	O2	73	THR
33	O2	75	LEU

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Mol	Chain	Res	Type
33	O2	82	LEU
33	O2	109	LEU
33	O2	125	ARG
33	O2	126	LEU
33	O2	128	LEU
34	O3	56	SER
34	O3	60	ARG
34	O3	70	LYS
34	O3	81	VAL
34	O3	86	ARG
34	O3	98	VAL
35	O4	18	ASN
35	O4	31	ARG
35	O4	44	CYS
35	O4	51	LEU
35	O4	57	LEU
35	O4	58	ARG
35	O4	65	VAL
35	O4	84	CYS
35	O4	102	LYS
35	O4	105	VAL
35	O4	110	GLU
36	O5	7	TYR
36	O5	10	ARG
36	O5	13	SER
36	O5	21	LEU
36	O5	46	THR
36	O5	68	GLN
36	O5	76	GLN
36	O5	89	ARG
36	O5	90	ARG
36	O5	93	THR
36	O5	94	LYS
36	O5	96	GLU
36	O5	104	GLN
36	O5	105	ARG
36	O5	115	LYS
36	O5	118	ILE
37	O6	13	LYS
37	O6	17	VAL
37	O6	20	MET
37	O6	29	LYS

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Mol	Chain	Res	Type
37	O6	36	ARG
37	O6	53	TYR
37	O6	56	ARG
37	O6	76	ARG
37	O6	94	ILE
37	O6	98	ARG
38	O7	24	ARG
38	O7	25	ARG
38	O7	33	THR
38	O7	43	LYS
38	O7	55	ARG
38	O7	58	THR
38	O7	67	LEU
38	O7	80	THR
39	O8	8	ILE
39	O8	13	GLU
39	O8	19	ASP
39	O8	24	THR
39	O8	31	LEU
39	O8	32	ASN
39	O8	48	SER
39	O8	53	THR
39	O8	64	LYS
39	O8	77	ARG
40	O9	4	GLN
40	O9	21	ARG
40	O9	23	LEU
40	O9	28	ARG
40	O9	45	ARG
40	O9	47	THR
41	Q0	78	ILE
41	Q0	79	GLU
41	Q0	113	ARG
41	Q0	120	GLN
41	Q0	127	LEU
42	Q1	1	MET
42	Q1	2	ARG
42	Q1	9	ARG
42	Q1	10	THR
43	Q2	8	ARG
43	Q2	21	THR
43	Q2	26	THR

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Mol	Chain	Res	Type
43	Q2	35	LEU
43	Q2	71	ARG
43	Q2	83	LEU
43	Q2	84	THR
43	Q2	85	LEU
43	Q2	93	LEU
44	Q3	11	THR
44	Q3	40	SER
44	Q3	45	LYS
44	Q3	60	CYS
44	Q3	82	THR
44	Q3	87	ARG
46	S0	8	ASP
46	S0	23	HIS
46	S0	27	ARG
46	S0	28	ASN
46	S0	59	LEU
46	S0	62	ARG
46	S0	101	ARG
46	S0	119	ARG
46	S0	153	SER
46	S0	172	LEU
46	S0	177	LEU
46	S0	185	ARG
46	S0	188	LEU
46	S0	189	VAL
46	S0	190	ASP
46	S0	191	ARG
46	S0	202	TYR
46	S0	203	PHE
46	S0	205	ARG
46	S0	206	ASP
47	S1	21	VAL
47	S1	30	PHE
47	S1	31	ASP
47	S1	36	SER
47	S1	38	PHE
47	S1	43	VAL
47	S1	46	THR
47	S1	49	ASN
47	S1	61	LEU
47	S1	62	LYS

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Mol	Chain	Res	Type
47	S1	78	ASP
47	S1	81	PHE
47	S1	84	ILE
47	S1	89	ASP
47	S1	96	LEU
47	S1	105	PHE
47	S1	108	ASP
47	S1	115	ARG
47	S1	117	TRP
47	S1	135	LEU
47	S1	148	ASN
47	S1	177	GLN
47	S1	180	THR
47	S1	181	LEU
47	S1	183	GLN
47	S1	194	ASN
47	S1	209	ASN
47	S1	218	LEU
47	S1	220	GLN
47	S1	223	PHE
48	S2	53	ILE
48	S2	69	ILE
48	S2	70	ASP
48	S2	76	LEU
48	S2	91	ARG
48	S2	97	ARG
48	S2	111	VAL
48	S2	117	THR
48	S2	140	ARG
48	S2	141	ARG
48	S2	152	HIS
48	S2	187	LEU
48	S2	226	THR
49	S3	20	GLU
49	S3	21	LEU
49	S3	64	ARG
49	S3	65	ARG
49	S3	74	GLN
49	S3	76	ARG
49	S3	113	LEU
49	S3	116	ARG
49	S3	117	ARG

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Mol	Chain	Res	Type
49	S3	143	ARG
49	S3	146	ARG
49	S3	148	LYS
49	S3	151	LYS
49	S3	158	ILE
49	S3	177	MET
49	S3	178	ARG
49	S3	190	ARG
49	S3	197	THR
49	S3	204	ASP
49	S3	218	LEU
50	S4	9	LEU
50	S4	38	LEU
50	S4	39	ARG
50	S4	40	GLU
50	S4	42	LEU
50	S4	45	ILE
50	S4	57	ASN
50	S4	77	ARG
50	S4	102	VAL
50	S4	104	ASP
50	S4	108	ARG
50	S4	116	ASP
50	S4	126	VAL
50	S4	131	LEU
50	S4	148	ARG
50	S4	180	LEU
50	S4	181	VAL
50	S4	182	TYR
50	S4	187	ARG
50	S4	198	LYS
50	S4	211	LYS
50	S4	215	ASP
50	S4	222	LEU
50	S4	226	PHE
50	S4	227	VAL
50	S4	231	GLN
51	S5	25	LEU
51	S5	44	ASN
51	S5	72	HIS
51	S5	79	ASN
51	S5	93	LEU

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Mol	Chain	Res	Type
51	S5	94	THR
51	S5	119	ASP
51	S5	123	VAL
51	S5	156	ARG
51	S5	157	ARG
51	S5	174	LEU
51	S5	186	ASN
51	S5	194	LEU
51	S5	203	LYS
51	S5	223	SER
52	S6	7	TYR
52	S6	10	ASN
52	S6	15	THR
52	S6	41	VAL
52	S6	56	ASN
52	S6	64	LYS
52	S6	69	LEU
52	S6	76	LEU
52	S6	78	THR
52	S6	109	LEU
52	S6	126	ASP
52	S6	132	ARG
52	S6	133	LEU
52	S6	137	ARG
52	S6	139	ASN
52	S6	143	LYS
52	S6	155	ASP
52	S6	157	VAL
52	S6	168	THR
52	S6	169	TYR
52	S6	177	ARG
52	S6	189	HIS
52	S6	211	LEU
52	S6	216	LEU
53	S7	24	PHE
53	S7	29	ASN
53	S7	50	ASP
53	S7	70	PHE
53	S7	76	LYS
53	S7	77	LEU
53	S7	85	PHE
53	S7	104	ARG

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Mol	Chain	Res	Type
53	S7	114	ARG
53	S7	126	LEU
53	S7	133	THR
53	S7	160	GLN
53	S7	161	GLN
53	S7	163	ASP
54	S8	4	SER
54	S8	8	ARG
54	S8	11	ARG
54	S8	21	PHE
54	S8	25	ARG
54	S8	36	THR
54	S8	45	SER
54	S8	47	ARG
54	S8	56	ARG
54	S8	58	LEU
54	S8	92	ARG
54	S8	107	THR
54	S8	123	LYS
54	S8	138	ASN
54	S8	178	ARG
54	S8	184	LEU
54	S8	189	LEU
54	S8	193	LEU
55	S9	3	ARG
55	S9	6	ARG
55	S9	21	SER
55	S9	28	LEU
55	S9	33	GLU
55	S9	38	ASN
55	S9	39	LYS
55	S9	49	LEU
55	S9	78	ARG
55	S9	93	LEU
55	S9	97	LEU
55	S9	99	LEU
55	S9	103	ASP
55	S9	118	LEU
55	S9	142	ASN
55	S9	150	LEU
55	S9	157	ASP
55	S9	175	ARG

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Mol	Chain	Res	Type
56	C0	8	ARG
56	C0	16	PHE
56	C0	32	HIS
56	C0	37	THR
56	C0	46	LEU
56	C0	47	GLN
56	C0	55	VAL
56	C0	56	LYS
56	C0	76	LEU
56	C0	78	GLU
56	C0	82	LEU
57	C1	5	LEU
57	C1	8	GLN
57	C1	18	HIS
57	C1	44	THR
57	C1	55	ASP
57	C1	67	ARG
57	C1	69	LYS
57	C1	74	THR
57	C1	83	THR
57	C1	136	ARG
58	C2	43	ARG
58	C2	45	LEU
58	C2	61	VAL
58	C2	103	LEU
58	C2	125	ASN
58	C2	126	TRP
58	C2	132	GLU
58	C2	140	PHE
59	C3	3	ARG
59	C3	13	SER
59	C3	27	LYS
59	C3	42	ARG
59	C3	64	ARG
59	C3	99	ARG
59	C3	105	ASN
59	C3	127	ARG
59	C3	138	ASN
59	C3	149	LEU
60	C4	25	ASP
60	C4	29	HIS
60	C4	41	ARG

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Mol	Chain	Res	Type
60	C4	43	THR
60	C4	51	ASP
60	C4	79	VAL
60	C4	81	VAL
60	C4	89	THR
60	C4	91	THR
60	C4	92	LYS
60	C4	137	LEU
61	C5	18	ARG
61	C5	21	ASP
61	C5	22	LEU
61	C5	36	LEU
61	C5	40	ARG
61	C5	50	THR
61	C5	89	MET
61	C5	108	ARG
61	C5	110	GLU
61	C5	130	ARG
62	C6	10	PHE
62	C6	12	LYS
62	C6	14	LYS
62	C6	34	SER
62	C6	40	GLU
62	C6	45	ARG
62	C6	46	PHE
62	C6	53	LEU
62	C6	59	LYS
62	C6	66	ARG
62	C6	69	VAL
62	C6	74	HIS
62	C6	106	LYS
62	C6	109	PHE
62	C6	114	ARG
62	C6	128	LYS
63	C7	3	ARG
63	C7	5	ARG
63	C7	6	THR
63	C7	7	LYS
63	C7	19	ARG
63	C7	23	LYS
63	C7	36	ASP
63	C7	38	ILE

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Mol	Chain	Res	Type
63	C7	40	THR
63	C7	43	SER
63	C7	46	LEU
63	C7	49	LYS
63	C7	59	LYS
63	C7	62	GLN
63	C7	83	GLN
63	C7	85	VAL
63	C7	87	GLU
63	C7	102	VAL
64	C8	7	GLU
64	C8	12	GLN
64	C8	25	ASN
64	C8	32	LEU
64	C8	47	CYS
64	C8	57	ARG
64	C8	71	GLN
64	C8	74	GLN
64	C8	88	ARG
64	C8	103	ASN
64	C8	111	ASP
64	C8	120	ARG
64	C8	143	ARG
64	C8	145	ARG
65	C9	6	VAL
65	C9	18	TYR
65	C9	22	LEU
65	C9	28	LEU
65	C9	35	ASP
65	C9	36	ILE
65	C9	43	ASN
65	C9	70	GLN
65	C9	84	LYS
65	C9	89	ARG
65	C9	126	GLU
65	C9	130	ARG
65	C9	144	GLU
66	D0	18	GLN
66	D0	23	ARG
66	D0	27	THR
66	D0	49	ASN
66	D0	66	SER

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Mol	Chain	Res	Type
66	D0	70	THR
66	D0	74	GLU
66	D0	81	THR
66	D0	85	ARG
66	D0	88	LYS
66	D0	118	VAL
67	D1	1	MET
67	D1	5	LYS
67	D1	22	ARG
67	D1	31	SER
67	D1	32	VAL
67	D1	33	GLN
67	D1	52	THR
67	D1	76	ASP
67	D1	87	ARG
68	D2	9	ASP
68	D2	22	LYS
68	D2	23	ARG
68	D2	31	SER
68	D2	37	PHE
68	D2	53	ILE
68	D2	65	LEU
68	D2	76	SER
68	D2	89	TRP
68	D2	93	LEU
68	D2	98	GLN
68	D2	121	VAL
68	D2	126	LEU
69	D3	3	LYS
69	D3	7	ARG
69	D3	19	ARG
69	D3	30	LYS
69	D3	57	LEU
69	D3	66	SER
69	D3	82	LYS
69	D3	89	ASN
69	D3	107	PHE
69	D3	110	LYS
69	D3	117	ILE
69	D3	133	LEU
70	D4	10	ARG
70	D4	34	ASN

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Mol	Chain	Res	Type
70	D4	49	LYS
70	D4	55	VAL
70	D4	57	VAL
70	D4	61	ARG
70	D4	63	GLN
70	D4	88	THR
70	D4	102	LYS
70	D4	104	SER
70	D4	124	ARG
70	D4	131	ARG
70	D4	132	ARG
71	D5	42	LEU
71	D5	48	ASP
71	D5	59	TYR
71	D5	60	VAL
71	D5	67	ASP
71	D5	70	LYS
71	D5	85	LYS
71	D5	95	HIS
71	D5	100	ILE
71	D5	102	THR
72	D6	3	LYS
72	D6	5	ARG
72	D6	7	SER
72	D6	12	LYS
72	D6	23	CYS
72	D6	38	ARG
72	D6	39	MET
72	D6	44	ILE
72	D6	52	ASP
72	D6	75	VAL
72	D6	82	ARG
72	D6	85	ARG
73	D7	3	LEU
73	D7	11	THR
73	D7	29	ARG
73	D7	33	LEU
73	D7	54	VAL
73	D7	72	LYS
73	D7	77	THR
73	D7	79	PHE
74	D8	14	LYS

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Mol	Chain	Res	Type
74	D8	19	THR
74	D8	32	PHE
74	D8	49	ARG
74	D8	64	ARG
74	D8	67	ARG
75	D9	5	ASN
75	D9	12	ARG
75	D9	14	TYR
75	D9	19	ARG
75	D9	21	CYS
75	D9	30	LEU
75	D9	32	ARG
75	D9	41	GLN
76	E0	15	LYS
76	E0	28	LYS
76	E0	39	LEU
76	E0	53	LYS
76	E0	55	ARG
77	E1	89	LYS
77	E1	138	ARG
77	E1	140	TYR
77	E1	144	CYS
77	E1	150	VAL
77	E1	151	ASN
78	SR	16	HIS
78	SR	44	SER
78	SR	50	ASP
78	SR	52	GLN
78	SR	59	ARG
78	SR	66	HIS
78	SR	73	LEU
78	SR	76	ASP
78	SR	106	HIS
78	SR	117	LYS
78	SR	141	LEU
78	SR	147	HIS
78	SR	149	ASP
78	SR	165	ASP
78	SR	191	ASP
78	SR	202	LEU
78	SR	207	ASP
78	SR	238	ASP

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Mol	Chain	Res	Type
78	SR	250	TYR
78	SR	265	LEU
78	SR	268	GLN
79	SM	23	LYS
79	SM	24	GLU
79	SM	27	LYS
79	SM	28	SER
79	SM	30	THR
79	SM	34	LYS
79	SM	46	LYS
79	SM	61	ILE
79	SM	70	ASN
79	SM	78	ASP
79	SM	88	ARG
79	SM	89	ARG
79	SM	91	THR
79	SM	102	THR
79	SM	116	GLU
79	SM	117	LEU
4	l2	14	SER
4	l2	31	THR
4	l2	32	LEU
4	l2	45	VAL
4	l2	79	ASN
4	l2	101	VAL
4	l2	104	LEU
4	l2	109	GLU
4	l2	113	VAL
4	l2	114	SER
4	l2	147	ARG
4	l2	159	SER
4	l2	165	VAL
4	l2	179	LEU
4	l2	181	LYS
4	l2	193	ARG
4	l2	243	THR
5	l3	3	HIS
5	l3	4	ARG
5	l3	5	LYS
5	l3	7	GLU
5	l3	10	ARG
5	l3	19	ARG

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Mol	Chain	Res	Type
5	13	24	SER
5	13	34	LYS
5	13	37	ARG
5	13	44	THR
5	13	47	LEU
5	13	53	MET
5	13	77	THR
5	13	85	VAL
5	13	103	THR
5	13	104	THR
5	13	111	SER
5	13	112	ASP
5	13	113	GLU
5	13	114	VAL
5	13	120	LYS
5	13	121	ASN
5	13	139	GLN
5	13	146	ARG
5	13	148	LEU
5	13	169	THR
5	13	192	VAL
5	13	196	ARG
5	13	202	THR
5	13	205	VAL
5	13	207	SER
5	13	211	GLN
5	13	222	LYS
5	13	229	VAL
5	13	232	ARG
5	13	242	THR
5	13	252	ILE
5	13	260	VAL
5	13	284	ARG
5	13	297	SER
5	13	316	GLU
5	13	320	ASP
5	13	332	ARG
5	13	369	ARG
5	13	386	ASP
6	14	10	SER
6	14	14	GLU
6	14	25	VAL

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Mol	Chain	Res	Type
6	14	33	ASP
6	14	37	THR
6	14	52	VAL
6	14	54	GLU
6	14	60	THR
6	14	64	SER
6	14	73	ARG
6	14	93	MET
6	14	105	THR
6	14	112	LYS
6	14	120	TYR
6	14	138	ARG
6	14	144	LYS
6	14	150	LEU
6	14	156	LEU
6	14	177	ASP
6	14	179	LEU
6	14	186	LYS
6	14	187	LEU
6	14	191	LYS
6	14	194	TYR
6	14	197	ARG
6	14	200	THR
6	14	206	LEU
6	14	220	ARG
6	14	230	VAL
6	14	246	ARG
6	14	258	LEU
6	14	287	THR
6	14	313	LEU
6	14	327	LEU
6	14	338	LYS
7	15	8	LYS
7	15	25	GLU
7	15	35	ARG
7	15	51	LEU
7	15	56	THR
7	15	70	THR
7	15	74	VAL
7	15	75	LEU
7	15	81	HIS
7	15	85	ARG

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Mol	Chain	Res	Type
7	15	110	LEU
7	15	111	GLN
7	15	112	LYS
7	15	117	GLU
7	15	133	GLU
7	15	146	LEU
7	15	152	ARG
7	15	155	THR
7	15	178	ASN
7	15	183	TRP
7	15	185	PHE
7	15	194	LEU
7	15	205	SER
7	15	210	GLU
7	15	211	LEU
7	15	220	SER
7	15	227	LEU
7	15	230	ASP
7	15	232	ASP
7	15	234	ASP
7	15	236	LEU
7	15	237	GLU
7	15	241	THR
7	15	259	LYS
7	15	271	LYS
7	15	273	ARG
8	16	2	SER
8	16	5	LYS
8	16	8	LYS
8	16	21	THR
8	16	26	ARG
8	16	30	LEU
8	16	46	ARG
8	16	50	LYS
8	16	52	VAL
8	16	64	LEU
8	16	65	ILE
8	16	66	SER
8	16	78	ARG
8	16	79	VAL
8	16	88	SER
8	16	89	THR

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Mol	Chain	Res	Type
8	16	96	VAL
8	16	98	VAL
8	16	109	GLU
8	16	129	GLU
8	16	152	THR
8	16	155	LEU
8	16	162	SER
9	17	22	THR
9	17	24	GLU
9	17	45	LEU
9	17	60	ARG
9	17	78	GLU
9	17	87	VAL
9	17	88	ARG
9	17	98	LYS
9	17	110	ARG
9	17	124	LEU
9	17	130	ILE
9	17	158	LYS
9	17	159	GLN
9	17	175	LYS
9	17	179	LEU
9	17	180	SER
9	17	184	LEU
9	17	229	PHE
9	17	232	ARG
10	18	68	ARG
10	18	74	THR
10	18	79	GLN
10	18	81	THR
10	18	83	ASP
10	18	108	ARG
10	18	132	VAL
10	18	136	LEU
10	18	149	LYS
10	18	162	LEU
10	18	164	VAL
10	18	169	LEU
10	18	172	LYS
10	18	192	GLN
10	18	200	LEU
10	18	203	VAL

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Mol	Chain	Res	Type
10	l8	246	MET
10	l8	248	LYS
11	l9	2	LYS
11	l9	6	THR
11	l9	18	VAL
11	l9	31	ARG
11	l9	48	VAL
11	l9	52	LEU
11	l9	68	LEU
11	l9	70	THR
11	l9	92	TYR
11	l9	93	VAL
11	l9	105	GLU
11	l9	133	THR
11	l9	140	VAL
11	l9	151	VAL
11	l9	157	ASN
11	l9	161	LEU
11	l9	169	ASN
11	l9	177	ASP
12	m0	3	ARG
12	m0	4	ARG
12	m0	20	SER
12	m0	21	ARG
12	m0	26	VAL
12	m0	28	ASP
12	m0	35	ASP
12	m0	42	THR
12	m0	48	LEU
12	m0	50	VAL
12	m0	52	LEU
12	m0	58	GLU
12	m0	59	GLN
12	m0	63	GLU
12	m0	71	CYS
12	m0	74	LYS
12	m0	76	MET
12	m0	85	PHE
12	m0	87	LEU
12	m0	95	HIS
12	m0	101	LYS
12	m0	129	VAL

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Mol	Chain	Res	Type
12	m0	138	VAL
12	m0	139	ARG
12	m0	142	ASP
12	m0	143	SER
12	m0	154	ARG
12	m0	156	ARG
12	m0	163	GLN
12	m0	167	LEU
12	m0	169	LYS
12	m0	176	LEU
12	m0	177	ASP
12	m0	200	LEU
12	m0	205	SER
12	m0	217	PHE
12	m0	220	GLN
13	m1	7	ASN
13	m1	9	MET
13	m1	13	LYS
13	m1	16	LYS
13	m1	29	ARG
13	m1	30	LEU
13	m1	34	SER
13	m1	44	THR
13	m1	55	ARG
13	m1	56	THR
13	m1	92	ARG
13	m1	101	ASN
13	m1	107	ASP
13	m1	109	HIS
13	m1	112	LEU
13	m1	129	VAL
13	m1	130	VAL
13	m1	137	ARG
13	m1	148	VAL
13	m1	152	HIS
13	m1	157	GLU
13	m1	159	THR
14	m3	13	HIS
14	m3	15	ARG
14	m3	23	LYS
14	m3	54	LEU
14	m3	57	VAL

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Mol	Chain	Res	Type
14	m3	58	VAL
14	m3	67	ARG
14	m3	69	VAL
14	m3	76	THR
14	m3	80	VAL
14	m3	85	LEU
14	m3	86	THR
14	m3	149	GLN
14	m3	152	THR
14	m3	168	ARG
14	m3	184	GLU
14	m3	194	GLU
15	m4	4	ASP
15	m4	13	ARG
15	m4	20	VAL
15	m4	21	VAL
15	m4	28	SER
15	m4	42	LYS
15	m4	62	GLN
15	m4	72	LEU
15	m4	80	THR
15	m4	82	SER
15	m4	90	VAL
15	m4	108	ARG
16	m5	7	LEU
16	m5	19	LEU
16	m5	22	LEU
16	m5	24	ARG
16	m5	49	ARG
16	m5	62	TYR
16	m5	65	ARG
16	m5	68	ARG
16	m5	71	ARG
16	m5	75	VAL
16	m5	80	THR
16	m5	83	LYS
16	m5	97	SER
16	m5	98	LEU
16	m5	99	ARG
16	m5	114	ARG
16	m5	117	ASN
16	m5	138	GLN

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Mol	Chain	Res	Type
16	m5	147	ARG
16	m5	153	ASP
16	m5	178	HIS
16	m5	180	PHE
16	m5	182	ASN
16	m5	204	LYS
17	m6	22	VAL
17	m6	25	LYS
17	m6	41	LEU
17	m6	56	ASP
17	m6	67	THR
17	m6	68	ARG
17	m6	78	ARG
17	m6	84	LEU
17	m6	85	ARG
17	m6	106	GLU
17	m6	108	ILE
17	m6	116	LYS
17	m6	119	VAL
17	m6	124	LEU
17	m6	128	ARG
17	m6	142	SER
17	m6	143	THR
17	m6	182	ASN
17	m6	184	THR
18	m7	3	ARG
18	m7	7	THR
18	m7	20	SER
18	m7	25	SER
18	m7	32	THR
18	m7	40	GLU
18	m7	52	LEU
18	m7	56	ARG
18	m7	69	ARG
18	m7	94	LEU
18	m7	107	LEU
18	m7	112	LEU
18	m7	115	SER
18	m7	116	HIS
18	m7	121	GLN
18	m7	126	ARG
18	m7	127	ARG

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Mol	Chain	Res	Type
18	m7	142	SER
18	m7	144	SER
18	m7	148	LEU
18	m7	155	GLU
19	m8	3	ILE
19	m8	7	SER
19	m8	12	ARG
19	m8	21	SER
19	m8	26	LEU
19	m8	32	LEU
19	m8	33	TYR
19	m8	49	LEU
19	m8	57	ILE
19	m8	64	VAL
19	m8	81	VAL
19	m8	86	THR
19	m8	93	ILE
19	m8	99	THR
19	m8	127	LEU
19	m8	135	GLN
19	m8	138	LEU
19	m8	141	ARG
19	m8	148	GLU
19	m8	168	THR
19	m8	170	ARG
19	m8	178	ARG
20	m9	10	LEU
20	m9	17	VAL
20	m9	27	ASN
20	m9	29	THR
20	m9	63	THR
20	m9	74	ARG
20	m9	84	THR
20	m9	88	ARG
20	m9	106	LEU
20	m9	114	LYS
20	m9	128	LYS
20	m9	130	ASN
20	m9	134	HIS
20	m9	138	LEU
20	m9	171	ASP
21	n0	1	MET

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Mol	Chain	Res	Type
21	n0	3	HIS
21	n0	17	GLU
21	n0	23	LYS
21	n0	32	SER
21	n0	50	LYS
21	n0	80	ARG
21	n0	87	THR
21	n0	88	HIS
21	n0	96	ASP
21	n0	97	VAL
21	n0	104	GLU
21	n0	117	ARG
21	n0	132	THR
21	n0	137	ARG
21	n0	148	LEU
21	n0	149	LYS
21	n0	155	ARG
21	n0	162	THR
21	n0	172	TYR
22	n1	3	LYS
22	n1	9	SER
22	n1	17	ARG
22	n1	25	VAL
22	n1	26	HIS
22	n1	28	SER
22	n1	60	LYS
22	n1	64	VAL
22	n1	78	LYS
22	n1	83	ARG
22	n1	88	ARG
22	n1	89	LEU
22	n1	101	CYS
22	n1	102	ARG
22	n1	107	GLU
22	n1	116	ARG
22	n1	118	GLU
22	n1	127	GLN
22	n1	131	GLN
22	n1	136	ARG
22	n1	139	ARG
22	n1	143	THR
22	n1	157	GLU

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Mol	Chain	Res	Type
23	n2	28	PHE
23	n2	50	LEU
23	n2	55	THR
23	n2	57	THR
23	n2	74	LYS
23	n2	75	TYR
23	n2	93	ILE
23	n2	100	THR
23	n2	104	ARG
24	n3	9	THR
24	n3	13	ILE
24	n3	32	ARG
24	n3	44	SER
24	n3	45	ARG
24	n3	68	GLU
24	n3	81	GLN
24	n3	131	SER
24	n3	135	VAL
81	n4	1	MET
81	n4	19	THR
81	n4	25	ASP
81	n4	36	SER
81	n4	39	LEU
81	n4	80	ARG
81	n4	96	LEU
81	n4	107	GLU
81	n4	127	LYS
26	n5	24	LEU
26	n5	27	ARG
26	n5	37	THR
26	n5	56	ARG
26	n5	59	SER
26	n5	71	THR
26	n5	102	LEU
26	n5	115	ARG
26	n5	125	ARG
26	n5	142	ILE
27	n6	3	LYS
27	n6	6	LEU
27	n6	12	ARG
27	n6	16	ARG
27	n6	21	THR

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Mol	Chain	Res	Type
27	n6	37	LYS
27	n6	40	ARG
27	n6	45	ILE
27	n6	48	LEU
27	n6	51	ARG
27	n6	56	VAL
27	n6	66	GLN
27	n6	71	SER
27	n6	74	TYR
27	n6	115	ARG
27	n6	120	GLN
27	n6	122	LYS
28	n7	3	LYS
28	n7	14	VAL
28	n7	29	HIS
28	n7	46	ILE
28	n7	81	LEU
28	n7	95	VAL
28	n7	99	GLU
28	n7	100	THR
28	n7	102	GLU
28	n7	108	GLU
28	n7	128	GLN
28	n7	134	LEU
29	n8	3	SER
29	n8	4	ARG
29	n8	8	THR
29	n8	10	LYS
29	n8	14	HIS
29	n8	15	VAL
29	n8	25	HIS
29	n8	32	ARG
29	n8	34	MET
29	n8	46	ASP
29	n8	47	LYS
29	n8	59	ARG
29	n8	60	TYR
29	n8	77	LYS
29	n8	82	ILE
29	n8	88	ASP
29	n8	115	LYS
29	n8	133	LEU

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Mol	Chain	Res	Type
30	n9	3	LYS
30	n9	13	THR
30	n9	17	HIS
30	n9	19	ASN
30	n9	21	ILE
30	n9	22	LYS
30	n9	58	LYS
31	o0	11	ASN
31	o0	12	GLN
31	o0	34	LEU
31	o0	41	LEU
31	o0	52	ARG
31	o0	54	SER
31	o0	59	TYR
31	o0	61	MET
31	o0	68	TYR
31	o0	76	GLU
31	o0	91	SER
31	o0	97	ASP
31	o0	104	LEU
32	o1	4	LEU
32	o1	5	LYS
32	o1	16	LEU
32	o1	26	LYS
32	o1	31	ARG
32	o1	44	MET
32	o1	46	THR
32	o1	55	LEU
32	o1	64	VAL
32	o1	76	SER
32	o1	89	LEU
32	o1	91	SER
32	o1	96	VAL
32	o1	106	THR
32	o1	107	VAL
32	o1	112	ASP
33	o2	6	HIS
33	o2	16	LYS
33	o2	18	LYS
33	o2	24	ARG
33	o2	27	ARG
33	o2	30	GLU

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Mol	Chain	Res	Type
33	o2	34	LYS
33	o2	35	GLN
33	o2	41	VAL
33	o2	51	SER
33	o2	73	THR
33	o2	75	LEU
33	o2	82	LEU
33	o2	100	ILE
33	o2	103	LYS
33	o2	125	ARG
34	o3	10	LYS
34	o3	20	LYS
34	o3	59	VAL
34	o3	60	ARG
34	o3	62	SER
34	o3	74	THR
34	o3	92	LYS
34	o3	98	VAL
34	o3	105	SER
35	o4	58	ARG
35	o4	64	THR
35	o4	66	SER
35	o4	68	THR
35	o4	71	THR
35	o4	81	CYS
35	o4	83	ASN
36	o5	20	GLN
36	o5	21	LEU
36	o5	27	GLU
36	o5	36	LEU
36	o5	38	ARG
36	o5	41	LEU
36	o5	46	THR
36	o5	67	ARG
36	o5	79	ASP
36	o5	86	ARG
36	o5	89	ARG
36	o5	90	ARG
36	o5	98	SER
37	o6	2	THR
37	o6	15	LYS
37	o6	19	SER

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Mol	Chain	Res	Type
37	o6	21	THR
37	o6	29	LYS
37	o6	34	SER
37	o6	35	ASN
37	o6	36	ARG
37	o6	38	LYS
37	o6	68	ARG
37	o6	99	ARG
38	o7	3	LYS
38	o7	11	ARG
38	o7	16	HIS
38	o7	25	ARG
38	o7	28	HIS
38	o7	33	THR
38	o7	44	THR
38	o7	46	SER
38	o7	58	THR
38	o7	59	THR
38	o7	65	ARG
38	o7	80	THR
39	o8	16	ARG
39	o8	17	ARG
39	o8	28	ASN
39	o8	41	THR
39	o8	46	ARG
39	o8	52	TYR
39	o8	63	LYS
39	o8	64	LYS
40	o9	6	SER
40	o9	15	LYS
40	o9	21	ARG
40	o9	42	ARG
40	o9	45	ARG
40	o9	49	MET
40	o9	51	ILE
82	p0	5	ARG
82	p0	10	GLU
82	p0	15	LEU
82	p0	26	PHE
82	p0	31	ASP
82	p0	46	ARG
82	p0	48	ARG

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Mol	Chain	Res	Type
82	p0	51	VAL
82	p0	55	LYS
82	p0	67	LEU
82	p0	72	ASP
82	p0	73	PHE
82	p0	93	LEU
82	p0	104	ARG
82	p0	196	VAL
41	q0	79	GLU
41	q0	91	CYS
41	q0	98	LYS
41	q0	112	LYS
41	q0	113	ARG
41	q0	114	LYS
41	q0	127	LEU
41	q0	128	LYS
42	q1	8	LYS
42	q1	24	SER
42	q1	25	LYS
43	q2	2	VAL
43	q2	7	THR
43	q2	8	ARG
43	q2	17	CYS
43	q2	18	ARG
43	q2	26	THR
43	q2	28	TYR
43	q2	34	SER
43	q2	48	SER
43	q2	61	LYS
43	q2	71	ARG
43	q2	78	LYS
43	q2	80	ARG
43	q2	85	LEU
43	q2	93	LEU
43	q2	96	GLU
43	q2	105	GLN
43	q2	106	PHE
44	q3	4	ARG
44	q3	24	ARG
44	q3	25	GLN
44	q3	26	VAL
44	q3	54	ILE

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Mol	Chain	Res	Type
44	q3	60	CYS
46	s0	3	LEU
46	s0	22	THR
46	s0	30	GLN
46	s0	50	VAL
46	s0	59	LEU
46	s0	83	GLN
46	s0	87	LEU
46	s0	103	THR
46	s0	135	GLU
46	s0	139	VAL
46	s0	153	SER
46	s0	157	ASP
46	s0	164	ASN
46	s0	172	LEU
46	s0	185	ARG
46	s0	190	ASP
46	s0	200	ASP
46	s0	202	TYR
46	s0	203	PHE
47	s1	47	LEU
47	s1	54	LEU
47	s1	61	LEU
47	s1	62	LYS
47	s1	70	LEU
47	s1	78	ASP
47	s1	81	PHE
47	s1	96	LEU
47	s1	98	THR
47	s1	103	MET
47	s1	115	ARG
47	s1	169	SER
47	s1	173	THR
47	s1	183	GLN
47	s1	185	THR
47	s1	194	ASN
47	s1	223	PHE
47	s1	234	GLU
48	s2	55	GLU
48	s2	69	ILE
48	s2	72	LEU
48	s2	73	LEU

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Mol	Chain	Res	Type
48	s2	89	GLN
48	s2	90	THR
48	s2	91	ARG
48	s2	94	GLN
48	s2	97	ARG
48	s2	111	VAL
48	s2	117	THR
48	s2	137	ILE
48	s2	139	ILE
48	s2	141	ARG
48	s2	146	THR
48	s2	152	HIS
48	s2	161	LYS
48	s2	164	SER
48	s2	185	LYS
48	s2	186	LYS
48	s2	225	LEU
48	s2	229	LEU
49	s3	7	LYS
49	s3	21	LEU
49	s3	35	SER
49	s3	40	ARG
49	s3	44	THR
49	s3	55	THR
49	s3	61	GLU
49	s3	64	ARG
49	s3	65	ARG
49	s3	71	LEU
49	s3	74	GLN
49	s3	109	LEU
49	s3	111	ASN
49	s3	113	LEU
49	s3	116	ARG
49	s3	117	ARG
49	s3	127	MET
49	s3	132	LYS
49	s3	139	SER
49	s3	162	GLN
49	s3	168	ILE
49	s3	169	ASP
49	s3	170	THR
49	s3	172	THR

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Mol	Chain	Res	Type
49	s3	176	LEU
49	s3	177	MET
49	s3	178	ARG
49	s3	179	GLN
49	s3	185	LYS
49	s3	212	LYS
49	s3	213	GLU
49	s3	218	LEU
50	s4	9	LEU
50	s4	11	ARG
50	s4	12	LEU
50	s4	38	LEU
50	s4	45	ILE
50	s4	57	ASN
50	s4	66	MET
50	s4	67	GLN
50	s4	100	ARG
50	s4	104	ASP
50	s4	113	ARG
50	s4	116	ASP
50	s4	126	VAL
50	s4	131	LEU
50	s4	138	TYR
50	s4	148	ARG
50	s4	170	THR
50	s4	180	LEU
50	s4	182	TYR
50	s4	187	ARG
50	s4	194	THR
50	s4	216	ASN
50	s4	217	THR
50	s4	221	ARG
50	s4	246	LEU
50	s4	252	ARG
51	s5	25	LEU
51	s5	27	THR
51	s5	31	GLU
51	s5	37	GLN
51	s5	38	THR
51	s5	42	LEU
51	s5	51	VAL
51	s5	60	ASP

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Mol	Chain	Res	Type
51	s5	63	GLN
51	s5	66	GLN
51	s5	79	ASN
51	s5	89	ILE
51	s5	93	LEU
51	s5	112	ARG
51	s5	148	ARG
51	s5	156	ARG
51	s5	157	ARG
51	s5	167	ARG
51	s5	190	ILE
51	s5	194	LEU
51	s5	208	SER
51	s5	213	LYS
51	s5	225	ARG
52	s6	1	MET
52	s6	6	SER
52	s6	7	TYR
52	s6	14	LYS
52	s6	15	THR
52	s6	22	HIS
52	s6	30	LYS
52	s6	31	ARG
52	s6	34	GLN
52	s6	50	PHE
52	s6	57	ASP
52	s6	71	THR
52	s6	76	LEU
52	s6	80	ASN
52	s6	92	ARG
52	s6	93	LYS
52	s6	97	VAL
52	s6	98	ARG
52	s6	111	LEU
52	s6	121	LEU
52	s6	126	ASP
52	s6	127	THR
52	s6	128	THR
52	s6	151	ASP
52	s6	166	GLU
52	s6	215	ARG
52	s6	216	LEU

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Mol	Chain	Res	Type
53	s7	8	ILE
53	s7	11	GLN
53	s7	35	LYS
53	s7	42	GLN
53	s7	50	ASP
53	s7	62	VAL
53	s7	67	LEU
53	s7	79	ARG
53	s7	108	GLN
53	s7	117	THR
53	s7	157	LYS
53	s7	160	GLN
53	s7	166	LEU
54	s8	20	GLN
54	s8	28	GLU
54	s8	29	LEU
54	s8	36	THR
54	s8	59	ARG
54	s8	69	SER
54	s8	76	THR
54	s8	116	HIS
54	s8	137	LYS
54	s8	155	SER
54	s8	168	CYS
55	s9	6	ARG
55	s9	11	THR
55	s9	22	SER
55	s9	28	LEU
55	s9	39	LYS
55	s9	46	SER
55	s9	90	LYS
55	s9	93	LEU
55	s9	94	ASP
55	s9	105	LEU
55	s9	109	LEU
55	s9	130	THR
55	s9	133	HIS
55	s9	134	ILE
55	s9	147	MET
56	c0	3	MET
56	c0	15	LEU
56	c0	33	GLU

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Mol	Chain	Res	Type
56	c0	36	ASP
56	c0	37	THR
56	c0	40	LEU
56	c0	58	GLN
56	c0	79	TYR
57	c1	20	PHE
57	c1	21	ASN
57	c1	22	ASN
57	c1	25	VAL
57	c1	33	ARG
57	c1	40	LEU
57	c1	60	PHE
57	c1	61	THR
57	c1	67	ARG
57	c1	72	THR
57	c1	74	THR
57	c1	83	THR
57	c1	90	TYR
57	c1	115	PHE
57	c1	117	VAL
57	c1	122	ILE
57	c1	129	ARG
58	c2	26	ASP
58	c2	28	LEU
58	c2	52	LEU
58	c2	58	LEU
58	c2	61	VAL
58	c2	103	LEU
58	c2	121	VAL
58	c2	126	TRP
58	c2	129	GLU
58	c2	131	ASP
58	c2	139	HIS
58	c2	140	PHE
59	c3	12	SER
59	c3	19	SER
59	c3	40	TYR
59	c3	58	HIS
59	c3	64	ARG
59	c3	66	ILE
59	c3	72	MET
59	c3	73	ARG

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Mol	Chain	Res	Type
59	c3	80	LEU
59	c3	87	ASP
59	c3	94	LYS
59	c3	104	ARG
59	c3	106	ARG
59	c3	115	LEU
59	c3	125	LEU
59	c3	131	THR
59	c3	134	VAL
60	c4	14	PHE
60	c4	28	VAL
60	c4	32	ASP
60	c4	55	SER
60	c4	71	CYS
60	c4	82	LYS
60	c4	89	THR
60	c4	92	LYS
60	c4	114	ARG
60	c4	123	SER
60	c4	132	ARG
60	c4	136	ARG
60	c4	137	LEU
61	c5	21	ASP
61	c5	22	LEU
61	c5	71	GLU
61	c5	92	SER
61	c5	97	TYR
61	c5	107	ILE
61	c5	121	ILE
61	c5	122	THR
61	c5	124	THR
61	c5	127	ARG
62	c6	13	LYS
62	c6	17	THR
62	c6	23	LYS
62	c6	40	GLU
62	c6	48	VAL
62	c6	53	LEU
62	c6	57	LEU
62	c6	69	VAL
62	c6	111	SER
62	c6	113	ASP

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Mol	Chain	Res	Type
62	c6	117	LEU
62	c6	121	SER
62	c6	128	LYS
62	c6	137	ARG
62	c6	141	SER
63	c7	5	ARG
63	c7	6	THR
63	c7	7	LYS
63	c7	30	THR
63	c7	34	LEU
63	c7	46	LEU
63	c7	54	THR
63	c7	75	GLU
63	c7	103	ASP
63	c7	108	ASP
64	c8	2	SER
64	c8	3	LEU
64	c8	5	VAL
64	c8	12	GLN
64	c8	13	HIS
64	c8	26	ILE
64	c8	28	ILE
64	c8	36	LYS
64	c8	40	ARG
64	c8	57	ARG
64	c8	61	LEU
64	c8	73	MET
64	c8	85	PHE
64	c8	100	THR
64	c8	101	LEU
64	c8	116	LEU
64	c8	134	ARG
64	c8	138	THR
64	c8	140	THR
64	c8	143	ARG
65	c9	6	VAL
65	c9	25	GLN
65	c9	28	LEU
65	c9	33	TYR
65	c9	36	ILE
65	c9	57	ARG
65	c9	68	ARG

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Mol	Chain	Res	Type
65	c9	86	ARG
65	c9	88	VAL
65	c9	89	ARG
65	c9	99	SER
65	c9	116	ILE
65	c9	123	ARG
65	c9	125	SER
65	c9	126	GLU
66	d0	19	ILE
66	d0	23	ARG
66	d0	27	THR
66	d0	30	LYS
66	d0	34	LEU
66	d0	42	VAL
66	d0	44	ASN
66	d0	57	ARG
66	d0	70	THR
66	d0	77	LYS
66	d0	98	GLN
66	d0	103	ILE
66	d0	109	GLU
66	d0	115	GLU
67	d1	2	GLU
67	d1	3	ASN
67	d1	12	TYR
67	d1	21	ASN
67	d1	52	THR
67	d1	62	ARG
67	d1	68	SER
67	d1	75	ASN
67	d1	81	ASN
68	d2	3	ARG
68	d2	4	SER
68	d2	6	VAL
68	d2	7	LEU
68	d2	9	ASP
68	d2	20	THR
68	d2	22	LYS
68	d2	23	ARG
68	d2	28	ARG
68	d2	65	LEU
68	d2	68	ARG

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Mol	Chain	Res	Type
68	d2	98	GLN
68	d2	126	LEU
69	d3	3	LYS
69	d3	16	ARG
69	d3	19	ARG
69	d3	28	ASN
69	d3	69	ARG
69	d3	73	ARG
69	d3	84	THR
69	d3	100	ASP
69	d3	107	PHE
69	d3	144	ARG
70	d4	10	ARG
70	d4	35	VAL
70	d4	43	LYS
70	d4	49	LYS
70	d4	53	ASP
70	d4	57	VAL
70	d4	58	PHE
70	d4	62	THR
70	d4	88	THR
70	d4	124	ARG
70	d4	132	ARG
71	d5	68	ARG
71	d5	70	LYS
71	d5	85	LYS
71	d5	97	LYS
72	d6	7	SER
72	d6	10	ARG
72	d6	11	ASN
72	d6	18	VAL
72	d6	33	ASP
72	d6	46	GLU
72	d6	52	ASP
72	d6	82	ARG
72	d6	84	VAL
72	d6	88	SER
72	d6	91	ASP
73	d7	3	LEU
73	d7	37	CYS
73	d7	52	THR
73	d7	56	CYS

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Mol	Chain	Res	Type
73	d7	81	ARG
74	d8	15	VAL
74	d8	22	ARG
74	d8	31	GLU
74	d8	32	PHE
74	d8	33	LEU
74	d8	34	GLU
74	d8	38	ARG
74	d8	40	ILE
74	d8	49	ARG
74	d8	52	ASP
74	d8	58	GLU
74	d8	60	GLU
74	d8	62	GLU
74	d8	64	ARG
74	d8	65	ARG
75	d9	7	TRP
75	d9	8	PHE
75	d9	10	HIS
75	d9	12	ARG
75	d9	16	LYS
75	d9	30	LEU
75	d9	32	ARG
75	d9	36	LEU
75	d9	39	CYS
75	d9	49	ASP
75	d9	55	PHE
76	e0	3	LYS
76	e0	4	VAL
76	e0	5	HIS
76	e0	13	LYS
76	e0	28	LYS
76	e0	29	LYS
76	e0	44	PHE
76	e0	48	THR
76	e0	55	ARG
77	e1	84	VAL
77	e1	90	LYS
77	e1	91	ILE
77	e1	99	LYS
77	e1	100	LEU
77	e1	106	TYR

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Mol	Chain	Res	Type
77	e1	108	VAL
77	e1	113	LYS
77	e1	130	VAL
77	e1	137	ASP
77	e1	144	CYS
77	e1	150	VAL
78	sR	4	ASN
78	sR	10	ARG
78	sR	22	SER
78	sR	60	SER
78	sR	70	ASP
78	sR	76	ASP
78	sR	96	THR
78	sR	109	ASP
78	sR	123	ILE
78	sR	126	SER
78	sR	145	LEU
78	sR	167	VAL
78	sR	195	HIS
78	sR	197	SER
78	sR	238	ASP
78	sR	258	THR
78	sR	266	ASP
78	sR	275	ARG
78	sR	282	SER
79	sM	30	THR
79	sM	33	LYS
79	sM	53	ARG
79	sM	61	ILE
79	sM	77	THR
79	sM	84	LYS
79	sM	102	THR
79	sM	103	LYS
79	sM	104	LYS
79	sM	110	TRP
79	sM	116	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
4	L2	86	GLN
7	L5	40	HIS

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Mol	Chain	Res	Type
7	L5	264	GLN
11	L9	49	ASN
12	M0	59	GLN
13	M1	68	HIS
13	M1	109	HIS
19	M8	136	ASN
21	N0	88	HIS
23	N2	52	ASN
24	N3	98	ASN
28	N7	57	HIS
29	N8	62	HIS
38	O7	30	GLN
47	S1	118	GLN
47	S1	209	ASN
50	S4	188	ASN
50	S4	209	HIS
53	S7	71	HIS
53	S7	160	GLN
54	S8	103	GLN
55	S9	38	ASN
55	S9	139	GLN
56	C0	28	ASN
57	C1	81	HIS
61	C5	103	ASN
70	D4	63	GLN
71	D5	95	HIS
75	D9	5	ASN
5	l3	211	GLN
6	l4	279	HIS
7	l5	17	GLN
7	l5	81	HIS
9	l7	166	ASN
11	l9	162	GLN
12	m0	23	ASN
16	m5	138	GLN
20	m9	7	GLN
20	m9	36	ASN
20	m9	118	HIS
26	n5	111	ASN
27	n6	120	GLN
28	n7	57	HIS
28	n7	128	GLN

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Mol	Chain	Res	Type
47	s1	232	HIS
50	s4	69	HIS
52	s6	182	GLN
53	s7	71	HIS
56	c0	32	HIS
57	c1	138	ASN
62	c6	83	GLN
64	c8	44	ASN
66	d0	72	ASN
67	d1	3	ASN
70	d4	22	GLN
73	d7	51	GLN
76	e0	17	GLN
78	sR	248	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3095/3396 (91%)	696 (22%)	86 (2%)
1	5	3129/3396 (92%)	752 (24%)	83 (2%)
2	3	120/121 (99%)	22 (18%)	1 (0%)
2	7	120/121 (99%)	24 (20%)	1 (0%)
3	4	154/158 (97%)	36 (23%)	2 (1%)
3	8	157/158 (99%)	43 (27%)	1 (0%)
45	2	1708/1800 (94%)	481 (28%)	59 (3%)
45	6	1733/1800 (96%)	485 (27%)	62 (3%)
All	All	10216/10950 (93%)	2539 (24%)	295 (2%)

All (2539) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	14	U
1	1	16	A
1	1	26	A
1	1	30	G
1	1	40	A
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A

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Mol	Chain	Res	Type
1	1	65	A
1	1	66	A
1	1	68	C
1	1	73	C
1	1	74	G
1	1	76	G
1	1	92	G
1	1	101	G
1	1	109	A
1	1	110	G
1	1	111	C
1	1	113	C
1	1	118	U
1	1	121	A
1	1	122	A
1	1	123	A
1	1	133	U
1	1	135	C
1	1	136	G
1	1	146	U
1	1	147	U
1	1	148	G
1	1	156	G
1	1	157	A
1	1	166	C
1	1	169	U
1	1	170	G
1	1	187	A
1	1	190	U
1	1	191	U
1	1	192	C
1	1	200	C
1	1	210	U
1	1	211	A
1	1	218	G
1	1	219	A
1	1	227	G
1	1	228	U
1	1	237	G
1	1	238	A
1	1	240	U
1	1	241	G

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Mol	Chain	Res	Type
1	1	244	G
1	1	245	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	269	G
1	1	286	U
1	1	295	A
1	1	298	U
1	1	305	U
1	1	315	C
1	1	316	U
1	1	323	A
1	1	329	U
1	1	334	A
1	1	338	A
1	1	339	C
1	1	349	A
1	1	350	C
1	1	373	A
1	1	374	A
1	1	376	G
1	1	378	A
1	1	390	G
1	1	397	A
1	1	398	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	404	G
1	1	420	G
1	1	421	G
1	1	422	A
1	1	437	G
1	1	439	C
1	1	440	A
1	1	495	G
1	1	496	C
1	1	498	A
1	1	511	G
1	1	519	A
1	1	521	A

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Mol	Chain	Res	Type
1	1	535	G
1	1	543	C
1	1	544	C
1	1	546	C
1	1	547	G
1	1	548	G
1	1	549	U
1	1	552	G
1	1	555	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	566	G
1	1	568	G
1	1	578	A
1	1	579	G
1	1	592	A
1	1	594	U
1	1	595	G
1	1	597	G
1	1	600	G
1	1	603	A
1	1	604	G
1	1	609	G
1	1	611	A
1	1	619	A
1	1	620	U
1	1	621	A
1	1	622	A
1	1	623	U
1	1	636	C
1	1	637	C
1	1	638	C
1	1	641	C
1	1	642	U
1	1	646	A
1	1	649	A
1	1	651	G
1	1	660	A
1	1	661	G
1	1	662	U
1	1	677	A

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Mol	Chain	Res	Type
1	1	681	U
1	1	683	U
1	1	691	A
1	1	696	C
1	1	698	U
1	1	705	A
1	1	712	G
1	1	715	A
1	1	716	A
1	1	719	U
1	1	725	G
1	1	726	G
1	1	758	C
1	1	764	U
1	1	766	U
1	1	767	U
1	1	776	U
1	1	777	U
1	1	778	U
1	1	781	G
1	1	785	G
1	1	786	A
1	1	806	A
1	1	816	A
1	1	817	A
1	1	823	C
1	1	830	A
1	1	832	G
1	1	849	C
1	1	857	G
1	1	861	C
1	1	874	U
1	1	875	G
1	1	879	U
1	1	883	A
1	1	890	C
1	1	894	G
1	1	896	A
1	1	905	U
1	1	907	G
1	1	908	G
1	1	913	A

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Mol	Chain	Res	Type
1	1	914	A
1	1	916	G
1	1	917	A
1	1	920	A
1	1	921	A
1	1	924	G
1	1	937	G
1	1	944	C
1	1	953	G
1	1	959	C
1	1	960	U
1	1	962	A
1	1	974	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	994	G
1	1	1001	G
1	1	1002	A
1	1	1010	G
1	1	1015	U
1	1	1016	C
1	1	1017	C
1	1	1018	G
1	1	1020	G
1	1	1021	G
1	1	1024	G
1	1	1025	A
1	1	1026	A
1	1	1028	U
1	1	1029	G
1	1	1030	A
1	1	1036	A
1	1	1037	C
1	1	1045	C
1	1	1047	A
1	1	1049	C
1	1	1057	A
1	1	1064	A
1	1	1065	A
1	1	1071	U

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Mol	Chain	Res	Type
1	1	1072	G
1	1	1081	U
1	1	1082	U
1	1	1083	G
1	1	1087	G
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1096	U
1	1	1097	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1117	G
1	1	1131	G
1	1	1153	A
1	1	1159	A
1	1	1178	G
1	1	1180	A
1	1	1181	U
1	1	1186	G
1	1	1190	A
1	1	1191	U
1	1	1192	C
1	1	1201	C
1	1	1209	G
1	1	1211	U
1	1	1213	G
1	1	1216	C
1	1	1218	U
1	1	1220	U
1	1	1221	A
1	1	1222	G
1	1	1227	C
1	1	1279	C
1	1	1281	G
1	1	1284	C
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1288	U
1	1	1292	C

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Mol	Chain	Res	Type
1	1	1303	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1318	A
1	1	1325	U
1	1	1326	A
1	1	1330	A
1	1	1332	A
1	1	1345	G
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1377	G
1	1	1386	A
1	1	1395	G
1	1	1399	A
1	1	1400	G
1	1	1407	A
1	1	1408	G
1	1	1419	A
1	1	1421	G
1	1	1431	G
1	1	1433	A
1	1	1434	G
1	1	1437	C
1	1	1446	A
1	1	1450	G
1	1	1454	A
1	1	1455	U
1	1	1467	A
1	1	1481	A
1	1	1482	A
1	1	1485	G
1	1	1506	A

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Mol	Chain	Res	Type
1	1	1508	C
1	1	1514	G
1	1	1527	C
1	1	1546	A
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1558	A
1	1	1560	G
1	1	1561	G
1	1	1562	C
1	1	1563	C
1	1	1564	U
1	1	1565	G
1	1	1566	A
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1570	U
1	1	1576	G
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1583	A
1	1	1587	A
1	1	1589	A
1	1	1593	A
1	1	1605	A
1	1	1607	U
1	1	1608	C
1	1	1619	A
1	1	1620	U
1	1	1629	U
1	1	1639	C
1	1	1643	A
1	1	1644	C
1	1	1645	U
1	1	1655	G
1	1	1657	C
1	1	1658	G
1	1	1683	A
1	1	1686	U

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Mol	Chain	Res	Type
1	1	1701	C
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1729	A
1	1	1736	G
1	1	1741	A
1	1	1742	U
1	1	1746	U
1	1	1750	A
1	1	1751	G
1	1	1752	A
1	1	1759	C
1	1	1760	A
1	1	1761	C
1	1	1762	C
1	1	1763	U
1	1	1764	U
1	1	1765	U
1	1	1770	G
1	1	1773	C
1	1	1780	G
1	1	1781	C
1	1	1797	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1819	U
1	1	1820	U
1	1	1821	U
1	1	1834	U
1	1	1835	A
1	1	1839	A
1	1	1841	A
1	1	1842	A
1	1	1845	G
1	1	1846	C
1	1	1849	C
1	1	1850	A
1	1	1864	A

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Mol	Chain	Res	Type
1	1	1871	U
1	1	1878	G
1	1	1879	A
1	1	1880	U
1	1	1886	A
1	1	1892	G
1	1	1906	G
1	1	1926	C
1	1	1927	G
1	1	1948	G
1	1	1951	C
1	1	1952	G
1	1	1953	G
1	1	1954	G
1	1	2094	C
1	1	2095	G
1	1	2100	A
1	1	2101	C
1	1	2102	U
1	1	2111	G
1	1	2112	U
1	1	2113	A
1	1	2114	C
1	1	2121	G
1	1	2122	G
1	1	2131	A
1	1	2140	U
1	1	2158	A
1	1	2164	A
1	1	2169	G
1	1	2170	U
1	1	2171	G
1	1	2177	G
1	1	2179	C
1	1	2188	A
1	1	2190	U
1	1	2194	G
1	1	2198	A
1	1	2200	U
1	1	2201	G
1	1	2205	U
1	1	2206	G

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Mol	Chain	Res	Type
1	1	2207	A
1	1	2208	A
1	1	2209	U
1	1	2223	A
1	1	2228	A
1	1	2230	C
1	1	2244	A
1	1	2249	G
1	1	2250	G
1	1	2252	A
1	1	2255	A
1	1	2256	A
1	1	2257	C
1	1	2272	G
1	1	2273	G
1	1	2279	A
1	1	2280	A
1	1	2281	A
1	1	2282	U
1	1	2284	C
1	1	2288	G
1	1	2307	G
1	1	2310	U
1	1	2311	G
1	1	2313	A
1	1	2314	U
1	1	2315	G
1	1	2334	U
1	1	2336	U
1	1	2364	G
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2385	G
1	1	2393	G
1	1	2397	A
1	1	2401	A
1	1	2402	A
1	1	2403	G
1	1	2404	A
1	1	2405	C

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Mol	Chain	Res	Type
1	1	2411	U
1	1	2412	G
1	1	2418	G
1	1	2419	A
1	1	2434	U
1	1	2440	G
1	1	2444	C
1	1	2503	G
1	1	2504	U
1	1	2507	C
1	1	2508	U
1	1	2511	A
1	1	2514	U
1	1	2515	A
1	1	2522	G
1	1	2523	A
1	1	2532	U
1	1	2533	G
1	1	2537	U
1	1	2538	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2546	C
1	1	2547	A
1	1	2549	G
1	1	2552	C
1	1	2554	A
1	1	2555	G
1	1	2559	U
1	1	2561	A
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2574	G
1	1	2576	G
1	1	2581	U
1	1	2585	G

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Mol	Chain	Res	Type
1	1	2593	A
1	1	2594	C
1	1	2606	G
1	1	2607	G
1	1	2614	G
1	1	2619	G
1	1	2636	A
1	1	2638	C
1	1	2652	U
1	1	2656	A
1	1	2658	G
1	1	2673	A
1	1	2674	A
1	1	2675	C
1	1	2677	G
1	1	2681	U
1	1	2689	A
1	1	2691	A
1	1	2694	A
1	1	2696	A
1	1	2705	A
1	1	2714	G
1	1	2719	U
1	1	2720	G
1	1	2723	U
1	1	2728	G
1	1	2737	C
1	1	2752	U
1	1	2753	G
1	1	2760	C
1	1	2766	U
1	1	2769	A
1	1	2772	C
1	1	2773	C
1	1	2776	C
1	1	2777	G
1	1	2778	G
1	1	2796	G
1	1	2799	A
1	1	2800	G
1	1	2801	A
1	1	2802	A

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Mol	Chain	Res	Type
1	1	2803	A
1	1	2810	C
1	1	2814	G
1	1	2815	G
1	1	2816	G
1	1	2817	A
1	1	2818	U
1	1	2836	C
1	1	2839	G
1	1	2842	U
1	1	2845	A
1	1	2847	A
1	1	2853	A
1	1	2860	U
1	1	2868	U
1	1	2871	G
1	1	2872	A
1	1	2875	U
1	1	2876	C
1	1	2887	A
1	1	2896	A
1	1	2898	G
1	1	2899	C
1	1	2914	G
1	1	2923	U
1	1	2935	U
1	1	2936	A
1	1	2942	C
1	1	2946	A
1	1	2947	G
1	1	2965	U
1	1	2971	A
1	1	2973	G
1	1	2983	C
1	1	2985	C
1	1	2986	U
1	1	2987	A
1	1	2990	G
1	1	2997	G
1	1	3011	A
1	1	3012	A
1	1	3030	G

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Mol	Chain	Res	Type
1	1	3046	A
1	1	3057	U
1	1	3059	G
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3086	A
1	1	3092	C
1	1	3094	A
1	1	3101	G
1	1	3117	C
1	1	3120	C
1	1	3122	A
1	1	3128	G
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3152	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U
1	1	3157	U
1	1	3164	C
1	1	3165	A
1	1	3168	A
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3181	C
1	1	3187	A
1	1	3195	U
1	1	3196	U
1	1	3206	C
1	1	3207	U
1	1	3210	A
1	1	3217	C
1	1	3218	A

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Mol	Chain	Res	Type
1	1	3219	G
1	1	3234	A
1	1	3235	C
1	1	3244	A
1	1	3245	A
1	1	3246	G
1	1	3247	G
1	1	3256	G
1	1	3259	U
1	1	3270	U
1	1	3273	A
1	1	3276	G
1	1	3277	U
1	1	3279	A
1	1	3280	U
1	1	3281	U
1	1	3286	G
1	1	3288	G
1	1	3289	G
1	1	3293	U
1	1	3294	A
1	1	3295	A
1	1	3303	G
1	1	3304	U
1	1	3307	A
1	1	3316	A
1	1	3318	G
1	1	3320	A
1	1	3323	A
1	1	3335	A
1	1	3341	U
1	1	3342	A
1	1	3344	A
1	1	3345	G
1	1	3346	U
1	1	3347	A
1	1	3349	C
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3354	U
1	1	3355	U

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Mol	Chain	Res	Type
1	1	3358	U
1	1	3359	A
1	1	3360	C
1	1	3363	U
1	1	3368	U
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3382	U
1	1	3383	G
1	1	3384	U
1	1	3386	G
1	1	3389	U
1	1	3396	U
2	3	5	G
2	3	7	G
2	3	10	C
2	3	13	A
2	3	22	A
2	3	29	C
2	3	41	G
2	3	49	G
2	3	51	A
2	3	53	U
2	3	54	U
2	3	55	A
2	3	65	G
2	3	73	C
2	3	74	C
2	3	75	G
2	3	76	A
2	3	91	G
2	3	95	A
2	3	102	A
2	3	112	G
2	3	114	U
3	4	2	A
3	4	20	U
3	4	23	U
3	4	34	U
3	4	35	C
3	4	39	G

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Mol	Chain	Res	Type
3	4	43	A
3	4	51	G
3	4	59	A
3	4	62	C
3	4	63	G
3	4	75	G
3	4	84	C
3	4	85	G
3	4	86	U
3	4	87	G
3	4	90	U
3	4	95	G
3	4	104	A
3	4	105	A
3	4	106	C
3	4	110	C
3	4	111	A
3	4	113	U
3	4	120	C
3	4	125	U
3	4	126	A
3	4	128	U
3	4	146	U
3	4	148	G
3	4	151	C
3	4	152	G
3	4	155	A
3	4	156	U
3	4	157	U
3	4	158	U
45	2	2	A
45	2	4	C
45	2	17	C
45	2	25	C
45	2	26	A
45	2	27	U
45	2	34	G
45	2	39	A
45	2	42	G
45	2	45	U
45	2	46	A
45	2	47	A

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Mol	Chain	Res	Type
45	2	50	C
45	2	57	G
45	2	59	C
45	2	60	U
45	2	67	A
45	2	68	A
45	2	69	G
45	2	72	A
45	2	73	U
45	2	74	U
45	2	75	U
45	2	76	A
45	2	77	U
45	2	95	G
45	2	100	A
45	2	104	A
45	2	105	A
45	2	106	U
45	2	111	U
45	2	114	C
45	2	140	A
45	2	141	U
45	2	144	U
45	2	145	A
45	2	146	U
45	2	153	G
45	2	159	U
45	2	160	C
45	2	178	U
45	2	179	A
45	2	181	A
45	2	185	U
45	2	186	C
45	2	190	C
45	2	191	C
45	2	194	U
45	2	195	G
45	2	196	G
45	2	197	A
45	2	198	A
45	2	199	G
45	2	200	A

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Mol	Chain	Res	Type
45	2	215	A
45	2	218	A
45	2	219	A
45	2	222	A
45	2	226	A
45	2	227	U
45	2	228	G
45	2	229	U
45	2	230	C
45	2	231	U
45	2	233	C
45	2	234	G
45	2	235	G
45	2	238	U
45	2	239	C
45	2	240	U
45	2	241	U
45	2	242	U
45	2	250	C
45	2	260	U
45	2	261	U
45	2	262	U
45	2	265	A
45	2	266	A
45	2	267	U
45	2	271	A
45	2	272	U
45	2	273	G
45	2	275	C
45	2	276	C
45	2	277	U
45	2	278	U
45	2	279	G
45	2	280	U
45	2	281	G
45	2	288	A
45	2	290	G
45	2	299	A
45	2	308	C
45	2	309	C
45	2	314	C
45	2	316	A

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Mol	Chain	Res	Type
45	2	320	U
45	2	321	C
45	2	322	G
45	2	333	A
45	2	337	G
45	2	338	C
45	2	341	A
45	2	352	A
45	2	359	A
45	2	360	A
45	2	361	C
45	2	370	A
45	2	380	U
45	2	390	G
45	2	393	C
45	2	399	A
45	2	400	A
45	2	401	A
45	2	402	C
45	2	404	G
45	2	409	C
45	2	412	A
45	2	416	A
45	2	418	G
45	2	424	C
45	2	425	A
45	2	426	G
45	2	428	A
45	2	434	G
45	2	435	C
45	2	437	A
45	2	438	A
45	2	439	U
45	2	444	C
45	2	448	C
45	2	452	A
45	2	459	G
45	2	468	A
45	2	469	C
45	2	475	A
45	2	477	A
45	2	484	C

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Mol	Chain	Res	Type
45	2	485	A
45	2	487	G
45	2	500	C
45	2	502	U
45	2	504	U
45	2	505	A
45	2	506	A
45	2	507	U
45	2	508	U
45	2	510	G
45	2	512	A
45	2	513	U
45	2	515	A
45	2	516	G
45	2	519	C
45	2	527	A
45	2	532	U
45	2	538	A
45	2	539	G
45	2	540	G
45	2	541	A
45	2	542	A
45	2	543	C
45	2	544	A
45	2	545	A
45	2	548	G
45	2	549	G
45	2	554	C
45	2	555	A
45	2	556	A
45	2	557	G
45	2	558	U
45	2	559	C
45	2	565	C
45	2	571	G
45	2	577	G
45	2	579	A
45	2	580	A
45	2	594	A
45	2	595	G
45	2	609	U
45	2	611	U

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Mol	Chain	Res	Type
45	2	619	A
45	2	620	A
45	2	621	A
45	2	622	A
45	2	623	A
45	2	635	A
45	2	639	U
45	2	640	U
45	2	650	U
45	2	652	G
45	2	653	C
45	2	655	G
45	2	656	G
45	2	657	U
45	2	658	C
45	2	677	G
45	2	680	U
45	2	684	A
45	2	685	A
45	2	686	C
45	2	687	G
45	2	688	G
45	2	690	G
45	2	692	C
45	2	693	U
45	2	694	U
45	2	696	C
45	2	697	C
45	2	698	U
45	2	700	C
45	2	701	U
45	2	702	G
45	2	703	G
45	2	704	C
45	2	705	U
45	2	735	C
45	2	736	C
45	2	737	A
45	2	738	G
45	2	741	C
45	2	742	U
45	2	743	U

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Mol	Chain	Res	Type
45	2	754	A
45	2	755	A
45	2	756	A
45	2	757	A
45	2	765	G
45	2	766	U
45	2	774	A
45	2	775	G
45	2	778	G
45	2	781	U
45	2	782	U
45	2	783	G
45	2	784	C
45	2	787	G
45	2	789	A
45	2	794	U
45	2	795	U
45	2	796	A
45	2	803	A
45	2	812	A
45	2	815	G
45	2	816	G
45	2	819	G
45	2	820	U
45	2	821	U
45	2	823	G
45	2	829	A
45	2	831	U
45	2	832	U
45	2	833	U
45	2	835	U
45	2	836	U
45	2	837	G
45	2	846	G
45	2	852	C
45	2	854	U
45	2	856	A
45	2	857	U
45	2	860	U
45	2	863	A
45	2	873	U
45	2	886	U

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Mol	Chain	Res	Type
45	2	898	A
45	2	906	A
45	2	912	U
45	2	914	G
45	2	915	A
45	2	921	U
45	2	926	A
45	2	933	A
45	2	935	U
45	2	942	G
45	2	944	A
45	2	951	A
45	2	960	U
45	2	992	A
45	2	993	A
45	2	996	U
45	2	997	G
45	2	1003	A
45	2	1004	U
45	2	1005	A
45	2	1010	C
45	2	1020	A
45	2	1021	C
45	2	1025	A
45	2	1026	A
45	2	1028	C
45	2	1029	U
45	2	1039	A
45	2	1040	G
45	2	1052	U
45	2	1053	G
45	2	1055	U
45	2	1056	U
45	2	1057	U
45	2	1058	U
45	2	1059	U
45	2	1060	U
45	2	1061	A
45	2	1064	G
45	2	1075	C
45	2	1076	A
45	2	1079	U

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Mol	Chain	Res	Type
45	2	1081	A
45	2	1082	C
45	2	1085	G
45	2	1092	A
45	2	1095	U
45	2	1096	C
45	2	1097	U
45	2	1100	G
45	2	1101	G
45	2	1109	G
45	2	1138	A
45	2	1146	G
45	2	1150	G
45	2	1151	A
45	2	1155	G
45	2	1157	A
45	2	1158	C
45	2	1160	A
45	2	1164	G
45	2	1167	G
45	2	1175	U
45	2	1185	U
45	2	1194	A
45	2	1196	A
45	2	1197	C
45	2	1198	G
45	2	1199	G
45	2	1200	G
45	2	1202	A
45	2	1207	C
45	2	1208	A
45	2	1209	C
45	2	1217	A
45	2	1218	G
45	2	1226	A
45	2	1227	A
45	2	1228	G
45	2	1229	G
45	2	1244	A
45	2	1245	G
45	2	1250	U
45	2	1251	U

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Mol	Chain	Res	Type
45	2	1259	U
45	2	1284	C
45	2	1287	A
45	2	1288	G
45	2	1301	U
45	2	1311	U
45	2	1312	A
45	2	1314	U
45	2	1315	U
45	2	1321	A
45	2	1337	A
45	2	1339	C
45	2	1340	U
45	2	1341	A
45	2	1344	A
45	2	1345	A
45	2	1349	G
45	2	1354	G
45	2	1360	A
45	2	1361	U
45	2	1363	U
45	2	1364	G
45	2	1369	U
45	2	1370	U
45	2	1371	A
45	2	1372	U
45	2	1378	U
45	2	1385	G
45	2	1388	A
45	2	1390	U
45	2	1398	U
45	2	1399	C
45	2	1413	U
45	2	1414	U
45	2	1415	U
45	2	1416	G
45	2	1422	A
45	2	1426	C
45	2	1427	A
45	2	1428	G
45	2	1439	C
45	2	1440	C

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Mol	Chain	Res	Type
45	2	1443	U
45	2	1444	A
45	2	1445	G
45	2	1446	A
45	2	1448	G
45	2	1456	C
45	2	1457	C
45	2	1458	G
45	2	1459	C
45	2	1461	C
45	2	1471	A
45	2	1473	U
45	2	1474	G
45	2	1482	C
45	2	1486	G
45	2	1489	U
45	2	1490	C
45	2	1491	U
45	2	1492	A
45	2	1493	A
45	2	1494	C
45	2	1496	U
45	2	1500	C
45	2	1506	G
45	2	1514	U
45	2	1516	A
45	2	1517	U
45	2	1521	G
45	2	1523	G
45	2	1524	A
45	2	1526	A
45	2	1529	C
45	2	1533	C
45	2	1535	U
45	2	1536	G
45	2	1537	C
45	2	1538	U
45	2	1540	G
45	2	1542	G
45	2	1546	G
45	2	1552	U
45	2	1557	U

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Mol	Chain	Res	Type
45	2	1559	A
45	2	1569	A
45	2	1573	A
45	2	1574	G
45	2	1577	A
45	2	1582	U
45	2	1584	G
45	2	1593	A
45	2	1601	G
45	2	1607	G
45	2	1614	A
45	2	1615	C
45	2	1616	G
45	2	1618	C
45	2	1623	C
45	2	1624	C
45	2	1625	C
45	2	1626	U
45	2	1631	A
45	2	1636	C
45	2	1656	U
45	2	1657	U
45	2	1658	G
45	2	1680	G
45	2	1681	A
45	2	1682	U
45	2	1683	C
45	2	1684	U
45	2	1712	A
45	2	1713	G
45	2	1715	G
45	2	1717	G
45	2	1731	A
45	2	1736	G
45	2	1755	A
45	2	1756	A
45	2	1757	G
45	2	1762	A
45	2	1766	A
45	2	1769	U
45	2	1780	G
45	2	1782	A

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Mol	Chain	Res	Type
45	2	1783	C
45	2	1790	A
45	2	1792	G
45	2	1793	G
45	2	1794	A
45	2	1795	U
45	2	1796	C
1	5	15	C
1	5	16	A
1	5	26	A
1	5	28	C
1	5	40	A
1	5	43	A
1	5	49	A
1	5	57	A
1	5	59	G
1	5	60	A
1	5	65	A
1	5	66	A
1	5	73	C
1	5	74	G
1	5	76	G
1	5	92	G
1	5	96	G
1	5	97	U
1	5	99	A
1	5	109	A
1	5	110	G
1	5	111	C
1	5	113	C
1	5	116	A
1	5	121	A
1	5	122	A
1	5	132	C
1	5	133	U
1	5	134	U
1	5	136	G
1	5	146	U
1	5	152	U
1	5	156	G
1	5	157	A
1	5	161	G

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Mol	Chain	Res	Type
1	5	170	G
1	5	171	G
1	5	172	G
1	5	174	C
1	5	175	C
1	5	180	C
1	5	181	U
1	5	182	U
1	5	187	A
1	5	188	U
1	5	190	U
1	5	191	U
1	5	200	C
1	5	210	U
1	5	213	A
1	5	218	G
1	5	219	A
1	5	220	G
1	5	221	A
1	5	231	G
1	5	239	G
1	5	240	U
1	5	241	G
1	5	243	G
1	5	247	C
1	5	248	U
1	5	249	U
1	5	250	U
1	5	251	G
1	5	252	U
1	5	253	A
1	5	254	A
1	5	269	G
1	5	282	G
1	5	283	G
1	5	284	A
1	5	285	A
1	5	286	U
1	5	287	G
1	5	295	A
1	5	299	G
1	5	310	U

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Mol	Chain	Res	Type
1	5	323	A
1	5	329	U
1	5	334	A
1	5	339	C
1	5	349	A
1	5	350	C
1	5	370	U
1	5	376	G
1	5	378	A
1	5	398	A
1	5	399	A
1	5	401	U
1	5	402	A
1	5	403	C
1	5	419	G
1	5	421	G
1	5	422	A
1	5	436	A
1	5	437	G
1	5	439	C
1	5	440	A
1	5	442	G
1	5	443	G
1	5	492	U
1	5	494	G
1	5	495	G
1	5	503	C
1	5	514	G
1	5	515	C
1	5	521	A
1	5	530	G
1	5	535	G
1	5	542	G
1	5	544	C
1	5	545	U
1	5	546	C
1	5	547	G
1	5	548	G
1	5	549	U
1	5	555	U
1	5	557	A
1	5	558	U

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Mol	Chain	Res	Type
1	5	559	A
1	5	565	U
1	5	578	A
1	5	579	G
1	5	581	U
1	5	588	G
1	5	592	A
1	5	603	A
1	5	604	G
1	5	609	G
1	5	610	G
1	5	611	A
1	5	619	A
1	5	620	U
1	5	622	A
1	5	636	C
1	5	649	A
1	5	660	A
1	5	662	U
1	5	676	G
1	5	677	A
1	5	681	U
1	5	683	U
1	5	697	A
1	5	699	A
1	5	702	C
1	5	705	A
1	5	712	G
1	5	715	A
1	5	716	A
1	5	720	A
1	5	725	G
1	5	727	G
1	5	736	A
1	5	751	A
1	5	752	C
1	5	765	C
1	5	766	U
1	5	767	U
1	5	776	U
1	5	777	U
1	5	781	G

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Mol	Chain	Res	Type
1	5	785	G
1	5	786	A
1	5	801	A
1	5	806	A
1	5	816	A
1	5	817	A
1	5	818	C
1	5	820	A
1	5	830	A
1	5	851	C
1	5	860	G
1	5	861	C
1	5	874	U
1	5	879	U
1	5	895	A
1	5	896	A
1	5	907	G
1	5	908	G
1	5	914	A
1	5	916	G
1	5	917	A
1	5	921	A
1	5	924	G
1	5	925	A
1	5	937	G
1	5	944	C
1	5	953	G
1	5	959	C
1	5	960	U
1	5	979	U
1	5	980	A
1	5	981	U
1	5	983	A
1	5	994	G
1	5	1001	G
1	5	1002	A
1	5	1006	A
1	5	1010	G
1	5	1014	U
1	5	1015	U
1	5	1016	C
1	5	1017	C

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Mol	Chain	Res	Type
1	5	1018	G
1	5	1019	G
1	5	1021	G
1	5	1022	U
1	5	1023	C
1	5	1024	G
1	5	1033	U
1	5	1035	G
1	5	1041	U
1	5	1047	A
1	5	1049	C
1	5	1051	U
1	5	1064	A
1	5	1065	A
1	5	1071	U
1	5	1072	G
1	5	1081	U
1	5	1082	U
1	5	1083	G
1	5	1084	A
1	5	1085	A
1	5	1092	C
1	5	1093	A
1	5	1094	U
1	5	1095	U
1	5	1096	U
1	5	1097	G
1	5	1098	A
1	5	1103	A
1	5	1104	G
1	5	1117	G
1	5	1131	G
1	5	1140	G
1	5	1141	C
1	5	1143	A
1	5	1152	G
1	5	1153	A
1	5	1159	A
1	5	1160	C
1	5	1161	G
1	5	1177	G
1	5	1179	A

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Mol	Chain	Res	Type
1	5	1180	A
1	5	1181	U
1	5	1182	A
1	5	1191	U
1	5	1201	C
1	5	1202	A
1	5	1209	G
1	5	1210	U
1	5	1211	U
1	5	1221	A
1	5	1222	G
1	5	1225	A
1	5	1232	C
1	5	1235	U
1	5	1236	G
1	5	1237	G
1	5	1239	C
1	5	1241	U
1	5	1242	G
1	5	1243	G
1	5	1244	A
1	5	1245	A
1	5	1246	G
1	5	1252	A
1	5	1258	U
1	5	1259	A
1	5	1261	G
1	5	1262	G
1	5	1263	A
1	5	1264	G
1	5	1285	G
1	5	1295	G
1	5	1299	U
1	5	1307	G
1	5	1308	A
1	5	1309	U
1	5	1311	G
1	5	1313	G
1	5	1324	U
1	5	1330	A
1	5	1331	U
1	5	1332	A

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Mol	Chain	Res	Type
1	5	1337	A
1	5	1345	G
1	5	1348	U
1	5	1349	G
1	5	1355	A
1	5	1356	U
1	5	1357	G
1	5	1359	C
1	5	1360	C
1	5	1386	A
1	5	1390	A
1	5	1399	A
1	5	1400	G
1	5	1417	G
1	5	1418	A
1	5	1419	A
1	5	1421	G
1	5	1428	A
1	5	1431	G
1	5	1434	G
1	5	1435	A
1	5	1437	C
1	5	1446	A
1	5	1450	G
1	5	1451	C
1	5	1452	A
1	5	1472	U
1	5	1475	A
1	5	1481	A
1	5	1482	A
1	5	1483	G
1	5	1485	G
1	5	1495	U
1	5	1502	C
1	5	1503	A
1	5	1505	C
1	5	1508	C
1	5	1511	U
1	5	1514	G
1	5	1515	A
1	5	1528	G
1	5	1533	U

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Mol	Chain	Res	Type
1	5	1536	G
1	5	1541	G
1	5	1548	C
1	5	1554	U
1	5	1555	U
1	5	1556	C
1	5	1557	A
1	5	1560	G
1	5	1561	G
1	5	1562	C
1	5	1563	C
1	5	1575	A
1	5	1576	G
1	5	1577	G
1	5	1578	C
1	5	1579	C
1	5	1580	A
1	5	1581	C
1	5	1582	C
1	5	1583	A
1	5	1587	A
1	5	1589	A
1	5	1605	A
1	5	1607	U
1	5	1619	A
1	5	1622	U
1	5	1629	U
1	5	1630	U
1	5	1632	A
1	5	1639	C
1	5	1641	U
1	5	1643	A
1	5	1644	C
1	5	1645	U
1	5	1651	U
1	5	1656	A
1	5	1658	G
1	5	1677	G
1	5	1683	A
1	5	1688	U
1	5	1716	U
1	5	1717	U

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Mol	Chain	Res	Type
1	5	1724	U
1	5	1750	A
1	5	1751	G
1	5	1752	A
1	5	1754	G
1	5	1756	C
1	5	1760	A
1	5	1761	C
1	5	1762	C
1	5	1763	U
1	5	1764	U
1	5	1765	U
1	5	1766	G
1	5	1767	C
1	5	1768	U
1	5	1770	G
1	5	1772	U
1	5	1776	G
1	5	1777	U
1	5	1778	G
1	5	1779	C
1	5	1780	G
1	5	1797	A
1	5	1808	G
1	5	1810	A
1	5	1814	A
1	5	1815	U
1	5	1816	A
1	5	1818	U
1	5	1821	U
1	5	1834	U
1	5	1839	A
1	5	1841	A
1	5	1842	A
1	5	1846	C
1	5	1849	C
1	5	1859	A
1	5	1866	C
1	5	1868	G
1	5	1878	G
1	5	1879	A
1	5	1880	U

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Mol	Chain	Res	Type
1	5	1881	A
1	5	1886	A
1	5	1890	U
1	5	1891	A
1	5	1892	G
1	5	1906	G
1	5	1931	U
1	5	1935	G
1	5	1949	G
1	5	1950	U
1	5	1951	C
1	5	1952	G
1	5	1953	G
1	5	2094	C
1	5	2095	G
1	5	2096	A
1	5	2097	U
1	5	2098	C
1	5	2099	A
1	5	2100	A
1	5	2102	U
1	5	2103	U
1	5	2113	A
1	5	2121	G
1	5	2122	G
1	5	2131	A
1	5	2140	U
1	5	2144	A
1	5	2158	A
1	5	2168	A
1	5	2169	G
1	5	2170	U
1	5	2175	U
1	5	2177	G
1	5	2188	A
1	5	2193	U
1	5	2198	A
1	5	2205	U
1	5	2206	G
1	5	2207	A
1	5	2208	A
1	5	2210	G

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Mol	Chain	Res	Type
1	5	2218	G
1	5	2222	A
1	5	2223	A
1	5	2225	U
1	5	2244	A
1	5	2245	C
1	5	2246	G
1	5	2249	G
1	5	2250	G
1	5	2251	G
1	5	2253	G
1	5	2255	A
1	5	2256	A
1	5	2257	C
1	5	2258	U
1	5	2268	U
1	5	2269	U
1	5	2270	A
1	5	2273	G
1	5	2279	A
1	5	2281	A
1	5	2288	G
1	5	2303	A
1	5	2307	G
1	5	2310	U
1	5	2313	A
1	5	2315	G
1	5	2327	U
1	5	2334	U
1	5	2336	U
1	5	2372	A
1	5	2373	A
1	5	2374	C
1	5	2375	G
1	5	2382	G
1	5	2385	G
1	5	2388	U
1	5	2393	G
1	5	2394	G
1	5	2397	A
1	5	2400	G
1	5	2401	A

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Mol	Chain	Res	Type
1	5	2402	A
1	5	2403	G
1	5	2404	A
1	5	2411	U
1	5	2412	G
1	5	2413	A
1	5	2418	G
1	5	2419	A
1	5	2434	U
1	5	2435	G
1	5	2437	G
1	5	2439	A
1	5	2440	G
1	5	2441	A
1	5	2442	G
1	5	2443	A
1	5	2444	C
1	5	2504	U
1	5	2505	U
1	5	2506	U
1	5	2507	C
1	5	2508	U
1	5	2510	U
1	5	2511	A
1	5	2514	U
1	5	2515	A
1	5	2523	A
1	5	2526	C
1	5	2530	G
1	5	2531	C
1	5	2532	U
1	5	2534	G
1	5	2535	A
1	5	2536	A
1	5	2537	U
1	5	2538	U
1	5	2539	C
1	5	2540	A
1	5	2541	U
1	5	2542	U
1	5	2543	U
1	5	2549	G

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Mol	Chain	Res	Type
1	5	2550	U
1	5	2552	C
1	5	2553	U
1	5	2555	G
1	5	2566	C
1	5	2567	C
1	5	2569	A
1	5	2570	U
1	5	2571	U
1	5	2572	C
1	5	2573	G
1	5	2574	G
1	5	2583	C
1	5	2584	G
1	5	2585	G
1	5	2593	A
1	5	2594	C
1	5	2600	C
1	5	2606	G
1	5	2614	G
1	5	2619	G
1	5	2637	A
1	5	2638	C
1	5	2647	A
1	5	2652	U
1	5	2656	A
1	5	2657	A
1	5	2658	G
1	5	2663	G
1	5	2674	A
1	5	2677	G
1	5	2681	U
1	5	2683	U
1	5	2689	A
1	5	2691	A
1	5	2694	A
1	5	2695	A
1	5	2696	A
1	5	2704	A
1	5	2714	G
1	5	2717	U
1	5	2719	U

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Mol	Chain	Res	Type
1	5	2720	G
1	5	2728	G
1	5	2729	U
1	5	2737	C
1	5	2748	A
1	5	2749	G
1	5	2752	U
1	5	2753	G
1	5	2755	C
1	5	2772	C
1	5	2773	C
1	5	2777	G
1	5	2778	G
1	5	2783	U
1	5	2796	G
1	5	2797	C
1	5	2799	A
1	5	2800	G
1	5	2801	A
1	5	2802	A
1	5	2805	G
1	5	2810	C
1	5	2814	G
1	5	2816	G
1	5	2817	A
1	5	2818	U
1	5	2819	A
1	5	2821	C
1	5	2838	A
1	5	2842	U
1	5	2843	U
1	5	2845	A
1	5	2847	A
1	5	2849	C
1	5	2853	A
1	5	2863	G
1	5	2865	U
1	5	2871	G
1	5	2872	A
1	5	2873	U
1	5	2875	U
1	5	2876	C

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Mol	Chain	Res	Type
1	5	2887	A
1	5	2899	C
1	5	2913	C
1	5	2914	G
1	5	2923	U
1	5	2935	U
1	5	2936	A
1	5	2941	A
1	5	2942	C
1	5	2947	G
1	5	2954	U
1	5	2957	G
1	5	2970	C
1	5	2971	A
1	5	2972	G
1	5	2982	A
1	5	2983	C
1	5	2986	U
1	5	2990	G
1	5	2992	U
1	5	2993	G
1	5	2995	A
1	5	2996	U
1	5	2997	G
1	5	3003	G
1	5	3012	A
1	5	3028	G
1	5	3056	U
1	5	3057	U
1	5	3059	G
1	5	3062	G
1	5	3065	G
1	5	3078	U
1	5	3079	U
1	5	3080	G
1	5	3086	A
1	5	3087	A
1	5	3092	C
1	5	3104	U
1	5	3122	A
1	5	3123	A
1	5	3126	C

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Mol	Chain	Res	Type
1	5	3129	A
1	5	3131	U
1	5	3142	A
1	5	3143	C
1	5	3145	C
1	5	3153	U
1	5	3154	C
1	5	3155	U
1	5	3156	U
1	5	3157	U
1	5	3158	G
1	5	3159	C
1	5	3164	C
1	5	3165	A
1	5	3166	C
1	5	3168	A
1	5	3172	A
1	5	3173	G
1	5	3174	A
1	5	3176	G
1	5	3181	C
1	5	3187	A
1	5	3188	G
1	5	3195	U
1	5	3196	U
1	5	3197	G
1	5	3207	U
1	5	3210	A
1	5	3217	C
1	5	3218	A
1	5	3219	G
1	5	3223	A
1	5	3224	G
1	5	3227	A
1	5	3229	G
1	5	3233	C
1	5	3234	A
1	5	3238	G
1	5	3245	A
1	5	3246	G
1	5	3247	G
1	5	3253	G

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Mol	Chain	Res	Type
1	5	3258	U
1	5	3259	U
1	5	3260	G
1	5	3265	C
1	5	3266	G
1	5	3268	A
1	5	3269	U
1	5	3270	U
1	5	3273	A
1	5	3275	U
1	5	3276	G
1	5	3277	U
1	5	3278	C
1	5	3281	U
1	5	3282	U
1	5	3285	C
1	5	3286	G
1	5	3287	U
1	5	3288	G
1	5	3294	A
1	5	3295	A
1	5	3304	U
1	5	3318	G
1	5	3319	U
1	5	3320	A
1	5	3322	A
1	5	3335	A
1	5	3341	U
1	5	3342	A
1	5	3345	G
1	5	3350	C
1	5	3351	U
1	5	3352	U
1	5	3354	U
1	5	3355	U
1	5	3356	G
1	5	3358	U
1	5	3368	U
1	5	3369	G
1	5	3378	C
1	5	3382	U
1	5	3383	G

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Mol	Chain	Res	Type
1	5	3389	U
1	5	3390	G
1	5	3396	U
2	7	7	G
2	7	13	A
2	7	22	A
2	7	33	U
2	7	41	G
2	7	53	U
2	7	54	U
2	7	55	A
2	7	59	U
2	7	65	G
2	7	73	C
2	7	74	C
2	7	75	G
2	7	76	A
2	7	89	G
2	7	93	C
2	7	94	C
2	7	99	G
2	7	102	A
2	7	108	A
2	7	110	G
2	7	112	G
2	7	114	U
2	7	121	U
3	8	11	C
3	8	21	C
3	8	34	U
3	8	35	C
3	8	48	A
3	8	53	A
3	8	59	A
3	8	62	C
3	8	63	G
3	8	70	G
3	8	78	G
3	8	79	A
3	8	80	A
3	8	81	U
3	8	83	C

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Mol	Chain	Res	Type
3	8	84	C
3	8	86	U
3	8	87	G
3	8	91	C
3	8	92	A
3	8	95	G
3	8	97	A
3	8	100	U
3	8	104	A
3	8	105	A
3	8	106	C
3	8	107	G
3	8	109	A
3	8	111	A
3	8	113	U
3	8	114	G
3	8	116	G
3	8	117	C
3	8	123	G
3	8	125	U
3	8	126	A
3	8	127	U
3	8	138	A
3	8	152	G
3	8	155	A
3	8	156	U
3	8	157	U
3	8	158	U
45	6	2	A
45	6	4	C
45	6	13	C
45	6	17	C
45	6	23	G
45	6	25	C
45	6	26	A
45	6	27	U
45	6	34	G
45	6	40	A
45	6	42	G
45	6	47	A
45	6	57	G
45	6	61	A

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Mol	Chain	Res	Type
45	6	63	G
45	6	66	U
45	6	67	A
45	6	68	A
45	6	69	G
45	6	70	C
45	6	71	A
45	6	72	A
45	6	73	U
45	6	74	U
45	6	75	U
45	6	76	A
45	6	77	U
45	6	78	A
45	6	84	A
45	6	94	U
45	6	103	A
45	6	104	A
45	6	114	C
45	6	115	G
45	6	128	U
45	6	130	C
45	6	137	U
45	6	138	A
45	6	140	A
45	6	141	U
45	6	142	G
45	6	143	G
45	6	144	U
45	6	145	A
45	6	146	U
45	6	153	G
45	6	158	U
45	6	159	U
45	6	166	C
45	6	174	U
45	6	178	U
45	6	179	A
45	6	182	A
45	6	185	U
45	6	186	C
45	6	187	G

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Mol	Chain	Res	Type
45	6	188	A
45	6	190	C
45	6	191	C
45	6	192	U
45	6	193	U
45	6	194	U
45	6	195	G
45	6	196	G
45	6	197	A
45	6	198	A
45	6	199	G
45	6	200	A
45	6	212	U
45	6	215	A
45	6	216	U
45	6	217	A
45	6	218	A
45	6	219	A
45	6	220	A
45	6	221	A
45	6	224	C
45	6	226	A
45	6	227	U
45	6	228	G
45	6	230	C
45	6	232	U
45	6	233	C
45	6	234	G
45	6	235	G
45	6	236	A
45	6	238	U
45	6	239	C
45	6	240	U
45	6	242	U
45	6	246	G
45	6	249	U
45	6	250	C
45	6	261	U
45	6	265	A
45	6	266	A
45	6	270	C
45	6	271	A

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Mol	Chain	Res	Type
45	6	272	U
45	6	273	G
45	6	275	C
45	6	277	U
45	6	278	U
45	6	280	U
45	6	281	G
45	6	287	G
45	6	295	A
45	6	299	A
45	6	302	U
45	6	308	C
45	6	314	C
45	6	316	A
45	6	319	U
45	6	320	U
45	6	321	C
45	6	322	G
45	6	333	A
45	6	337	G
45	6	338	C
45	6	343	C
45	6	345	U
45	6	352	A
45	6	359	A
45	6	360	A
45	6	361	C
45	6	364	G
45	6	369	A
45	6	380	U
45	6	390	G
45	6	400	A
45	6	401	A
45	6	402	C
45	6	404	G
45	6	416	A
45	6	418	G
45	6	419	G
45	6	424	C
45	6	425	A
45	6	426	G
45	6	428	A

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Mol	Chain	Res	Type
45	6	434	G
45	6	437	A
45	6	439	U
45	6	443	C
45	6	444	C
45	6	448	C
45	6	452	A
45	6	454	U
45	6	455	C
45	6	464	A
45	6	468	A
45	6	475	A
45	6	477	A
45	6	480	G
45	6	484	C
45	6	486	G
45	6	504	U
45	6	505	A
45	6	506	A
45	6	507	U
45	6	508	U
45	6	510	G
45	6	511	A
45	6	512	A
45	6	513	U
45	6	515	A
45	6	516	G
45	6	518	A
45	6	519	C
45	6	520	A
45	6	521	A
45	6	526	A
45	6	527	A
45	6	532	U
45	6	533	U
45	6	538	A
45	6	539	G
45	6	542	A
45	6	543	C
45	6	548	G
45	6	549	G
45	6	555	A

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Mol	Chain	Res	Type
45	6	556	A
45	6	557	G
45	6	558	U
45	6	559	C
45	6	565	C
45	6	568	G
45	6	571	G
45	6	574	G
45	6	578	U
45	6	579	A
45	6	580	A
45	6	583	C
45	6	593	U
45	6	594	A
45	6	595	G
45	6	606	A
45	6	609	U
45	6	610	G
45	6	611	U
45	6	617	U
45	6	619	A
45	6	620	A
45	6	622	A
45	6	623	A
45	6	624	G
45	6	630	A
45	6	639	U
45	6	645	C
45	6	650	U
45	6	651	G
45	6	652	G
45	6	653	C
45	6	677	G
45	6	678	A
45	6	679	U
45	6	680	U
45	6	681	U
45	6	682	C
45	6	683	C
45	6	684	A
45	6	685	A
45	6	687	G

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Mol	Chain	Res	Type
45	6	691	C
45	6	696	C
45	6	701	U
45	6	702	G
45	6	704	C
45	6	708	C
45	6	730	G
45	6	731	C
45	6	740	A
45	6	742	U
45	6	751	G
45	6	754	A
45	6	755	A
45	6	756	A
45	6	765	G
45	6	767	U
45	6	771	A
45	6	774	A
45	6	775	G
45	6	779	U
45	6	780	A
45	6	782	U
45	6	783	G
45	6	787	G
45	6	789	A
45	6	793	A
45	6	794	U
45	6	795	U
45	6	803	A
45	6	810	G
45	6	811	A
45	6	812	A
45	6	814	A
45	6	815	G
45	6	816	G
45	6	821	U
45	6	822	U
45	6	823	G
45	6	825	U
45	6	826	U
45	6	828	U
45	6	829	A

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Mol	Chain	Res	Type
45	6	830	U
45	6	831	U
45	6	832	U
45	6	833	U
45	6	834	G
45	6	835	U
45	6	855	A
45	6	856	A
45	6	861	U
45	6	862	A
45	6	863	A
45	6	864	U
45	6	865	A
45	6	886	U
45	6	892	A
45	6	893	U
45	6	906	A
45	6	913	G
45	6	914	G
45	6	933	A
45	6	935	U
45	6	942	G
45	6	943	C
45	6	944	A
45	6	945	U
45	6	959	U
45	6	960	U
45	6	966	A
45	6	969	C
45	6	970	A
45	6	971	A
45	6	983	A
45	6	988	A
45	6	992	A
45	6	993	A
45	6	1003	A
45	6	1004	U
45	6	1005	A
45	6	1021	C
45	6	1026	A
45	6	1028	C
45	6	1029	U

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Mol	Chain	Res	Type
45	6	1039	A
45	6	1040	G
45	6	1042	G
45	6	1051	G
45	6	1052	U
45	6	1053	G
45	6	1057	U
45	6	1058	U
45	6	1059	U
45	6	1060	U
45	6	1061	A
45	6	1062	A
45	6	1072	C
45	6	1074	G
45	6	1076	A
45	6	1081	A
45	6	1082	C
45	6	1083	G
45	6	1091	A
45	6	1092	A
45	6	1095	U
45	6	1096	C
45	6	1097	U
45	6	1098	U
45	6	1100	G
45	6	1138	A
45	6	1150	G
45	6	1151	A
45	6	1155	G
45	6	1158	C
45	6	1159	C
45	6	1160	A
45	6	1164	G
45	6	1167	G
45	6	1185	U
45	6	1194	A
45	6	1196	A
45	6	1199	G
45	6	1200	G
45	6	1202	A
45	6	1208	A
45	6	1217	A

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Mol	Chain	Res	Type
45	6	1218	G
45	6	1223	A
45	6	1226	A
45	6	1227	A
45	6	1229	G
45	6	1232	U
45	6	1236	A
45	6	1239	U
45	6	1240	U
45	6	1241	G
45	6	1243	G
45	6	1244	A
45	6	1245	G
45	6	1246	C
45	6	1256	A
45	6	1257	U
45	6	1258	U
45	6	1275	A
45	6	1285	U
45	6	1286	U
45	6	1289	U
45	6	1291	G
45	6	1307	U
45	6	1314	U
45	6	1315	U
45	6	1316	G
45	6	1321	A
45	6	1337	A
45	6	1338	C
45	6	1341	A
45	6	1344	A
45	6	1345	A
45	6	1354	G
45	6	1361	U
45	6	1362	U
45	6	1363	U
45	6	1364	G
45	6	1370	U
45	6	1371	A
45	6	1372	U
45	6	1373	C
45	6	1382	A

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Mol	Chain	Res	Type
45	6	1390	U
45	6	1393	C
45	6	1396	U
45	6	1398	U
45	6	1399	C
45	6	1400	A
45	6	1402	G
45	6	1413	U
45	6	1414	U
45	6	1415	U
45	6	1424	A
45	6	1427	A
45	6	1428	G
45	6	1440	C
45	6	1445	G
45	6	1446	A
45	6	1459	C
45	6	1461	C
45	6	1465	C
45	6	1466	G
45	6	1469	A
45	6	1471	A
45	6	1481	C
45	6	1482	C
45	6	1486	G
45	6	1490	C
45	6	1491	U
45	6	1492	A
45	6	1493	A
45	6	1506	G
45	6	1514	U
45	6	1516	A
45	6	1517	U
45	6	1521	G
45	6	1523	G
45	6	1524	A
45	6	1535	U
45	6	1536	G
45	6	1537	C
45	6	1538	U
45	6	1539	G
45	6	1540	G

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Mol	Chain	Res	Type
45	6	1554	U
45	6	1557	U
45	6	1559	A
45	6	1569	A
45	6	1572	G
45	6	1573	A
45	6	1574	G
45	6	1575	G
45	6	1582	U
45	6	1584	G
45	6	1590	G
45	6	1596	C
45	6	1601	G
45	6	1607	G
45	6	1616	G
45	6	1629	G
45	6	1631	A
45	6	1637	C
45	6	1638	G
45	6	1657	U
45	6	1658	G
45	6	1666	U
45	6	1680	G
45	6	1681	A
45	6	1684	U
45	6	1688	U
45	6	1689	A
45	6	1707	A
45	6	1708	U
45	6	1712	A
45	6	1715	G
45	6	1717	G
45	6	1732	A
45	6	1736	G
45	6	1755	A
45	6	1756	A
45	6	1760	G
45	6	1762	A
45	6	1766	A
45	6	1767	G
45	6	1769	U
45	6	1780	G

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Mol	Chain	Res	Type
45	6	1782	A
45	6	1783	C
45	6	1790	A
45	6	1792	G
45	6	1793	G
45	6	1794	A
45	6	1796	C
45	6	1799	U
45	6	1800	A

All (295) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	169	U
1	1	210	U
1	1	239	G
1	1	240	U
1	1	518	G
1	1	594	U
1	1	603	A
1	1	621	A
1	1	637	C
1	1	715	A
1	1	763	G
1	1	896	A
1	1	916	G
1	1	961	C
1	1	979	U
1	1	980	A
1	1	981	U
1	1	993	G
1	1	1015	U
1	1	1017	C
1	1	1064	A
1	1	1097	G
1	1	1103	A
1	1	1220	U
1	1	1285	G
1	1	1307	G
1	1	1317	A
1	1	1329	U

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Mol	Chain	Res	Type
1	1	1331	U
1	1	1348	U
1	1	1349	G
1	1	1352	A
1	1	1355	A
1	1	1484	U
1	1	1554	U
1	1	1562	C
1	1	1568	U
1	1	1580	A
1	1	1607	U
1	1	1716	U
1	1	1724	U
1	1	1815	U
1	1	1816	A
1	1	1820	U
1	1	1845	G
1	1	1846	C
1	1	2101	C
1	1	2112	U
1	1	2205	U
1	1	2208	A
1	1	2227	C
1	1	2249	G
1	1	2256	A
1	1	2281	A
1	1	2372	A
1	1	2400	G
1	1	2418	G
1	1	2513	U
1	1	2522	G
1	1	2537	U
1	1	2538	U
1	1	2541	U
1	1	2554	A
1	1	2570	U
1	1	2585	G
1	1	2593	A
1	1	2677	G
1	1	2772	C
1	1	2801	A
1	1	2817	A

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Mol	Chain	Res	Type
1	1	2818	U
1	1	2875	U
1	1	3056	U
1	1	3078	U
1	1	3121	U
1	1	3195	U
1	1	3218	A
1	1	3245	A
1	1	3269	U
1	1	3280	U
1	1	3317	U
1	1	3344	A
1	1	3350	C
1	1	3353	G
1	1	3375	A
2	3	52	G
3	4	71	A
3	4	85	G
45	2	25	C
45	2	45	U
45	2	68	A
45	2	73	U
45	2	75	U
45	2	76	A
45	2	103	A
45	2	114	C
45	2	139	C
45	2	140	A
45	2	144	U
45	2	158	U
45	2	218	A
45	2	233	C
45	2	278	U
45	2	280	U
45	2	321	C
45	2	417	A
45	2	484	C
45	2	499	U
45	2	501	U
45	2	503	G
45	2	512	A
45	2	539	G

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Mol	Chain	Res	Type
45	2	540	G
45	2	555	A
45	2	558	U
45	2	685	A
45	2	696	C
45	2	697	C
45	2	704	C
45	2	781	U
45	2	782	U
45	2	794	U
45	2	795	U
45	2	831	U
45	2	913	G
45	2	1059	U
45	2	1081	A
45	2	1095	U
45	2	1150	G
45	2	1157	A
45	2	1196	A
45	2	1207	C
45	2	1226	A
45	2	1244	A
45	2	1250	U
45	2	1339	C
45	2	1344	A
45	2	1481	C
45	2	1491	U
45	2	1568	C
45	2	1573	A
45	2	1600	A
45	2	1615	C
45	2	1711	C
45	2	1755	A
45	2	1756	A
45	2	1761	U
1	5	151	A
1	5	242	C
1	5	282	G
1	5	438	A
1	5	545	U
1	5	588	G
1	5	594	U

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Mol	Chain	Res	Type
1	5	602	A
1	5	765	C
1	5	873	C
1	5	916	G
1	5	978	G
1	5	980	A
1	5	993	G
1	5	1064	A
1	5	1103	A
1	5	1152	G
1	5	1160	C
1	5	1192	C
1	5	1200	A
1	5	1238	C
1	5	1241	U
1	5	1307	G
1	5	1329	U
1	5	1354	G
1	5	1355	A
1	5	1356	U
1	5	1451	C
1	5	1481	A
1	5	1554	U
1	5	1560	G
1	5	1576	G
1	5	1589	A
1	5	1716	U
1	5	1776	G
1	5	1815	U
1	5	1878	G
1	5	1879	A
1	5	1950	U
1	5	1951	C
1	5	2095	G
1	5	2096	A
1	5	2098	C
1	5	2099	A
1	5	2112	U
1	5	2204	C
1	5	2207	A
1	5	2209	U
1	5	2249	G

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Mol	Chain	Res	Type
1	5	2255	A
1	5	2372	A
1	5	2400	G
1	5	2404	A
1	5	2418	G
1	5	2442	G
1	5	2503	G
1	5	2505	U
1	5	2513	U
1	5	2531	C
1	5	2583	C
1	5	2662	G
1	5	2682	C
1	5	2772	C
1	5	2801	A
1	5	2818	U
1	5	2842	U
1	5	2970	C
1	5	2971	A
1	5	3056	U
1	5	3078	U
1	5	3121	U
1	5	3154	C
1	5	3157	U
1	5	3167	A
1	5	3195	U
1	5	3218	A
1	5	3269	U
1	5	3276	G
1	5	3303	G
1	5	3317	U
1	5	3340	G
1	5	3341	U
1	5	3357	U
2	7	76	A
3	8	82	U
45	6	25	C
45	6	66	U
45	6	73	U
45	6	75	U
45	6	76	A
45	6	103	A

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Mol	Chain	Res	Type
45	6	114	C
45	6	139	C
45	6	144	U
45	6	145	A
45	6	158	U
45	6	187	G
45	6	217	A
45	6	218	A
45	6	237	C
45	6	238	U
45	6	239	C
45	6	272	U
45	6	277	U
45	6	280	U
45	6	319	U
45	6	320	U
45	6	321	C
45	6	322	G
45	6	417	A
45	6	512	A
45	6	525	A
45	6	542	A
45	6	555	A
45	6	557	G
45	6	558	U
45	6	681	U
45	6	682	C
45	6	695	U
45	6	755	A
45	6	794	U
45	6	815	G
45	6	829	A
45	6	831	U
45	6	832	U
45	6	834	G
45	6	914	G
45	6	1051	G
45	6	1058	U
45	6	1081	A
45	6	1097	U
45	6	1185	U
45	6	1238	A

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Mol	Chain	Res	Type
45	6	1244	A
45	6	1255	G
45	6	1344	A
45	6	1481	C
45	6	1490	C
45	6	1491	U
45	6	1535	U
45	6	1537	C
45	6	1568	C
45	6	1573	A
45	6	1600	A
45	6	1615	C
45	6	1637	C
45	6	1657	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 2153 ligands modelled in this entry, 2084 are monoatomic - leaving 69 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	$\# Z > 2$
85	LLL	7	233	-	29,33,33	0.22	0	34,49,49	0.93	2 (5%)
85	LLL	5	4165	-	29,33,33	0.16	0	34,49,49	1.04	2 (5%)
85	LLL	1	3994	-	29,33,33	0.20	0	34,49,49	1.14	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	LLL	1	3990	-	29,33,33	0.25	0	34,49,49	1.82	1 (2%)
85	LLL	2	2043	-	29,33,33	0.17	0	34,49,49	0.79	3 (8%)
85	LLL	5	4166	-	29,33,33	0.15	0	34,49,49	1.16	2 (5%)
85	LLL	5	4164	-	29,33,33	0.21	0	34,49,49	1.93	3 (8%)
85	LLL	7	232	-	29,33,33	0.17	0	34,49,49	0.90	2 (5%)
85	LLL	8	222	-	29,33,33	0.16	0	34,49,49	0.79	1 (2%)
85	LLL	5	4174	-	29,33,33	0.24	0	34,49,49	1.58	4 (11%)
85	LLL	5	4170	-	29,33,33	0.24	0	34,49,49	1.52	2 (5%)
85	LLL	1	3996	-	29,33,33	0.21	0	34,49,49	0.89	2 (5%)
85	LLL	1	3995	-	29,33,33	0.16	0	34,49,49	2.08	2 (5%)
85	LLL	5	4153	-	29,33,33	0.25	0	34,49,49	1.79	2 (5%)
85	LLL	6	2175	-	29,33,33	0.19	0	34,49,49	1.37	2 (5%)
85	LLL	5	4175	-	29,33,33	0.23	0	34,49,49	1.44	3 (8%)
85	LLL	2	2045	-	29,33,33	0.19	0	34,49,49	1.53	4 (11%)
85	LLL	1	4004	-	29,33,33	0.19	0	34,49,49	1.08	1 (2%)
85	LLL	1	3989	-	29,33,33	0.21	0	34,49,49	1.43	3 (8%)
85	LLL	5	4152	-	29,33,33	0.18	0	34,49,49	1.48	2 (5%)
85	LLL	5	4157	-	29,33,33	0.25	0	34,49,49	1.13	2 (5%)
85	LLL	2	2044	-	29,33,33	0.20	0	34,49,49	1.50	4 (11%)
85	LLL	5	4159	-	29,33,33	0.21	0	34,49,49	1.06	3 (8%)
85	LLL	5	4171	-	29,33,33	0.19	0	34,49,49	0.97	1 (2%)
85	LLL	5	4173	-	29,33,33	0.17	0	34,49,49	1.12	3 (8%)
85	LLL	6	2167	-	29,33,33	0.21	0	34,49,49	1.96	5 (14%)
85	LLL	L3	404	-	29,33,33	0.22	0	34,49,49	1.33	3 (8%)
85	LLL	6	2169	-	29,33,33	0.14	0	34,49,49	0.89	2 (5%)
85	LLL	6	2174	-	29,33,33	0.27	0	34,49,49	1.27	3 (8%)
85	LLL	1	3991	-	29,33,33	0.20	0	34,49,49	0.82	3 (8%)
85	LLL	5	4161	-	29,33,33	0.19	0	34,49,49	1.25	3 (8%)
85	LLL	1	3992	-	29,33,33	0.21	0	34,49,49	1.23	2 (5%)
85	LLL	5	4156	-	29,33,33	0.22	0	34,49,49	1.29	3 (8%)
85	LLL	1	3993	-	29,33,33	0.24	0	34,49,49	1.47	5 (14%)
85	LLL	13	412	-	29,33,33	0.25	0	34,49,49	1.88	3 (8%)
85	LLL	6	2173	-	29,33,33	0.19	0	34,49,49	1.11	3 (8%)
85	LLL	5	4169	-	29,33,33	0.20	0	34,49,49	1.46	4 (11%)
85	LLL	5	4168	-	29,33,33	0.20	0	34,49,49	1.67	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	LLL	1	4000	-	29,33,33	0.18	0	34,49,49	2.11	5 (14%)
85	LLL	5	4163	-	29,33,33	0.15	0	34,49,49	1.06	3 (8%)
85	LLL	6	2168	-	29,33,33	0.21	0	34,49,49	1.28	3 (8%)
85	LLL	6	2176	-	29,33,33	0.22	0	34,49,49	1.29	3 (8%)
85	LLL	1	3997	-	29,33,33	0.19	0	34,49,49	1.22	3 (8%)
85	LLL	1	3999	-	29,33,33	0.17	0	34,49,49	0.97	2 (5%)
85	LLL	5	4151	-	29,33,33	0.32	0	34,49,49	1.46	2 (5%)
85	LLL	5	4154	-	29,33,33	0.25	0	34,49,49	0.68	0
85	LLL	1	4001	-	29,33,33	0.17	0	34,49,49	1.08	2 (5%)
85	LLL	6	2171	-	29,33,33	0.14	0	34,49,49	1.14	1 (2%)
85	LLL	6	2170	-	29,33,33	0.23	0	34,49,49	1.25	2 (5%)
85	LLL	5	4167	-	29,33,33	0.15	0	34,49,49	1.00	2 (5%)
85	LLL	7	231	-	29,33,33	0.17	0	34,49,49	2.01	7 (20%)
85	LLL	1	4003	-	29,33,33	0.18	0	34,49,49	1.37	3 (8%)
85	LLL	5	4160	-	29,33,33	0.24	0	34,49,49	1.86	3 (8%)
85	LLL	6	2166	-	29,33,33	0.20	0	34,49,49	1.11	3 (8%)
85	LLL	6	2165	-	29,33,33	0.21	0	34,49,49	1.14	2 (5%)
85	LLL	4	224	-	29,33,33	0.20	0	34,49,49	1.46	2 (5%)
85	LLL	5	4176	-	29,33,33	0.22	0	34,49,49	1.26	3 (8%)
85	LLL	5	4178	-	29,33,33	0.20	0	34,49,49	0.86	1 (2%)
85	LLL	3	220	-	29,33,33	0.21	0	34,49,49	1.50	3 (8%)
85	LLL	5	4158	-	29,33,33	0.21	0	34,49,49	1.99	5 (14%)
85	LLL	5	4162	-	29,33,33	0.18	0	34,49,49	0.86	1 (2%)
85	LLL	6	2164	-	29,33,33	0.18	0	34,49,49	1.82	2 (5%)
85	LLL	1	3998	-	29,33,33	0.15	0	34,49,49	0.76	1 (2%)
85	LLL	1	4002	-	29,33,33	0.20	0	34,49,49	2.11	3 (8%)
85	LLL	5	4172	-	29,33,33	0.22	0	34,49,49	1.36	3 (8%)
85	LLL	6	2172	-	29,33,33	0.19	0	34,49,49	1.12	2 (5%)
85	LLL	5	4177	-	29,33,33	0.26	0	34,49,49	1.79	6 (17%)
85	LLL	8	221	-	29,33,33	0.21	0	34,49,49	1.73	2 (5%)
85	LLL	5	4155	-	29,33,33	0.24	0	34,49,49	1.00	1 (2%)

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
85	LLL	7	233	-	-	3/11/65/65	2/3/3/3
85	LLL	5	4165	-	-	1/11/65/65	0/3/3/3
85	LLL	1	3994	-	-	1/11/65/65	0/3/3/3
85	LLL	1	3990	-	-	2/11/65/65	0/3/3/3
85	LLL	2	2043	-	-	3/11/65/65	1/3/3/3
85	LLL	5	4166	-	-	3/11/65/65	0/3/3/3
85	LLL	5	4164	-	-	4/11/65/65	0/3/3/3
85	LLL	7	232	-	-	2/11/65/65	0/3/3/3
85	LLL	8	222	-	-	3/11/65/65	2/3/3/3
85	LLL	5	4174	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4170	-	-	1/11/65/65	1/3/3/3
85	LLL	1	3996	-	-	3/11/65/65	0/3/3/3
85	LLL	1	3995	-	-	3/11/65/65	0/3/3/3
85	LLL	5	4153	-	-	4/11/65/65	0/3/3/3
85	LLL	6	2175	-	-	4/11/65/65	1/3/3/3
85	LLL	5	4175	-	-	1/11/65/65	0/3/3/3
85	LLL	2	2045	-	-	7/11/65/65	0/3/3/3
85	LLL	1	4004	-	-	3/11/65/65	1/3/3/3
85	LLL	1	3989	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4152	-	-	5/11/65/65	0/3/3/3
85	LLL	5	4157	-	-	1/11/65/65	0/3/3/3
85	LLL	2	2044	-	-	3/11/65/65	1/3/3/3
85	LLL	5	4159	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4171	-	-	4/11/65/65	0/3/3/3
85	LLL	5	4173	-	-	2/11/65/65	1/3/3/3
85	LLL	6	2167	-	-	4/11/65/65	0/3/3/3
85	LLL	L3	404	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2169	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2174	-	-	1/11/65/65	0/3/3/3
85	LLL	1	3991	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4161	-	-	2/11/65/65	1/3/3/3
85	LLL	1	3992	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4156	-	-	4/11/65/65	0/3/3/3
85	LLL	1	3993	-	-	1/11/65/65	0/3/3/3
85	LLL	13	412	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2173	-	-	5/11/65/65	1/3/3/3
85	LLL	5	4169	-	-	1/11/65/65	0/3/3/3
85	LLL	5	4168	-	-	0/11/65/65	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	LLL	1	4000	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4163	-	-	6/11/65/65	2/3/3/3
85	LLL	6	2168	-	-	5/11/65/65	1/3/3/3
85	LLL	6	2176	-	-	3/11/65/65	0/3/3/3
85	LLL	1	3997	-	-	1/11/65/65	0/3/3/3
85	LLL	1	3999	-	-	4/11/65/65	0/3/3/3
85	LLL	5	4151	-	-	8/11/65/65	0/3/3/3
85	LLL	5	4154	-	-	2/11/65/65	0/3/3/3
85	LLL	1	4001	-	-	2/11/65/65	0/3/3/3
85	LLL	6	2171	-	-	1/11/65/65	0/3/3/3
85	LLL	6	2170	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4167	-	-	2/11/65/65	0/3/3/3
85	LLL	7	231	-	-	4/11/65/65	0/3/3/3
85	LLL	1	4003	-	-	4/11/65/65	2/3/3/3
85	LLL	5	4160	-	-	3/11/65/65	0/3/3/3
85	LLL	6	2166	-	-	3/11/65/65	0/3/3/3
85	LLL	6	2165	-	-	3/11/65/65	0/3/3/3
85	LLL	4	224	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4176	-	-	2/11/65/65	0/3/3/3
85	LLL	5	4178	-	-	1/11/65/65	0/3/3/3
85	LLL	3	220	-	-	3/11/65/65	0/3/3/3
85	LLL	5	4158	-	-	5/11/65/65	0/3/3/3
85	LLL	5	4162	-	-	3/11/65/65	1/3/3/3
85	LLL	6	2164	-	-	2/11/65/65	0/3/3/3
85	LLL	1	3998	-	-	2/11/65/65	0/3/3/3
85	LLL	1	4002	-	-	5/11/65/65	0/3/3/3
85	LLL	5	4172	-	-	5/11/65/65	0/3/3/3
85	LLL	6	2172	-	-	3/11/65/65	1/3/3/3
85	LLL	5	4177	-	-	4/11/65/65	0/3/3/3
85	LLL	8	221	-	-	6/11/65/65	0/3/3/3
85	LLL	5	4155	-	-	5/11/65/65	1/3/3/3

There are no bond length outliers.

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	1	4002	LLL	C11-O51-C51	11.16	125.50	113.13
85	1	3995	LLL	C11-O51-C51	11.05	125.37	113.13
85	1	4000	LLL	C11-O51-C51	10.82	125.12	113.13
85	1	3990	LLL	C11-O51-C51	9.69	123.86	113.13
85	6	2164	LLL	C11-O51-C51	9.60	123.77	113.13
85	13	412	LLL	C11-O51-C51	9.45	123.60	113.13
85	5	4160	LLL	C11-O51-C51	9.41	123.55	113.13
85	5	4153	LLL	C11-O51-C51	9.22	123.34	113.13
85	5	4164	LLL	C11-O51-C51	9.20	123.32	113.13
85	5	4158	LLL	C11-O51-C51	8.98	123.08	113.13
85	6	2167	LLL	C11-O51-C51	8.74	122.81	113.13
85	5	4168	LLL	C11-O51-C51	8.54	122.59	113.13
85	8	221	LLL	C11-O51-C51	7.94	121.92	113.13
85	5	4170	LLL	C11-O51-C51	7.70	121.66	113.13
85	7	231	LLL	C11-O51-C51	7.50	121.44	113.13
85	5	4152	LLL	C11-O51-C51	7.49	121.43	113.13
85	5	4177	LLL	C11-O51-C51	6.98	120.86	113.13
85	3	220	LLL	C11-O51-C51	6.66	120.51	113.13
85	2	2044	LLL	C11-O51-C51	6.58	120.42	113.13
85	L3	404	LLL	C11-O51-C51	6.14	119.94	113.13
85	5	4175	LLL	C11-O51-C51	5.96	119.73	113.13
85	6	2175	LLL	C53-O53-C13	5.93	121.08	111.53
85	4	224	LLL	C11-O51-C51	5.86	119.62	113.13
85	1	3992	LLL	C11-O51-C51	5.85	119.61	113.13
85	6	2171	LLL	C11-O51-C51	5.82	119.58	113.13
85	5	4151	LLL	C11-O51-C51	5.70	119.44	113.13
85	1	4003	LLL	C11-O51-C51	5.53	119.26	113.13
85	1	3989	LLL	C11-O51-C51	5.52	119.25	113.13
85	1	4004	LLL	C11-O51-C51	5.46	119.18	113.13
85	1	3993	LLL	O11-C11-C21	-5.30	99.36	108.23
85	2	2045	LLL	O11-C42-C32	-5.26	96.64	109.18
85	5	4174	LLL	C11-O51-C51	5.16	118.85	113.13
85	1	3997	LLL	C11-O51-C51	5.02	118.69	113.13
85	6	2168	LLL	C53-O53-C13	5.01	119.61	111.53
85	5	4169	LLL	C11-O51-C51	5.00	118.67	113.13
85	5	4157	LLL	O11-C11-C21	-4.86	100.10	108.23
85	6	2170	LLL	C53-O53-C13	4.86	119.36	111.53
85	6	2165	LLL	C11-O51-C51	4.79	118.43	113.13
85	5	4161	LLL	C11-O51-C51	4.78	118.42	113.13
85	5	4169	LLL	C53-O53-C13	4.73	119.15	111.53
85	5	4171	LLL	C53-O53-C13	4.72	119.14	111.53
85	5	4177	LLL	C53-O53-C13	4.71	119.12	111.53
85	5	4176	LLL	C11-O51-C51	4.61	118.24	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	5	4173	LLL	C11-O51-C51	4.56	118.18	113.13
85	1	4001	LLL	C11-O51-C51	4.51	118.12	113.13
85	5	4172	LLL	C11-O51-C51	4.49	118.11	113.13
85	8	221	LLL	C53-O53-C13	4.48	118.74	111.53
85	7	231	LLL	O11-C42-C32	-4.47	98.51	109.18
85	6	2176	LLL	C53-O53-C13	4.47	118.73	111.53
85	5	4164	LLL	O11-C42-C32	-4.40	98.67	109.18
85	4	224	LLL	C53-O53-C13	4.32	118.49	111.53
85	6	2174	LLL	C11-O51-C51	4.24	117.83	113.13
85	7	231	LLL	O11-C11-C21	-4.23	101.16	108.23
85	5	4151	LLL	O11-C42-C32	-4.19	99.18	109.18
85	5	4172	LLL	C53-O53-C13	4.15	118.22	111.53
85	5	4156	LLL	C53-O53-C13	4.14	118.21	111.53
85	6	2176	LLL	O11-C42-C32	-4.14	99.30	109.18
85	2	2045	LLL	C53-O53-C13	4.13	118.18	111.53
85	5	4166	LLL	C53-O53-C13	4.12	118.17	111.53
85	5	4166	LLL	C11-O51-C51	4.11	117.69	113.13
85	5	4155	LLL	C11-O51-C51	4.05	117.61	113.13
85	5	4165	LLL	C11-O51-C51	4.05	117.61	113.13
85	5	4174	LLL	C53-O53-C13	4.04	118.04	111.53
85	6	2167	LLL	C53-O53-C13	4.00	117.97	111.53
85	1	4003	LLL	C53-O53-C13	3.99	117.96	111.53
85	6	2172	LLL	C11-O51-C51	3.86	117.41	113.13
85	6	2169	LLL	C11-O51-C51	3.85	117.39	113.13
85	6	2172	LLL	C53-O53-C13	3.85	117.73	111.53
85	1	3995	LLL	C53-O53-C13	3.83	117.70	111.53
85	3	220	LLL	O11-C42-C32	-3.82	100.06	109.18
85	1	3989	LLL	O11-C42-C32	-3.79	100.13	109.18
85	6	2170	LLL	C11-O51-C51	3.78	117.32	113.13
85	5	4175	LLL	C53-O53-C13	3.77	117.61	111.53
85	2	2045	LLL	C11-O51-C51	3.77	117.31	113.13
85	5	4158	LLL	O11-C42-C32	-3.72	100.30	109.18
85	5	4162	LLL	C11-O51-C51	3.71	117.24	113.13
85	1	3994	LLL	C53-O53-C13	3.70	117.50	111.53
85	6	2166	LLL	O11-C42-C32	-3.69	100.39	109.18
85	6	2173	LLL	C11-O51-C51	3.68	117.21	113.13
85	6	2174	LLL	C53-O53-C13	3.67	117.44	111.53
85	7	231	LLL	C53-O53-C13	3.65	117.41	111.53
85	5	4176	LLL	O11-C42-C32	3.62	117.81	109.18
85	6	2167	LLL	O11-C11-C21	-3.60	102.21	108.23
85	5	4167	LLL	C11-O51-C51	3.59	117.11	113.13
85	5	4153	LLL	O11-C42-C32	-3.58	100.64	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	7	233	LLL	C11-O51-C51	3.57	117.08	113.13
85	5	4172	LLL	O11-C11-C21	3.52	114.13	108.23
85	6	2174	LLL	O11-C11-C21	3.51	114.11	108.23
85	5	4178	LLL	C11-O51-C51	3.47	116.97	113.13
85	1	3993	LLL	O11-C42-C32	-3.45	100.94	109.18
85	5	4174	LLL	O11-C11-C21	-3.43	102.50	108.23
85	5	4158	LLL	O62-C62-C12	-3.41	101.03	109.18
85	5	4156	LLL	O62-C62-C12	-3.39	101.10	109.18
85	13	412	LLL	O11-C11-C21	3.38	113.88	108.23
85	5	4156	LLL	O11-C42-C32	-3.35	101.18	109.18
85	5	4157	LLL	C11-O51-C51	3.33	116.82	113.13
85	1	3994	LLL	C11-O51-C51	3.29	116.78	113.13
85	6	2168	LLL	C11-O51-C51	3.28	116.77	113.13
85	6	2166	LLL	C11-O51-C51	3.27	116.75	113.13
85	5	4163	LLL	C11-O51-C51	3.24	116.72	113.13
85	6	2167	LLL	O11-C42-C32	-3.18	101.58	109.18
85	5	4177	LLL	O62-C62-C52	3.15	115.66	107.28
85	5	4163	LLL	O11-C42-C32	-3.13	101.72	109.18
85	5	4159	LLL	C11-O51-C51	3.08	116.55	113.13
85	6	2165	LLL	O62-C62-C12	-3.07	101.85	109.18
85	7	231	LLL	O62-C62-C12	3.07	116.50	109.18
85	1	3996	LLL	C11-O51-C51	3.07	116.53	113.13
85	1	3993	LLL	C11-O51-C51	3.04	116.50	113.13
85	6	2164	LLL	C53-O53-C13	2.99	116.36	111.53
85	1	3999	LLL	O11-C42-C32	-2.97	102.09	109.18
85	5	4160	LLL	O11-C42-C32	-2.94	102.16	109.18
85	1	4000	LLL	C53-O53-C13	2.93	116.26	111.53
85	6	2175	LLL	O62-C62-C12	-2.90	102.26	109.18
85	2	2045	LLL	O11-C11-C21	-2.89	103.40	108.23
85	2	2044	LLL	C53-O53-C13	2.88	116.17	111.53
85	1	4001	LLL	C53-O53-C13	2.87	116.16	111.53
85	5	4161	LLL	C53-O53-C13	2.86	116.14	111.53
85	1	4000	LLL	O62-C62-C12	-2.84	102.39	109.18
85	5	4167	LLL	C53-O53-C13	2.83	116.08	111.53
85	5	4176	LLL	C32-C22-C12	2.81	116.94	111.18
85	5	4161	LLL	O11-C42-C32	-2.80	102.49	109.18
85	6	2173	LLL	O62-C62-C12	-2.79	102.53	109.18
85	6	2176	LLL	C11-O51-C51	2.79	116.22	113.13
85	5	4159	LLL	C53-O53-C13	2.77	115.99	111.53
85	6	2173	LLL	O11-C42-C32	-2.76	102.60	109.18
85	7	232	LLL	O11-C42-C32	-2.70	102.72	109.18
85	1	3999	LLL	C11-O51-C51	2.68	116.10	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	6	2166	LLL	C32-C22-C12	-2.67	105.69	111.18
85	1	3998	LLL	O62-C62-C12	-2.65	102.85	109.18
85	1	4002	LLL	O11-C42-C32	-2.65	102.85	109.18
85	8	222	LLL	C53-O53-C13	2.65	115.80	111.53
85	1	3991	LLL	O11-C42-C32	-2.64	102.88	109.18
85	1	3996	LLL	O11-C11-C21	2.64	112.65	108.23
85	1	3997	LLL	O11-C11-C21	2.63	112.63	108.23
85	1	4000	LLL	O11-C11-C21	-2.61	103.86	108.23
85	5	4163	LLL	C53-O53-C13	2.61	115.74	111.53
85	1	4002	LLL	C53-O53-C13	2.61	115.73	111.53
85	5	4152	LLL	C53-O53-C13	2.58	115.69	111.53
85	5	4158	LLL	C62-C52-C42	2.56	114.27	108.96
85	2	2044	LLL	O11-C42-C32	-2.52	103.17	109.18
85	5	4169	LLL	C32-C22-C12	2.51	116.34	111.18
85	6	2169	LLL	C53-O53-C13	2.50	115.55	111.53
85	1	3992	LLL	C53-O53-C13	2.47	115.51	111.53
85	5	4173	LLL	C53-O53-C13	2.47	115.51	111.53
85	1	3997	LLL	C53-O53-C13	2.46	115.50	111.53
85	5	4173	LLL	O11-C42-C32	-2.46	103.30	109.18
85	5	4177	LLL	O11-C42-C52	2.45	113.81	107.28
85	1	3993	LLL	C32-C22-C12	2.44	116.20	111.18
85	1	3993	LLL	O62-C62-C12	-2.44	103.36	109.18
85	1	3991	LLL	C53-O53-C13	2.41	115.41	111.53
85	2	2043	LLL	C53-O53-C13	2.40	115.39	111.53
85	2	2044	LLL	O62-C62-C12	-2.39	103.47	109.18
85	L3	404	LLL	C13-C23-C33	2.39	113.30	109.34
85	7	233	LLL	C53-O53-C13	2.39	115.38	111.53
85	5	4158	LLL	C53-O53-C13	2.39	115.38	111.53
85	5	4170	LLL	C53-O53-C13	2.35	115.32	111.53
85	5	4165	LLL	C53-O53-C13	2.35	115.31	111.53
85	7	231	LLL	C41-C51-C61	-2.34	108.35	112.83
85	L3	404	LLL	O11-C42-C32	-2.34	103.61	109.18
85	1	4003	LLL	O62-C62-C12	-2.30	103.68	109.18
85	6	2167	LLL	O62-C62-C12	-2.30	103.69	109.18
85	3	220	LLL	O11-C42-C52	2.28	113.34	107.28
85	5	4164	LLL	C53-O53-C13	2.23	115.13	111.53
85	5	4168	LLL	C13-C23-C33	2.22	113.01	109.34
85	l3	412	LLL	O11-C42-C32	-2.19	103.94	109.18
85	1	3994	LLL	O62-C62-C12	-2.16	104.02	109.18
85	1	3989	LLL	C13-C23-C33	2.15	112.91	109.34
85	5	4159	LLL	O11-C42-C32	-2.13	104.09	109.18
85	2	2043	LLL	C11-O51-C51	2.12	115.48	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	6	2168	LLL	O11-C42-C52	2.12	112.91	107.28
85	5	4175	LLL	O11-C11-C21	2.11	111.76	108.23
85	5	4168	LLL	O11-C11-C21	2.10	111.75	108.23
85	5	4177	LLL	O11-C11-C21	-2.09	104.74	108.23
85	5	4160	LLL	C41-C51-C61	-2.08	108.86	112.83
85	5	4177	LLL	C32-C22-C12	-2.07	106.93	111.18
85	7	232	LLL	C53-O53-C13	2.07	114.87	111.53
85	7	231	LLL	C32-C22-C12	2.06	115.40	111.18
85	2	2043	LLL	O11-C42-C32	-2.05	104.28	109.18
85	5	4169	LLL	C62-C52-C42	-2.04	104.72	108.96
85	1	4000	LLL	O11-C42-C32	-2.03	104.34	109.18
85	5	4174	LLL	O62-C62-C52	2.01	112.62	107.28
85	1	3991	LLL	O62-C62-C12	-2.01	104.39	109.18

There are no chirality outliers.

All (195) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	1	3990	LLL	C23-C33-N33-C93
85	1	3991	LLL	O51-C51-C61-N61
85	1	3991	LLL	C23-C33-N33-C93
85	1	3992	LLL	C23-C33-N33-C93
85	1	3993	LLL	C23-C33-N33-C93
85	1	3994	LLL	C23-C33-N33-C93
85	1	3995	LLL	O51-C51-C61-N61
85	1	3995	LLL	C23-C33-N33-C93
85	1	3996	LLL	C41-C51-C61-N61
85	1	3996	LLL	O51-C51-C61-N61
85	1	3996	LLL	C23-C33-N33-C93
85	1	3997	LLL	C23-C33-N33-C93
85	1	3998	LLL	C23-C33-N33-C93
85	1	3999	LLL	O51-C51-C61-N61
85	1	3999	LLL	C23-C33-N33-C93
85	1	4000	LLL	O51-C51-C61-N61
85	1	4000	LLL	C23-C33-N33-C93
85	1	4001	LLL	C23-C33-N33-C93
85	1	4002	LLL	C21-C11-O11-C42
85	1	4002	LLL	O51-C51-C61-N61
85	1	4003	LLL	C21-C11-O11-C42
85	1	4003	LLL	C41-C51-C61-N61
85	1	4003	LLL	C23-C33-N33-C93
85	1	4004	LLL	C41-C51-C61-N61

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Mol	Chain	Res	Type	Atoms
85	1	4004	LLL	C23-C33-N33-C93
85	3	220	LLL	C23-C33-N33-C93
85	4	224	LLL	O51-C51-C61-N61
85	4	224	LLL	C23-C33-N33-C93
85	L3	404	LLL	C23-C33-N33-C93
85	2	2043	LLL	C41-C51-C61-N61
85	2	2043	LLL	O51-C51-C61-N61
85	2	2043	LLL	C23-C33-N33-C93
85	2	2044	LLL	C41-C51-C61-N61
85	2	2044	LLL	O51-C51-C61-N61
85	2	2044	LLL	C23-C33-N33-C93
85	2	2045	LLL	O51-C51-C61-N61
85	2	2045	LLL	C23-C33-N33-C93
85	5	4151	LLL	C41-C51-C61-N61
85	5	4151	LLL	O51-C51-C61-N61
85	5	4151	LLL	C23-C33-N33-C93
85	5	4152	LLL	C21-C11-O11-C42
85	5	4152	LLL	C41-C51-C61-N61
85	5	4152	LLL	O51-C51-C61-N61
85	5	4152	LLL	C23-C33-N33-C93
85	5	4153	LLL	C41-C51-C61-N61
85	5	4153	LLL	O51-C51-C61-N61
85	5	4153	LLL	C23-C33-N33-C93
85	5	4154	LLL	C23-C33-N33-C93
85	5	4155	LLL	C21-C11-O11-C42
85	5	4155	LLL	O51-C51-C61-N61
85	5	4155	LLL	C23-C33-N33-C93
85	5	4156	LLL	C23-C33-N33-C93
85	5	4157	LLL	C23-C33-N33-C93
85	5	4158	LLL	C41-C51-C61-N61
85	5	4158	LLL	O51-C51-C61-N61
85	5	4158	LLL	C23-C33-N33-C93
85	5	4159	LLL	C23-C33-N33-C93
85	5	4160	LLL	O51-C51-C61-N61
85	5	4160	LLL	C23-C33-N33-C93
85	5	4161	LLL	C23-C33-N33-C93
85	5	4162	LLL	C21-C11-O11-C42
85	5	4162	LLL	O51-C51-C61-N61
85	5	4163	LLL	C21-C11-O11-C42
85	5	4163	LLL	C41-C51-C61-N61
85	5	4163	LLL	O51-C51-C61-N61
85	5	4164	LLL	C23-C33-N33-C93

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Mol	Chain	Res	Type	Atoms
85	5	4166	LLL	C23-C33-N33-C93
85	5	4167	LLL	C23-C33-N33-C93
85	5	4169	LLL	C23-C33-N33-C93
85	5	4170	LLL	C23-C33-N33-C93
85	5	4171	LLL	C41-C51-C61-N61
85	5	4171	LLL	O51-C51-C61-N61
85	5	4171	LLL	C23-C33-N33-C93
85	5	4172	LLL	C21-C11-O11-C42
85	5	4172	LLL	O51-C51-C61-N61
85	5	4172	LLL	C23-C33-N33-C93
85	5	4173	LLL	C23-C33-N33-C93
85	5	4174	LLL	C23-C33-N33-C93
85	5	4176	LLL	C32-C42-O11-C11
85	5	4176	LLL	C23-C33-N33-C93
85	5	4177	LLL	O51-C51-C61-N61
85	5	4177	LLL	C23-C33-N33-C93
85	5	4178	LLL	C23-C33-N33-C93
85	7	231	LLL	C12-C62-O62-C13
85	7	231	LLL	C23-C33-N33-C93
85	7	232	LLL	C23-C33-N33-C93
85	7	233	LLL	C23-C33-N33-C93
85	8	221	LLL	C21-C11-O11-C42
85	8	221	LLL	C41-C51-C61-N61
85	8	221	LLL	C23-C33-N33-C93
85	8	222	LLL	C21-C11-O11-C42
85	8	222	LLL	C23-C33-N33-C93
85	6	2165	LLL	C23-C33-N33-C93
85	6	2166	LLL	O51-C51-C61-N61
85	6	2166	LLL	C23-C33-N33-C93
85	6	2167	LLL	C41-C51-C61-N61
85	6	2167	LLL	C23-C33-N33-C93
85	6	2168	LLL	C21-C11-O11-C42
85	6	2168	LLL	C41-C51-C61-N61
85	6	2168	LLL	O51-C51-C61-N61
85	6	2168	LLL	C23-C33-N33-C93
85	6	2169	LLL	C23-C33-N33-C93
85	6	2170	LLL	O51-C51-C61-N61
85	6	2170	LLL	C23-C33-N33-C93
85	6	2171	LLL	C23-C33-N33-C93
85	6	2172	LLL	O51-C51-C61-N61
85	6	2172	LLL	C23-C33-N33-C93
85	6	2173	LLL	C21-C11-O11-C42

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Mol	Chain	Res	Type	Atoms
85	6	2173	LLL	O51-C51-C61-N61
85	6	2173	LLL	C23-C33-N33-C93
85	6	2174	LLL	C23-C33-N33-C93
85	6	2175	LLL	C21-C11-O11-C42
85	6	2175	LLL	C23-C33-N33-C93
85	6	2176	LLL	C23-C33-N33-C93
85	1	3990	LLL	O51-C11-O11-C42
85	6	2175	LLL	O51-C11-O11-C42
85	5	4177	LLL	C52-C42-O11-C11
85	6	2173	LLL	C52-C62-O62-C13
85	1	4002	LLL	O51-C11-O11-C42
85	5	4155	LLL	O51-C11-O11-C42
85	1	3999	LLL	O51-C11-O11-C42
85	5	4164	LLL	O51-C11-O11-C42
85	1	3989	LLL	O51-C11-O11-C42
85	5	4153	LLL	O51-C11-O11-C42
85	5	4158	LLL	O53-C13-O62-C62
85	1	4004	LLL	O51-C11-O11-C42
85	5	4151	LLL	O51-C11-O11-C42
85	3	220	LLL	C52-C42-O11-C11
85	5	4177	LLL	O53-C13-O62-C62
85	8	221	LLL	O51-C11-O11-C42
85	5	4171	LLL	O53-C13-O62-C62
85	8	221	LLL	C52-C62-O62-C13
85	6	2168	LLL	O51-C11-O11-C42
85	5	4172	LLL	O51-C11-O11-C42
85	7	233	LLL	C52-C62-O62-C13
85	5	4172	LLL	C52-C42-O11-C11
85	2	2045	LLL	O53-C13-O62-C62
85	5	4164	LLL	C52-C42-O11-C11
85	5	4158	LLL	C52-C42-O11-C11
85	6	2176	LLL	C52-C42-O11-C11
85	2	2045	LLL	C52-C42-O11-C11
85	6	2173	LLL	C52-C42-O11-C11
85	5	4163	LLL	O51-C11-O11-C42
85	5	4173	LLL	O51-C11-O11-C42
85	5	4166	LLL	O53-C13-O62-C62
85	5	4151	LLL	O53-C13-O62-C62
85	3	220	LLL	C32-C42-O11-C11
85	6	2175	LLL	O51-C51-C61-N61
85	7	233	LLL	C52-C42-O11-C11
85	5	4155	LLL	C52-C62-O62-C13

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Mol	Chain	Res	Type	Atoms
85	2	2045	LLL	C23-C13-O62-C62
85	1	4003	LLL	C52-C62-O62-C13
85	5	4160	LLL	O51-C11-O11-C42
85	1	3999	LLL	C41-C51-C61-N61
85	1	4002	LLL	C41-C51-C61-N61
85	5	4154	LLL	C41-C51-C61-N61
85	5	4165	LLL	C41-C51-C61-N61
85	1	3989	LLL	C52-C42-O11-C11
85	5	4152	LLL	O51-C11-O11-C42
85	5	4161	LLL	O51-C11-O11-C42
85	6	2167	LLL	C52-C62-O62-C13
85	5	4156	LLL	C52-C42-O11-C11
85	6	2165	LLL	C52-C62-O62-C13
85	6	2164	LLL	O51-C11-O11-C42
85	1	3995	LLL	C21-C11-O11-C42
85	5	4174	LLL	C21-C11-O11-C42
85	5	4175	LLL	C21-C11-O11-C42
85	6	2167	LLL	O51-C11-O11-C42
85	5	4166	LLL	C23-C13-O62-C62
85	1	3998	LLL	C52-C62-O62-C13
85	6	2165	LLL	O51-C11-O11-C42
85	6	2172	LLL	O51-C11-O11-C42
85	5	4156	LLL	C52-C62-O62-C13
85	6	2176	LLL	O51-C11-O11-C42
85	6	2166	LLL	C52-C42-O11-C11
85	7	231	LLL	O51-C11-O11-C42
85	8	222	LLL	O51-C11-O11-C42
85	5	4163	LLL	O53-C13-O62-C62
85	5	4151	LLL	C52-C62-O62-C13
85	5	4151	LLL	C23-C13-O62-C62
85	5	4156	LLL	O51-C11-O11-C42
85	5	4163	LLL	C23-C13-O62-C62
85	1	4002	LLL	C23-C33-N33-C93
85	5	4162	LLL	C23-C33-N33-C93
85	13	412	LLL	C23-C33-N33-C93
85	6	2164	LLL	C23-C33-N33-C93
85	2	2045	LLL	C52-C62-O62-C13
85	7	232	LLL	C52-C62-O62-C13
85	2	2045	LLL	C32-C42-O11-C11
85	5	4164	LLL	C32-C42-O11-C11
85	8	221	LLL	C12-C62-O62-C13
85	5	4151	LLL	C52-C42-O11-C11

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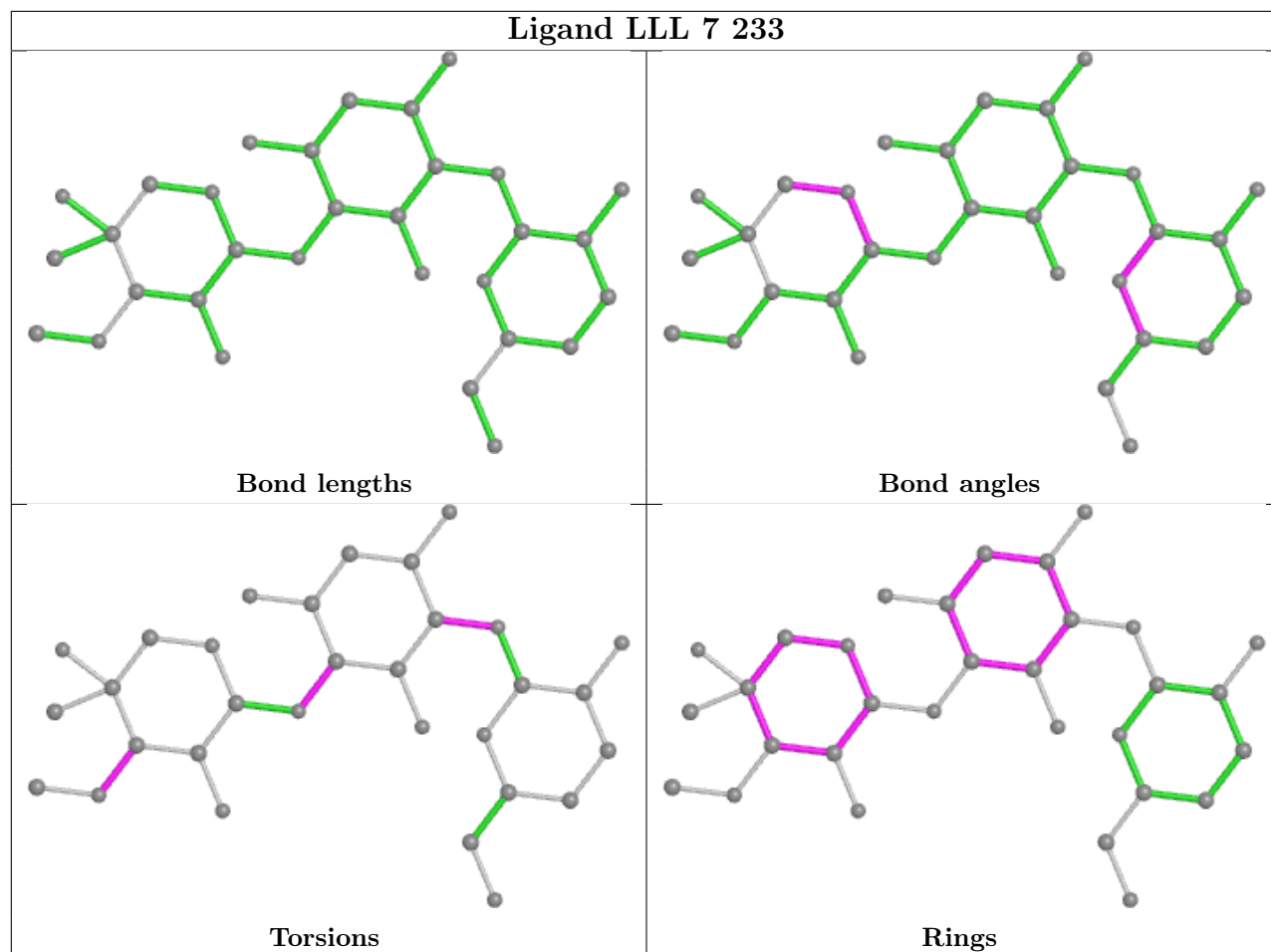
Mol	Chain	Res	Type	Atoms
85	1	4001	LLL	O53-C13-O62-C62
85	5	4167	LLL	C52-C62-O62-C13
85	7	231	LLL	C52-C62-O62-C13

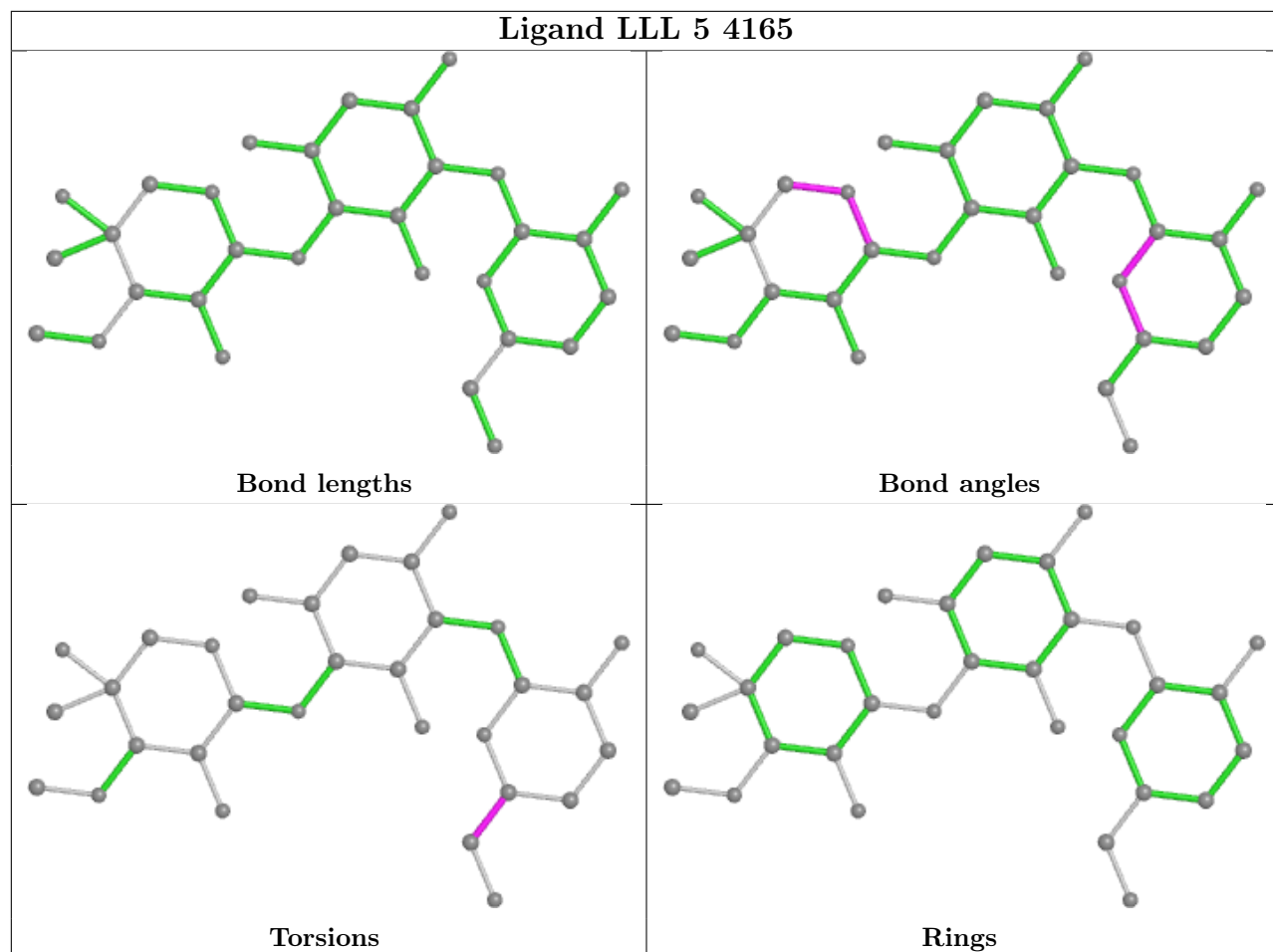
All (20) ring outliers are listed below:

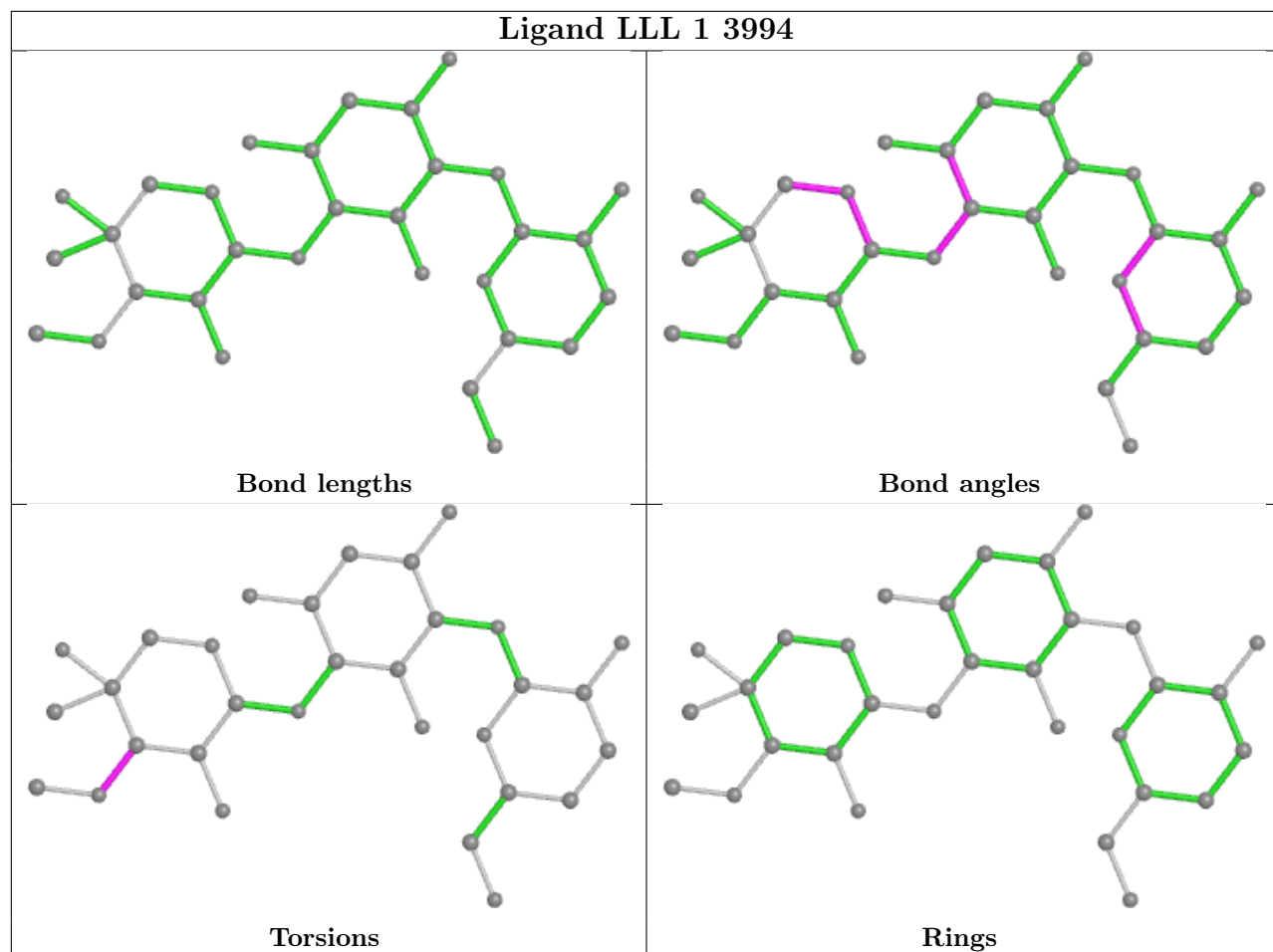
Mol	Chain	Res	Type	Atoms
85	6	2172	LLL	C12-C22-C32-C42-C52-C62
85	5	4155	LLL	C11-C21-C31-C41-C51-O51
85	1	4004	LLL	C11-C21-C31-C41-C51-O51
85	5	4170	LLL	C11-C21-C31-C41-C51-O51
85	6	2168	LLL	C11-C21-C31-C41-C51-O51
85	2	2043	LLL	C11-C21-C31-C41-C51-O51
85	2	2044	LLL	C11-C21-C31-C41-C51-O51
85	6	2175	LLL	C11-C21-C31-C41-C51-O51
85	1	4003	LLL	C13-C23-C33-C43-C53-O53
85	7	233	LLL	C12-C22-C32-C42-C52-C62
85	1	4003	LLL	C11-C21-C31-C41-C51-O51
85	6	2173	LLL	C11-C21-C31-C41-C51-O51
85	8	222	LLL	C12-C22-C32-C42-C52-C62
85	5	4163	LLL	C12-C22-C32-C42-C52-C62
85	7	233	LLL	C13-C23-C33-C43-C53-O53
85	5	4161	LLL	C11-C21-C31-C41-C51-O51
85	5	4162	LLL	C11-C21-C31-C41-C51-O51
85	5	4173	LLL	C12-C22-C32-C42-C52-C62
85	5	4163	LLL	C11-C21-C31-C41-C51-O51
85	8	222	LLL	C11-C21-C31-C41-C51-O51

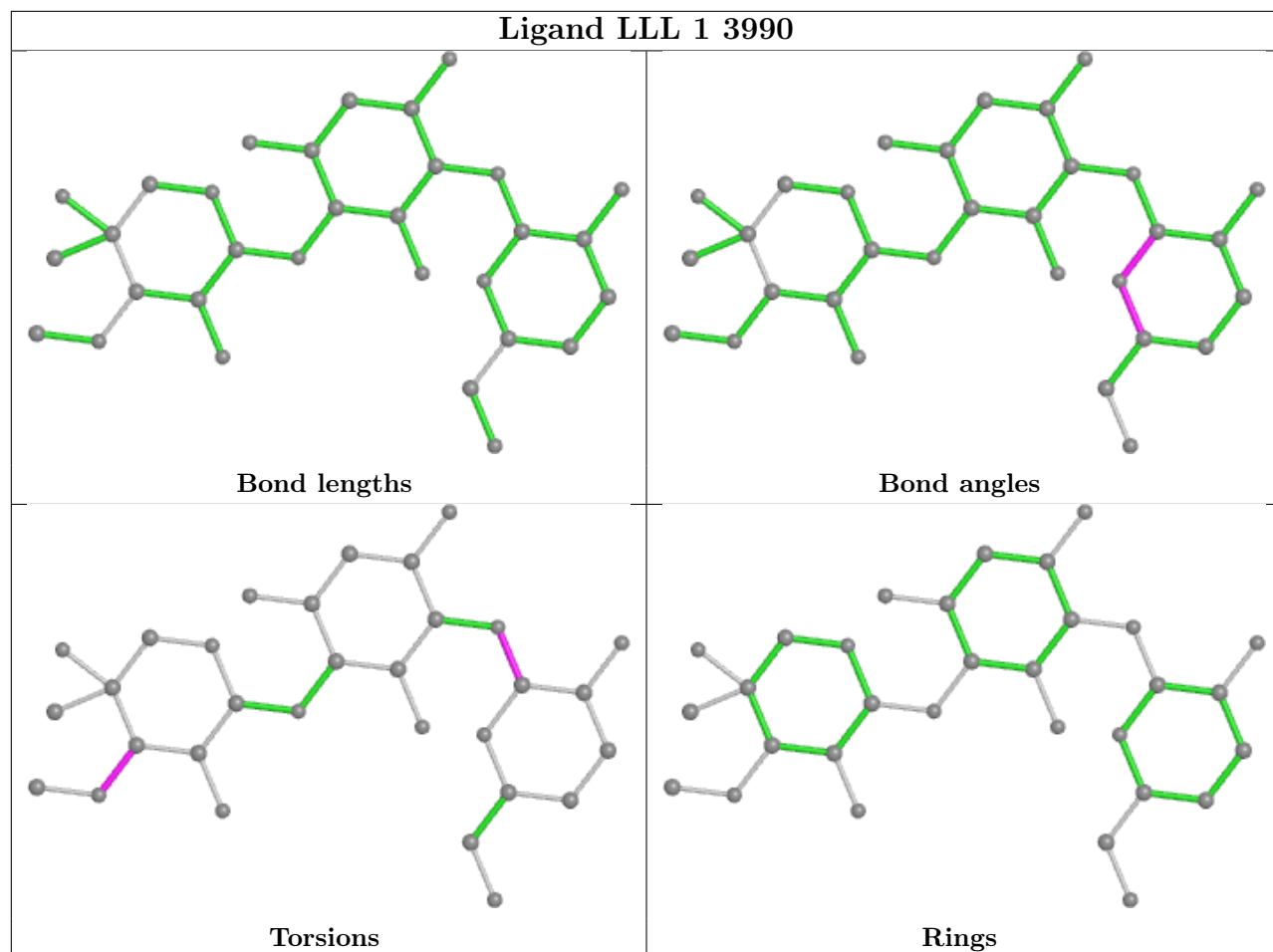
No monomer is involved in short contacts.

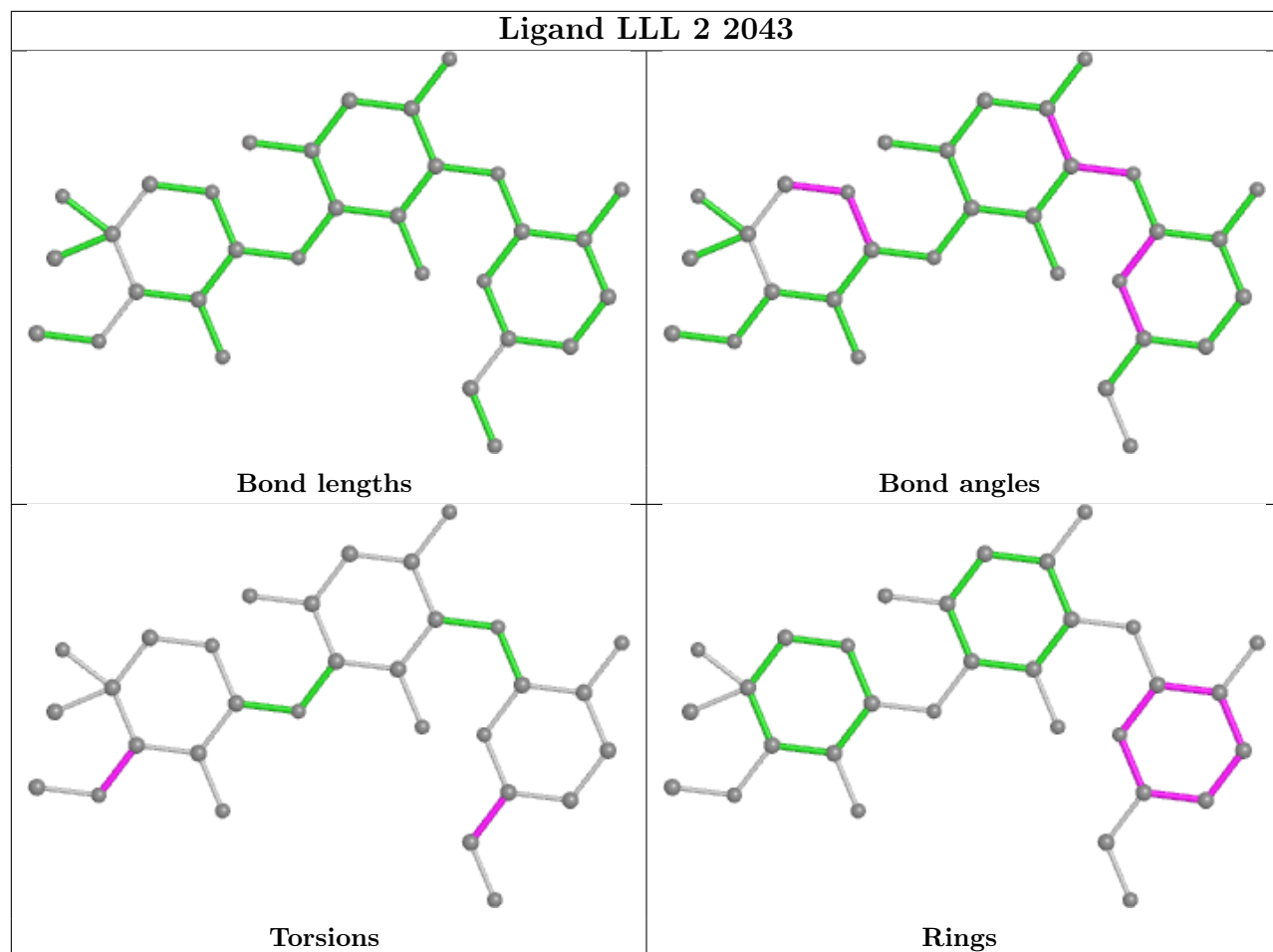
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

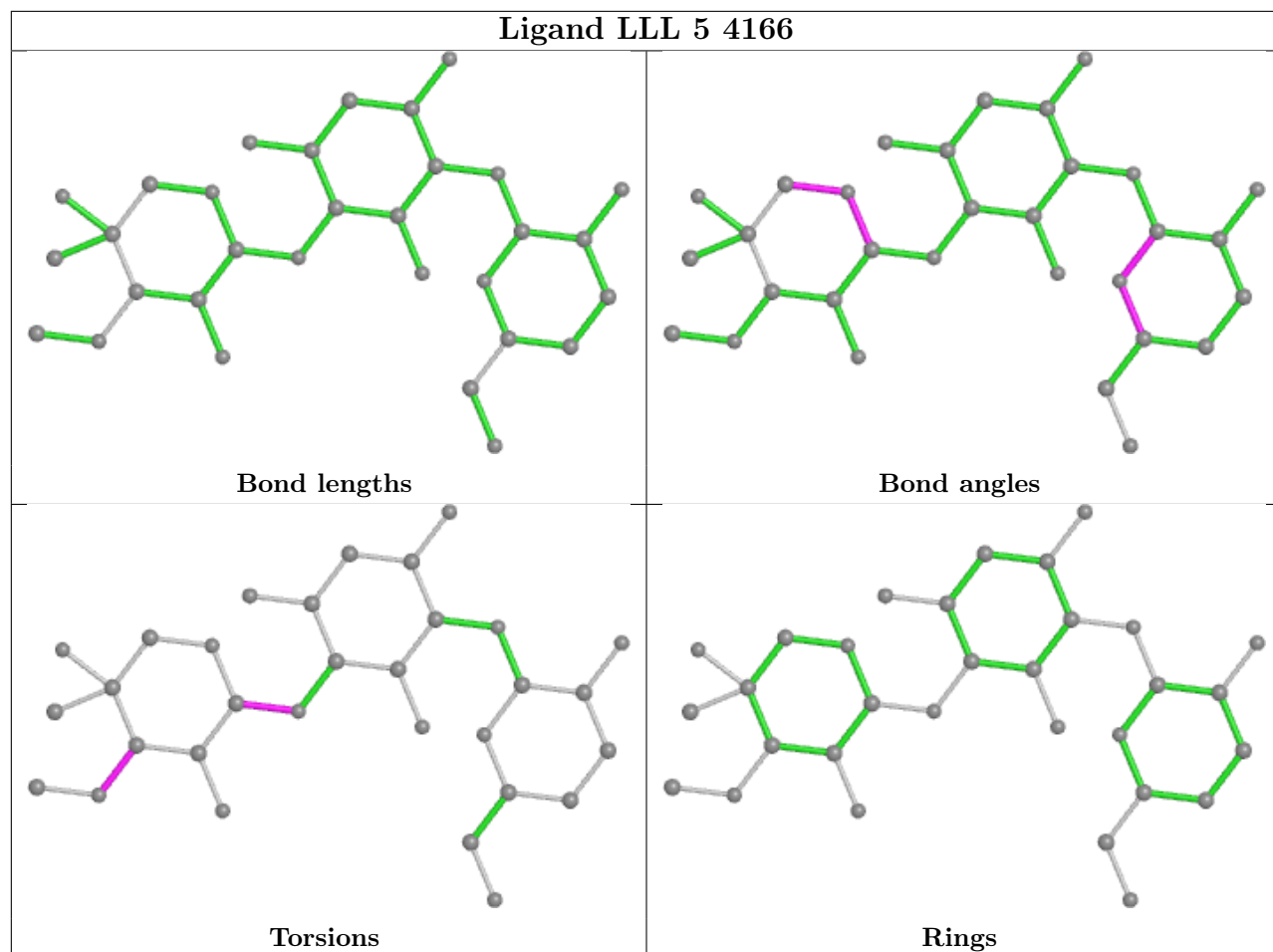


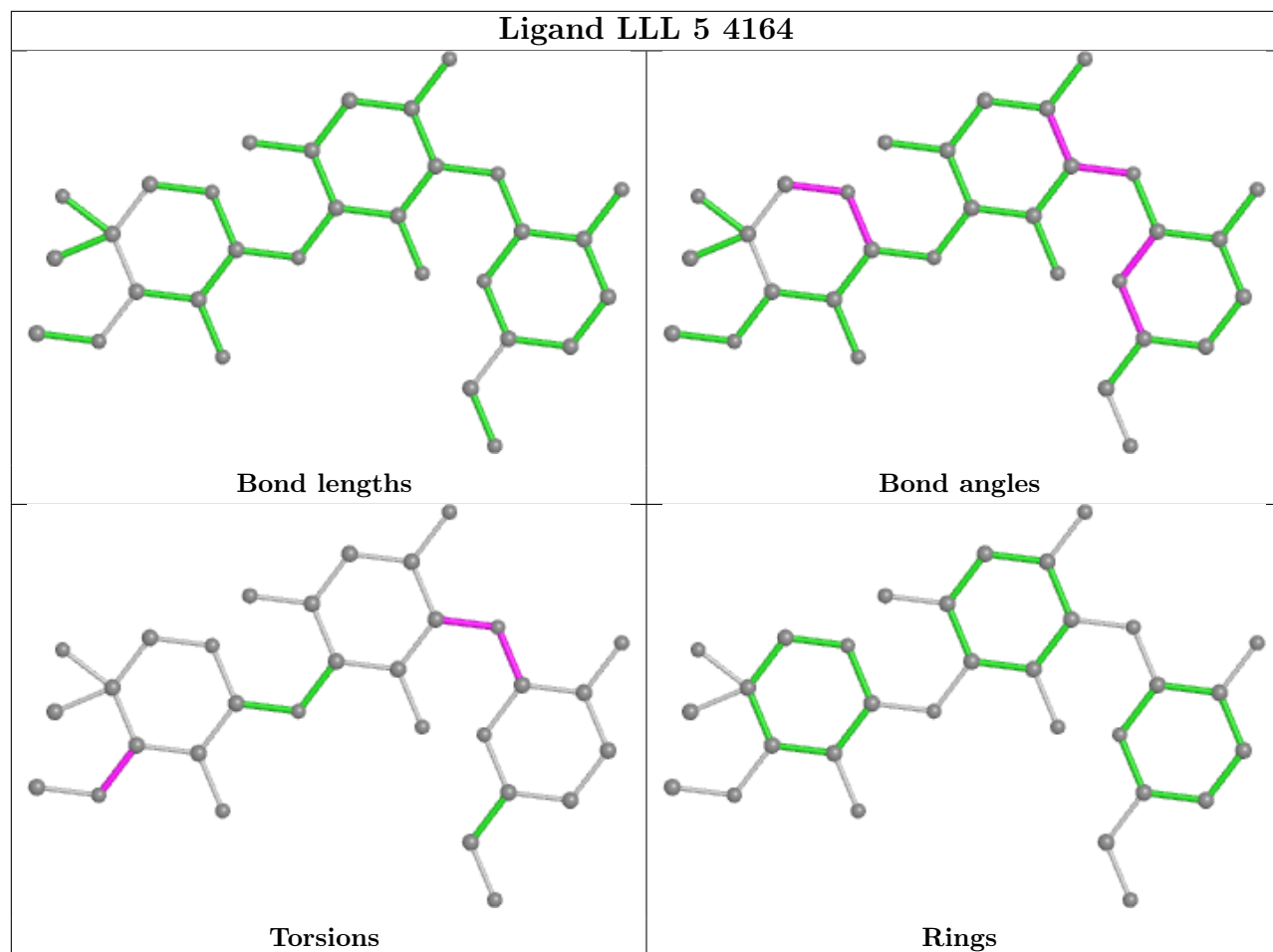


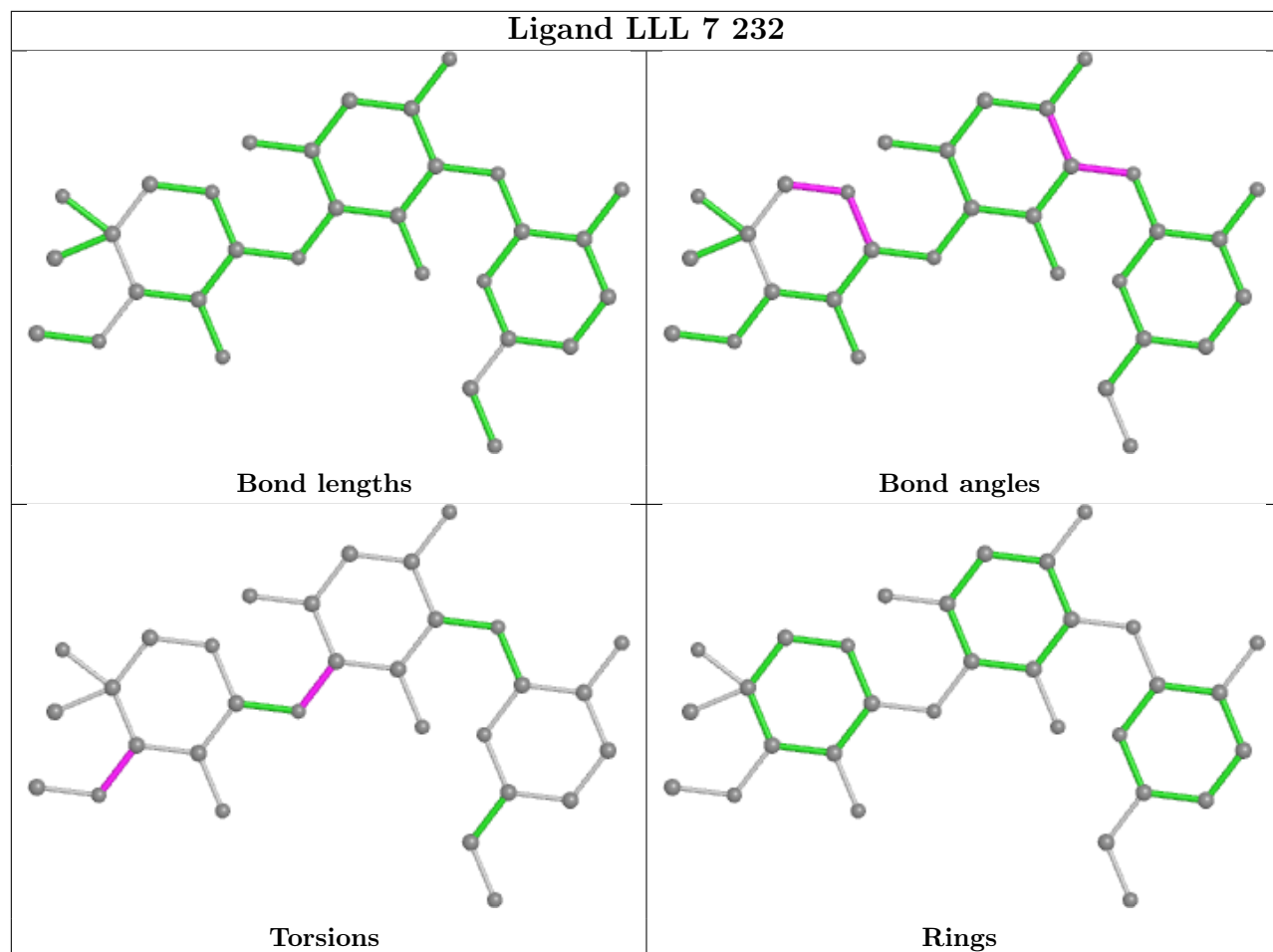


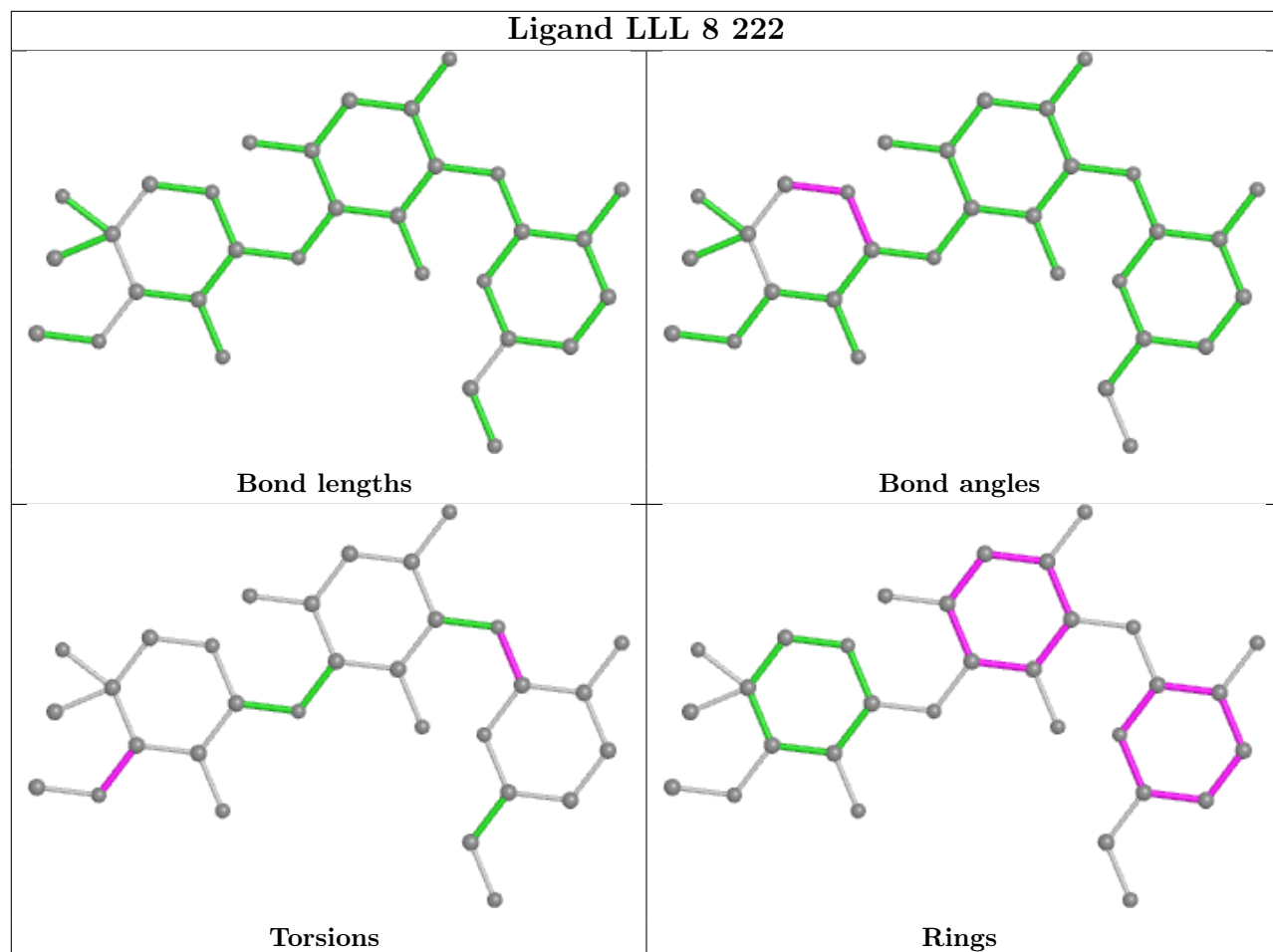


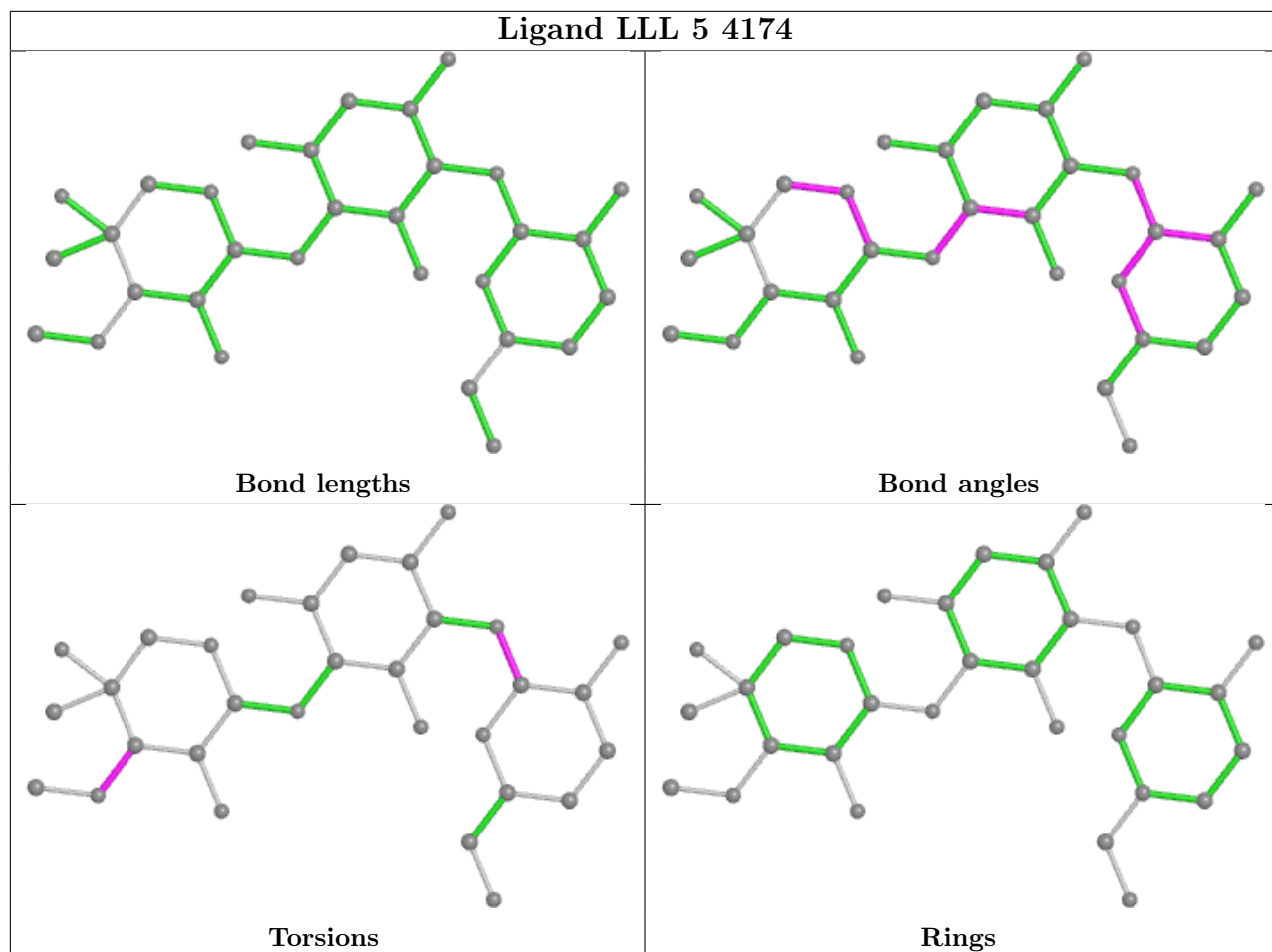


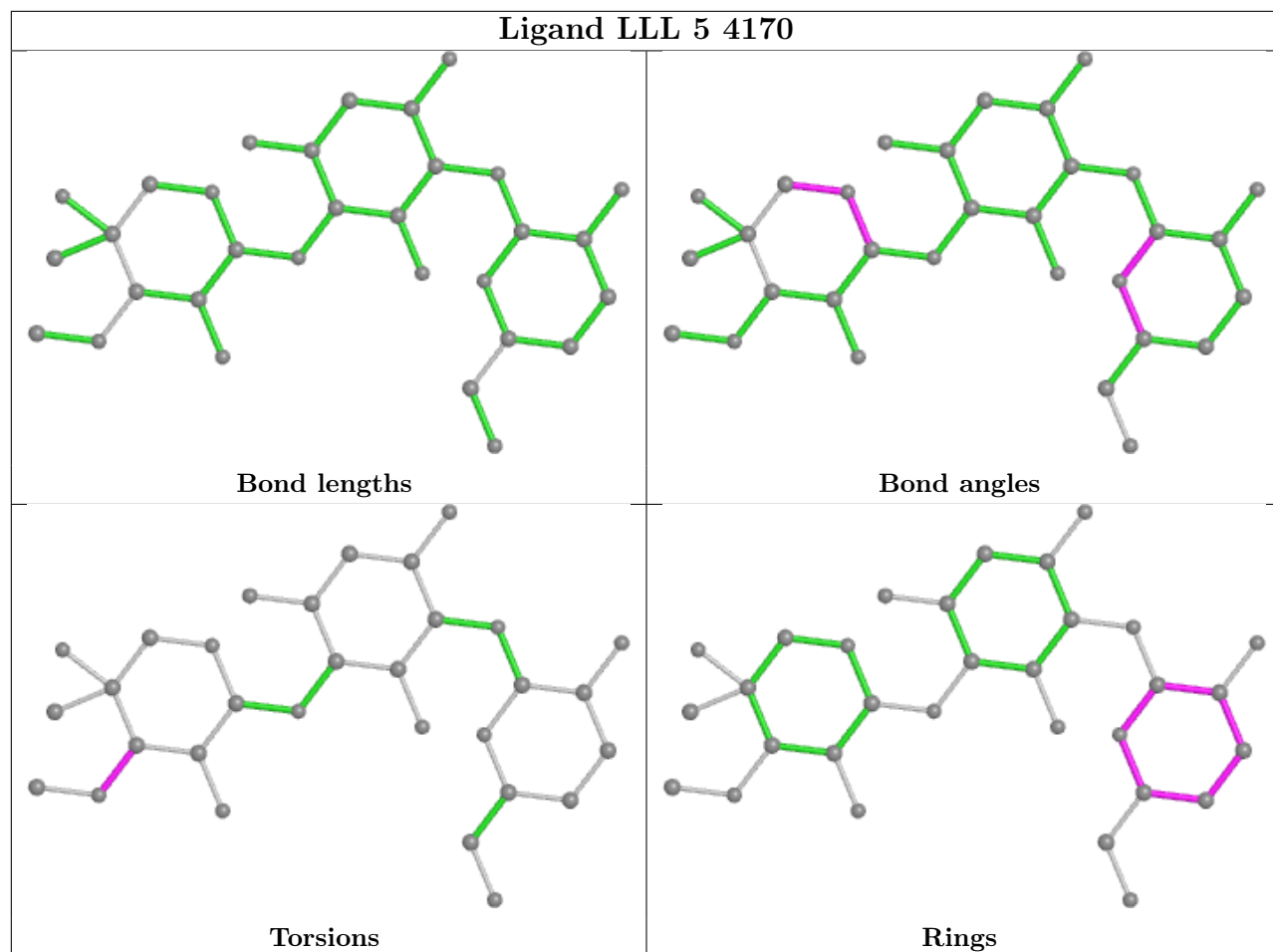


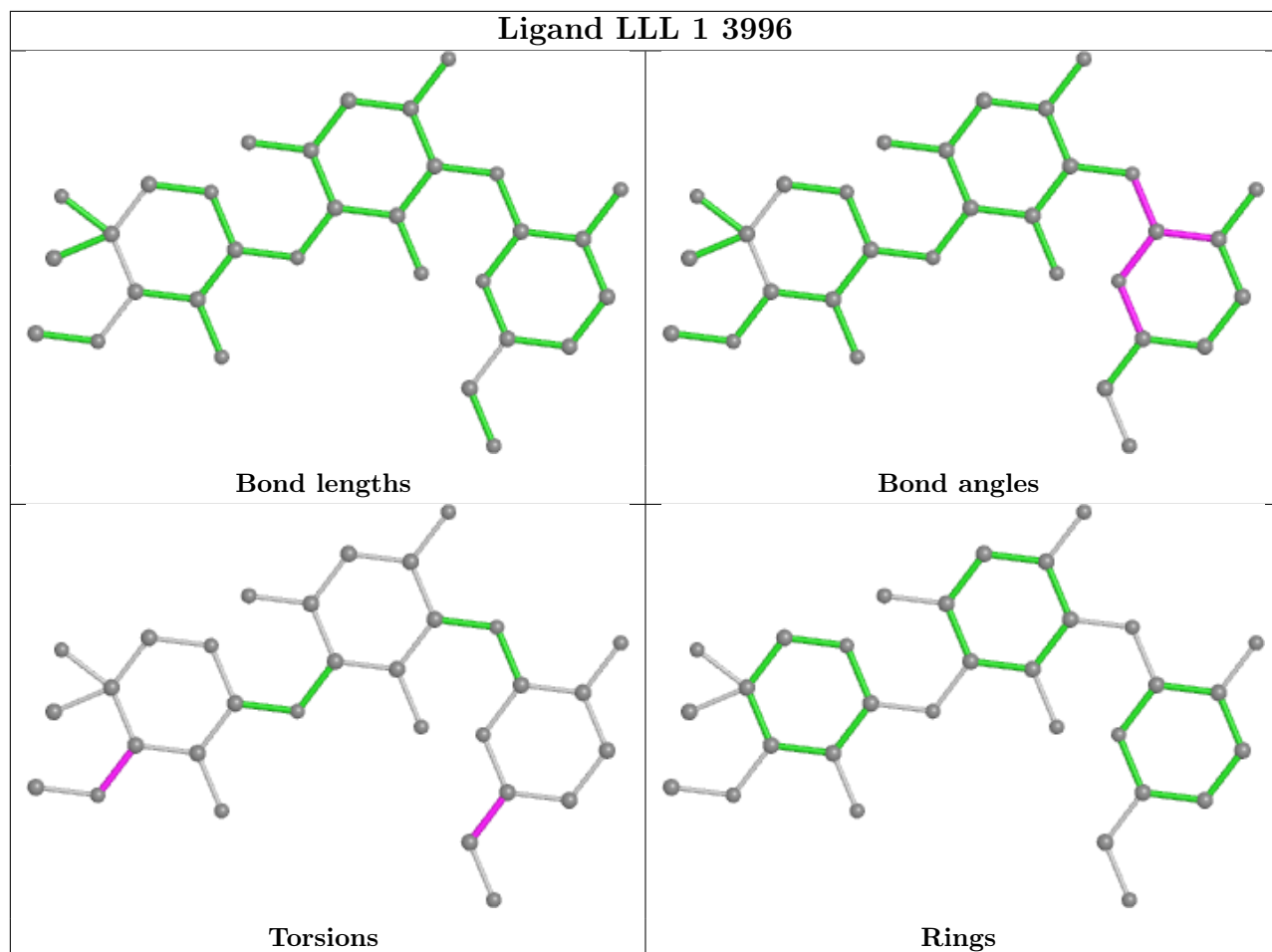


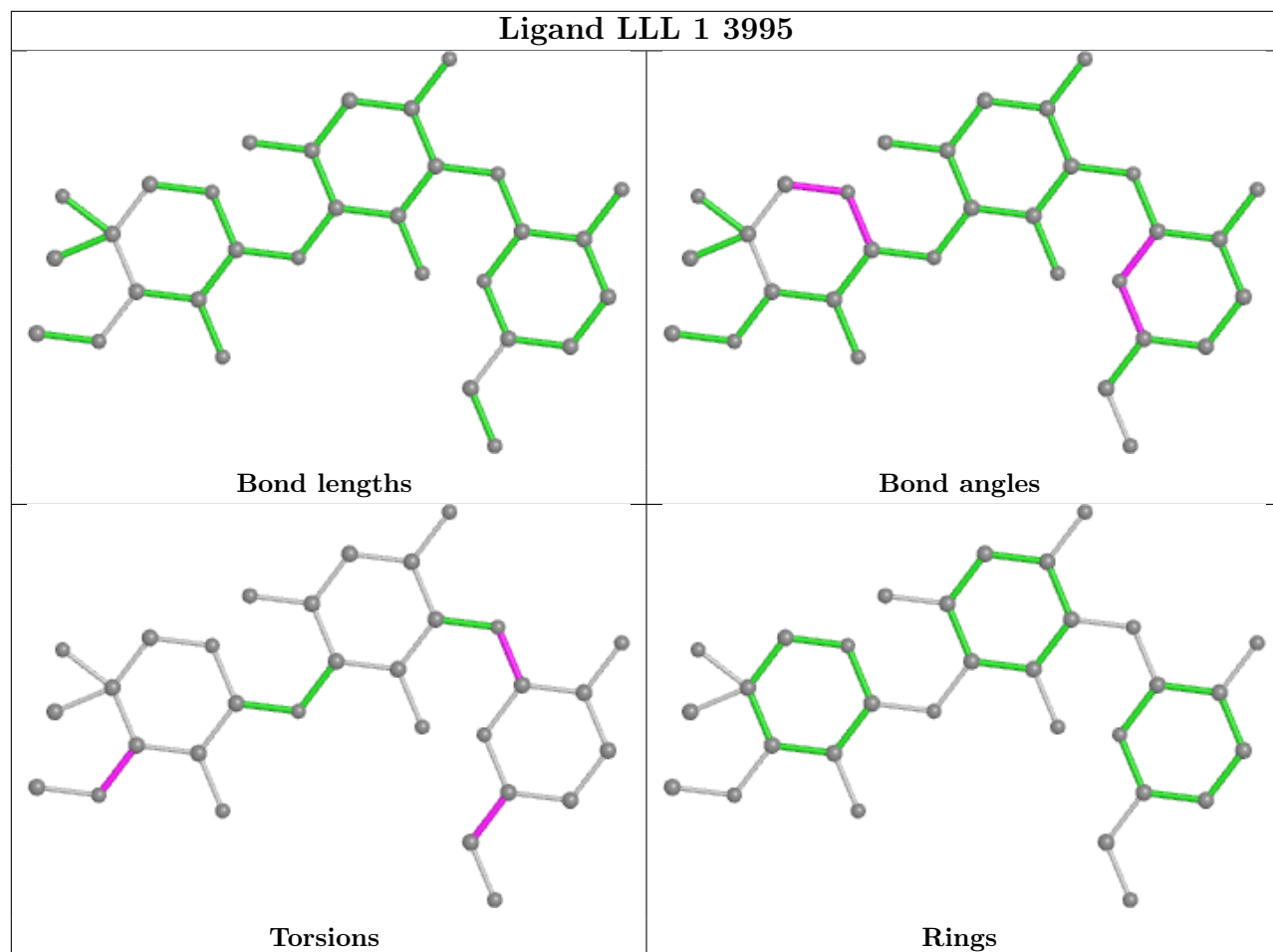


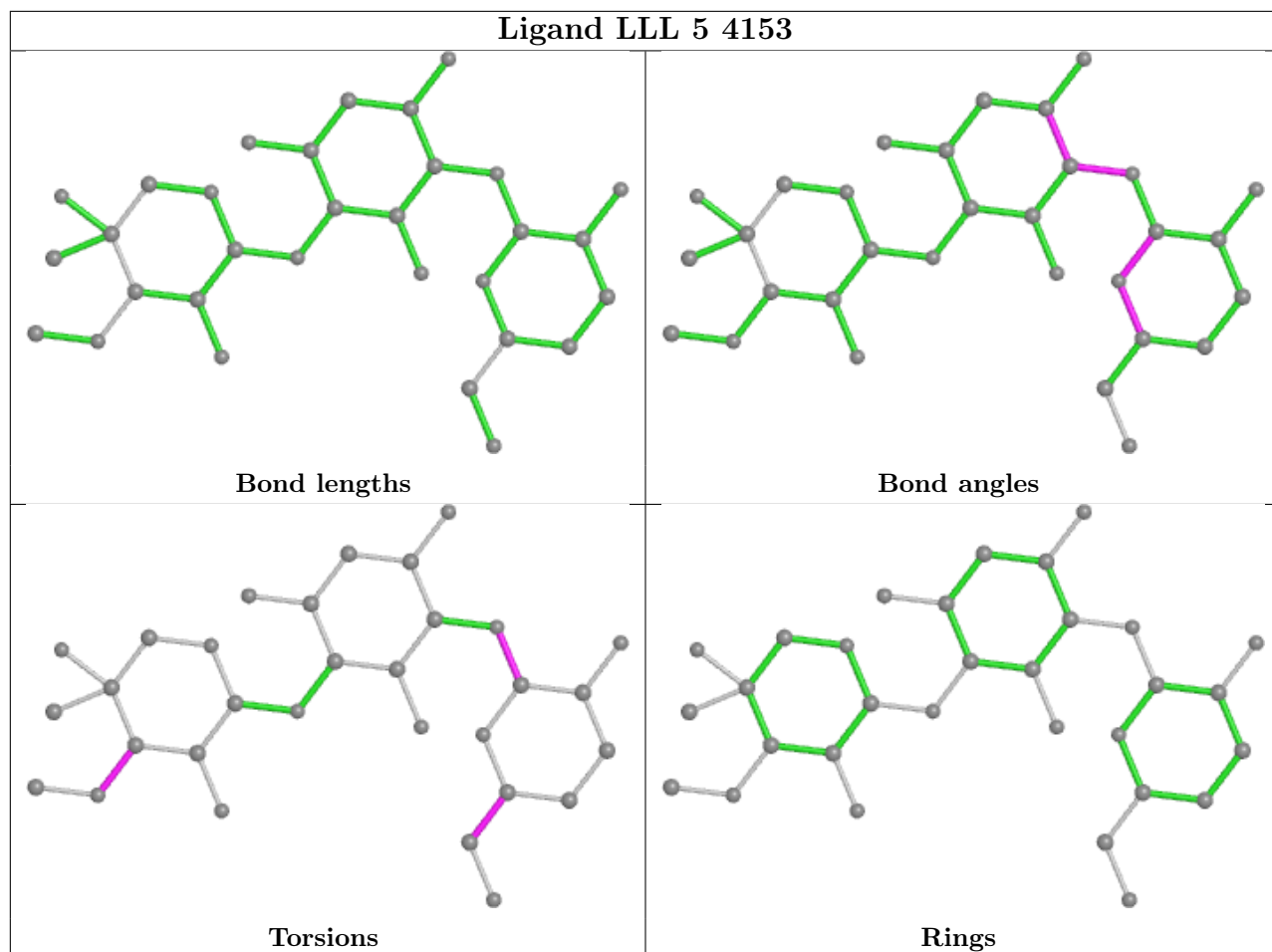


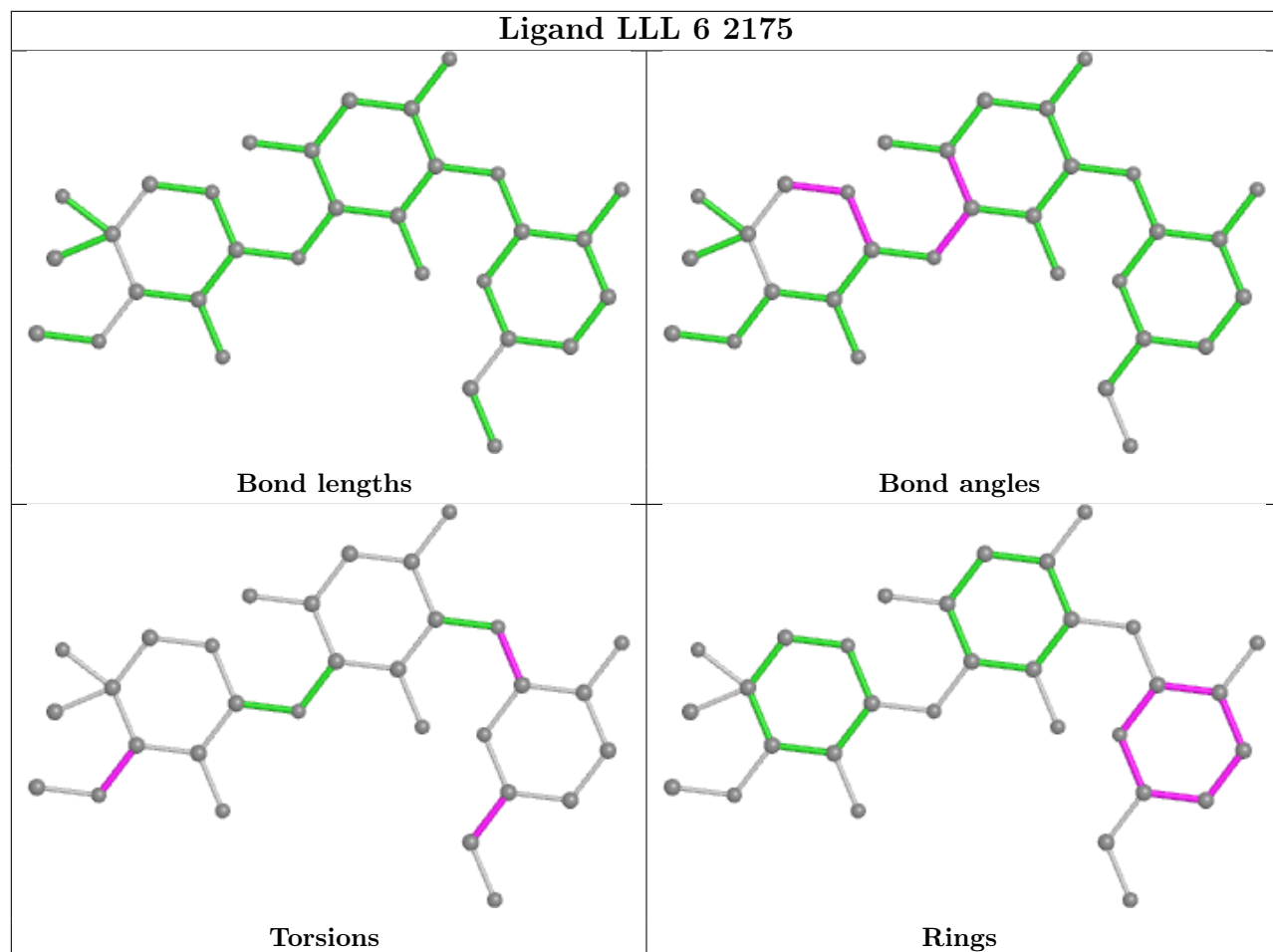


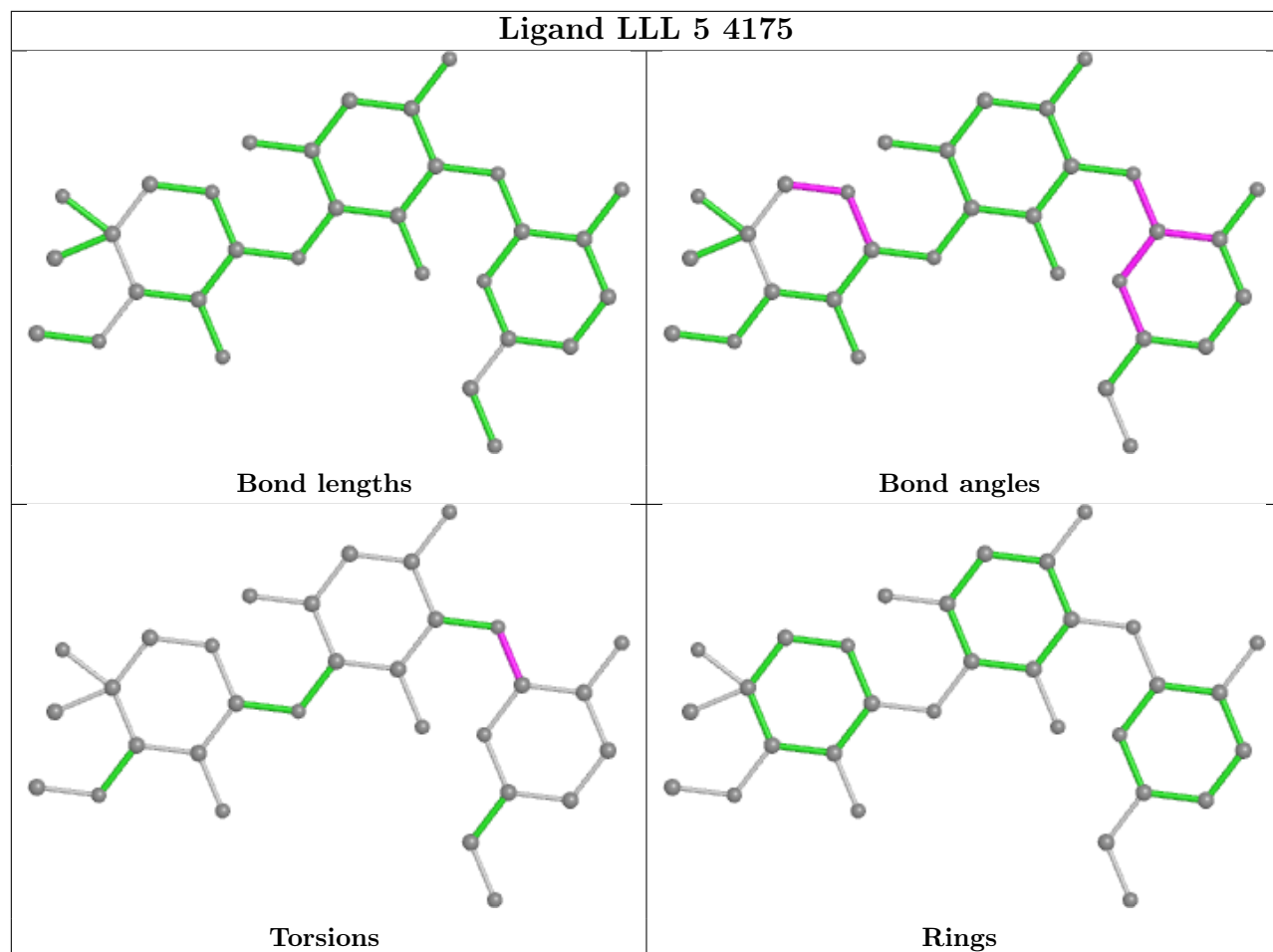


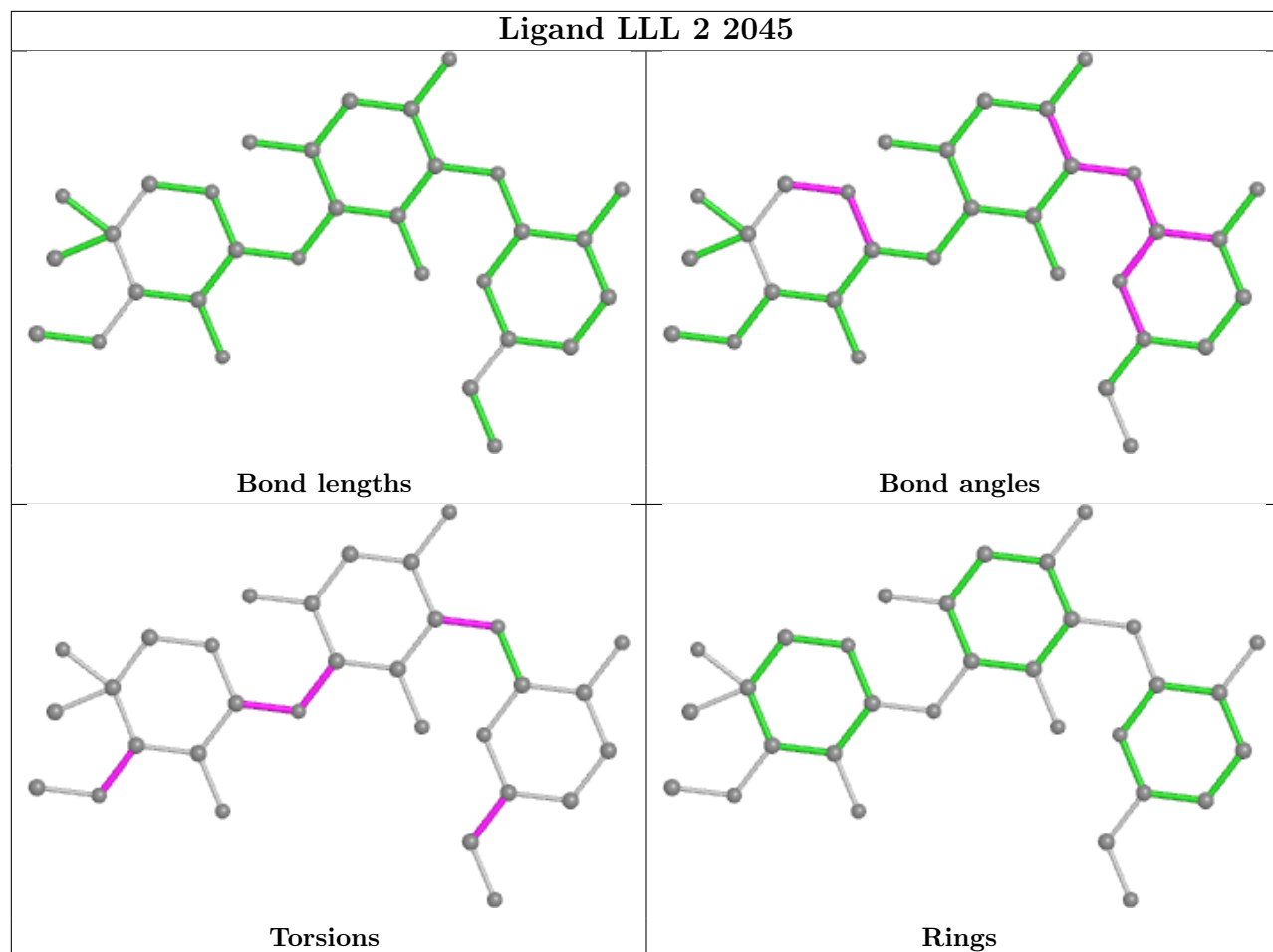


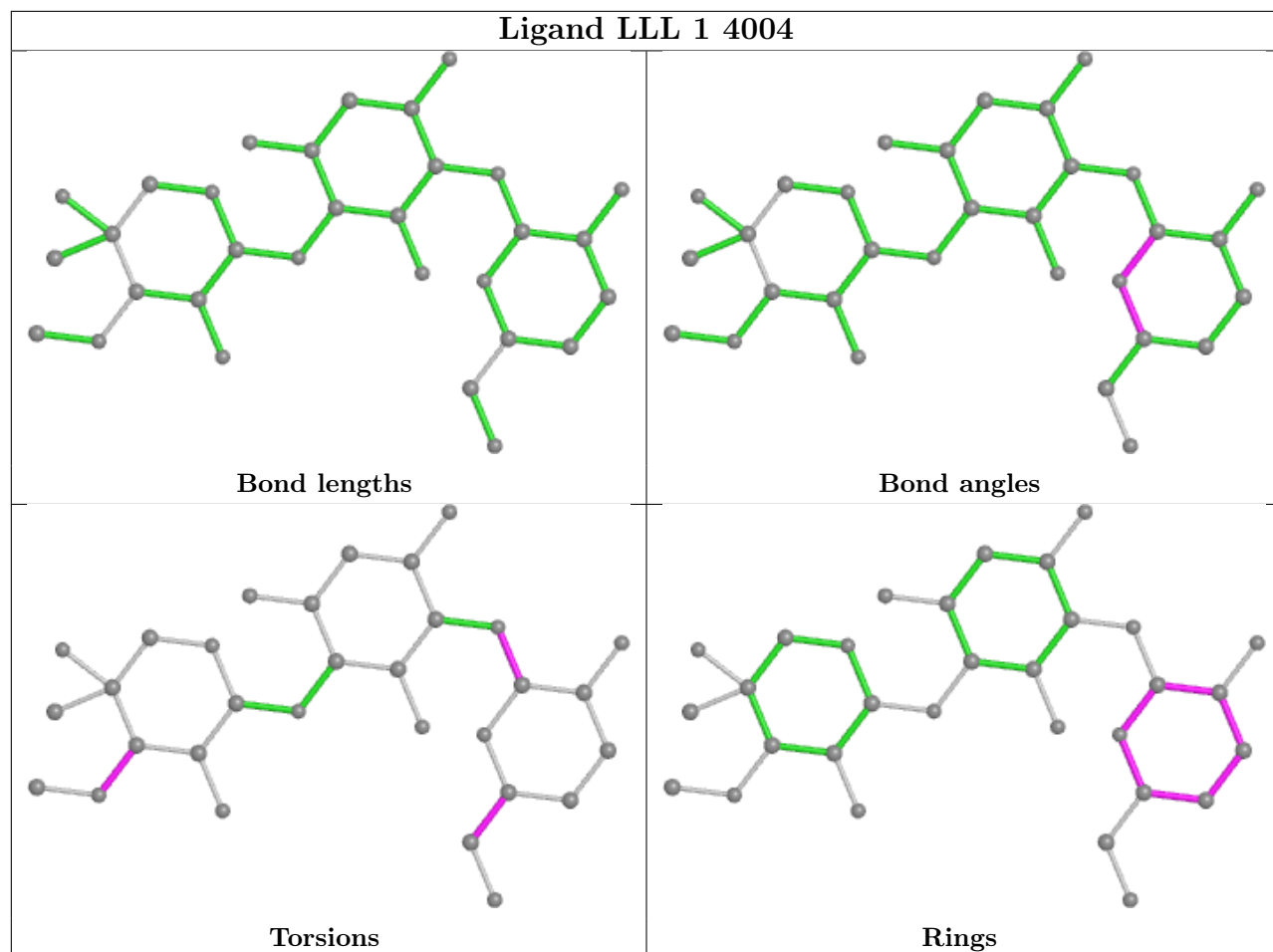


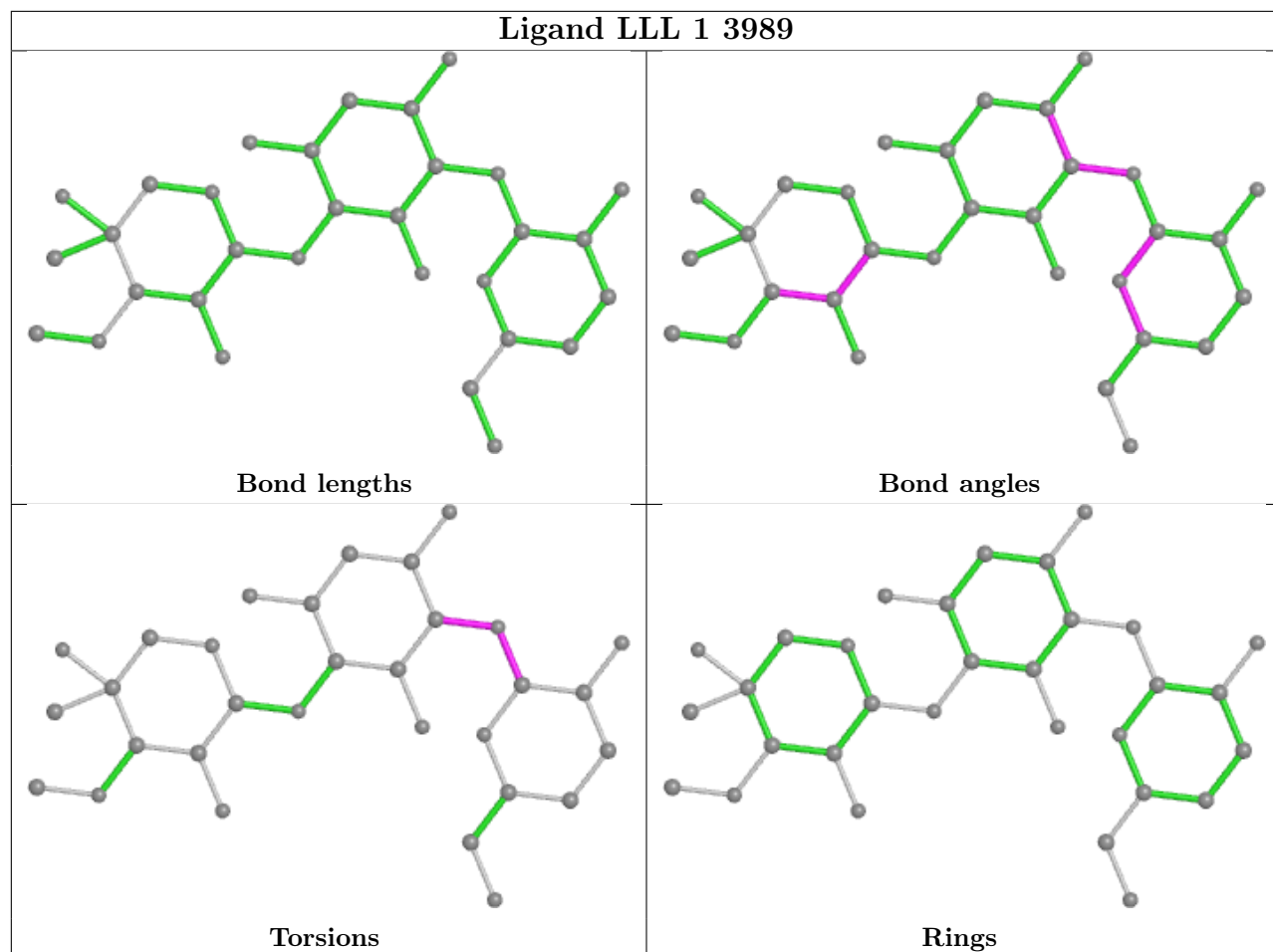


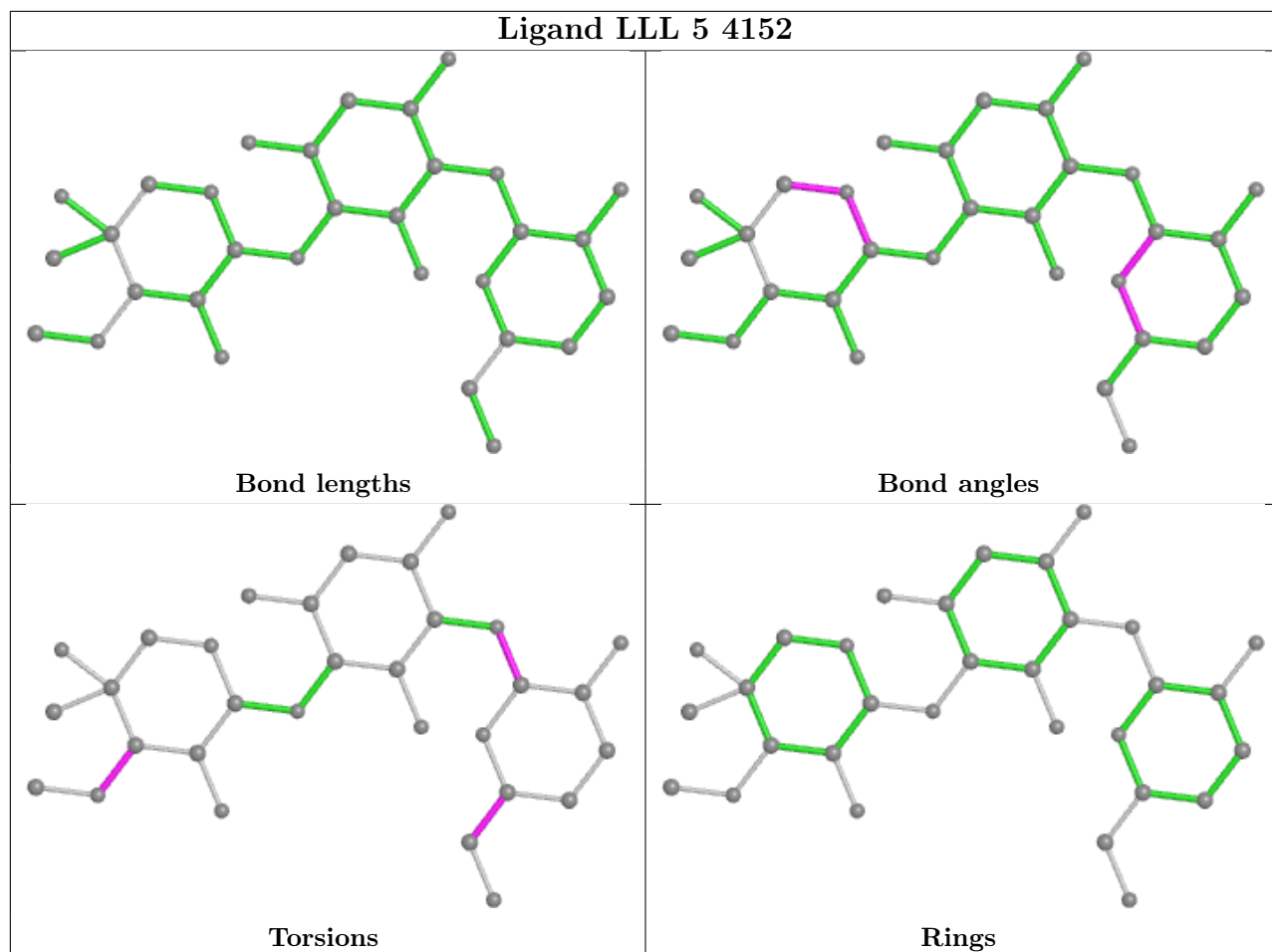


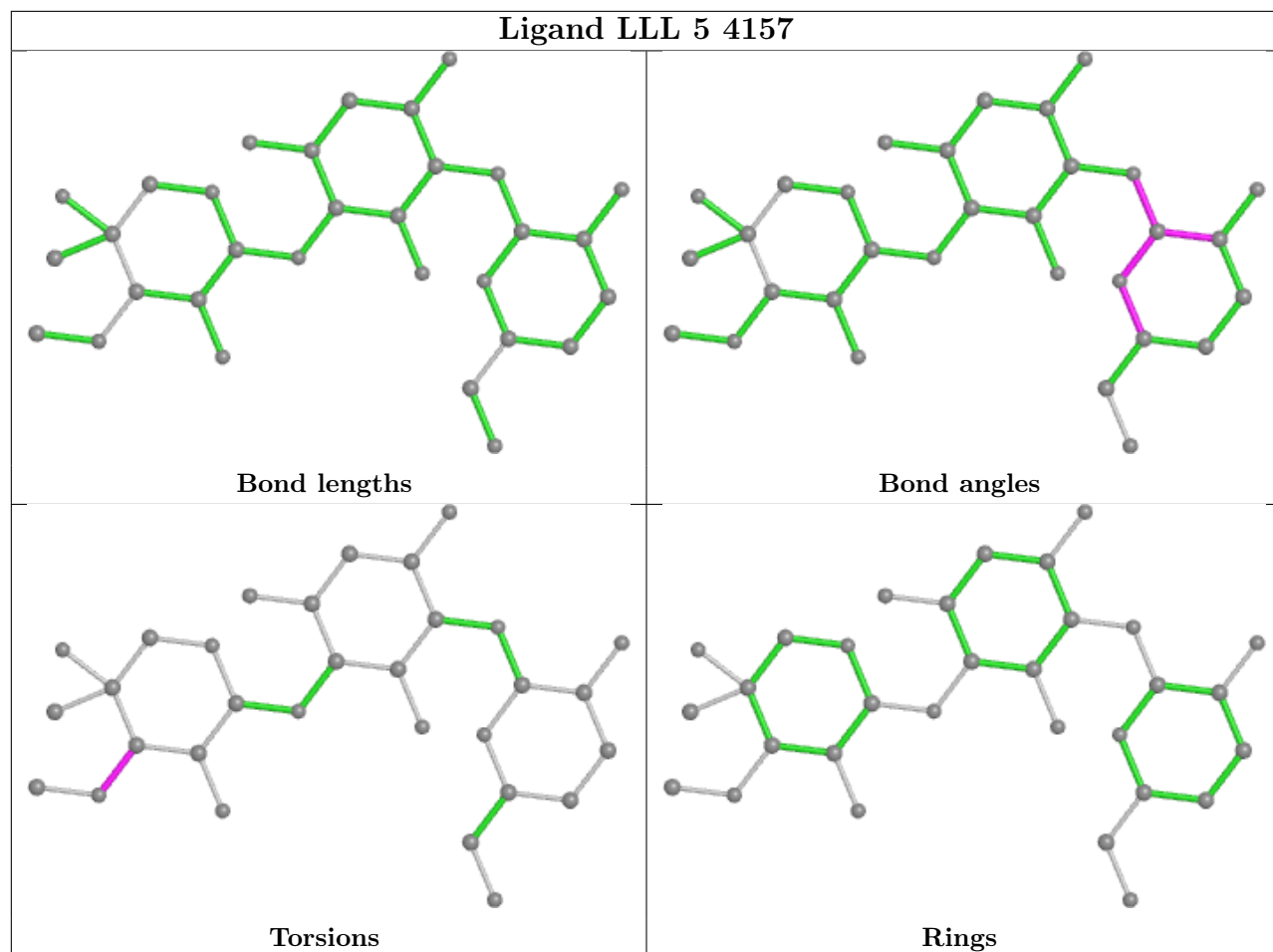


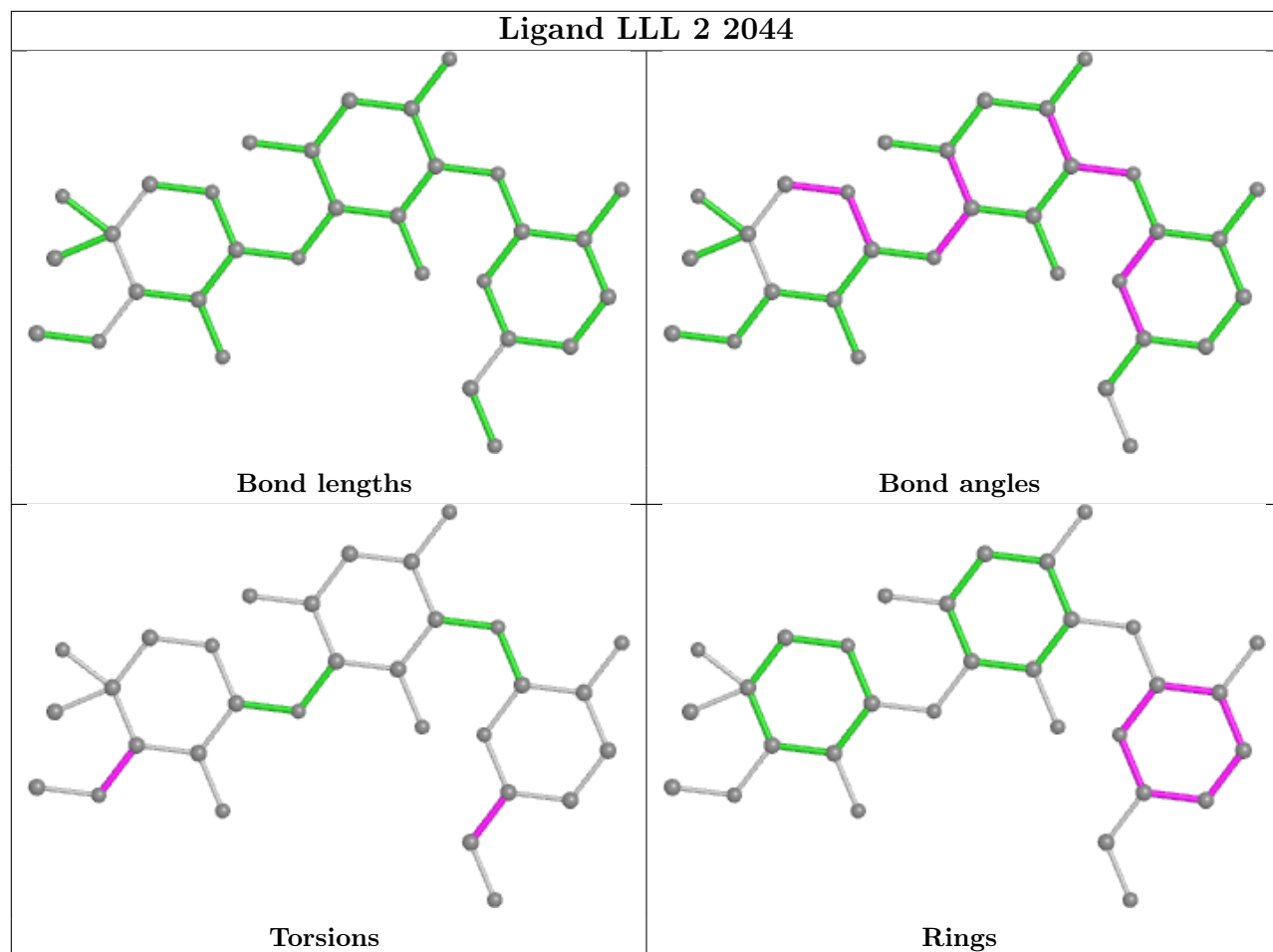


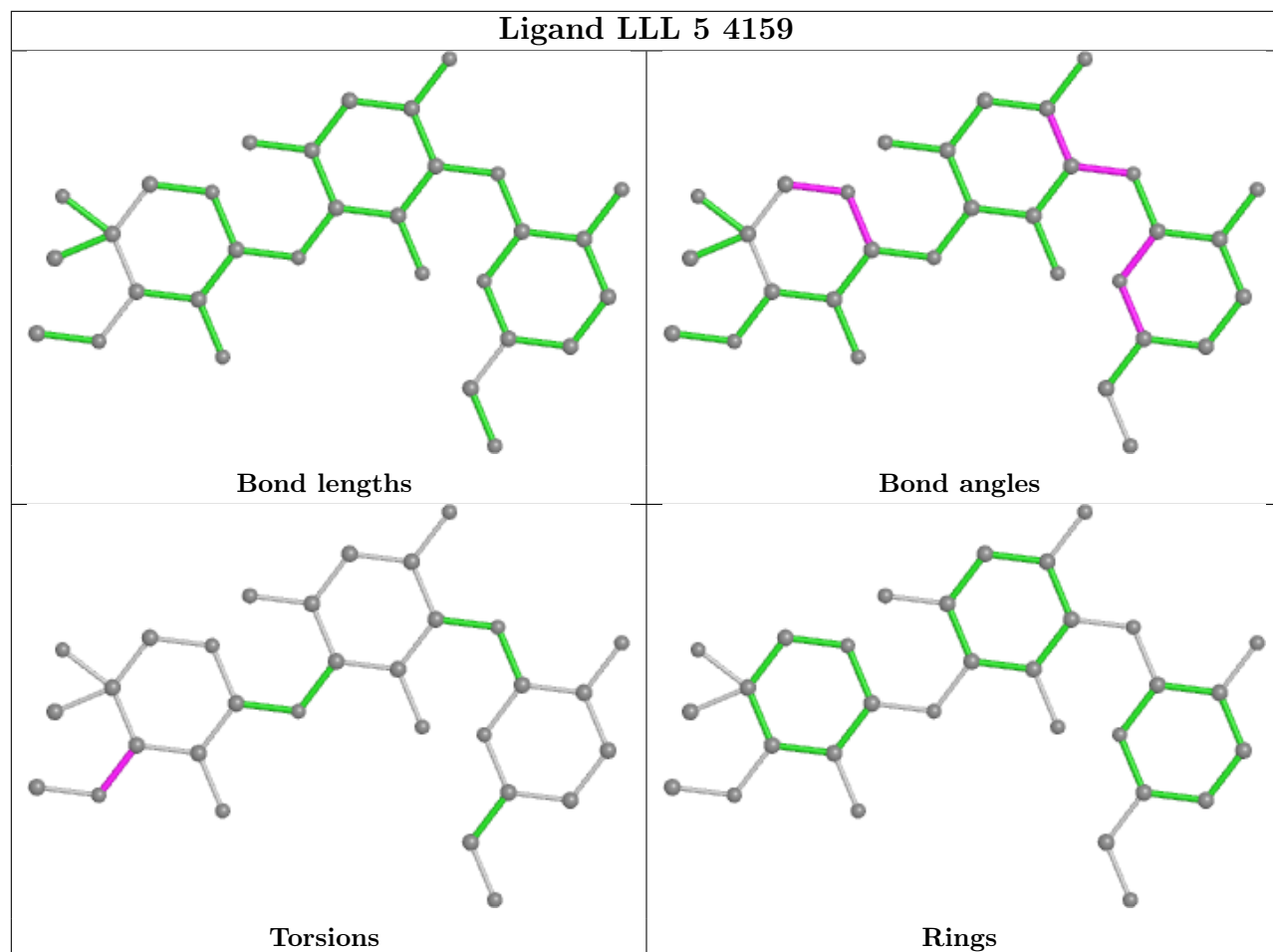


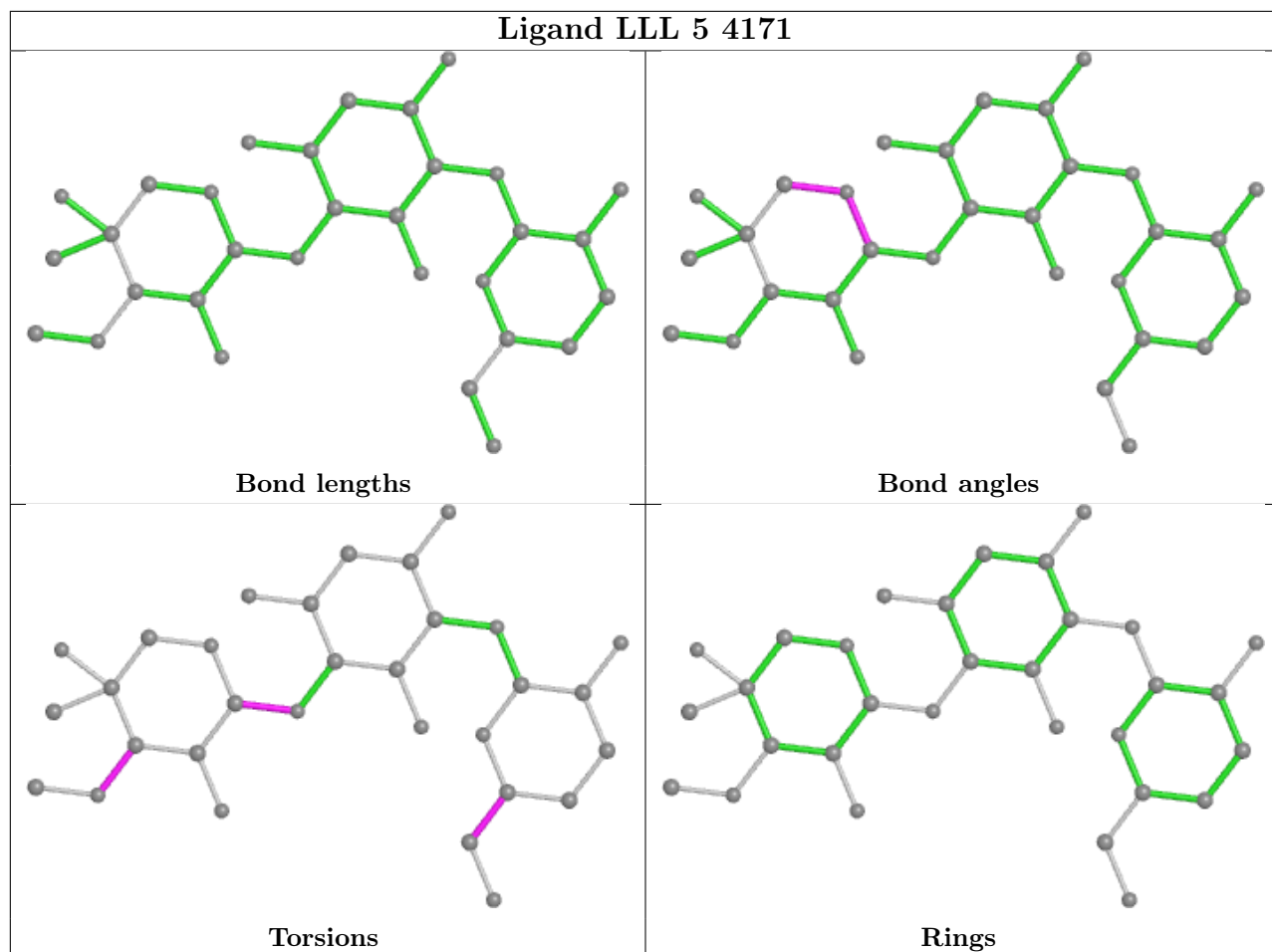


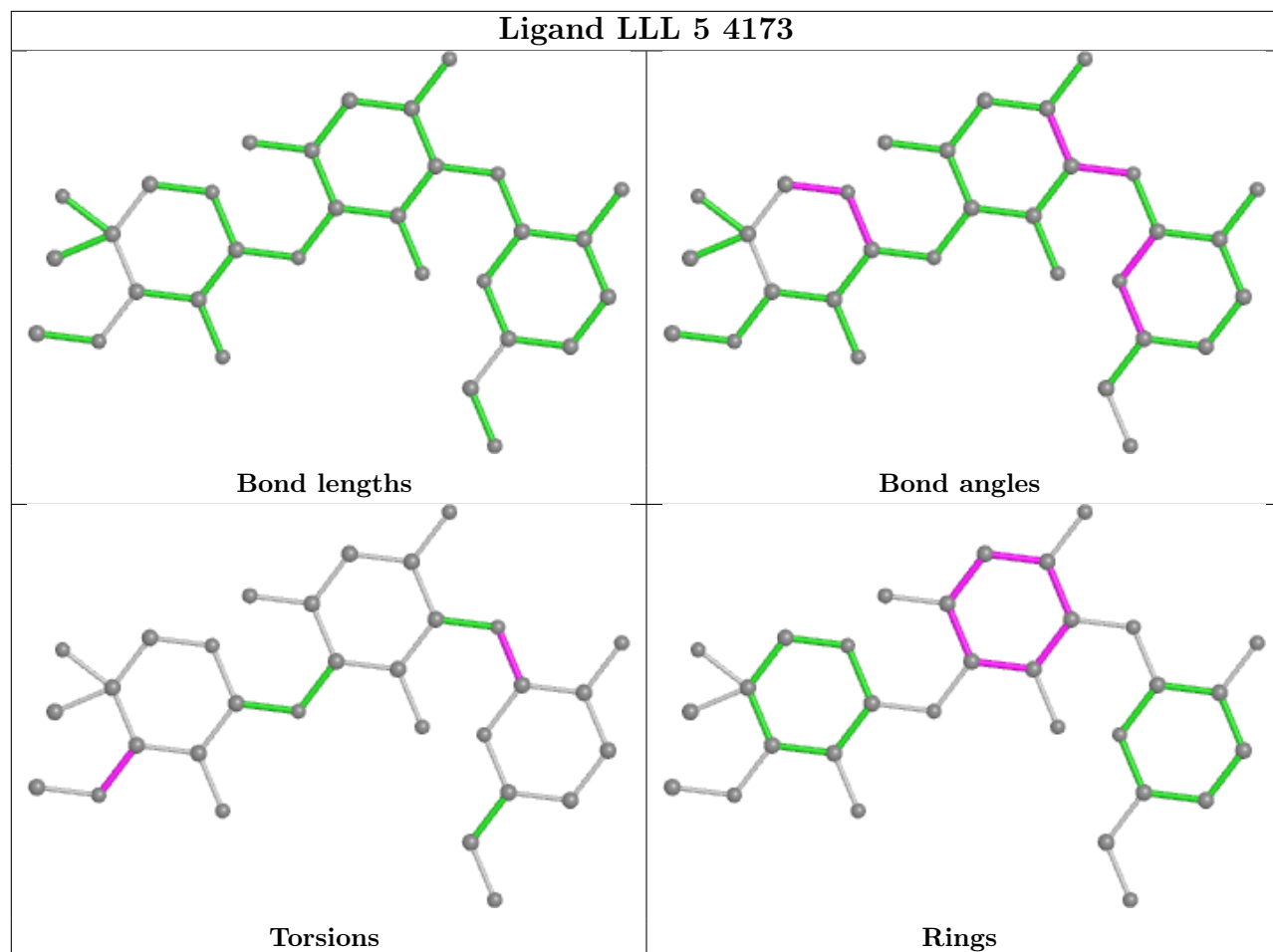


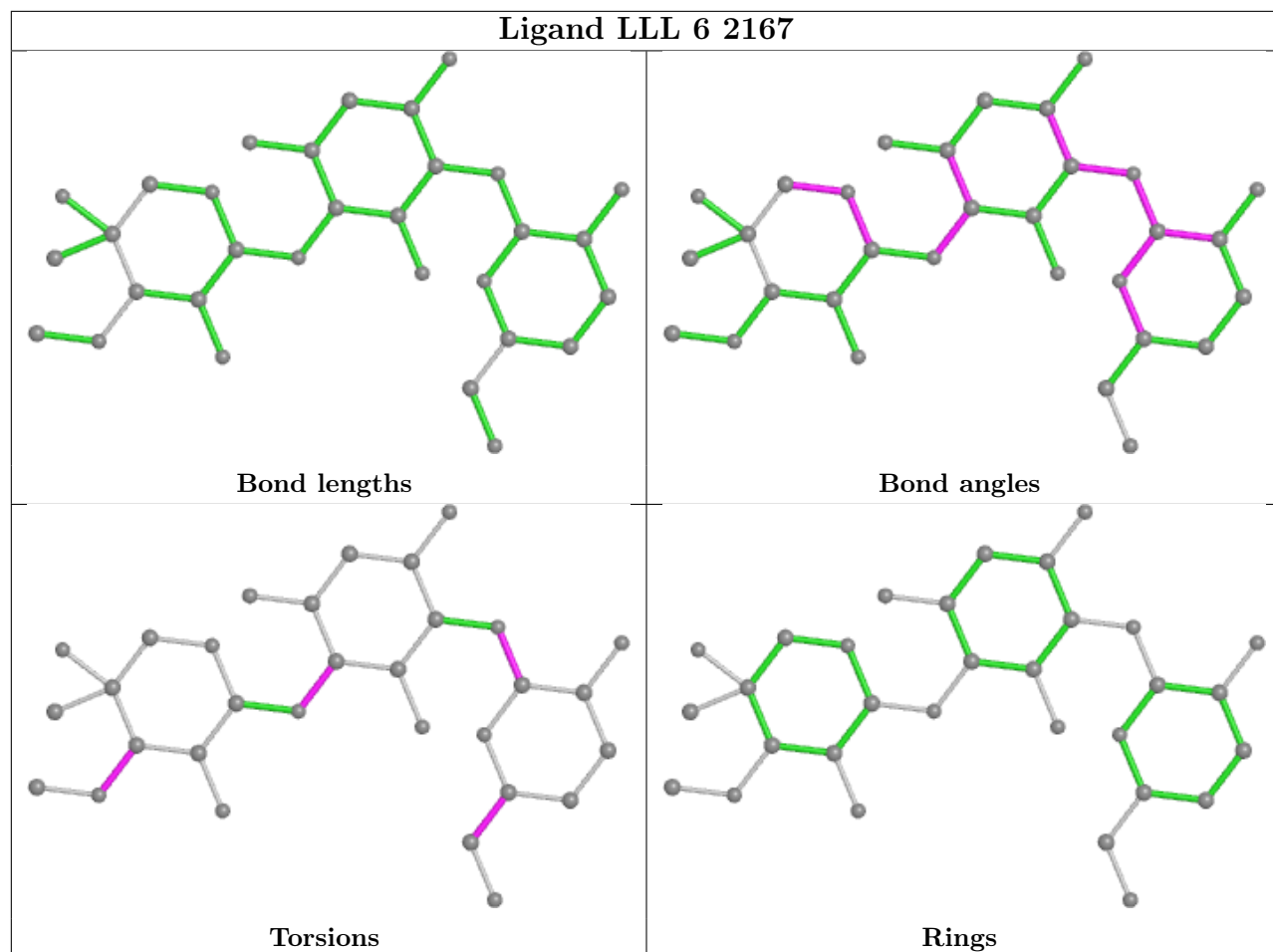


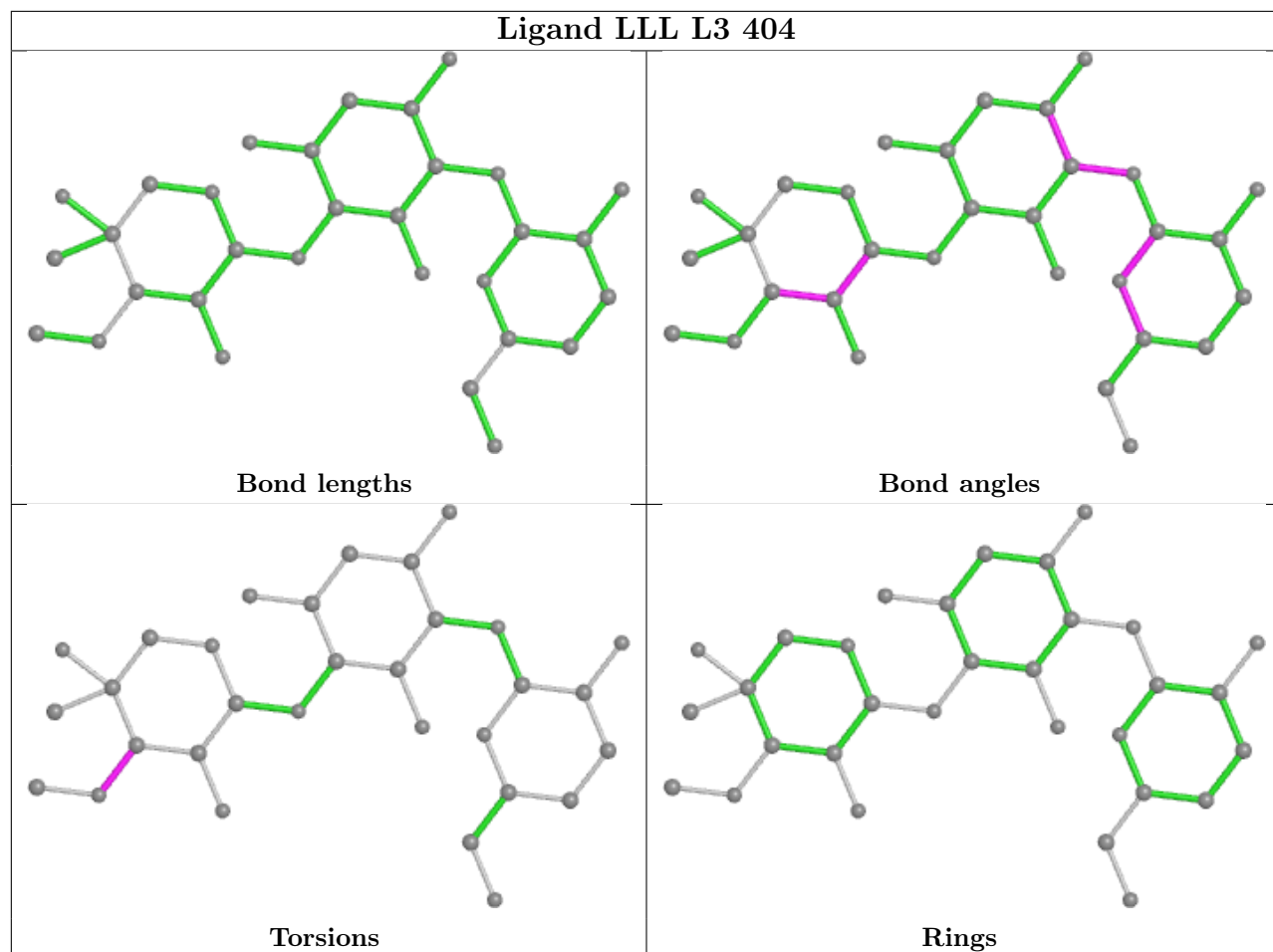


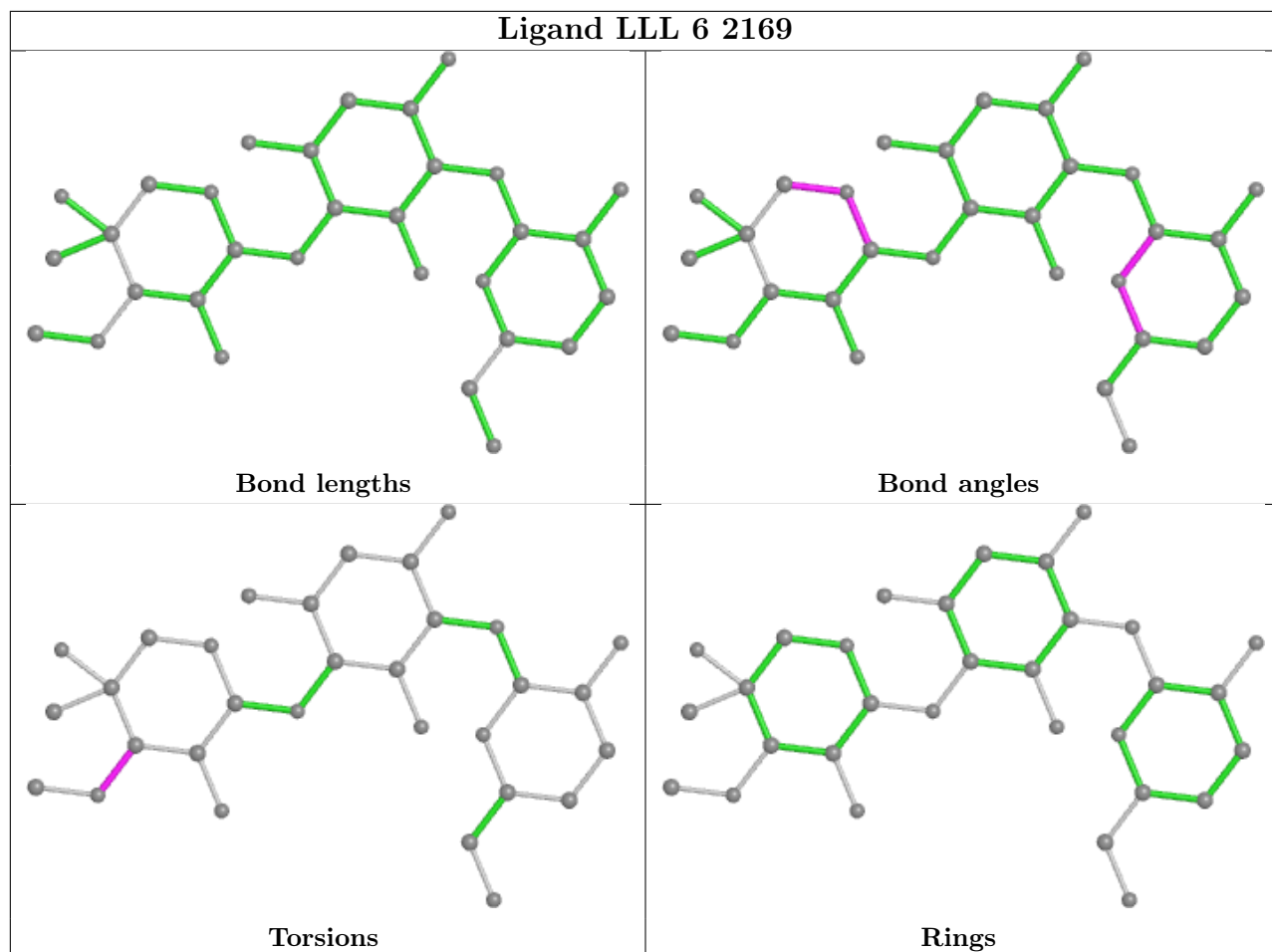


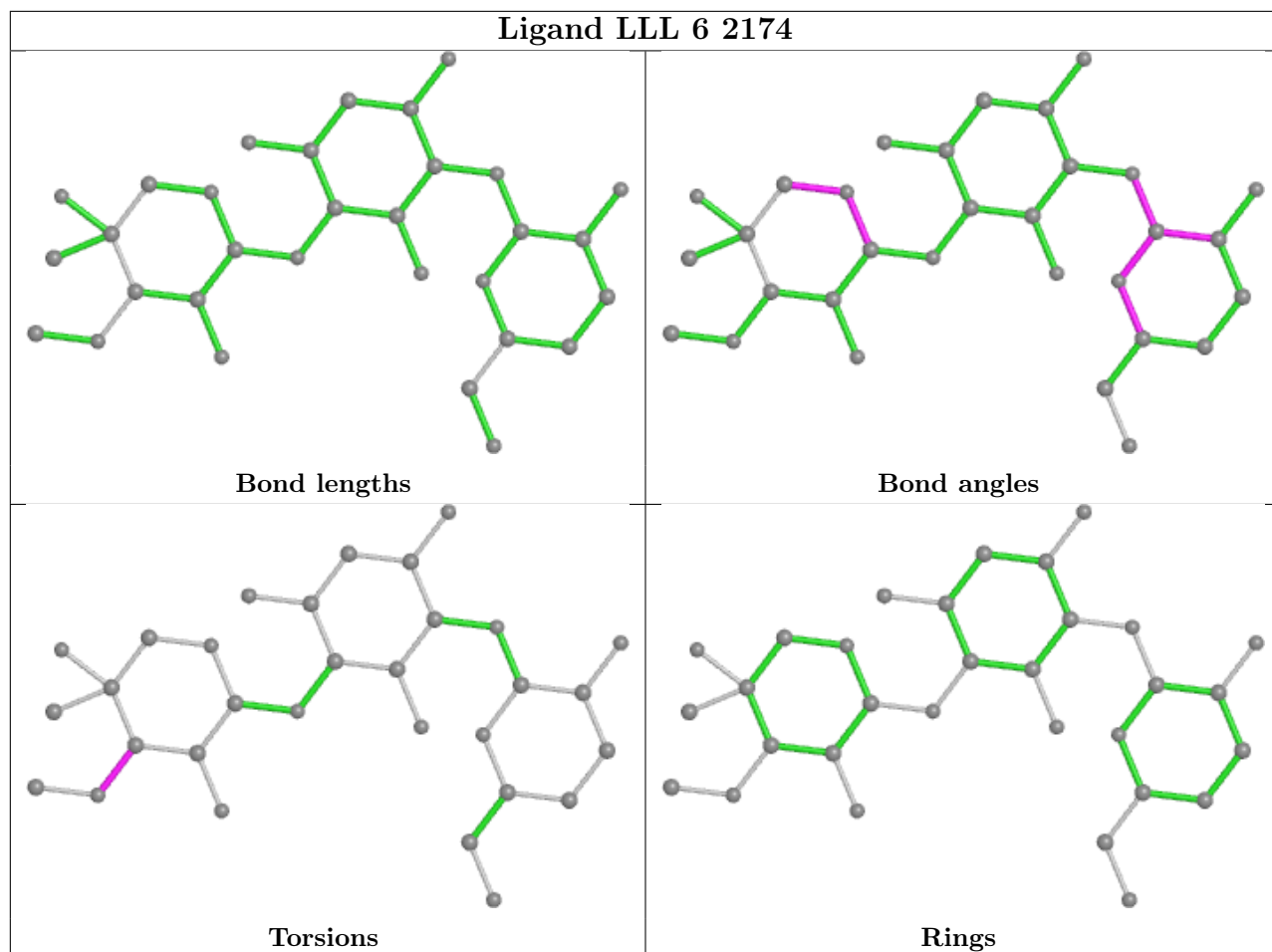


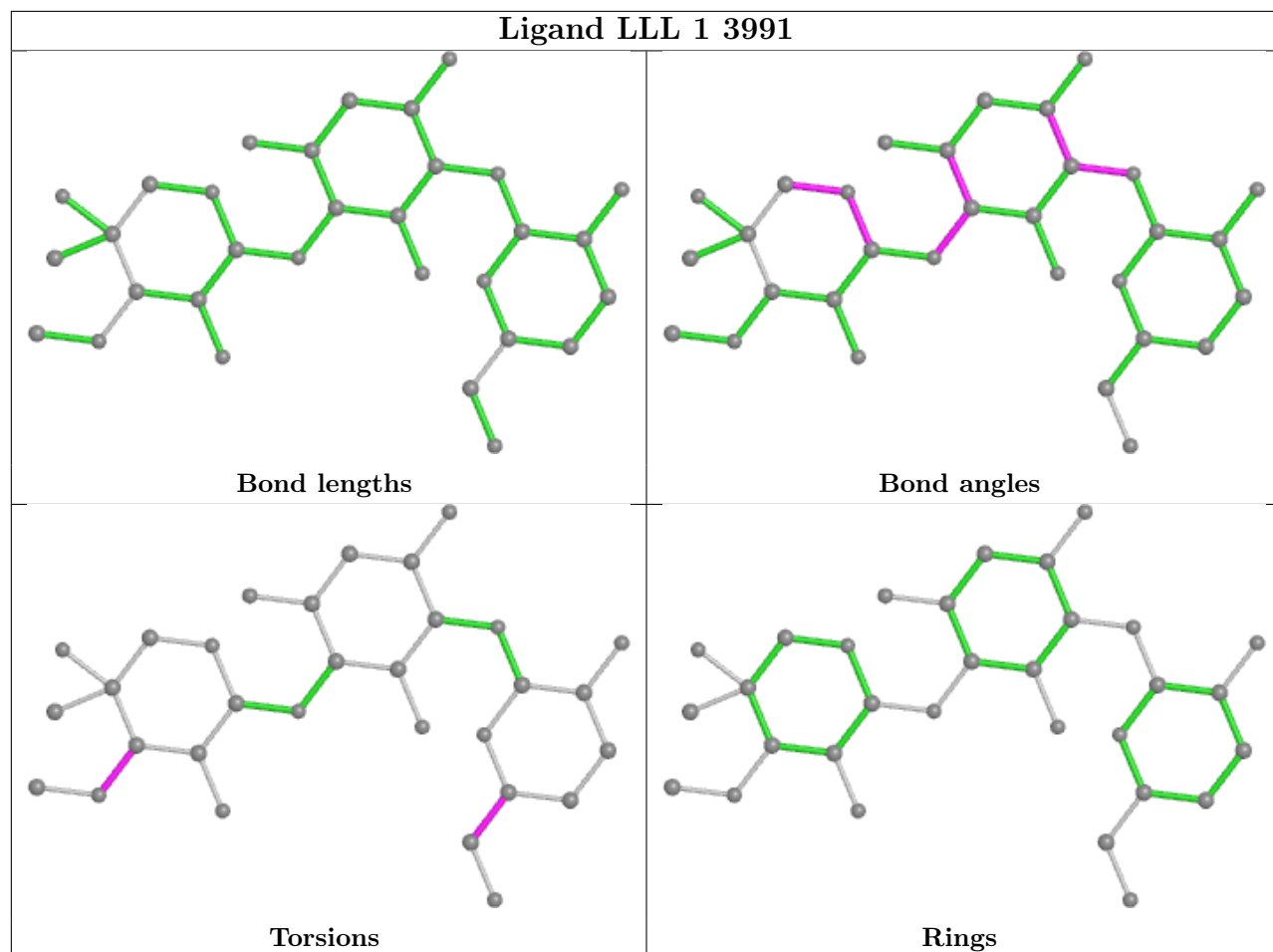


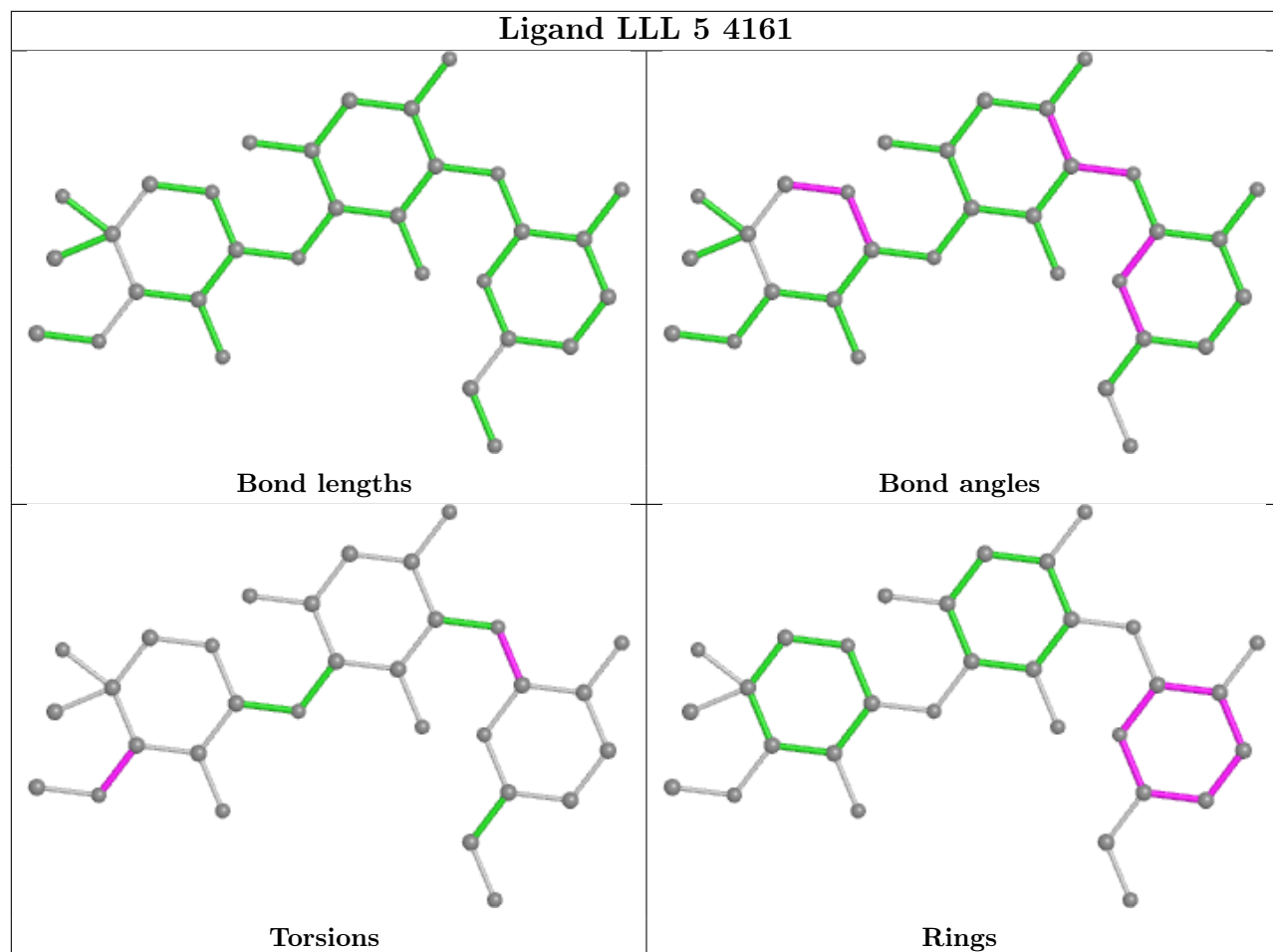


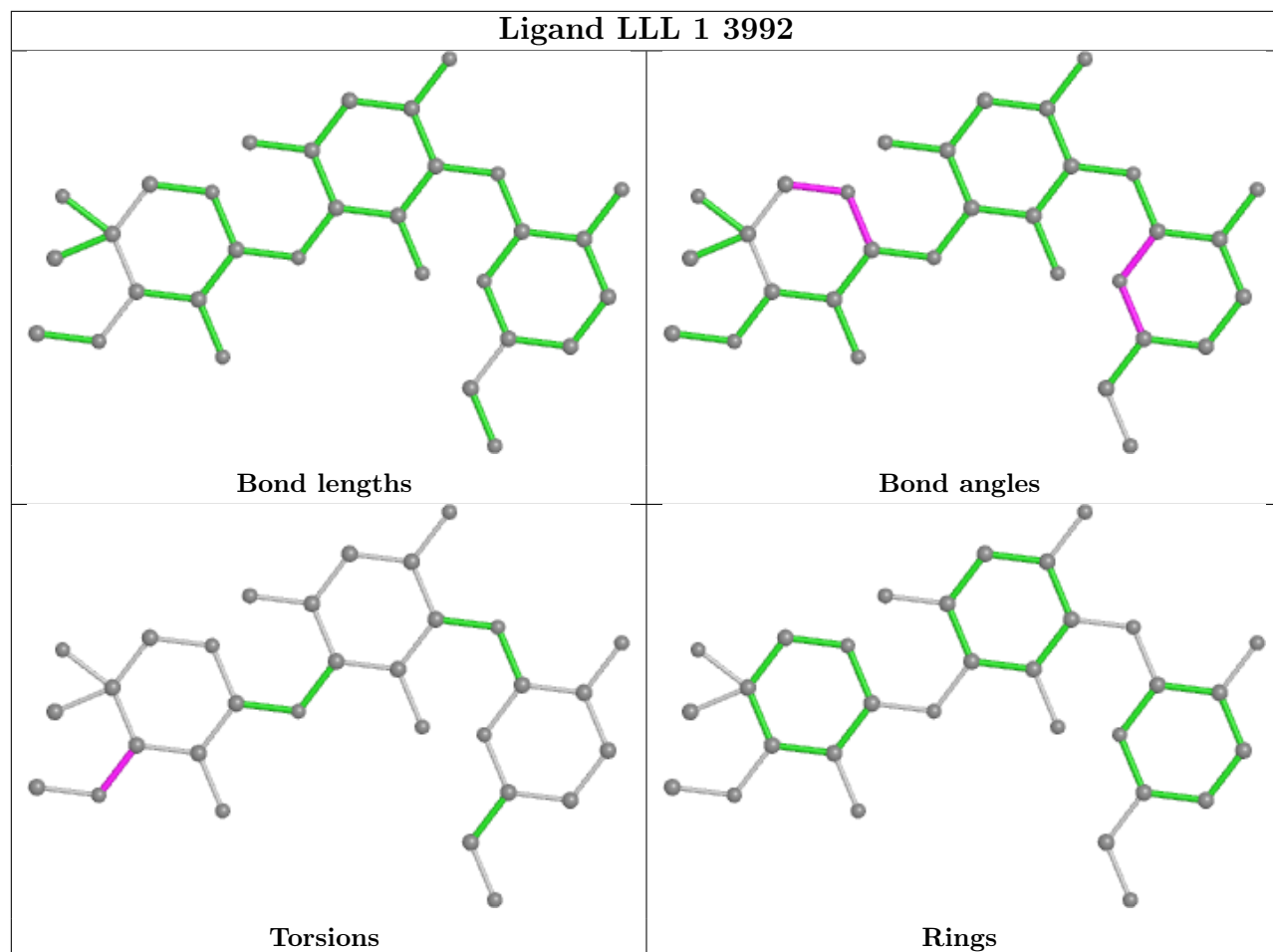


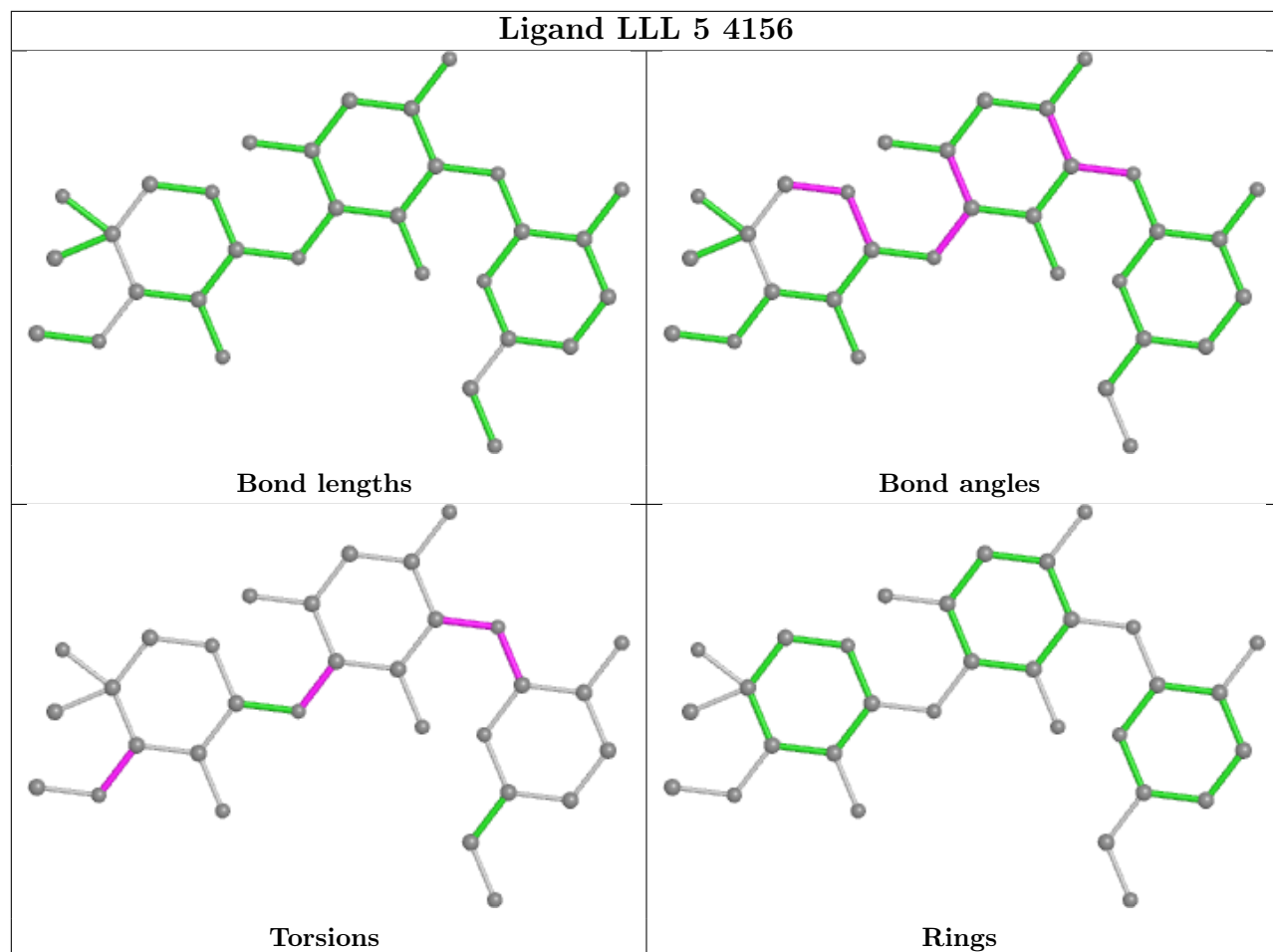


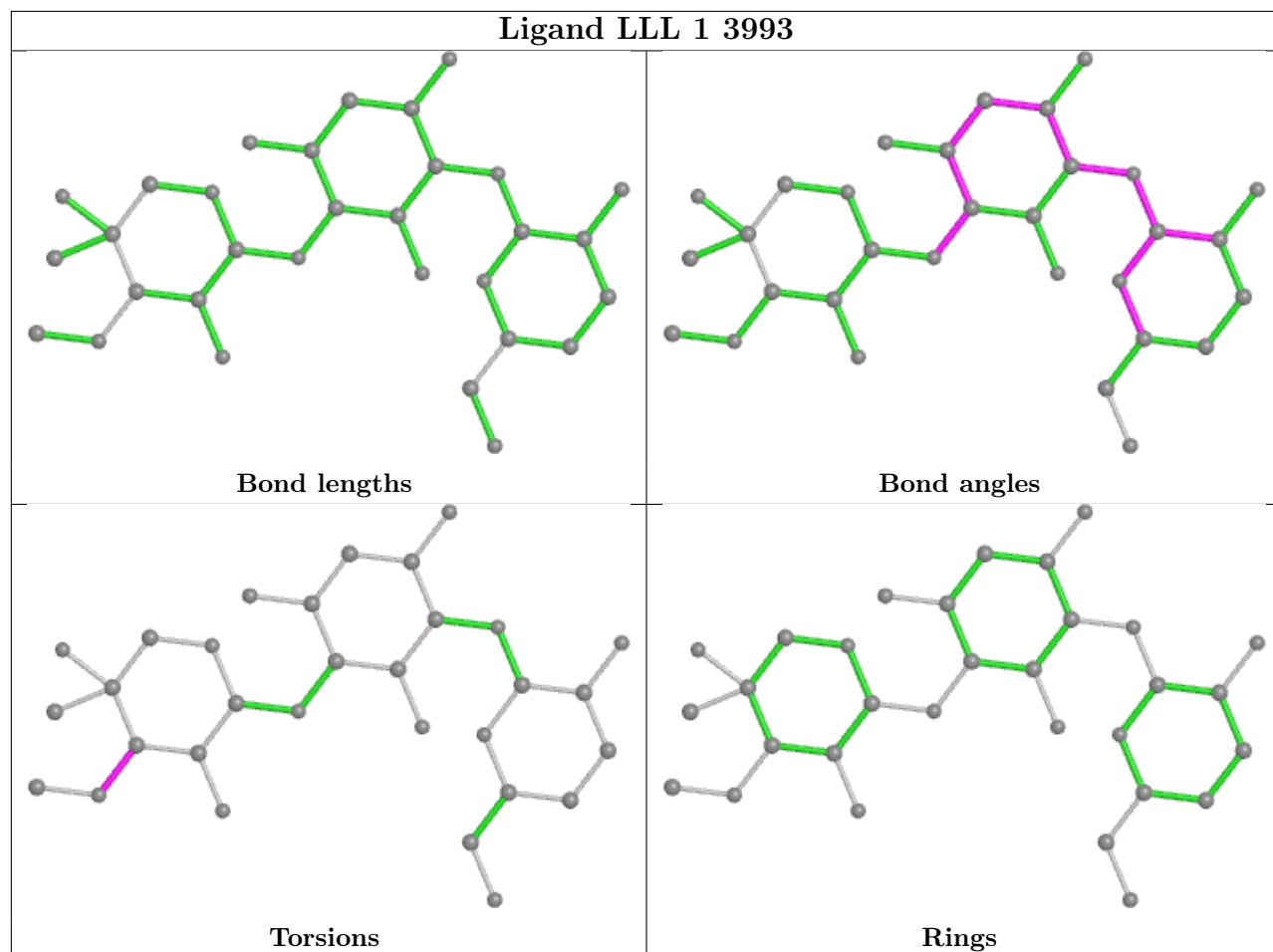


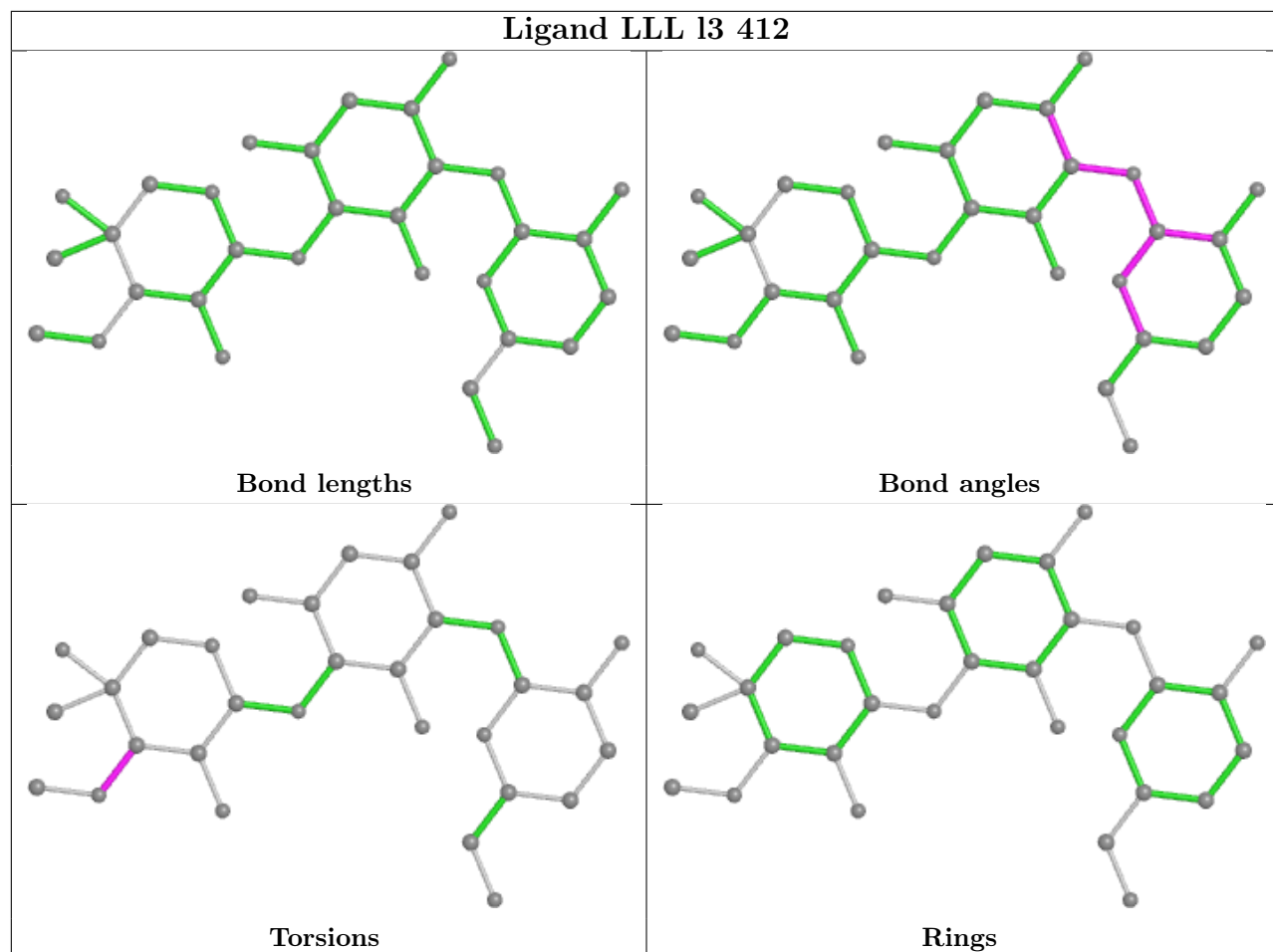


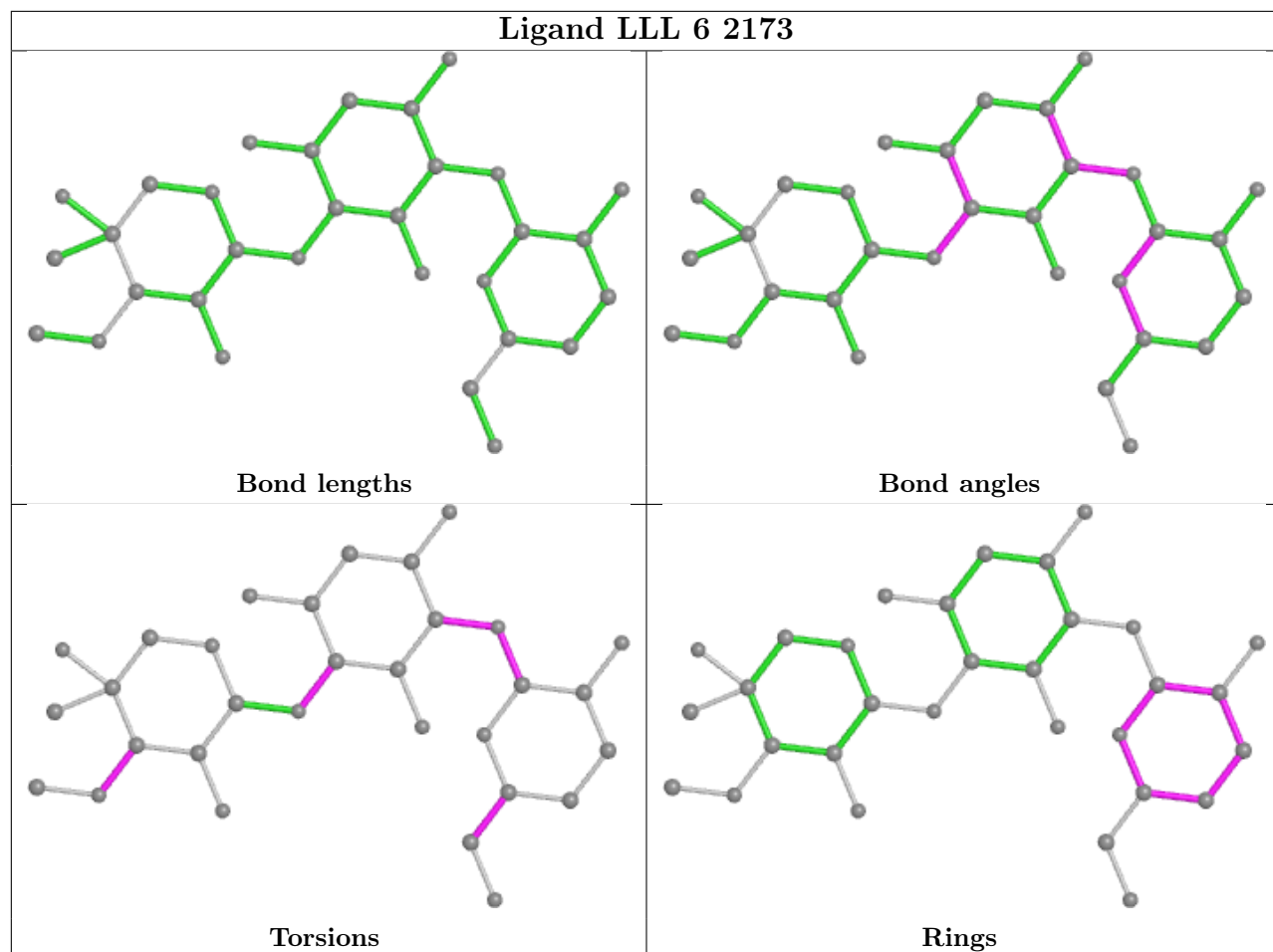


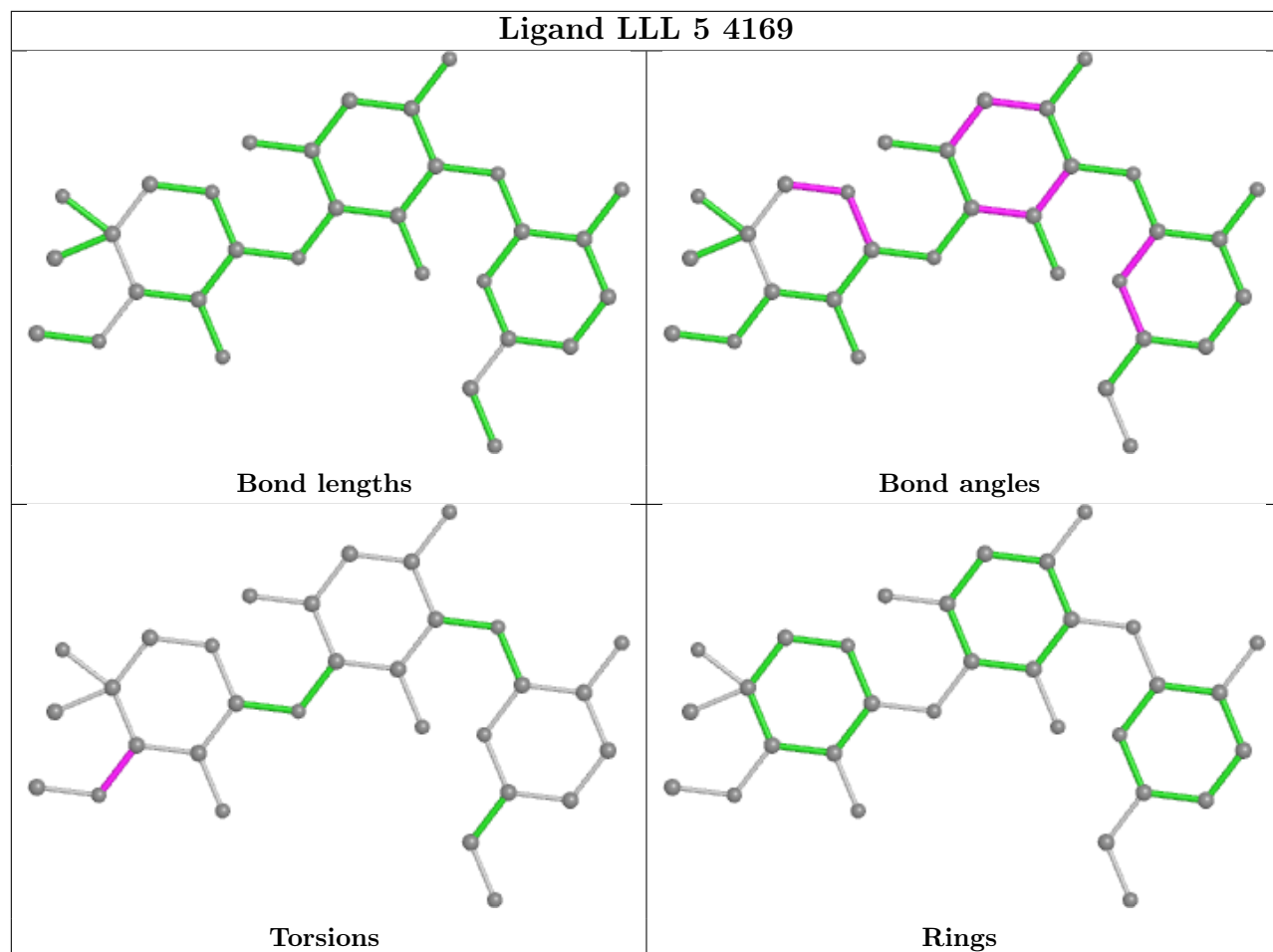


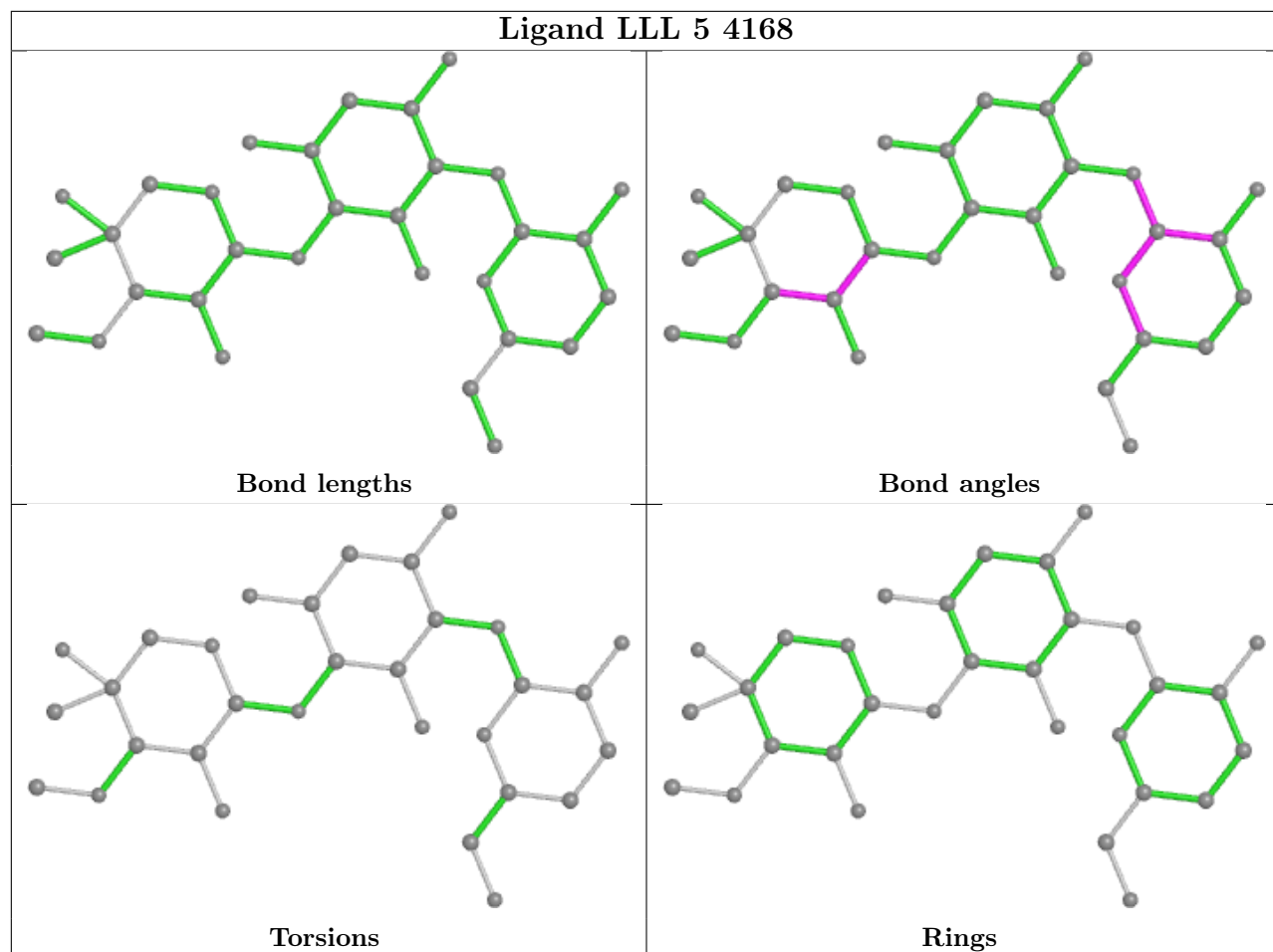


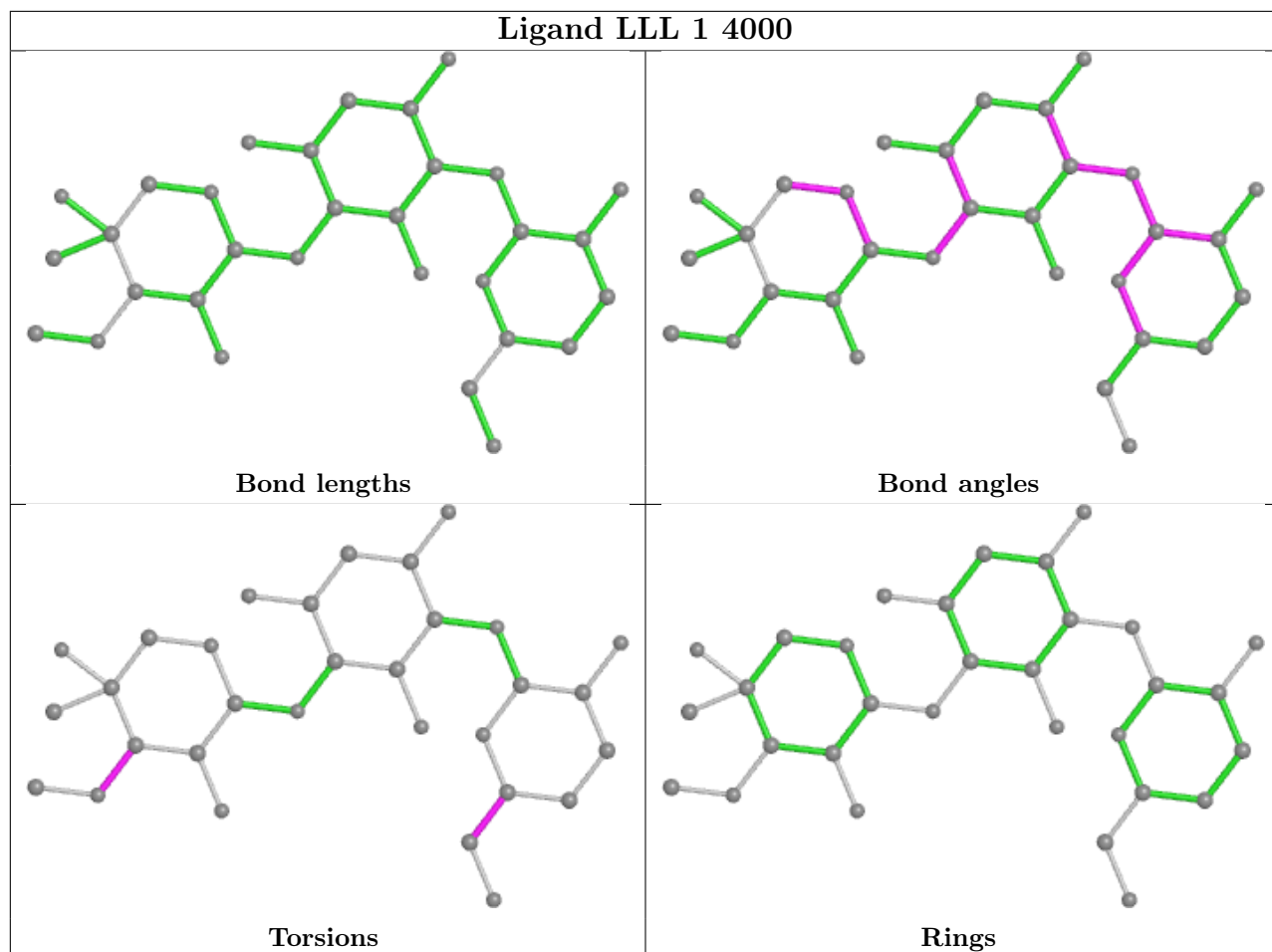


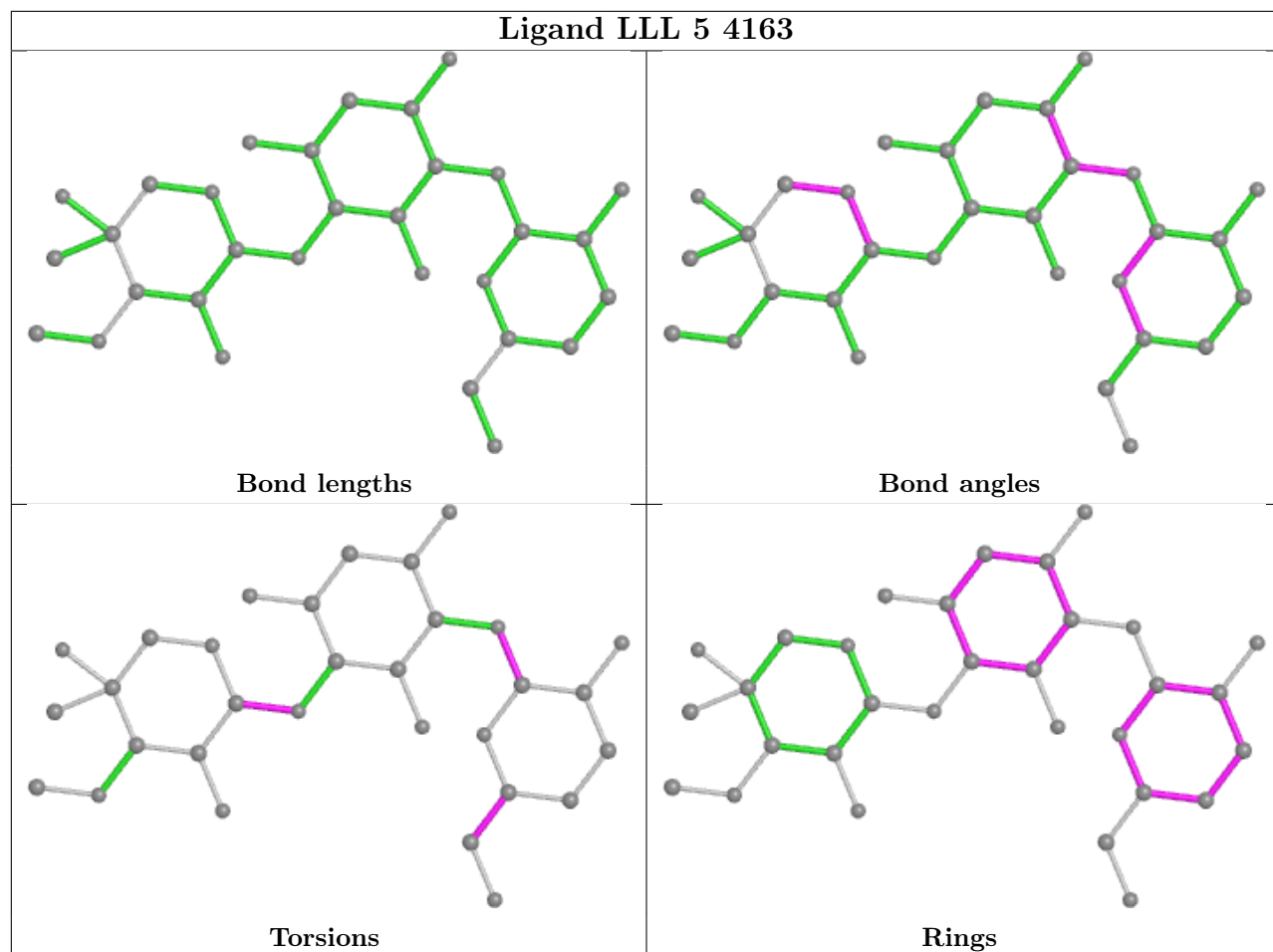


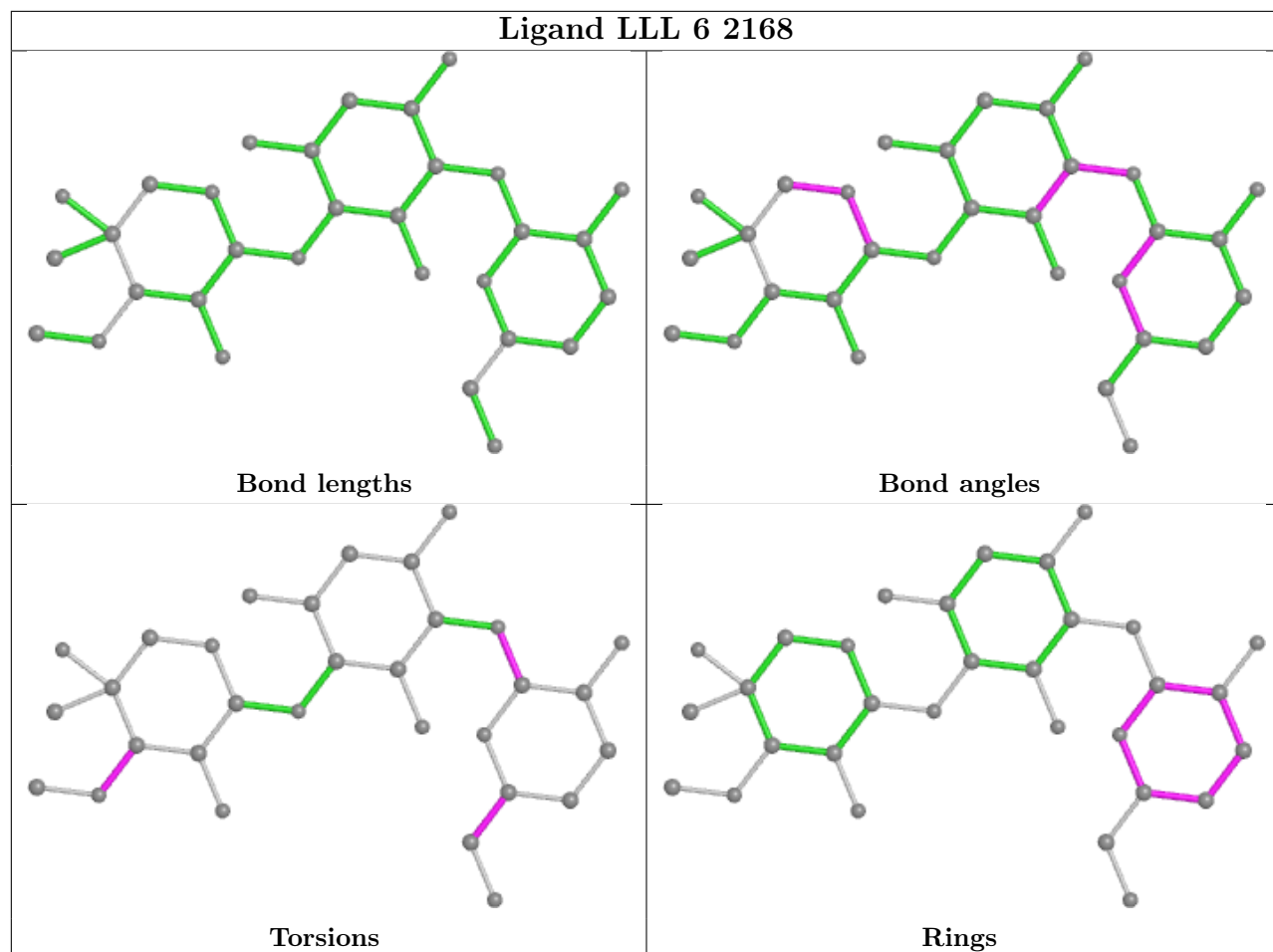


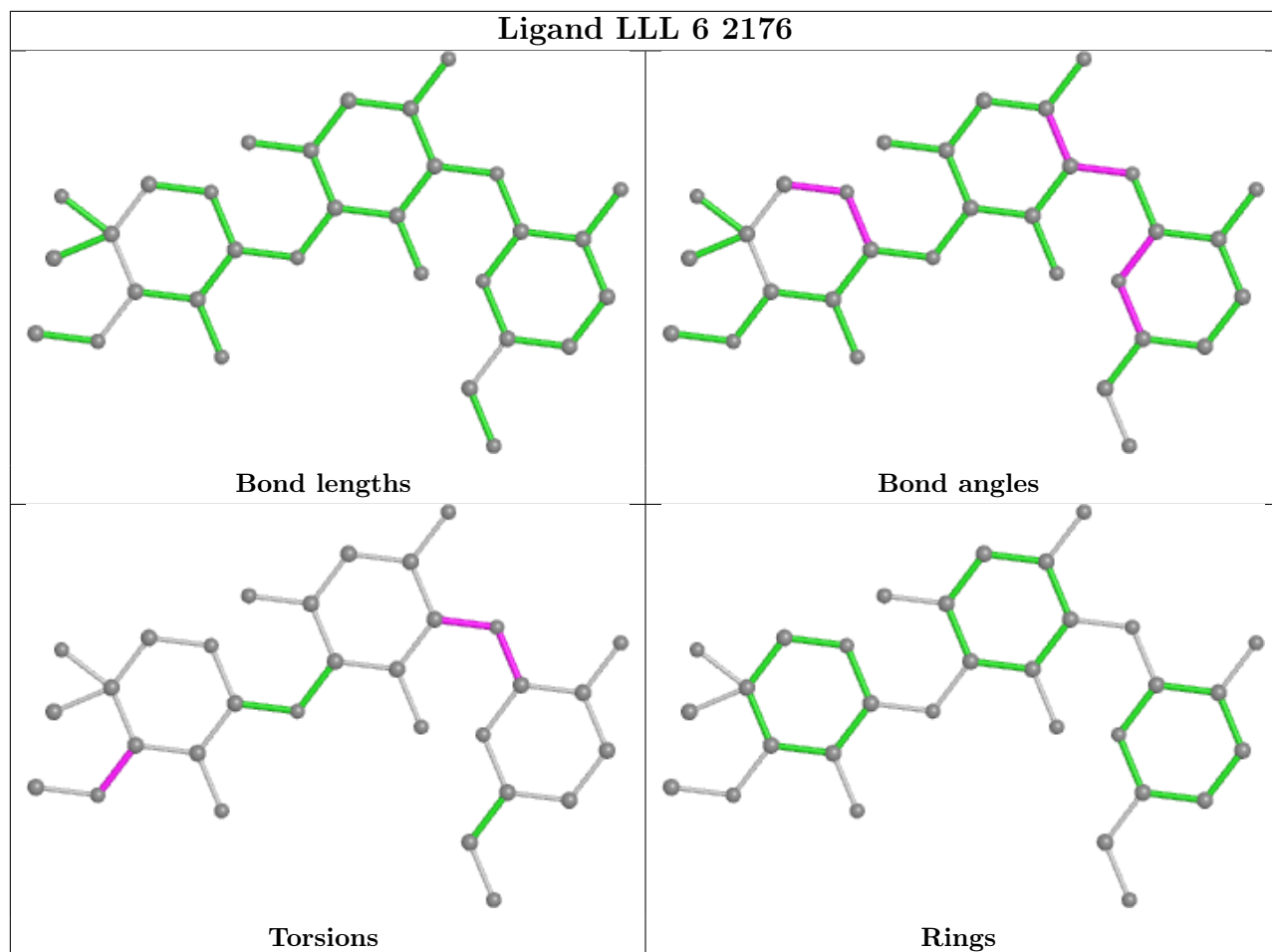


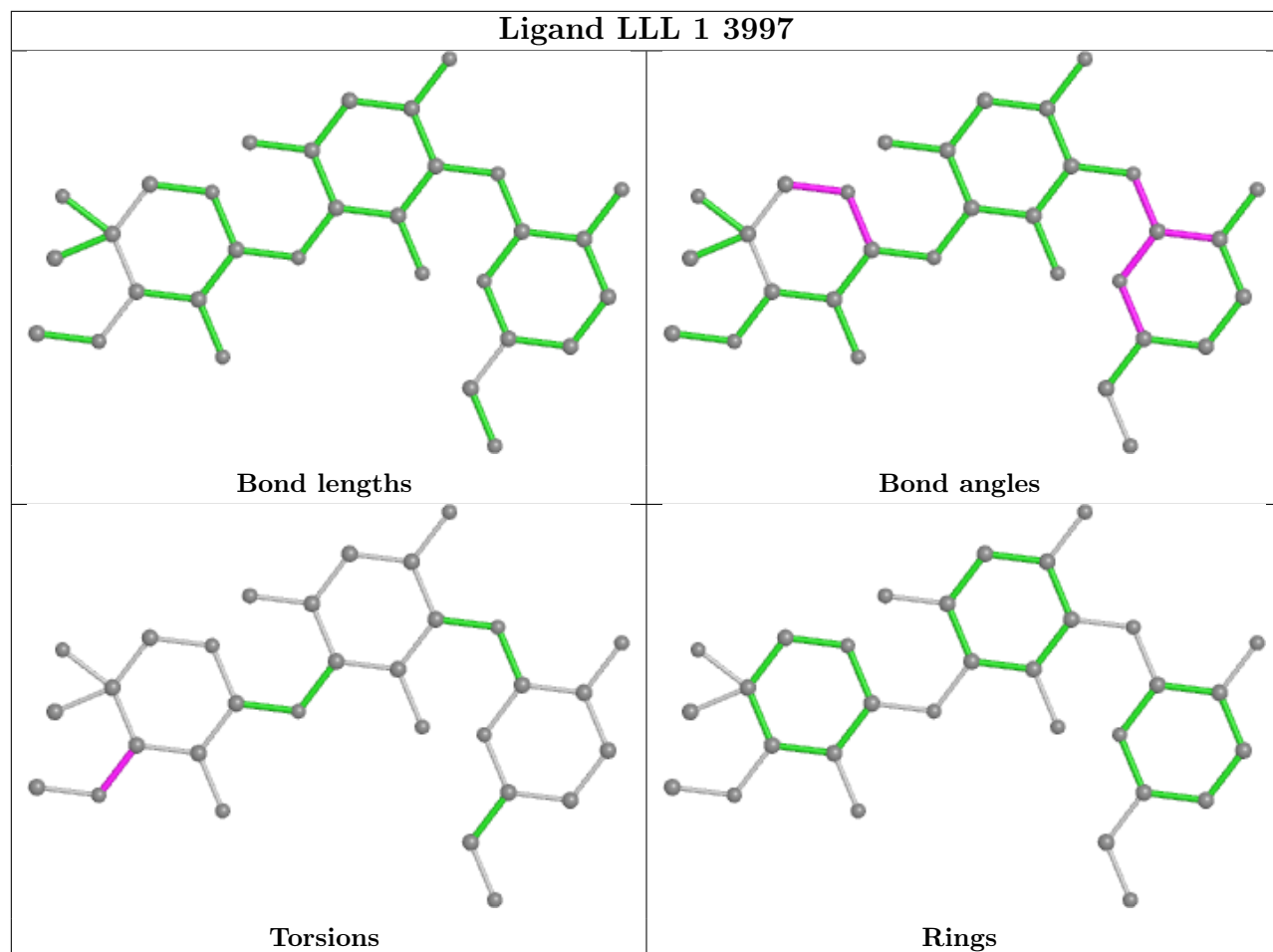


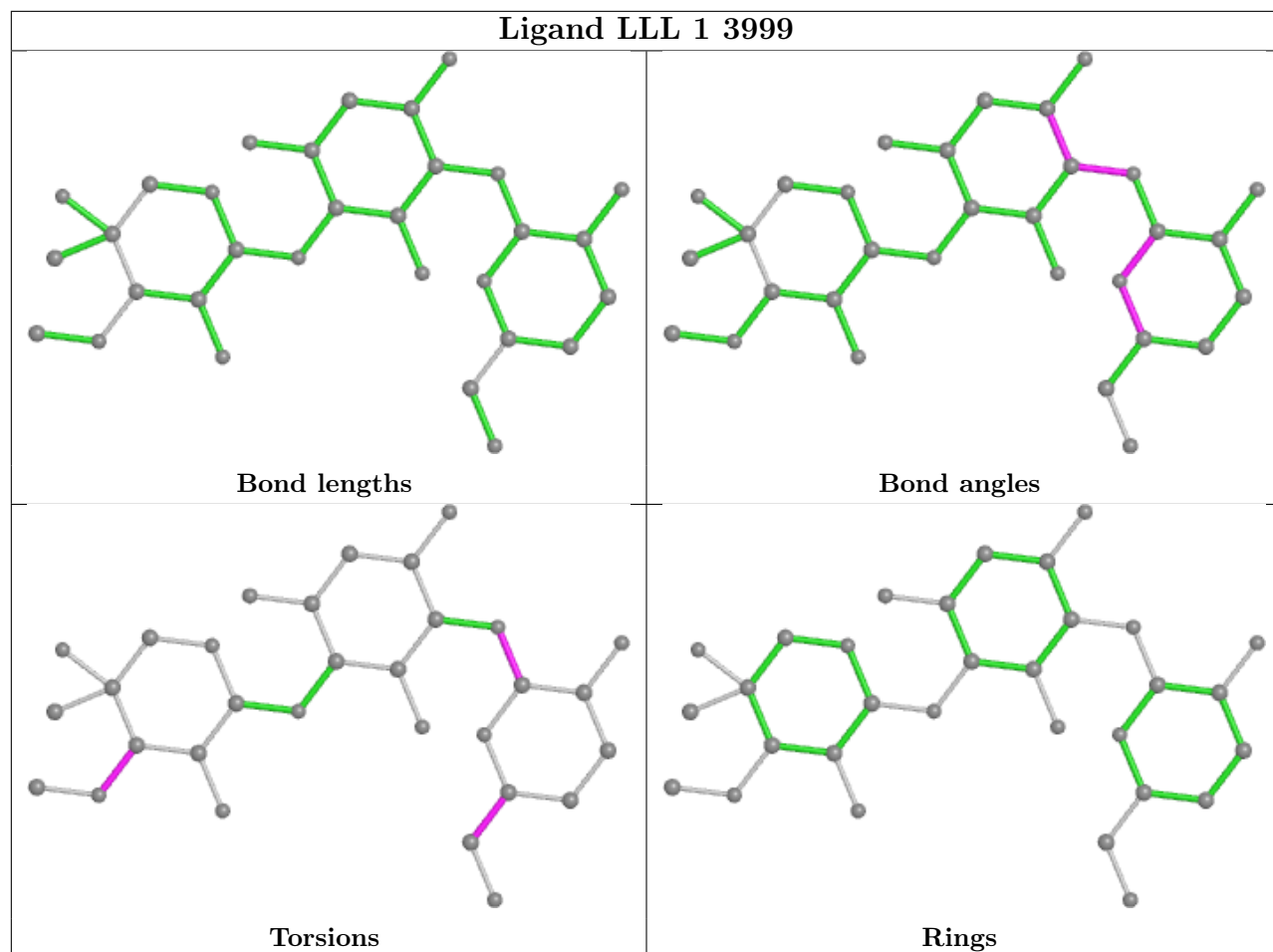


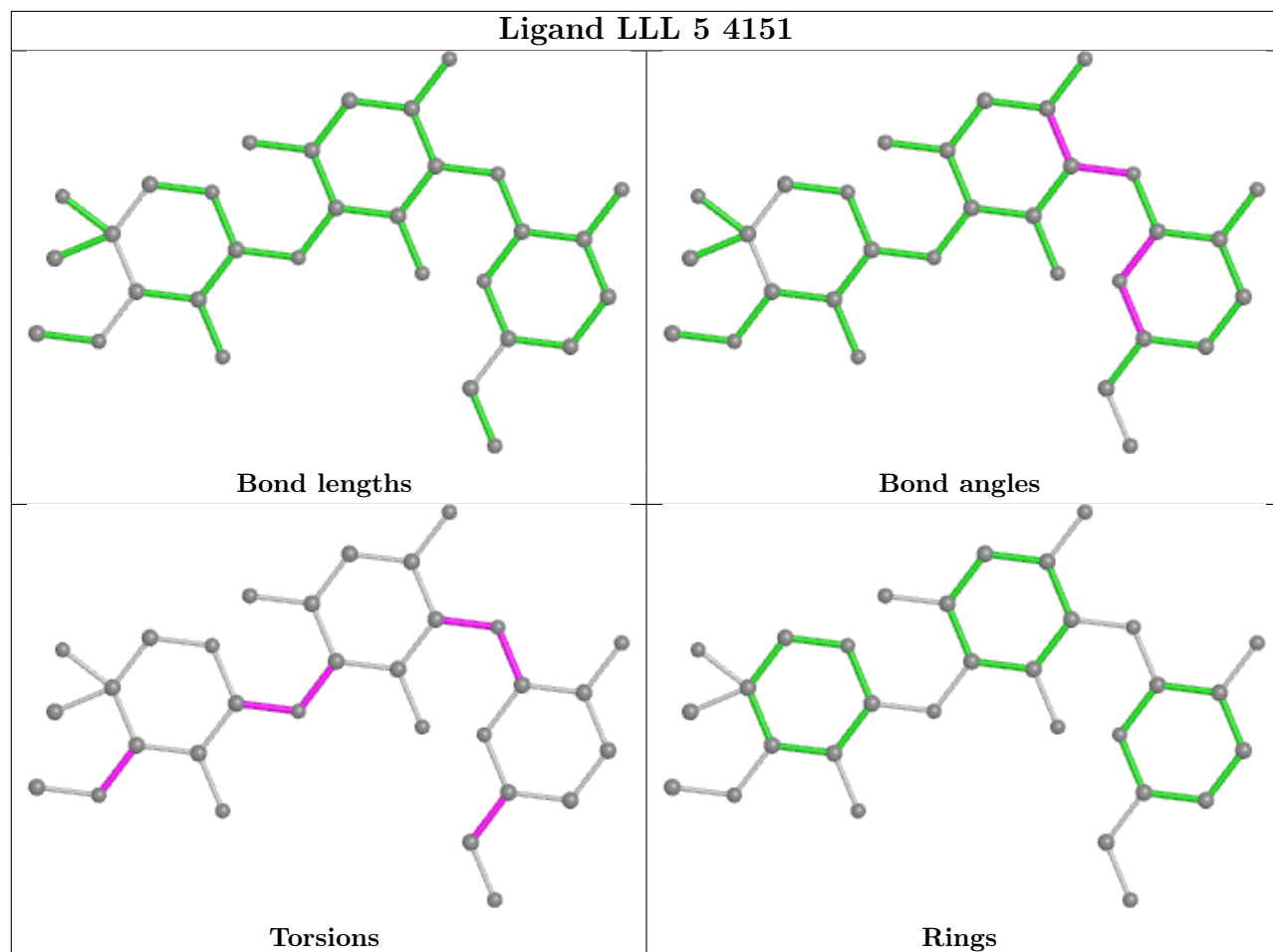


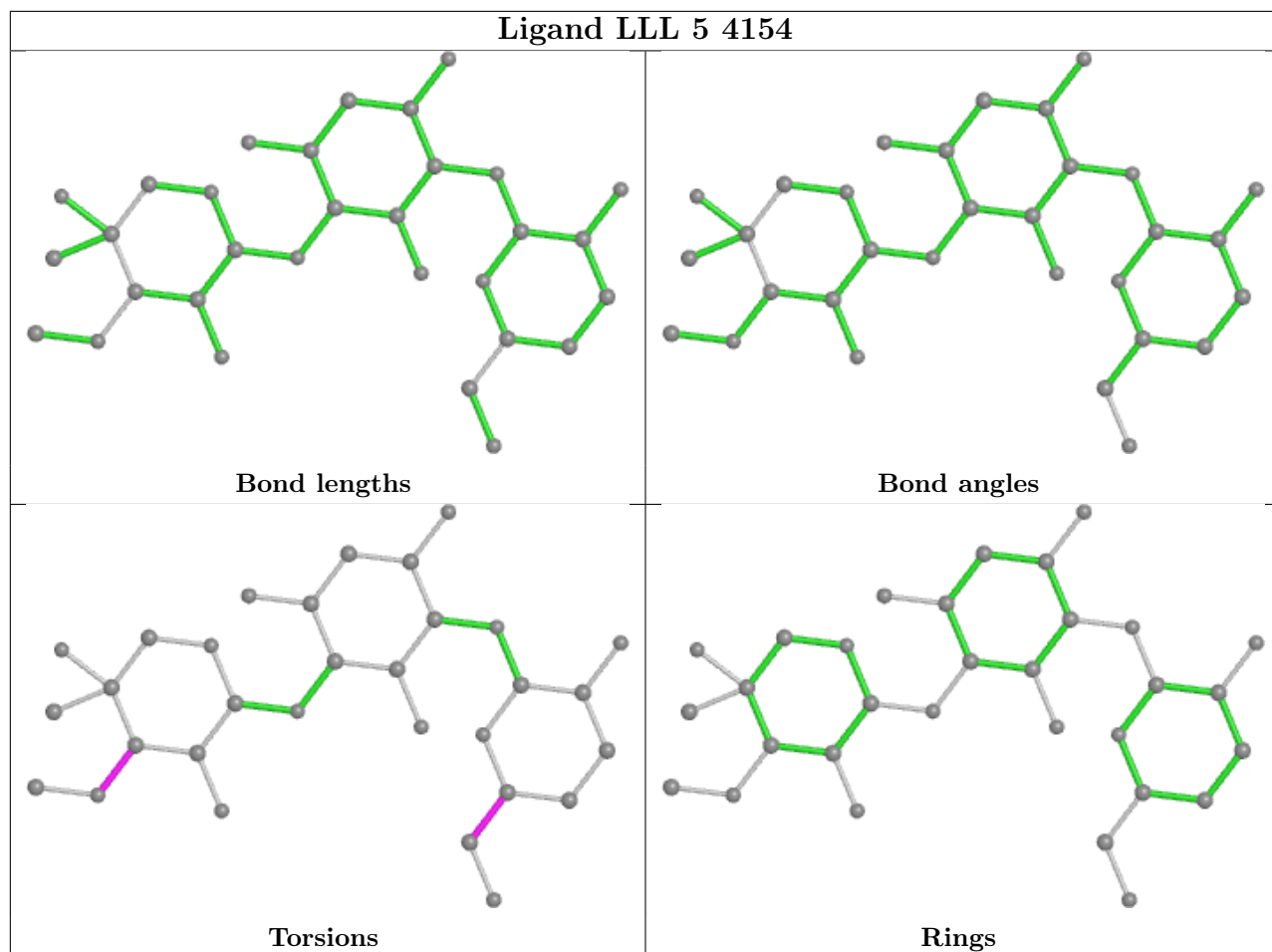


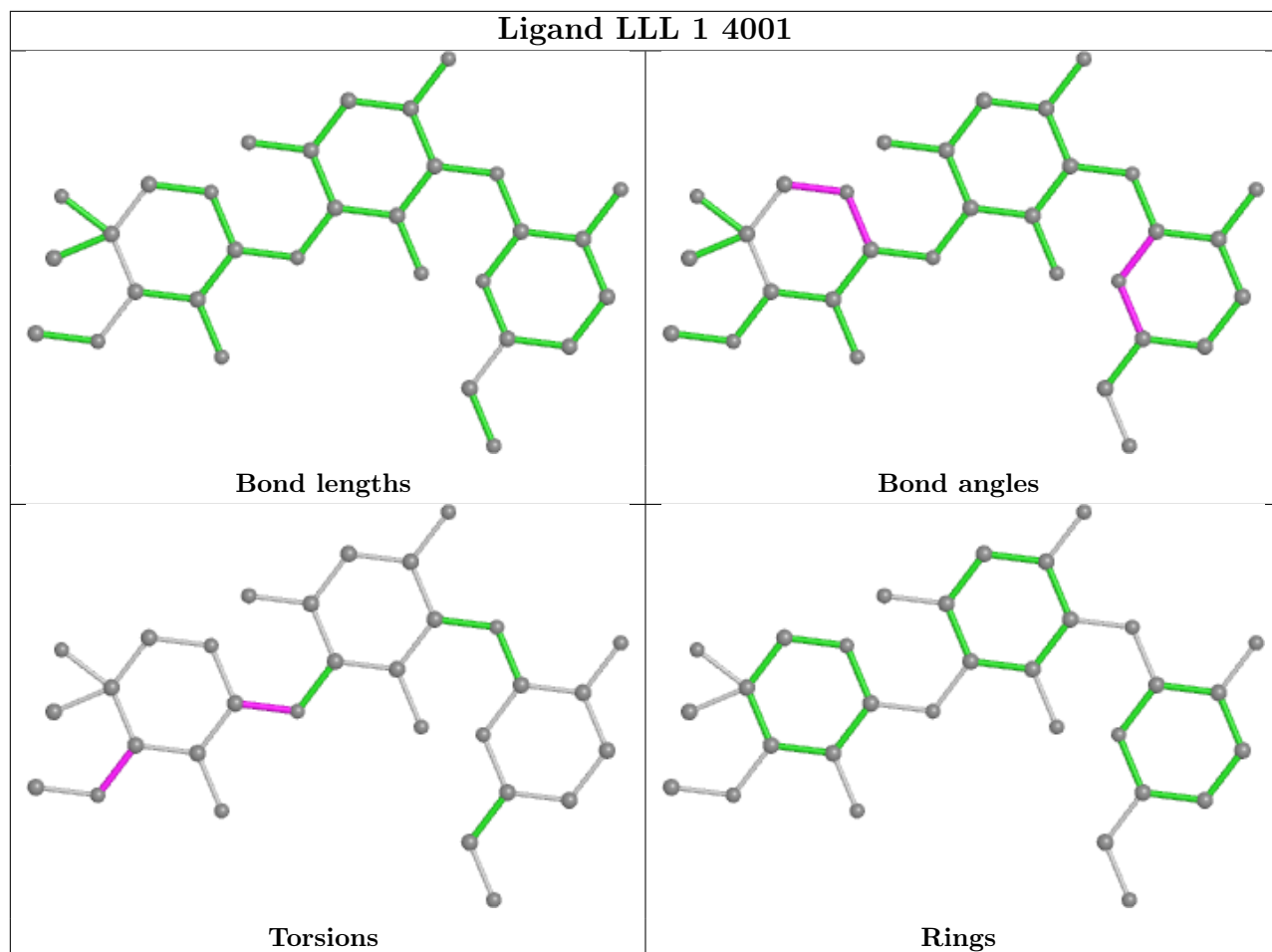


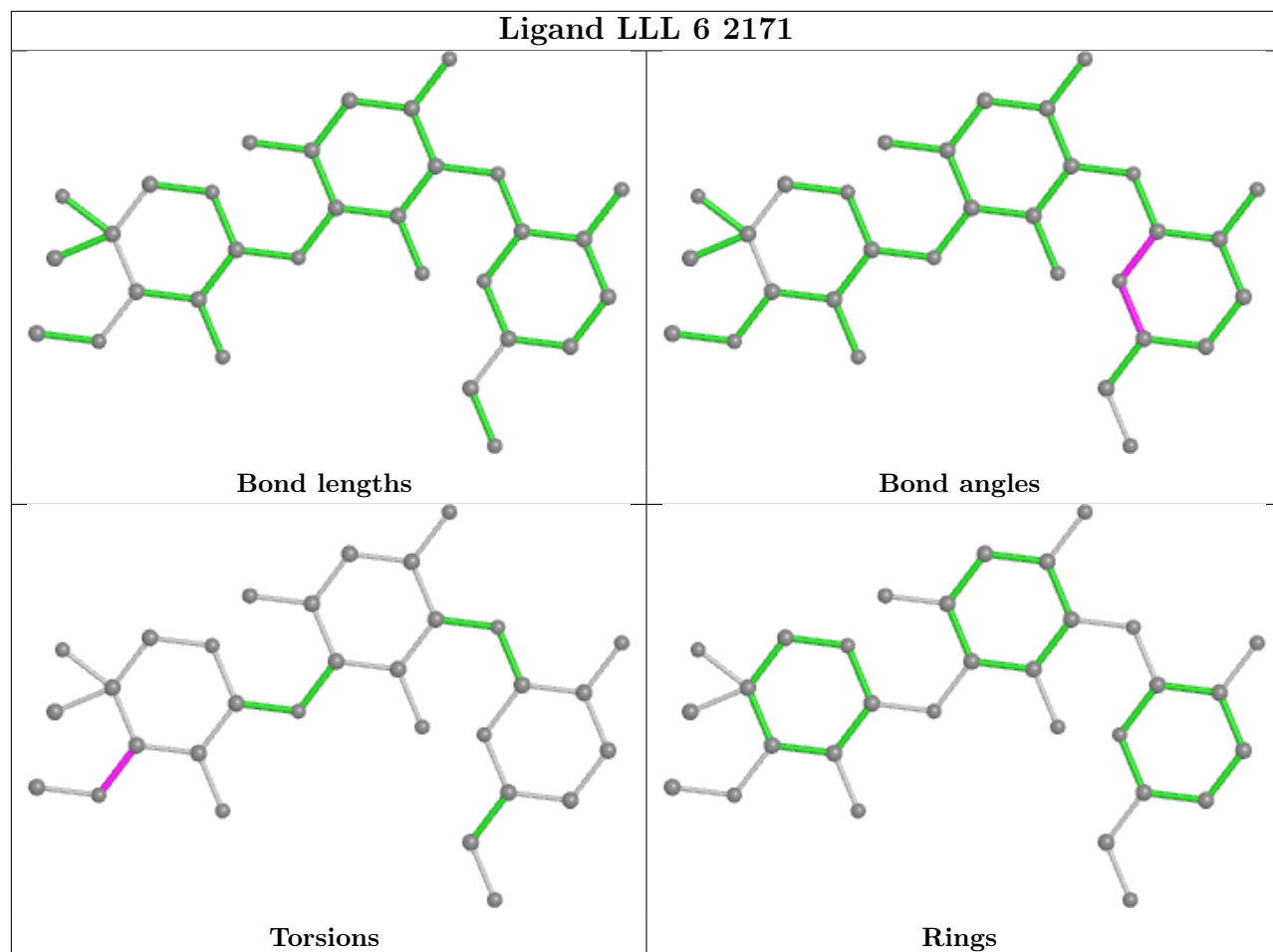


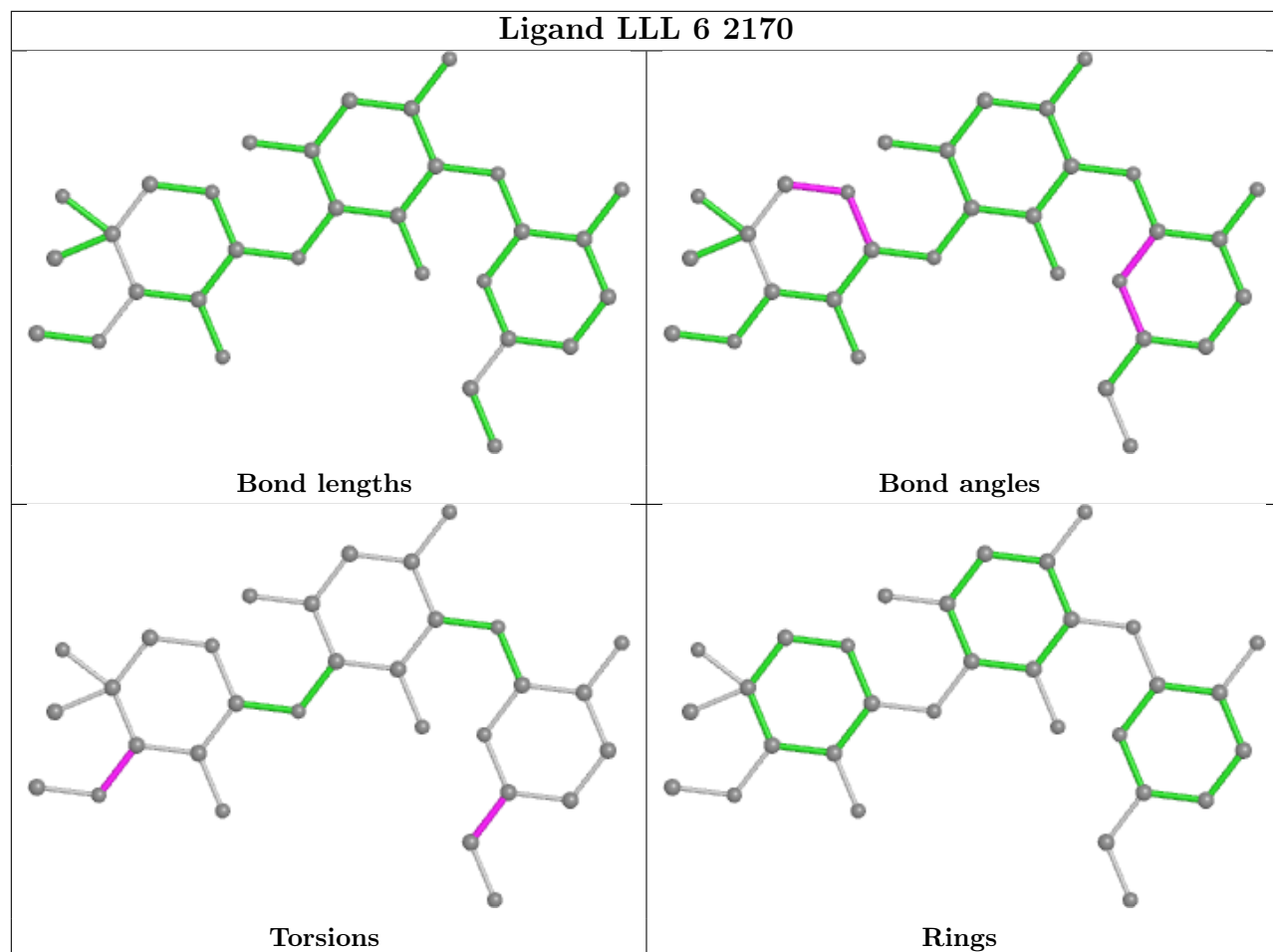


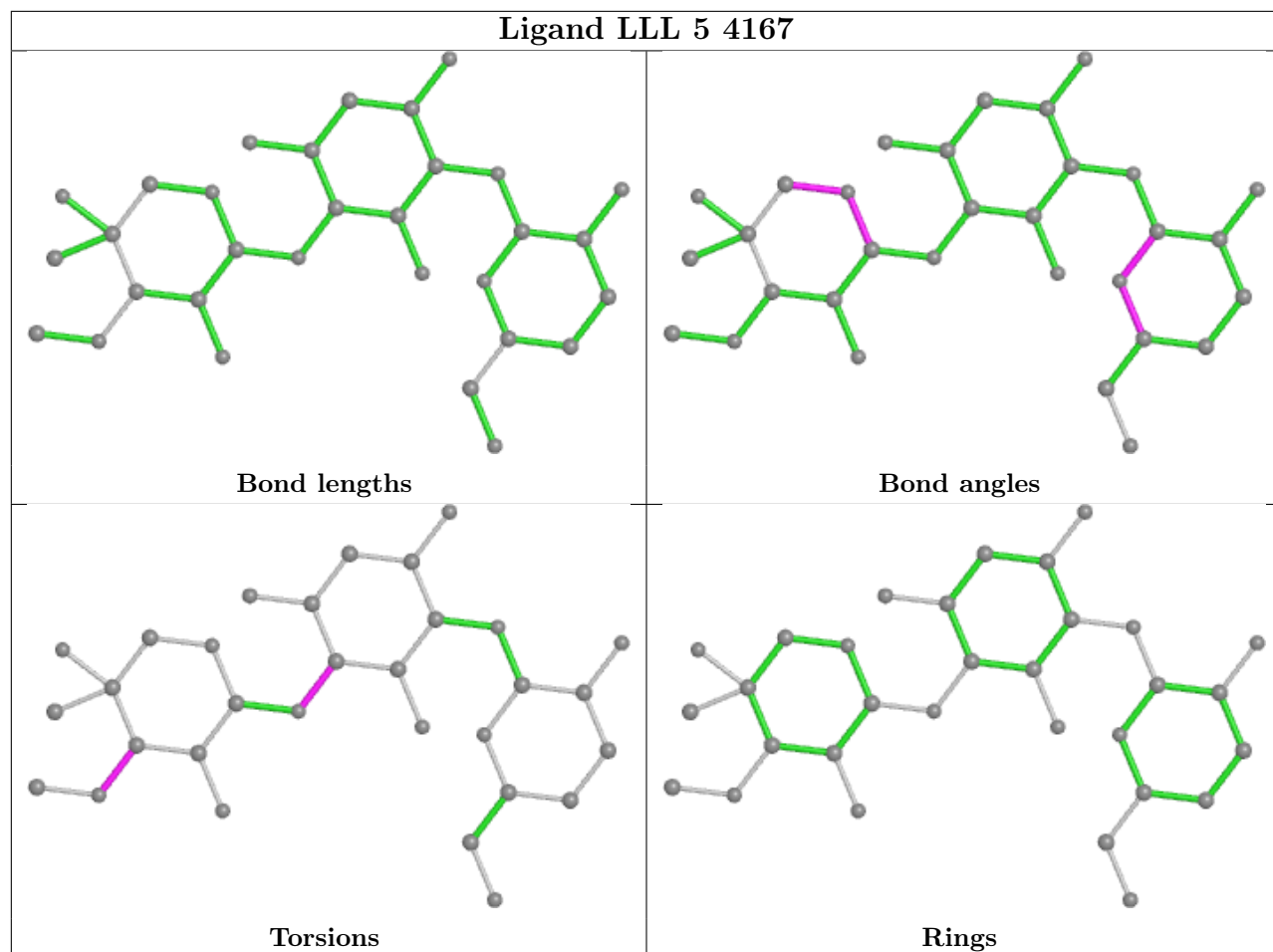


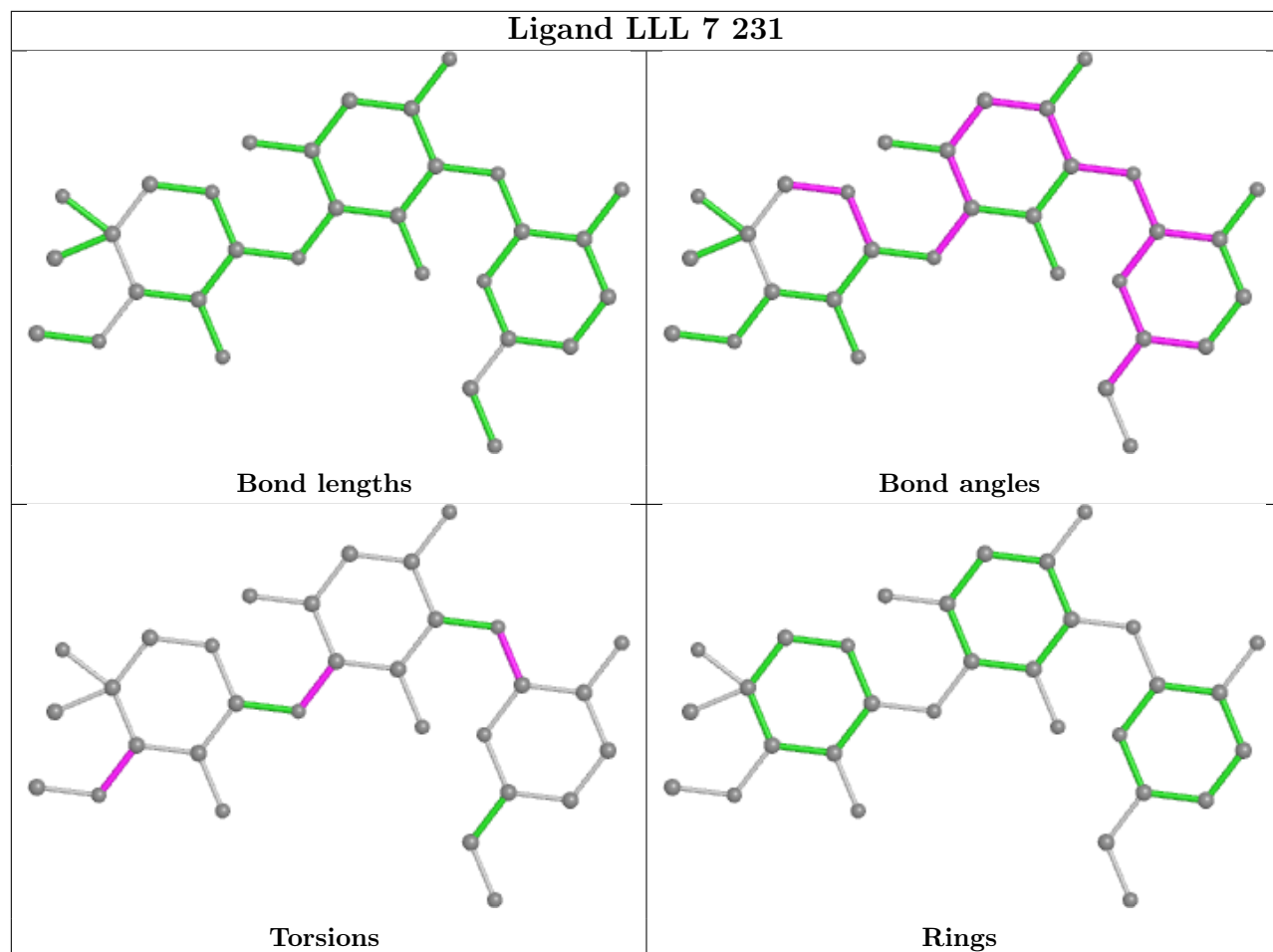


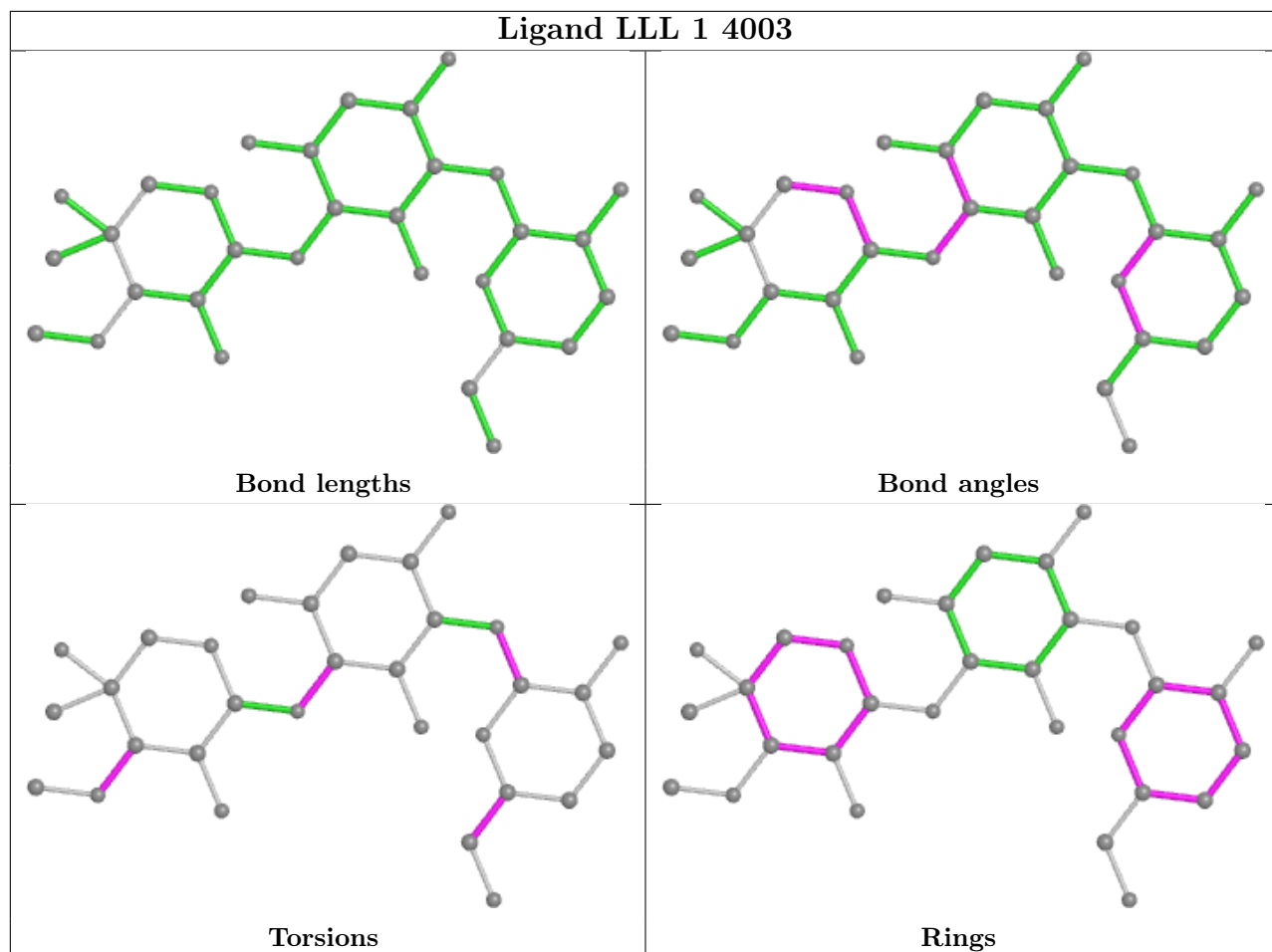


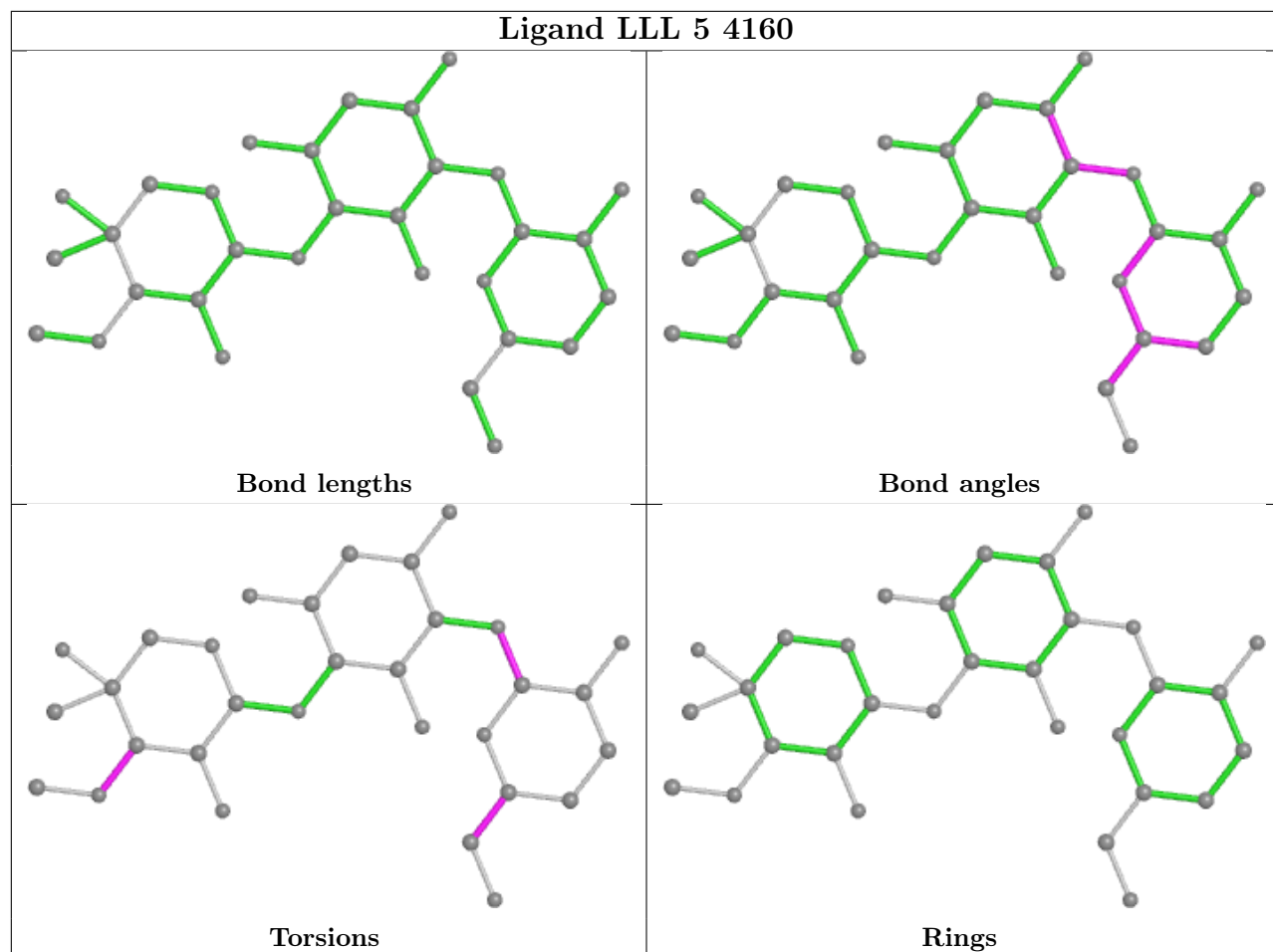


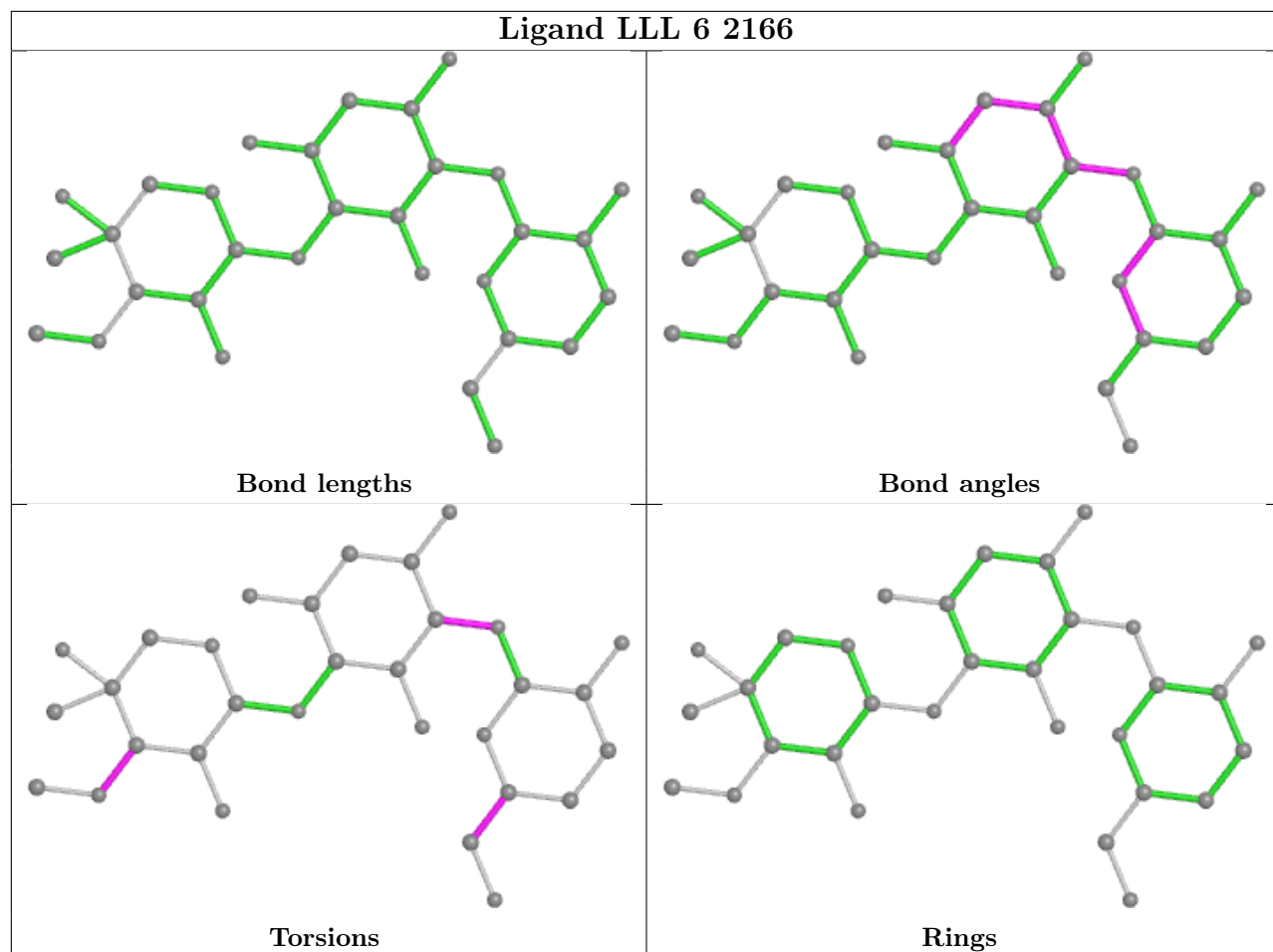


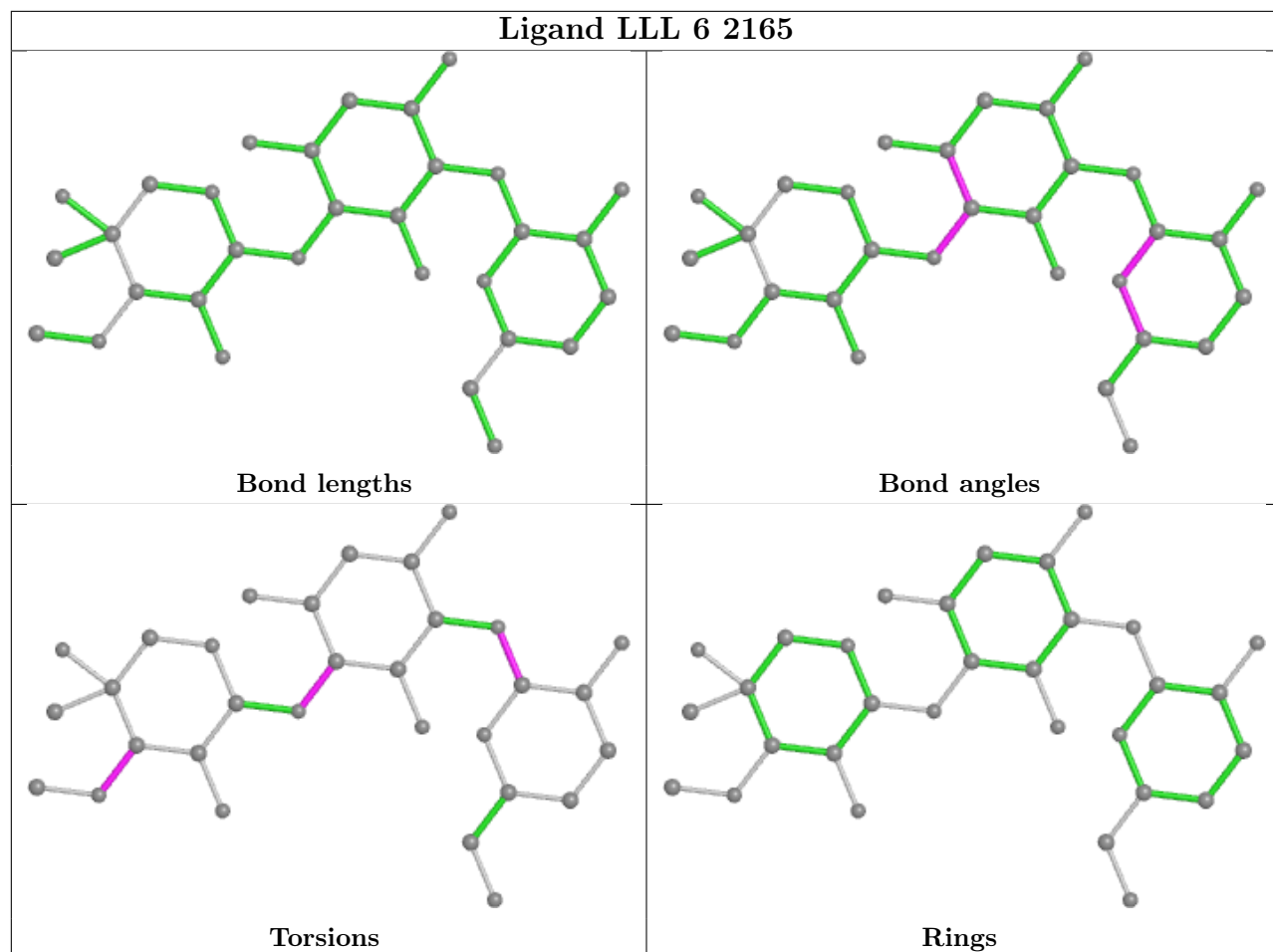


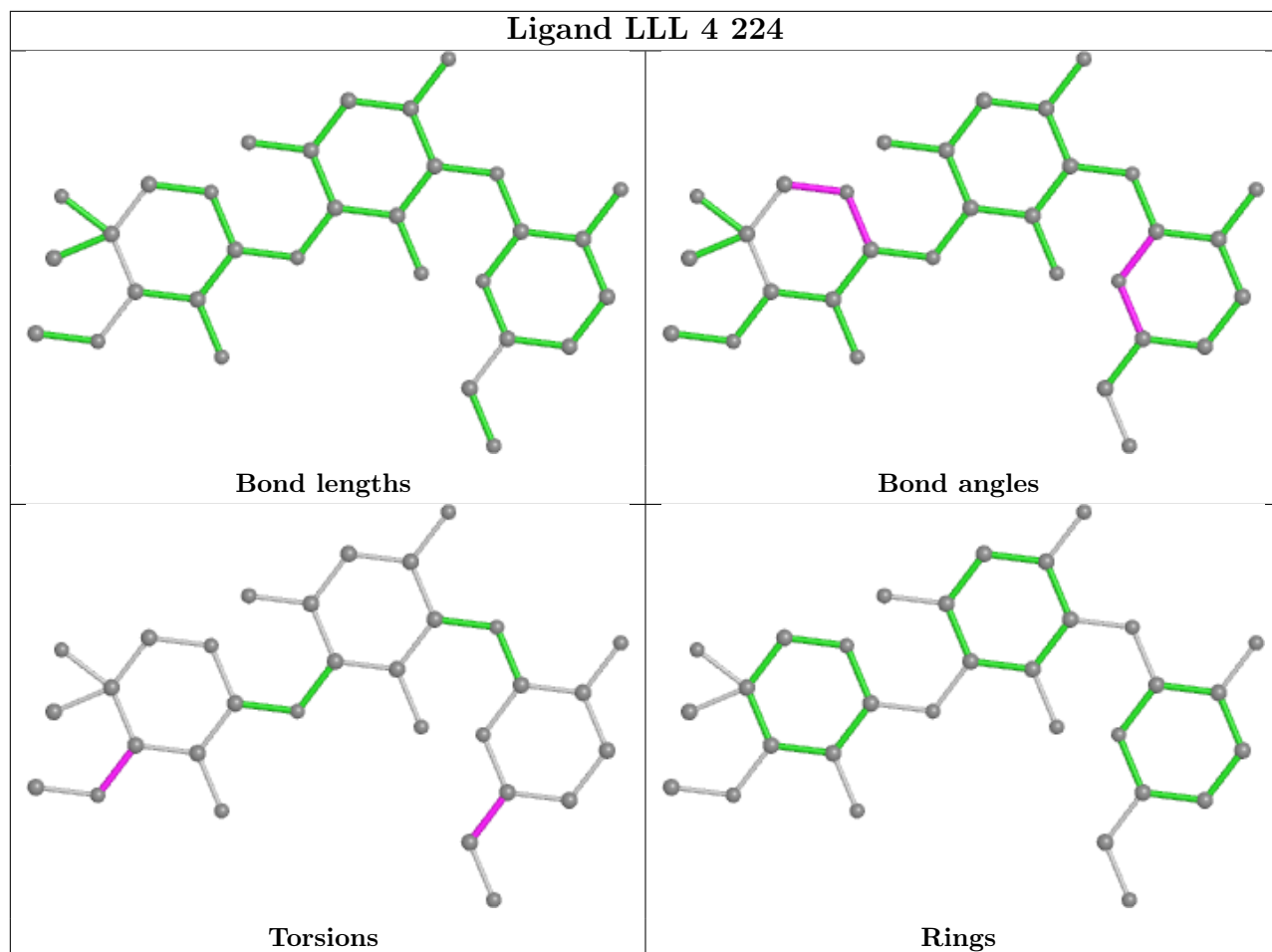


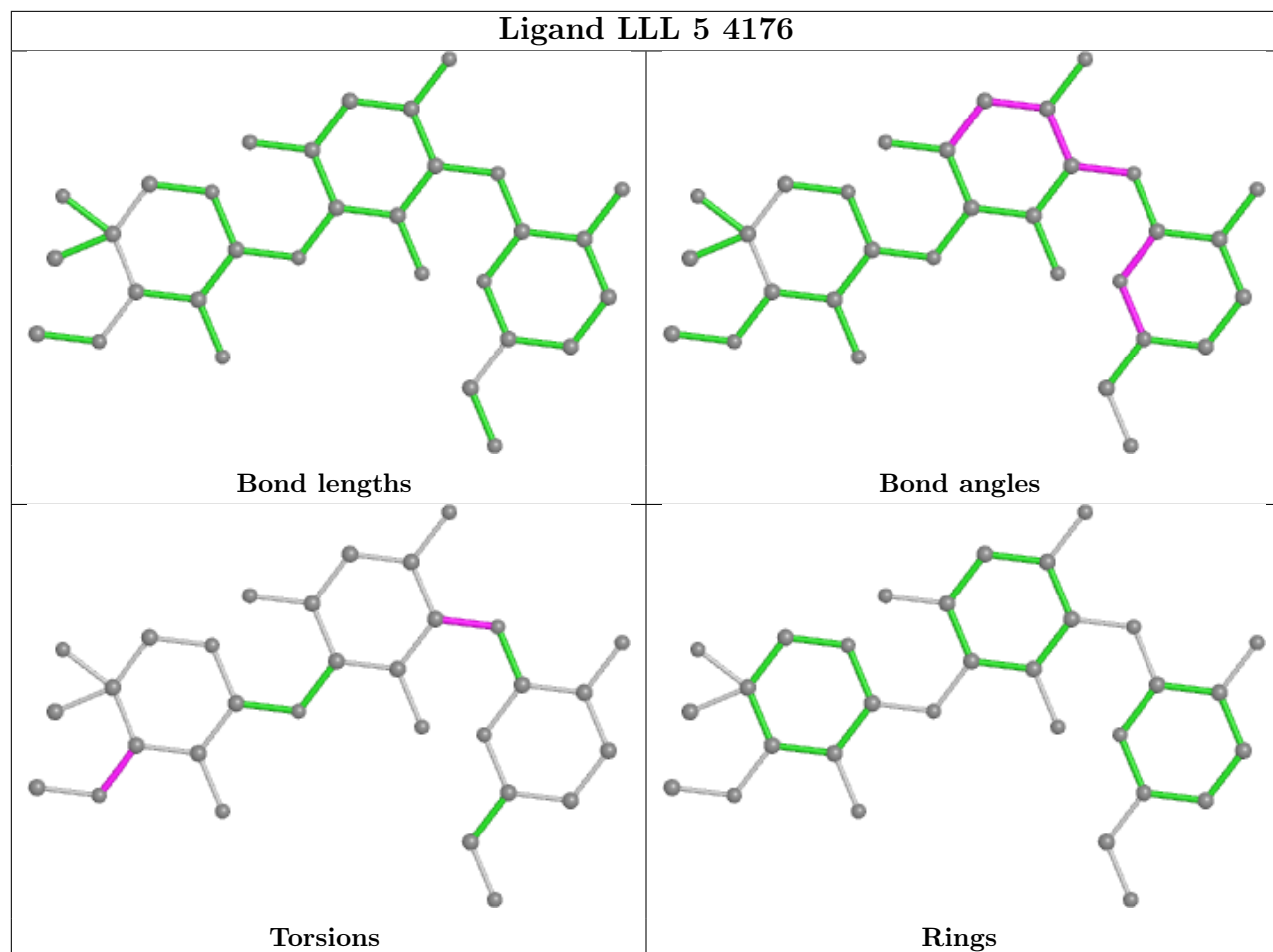


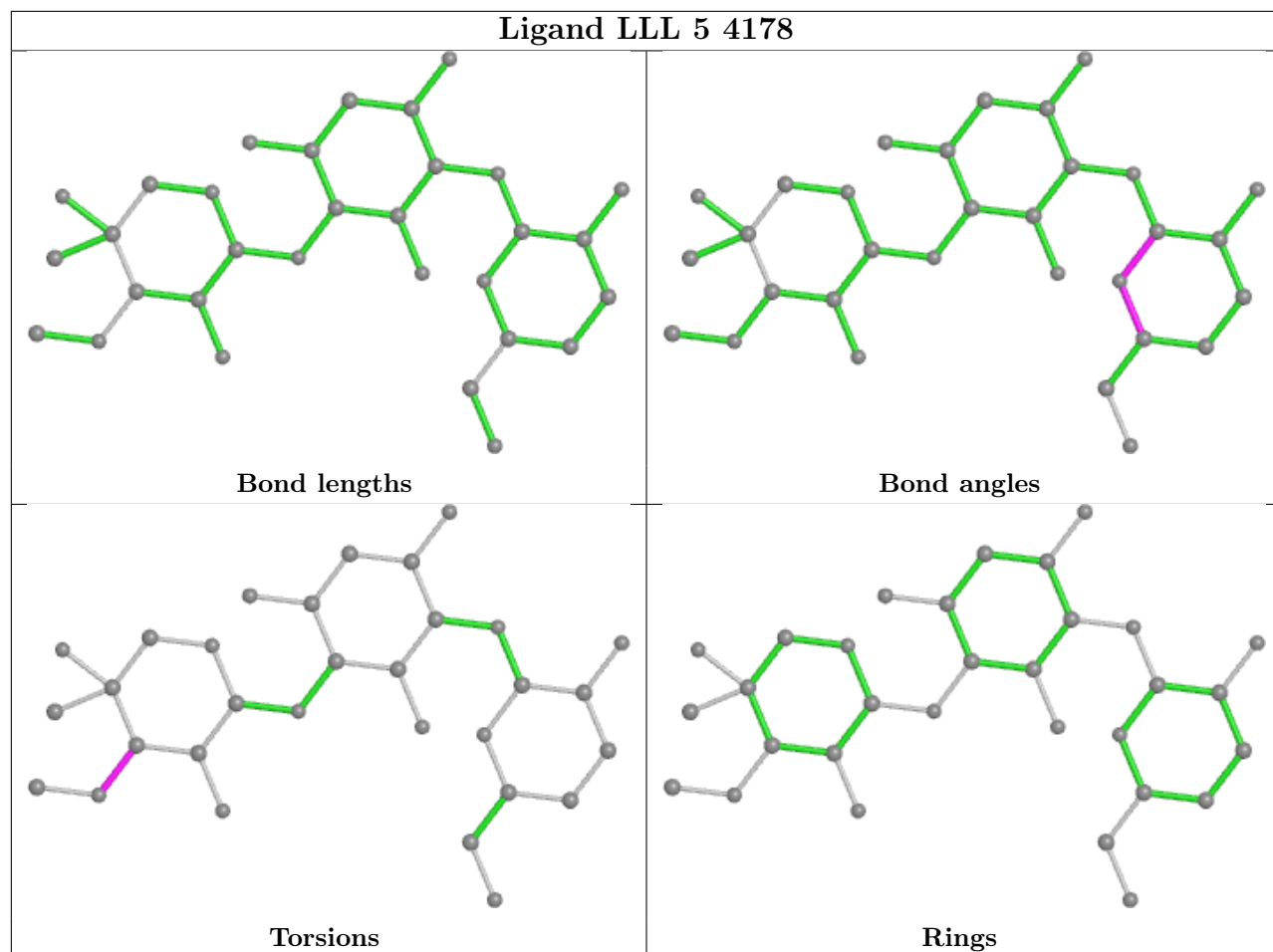


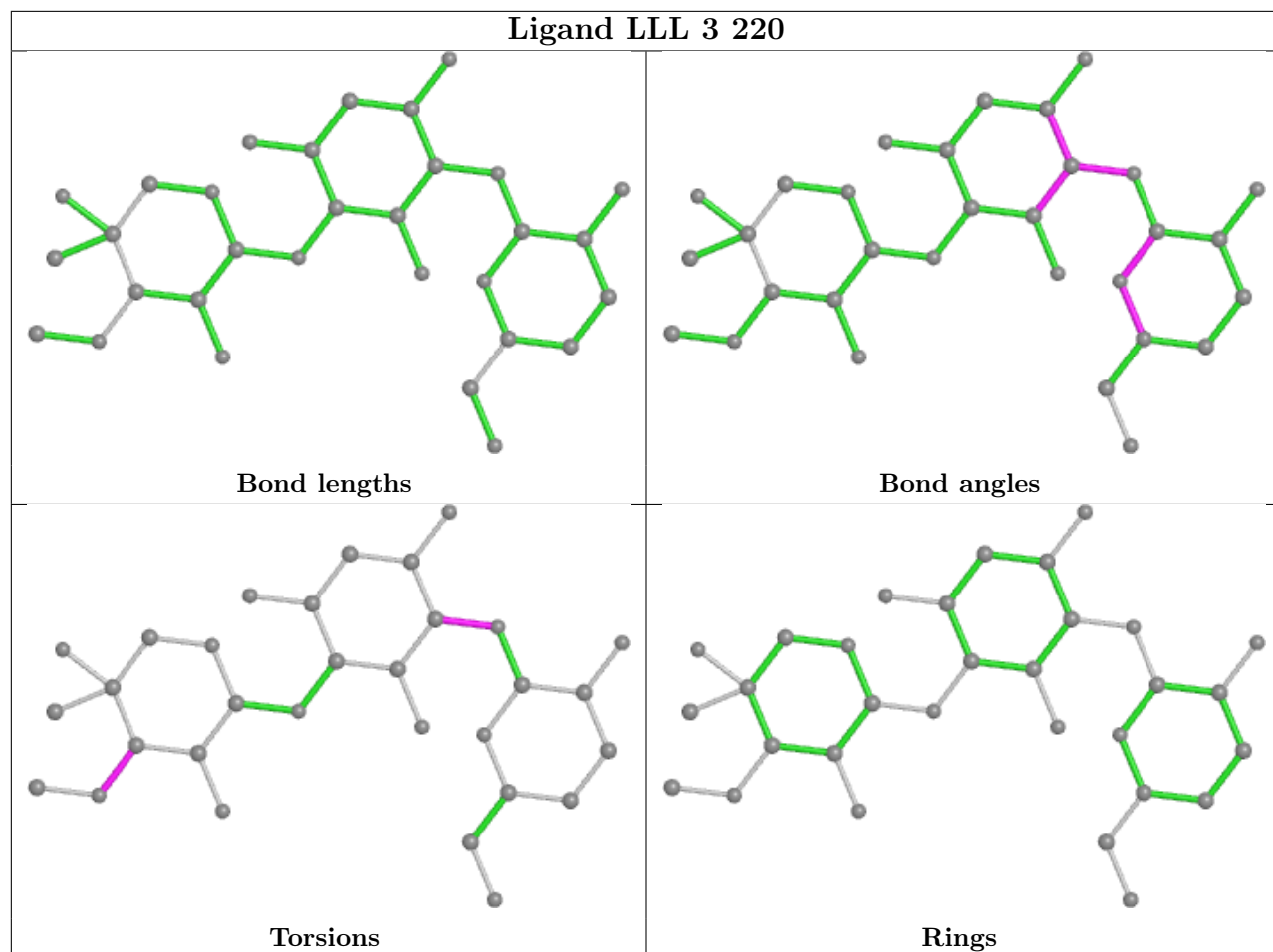


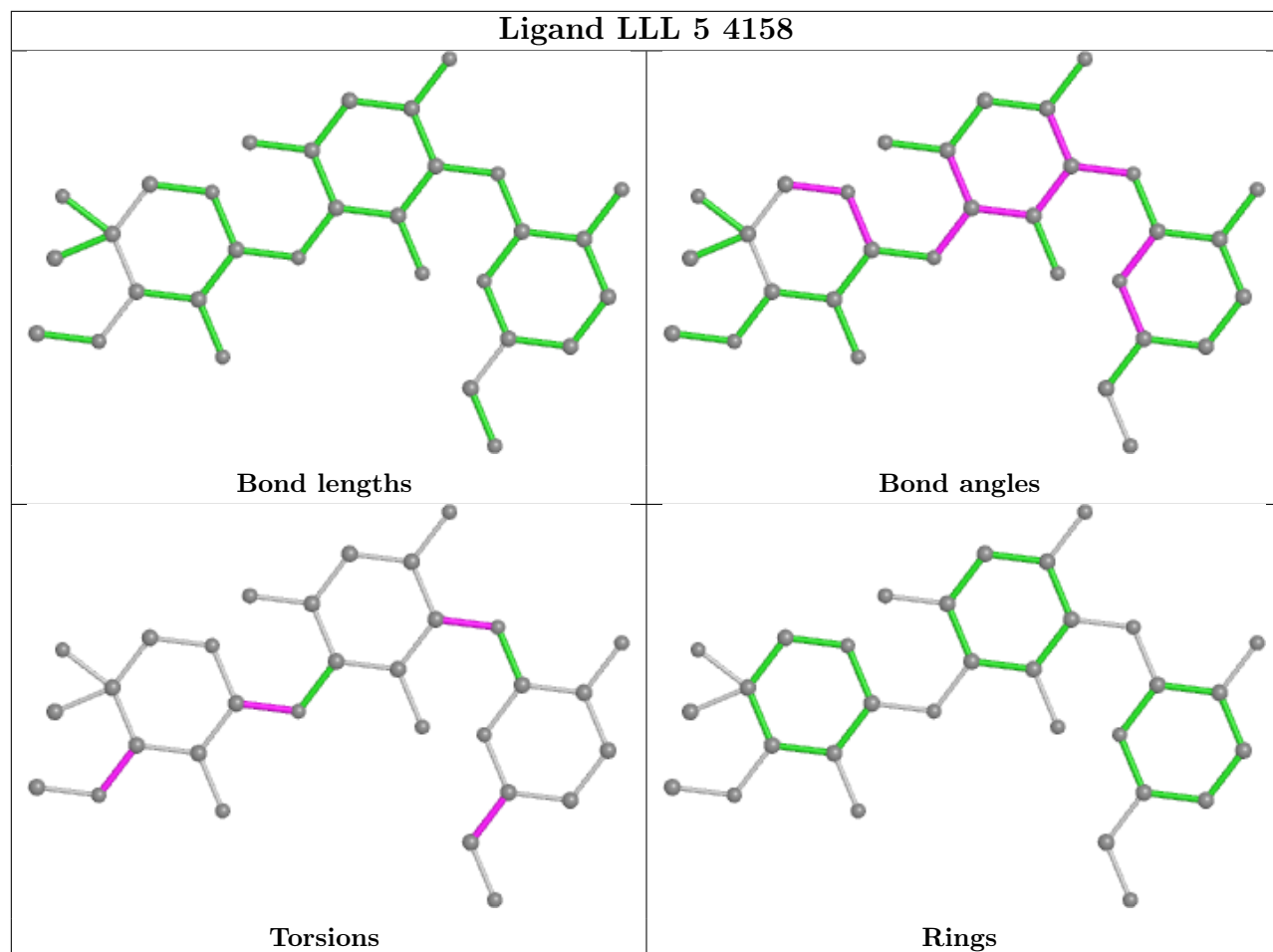


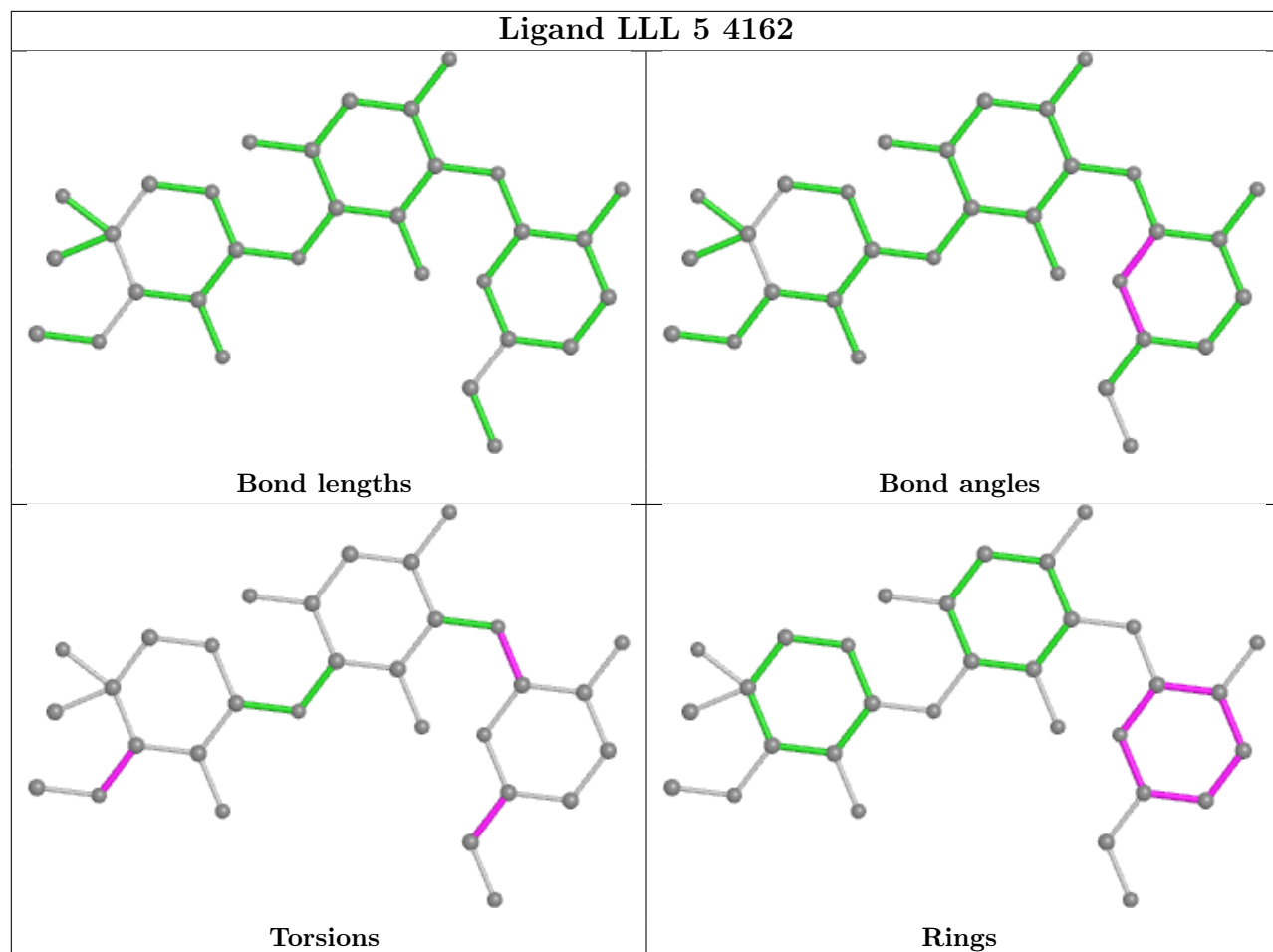


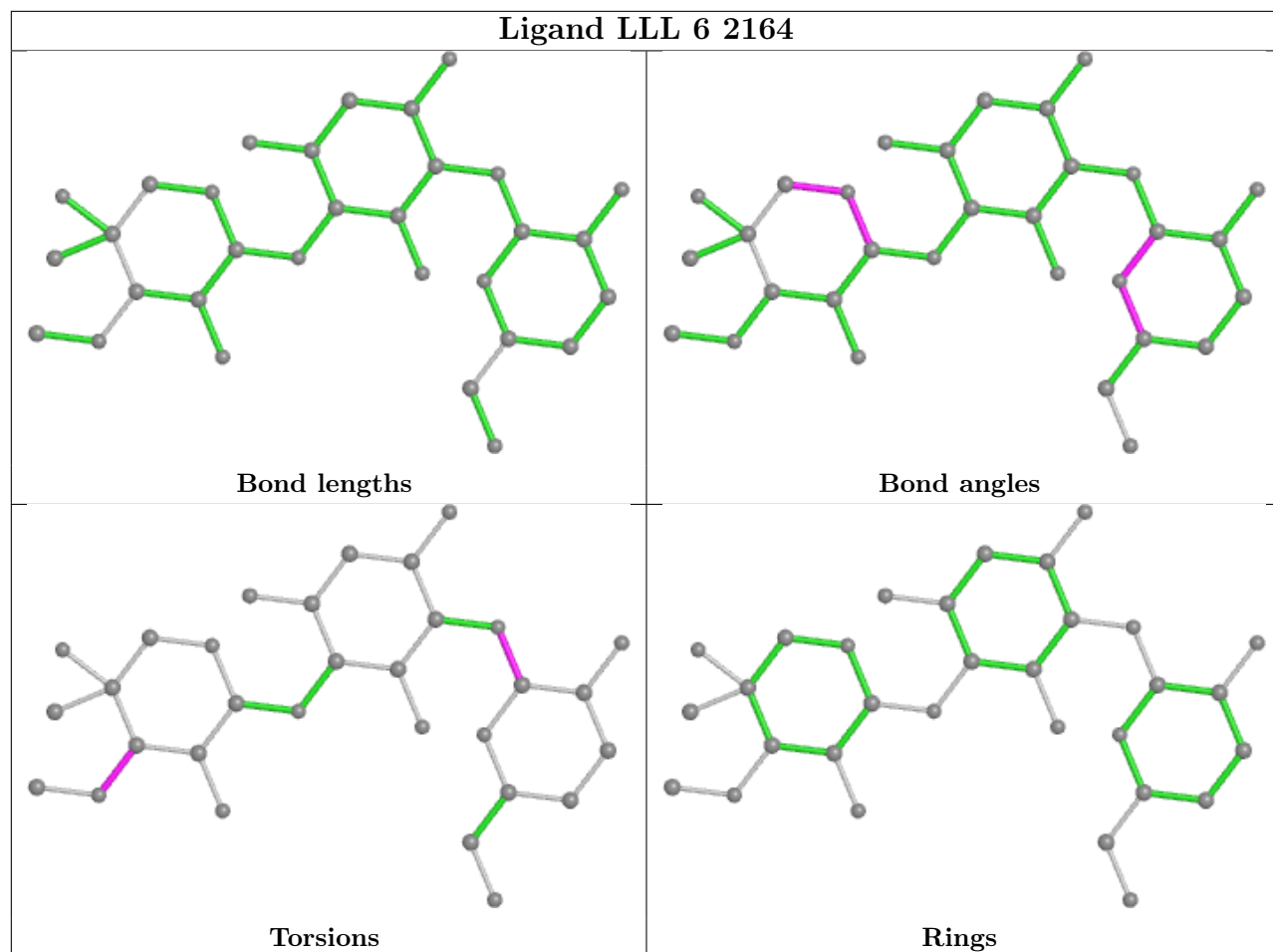


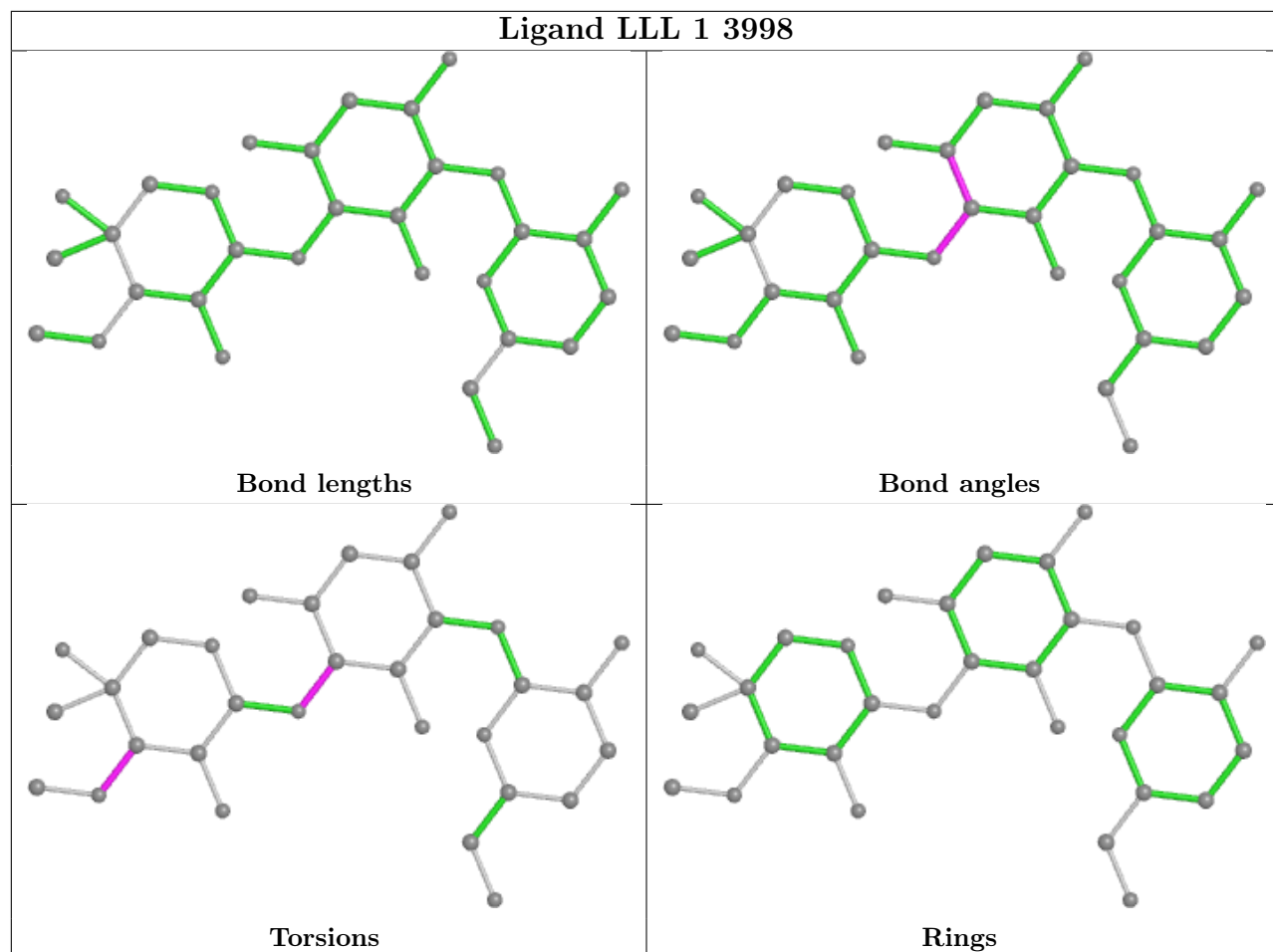


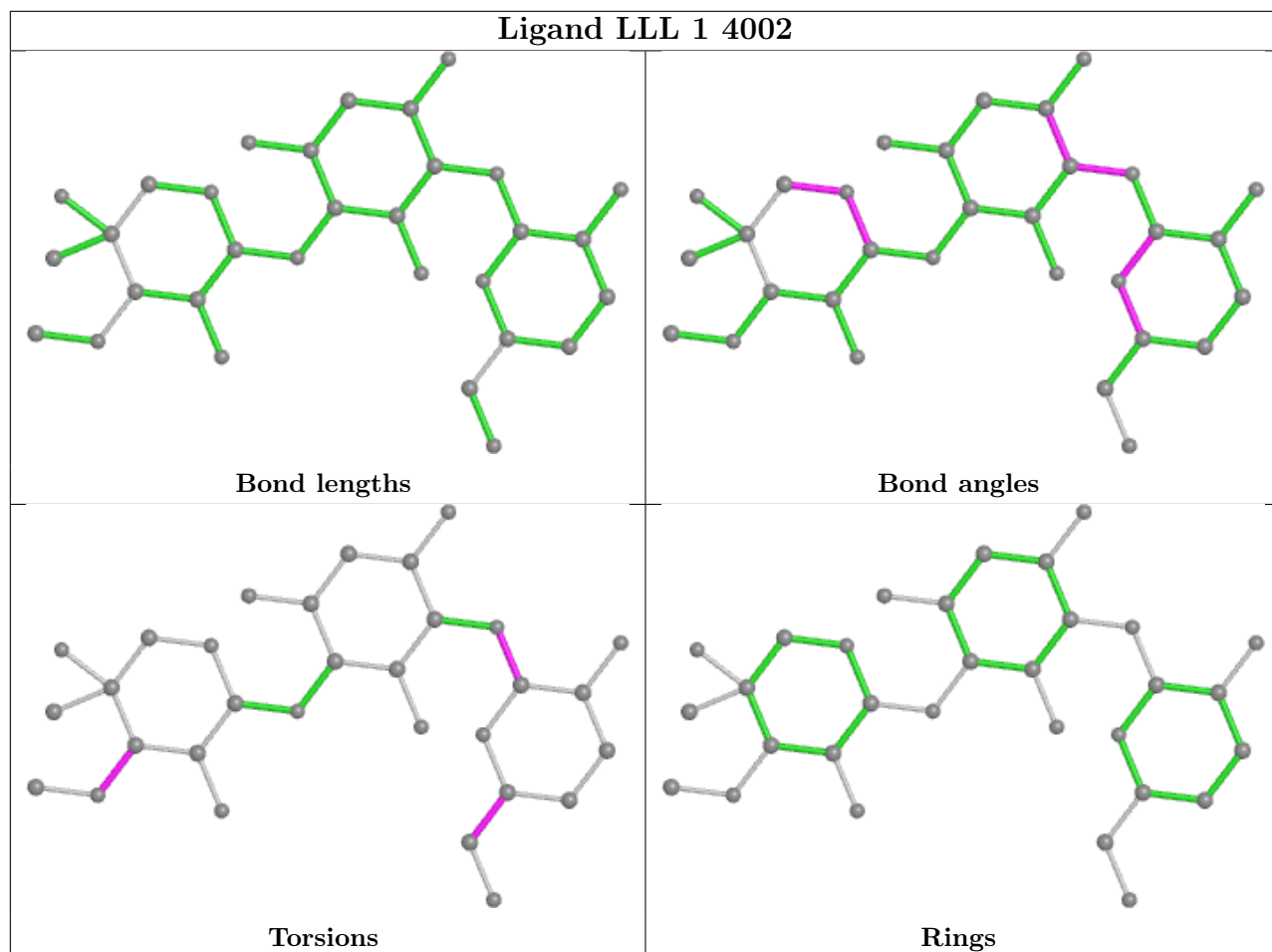


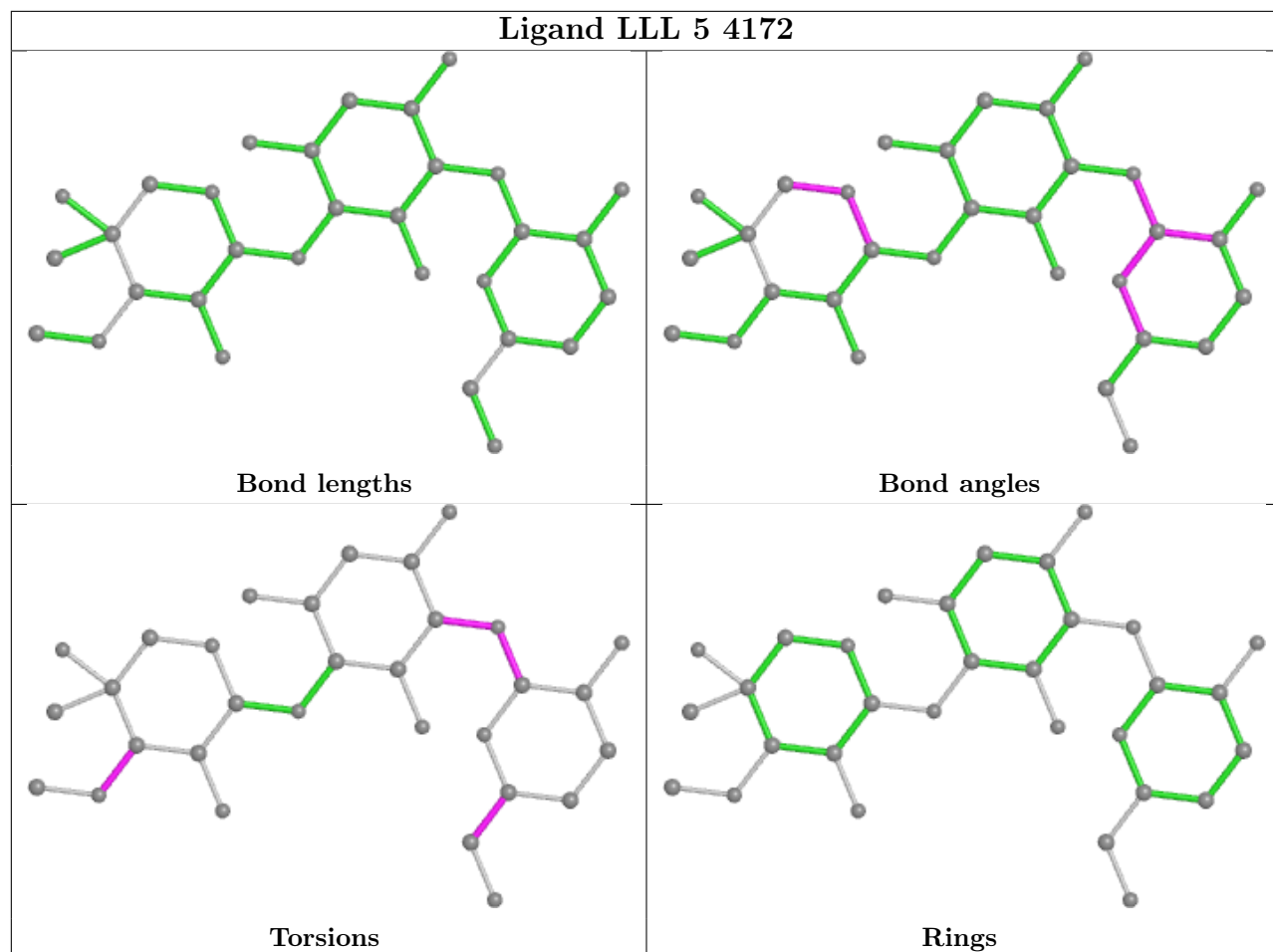


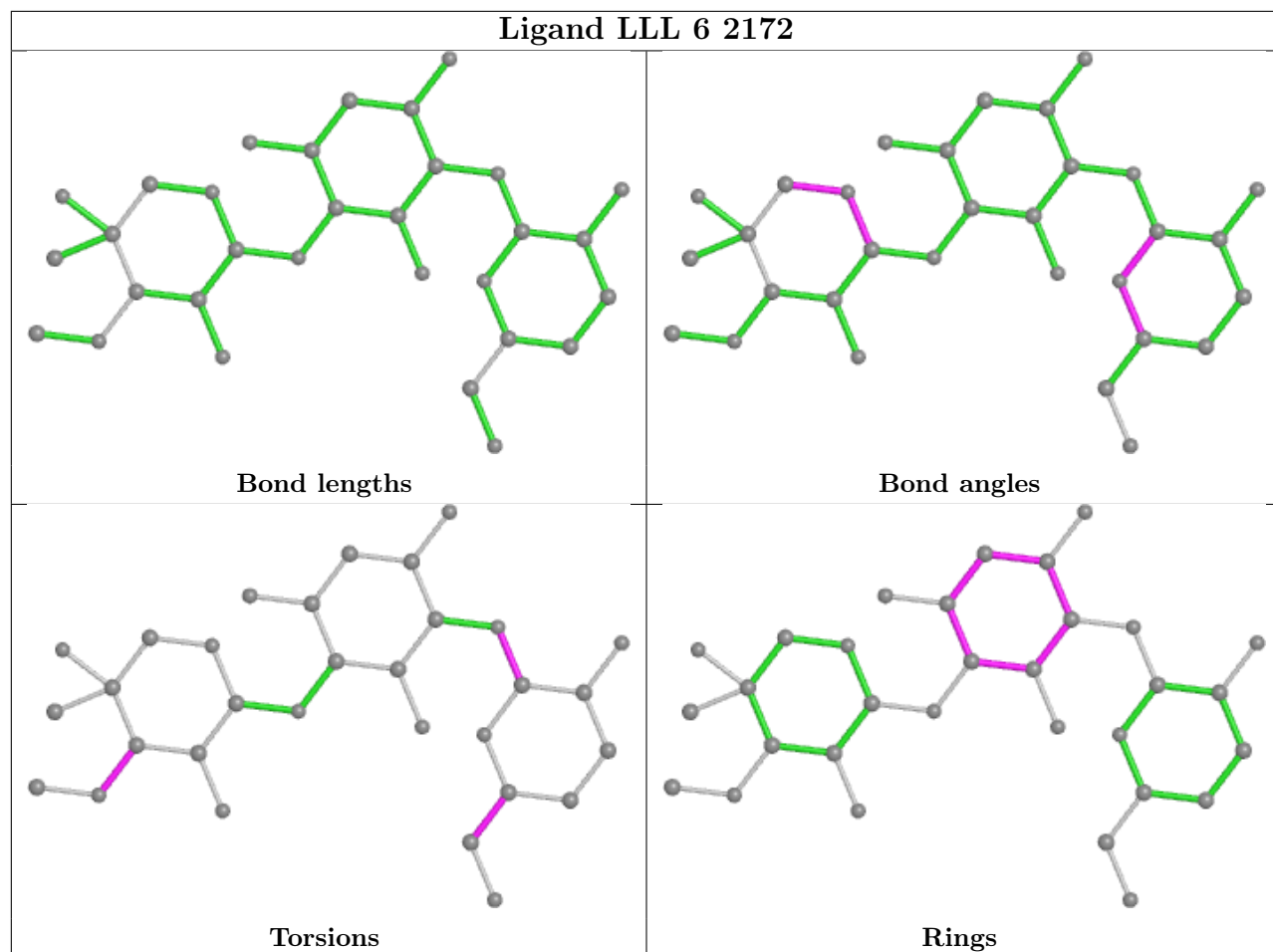


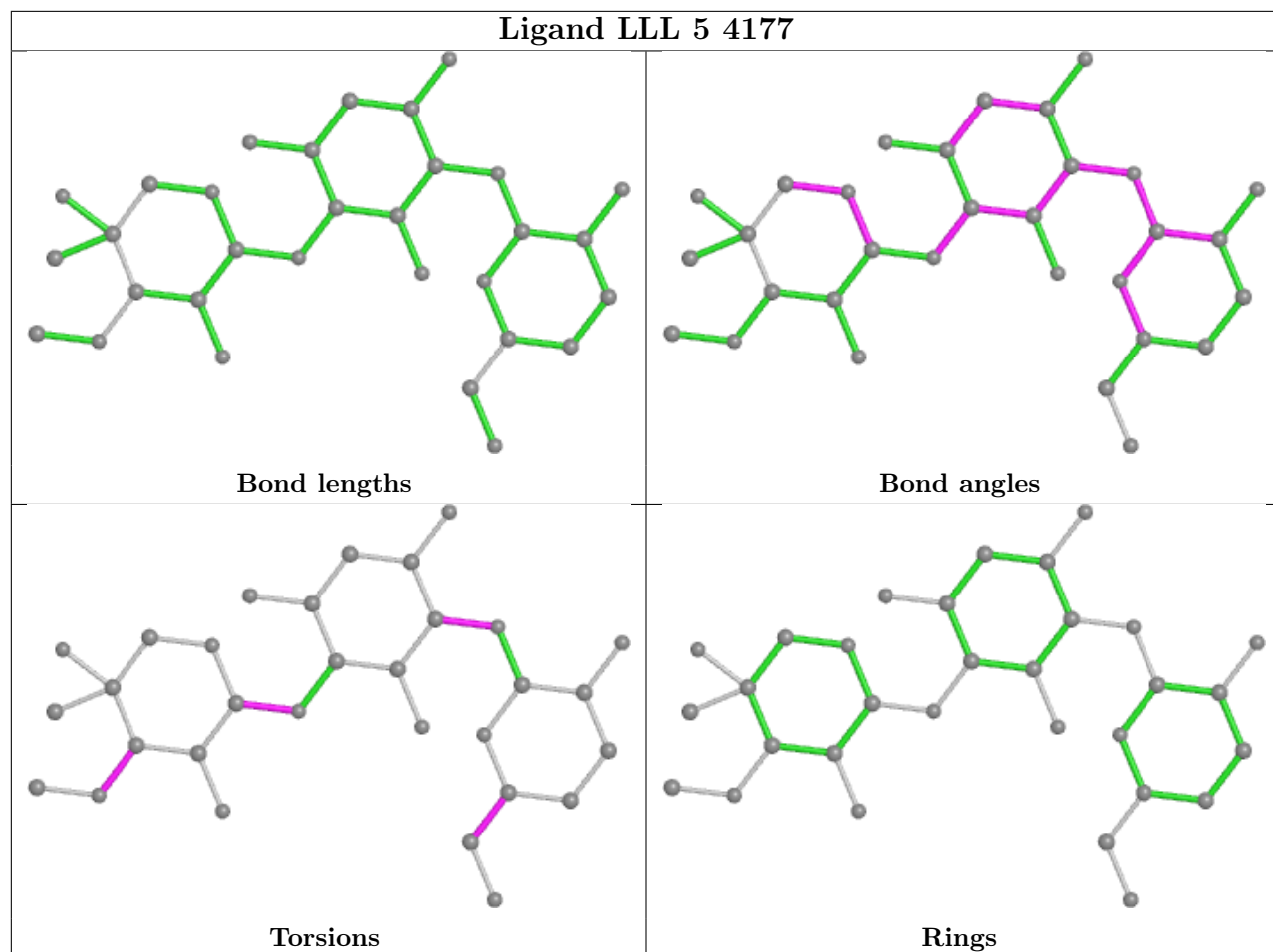


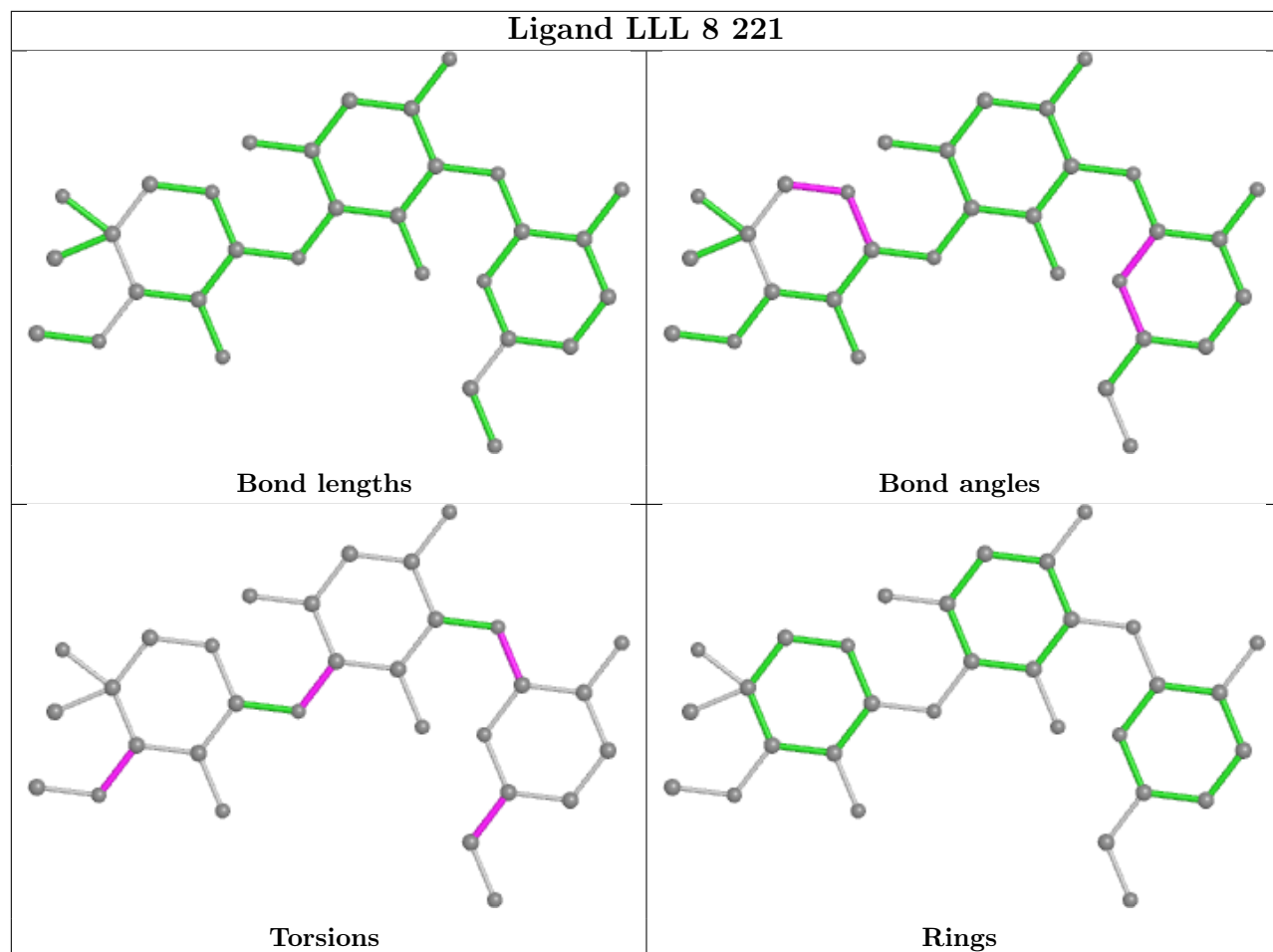


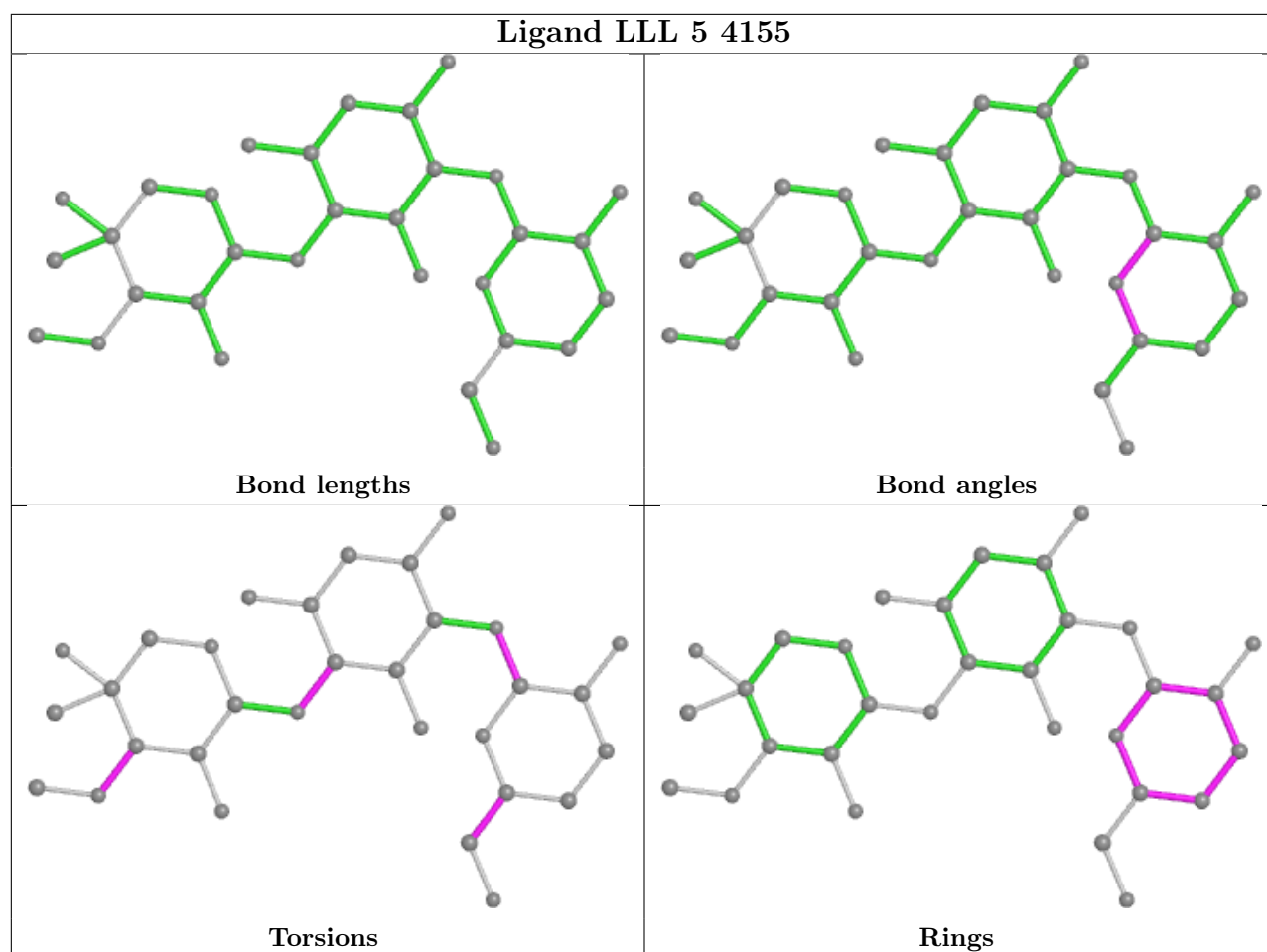












5.7 Other polymers [i](#)

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
80	m2	2
51	S5	1
10	l8	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m2	23:UNK	C	28:UNK	N	6.26
1	m2	52:UNK	C	54:UNK	N	3.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S5	21:THR	C	22:PRO	N	1.72
1	l8	51:LYS	C	52:TRP	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	1	3100/3396 (91%)	0.02	23 (0%) 87 87	47, 83, 190, 354	0
1	5	3134/3396 (92%)	0.06	13 (0%) 92 92	37, 76, 173, 292	0
2	3	121/121 (100%)	-0.29	0 100 100	58, 107, 135, 155	0
2	7	121/121 (100%)	-0.24	0 100 100	45, 72, 94, 160	0
3	4	156/158 (98%)	-0.02	0 100 100	54, 94, 152, 260	0
3	8	158/158 (100%)	0.02	0 100 100	61, 102, 164, 234	0
4	L2	252/252 (100%)	0.40	7 (2%) 53 51	51, 88, 124, 174	0
4	l2	252/252 (100%)	0.48	6 (2%) 59 57	51, 84, 121, 177	0
5	L3	386/386 (100%)	0.22	3 (0%) 86 85	41, 77, 104, 170	0
5	l3	386/386 (100%)	0.08	1 (0%) 94 93	34, 60, 91, 165	0
6	L4	361/361 (100%)	0.19	0 100 100	45, 85, 119, 142	0
6	l4	361/361 (100%)	0.23	6 (1%) 70 68	44, 90, 128, 167	0
7	L5	296/296 (100%)	0.59	22 (7%) 14 16	74, 120, 162, 214	0
7	l5	294/296 (99%)	0.21	5 (1%) 70 68	51, 80, 124, 155	0
8	L6	156/176 (88%)	0.14	1 (0%) 89 89	61, 84, 119, 149	0
8	l6	157/176 (89%)	0.18	1 (0%) 89 89	53, 81, 129, 204	0
9	L7	222/223 (99%)	0.14	3 (1%) 75 74	47, 76, 119, 219	0
9	l7	223/223 (100%)	0.03	0 100 100	39, 66, 123, 205	0
10	L8	233/233 (100%)	0.96	32 (13%) 3 3	96, 131, 183, 250	0
10	l8	231/233 (99%)	0.95	38 (16%) 1 2	96, 137, 184, 229	0
11	L9	191/191 (100%)	0.35	6 (3%) 49 48	60, 91, 121, 162	0
11	l9	191/191 (100%)	0.00	1 (0%) 91 90	41, 60, 92, 148	0
12	M0	212/221 (95%)	0.34	7 (3%) 46 45	52, 84, 129, 242	0
12	m0	211/221 (95%)	0.24	4 (1%) 66 65	32, 65, 120, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M1	169/169 (100%)	1.06	32 (18%) 1 1	88, 124, 153, 166	0
13	m1	169/169 (100%)	0.16	1 (0%) 89 89	51, 77, 104, 125	0
14	M3	193/194 (99%)	0.55	12 (6%) 20 21	55, 102, 161, 213	0
14	m3	194/194 (100%)	0.59	16 (8%) 11 13	53, 113, 167, 220	0
15	M4	136/137 (99%)	0.25	2 (1%) 73 72	61, 88, 115, 151	0
15	m4	137/137 (100%)	-0.10	1 (0%) 87 87	45, 67, 96, 170	0
16	M5	203/203 (100%)	0.79	19 (9%) 8 10	52, 88, 116, 130	0
16	m5	203/203 (100%)	0.88	19 (9%) 8 10	58, 97, 120, 136	0
17	M6	197/197 (100%)	0.14	1 (0%) 91 90	45, 64, 104, 140	0
17	m6	197/197 (100%)	-0.08	0 100 100	34, 50, 93, 123	0
18	M7	183/184 (99%)	0.91	25 (13%) 3 3	50, 70, 209, 262	0
18	m7	155/184 (84%)	0.12	1 (0%) 89 89	49, 67, 96, 136	0
19	M8	185/185 (100%)	0.48	3 (1%) 72 70	62, 83, 102, 160	0
19	m8	185/185 (100%)	0.42	3 (1%) 72 70	47, 83, 108, 135	0
20	M9	182/188 (96%)	0.42	7 (3%) 40 39	77, 106, 198, 250	0
20	m9	188/188 (100%)	0.46	11 (5%) 22 23	63, 95, 190, 264	0
21	N0	172/172 (100%)	0.56	12 (6%) 16 18	59, 80, 108, 150	0
21	n0	172/172 (100%)	0.08	2 (1%) 79 77	40, 57, 88, 123	0
22	N1	159/159 (100%)	0.53	8 (5%) 28 29	56, 84, 149, 195	0
22	n1	159/159 (100%)	0.32	5 (3%) 49 48	43, 68, 130, 165	0
23	N2	100/100 (100%)	0.79	14 (14%) 2 3	115, 150, 198, 212	0
23	n2	98/100 (98%)	1.42	26 (26%) 0 0	92, 136, 165, 200	0
24	N3	136/136 (100%)	0.41	4 (2%) 51 50	47, 75, 111, 159	0
24	n3	136/136 (100%)	0.44	2 (1%) 73 72	34, 55, 87, 130	0
25	N4	98/155 (63%)	1.76	27 (27%) 0 0	67, 97, 245, 294	0
26	N5	121/121 (100%)	0.92	12 (9%) 7 8	76, 107, 137, 228	0
26	n5	120/121 (99%)	0.69	9 (7%) 14 16	73, 116, 150, 171	0
27	N6	126/126 (100%)	0.98	15 (11%) 4 5	60, 96, 132, 163	0
27	n6	126/126 (100%)	0.73	11 (8%) 10 12	75, 110, 146, 183	0
28	N7	135/135 (100%)	2.24	70 (51%) 0 0	114, 145, 176, 223	0
28	n7	135/135 (100%)	1.48	36 (26%) 0 0	106, 144, 172, 207	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	N8	148/148 (100%)	0.74	21 (14%) 2 3	46, 84, 125, 154	0
29	n8	148/148 (100%)	0.40	6 (4%) 37 36	46, 85, 128, 156	0
30	N9	58/58 (100%)	0.75	8 (13%) 2 3	50, 90, 159, 165	0
30	n9	58/58 (100%)	0.36	1 (1%) 70 68	43, 87, 136, 176	0
31	O0	97/100 (97%)	0.79	13 (13%) 3 4	96, 132, 178, 188	0
31	o0	100/100 (100%)	0.61	8 (8%) 12 13	93, 124, 178, 229	0
32	O1	109/109 (100%)	1.04	12 (11%) 5 6	65, 92, 156, 210	0
32	o1	109/109 (100%)	0.58	5 (4%) 32 32	57, 80, 146, 186	0
33	O2	127/127 (100%)	0.14	3 (2%) 59 57	42, 67, 95, 128	0
33	o2	127/127 (100%)	0.13	1 (0%) 86 85	42, 76, 105, 157	0
34	O3	106/106 (100%)	0.11	0 100 100	51, 68, 106, 147	0
34	o3	106/106 (100%)	0.07	0 100 100	41, 60, 94, 133	0
35	O4	112/112 (100%)	0.85	15 (13%) 3 4	73, 114, 163, 223	0
35	o4	112/112 (100%)	0.60	8 (7%) 16 18	69, 104, 163, 198	0
36	O5	119/119 (100%)	0.61	5 (4%) 36 35	81, 111, 140, 163	0
36	o5	119/119 (100%)	0.60	5 (4%) 36 35	78, 123, 152, 162	0
37	O6	99/99 (100%)	0.44	7 (7%) 16 18	85, 111, 160, 197	0
37	o6	99/99 (100%)	0.88	15 (15%) 2 2	89, 117, 162, 193	0
38	O7	87/87 (100%)	0.32	2 (2%) 60 59	56, 76, 125, 211	0
38	o7	87/87 (100%)	0.47	2 (2%) 60 59	54, 82, 153, 163	0
39	O8	77/77 (100%)	0.79	9 (11%) 4 5	114, 147, 172, 230	0
39	o8	77/77 (100%)	1.37	22 (28%) 0 0	106, 136, 170, 181	0
40	O9	50/50 (100%)	0.50	2 (4%) 38 37	63, 84, 106, 116	0
40	o9	50/50 (100%)	0.48	1 (2%) 65 64	70, 91, 106, 108	0
41	Q0	52/52 (100%)	0.81	6 (11%) 4 5	61, 79, 108, 126	0
41	q0	52/52 (100%)	0.14	0 100 100	37, 51, 72, 118	0
42	Q1	25/25 (100%)	0.49	0 100 100	71, 84, 102, 104	0
42	q1	25/25 (100%)	-0.03	0 100 100	55, 70, 90, 100	0
43	Q2	105/105 (100%)	0.72	11 (10%) 6 7	59, 84, 123, 165	0
43	q2	105/105 (100%)	0.19	1 (0%) 82 81	45, 74, 105, 179	0
44	Q3	91/91 (100%)	0.26	2 (2%) 62 60	54, 96, 128, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	q3	91/91 (100%)	0.25	0 100 100	44, 85, 112, 130	0
45	2	1712/1800 (95%)	-0.02	23 (1%) 77 76	70, 132, 242, 320	0
45	6	1739/1800 (96%)	-0.05	22 (1%) 77 76	49, 95, 249, 344	0
46	S0	206/206 (100%)	1.38	57 (27%) 0 0	109, 161, 224, 271	0
46	s0	206/206 (100%)	0.54	10 (4%) 29 29	81, 124, 166, 215	0
47	S1	214/216 (99%)	1.07	47 (21%) 0 1	114, 173, 227, 252	0
47	s1	216/216 (100%)	0.59	18 (8%) 11 13	81, 117, 159, 193	0
48	S2	217/217 (100%)	0.89	31 (14%) 2 3	84, 130, 171, 200	0
48	s2	217/217 (100%)	0.49	12 (5%) 25 25	71, 104, 138, 174	0
49	S3	223/223 (100%)	1.21	48 (21%) 0 1	82, 139, 193, 260	0
49	s3	223/223 (100%)	0.89	29 (13%) 3 4	78, 116, 163, 223	0
50	S4	260/260 (100%)	1.46	84 (32%) 0 0	97, 142, 169, 225	0
50	s4	260/260 (100%)	0.86	38 (14%) 2 3	72, 127, 165, 189	0
51	S5	206/206 (100%)	1.64	56 (27%) 0 0	131, 172, 213, 237	0
51	s5	206/206 (100%)	0.49	13 (6%) 20 21	64, 97, 147, 197	0
52	S6	226/236 (95%)	0.88	30 (13%) 3 4	82, 145, 214, 373	0
52	s6	218/236 (92%)	0.69	18 (8%) 11 13	73, 120, 168, 213	0
53	S7	184/186 (98%)	0.96	29 (15%) 2 2	115, 179, 224, 251	0
53	s7	186/186 (100%)	0.77	21 (11%) 5 6	99, 157, 207, 271	0
54	S8	188/200 (94%)	1.59	64 (34%) 0 0	84, 125, 176, 199	0
54	s8	186/200 (93%)	0.73	20 (10%) 5 7	70, 113, 164, 198	0
55	S9	185/185 (100%)	1.51	59 (31%) 0 0	111, 152, 192, 244	0
55	s9	185/185 (100%)	0.83	20 (10%) 5 7	87, 134, 188, 215	0
56	C0	96/105 (91%)	1.32	25 (26%) 0 0	127, 170, 212, 235	0
56	c0	96/105 (91%)	1.22	21 (21%) 0 1	93, 137, 193, 217	0
57	C1	155/156 (99%)	1.90	61 (39%) 0 0	84, 122, 201, 267	0
57	c1	142/156 (91%)	0.98	14 (9%) 7 8	69, 111, 169, 198	0
58	C2	124/143 (86%)	2.47	62 (50%) 0 0	175, 223, 267, 294	0
58	c2	124/143 (86%)	1.74	51 (41%) 0 0	132, 190, 233, 259	0
59	C3	150/150 (100%)	0.72	12 (8%) 12 13	95, 139, 177, 206	0
59	c3	150/150 (100%)	0.10	2 (1%) 77 76	67, 111, 148, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	C4	127/128 (99%)	1.16	37 (29%) 0 0	93, 164, 207, 215	0
60	c4	128/128 (100%)	0.81	11 (8%) 10 12	63, 103, 135, 156	0
61	C5	124/141 (87%)	1.25	35 (28%) 0 0	108, 165, 211, 236	0
61	c5	135/141 (95%)	0.40	7 (5%) 27 27	61, 96, 162, 201	0
62	C6	141/142 (99%)	1.94	56 (39%) 0 0	105, 157, 196, 212	0
62	c6	142/142 (100%)	0.38	4 (2%) 53 51	59, 91, 128, 197	0
63	C7	120/136 (88%)	1.34	31 (25%) 0 0	110, 161, 290, 384	0
63	c7	117/136 (86%)	0.58	8 (6%) 17 19	81, 123, 194, 239	0
64	C8	145/145 (100%)	1.46	51 (35%) 0 0	102, 165, 211, 235	0
64	c8	145/145 (100%)	0.02	2 (1%) 75 74	64, 82, 128, 184	0
65	C9	143/143 (100%)	1.17	31 (21%) 0 1	128, 159, 204, 232	0
65	c9	143/143 (100%)	0.18	3 (2%) 63 62	61, 84, 117, 154	0
66	D0	107/110 (97%)	1.38	29 (27%) 0 0	101, 156, 232, 270	0
66	d0	110/110 (100%)	1.31	30 (27%) 0 0	68, 121, 203, 223	0
67	D1	87/87 (100%)	1.47	26 (29%) 0 0	112, 151, 183, 198	0
67	d1	87/87 (100%)	0.48	7 (8%) 12 13	87, 117, 158, 188	0
68	D2	129/129 (100%)	1.09	28 (21%) 0 1	99, 127, 155, 176	0
68	d2	129/129 (100%)	0.64	5 (3%) 39 38	74, 99, 120, 137	0
69	D3	144/144 (100%)	0.77	16 (11%) 5 6	76, 102, 127, 174	0
69	d3	144/144 (100%)	0.08	1 (0%) 87 87	51, 73, 99, 157	0
70	D4	134/134 (100%)	1.13	27 (20%) 1 1	106, 152, 191, 215	0
70	d4	133/134 (99%)	0.61	15 (11%) 5 6	80, 134, 173, 195	0
71	D5	70/70 (100%)	2.72	48 (68%) 0 0	151, 189, 233, 266	0
71	d5	69/70 (98%)	0.48	3 (4%) 35 35	77, 108, 142, 162	0
72	D6	97/97 (100%)	1.20	25 (25%) 0 0	86, 126, 189, 239	0
72	d6	97/97 (100%)	0.31	2 (2%) 63 62	63, 88, 136, 238	0
73	D7	81/81 (100%)	1.67	34 (41%) 0 0	117, 161, 215, 267	0
73	d7	81/81 (100%)	0.69	10 (12%) 4 5	92, 124, 199, 227	0
74	D8	63/63 (100%)	1.96	29 (46%) 0 0	136, 175, 215, 257	0
74	d8	63/63 (100%)	1.33	17 (26%) 0 0	81, 117, 146, 165	0
75	D9	53/53 (100%)	1.31	16 (30%) 0 0	104, 128, 154, 187	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	d9	53/53 (100%)	0.57	5 (9%) 8 10	64, 86, 109, 148	0
76	E0	60/62 (96%)	1.42	18 (30%) 0 0	98, 144, 215, 237	0
76	e0	62/62 (100%)	0.65	6 (9%) 7 9	64, 118, 179, 202	0
77	E1	71/72 (98%)	1.71	23 (32%) 0 0	143, 199, 243, 257	0
77	e1	72/72 (100%)	1.32	21 (29%) 0 0	125, 174, 212, 236	0
78	SR	318/318 (100%)	2.13	148 (46%) 0 0	131, 175, 225, 269	0
78	sR	318/318 (100%)	0.88	48 (15%) 2 2	88, 125, 174, 226	0
79	SM	159/272 (58%)	0.84	25 (15%) 2 2	88, 153, 237, 268	0
79	sM	129/272 (47%)	0.53	10 (7%) 13 14	76, 118, 187, 220	0
80	m2	0/165	-	-	-	-
81	n4	135/135 (100%)	1.00	23 (17%) 1 2	42, 139, 211, 238	0
82	p0	143/312 (45%)	0.94	22 (15%) 2 2	84, 138, 215, 261	0
83	p1	0/47	-	-	-	-
All	All	32909/34616 (95%)	0.50	2766 (8%) 11 13	32, 103, 196, 384	0

All (2766) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	N4	75	THR	15.5
25	N4	76	VAL	12.9
57	C1	146	ALA	12.4
18	M7	167	ARG	12.3
57	C1	145	ALA	11.4
25	N4	84	GLY	11.3
18	M7	161	ALA	10.6
58	C2	59	LEU	9.9
51	S5	151	GLY	9.7
18	M7	162	GLU	9.4
58	C2	60	VAL	9.4
57	C1	147	GLY	9.4
79	SM	17	VAL	9.2
78	SR	115	ILE	8.9
18	M7	183	ALA	8.8
18	M7	163	LYS	8.5
58	C2	121	VAL	8.3
25	N4	85	ALA	8.2
79	SM	18	VAL	8.2
51	S5	154	ALA	8.1

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Mol	Chain	Res	Type	RSRZ
51	S5	153	GLY	7.9
76	E0	61	SER	7.8
79	SM	16	ASP	7.7
25	N4	87	LEU	7.6
79	SM	19	VAL	7.6
78	SR	24	ALA	7.6
78	SR	79	TYR	7.5
78	SR	33	LEU	7.5
71	D5	71	ILE	7.5
51	S5	155	ALA	7.5
78	SR	302	PHE	7.5
81	n4	68	ALA	7.5
77	E1	86	THR	7.5
74	D8	17	GLY	7.3
18	M7	168	LEU	7.2
27	N6	127	GLU	7.2
28	N7	2	ALA	7.2
54	S8	200	LYS	7.2
62	C6	89	LEU	7.0
53	s7	2	SER	7.0
25	N4	86	SER	6.9
53	s7	43	PHE	6.9
77	E1	145	HIS	6.9
21	N0	1	MET	6.9
61	C5	104	GLN	6.8
62	C6	20	ALA	6.8
51	S5	152	GLY	6.7
53	S7	93	LEU	6.7
58	C2	28	LEU	6.7
62	C6	10	PHE	6.7
62	C6	29	ILE	6.6
78	SR	57	PRO	6.6
57	c1	30	ARG	6.6
47	S1	54	LEU	6.5
58	C2	82	PRO	6.5
81	n4	67	VAL	6.5
10	l8	150	LEU	6.5
78	SR	73	LEU	6.5
78	SR	212	ALA	6.4
51	S5	156	ARG	6.3
58	C2	126	TRP	6.3
23	n2	11	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
78	SR	32	LEU	6.2
58	C2	41	LEU	6.2
76	E0	48	THR	6.2
10	L8	198	ALA	6.2
50	S4	149	TYR	6.2
66	D0	121	ASN	6.2
18	M7	166	VAL	6.2
78	SR	81	LEU	6.1
58	C2	88	LEU	6.1
1	1	1025	A	6.1
28	N7	131	PHE	6.1
63	C7	99	VAL	6.1
78	SR	121	MET	6.1
67	D1	34	ILE	6.0
57	C1	50	GLU	6.0
58	C2	42	ALA	6.0
58	C2	87	PRO	5.9
54	S8	66	SER	5.9
55	s9	184	SER	5.9
51	S5	150	GLY	5.9
10	l8	199	ALA	5.8
25	N4	77	LYS	5.8
58	C2	120	VAL	5.8
55	S9	185	GLY	5.8
53	S7	38	LEU	5.8
25	N4	88	ASP	5.8
74	D8	19	THR	5.8
81	n4	66	GLU	5.7
78	SR	168	THR	5.7
71	D5	41	ILE	5.7
78	SR	94	VAL	5.7
64	C8	2	SER	5.7
55	S9	158	PHE	5.6
77	e1	87	THR	5.6
58	c2	104	GLY	5.6
78	SR	186	PHE	5.6
18	M7	178	ALA	5.5
70	D4	25	VAL	5.5
18	M7	182	ILE	5.5
71	D5	89	ILE	5.5
54	S8	152	ILE	5.5
58	c2	41	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
63	C7	120	SER	5.5
52	s6	169	TYR	5.5
57	C1	30	ARG	5.4
62	C6	36	ILE	5.4
63	C7	117	LEU	5.4
58	C2	102	GLY	5.4
47	S1	217	LEU	5.3
76	E0	49	LEU	5.3
39	o8	53	THR	5.3
18	M7	160	ALA	5.3
38	O7	86	ALA	5.3
58	C2	78	LEU	5.3
25	N4	83	THR	5.3
45	2	658	C	5.3
62	C6	85	ILE	5.3
51	s5	152	GLY	5.3
73	D7	33	LEU	5.3
28	N7	28	PRO	5.3
63	C7	121	VAL	5.3
5	L3	387	LEU	5.3
23	n2	63	VAL	5.3
47	S1	103	MET	5.3
28	N7	132	SER	5.3
10	l8	198	ALA	5.2
23	n2	15	PHE	5.2
47	S1	101	HIS	5.2
28	N7	22	LYS	5.2
25	N4	78	ALA	5.2
78	SR	204	ALA	5.2
77	E1	85	TYR	5.2
28	n7	118	PHE	5.2
23	N2	9	GLN	5.1
13	M1	127	PHE	5.1
29	N8	79	TRP	5.1
56	c0	98	THR	5.1
78	SR	23	LEU	5.1
55	S9	184	SER	5.1
36	O5	120	ALA	5.1
46	S0	24	LEU	5.1
58	C2	31	VAL	5.1
76	e0	63	GLN	5.1
78	SR	72	THR	5.1

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Mol	Chain	Res	Type	RSRZ
54	S8	179	CYS	5.1
67	D1	33	GLN	5.1
58	C2	89	ILE	5.1
78	SR	309	VAL	5.1
18	M7	179	GLN	5.1
1	1	1569	U	5.1
46	S0	198	MET	5.1
73	D7	41	LEU	5.0
76	E0	54	ARG	5.0
56	C0	56	LYS	5.0
55	S9	186	GLU	5.0
28	n7	2	ALA	5.0
70	D4	70	VAL	5.0
50	S4	123	LEU	5.0
66	d0	18	GLN	5.0
54	S8	199	LYS	5.0
56	c0	22	VAL	5.0
58	C2	85	LYS	5.0
79	SM	88	ARG	5.0
58	C2	37	VAL	5.0
28	N7	89	VAL	5.0
62	C6	55	VAL	5.0
28	N7	27	LYS	5.0
66	D0	64	LYS	5.0
28	N7	26	VAL	5.0
62	C6	9	THR	5.0
49	S3	214	GLU	5.0
78	SR	181	TRP	5.0
12	M0	220	GLN	4.9
78	SR	34	LEU	4.9
55	S9	181	ALA	4.9
47	S1	140	ILE	4.9
57	C1	155	LYS	4.9
47	S1	90	GLU	4.9
25	N4	81	PRO	4.9
23	n2	64	THR	4.9
56	C0	60	SER	4.9
1	1	1570	U	4.9
75	D9	43	PHE	4.9
28	N7	7	ALA	4.9
50	S4	261	LEU	4.8
61	c5	133	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
27	n6	45	ILE	4.8
1	5	2539	C	4.8
56	C0	12	HIS	4.8
68	D2	25	VAL	4.8
54	S8	167	ALA	4.8
45	2	241	U	4.8
66	D0	81	THR	4.8
1	1	1028	U	4.8
58	c2	59	LEU	4.8
47	S1	216	LYS	4.8
78	SR	77	GLY	4.8
67	D1	55	LEU	4.8
78	SR	180	ALA	4.8
78	SR	192	PHE	4.7
18	M7	164	LYS	4.7
58	C2	32	LEU	4.7
63	C7	123	ASN	4.7
76	E0	55	ARG	4.7
25	N4	92	GLU	4.7
18	M7	156	ALA	4.7
18	M7	165	VAL	4.7
51	S5	53	VAL	4.7
79	SM	13	GLU	4.7
56	c0	95	ARG	4.7
12	m0	221	ALA	4.7
27	N6	124	GLY	4.7
28	N7	106	GLN	4.7
57	C1	24	LYS	4.7
61	c5	132	GLY	4.7
51	S5	175	LEU	4.7
57	C1	149	ALA	4.6
25	N4	89	LEU	4.6
56	C0	65	TYR	4.6
81	n4	133	THR	4.6
23	n2	54	VAL	4.6
63	C7	124	VAL	4.6
58	c2	73	LYS	4.6
74	D8	45	LYS	4.6
21	n0	1	MET	4.6
50	S4	192	ILE	4.6
79	SM	85	SER	4.6
78	SR	92	TRP	4.6

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Mol	Chain	Res	Type	RSRZ
32	o1	4	LEU	4.6
46	S0	23	HIS	4.6
58	C2	61	VAL	4.6
74	D8	6	PRO	4.6
78	SR	262	VAL	4.6
56	c0	68	LEU	4.6
78	SR	45	TRP	4.6
51	S5	128	ASN	4.6
58	c2	28	LEU	4.6
57	C1	154	ALA	4.6
62	C6	7	VAL	4.6
27	N6	125	LYS	4.6
71	D5	98	GLN	4.6
28	N7	5	LEU	4.6
78	SR	25	THR	4.6
63	C7	102	VAL	4.5
78	sR	6	VAL	4.5
28	N7	25	ILE	4.5
23	n2	56	VAL	4.5
77	E1	149	LYS	4.5
28	N7	92	PHE	4.5
65	C9	92	LYS	4.5
78	SR	80	ALA	4.5
73	D7	42	ASN	4.5
71	D5	69	LEU	4.5
62	C6	65	ILE	4.5
56	C0	23	ALA	4.5
68	D2	26	LEU	4.5
74	D8	16	LEU	4.5
61	C5	90	ILE	4.5
74	D8	53	ILE	4.5
62	C6	60	PHE	4.5
65	C9	35	ASP	4.5
54	S8	149	SER	4.5
55	S9	138	LYS	4.5
53	S7	94	ALA	4.5
66	D0	63	LEU	4.5
24	n3	3	GLY	4.5
54	S8	151	LYS	4.5
78	SR	46	LYS	4.5
64	C8	5	VAL	4.5
46	S0	174	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
78	SR	167	VAL	4.4
78	sR	33	LEU	4.4
24	N3	2	SER	4.4
37	o6	100	HIS	4.4
54	S8	168	CYS	4.4
78	SR	117	LYS	4.4
47	S1	53	GLY	4.4
77	e1	88	PRO	4.4
61	C5	94	VAL	4.4
76	E0	45	VAL	4.4
18	M7	184	ALA	4.4
47	S1	139	ALA	4.4
63	C7	38	ILE	4.4
78	SR	131	ILE	4.4
78	SR	158	PRO	4.4
45	6	696	C	4.4
58	c2	42	ALA	4.4
62	C6	105	LEU	4.4
77	e1	92	LYS	4.4
20	m9	181	ARG	4.4
25	N4	97	LYS	4.4
47	S1	100	PHE	4.4
28	N7	124	ALA	4.4
74	d8	10	ALA	4.4
55	S9	180	LYS	4.4
58	c2	43	ARG	4.4
77	e1	97	LYS	4.4
58	c2	121	VAL	4.3
60	C4	83	ILE	4.3
57	C1	15	LYS	4.3
28	N7	96	VAL	4.3
46	S0	48	ILE	4.3
71	D5	82	HIS	4.3
54	S8	72	ILE	4.3
53	S7	61	PHE	4.3
58	C2	138	GLU	4.3
62	C6	6	SER	4.3
78	sR	3	SER	4.3
28	N7	44	ALA	4.3
45	6	1370	U	4.3
55	s9	183	ALA	4.3
78	SR	178	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
23	n2	14	THR	4.3
64	C8	32	LEU	4.3
71	D5	101	TYR	4.3
77	E1	148	TYR	4.3
55	S9	134	ILE	4.3
66	D0	54	GLY	4.3
74	D8	67	ARG	4.3
58	c2	102	GLY	4.3
46	S0	97	PRO	4.3
54	s8	102	VAL	4.3
60	C4	79	VAL	4.3
65	C9	4	VAL	4.3
65	C9	54	PHE	4.2
56	c0	94	GLU	4.2
58	c2	126	TRP	4.2
51	S5	149	VAL	4.2
78	SR	55	GLY	4.2
1	1	1572	U	4.2
46	S0	199	PRO	4.2
60	C4	27	PHE	4.2
10	l8	162	LEU	4.2
54	S8	67	TRP	4.2
54	S8	165	LEU	4.2
23	n2	71	PHE	4.2
71	D5	88	ILE	4.2
58	c2	21	GLU	4.2
28	N7	118	PHE	4.2
18	M7	181	ARG	4.2
72	D6	44	ILE	4.2
55	S9	97	LEU	4.2
55	S9	104	PHE	4.2
74	D8	7	VAL	4.2
81	n4	134	GLN	4.2
27	N6	126	LEU	4.2
76	E0	46	ASN	4.2
78	SR	74	THR	4.2
18	M7	180	LYS	4.2
27	n6	127	GLU	4.2
51	S5	71	ALA	4.2
39	o8	54	LEU	4.2
57	C1	35	TYR	4.2
28	n7	23	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
77	E1	116	LYS	4.2
54	S8	65	PHE	4.2
77	e1	85	TYR	4.2
66	D0	84	MET	4.1
64	C8	56	LYS	4.1
50	S4	54	TYR	4.1
49	s3	109	LEU	4.1
58	c2	103	LEU	4.1
78	sR	34	LEU	4.1
1	5	2569	A	4.1
62	C6	22	VAL	4.1
79	SM	84	LYS	4.1
12	M0	221	ALA	4.1
64	C8	17	LEU	4.1
71	D5	80	LEU	4.1
78	SR	190	ALA	4.1
78	SR	171	SER	4.1
53	s7	93	LEU	4.1
10	L8	121	SER	4.1
66	D0	82	TYR	4.1
49	s3	184	ILE	4.1
62	C6	21	HIS	4.1
78	sR	316	MET	4.1
50	S4	229	GLY	4.1
1	5	1103	A	4.1
75	D9	31	ILE	4.1
78	SR	30	PRO	4.1
79	sM	23	LYS	4.1
57	C1	138	ASN	4.1
49	s3	135	GLU	4.1
70	D4	18	LEU	4.1
53	s7	92	PHE	4.1
78	SR	82	SER	4.1
64	C8	25	ASN	4.1
23	n2	13	LYS	4.1
58	C2	140	PHE	4.0
38	O7	87	SER	4.0
63	C7	35	CYS	4.0
28	n7	42	LEU	4.0
73	D7	49	HIS	4.0
26	N5	26	VAL	4.0
38	o7	88	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
56	c0	23	ALA	4.0
48	S2	236	PRO	4.0
49	S3	49	ILE	4.0
51	S5	174	LEU	4.0
39	o8	61	LYS	4.0
58	c2	125	ASN	4.0
64	C8	22	VAL	4.0
71	D5	102	THR	4.0
53	S7	92	PHE	4.0
62	C6	57	LEU	4.0
48	S2	90	THR	4.0
58	c2	61	VAL	4.0
66	D0	120	SER	4.0
28	N7	91	ALA	4.0
51	S5	193	THR	4.0
50	s4	208	VAL	4.0
53	S7	90	VAL	4.0
57	C1	151	LYS	4.0
78	sR	117	LYS	4.0
50	S4	56	LEU	4.0
56	c0	96	ASN	4.0
74	d8	28	VAL	4.0
26	N5	50	ALA	4.0
28	N7	4	PHE	4.0
78	SR	56	VAL	4.0
78	sR	313	TRP	4.0
73	D7	73	LEU	4.0
71	D5	79	ALA	4.0
30	N9	53	ALA	4.0
37	O6	99	ARG	4.0
58	c2	105	LYS	4.0
78	SR	253	ALA	4.0
73	D7	7	LEU	3.9
53	S7	98	ILE	3.9
58	C2	91	VAL	3.9
63	C7	100	LEU	3.9
73	d7	64	CYS	3.9
76	E0	51	ASN	3.9
71	D5	99	ALA	3.9
48	s2	96	THR	3.9
49	S3	21	LEU	3.9
45	2	499	U	3.9

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Mol	Chain	Res	Type	RSRZ
77	E1	144	CYS	3.9
78	SR	160	GLU	3.9
10	l8	152	LEU	3.9
66	D0	85	ARG	3.9
18	M7	177	ALA	3.9
54	S8	135	LYS	3.9
51	S5	140	THR	3.9
79	SM	141	ALA	3.9
28	N7	42	LEU	3.9
31	O0	35	ARG	3.9
64	C8	146	ALA	3.9
78	SR	78	ALA	3.9
61	C5	105	VAL	3.9
82	p0	87	VAL	3.9
50	S4	130	GLN	3.9
53	S7	49	ILE	3.9
55	S9	105	LEU	3.9
58	C2	36	LEU	3.9
58	C2	123	VAL	3.9
47	S1	46	THR	3.9
62	C6	79	TYR	3.9
50	s4	226	PHE	3.9
57	C1	137	PHE	3.9
51	s5	37	GLN	3.9
63	C7	122	ILE	3.9
50	S4	55	ALA	3.9
10	L8	197	VAL	3.9
58	C2	49	THR	3.9
77	e1	102	VAL	3.8
25	N4	98	PRO	3.8
46	S0	50	VAL	3.8
71	D5	62	VAL	3.8
78	sR	32	LEU	3.8
28	N7	6	LYS	3.8
77	E1	91	ILE	3.8
46	S0	99	ALA	3.8
54	S8	116	HIS	3.8
79	SM	176	ALA	3.8
57	C1	68	GLY	3.8
28	N7	82	PRO	3.8
51	S5	211	ILE	3.8
65	C9	55	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
12	m0	220	GLN	3.8
63	C7	119	LEU	3.8
68	D2	129	VAL	3.8
50	S4	147	ILE	3.8
54	S8	60	ILE	3.8
1	1	2540	A	3.8
58	C2	43	ARG	3.8
57	C1	148	LYS	3.8
47	S1	25	THR	3.8
47	s1	46	THR	3.8
51	S5	183	ALA	3.8
77	E1	152	ALA	3.8
1	1	2502	A	3.8
51	S5	130	ILE	3.8
50	S4	44	LEU	3.8
52	S6	75	LEU	3.8
52	S6	166	GLU	3.8
81	n4	65	GLU	3.8
45	6	225	A	3.8
28	N7	74	VAL	3.8
61	C5	86	VAL	3.8
78	SR	293	ALA	3.8
66	d0	94	GLU	3.8
25	N4	90	ILE	3.8
57	C1	156	PHE	3.8
55	S9	72	GLU	3.8
55	s9	33	GLU	3.8
71	D5	52	LYS	3.8
25	N4	64	THR	3.8
26	N5	24	LEU	3.8
57	C1	116	ARG	3.8
13	M1	125	MET	3.8
71	D5	87	GLY	3.8
52	S6	65	GLN	3.8
54	S8	182	TYR	3.8
61	C5	84	ILE	3.8
51	S5	62	VAL	3.7
35	O4	77	GLY	3.7
79	SM	15	ALA	3.7
55	S9	95	TYR	3.7
18	M7	176	ILE	3.7
78	SR	263	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
67	D1	18	SER	3.7
7	L5	95	TRP	3.7
54	S8	183	ILE	3.7
71	D5	50	ILE	3.7
78	SR	26	SER	3.7
60	C4	12	GLN	3.7
54	S8	63	GLY	3.7
79	sM	83	LYS	3.7
28	N7	105	SER	3.7
73	D7	48	SER	3.7
47	S1	138	PHE	3.7
60	C4	120	PRO	3.7
66	D0	65	ILE	3.7
45	6	226	A	3.7
49	S3	186	VAL	3.7
28	N7	99	GLU	3.7
62	C6	54	LEU	3.7
67	D1	69	LEU	3.7
30	N9	59	LYS	3.7
39	O8	44	LYS	3.7
23	n2	57	THR	3.7
28	N7	129	TRP	3.7
10	L8	26	LEU	3.7
60	C4	102	LEU	3.7
78	SR	136	ILE	3.7
28	n7	14	VAL	3.7
50	s4	227	VAL	3.7
10	l8	161	GLU	3.7
28	n7	22	LYS	3.7
48	S2	240	LEU	3.7
67	D1	40	ASP	3.7
49	S3	223	LYS	3.6
66	D0	86	ILE	3.6
71	D5	59	TYR	3.6
16	M5	37	HIS	3.6
46	S0	28	ASN	3.6
46	S0	16	LEU	3.6
10	L8	199	ALA	3.6
10	l8	180	VAL	3.6
46	s0	170	ILE	3.6
62	C6	121	SER	3.6
55	S9	92	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
46	S0	186	GLY	3.6
46	S0	201	LEU	3.6
45	6	1693	A	3.6
54	S8	104	ILE	3.6
62	C6	30	LYS	3.6
65	C9	2	PRO	3.6
46	S0	15	GLN	3.6
21	N0	2	ALA	3.6
54	S8	74	LYS	3.6
60	C4	19	ILE	3.6
72	d6	69	ASN	3.6
67	D1	53	TYR	3.6
29	N8	117	ARG	3.6
37	o6	68	ARG	3.6
55	s9	164	PHE	3.6
26	N5	95	ILE	3.6
23	n2	12	ALA	3.6
51	s5	153	GLY	3.6
78	SR	118	LYS	3.6
7	l5	297	GLN	3.6
45	6	1695	G	3.6
49	S3	217	ILE	3.6
78	SR	156	VAL	3.6
50	S4	9	LEU	3.6
54	S8	143	TRP	3.6
52	S6	114	VAL	3.6
57	C1	2	SER	3.6
60	C4	28	VAL	3.6
48	S2	88	LYS	3.6
58	C2	133	LEU	3.6
78	SR	31	ASN	3.6
78	SR	214	ALA	3.6
26	N5	27	ARG	3.6
16	M5	58	GLY	3.6
31	o0	6	SER	3.6
53	s7	41	LEU	3.6
77	e1	145	HIS	3.6
1	5	2540	A	3.5
45	6	1694	A	3.5
47	S1	68	VAL	3.5
67	D1	23	ILE	3.5
70	D4	96	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
78	SR	292	LEU	3.5
52	S6	153	VAL	3.5
48	S2	95	ARG	3.5
43	q2	106	PHE	3.5
54	S8	109	PHE	3.5
13	M1	91	LEU	3.5
13	M1	102	PHE	3.5
18	M7	157	VAL	3.5
58	C2	122	VAL	3.5
26	N5	34	LEU	3.5
67	D1	16	LYS	3.5
55	S9	118	LEU	3.5
58	C2	74	LEU	3.5
62	C6	26	LYS	3.5
77	E1	106	TYR	3.5
1	5	2503	G	3.5
28	n7	96	VAL	3.5
39	O8	45	VAL	3.5
39	O8	72	THR	3.5
77	E1	87	THR	3.5
78	SR	179	LYS	3.5
65	C9	28	LEU	3.5
29	n8	127	ALA	3.5
49	S3	147	ALA	3.5
78	SR	223	TRP	3.5
46	S0	175	TYR	3.5
13	M1	132	ASN	3.5
78	SR	58	VAL	3.5
57	C1	19	ILE	3.5
47	S1	135	LEU	3.5
56	C0	67	THR	3.5
53	S7	183	PHE	3.5
56	C0	75	TYR	3.5
20	m9	184	LEU	3.5
50	S4	228	ILE	3.5
37	o6	64	SER	3.5
50	S4	101	LEU	3.5
16	m5	58	GLY	3.5
50	s4	15	PRO	3.5
61	c5	136	SER	3.5
70	D4	69	SER	3.5
77	e1	86	THR	3.5

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Mol	Chain	Res	Type	RSRZ
60	C4	81	VAL	3.5
25	N4	96	LEU	3.5
51	S5	157	ARG	3.5
57	C1	3	THR	3.5
49	s3	40	ARG	3.5
66	D0	26	LEU	3.5
26	N5	32	PHE	3.5
76	E0	44	PHE	3.5
58	c2	35	ALA	3.5
58	c2	128	ALA	3.5
60	c4	28	VAL	3.4
71	D5	60	VAL	3.4
54	S8	169	ILE	3.4
56	c0	76	LEU	3.4
52	S6	83	CYS	3.4
48	S2	224	PHE	3.4
55	s9	34	PHE	3.4
7	l5	125	VAL	3.4
46	S0	49	ASN	3.4
47	S1	89	ASP	3.4
54	S8	64	ASN	3.4
73	D7	35	VAL	3.4
28	N7	134	LEU	3.4
62	C6	8	GLN	3.4
78	SR	102	ARG	3.4
54	s8	67	TRP	3.4
51	S5	206	SER	3.4
81	n4	130	SER	3.4
61	C5	13	LYS	3.4
29	n8	109	TYR	3.4
48	S2	104	VAL	3.4
82	p0	217	VAL	3.4
73	D7	38	PRO	3.4
51	s5	154	ALA	3.4
10	L8	226	TYR	3.4
14	M3	138	VAL	3.4
78	SR	243	LEU	3.4
58	C2	77	GLY	3.4
10	l8	200	LEU	3.4
54	s8	58	LEU	3.4
78	SR	157	VAL	3.4
28	n7	6	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
54	S8	137	LYS	3.4
61	C5	89	MET	3.4
70	D4	26	ASP	3.4
29	N8	78	LEU	3.4
54	S8	148	ALA	3.4
54	S8	95	THR	3.4
74	D8	59	SER	3.4
67	d1	34	ILE	3.4
82	p0	88	PHE	3.4
45	2	227	U	3.4
1	5	2442	G	3.4
46	S0	47	VAL	3.4
62	C6	66	ARG	3.4
72	D6	37	LYS	3.4
76	E0	47	VAL	3.4
57	C1	153	PHE	3.4
78	SR	120	SER	3.4
58	c2	36	LEU	3.4
63	C7	65	PRO	3.4
28	N7	10	VAL	3.4
28	n7	72	ILE	3.4
28	N7	64	LYS	3.4
29	N8	119	PRO	3.4
64	C8	18	LEU	3.4
23	N2	52	ASN	3.4
46	S0	173	ILE	3.4
60	C4	29	HIS	3.4
26	n5	99	VAL	3.3
70	D4	57	VAL	3.3
48	S2	222	TYR	3.3
58	C2	71	ILE	3.3
24	N3	3	GLY	3.3
26	N5	25	LYS	3.3
58	C2	83	GLU	3.3
62	C6	12	LYS	3.3
46	S0	177	LEU	3.3
53	s7	16	LEU	3.3
57	C1	40	LEU	3.3
13	M1	104	PHE	3.3
46	S0	203	PHE	3.3
50	S4	137	PRO	3.3
71	D5	103	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
13	M1	128	TYR	3.3
57	C1	23	PRO	3.3
64	C8	48	LYS	3.3
31	O0	38	LYS	3.3
52	s6	22	HIS	3.3
57	C1	60	PHE	3.3
71	D5	61	SER	3.3
77	E1	93	HIS	3.3
78	sR	213	SER	3.3
64	C8	57	ARG	3.3
57	C1	127	GLN	3.3
74	D8	25	VAL	3.3
45	2	913	G	3.3
61	C5	85	ILE	3.3
78	SR	35	SER	3.3
58	c2	44	GLY	3.3
10	L8	152	LEU	3.3
28	n7	34	LYS	3.3
58	C2	81	ASP	3.3
51	S5	111	VAL	3.3
51	S5	225	ARG	3.3
56	C0	22	VAL	3.3
78	sR	24	ALA	3.3
60	C4	20	TYR	3.3
81	n4	75	THR	3.3
33	O2	128	LEU	3.3
40	o9	11	GLN	3.3
48	S2	235	LEU	3.3
82	p0	19	LEU	3.3
49	S3	37	VAL	3.3
57	C1	65	SER	3.3
46	S0	18	LEU	3.3
58	C2	45	LEU	3.3
1	1	1286	A	3.3
45	2	234	G	3.3
46	S0	197	ILE	3.3
59	C3	40	TYR	3.3
78	SR	182	ASN	3.3
55	s9	80	LEU	3.3
55	s9	180	LYS	3.3
58	C2	124	LYS	3.3
71	D5	53	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
16	m5	2	GLY	3.3
70	d4	67	GLY	3.3
30	N9	54	LEU	3.3
13	M1	43	GLN	3.3
61	C5	12	PHE	3.3
66	d0	27	THR	3.3
78	SR	62	LYS	3.3
32	O1	4	LEU	3.3
47	S1	91	VAL	3.3
49	s3	138	VAL	3.3
55	S9	96	VAL	3.3
50	s4	35	PRO	3.3
73	d7	38	PRO	3.3
78	SR	134	TRP	3.3
78	sR	82	SER	3.3
78	sR	72	THR	3.3
68	D2	69	LEU	3.3
39	o8	45	VAL	3.3
50	S4	111	VAL	3.3
63	C7	66	VAL	3.3
68	D2	22	LYS	3.3
50	S4	49	ARG	3.2
51	S5	90	ILE	3.2
60	c4	15	GLY	3.2
67	D1	52	THR	3.2
68	D2	73	GLY	3.2
78	SR	211	ILE	3.2
45	2	1711	C	3.2
50	s4	261	LEU	3.2
10	L8	132	VAL	3.2
48	s2	88	LYS	3.2
60	C4	18	ARG	3.2
25	N4	72	SER	3.2
35	O4	79	SER	3.2
51	S5	187	ILE	3.2
57	C1	150	ASN	3.2
64	C8	44	ASN	3.2
49	s3	151	LYS	3.2
50	S4	122	LYS	3.2
50	s4	54	TYR	3.2
71	D5	83	LEU	3.2
58	C2	86	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
48	S2	151	PRO	3.2
55	S9	110	GLN	3.2
62	C6	92	TYR	3.2
49	S3	25	PHE	3.2
66	d0	112	VAL	3.2
77	e1	98	VAL	3.2
14	M3	54	LEU	3.2
47	S1	50	LYS	3.2
49	s3	50	ILE	3.2
60	c4	112	ILE	3.2
45	2	656	G	3.2
74	d8	9	LEU	3.2
27	N6	43	TYR	3.2
48	S2	156	THR	3.2
49	s3	152	PHE	3.2
56	C0	64	TYR	3.2
58	C2	119	SER	3.2
54	S8	76	THR	3.2
58	c2	22	VAL	3.2
74	D8	5	THR	3.2
77	e1	84	VAL	3.2
78	SR	163	ASP	3.2
13	M1	59	ILE	3.2
53	s7	34	LEU	3.2
16	m5	6	TYR	3.2
23	N2	27	VAL	3.2
73	D7	32	PHE	3.2
4	L2	111	THR	3.2
20	m9	187	GLU	3.2
48	s2	90	THR	3.2
51	S5	54	LYS	3.2
71	D5	56	THR	3.2
28	n7	11	ALA	3.2
60	C4	40	ALA	3.2
35	O4	23	VAL	3.2
48	S2	196	VAL	3.2
64	C8	4	VAL	3.2
14	M3	194	GLU	3.2
73	D7	70	LYS	3.2
51	S5	93	LEU	3.2
78	SR	220	ILE	3.2
79	SM	75	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
20	M9	132	PHE	3.2
51	S5	179	ALA	3.2
78	SR	226	ALA	3.2
52	s6	164	LYS	3.2
58	c2	115	VAL	3.2
41	Q0	77	ILE	3.2
50	S4	38	LEU	3.2
50	S4	48	LEU	3.2
28	N7	126	LYS	3.2
28	n7	4	PHE	3.2
67	D1	39	VAL	3.2
71	D5	91	PRO	3.2
28	N7	135	ARG	3.2
47	S1	99	ASN	3.2
64	C8	73	MET	3.2
77	E1	132	LEU	3.2
78	sR	300	THR	3.2
50	S4	47	PHE	3.2
78	sR	214	ALA	3.2
78	sR	263	PHE	3.2
57	C1	25	VAL	3.2
62	C6	44	LEU	3.2
73	D7	36	LYS	3.2
78	SR	170	ILE	3.2
37	o6	2	THR	3.2
39	o8	43	PHE	3.2
46	S0	124	THR	3.2
49	S3	24	PHE	3.2
45	6	675	U	3.2
28	N7	45	GLY	3.2
31	O0	92	ILE	3.2
55	S9	120	LYS	3.2
71	D5	90	LYS	3.2
28	N7	95	VAL	3.2
49	s3	38	GLU	3.2
48	S2	234	PRO	3.1
16	M5	22	LEU	3.1
55	S9	91	LYS	3.1
51	s5	151	GLY	3.1
58	C2	75	VAL	3.1
82	p0	50	VAL	3.1
22	N1	34	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
78	SR	205	SER	3.1
62	C6	13	LYS	3.1
62	C6	64	ASP	3.1
1	1	1026	A	3.1
46	S0	54	TRP	3.1
50	S4	110	ALA	3.1
71	D5	37	GLN	3.1
61	c5	51	SER	3.1
67	d1	87	ARG	3.1
79	SM	175	ASP	3.1
19	M8	93	ILE	3.1
67	D1	14	PRO	3.1
29	n8	126	LYS	3.1
78	SR	20	VAL	3.1
78	SR	113	VAL	3.1
1	1	1563	C	3.1
30	N9	57	ALA	3.1
64	C8	58	ALA	3.1
14	m3	54	LEU	3.1
74	d8	66	LEU	3.1
78	SR	60	SER	3.1
78	SR	159	ASN	3.1
13	M1	44	THR	3.1
18	M7	169	THR	3.1
28	n7	20	GLY	3.1
78	SR	14	GLU	3.1
14	M3	139	LEU	3.1
10	l8	155	ASN	3.1
9	L7	27	ALA	3.1
37	o6	69	ALA	3.1
53	S7	129	LEU	3.1
74	D8	66	LEU	3.1
50	S4	22	LYS	3.1
57	c1	138	ASN	3.1
78	SR	43	ILE	3.1
81	n4	112	ASN	3.1
51	S5	143	ARG	3.1
58	c2	33	ARG	3.1
28	N7	11	ALA	3.1
54	S8	145	ALA	3.1
49	S3	87	TYR	3.1
56	C0	63	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
66	D0	20	ILE	3.1
71	D5	86	GLU	3.1
73	D7	30	SER	3.1
78	SR	319	ASN	3.1
30	N9	56	ALA	3.1
69	D3	24	TRP	3.1
46	S0	100	GLY	3.1
58	C2	44	GLY	3.1
7	L5	126	GLU	3.1
49	s3	150	MET	3.1
57	C1	75	VAL	3.1
62	C6	19	VAL	3.1
20	M9	49	THR	3.1
52	S6	100	ALA	3.1
53	S7	41	LEU	3.1
66	d0	64	LYS	3.1
74	d8	16	LEU	3.1
78	SR	7	LEU	3.1
65	C9	144	GLU	3.1
15	M4	138	ALA	3.1
23	N2	89	LEU	3.1
58	C2	101	ALA	3.1
50	s4	39	ARG	3.1
51	S5	209	TYR	3.1
57	C1	73	GLY	3.1
47	s1	20	VAL	3.1
49	S3	185	LYS	3.1
50	S4	180	LEU	3.1
61	C5	15	HIS	3.1
72	D6	38	ARG	3.1
10	l8	34	PHE	3.1
46	S0	38	PHE	3.1
52	S6	210	GLN	3.1
1	1	1350	A	3.1
16	M5	134	LEU	3.1
27	N6	48	LEU	3.1
28	n7	80	LEU	3.1
62	C6	117	LEU	3.1
78	SR	301	LEU	3.1
23	N2	69	ALA	3.1
78	SR	254	ALA	3.1
10	l8	94	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
66	d0	121	ASN	3.0
70	D4	3	ASP	3.0
53	S7	58	LEU	3.0
28	N7	29	HIS	3.0
46	S0	14	ALA	3.0
78	sR	253	ALA	3.0
75	D9	38	ILE	3.0
77	E1	90	LYS	3.0
19	M8	74	GLU	3.0
57	C1	4	GLU	3.0
20	m9	22	VAL	3.0
22	N1	126	VAL	3.0
74	D8	44	VAL	3.0
49	s3	178	ARG	3.0
7	L5	131	LEU	3.0
58	C2	62	LEU	3.0
41	Q0	128	LYS	3.0
46	S0	46	HIS	3.0
51	S5	182	ALA	3.0
22	n1	160	ILE	3.0
57	C1	59	PRO	3.0
57	C1	66	ILE	3.0
64	C8	69	ILE	3.0
70	d4	71	GLY	3.0
53	S7	95	GLU	3.0
50	S4	102	VAL	3.0
66	d0	17	GLN	3.0
64	C8	101	LEU	3.0
50	S4	236	ILE	3.0
72	D6	73	TYR	3.0
58	c2	122	VAL	3.0
7	L5	92	LEU	3.0
75	D9	36	LEU	3.0
82	p0	219	THR	3.0
49	s3	153	ALA	3.0
52	S6	165	GLY	3.0
59	C3	141	TYR	3.0
66	D0	87	HIS	3.0
16	m5	135	VAL	3.0
51	S5	70	VAL	3.0
71	D5	42	LEU	3.0
10	l8	121	SER	3.0

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Mol	Chain	Res	Type	RSRZ
61	C5	111	MET	3.0
75	D9	55	PHE	3.0
10	l8	197	VAL	3.0
58	c2	75	VAL	3.0
73	D7	2	VAL	3.0
46	s0	18	LEU	3.0
58	c2	74	LEU	3.0
69	D3	71	CYS	3.0
52	s6	215	ARG	3.0
70	D4	119	PHE	3.0
75	D9	44	ARG	3.0
7	L5	127	GLY	3.0
13	M1	122	ILE	3.0
22	n1	125	ALA	3.0
23	n2	70	LYS	3.0
43	Q2	79	THR	3.0
46	S0	192	THR	3.0
52	S6	198	ALA	3.0
58	C2	69	ALA	3.0
62	C6	104	GLU	3.0
50	S4	11	ARG	3.0
58	C2	128	ALA	3.0
63	C7	101	ASN	3.0
69	D3	49	ALA	3.0
71	D5	100	ILE	3.0
73	d7	42	ASN	3.0
52	S6	208	TYR	3.0
75	D9	45	GLU	3.0
71	D5	64	VAL	3.0
62	C6	109	PHE	3.0
35	O4	32	ALA	3.0
70	d4	120	GLY	3.0
65	C9	124	ILE	3.0
78	sR	51	ASP	3.0
68	D2	46	TYR	3.0
81	n4	131	ALA	3.0
55	s9	36	LEU	3.0
78	SR	144	LEU	3.0
30	N9	58	LYS	3.0
78	SR	314	GLN	3.0
50	s4	173	ILE	3.0
58	c2	106	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
78	SR	114	ASP	3.0
48	S2	174	ARG	3.0
74	D8	21	SER	3.0
79	SM	12	VAL	3.0
55	S9	93	LEU	3.0
57	C1	16	GLN	3.0
74	d8	27	GLN	3.0
78	SR	313	TRP	3.0
78	sR	5	GLU	3.0
29	N8	112	ILE	3.0
28	n7	10	VAL	3.0
36	O5	116	TYR	3.0
52	s6	160	ARG	3.0
58	C2	27	ALA	3.0
52	S6	111	LEU	3.0
23	N2	10	LYS	3.0
25	N4	79	GLN	3.0
37	O6	100	HIS	3.0
54	S8	62	THR	3.0
57	c1	31	THR	3.0
47	S1	45	LYS	2.9
49	S3	86	LEU	2.9
57	C1	71	LEU	2.9
66	d0	114	VAL	2.9
60	C4	117	ASP	2.9
61	C5	8	LYS	2.9
75	D9	33	LYS	2.9
78	sR	7	LEU	2.9
46	S0	196	SER	2.9
4	L2	253	GLN	2.9
57	C1	47	THR	2.9
57	C1	61	THR	2.9
66	D0	78	THR	2.9
81	n4	132	GLY	2.9
31	o0	42	ILE	2.9
10	L8	189	LEU	2.9
14	M3	135	ALA	2.9
28	n7	21	LYS	2.9
47	S1	94	LYS	2.9
49	S3	48	VAL	2.9
53	s7	3	ALA	2.9
58	c2	71	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
60	c4	19	ILE	2.9
59	C3	25	TRP	2.9
65	C9	6	VAL	2.9
67	D1	19	ALA	2.9
67	D1	32	VAL	2.9
54	S8	180	ASP	2.9
73	D7	58	SER	2.9
78	SR	311	ARG	2.9
52	s6	171	LYS	2.9
28	N7	24	VAL	2.9
61	C5	75	PRO	2.9
61	C5	66	ALA	2.9
78	sR	301	LEU	2.9
53	s7	70	PHE	2.9
49	S3	187	LYS	2.9
65	C9	45	MET	2.9
10	L8	93	LEU	2.9
38	o7	83	ALA	2.9
56	C0	66	TYR	2.9
52	S6	29	ASP	2.9
57	C1	46	LYS	2.9
23	n2	67	SER	2.9
60	C4	39	ILE	2.9
56	C0	30	ALA	2.9
66	d0	95	ALA	2.9
68	D2	104	LEU	2.9
71	D5	40	VAL	2.9
74	D8	28	VAL	2.9
35	O4	76	TYR	2.9
45	2	1686	C	2.9
54	S8	54	LYS	2.9
46	s0	158	VAL	2.9
68	d2	27	ILE	2.9
78	SR	225	LEU	2.9
14	m3	133	PRO	2.9
51	S5	22	PRO	2.9
56	C0	39	ASN	2.9
63	C7	39	ALA	2.9
72	D6	62	TYR	2.9
78	SR	213	SER	2.9
10	l8	203	VAL	2.9
19	m8	140	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
23	n2	65	VAL	2.9
49	s3	137	VAL	2.9
60	c4	110	LEU	2.9
76	e0	49	LEU	2.9
79	SM	174	LEU	2.9
31	o0	22	LYS	2.9
60	c4	60	ALA	2.9
21	N0	74	ASN	2.9
50	S4	124	GLY	2.9
28	N7	46	ILE	2.9
43	Q2	75	VAL	2.9
52	s6	147	LEU	2.9
58	C2	136	ILE	2.9
58	c2	32	LEU	2.9
14	m3	190	LYS	2.9
22	N1	125	ALA	2.9
55	S9	71	PHE	2.9
72	d6	68	TYR	2.9
78	SR	100	TYR	2.9
78	SR	17	ASN	2.9
46	S0	22	THR	2.9
8	L6	130	ILE	2.9
29	N8	73	LEU	2.9
46	S0	98	ILE	2.9
50	S4	52	LEU	2.9
57	C1	70	ILE	2.9
68	D2	61	ILE	2.9
73	D7	24	LEU	2.9
78	SR	183	LEU	2.9
66	D0	80	GLU	2.9
47	S1	233	GLY	2.9
71	D5	81	ARG	2.9
39	o8	55	VAL	2.9
47	s1	231	LEU	2.9
50	S4	66	MET	2.9
54	s8	165	LEU	2.9
56	c0	1	MET	2.9
59	C3	61	THR	2.9
78	sR	121	MET	2.9
50	s4	205	PHE	2.9
66	d0	15	GLN	2.9
82	p0	26	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
55	S9	8	TYR	2.9
50	s4	127	LYS	2.9
55	s9	185	GLY	2.9
56	C0	24	LYS	2.9
77	e1	93	HIS	2.9
43	Q2	70	LEU	2.9
56	c0	73	VAL	2.9
59	C3	139	TRP	2.9
60	C4	42	VAL	2.9
64	C8	47	CYS	2.9
78	SR	130	THR	2.9
18	m7	2	ALA	2.9
20	m9	183	ALA	2.9
46	S0	40	ALA	2.9
47	s1	47	LEU	2.9
23	N2	54	VAL	2.8
49	S3	175	VAL	2.8
67	D1	82	VAL	2.8
72	D6	45	VAL	2.8
64	C8	19	ASN	2.8
72	D6	43	ASN	2.8
76	E0	56	MET	2.8
78	sR	251	TRP	2.8
62	C6	37	THR	2.8
59	C3	107	LYS	2.8
60	C4	82	LYS	2.8
64	C8	8	GLN	2.8
55	S9	89	ASP	2.8
28	n7	26	VAL	2.8
66	D0	114	VAL	2.8
54	S8	141	ARG	2.8
58	c2	119	SER	2.8
33	O2	127	ALA	2.8
51	S5	41	LYS	2.8
55	S9	61	THR	2.8
55	S9	135	ALA	2.8
71	D5	76	ALA	2.8
76	E0	23	LYS	2.8
60	C4	119	THR	2.8
50	S4	65	LEU	2.8
35	o4	93	PHE	2.8
50	S4	45	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
57	c1	113	PRO	2.8
62	C6	39	VAL	2.8
71	d5	88	ILE	2.8
52	s6	218	GLU	2.8
54	S8	136	SER	2.8
53	s7	42	GLN	2.8
53	S7	176	LEU	2.8
14	m3	95	ILE	2.8
25	N4	91	LYS	2.8
28	n7	92	PHE	2.8
49	s3	188	ILE	2.8
50	S4	64	ILE	2.8
74	d8	30	VAL	2.8
78	sR	50	ASP	2.8
65	C9	142	GLU	2.8
52	s6	217	SER	2.8
50	S4	159	THR	2.8
75	D9	22	ARG	2.8
76	e0	53	LYS	2.8
7	L5	145	PHE	2.8
53	s7	89	HIS	2.8
66	d0	93	LEU	2.8
77	E1	146	SER	2.8
79	sM	41	SER	2.8
10	l8	151	VAL	2.8
45	6	506	A	2.8
49	S3	50	ILE	2.8
50	S4	46	VAL	2.8
57	C1	139	VAL	2.8
10	l8	196	ALA	2.8
45	6	233	C	2.8
14	M3	51	LEU	2.8
74	d8	33	LEU	2.8
75	D9	30	LEU	2.8
78	sR	92	TRP	2.8
11	L9	99	ILE	2.8
13	M1	123	PHE	2.8
49	S3	12	VAL	2.8
52	s6	145	PHE	2.8
58	c2	120	VAL	2.8
1	1	1351	U	2.8
28	N7	133	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
28	N7	80	LEU	2.8
54	s8	167	ALA	2.8
60	C4	78	ALA	2.8
78	SR	42	LEU	2.8
47	s1	84	ILE	2.8
52	S6	96	SER	2.8
64	C8	85	PHE	2.8
78	SR	193	ILE	2.8
58	c2	137	MET	2.8
77	e1	83	LYS	2.8
52	S6	212	LEU	2.8
78	SR	16	HIS	2.8
52	s6	27	PHE	2.8
73	D7	43	ILE	2.8
13	M1	108	GLU	2.8
73	D7	52	THR	2.8
13	M1	134	PRO	2.8
23	n2	105	LEU	2.8
46	S0	9	LEU	2.8
50	S4	8	HIS	2.8
58	c2	20	ALA	2.8
69	D3	132	LEU	2.8
50	s4	34	GLY	2.8
70	D4	58	PHE	2.8
46	s0	165	ARG	2.8
7	L5	2	ALA	2.8
10	L8	196	ALA	2.8
70	d4	44	LEU	2.8
13	M1	47	GLN	2.8
16	m5	59	PHE	2.8
25	N4	93	ARG	2.8
28	n7	13	VAL	2.8
32	O1	5	LYS	2.8
39	o8	42	LYS	2.8
47	S1	20	VAL	2.8
47	s1	140	ILE	2.8
58	C2	100	TRP	2.8
58	c2	76	GLU	2.8
24	n3	2	SER	2.8
49	S3	182	LEU	2.8
72	D6	64	LEU	2.8
78	sR	81	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
31	O0	105	ALA	2.8
51	S5	221	ALA	2.8
58	c2	118	ALA	2.8
59	C3	24	ALA	2.8
78	SR	119	ALA	2.8
47	S1	98	THR	2.8
45	6	1709	C	2.8
74	D8	14	LYS	2.8
78	sR	302	PHE	2.8
81	n4	69	LYS	2.8
59	c3	16	ILE	2.7
49	S3	23	GLU	2.7
63	C7	34	LEU	2.7
60	C4	100	ALA	2.7
60	C4	106	ALA	2.7
62	C6	142	TYR	2.7
51	S5	37	GLN	2.7
53	S7	181	ILE	2.7
55	S9	94	ASP	2.7
63	C7	83	GLN	2.7
50	S4	87	MET	2.7
52	S6	77	LEU	2.7
57	C1	115	PHE	2.7
60	C4	108	SER	2.7
28	N7	68	ILE	2.7
78	SR	294	TRP	2.7
27	n6	57	LEU	2.7
54	S8	96	LEU	2.7
58	c2	62	LEU	2.7
20	M9	51	VAL	2.7
54	S8	113	PHE	2.7
56	c0	20	VAL	2.7
68	D2	128	PHE	2.7
72	D6	6	ALA	2.7
78	SR	54	PHE	2.7
28	n7	68	ILE	2.7
50	S4	150	PRO	2.7
10	L8	122	LYS	2.7
28	N7	34	LYS	2.7
57	c1	24	LYS	2.7
77	e1	96	LYS	2.7
62	C6	52	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
49	s3	134	CYS	2.7
23	N2	28	PHE	2.7
10	L8	130	TYR	2.7
16	m5	3	ALA	2.7
16	m5	53	TYR	2.7
23	n2	17	VAL	2.7
49	S3	137	VAL	2.7
58	C2	92	ALA	2.7
25	N4	66	GLU	2.7
77	E1	104	SER	2.7
78	SR	169	ILE	2.7
49	S3	143	ARG	2.7
50	S4	15	PRO	2.7
68	D2	16	ASN	2.7
74	D8	27	GLN	2.7
37	o6	60	LEU	2.7
48	S2	225	LEU	2.7
49	s3	69	LEU	2.7
29	N8	110	GLY	2.7
50	s4	109	PHE	2.7
55	S9	146	PHE	2.7
60	C4	15	GLY	2.7
10	l8	140	VAL	2.7
14	m3	60	ALA	2.7
54	s8	168	CYS	2.7
56	c0	65	TYR	2.7
69	D3	92	CYS	2.7
74	D8	12	VAL	2.7
78	SR	6	VAL	2.7
29	N8	118	ILE	2.7
63	C7	41	ILE	2.7
54	S8	73	SER	2.7
48	S2	59	HIS	2.7
55	s9	59	LEU	2.7
47	S1	93	GLY	2.7
49	s3	167	PHE	2.7
49	s3	136	VAL	2.7
65	C9	18	TYR	2.7
78	sR	56	VAL	2.7
66	D0	22	ILE	2.7
66	d0	102	ARG	2.7
67	D1	42	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	1	1349	G	2.7
78	SR	222	LEU	2.7
50	s4	85	GLY	2.7
7	L5	125	VAL	2.7
23	n2	104	ARG	2.7
52	S6	97	VAL	2.7
57	C1	144	ALA	2.7
60	C4	118	VAL	2.7
27	N6	88	GLU	2.7
65	C9	50	ALA	2.7
78	sR	2	ALA	2.7
28	N7	72	ILE	2.7
66	d0	63	LEU	2.7
50	s4	245	LYS	2.7
54	s8	195	ARG	2.7
57	C1	29	LYS	2.7
45	2	228	G	2.7
45	2	501	U	2.7
56	C0	61	TRP	2.7
58	C2	30	VAL	2.7
4	l2	41	ILE	2.7
58	c2	23	THR	2.7
78	SR	188	ILE	2.7
13	M1	40	LEU	2.7
51	s5	156	ARG	2.7
67	d1	7	GLN	2.7
54	S8	186	GLY	2.7
61	C5	109	PRO	2.7
62	C6	74	HIS	2.7
10	l8	252	ASN	2.7
62	C6	63	ILE	2.7
70	D4	48	TYR	2.7
78	sR	303	ALA	2.7
5	l3	387	LEU	2.7
23	n2	16	THR	2.7
39	O8	15	THR	2.7
45	2	488	G	2.7
49	S3	218	LEU	2.7
72	D6	66	LYS	2.7
53	S7	22	GLN	2.7
63	c7	62	GLN	2.7
29	N8	83	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
55	S9	133	HIS	2.7
78	sR	240	VAL	2.7
41	Q0	78	ILE	2.7
1	5	2538	U	2.7
10	L8	32	LYS	2.7
10	l8	254	ASP	2.7
13	M1	172	LEU	2.7
50	S4	207	LEU	2.7
64	C8	145	ARG	2.7
43	Q2	106	PHE	2.7
28	N7	43	VAL	2.7
49	s3	39	VAL	2.7
54	S8	153	GLU	2.7
63	C7	118	PRO	2.7
78	sR	94	VAL	2.7
54	S8	106	ALA	2.7
60	C4	112	ILE	2.7
74	D8	10	ALA	2.7
78	SR	252	LEU	2.6
12	M0	199	PHE	2.6
23	n2	68	THR	2.6
69	d3	2	GLY	2.6
50	S4	71	LYS	2.6
52	S6	164	LYS	2.6
16	m5	55	ALA	2.6
49	S3	69	LEU	2.6
50	s4	92	LEU	2.6
60	C4	103	ARG	2.6
60	C4	105	LEU	2.6
73	D7	31	TYR	2.6
10	L8	94	PHE	2.6
57	C1	22	ASN	2.6
54	S8	181	GLY	2.6
62	C6	56	GLY	2.6
70	D4	67	GLY	2.6
49	S3	38	GLU	2.6
73	D7	45	THR	2.6
76	e0	45	VAL	2.6
76	e0	48	THR	2.6
16	M5	148	TYR	2.6
48	S2	178	ILE	2.6
49	S3	76	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
64	C8	54	LEU	2.6
72	D6	83	ILE	2.6
28	N7	122	HIS	2.6
78	SR	251	TRP	2.6
28	N7	12	VAL	2.6
45	6	656	G	2.6
47	S1	215	VAL	2.6
61	C5	70	ASN	2.6
62	C6	90	VAL	2.6
79	SM	86	ASN	2.6
46	S0	17	LEU	2.6
50	s4	162	ILE	2.6
61	C5	96	ILE	2.6
65	C9	66	TYR	2.6
66	d0	26	LEU	2.6
5	L3	294	GLY	2.6
47	S1	226	GLY	2.6
55	S9	85	VAL	2.6
13	M1	90	GLN	2.6
29	n8	118	ILE	2.6
50	s4	84	ALA	2.6
52	S6	52	ILE	2.6
53	S7	81	LEU	2.6
61	C5	112	LEU	2.6
78	SR	310	ILE	2.6
7	L5	175	HIS	2.6
52	S6	112	VAL	2.6
70	D4	2	SER	2.6
45	2	500	C	2.6
64	C8	6	GLN	2.6
52	s6	3	LEU	2.6
62	C6	43	ILE	2.6
79	SM	151	LEU	2.6
11	L9	88	TYR	2.6
70	D4	72	PHE	2.6
28	n7	74	VAL	2.6
29	N8	72	VAL	2.6
51	S5	133	VAL	2.6
54	S8	102	VAL	2.6
54	s8	63	GLY	2.6
65	C9	71	VAL	2.6
16	M5	36	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
27	n6	35	LEU	2.6
31	o0	43	ILE	2.6
33	o2	128	LEU	2.6
49	s3	185	LYS	2.6
73	d7	41	LEU	2.6
78	SR	122	ILE	2.6
54	S8	144	ALA	2.6
14	M3	126	PHE	2.6
56	c0	66	TYR	2.6
46	S0	185	ARG	2.6
61	C5	45	PHE	2.6
49	s3	216	PRO	2.6
37	o6	66	GLU	2.6
58	C2	21	GLU	2.6
14	M3	95	ILE	2.6
14	m3	68	LYS	2.6
46	S0	144	ILE	2.6
46	S0	170	ILE	2.6
47	S1	228	LEU	2.6
52	S6	30	LYS	2.6
52	s6	113	ILE	2.6
55	S9	36	LEU	2.6
79	SM	23	LYS	2.6
20	m9	39	ASN	2.6
39	O8	41	THR	2.6
45	6	678	A	2.6
51	S5	176	THR	2.6
67	D1	20	THR	2.6
28	n7	45	GLY	2.6
78	SR	15	GLY	2.6
50	S4	128	LYS	2.6
36	O5	118	ILE	2.6
51	S5	194	LEU	2.6
53	S7	91	ILE	2.6
71	D5	65	LEU	2.6
55	S9	132	ARG	2.6
11	L9	190	ASP	2.6
21	N0	75	PHE	2.6
28	N7	130	PHE	2.6
75	d9	52	PHE	2.6
78	SR	172	ALA	2.6
10	l8	146	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
28	N7	23	VAL	2.6
28	N7	116	LYS	2.6
28	n7	28	PRO	2.6
35	O4	78	GLY	2.6
58	C2	80	ASN	2.6
52	s6	36	VAL	2.6
66	D0	62	VAL	2.6
7	L5	171	LEU	2.6
18	M7	175	ARG	2.6
26	n5	82	LEU	2.6
36	O5	92	LEU	2.6
49	S3	84	ILE	2.6
63	C7	115	LEU	2.6
68	d2	14	ILE	2.6
47	S1	92	GLN	2.6
55	S9	145	SER	2.6
55	S9	177	ALA	2.6
70	d4	119	PHE	2.6
49	s3	175	VAL	2.6
71	D5	94	LYS	2.6
10	L8	129	PRO	2.6
13	M1	19	LEU	2.6
49	S3	90	ARG	2.6
78	SR	99	THR	2.6
22	N1	122	GLN	2.6
32	O1	90	PHE	2.6
28	n7	73	LYS	2.6
31	O0	69	TYR	2.6
58	c2	143	GLN	2.6
61	C5	74	ALA	2.6
73	D7	51	GLN	2.6
45	2	194	U	2.6
78	SR	318	ALA	2.6
51	S5	212	LYS	2.6
7	L5	53	VAL	2.6
56	c0	21	VAL	2.6
57	c1	140	VAL	2.6
58	c2	117	GLY	2.6
69	D3	130	VAL	2.6
78	SR	116	ASP	2.6
82	p0	104	ARG	2.6
23	n2	101	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
28	n7	5	LEU	2.6
46	s0	177	LEU	2.6
57	c1	40	LEU	2.6
67	D1	8	LEU	2.6
27	N6	45	ILE	2.6
37	O6	94	ILE	2.6
59	C3	16	ILE	2.6
72	D6	30	ILE	2.6
30	n9	59	LYS	2.5
78	SR	137	LYS	2.5
58	C2	132	GLU	2.5
50	S4	100	ARG	2.5
55	S9	113	VAL	2.5
53	s7	67	LEU	2.5
79	SM	14	ASP	2.5
7	l5	290	ILE	2.5
23	n2	41	ILE	2.5
71	D5	55	PRO	2.5
51	S5	69	PHE	2.5
37	o6	99	ARG	2.5
72	D6	89	ARG	2.5
28	N7	87	LEU	2.5
29	N8	111	LYS	2.5
62	C6	51	PRO	2.5
64	C8	14	ILE	2.5
71	D5	85	LYS	2.5
14	M3	192	GLU	2.5
47	S1	136	ARG	2.5
21	N0	78	TRP	2.5
35	O4	33	GLN	2.5
37	O6	66	GLU	2.5
73	D7	64	CYS	2.5
79	SM	87	THR	2.5
10	l8	132	VAL	2.5
57	c1	147	GLY	2.5
58	C2	40	GLY	2.5
55	S9	76	LEU	2.5
60	c4	33	LEU	2.5
64	C8	3	LEU	2.5
72	D6	3	LYS	2.5
35	O4	7	PHE	2.5
57	c1	115	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
14	m3	152	THR	2.5
16	M5	30	TYR	2.5
36	o5	2	ALA	2.5
48	S2	143	TYR	2.5
5	L3	91	GLY	2.5
32	O1	49	VAL	2.5
55	s9	85	VAL	2.5
62	C6	11	GLY	2.5
66	D0	42	VAL	2.5
67	d1	82	VAL	2.5
27	n6	126	LEU	2.5
36	o5	115	LYS	2.5
64	C8	80	LYS	2.5
55	S9	3	ARG	2.5
64	C8	11	PHE	2.5
10	l8	167	PRO	2.5
1	1	1571	A	2.5
55	S9	68	LYS	2.5
56	C0	57	THR	2.5
58	c2	116	VAL	2.5
60	c4	42	VAL	2.5
11	l9	191	LEU	2.5
20	M9	142	ILE	2.5
29	N8	82	ILE	2.5
47	s1	100	PHE	2.5
50	s4	47	PHE	2.5
57	C1	128	CYS	2.5
67	D1	24	ILE	2.5
75	d9	50	ILE	2.5
77	E1	131	PHE	2.5
47	s1	23	PRO	2.5
49	S3	216	PRO	2.5
78	SR	166	SER	2.5
58	c2	91	VAL	2.5
66	d0	97	VAL	2.5
82	p0	49	ALA	2.5
37	o6	77	LEU	2.5
50	s4	164	LEU	2.5
82	p0	45	LEU	2.5
50	s4	146	THR	2.5
51	S5	185	ARG	2.5
55	S9	147	MET	2.5

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Mol	Chain	Res	Type	RSRZ
62	c6	29	ILE	2.5
50	S4	62	LYS	2.5
77	e1	149	LYS	2.5
13	M1	45	PRO	2.5
47	S1	43	VAL	2.5
49	S3	35	SER	2.5
52	S6	33	GLY	2.5
56	c0	64	TYR	2.5
60	C4	50	ALA	2.5
16	m5	15	GLN	2.5
32	O1	71	LEU	2.5
43	Q2	72	LEU	2.5
43	Q2	102	GLN	2.5
45	2	240	U	2.5
47	s1	64	ARG	2.5
64	C8	120	ARG	2.5
81	n4	96	LEU	2.5
46	S0	107	PHE	2.5
70	D4	34	ASN	2.5
78	sR	294	TRP	2.5
55	S9	77	ILE	2.5
75	D9	50	ILE	2.5
32	O1	78	LYS	2.5
1	5	2441	A	2.5
28	N7	125	GLY	2.5
54	s8	192	TYR	2.5
55	S9	148	VAL	2.5
39	o8	73	LEU	2.5
65	C9	41	SER	2.5
79	sM	52	PRO	2.5
13	M1	109	HIS	2.5
52	S6	27	PHE	2.5
13	M1	106	ILE	2.5
39	o8	5	ILE	2.5
50	S4	245	LYS	2.5
74	d8	43	ASN	2.5
66	d0	13	GLU	2.5
76	e0	56	MET	2.5
55	S9	174	ARG	2.5
11	L9	191	LEU	2.5
23	N2	33	TYR	2.5
32	o1	71	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
39	o8	31	LEU	2.5
65	C9	9	VAL	2.5
35	o4	19	LYS	2.5
58	C2	139	HIS	2.5
47	S1	52	THR	2.5
18	M7	158	ALA	2.5
46	S0	74	VAL	2.5
49	s3	72	LEU	2.5
61	C5	93	VAL	2.5
70	d4	25	VAL	2.5
74	d8	54	LEU	2.5
43	Q2	76	LYS	2.5
60	c4	96	PRO	2.5
66	d0	14	GLN	2.5
71	D5	97	LYS	2.5
32	o1	75	ILE	2.5
51	s5	29	ILE	2.5
53	S7	60	ILE	2.5
50	S4	191	ARG	2.5
13	M1	148	VAL	2.5
16	M5	135	VAL	2.5
29	N8	123	VAL	2.5
10	l8	245	LYS	2.5
28	N7	60	LYS	2.5
29	N8	127	ALA	2.5
32	O1	92	TYR	2.5
46	S0	138	TYR	2.5
47	S1	86	LEU	2.5
60	C4	121	VAL	2.5
47	S1	141	ALA	2.5
55	S9	119	ALA	2.5
78	SR	210	LEU	2.5
16	m5	45	PRO	2.5
56	C0	17	GLN	2.5
7	L5	60	ILE	2.5
47	s1	82	ARG	2.5
60	C4	84	ARG	2.5
68	D2	14	ILE	2.5
69	D3	145	SER	2.5
20	m9	53	LYS	2.4
26	n5	107	VAL	2.4
60	C4	98	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
64	C8	52	VAL	2.4
64	C8	116	LEU	2.4
70	d4	57	VAL	2.4
73	D7	40	CYS	2.4
74	D8	54	LEU	2.4
64	C8	79	TYR	2.4
35	O4	93	PHE	2.4
69	D3	95	PHE	2.4
61	C5	106	GLU	2.4
20	m9	23	TRP	2.4
28	n7	87	LEU	2.4
52	s6	79	LYS	2.4
55	S9	86	LEU	2.4
62	c6	54	LEU	2.4
70	D4	35	VAL	2.4
70	d4	35	VAL	2.4
45	2	506	A	2.4
54	S8	138	ASN	2.4
79	SM	154	TYR	2.4
82	p0	60	ARG	2.4
50	S4	173	ILE	2.4
54	S8	103	GLN	2.4
78	SR	283	LYS	2.4
10	l8	169	LEU	2.4
13	M1	129	VAL	2.4
14	m3	57	VAL	2.4
50	S4	160	VAL	2.4
53	S7	62	VAL	2.4
65	C9	53	TRP	2.4
14	m3	193	ALA	2.4
48	S2	231	ALA	2.4
48	s2	97	ARG	2.4
49	S3	153	ALA	2.4
54	S8	150	ALA	2.4
13	M1	79	ILE	2.4
27	N6	116	LYS	2.4
28	N7	102	GLU	2.4
32	O1	75	ILE	2.4
45	6	679	U	2.4
47	S1	171	ILE	2.4
61	C5	107	ILE	2.4
71	d5	50	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
75	d9	31	ILE	2.4
46	S0	166	GLY	2.4
58	c2	45	LEU	2.4
62	C6	120	ASP	2.4
54	S8	22	ARG	2.4
54	S8	112	TRP	2.4
74	D8	22	ARG	2.4
16	M5	59	PHE	2.4
50	s4	182	TYR	2.4
31	O0	94	GLU	2.4
32	o1	61	LYS	2.4
54	S8	61	GLU	2.4
66	D0	83	GLU	2.4
10	L8	123	GLN	2.4
35	o4	105	VAL	2.4
46	S0	188	LEU	2.4
55	S9	179	ARG	2.4
56	c0	19	GLY	2.4
77	E1	102	VAL	2.4
63	C7	103	ASP	2.4
64	C8	23	ASP	2.4
79	sM	101	ASP	2.4
28	n7	131	PHE	2.4
50	S4	235	TYR	2.4
53	S7	70	PHE	2.4
54	S8	147	ALA	2.4
77	e1	104	SER	2.4
39	o8	27	ILE	2.4
56	c0	70	GLU	2.4
10	l8	186	LEU	2.4
61	C5	10	ARG	2.4
67	D1	15	ARG	2.4
68	D2	126	LEU	2.4
72	D6	86	VAL	2.4
78	sR	74	THR	2.4
78	sR	141	LEU	2.4
14	m3	179	PHE	2.4
47	S1	219	LYS	2.4
63	C7	116	LYS	2.4
49	S3	19	ALA	2.4
75	D9	7	TRP	2.4
28	N7	120	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
54	s8	38	ILE	2.4
53	S7	99	LEU	2.4
56	C0	3	MET	2.4
63	C7	16	LEU	2.4
63	C7	24	LEU	2.4
61	C5	95	GLY	2.4
68	D2	63	VAL	2.4
73	D7	4	VAL	2.4
78	SR	177	MET	2.4
15	M4	137	LYS	2.4
32	o1	5	LYS	2.4
79	SM	167	PRO	2.4
31	O0	59	TYR	2.4
39	o8	52	TYR	2.4
48	s2	110	HIS	2.4
51	s5	155	ALA	2.4
53	S7	134	GLU	2.4
65	C9	49	ASP	2.4
14	M3	140	SER	2.4
29	N8	124	ILE	2.4
51	S5	114	ILE	2.4
52	s6	5	ILE	2.4
54	S8	171	SER	2.4
63	C7	112	SER	2.4
66	d0	19	ILE	2.4
74	d8	22	ARG	2.4
77	e1	91	ILE	2.4
10	L8	142	LEU	2.4
49	S3	109	LEU	2.4
7	L5	170	GLY	2.4
10	L8	151	VAL	2.4
18	M7	172	GLN	2.4
21	N0	141	LYS	2.4
49	S3	206	VAL	2.4
56	C0	82	LEU	2.4
50	s4	124	GLY	2.4
57	C1	126	GLY	2.4
10	l8	80	TYR	2.4
27	N6	115	ARG	2.4
64	C8	16	ARG	2.4
69	D3	48	HIS	2.4
78	SR	303	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
54	s8	60	ILE	2.4
65	C9	15	ILE	2.4
1	1	1017	C	2.4
1	5	1762	C	2.4
63	C7	109	LEU	2.4
73	D7	3	LEU	2.4
72	D6	65	PRO	2.4
46	S0	110	TYR	2.4
13	M1	152	HIS	2.4
21	n0	2	ALA	2.4
61	c5	101	ALA	2.4
76	E0	43	ARG	2.4
82	p0	44	GLU	2.4
6	l4	150	LEU	2.4
20	m9	21	LYS	2.4
25	N4	74	LYS	2.4
49	S3	7	LYS	2.4
49	s3	86	LEU	2.4
51	S5	25	LEU	2.4
53	s7	44	LYS	2.4
66	d0	88	LYS	2.4
69	D3	2	GLY	2.4
78	SR	194	GLY	2.4
1	1	1284	C	2.4
50	S4	26	CYS	2.4
54	s8	179	CYS	2.4
10	l8	240	ASN	2.4
35	O4	6	THR	2.4
50	s4	128	LYS	2.4
51	S5	195	ALA	2.4
61	C5	14	THR	2.4
65	C9	59	ALA	2.4
77	E1	151	ASN	2.4
49	S3	184	ILE	2.4
52	s6	18	ILE	2.4
81	n4	90	ILE	2.4
16	m5	10	LEU	2.4
50	s4	131	LEU	2.4
23	n2	66	VAL	2.4
45	6	238	U	2.4
52	S6	31	ARG	2.4
54	S8	146	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
12	M0	219	ALA	2.4
28	N7	21	LYS	2.4
57	c1	36	LYS	2.4
57	c1	59	PRO	2.4
64	C8	7	GLU	2.4
36	o5	75	TYR	2.4
39	o8	2	ALA	2.4
76	E0	58	PRO	2.4
23	n2	61	THR	2.4
40	O9	43	ASN	2.4
51	S5	79	ASN	2.4
58	c2	34	THR	2.4
23	N2	56	VAL	2.3
47	S1	102	GLY	2.3
62	C6	46	PHE	2.3
70	D4	66	GLY	2.3
28	N7	128	GLN	2.3
49	S3	179	GLN	2.3
66	d0	98	GLN	2.3
74	d8	32	PHE	2.3
45	2	73	U	2.3
49	s3	75	LYS	2.3
78	SR	124	SER	2.3
16	M5	137	PRO	2.3
28	N7	49	TYR	2.3
47	S1	193	ILE	2.3
54	S8	101	ILE	2.3
58	c2	112	ALA	2.3
69	D3	85	ALA	2.3
72	D6	35	ALA	2.3
64	C8	15	LEU	2.3
66	D0	93	LEU	2.3
76	E0	39	LEU	2.3
4	l2	252	THR	2.3
60	c4	29	HIS	2.3
78	SR	184	ASN	2.3
56	C0	29	GLN	2.3
57	C1	118	GLN	2.3
58	C2	90	LYS	2.3
66	D0	69	LYS	2.3
75	D9	54	LYS	2.3
81	n4	102	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
4	l2	112	ILE	2.3
31	o0	41	LEU	2.3
35	o4	2	ALA	2.3
46	S0	122	ILE	2.3
50	S4	27	TYR	2.3
50	s4	147	ILE	2.3
77	e1	148	TYR	2.3
78	SR	284	ALA	2.3
78	sR	73	LEU	2.3
78	sR	115	ILE	2.3
78	sR	193	ILE	2.3
7	L5	3	PHE	2.3
13	M1	36	VAL	2.3
13	M1	155	THR	2.3
14	m3	94	GLY	2.3
28	N7	40	HIS	2.3
46	S0	21	ASN	2.3
48	s2	63	VAL	2.3
50	S4	57	ASN	2.3
55	s9	148	VAL	2.3
62	C6	48	VAL	2.3
57	C1	26	LYS	2.3
57	C1	42	PHE	2.3
62	C6	88	GLY	2.3
64	C8	133	VAL	2.3
74	d8	41	VAL	2.3
82	p0	86	PHE	2.3
26	n5	50	ALA	2.3
45	6	707	A	2.3
50	S4	162	ILE	2.3
54	S8	170	SER	2.3
75	d9	36	LEU	2.3
78	sR	254	ALA	2.3
35	O4	65	VAL	2.3
39	o8	35	GLY	2.3
54	S8	46	VAL	2.3
55	s9	158	PHE	2.3
57	C1	64	VAL	2.3
69	D3	4	GLY	2.3
78	SR	315	VAL	2.3
6	l4	262	TRP	2.3
72	D6	39	MET	2.3

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Mol	Chain	Res	Type	RSRZ
73	D7	19	HIS	2.3
64	C8	12	GLN	2.3
70	D4	22	GLN	2.3
74	D8	26	THR	2.3
1	1	1226	G	2.3
16	m5	129	TYR	2.3
26	N5	103	TYR	2.3
29	N8	109	TYR	2.3
31	O0	62	LEU	2.3
48	S2	69	ILE	2.3
54	S8	198	ALA	2.3
54	s8	100	ALA	2.3
55	S9	4	ALA	2.3
55	s9	128	LEU	2.3
68	D2	125	ILE	2.3
74	D8	40	ILE	2.3
20	M9	52	LYS	2.3
28	N7	75	VAL	2.3
50	S4	181	VAL	2.3
55	s9	101	VAL	2.3
52	S6	1	MET	2.3
28	N7	100	THR	2.3
66	D0	15	GLN	2.3
66	d0	16	GLN	2.3
72	D6	5	ARG	2.3
51	S5	119	ASP	2.3
6	l4	249	ILE	2.3
10	L8	166	LEU	2.3
26	N5	121	LYS	2.3
37	O6	95	ALA	2.3
50	S4	90	ILE	2.3
51	s5	84	LYS	2.3
54	S8	166	TYR	2.3
64	C8	42	TYR	2.3
64	C8	66	LEU	2.3
81	n4	128	ALA	2.3
50	S4	226	PHE	2.3
55	S9	34	PHE	2.3
55	S9	121	SER	2.3
65	C9	21	PHE	2.3
66	d0	31	VAL	2.3
73	D7	39	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
60	C4	99	GLN	2.3
78	SR	150	TRP	2.3
10	l8	136	LEU	2.3
23	N2	11	ILE	2.3
27	n6	104	LEU	2.3
29	N8	75	LEU	2.3
41	Q0	82	LEU	2.3
28	n7	41	ALA	2.3
62	C6	24	ALA	2.3
70	D4	13	ILE	2.3
71	D5	48	ASP	2.3
28	N7	136	PHE	2.3
55	S9	122	VAL	2.3
48	s2	95	ARG	2.3
53	S7	48	GLU	2.3
65	C9	47	PRO	2.3
72	D6	92	ARG	2.3
26	n5	36	LYS	2.3
49	S3	105	MET	2.3
1	1	3275	U	2.3
10	L8	52	TRP	2.3
36	o5	9	LEU	2.3
49	S3	110	LEU	2.3
50	s4	18	TRP	2.3
51	S5	46	TRP	2.3
52	S6	5	ILE	2.3
64	C8	61	LEU	2.3
57	c1	124	THR	2.3
50	S4	105	VAL	2.3
74	d8	67	ARG	2.3
75	D9	40	ARG	2.3
4	l2	36	GLU	2.3
10	l8	89	GLU	2.3
31	O0	64	LYS	2.3
49	S3	213	GLU	2.3
77	E1	88	PRO	2.3
50	S4	41	SER	2.3
67	d1	1	MET	2.3
68	D2	72	CYS	2.3
36	o5	80	LEU	2.3
70	d4	28	LEU	2.3
27	n6	43	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
50	S4	86	PHE	2.3
50	s4	82	TYR	2.3
78	sR	136	ILE	2.3
28	N7	88	ASP	2.3
28	n7	12	VAL	2.3
74	d8	29	ARG	2.3
78	SR	2	ALA	2.3
47	s1	98	THR	2.3
66	d0	107	THR	2.3
74	D8	31	GLU	2.3
23	n2	76	LEU	2.3
23	n2	97	SER	2.3
54	s8	66	SER	2.3
13	M1	21	ILE	2.3
51	S5	137	ILE	2.3
1	5	3154	C	2.3
28	N7	114	VAL	2.3
48	S2	103	VAL	2.3
50	s4	225	VAL	2.3
51	s5	148	ARG	2.3
55	S9	53	ARG	2.3
55	s9	104	PHE	2.3
58	C2	22	VAL	2.3
65	C9	58	ALA	2.3
78	SR	154	VAL	2.3
27	N6	107	THR	2.3
27	n6	44	GLY	2.3
50	S4	74	GLY	2.3
50	s4	260	GLY	2.3
56	C0	25	LYS	2.3
69	D3	3	LYS	2.3
78	SR	261	LYS	2.3
50	S4	230	GLU	2.3
72	D6	61	GLU	2.3
22	N1	148	PRO	2.3
1	5	2443	A	2.3
37	o6	11	LEU	2.3
64	C8	76	PRO	2.3
68	D2	94	LEU	2.3
29	N8	87	ARG	2.3
47	S1	213	ARG	2.3
66	D0	68	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
6	l4	207	VAL	2.3
10	l8	164	VAL	2.3
13	M1	96	PHE	2.3
48	S2	111	VAL	2.3
49	S3	174	HIS	2.3
50	S4	70	VAL	2.3
61	C5	9	LYS	2.3
82	p0	216	ALA	2.3
20	m9	188	ASP	2.3
47	S1	42	ASN	2.3
17	M6	110	PRO	2.3
47	s1	188	LEU	2.3
68	D2	41	MET	2.3
71	D5	51	LEU	2.3
4	L2	76	PHE	2.3
66	d0	65	ILE	2.3
35	o4	23	VAL	2.3
49	S3	221	SER	2.3
66	D0	51	VAL	2.3
62	C6	25	GLY	2.2
73	D7	53	ALA	2.3
48	S2	55	GLU	2.2
71	D5	84	GLU	2.2
20	M9	138	LEU	2.2
48	S2	44	LEU	2.2
58	C2	107	ASP	2.2
1	1	1016	C	2.2
11	L9	144	ILE	2.2
39	o8	37	PRO	2.2
57	C1	141	LYS	2.2
68	D2	103	ILE	2.2
70	d4	7	ILE	2.2
7	L5	100	ALA	2.2
26	n5	46	TYR	2.2
58	c2	63	VAL	2.2
70	D4	24	VAL	2.2
54	s8	84	HIS	2.2
70	D4	71	GLY	2.2
78	SR	227	ALA	2.2
72	D6	82	ARG	2.2
39	o8	36	LYS	2.2
55	S9	59	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
60	C4	33	LEU	2.2
7	l5	109	THR	2.2
23	N2	68	THR	2.2
45	6	228	G	2.2
57	C1	124	THR	2.2
79	sM	50	ASN	2.2
82	p0	38	MET	2.2
64	C8	81	ILE	2.2
82	p0	100	ILE	2.2
4	l2	118	GLU	2.2
26	N5	23	ALA	2.2
27	n6	66	GLN	2.2
60	C4	101	ALA	2.2
68	d2	122	SER	2.2
74	d8	21	SER	2.2
82	p0	215	SER	2.2
30	N9	32	LEU	2.2
50	S4	42	LEU	2.2
65	c9	28	LEU	2.2
73	d7	8	LEU	2.2
77	E1	143	LYS	2.2
78	SR	13	LEU	2.2
24	N3	4	ASN	2.2
10	l8	159	PRO	2.2
70	d4	24	VAL	2.2
78	sR	271	VAL	2.2
7	L5	129	TYR	2.2
35	o4	33	GLN	2.2
36	O5	75	TYR	2.2
49	S3	119	ALA	2.2
67	D1	12	TYR	2.2
81	n4	85	ALA	2.2
21	N0	136	LYS	2.2
28	N7	93	LYS	2.2
10	L8	150	LEU	2.2
55	S9	162	SER	2.2
63	C7	125	SER	2.2
46	s0	48	ILE	2.2
54	s8	156	VAL	2.2
56	C0	86	ILE	2.2
73	D7	79	PHE	2.2
49	S3	41	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
60	C4	16	VAL	2.2
63	c7	9	VAL	2.2
75	D9	23	VAL	2.2
78	SR	123	ILE	2.2
32	O1	50	ARG	2.2
45	2	505	A	2.2
49	S3	173	ARG	2.2
53	s7	48	GLU	2.2
78	SR	317	THR	2.2
78	SR	71	CYS	2.2
78	SR	187	GLN	2.2
82	p0	18	TYR	2.2
22	n1	31	LEU	2.2
71	D5	75	LEU	2.2
1	1	1024	G	2.2
14	M3	93	ILE	2.2
16	m5	21	PHE	2.2
12	M0	50	VAL	2.2
14	m3	58	VAL	2.2
19	m8	93	ILE	2.2
26	n5	95	ILE	2.2
63	c7	71	PHE	2.2
49	s3	58	VAL	2.2
57	C1	125	VAL	2.2
61	C5	76	VAL	2.2
68	D2	74	VAL	2.2
16	M5	56	LYS	2.2
18	M7	159	LYS	2.2
22	N1	65	TYR	2.2
39	O8	21	LYS	2.2
46	s0	161	PRO	2.2
50	S4	167	GLY	2.2
50	S4	239	PRO	2.2
68	D2	21	GLY	2.2
77	e1	127	GLY	2.2
58	C2	142	GLN	2.2
73	d7	40	CYS	2.2
82	p0	77	LEU	2.2
64	C8	55	HIS	2.2
26	N5	84	PHE	2.2
10	L8	128	LYS	2.2
24	N3	137	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
31	O0	39	SER	2.2
37	O6	9	ILE	2.2
64	C8	43	SER	2.2
71	D5	49	ARG	2.2
72	D6	36	ILE	2.2
71	D5	73	GLY	2.2
26	n5	90	ALA	2.2
37	o6	8	ALA	2.2
78	SR	36	ALA	2.2
23	n2	79	LEU	2.2
39	o8	14	LEU	2.2
47	S1	95	ASN	2.2
58	C2	84	ASN	2.2
62	C6	28	LEU	2.2
65	C9	105	LEU	2.2
10	L8	120	LYS	2.2
46	s0	23	HIS	2.2
50	S4	6	LYS	2.2
57	c1	57	LYS	2.2
79	SM	89	ARG	2.2
21	N0	77	VAL	2.2
28	N7	53	VAL	2.2
46	S0	139	VAL	2.2
51	s5	137	ILE	2.2
52	s6	158	ILE	2.2
51	S5	181	GLU	2.2
57	C1	117	VAL	2.2
60	c4	79	VAL	2.2
39	O8	2	ALA	2.2
56	c0	41	TYR	2.2
48	s2	58	LEU	2.2
59	C3	135	LEU	2.2
63	c7	83	GLN	2.2
39	o8	44	LYS	2.2
61	C5	59	LYS	2.2
72	D6	8	ASN	2.2
28	n7	57	HIS	2.2
50	S4	244	ILE	2.2
12	m0	207	GLU	2.2
16	m5	66	VAL	2.2
59	C3	123	HIS	2.2
63	c7	66	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
65	C9	64	HIS	2.2
74	D8	55	VAL	2.2
78	sR	134	TRP	2.2
79	sM	110	TRP	2.2
10	l8	177	TYR	2.2
51	S5	61	TYR	2.2
16	M5	10	LEU	2.2
25	N4	54	LEU	2.2
31	O0	93	LEU	2.2
31	O0	101	LEU	2.2
54	S8	79	ALA	2.2
20	M9	117	LYS	2.2
32	O1	10	ARG	2.2
35	o4	51	LEU	2.2
37	O6	98	ARG	2.2
55	S9	90	LYS	2.2
63	c7	103	ASP	2.2
73	d7	51	GLN	2.2
78	sR	46	LYS	2.2
10	L8	27	THR	2.2
50	S4	91	THR	2.2
57	c1	19	ILE	2.2
58	c2	123	VAL	2.2
72	D6	90	GLU	2.2
70	d4	66	GLY	2.2
10	L8	113	ALA	2.2
10	l8	29	SER	2.2
27	N6	35	LEU	2.2
39	o8	33	LYS	2.2
45	6	1708	U	2.2
46	S0	146	LEU	2.2
48	s2	229	LEU	2.2
51	S5	180	ARG	2.2
55	s9	118	LEU	2.2
56	c0	15	LEU	2.2
10	l8	77	GLN	2.2
37	o6	52	PRO	2.2
55	S9	157	ASP	2.2
70	D4	135	ASP	2.2
78	SR	61	PHE	2.2
50	S4	76	VAL	2.2
63	C7	17	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
63	c7	61	ILE	2.2
47	S1	33	LYS	2.2
81	n4	110	LYS	2.2
28	N7	94	SER	2.2
45	6	655	G	2.2
66	d0	12	GLN	2.2
48	S2	171	PRO	2.2
78	sR	54	PHE	2.2
12	M0	190	VAL	2.2
74	d8	53	ILE	2.2
35	O4	70	LYS	2.2
50	S4	198	LYS	2.2
50	s4	16	HIS	2.2
50	s4	161	LYS	2.2
71	D5	70	LYS	2.2
78	SR	106	HIS	2.2
78	SR	138	GLY	2.2
47	s1	184	LEU	2.1
50	S4	92	LEU	2.1
55	S9	49	LEU	2.1
64	c8	18	LEU	2.1
7	l5	291	ALA	2.1
45	2	484	C	2.1
67	d1	54	ALA	2.1
10	L8	218	ILE	2.1
25	N4	82	ILE	2.1
35	O4	22	VAL	2.1
55	s9	136	VAL	2.1
62	C6	40	GLU	2.1
64	C8	28	ILE	2.1
76	E0	50	VAL	2.1
79	sM	49	LYS	2.1
22	N1	30	TYR	2.1
32	O1	73	LEU	2.1
46	S0	176	LEU	2.1
47	s1	54	LEU	2.1
48	S2	41	LEU	2.1
54	S8	192	TYR	2.1
56	C0	40	LEU	2.1
57	C1	5	LEU	2.1
53	s7	94	ALA	2.1
62	C6	3	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
54	S8	21	PHE	2.1
70	D4	85	PHE	2.1
43	Q2	99	GLN	2.1
14	m3	180	ARG	2.1
25	N4	95	SER	2.1
28	n7	62	VAL	2.1
50	S4	256	ARG	2.1
51	s5	157	ARG	2.1
54	s8	183	ILE	2.1
45	2	836	U	2.1
64	C8	24	GLY	2.1
10	L8	65	LEU	2.1
9	L7	244	ASN	2.1
28	n7	83	THR	2.1
31	o0	68	TYR	2.1
46	S0	195	TRP	2.1
53	S7	71	HIS	2.1
1	1	1285	G	2.1
48	s2	224	PHE	2.1
53	S7	171	ALA	2.1
67	D1	54	ALA	2.1
67	d1	81	ASN	2.1
68	D2	70	ASN	2.1
73	D7	71	ALA	2.1
56	c0	25	LYS	2.1
57	C1	88	ARG	2.1
16	M5	61	ILE	2.1
29	N8	102	ILE	2.1
49	s3	123	VAL	2.1
58	c2	129	GLU	2.1
74	D8	34	GLU	2.1
82	p0	4	ILE	2.1
28	n7	70	PRO	2.1
1	1	1353	U	2.1
6	l4	187	LEU	2.1
50	S4	19	LEU	2.1
65	C9	143	ASP	2.1
78	SR	191	ASP	2.1
79	SM	155	LEU	2.1
13	M1	163	PHE	2.1
28	N7	101	PHE	2.1
56	C0	59	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
65	c9	14	PHE	2.1
65	c9	18	TYR	2.1
50	S4	252	ARG	2.1
66	d0	21	LYS	2.1
67	D1	17	CYS	2.1
68	D2	60	LYS	2.1
78	SR	224	ASN	2.1
7	L5	296	GLN	2.1
31	o0	39	SER	2.1
45	6	1228	G	2.1
57	C1	91	LEU	2.1
79	SM	28	SER	2.1
28	n7	135	ARG	2.1
44	Q3	36	ARG	2.1
50	S4	175	PHE	2.1
54	s8	57	ALA	2.1
58	c2	101	ALA	2.1
66	d0	45	ALA	2.1
4	L2	146	THR	2.1
41	Q0	90	ASN	2.1
22	N1	39	ILE	2.1
46	S0	156	VAL	2.1
61	C5	50	THR	2.1
68	D2	18	GLU	2.1
68	D2	40	VAL	2.1
77	E1	125	THR	2.1
81	n4	106	GLU	2.1
48	s2	89	GLN	2.1
53	s7	5	GLN	2.1
55	s9	112	GLN	2.1
58	C2	143	GLN	2.1
58	c2	89	ILE	2.1
82	p0	51	VAL	2.1
39	O8	73	LEU	2.1
61	C5	57	MET	2.1
61	C5	73	PRO	2.1
14	m3	115	ARG	2.1
66	d0	52	LYS	2.1
69	D3	11	SER	2.1
77	E1	119	ARG	2.1
77	e1	90	LYS	2.1
27	n6	33	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
33	O2	2	ALA	2.1
61	c5	4	ALA	2.1
44	Q3	71	VAL	2.1
55	S9	124	HIS	2.1
7	L5	4	GLN	2.1
39	o8	15	THR	2.1
51	S5	186	ASN	2.1
58	c2	72	ILE	2.1
70	d4	118	ILE	2.1
4	L2	32	LEU	2.1
10	l8	211	LEU	2.1
21	N0	76	GLY	2.1
58	C2	104	GLY	2.1
64	C8	144	ARG	2.1
78	SR	202	LEU	2.1
10	l8	176	PRO	2.1
60	C4	11	SER	2.1
28	N7	117	ALA	2.1
62	c6	92	TYR	2.1
46	S0	12	GLU	2.1
16	m5	142	ILE	2.1
19	m8	81	VAL	2.1
21	N0	130	GLU	2.1
78	SR	76	ASP	2.1
14	m3	93	ILE	2.1
50	s4	183	VAL	2.1
65	C9	36	ILE	2.1
67	D1	36	VAL	2.1
68	D2	27	ILE	2.1
71	d5	60	VAL	2.1
78	SR	271	VAL	2.1
78	sR	220	ILE	2.1
7	L5	196	ARG	2.1
22	n1	89	LEU	2.1
48	S2	192	GLY	2.1
63	C7	105	GLN	2.1
63	c7	58	MET	2.1
74	D8	20	GLY	2.1
77	e1	94	LYS	2.1
78	SR	47	LEU	2.1
78	sR	23	LEU	2.1
81	n4	64	THR	2.1

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Mol	Chain	Res	Type	RSRZ
56	C0	27	PHE	2.1
70	D4	30	PRO	2.1
10	L8	80	TYR	2.1
46	s0	110	TYR	2.1
54	S8	117	TYR	2.1
50	S4	60	GLU	2.1
57	C1	114	ALA	2.1
66	D0	66	SER	2.1
78	SR	22	SER	2.1
78	sR	244	ALA	2.1
13	m1	65	ILE	2.1
46	S0	181	VAL	2.1
16	M5	38	ARG	2.1
53	s7	179	LYS	2.1
66	d0	113	ASP	2.1
81	n4	2	LYS	2.1
47	S1	218	LEU	2.1
53	s7	38	LEU	2.1
59	C3	53	LEU	2.1
73	d7	24	LEU	2.1
78	sR	314	GLN	2.1
28	N7	71	PHE	2.1
53	S7	85	PHE	2.1
45	2	235	G	2.1
50	S4	35	PRO	2.1
64	c8	76	PRO	2.1
58	C2	35	ALA	2.1
27	N6	70	ILE	2.1
35	o4	91	ARG	2.1
47	S1	225	VAL	2.1
68	D2	71	LYS	2.1
70	D4	61	ARG	2.1
71	D5	66	VAL	2.1
73	D7	82	LYS	2.1
55	S9	58	ASP	2.1
66	D0	24	ILE	2.1
78	SR	3	SER	2.1
10	l8	69	LEU	2.1
12	m0	206	LEU	2.1
50	S4	4	GLY	2.1
53	s7	58	LEU	2.1
58	C2	127	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
68	d2	104	LEU	2.1
82	p0	15	LEU	2.1
21	N0	110	MET	2.1
63	C7	62	GLN	2.1
1	5	2504	U	2.1
7	L5	55	PHE	2.1
39	O8	11	PHE	2.1
46	S0	81	PHE	2.1
30	N9	26	THR	2.1
43	Q2	26	THR	2.1
46	S0	163	ASN	2.1
64	C8	100	THR	2.1
27	N6	89	LYS	2.1
31	o0	59	TYR	2.1
45	6	673	A	2.1
16	M5	60	VAL	2.1
28	n7	75	VAL	2.1
35	O4	2	ALA	2.1
46	S0	191	ARG	2.1
52	S6	224	ALA	2.1
60	C4	47	LYS	2.1
70	D4	101	GLU	2.1
62	C6	67	VAL	2.1
16	M5	133	ILE	2.1
37	o6	57	LEU	2.1
39	o8	51	LEU	2.1
52	S6	68	LEU	2.1
53	S7	45	SER	2.1
55	S9	140	ILE	2.1
62	C6	61	SER	2.1
69	D3	133	LEU	2.1
73	D7	63	LEU	2.1
75	d9	30	LEU	2.1
78	SR	165	ASP	2.1
7	L5	99	TYR	2.1
29	N8	80	THR	2.1
50	S4	77	ARG	2.1
50	S4	103	TYR	2.1
50	s4	145	ARG	2.1
68	d2	130	TYR	2.1
70	D4	32	ARG	2.1
76	E0	42	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
51	S5	64	VAL	2.1
55	S9	141	VAL	2.1
62	C6	78	VAL	2.1
64	C8	82	PRO	2.1
73	D7	50	ALA	2.1
4	l2	167	GLY	2.1
48	s2	154	LEU	2.1
62	c6	52	LEU	2.1
11	L9	54	LYS	2.0
28	N7	79	HIS	2.1
29	n8	79	TRP	2.0
39	o8	11	PHE	2.0
47	S1	232	HIS	2.1
49	S3	224	ASP	2.1
51	S5	43	PHE	2.0
66	D0	105	GLN	2.0
67	D1	1	MET	2.1
74	D8	35	ASP	2.1
14	m3	195	ALA	2.0
16	m5	43	THR	2.0
49	S3	138	VAL	2.0
76	E0	2	ALA	2.0
4	L2	104	LEU	2.0
62	C6	53	LEU	2.0
64	C8	59	GLY	2.0
10	L8	225	LYS	2.0
54	s8	53	LYS	2.0
40	O9	46	ARG	2.0
41	Q0	92	ASP	2.0
50	s4	17	HIS	2.0
65	C9	12	GLN	2.0
66	d0	105	GLN	2.0
1	5	1201	C	2.0
54	S8	140	GLU	2.0
16	M5	39	ALA	2.0
50	S4	82	TYR	2.0
61	c5	105	VAL	2.0
79	sM	47	ALA	2.0
16	M5	42	PRO	2.0
29	n8	147	LEU	2.0
46	s0	146	LEU	2.0
50	s4	101	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
81	n4	87	LEU	2.0
20	m9	52	LYS	2.0
45	2	502	U	2.0
45	6	676	G	2.0
75	D9	52	PHE	2.0
78	SR	103	PHE	2.0
48	S2	144	TRP	2.0
71	D5	43	ASP	2.0
16	M5	62	TYR	2.0
28	N7	85	TYR	2.0
47	S1	212	VAL	2.0
4	L2	136	ILE	2.0
10	L8	214	LEU	2.0
12	M0	166	ILE	2.0
16	m5	39	ALA	2.0
27	N6	111	LEU	2.0
27	n6	118	LEU	2.0
35	O4	63	ALA	2.0
48	S2	190	LEU	2.0
49	s3	49	ILE	2.0
50	S4	12	LEU	2.0
51	s5	36	ALA	2.0
55	s9	109	LEU	2.0
58	c2	94	ALA	2.0
58	c2	124	LYS	2.0
59	c3	149	LEU	2.0
61	C5	67	ALA	2.0
73	D7	46	VAL	2.0
68	D2	75	ILE	2.0
70	d4	40	LEU	2.0
70	d4	96	LEU	2.0
71	D5	36	ALA	2.0
73	d7	33	LEU	2.0
73	d7	73	LEU	2.0
29	N8	98	THR	2.0
47	s1	105	PHE	2.0
50	S4	50	ASN	2.0
56	c0	57	THR	2.0
65	C9	46	PRO	2.0
78	SR	28	GLY	2.0
45	2	1534	G	2.0
46	S0	83	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
48	S2	208	GLU	2.0
9	L7	75	TYR	2.0
37	o6	53	TYR	2.0
49	s3	48	VAL	2.0
79	sM	112	ASP	2.0
13	M1	14	ILE	2.0
26	n5	142	ILE	2.0
1	1	1352	A	2.0
37	o6	56	ARG	2.0
43	Q2	71	ARG	2.0
47	S1	137	ILE	2.0
78	SR	83	ALA	2.0
52	S6	54	GLY	2.0
59	C3	59	GLY	2.0
74	D8	18	ARG	2.0
6	l4	26	PHE	2.0
21	N0	25	PHE	2.0
22	n1	77	ASN	2.0
15	m4	2	SER	2.0
16	m5	106	VAL	2.0
43	Q2	25	VAL	2.0
7	L5	78	ALA	2.0
10	L8	162	LEU	2.0
23	N2	79	LEU	2.0
31	O0	51	LEU	2.0
32	O1	91	SER	2.0
47	s1	104	ASP	2.0
50	S4	227	VAL	2.0
50	s4	36	HIS	2.0
54	S8	82	VAL	2.0
54	s8	44	HIS	2.0
28	n7	46	ILE	2.0
48	S2	113	LEU	2.0
50	s4	90	ILE	2.0
53	S7	77	LEU	2.0
67	D1	44	ARG	2.0
78	sR	13	LEU	2.0
81	n4	135	SER	2.0
47	s1	235	GLY	2.0
53	s7	91	ILE	2.0
57	C1	49	ILE	2.0
23	N2	71	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
47	s1	30	PHE	2.0
53	s7	24	PHE	2.0
49	S3	211	PRO	2.0
8	l6	8	LYS	2.0
14	M3	86	THR	2.0
69	D3	141	GLU	2.0
51	S5	158	GLN	2.0
78	SR	216	LYS	2.0
10	l8	134	TYR	2.0
16	m5	60	VAL	2.0
19	M8	140	LEU	2.0
52	S6	102	VAL	2.0
55	S9	80	LEU	2.0
57	C1	109	VAL	2.0
61	C5	17	TYR	2.0
77	e1	108	VAL	2.0

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

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	3634	1/1	-0.07	1.24	57,57,57,57	0
84	MG	1	3950	1/1	0.03	0.55	85,85,85,85	0
84	MG	6	2162	1/1	0.22	0.21	96,96,96,96	0
84	MG	1	3917	1/1	0.42	0.35	74,74,74,74	0
84	MG	1	3628	1/1	0.42	0.69	80,80,80,80	0
84	MG	1	3637	1/1	0.43	0.37	91,91,91,91	0
84	MG	6	2072	1/1	0.43	0.26	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	1	3759	1/1	0.43	0.82	73,73,73,73	0
84	MG	S2	301	1/1	0.44	0.55	107,107,107,107	0
84	MG	2	1961	1/1	0.44	0.17	109,109,109,109	0
84	MG	1	3842	1/1	0.45	0.98	92,92,92,92	0
84	MG	1	3493	1/1	0.46	0.65	76,76,76,76	0
84	MG	2	1980	1/1	0.46	0.54	77,77,77,77	0
84	MG	5	3611	1/1	0.47	0.38	104,104,104,104	0
84	MG	M3	203	1/1	0.47	0.24	92,92,92,92	0
84	MG	5	4097	1/1	0.49	0.48	68,68,68,68	0
84	MG	N3	204	1/1	0.49	0.39	87,87,87,87	0
84	MG	5	3970	1/1	0.49	0.72	75,75,75,75	0
84	MG	5	3654	1/1	0.50	0.39	79,79,79,79	0
84	MG	5	3695	1/1	0.50	0.35	93,93,93,93	0
84	MG	6	2090	1/1	0.50	0.40	91,91,91,91	0
84	MG	1	3510	1/1	0.50	0.51	57,57,57,57	0
84	MG	d6	102	1/1	0.50	0.28	76,76,76,76	0
84	MG	2	1940	1/1	0.51	0.64	82,82,82,82	0
84	MG	1	3636	1/1	0.51	0.22	104,104,104,104	0
84	MG	1	3902	1/1	0.52	0.19	77,77,77,77	0
84	MG	4	221	1/1	0.52	0.45	75,75,75,75	0
84	MG	6	2120	1/1	0.52	0.14	110,110,110,110	0
84	MG	8	213	1/1	0.52	0.58	68,68,68,68	0
84	MG	6	1924	1/1	0.52	0.29	70,70,70,70	0
84	MG	6	1944	1/1	0.53	0.86	71,71,71,71	0
84	MG	6	2121	1/1	0.53	0.61	97,97,97,97	0
84	MG	6	2141	1/1	0.53	0.32	99,99,99,99	0
84	MG	5	4057	1/1	0.53	0.15	99,99,99,99	1
84	MG	1	3876	1/1	0.53	0.67	76,76,76,76	0
84	MG	3	202	1/1	0.54	0.24	89,89,89,89	0
84	MG	O6	201	1/1	0.54	0.26	78,78,78,78	0
84	MG	6	1901	1/1	0.54	0.72	55,55,55,55	0
84	MG	1	3667	1/1	0.55	0.53	73,73,73,73	0
84	MG	6	1991	1/1	0.55	0.54	71,71,71,71	0
84	MG	s2	302	1/1	0.55	0.34	81,81,81,81	0
84	MG	2	1931	1/1	0.55	0.47	90,90,90,90	0
84	MG	4	212	1/1	0.56	0.38	84,84,84,84	0
84	MG	6	2129	1/1	0.56	0.36	88,88,88,88	0
84	MG	5	4031	1/1	0.56	0.37	65,65,65,65	0
84	MG	1	3483	1/1	0.56	0.59	68,68,68,68	0
84	MG	6	2106	1/1	0.56	0.58	91,91,91,91	0
84	MG	5	3751	1/1	0.56	0.59	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	6	1967	1/1	0.57	0.85	74,74,74,74	0
84	MG	5	3645	1/1	0.57	0.55	59,59,59,59	0
84	MG	2	2023	1/1	0.57	0.15	132,132,132,132	0
86	ZN	D7	101	1/1	0.57	0.22	264,264,264,264	0
84	MG	3	206	1/1	0.58	0.50	72,72,72,72	0
84	MG	n5	201	1/1	0.59	0.13	96,96,96,96	0
84	MG	q2	506	1/1	0.59	0.33	68,68,68,68	0
84	MG	2	1929	1/1	0.59	0.60	88,88,88,88	0
84	MG	5	4030	1/1	0.60	0.50	99,99,99,99	0
84	MG	4	206	1/1	0.60	0.53	60,60,60,60	0
84	MG	1	3744	1/1	0.60	0.17	82,82,82,82	0
84	MG	5	4080	1/1	0.60	0.16	67,67,67,67	0
84	MG	1	3980	1/1	0.60	0.14	91,91,91,91	0
84	MG	1	3490	1/1	0.60	0.16	80,80,80,80	0
84	MG	5	3886	1/1	0.60	0.36	77,77,77,77	0
84	MG	1	3927	1/1	0.60	0.17	77,77,77,77	1
84	MG	6	2024	1/1	0.61	0.23	80,80,80,80	0
84	MG	6	2030	1/1	0.61	0.30	82,82,82,82	0
84	MG	1	3726	1/1	0.61	0.47	69,69,69,69	0
84	MG	5	3966	1/1	0.61	0.63	95,95,95,95	0
84	MG	1	3803	1/1	0.61	0.45	76,76,76,76	0
84	MG	6	2119	1/1	0.61	0.35	91,91,91,91	0
84	MG	1	3442	1/1	0.61	0.39	83,83,83,83	0
84	MG	1	3630	1/1	0.62	0.12	106,106,106,106	0
84	MG	2	1965	1/1	0.62	0.32	91,91,91,91	0
84	MG	6	2107	1/1	0.62	0.45	90,90,90,90	0
84	MG	1	3758	1/1	0.62	0.59	74,74,74,74	0
84	MG	1	3521	1/1	0.63	0.43	69,69,69,69	0
84	MG	1	3816	1/1	0.63	0.46	78,78,78,78	0
84	MG	1	3888	1/1	0.63	0.38	68,68,68,68	0
84	MG	5	3984	1/1	0.63	0.49	62,62,62,62	0
84	MG	2	2015	1/1	0.64	0.59	84,84,84,84	0
84	MG	1	3952	1/1	0.64	1.00	88,88,88,88	0
84	MG	5	3813	1/1	0.64	0.55	58,58,58,58	0
84	MG	5	4106	1/1	0.64	0.32	49,49,49,49	0
84	MG	5	3836	1/1	0.64	0.29	79,79,79,79	0
84	MG	M5	305	1/1	0.64	0.33	72,72,72,72	0
84	MG	5	3904	1/1	0.64	0.62	59,59,59,59	0
84	MG	5	3591	1/1	0.64	0.54	61,61,61,61	0
84	MG	1	3639	1/1	0.64	0.29	96,96,96,96	0
84	MG	6	1933	1/1	0.64	0.57	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3985	1/1	0.64	0.40	77,77,77,77	0
84	MG	2	1966	1/1	0.64	0.28	106,106,106,106	0
84	MG	c3	204	1/1	0.64	0.14	107,107,107,107	0
84	MG	1	3650	1/1	0.64	0.40	53,53,53,53	0
84	MG	d7	102	1/1	0.64	0.40	78,78,78,78	0
84	MG	5	4049	1/1	0.64	0.20	79,79,79,79	0
84	MG	2	1955	1/1	0.65	0.33	86,86,86,86	0
84	MG	5	3937	1/1	0.65	0.35	60,60,60,60	0
84	MG	1	3590	1/1	0.65	0.39	58,58,58,58	0
84	MG	2	2036	1/1	0.65	0.18	113,113,113,113	0
84	MG	6	2149	1/1	0.65	0.18	73,73,73,73	0
84	MG	m8	203	1/1	0.65	0.39	69,69,69,69	0
84	MG	4	202	1/1	0.65	0.31	59,59,59,59	0
84	MG	1	3818	1/1	0.65	0.54	88,88,88,88	0
84	MG	1	3955	1/1	0.65	0.47	69,69,69,69	0
84	MG	2	2007	1/1	0.65	0.24	88,88,88,88	0
84	MG	5	3896	1/1	0.65	0.83	71,71,71,71	0
84	MG	5	3975	1/1	0.66	0.57	71,71,71,71	0
84	MG	O7	104	1/1	0.66	0.22	88,88,88,88	0
84	MG	n5	202	1/1	0.66	0.32	78,78,78,78	0
84	MG	5	3840	1/1	0.66	0.30	61,61,61,61	0
84	MG	5	3863	1/1	0.66	0.53	76,76,76,76	0
84	MG	S4	301	1/1	0.66	0.20	120,120,120,120	0
84	MG	1	3658	1/1	0.66	0.37	70,70,70,70	0
84	MG	5	3711	1/1	0.66	0.34	70,70,70,70	0
84	MG	1	3769	1/1	0.66	0.89	65,65,65,65	0
84	MG	6	1968	1/1	0.66	0.55	65,65,65,65	0
84	MG	5	3803	1/1	0.66	0.17	76,76,76,76	0
84	MG	2	2001	1/1	0.66	0.61	146,146,146,146	0
84	MG	d1	101	1/1	0.66	0.40	93,93,93,93	0
84	MG	l8	301	1/1	0.66	0.45	99,99,99,99	0
84	MG	6	2034	1/1	0.66	0.39	69,69,69,69	0
84	MG	m6	208	1/1	0.66	0.50	56,56,56,56	0
84	MG	5	3825	1/1	0.67	0.35	58,58,58,58	0
84	MG	4	211	1/1	0.67	0.27	86,86,86,86	0
84	MG	6	1989	1/1	0.67	0.44	67,67,67,67	0
84	MG	4	208	1/1	0.67	0.40	60,60,60,60	0
84	MG	c1	201	1/1	0.67	0.40	78,78,78,78	0
84	MG	6	1993	1/1	0.67	0.72	71,71,71,71	0
84	MG	5	3794	1/1	0.67	0.23	61,61,61,61	0
84	MG	2	1906	1/1	0.67	0.40	86,86,86,86	0
84	MG	O4	503	1/1	0.67	0.13	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	6	2134	1/1	0.67	0.14	99,99,99,99	0
84	MG	1	3447	1/1	0.68	0.45	58,58,58,58	0
84	MG	5	3664	1/1	0.68	0.41	56,56,56,56	0
84	MG	5	4129	1/1	0.68	0.57	90,90,90,90	0
84	MG	6	2128	1/1	0.68	0.32	77,77,77,77	0
84	MG	5	4135	1/1	0.68	0.32	77,77,77,77	0
84	MG	8	209	1/1	0.68	0.23	80,80,80,80	0
84	MG	5	3999	1/1	0.68	0.31	52,52,52,52	0
84	MG	6	2148	1/1	0.68	0.26	78,78,78,78	0
84	MG	5	4003	1/1	0.68	0.26	77,77,77,77	0
84	MG	5	3808	1/1	0.68	0.23	66,66,66,66	0
84	MG	1	3788	1/1	0.68	0.19	76,76,76,76	1
84	MG	L2	303	1/1	0.68	0.27	88,88,88,88	0
84	MG	2	1905	1/1	0.68	0.09	127,127,127,127	0
84	MG	5	4071	1/1	0.68	0.13	103,103,103,103	0
84	MG	5	3768	1/1	0.68	0.41	73,73,73,73	0
84	MG	6	1903	1/1	0.68	0.77	67,67,67,67	0
84	MG	6	1918	1/1	0.68	0.22	84,84,84,84	0
84	MG	5	3795	1/1	0.69	0.22	74,74,74,74	0
84	MG	1	3958	1/1	0.69	0.19	88,88,88,88	0
84	MG	1	3481	1/1	0.69	0.79	73,73,73,73	0
84	MG	N0	201	1/1	0.69	0.35	67,67,67,67	0
84	MG	5	4040	1/1	0.69	0.29	74,74,74,74	0
84	MG	1	3865	1/1	0.69	0.55	81,81,81,81	0
84	MG	6	2059	1/1	0.69	0.18	76,76,76,76	0
84	MG	1	3804	1/1	0.69	0.57	91,91,91,91	0
84	MG	m4	201	1/1	0.69	0.21	69,69,69,69	1
84	MG	1	3461	1/1	0.69	0.43	59,59,59,59	0
84	MG	6	1945	1/1	0.69	0.49	70,70,70,70	0
84	MG	6	1951	1/1	0.69	0.21	74,74,74,74	0
84	MG	1	3579	1/1	0.69	0.25	71,71,71,71	0
84	MG	n0	204	1/1	0.69	0.28	57,57,57,57	0
84	MG	3	215	1/1	0.70	0.17	74,74,74,74	0
84	MG	5	4086	1/1	0.70	0.17	96,96,96,96	0
84	MG	5	3868	1/1	0.70	0.74	57,57,57,57	0
84	MG	6	1983	1/1	0.70	0.18	100,100,100,100	0
84	MG	2	1997	1/1	0.70	0.36	98,98,98,98	0
84	MG	5	4007	1/1	0.70	0.46	63,63,63,63	0
84	MG	5	4134	1/1	0.70	0.30	73,73,73,73	0
84	MG	1	3934	1/1	0.70	0.48	65,65,65,65	0
84	MG	5	3558	1/1	0.70	0.46	60,60,60,60	0
84	MG	5	3704	1/1	0.70	0.38	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	1	3627	1/1	0.70	0.44	81,81,81,81	0
84	MG	6	1942	1/1	0.70	0.40	60,60,60,60	0
84	MG	6	1943	1/1	0.70	0.35	65,65,65,65	0
84	MG	1	3545	1/1	0.70	0.55	62,62,62,62	0
84	MG	2	1979	1/1	0.70	0.84	68,68,68,68	0
84	MG	6	2108	1/1	0.70	0.33	79,79,79,79	0
84	MG	6	2114	1/1	0.70	0.23	96,96,96,96	0
84	MG	2	1913	1/1	0.71	0.62	81,81,81,81	0
84	MG	1	3823	1/1	0.71	0.69	89,89,89,89	0
84	MG	1	3904	1/1	0.71	0.27	76,76,76,76	0
84	MG	N1	202	1/1	0.71	0.34	98,98,98,98	0
84	MG	6	2118	1/1	0.71	0.33	148,148,148,148	0
84	MG	2	1977	1/1	0.71	1.32	77,77,77,77	0
84	MG	5	3936	1/1	0.71	0.45	55,55,55,55	0
84	MG	5	3594	1/1	0.71	0.47	77,77,77,77	0
84	MG	5	3948	1/1	0.71	0.65	58,58,58,58	0
84	MG	2	2017	1/1	0.71	0.57	86,86,86,86	0
84	MG	2	1954	1/1	0.71	0.29	106,106,106,106	0
84	MG	5	3601	1/1	0.72	0.46	89,89,89,89	0
84	MG	1	3723	1/1	0.72	0.32	47,47,47,47	0
84	MG	7	219	1/1	0.72	0.17	62,62,62,62	0
84	MG	6	2100	1/1	0.72	0.28	84,84,84,84	0
84	MG	1	3815	1/1	0.72	0.74	77,77,77,77	0
84	MG	5	4073	1/1	0.72	0.12	97,97,97,97	0
84	MG	12	304	1/1	0.72	0.39	76,76,76,76	0
84	MG	C3	201	1/1	0.72	0.20	102,102,102,102	0
84	MG	M8	201	1/1	0.72	0.23	67,67,67,67	0
84	MG	6	2018	1/1	0.72	0.31	81,81,81,81	0
84	MG	1	3571	1/1	0.72	0.27	71,71,71,71	0
84	MG	5	3867	1/1	0.72	0.39	55,55,55,55	0
84	MG	1	3854	1/1	0.72	0.31	60,60,60,60	0
84	MG	5	3690	1/1	0.73	0.31	65,65,65,65	0
84	MG	5	3942	1/1	0.73	0.39	79,79,79,79	0
84	MG	1	3782	1/1	0.73	0.74	69,69,69,69	0
84	MG	1	3960	1/1	0.73	0.20	79,79,79,79	0
84	MG	6	2139	1/1	0.73	0.19	82,82,82,82	0
84	MG	6	2070	1/1	0.73	0.17	128,128,128,128	0
84	MG	1	3456	1/1	0.73	0.36	67,67,67,67	0
84	MG	5	3974	1/1	0.73	0.43	67,67,67,67	0
84	MG	6	2161	1/1	0.73	0.27	75,75,75,75	0
84	MG	1	3467	1/1	0.73	0.38	58,58,58,58	0
84	MG	5	3764	1/1	0.73	0.32	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3900	1/1	0.73	0.11	85,85,85,85	0
84	MG	1	3763	1/1	0.73	0.42	66,66,66,66	0
84	MG	3	208	1/1	0.73	0.46	64,64,64,64	0
84	MG	1	3495	1/1	0.73	0.62	75,75,75,75	0
84	MG	D3	204	1/1	0.73	0.51	94,94,94,94	0
84	MG	7	223	1/1	0.73	0.22	75,75,75,75	0
84	MG	5	4130	1/1	0.74	0.21	81,81,81,81	0
84	MG	m7	207	1/1	0.74	0.53	66,66,66,66	0
84	MG	1	3565	1/1	0.74	0.20	71,71,71,71	0
84	MG	2	2000	1/1	0.74	0.36	164,164,164,164	0
84	MG	6	2142	1/1	0.74	0.24	89,89,89,89	0
84	MG	6	1960	1/1	0.74	0.41	62,62,62,62	0
84	MG	5	3934	1/1	0.74	0.46	48,48,48,48	1
84	MG	2	2037	1/1	0.74	0.35	99,99,99,99	0
84	MG	6	1977	1/1	0.74	0.26	103,103,103,103	0
84	MG	8	202	1/1	0.74	0.19	90,90,90,90	0
84	MG	5	3856	1/1	0.74	0.34	61,61,61,61	0
84	MG	1	3580	1/1	0.74	0.24	75,75,75,75	0
84	MG	1	3738	1/1	0.74	0.73	75,75,75,75	0
84	MG	l5	302	1/1	0.74	0.14	78,78,78,78	0
84	MG	1	3694	1/1	0.74	0.38	62,62,62,62	0
84	MG	d9	102	1/1	0.74	0.22	94,94,94,94	0
84	MG	2	1984	1/1	0.74	0.43	113,113,113,113	0
84	MG	1	3681	1/1	0.75	0.36	62,62,62,62	0
84	MG	2	2004	1/1	0.75	0.72	81,81,81,81	0
84	MG	6	1920	1/1	0.75	0.23	81,81,81,81	0
84	MG	2	1953	1/1	0.75	0.33	96,96,96,96	0
84	MG	1	3893	1/1	0.75	0.30	57,57,57,57	0
84	MG	1	3560	1/1	0.75	0.20	78,78,78,78	0
84	MG	8	201	1/1	0.75	0.42	81,81,81,81	0
84	MG	5	3651	1/1	0.75	0.38	77,77,77,77	0
84	MG	8	208	1/1	0.75	0.21	79,79,79,79	0
84	MG	4	210	1/1	0.75	0.14	90,90,90,90	0
84	MG	1	3764	1/1	0.75	0.57	69,69,69,69	0
84	MG	8	216	1/1	0.75	0.68	67,67,67,67	0
84	MG	1	3584	1/1	0.75	0.36	76,76,76,76	0
84	MG	6	1974	1/1	0.75	0.17	90,90,90,90	0
84	MG	l3	410	1/1	0.75	0.17	73,73,73,73	0
84	MG	Q2	504	1/1	0.75	0.37	59,59,59,59	0
84	MG	5	4046	1/1	0.75	0.43	67,67,67,67	0
84	MG	1	3454	1/1	0.75	0.37	61,61,61,61	0
84	MG	m4	206	1/1	0.75	0.35	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	C1	201	1/1	0.75	0.20	103,103,103,103	0
84	MG	1	3566	1/1	0.75	0.22	74,74,74,74	0
84	MG	1	3426	1/1	0.75	0.31	45,45,45,45	0
84	MG	1	3948	1/1	0.75	0.51	82,82,82,82	0
84	MG	5	3780	1/1	0.75	0.30	64,64,64,64	0
84	MG	5	3793	1/1	0.75	0.37	68,68,68,68	0
84	MG	5	3577	1/1	0.75	0.57	54,54,54,54	0
84	MG	sR	401	1/1	0.75	0.18	76,76,76,76	0
84	MG	1	3555	1/1	0.75	0.16	92,92,92,92	0
84	MG	5	3755	1/1	0.76	0.44	59,59,59,59	0
84	MG	6	2064	1/1	0.76	0.15	126,126,126,126	0
84	MG	1	3879	1/1	0.76	0.69	63,63,63,63	0
84	MG	1	3977	1/1	0.76	0.16	87,87,87,87	0
84	MG	q2	502	1/1	0.76	0.27	63,63,63,63	0
84	MG	5	4117	1/1	0.76	0.18	82,82,82,82	0
84	MG	q2	507	1/1	0.76	0.20	51,51,51,51	0
84	MG	q3	503	1/1	0.76	0.26	79,79,79,79	0
84	MG	5	4120	1/1	0.76	0.10	90,90,90,90	0
84	MG	5	3775	1/1	0.76	0.45	120,120,120,120	0
84	MG	1	3827	1/1	0.76	0.47	61,61,61,61	0
84	MG	5	3954	1/1	0.76	0.62	58,58,58,58	0
84	MG	5	3617	1/1	0.76	0.30	75,75,75,75	0
84	MG	5	3622	1/1	0.76	0.19	84,84,84,84	0
84	MG	5	3624	1/1	0.76	0.57	65,65,65,65	0
84	MG	1	3668	1/1	0.76	0.32	74,74,74,74	0
84	MG	1	3499	1/1	0.76	0.46	61,61,61,61	0
84	MG	1	3859	1/1	0.76	0.16	67,67,67,67	0
84	MG	5	3469	1/1	0.76	0.46	54,54,54,54	0
84	MG	5	3526	1/1	0.76	0.62	61,61,61,61	0
84	MG	5	3675	1/1	0.76	0.25	67,67,67,67	0
84	MG	l2	303	1/1	0.76	0.36	72,72,72,72	0
84	MG	5	3855	1/1	0.76	0.57	69,69,69,69	0
84	MG	5	4033	1/1	0.76	0.13	74,74,74,74	0
84	MG	1	3578	1/1	0.76	0.21	78,78,78,78	0
84	MG	5	3693	1/1	0.76	0.32	81,81,81,81	0
84	MG	5	3563	1/1	0.76	0.46	55,55,55,55	0
84	MG	1	3514	1/1	0.76	0.61	63,63,63,63	0
84	MG	6	1996	1/1	0.76	0.32	74,74,74,74	0
84	MG	d6	104	1/1	0.76	0.30	76,76,76,76	0
84	MG	m6	202	1/1	0.76	0.29	47,47,47,47	0
84	MG	O7	102	1/1	0.76	0.39	61,61,61,61	0
84	MG	5	3722	1/1	0.76	0.38	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3593	1/1	0.76	0.50	68,68,68,68	0
84	MG	2	1978	1/1	0.77	0.50	64,64,64,64	0
84	MG	15	305	1/1	0.77	0.08	77,77,77,77	0
84	MG	16	202	1/1	0.77	0.39	66,66,66,66	0
84	MG	1	3886	1/1	0.77	0.22	83,83,83,83	0
84	MG	19	208	1/1	0.77	0.18	54,54,54,54	0
84	MG	5	3492	1/1	0.77	0.42	74,74,74,74	0
84	MG	5	3524	1/1	0.77	0.48	53,53,53,53	0
84	MG	5	3802	1/1	0.77	0.15	75,75,75,75	0
84	MG	1	3444	1/1	0.77	0.68	70,70,70,70	0
84	MG	1	3741	1/1	0.77	0.34	80,80,80,80	0
84	MG	m8	202	1/1	0.77	0.53	63,63,63,63	0
84	MG	1	3873	1/1	0.77	0.44	65,65,65,65	0
84	MG	5	4041	1/1	0.77	0.30	79,79,79,79	0
84	MG	5	3819	1/1	0.77	0.24	57,57,57,57	0
84	MG	1	3663	1/1	0.77	0.29	69,69,69,69	0
84	MG	8	205	1/1	0.77	0.17	111,111,111,111	0
84	MG	8	207	1/1	0.77	0.31	74,74,74,74	0
84	MG	5	3828	1/1	0.77	0.32	46,46,46,46	0
84	MG	5	4063	1/1	0.77	0.17	94,94,94,94	0
84	MG	c3	201	1/1	0.77	0.61	89,89,89,89	0
84	MG	4	223	1/1	0.77	0.26	72,72,72,72	0
84	MG	8	214	1/1	0.77	0.39	54,54,54,54	0
84	MG	5	3766	1/1	0.77	0.49	57,57,57,57	0
84	MG	1	3746	1/1	0.77	0.39	69,69,69,69	0
84	MG	6	2085	1/1	0.77	0.15	88,88,88,88	0
84	MG	L5	301	1/1	0.77	0.13	89,89,89,89	0
84	MG	5	3857	1/1	0.77	0.21	65,65,65,65	0
84	MG	6	1940	1/1	0.77	0.80	69,69,69,69	0
84	MG	5	3838	1/1	0.78	0.31	57,57,57,57	0
84	MG	5	3960	1/1	0.78	0.18	74,74,74,74	0
84	MG	5	3574	1/1	0.78	0.61	58,58,58,58	0
84	MG	6	1988	1/1	0.78	0.39	66,66,66,66	0
84	MG	3	211	1/1	0.78	0.24	71,71,71,71	0
84	MG	1	3515	1/1	0.78	1.17	64,64,64,64	0
84	MG	6	1992	1/1	0.78	0.47	78,78,78,78	0
84	MG	N4	201	1/1	0.78	0.39	70,70,70,70	0
84	MG	2	2013	1/1	0.78	0.12	120,120,120,120	0
84	MG	6	1997	1/1	0.78	0.28	78,78,78,78	0
84	MG	5	4112	1/1	0.78	0.18	52,52,52,52	0
84	MG	1	3805	1/1	0.78	0.32	74,74,74,74	0
84	MG	1	3742	1/1	0.78	0.51	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	3706	1/1	0.78	0.62	71,71,71,71	0
84	MG	5	3805	1/1	0.78	0.15	75,75,75,75	0
84	MG	1	3711	1/1	0.78	0.19	84,84,84,84	0
84	MG	5	3915	1/1	0.78	0.49	78,78,78,78	0
84	MG	5	4149	1/1	0.78	0.32	74,74,74,74	0
84	MG	1	3577	1/1	0.78	0.23	81,81,81,81	0
84	MG	d3	201	1/1	0.78	0.48	65,65,65,65	0
84	MG	5	3542	1/1	0.78	0.42	54,54,54,54	0
84	MG	m6	203	1/1	0.78	0.34	55,55,55,55	0
84	MG	7	225	1/1	0.78	0.20	71,71,71,71	0
84	MG	1	3665	1/1	0.78	0.22	67,67,67,67	0
84	MG	1	3686	1/1	0.78	0.34	57,57,57,57	0
84	MG	5	3564	1/1	0.78	0.47	59,59,59,59	0
84	MG	6	2026	1/1	0.79	0.28	78,78,78,78	0
84	MG	5	3588	1/1	0.79	0.94	62,62,62,62	0
84	MG	1	3949	1/1	0.79	0.14	79,79,79,79	0
84	MG	6	2035	1/1	0.79	0.21	82,82,82,82	0
84	MG	6	2058	1/1	0.79	0.30	81,81,81,81	0
84	MG	2	2024	1/1	0.79	0.07	130,130,130,130	0
84	MG	2	2026	1/1	0.79	0.22	126,126,126,126	0
84	MG	6	2066	1/1	0.79	0.10	121,121,121,121	0
84	MG	1	3820	1/1	0.79	0.45	76,76,76,76	0
84	MG	1	3880	1/1	0.79	0.45	73,73,73,73	0
84	MG	1	3953	1/1	0.79	0.30	72,72,72,72	0
84	MG	5	3965	1/1	0.79	0.57	65,65,65,65	0
84	MG	1	3508	1/1	0.79	0.89	60,60,60,60	0
84	MG	1	3792	1/1	0.79	0.23	94,94,94,94	0
84	MG	4	215	1/1	0.79	0.38	69,69,69,69	0
84	MG	D3	201	1/1	0.79	0.32	72,72,72,72	0
84	MG	1	3829	1/1	0.79	0.53	71,71,71,71	0
84	MG	6	1913	1/1	0.79	0.15	107,107,107,107	0
84	MG	5	3434	1/1	0.79	0.27	60,60,60,60	0
84	MG	5	3437	1/1	0.79	0.25	59,59,59,59	0
84	MG	5	3833	1/1	0.79	0.36	53,53,53,53	0
84	MG	5	4012	1/1	0.79	0.31	61,61,61,61	0
84	MG	5	4024	1/1	0.79	0.39	68,68,68,68	0
84	MG	5	3442	1/1	0.79	0.45	53,53,53,53	0
84	MG	2	1992	1/1	0.79	0.14	98,98,98,98	0
84	MG	5	3483	1/1	0.79	0.36	57,57,57,57	0
84	MG	8	219	1/1	0.79	0.38	90,90,90,90	0
84	MG	1	3465	1/1	0.79	0.37	56,56,56,56	0
84	MG	5	3697	1/1	0.79	0.44	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	l3	406	1/1	0.79	0.44	63,63,63,63	0
84	MG	l3	408	1/1	0.79	0.41	64,64,64,64	0
84	MG	1	3847	1/1	0.79	0.51	53,53,53,53	0
84	MG	1	3634	1/1	0.79	0.26	105,105,105,105	0
84	MG	1	3541	1/1	0.79	0.32	58,58,58,58	0
84	MG	1	3501	1/1	0.79	0.24	64,64,64,64	0
84	MG	5	3878	1/1	0.79	0.47	79,79,79,79	0
84	MG	2	2010	1/1	0.79	0.29	98,98,98,98	0
84	MG	m3	202	1/1	0.79	0.23	82,82,82,82	0
84	MG	1	3932	1/1	0.79	0.69	71,71,71,71	0
84	MG	1	3704	1/1	0.79	0.32	55,55,55,55	0
84	MG	1	3707	1/1	0.79	0.37	59,59,59,59	0
84	MG	5	4098	1/1	0.79	0.36	81,81,81,81	0
85	LLL	5	4178	31/31	0.79	0.35	69,69,69,69	31
84	MG	m6	207	1/1	0.79	0.29	47,47,47,47	0
84	MG	5	3458	1/1	0.80	0.29	57,57,57,57	0
84	MG	1	3975	1/1	0.80	0.28	63,63,63,63	0
84	MG	5	3967	1/1	0.80	0.62	71,71,71,71	0
84	MG	O2	203	1/1	0.80	0.35	57,57,57,57	0
84	MG	6	1934	1/1	0.80	0.36	67,67,67,67	0
84	MG	1	3430	1/1	0.80	0.39	54,54,54,54	0
84	MG	5	4114	1/1	0.80	0.20	83,83,83,83	0
84	MG	5	3859	1/1	0.80	0.56	71,71,71,71	0
84	MG	1	3928	1/1	0.80	0.23	64,64,64,64	0
84	MG	6	2111	1/1	0.80	0.19	113,113,113,113	0
84	MG	l9	206	1/1	0.80	0.32	68,68,68,68	0
84	MG	1	3469	1/1	0.80	0.21	59,59,59,59	1
84	MG	m3	201	1/1	0.80	0.28	88,88,88,88	0
84	MG	2	2034	1/1	0.80	0.19	92,92,92,92	0
84	MG	5	3869	1/1	0.80	0.87	67,67,67,67	0
84	MG	6	2124	1/1	0.80	0.26	76,76,76,76	0
84	MG	1	3881	1/1	0.80	0.18	78,78,78,78	0
84	MG	m5	303	1/1	0.80	0.17	79,79,79,79	0
84	MG	1	3457	1/1	0.80	0.25	63,63,63,63	0
84	MG	7	203	1/1	0.80	0.36	52,52,52,52	0
84	MG	L4	405	1/1	0.80	0.43	63,63,63,63	0
84	MG	5	3899	1/1	0.80	0.81	59,59,59,59	0
84	MG	1	3853	1/1	0.80	0.29	60,60,60,60	0
84	MG	7	227	1/1	0.80	0.28	76,76,76,76	0
84	MG	M0	303	1/1	0.80	0.33	66,66,66,66	0
84	MG	5	3583	1/1	0.80	0.59	59,59,59,59	0
84	MG	6	2014	1/1	0.80	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	1	3696	1/1	0.80	0.50	55,55,55,55	0
84	MG	1	3662	1/1	0.80	0.28	78,78,78,78	0
84	MG	5	4052	1/1	0.80	0.43	77,77,77,77	0
84	MG	5	4056	1/1	0.80	0.16	95,95,95,95	0
84	MG	1	3669	1/1	0.80	0.30	78,78,78,78	0
84	MG	1	3670	1/1	0.80	0.31	76,76,76,76	0
84	MG	6	2049	1/1	0.80	0.14	78,78,78,78	0
84	MG	1	3909	1/1	0.80	0.29	73,73,73,73	0
84	MG	5	3958	1/1	0.80	0.62	66,66,66,66	0
84	MG	6	2062	1/1	0.80	0.11	111,111,111,111	0
84	MG	6	2063	1/1	0.80	0.13	117,117,117,117	0
84	MG	1	3715	1/1	0.80	0.18	83,83,83,83	0
84	MG	1	3817	1/1	0.81	0.66	72,72,72,72	0
84	MG	5	4008	1/1	0.81	0.36	56,56,56,56	0
84	MG	M0	302	1/1	0.81	0.83	64,64,64,64	0
84	MG	5	4018	1/1	0.81	0.50	66,66,66,66	0
84	MG	5	4019	1/1	0.81	0.63	66,66,66,66	0
84	MG	5	3725	1/1	0.81	0.37	71,71,71,71	0
84	MG	8	206	1/1	0.81	0.25	81,81,81,81	0
84	MG	2	1990	1/1	0.81	0.21	116,116,116,116	0
84	MG	1	3556	1/1	0.81	0.35	73,73,73,73	0
84	MG	1	3698	1/1	0.81	0.54	69,69,69,69	0
84	MG	1	3800	1/1	0.81	0.52	67,67,67,67	0
84	MG	D3	202	1/1	0.81	0.51	67,67,67,67	0
84	MG	5	3772	1/1	0.81	0.32	128,128,128,128	0
84	MG	6	1937	1/1	0.81	0.93	62,62,62,62	0
84	MG	1	3506	1/1	0.81	0.35	57,57,57,57	0
84	MG	5	3419	1/1	0.81	0.37	49,49,49,49	0
84	MG	6	2115	1/1	0.81	0.12	93,93,93,93	0
84	MG	5	3792	1/1	0.81	0.26	63,63,63,63	1
84	MG	1	3739	1/1	0.81	0.42	72,72,72,72	0
84	MG	1	3840	1/1	0.81	0.67	67,67,67,67	0
84	MG	1	3409	1/1	0.81	0.40	49,49,49,49	0
84	MG	1	3937	1/1	0.81	0.42	73,73,73,73	0
84	MG	5	4078	1/1	0.81	0.25	67,67,67,67	0
84	MG	5	3946	1/1	0.81	0.69	64,64,64,64	0
84	MG	5	4085	1/1	0.81	0.16	79,79,79,79	0
84	MG	5	3635	1/1	0.81	0.29	55,55,55,55	0
84	MG	N8	203	1/1	0.81	0.44	63,63,63,63	0
84	MG	6	1987	1/1	0.81	0.31	79,79,79,79	0
84	MG	2	2016	1/1	0.81	0.39	72,72,72,72	0
84	MG	5	4104	1/1	0.81	0.30	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3810	1/1	0.81	0.27	70,70,70,70	0
84	MG	5	3520	1/1	0.81	0.36	54,54,54,54	0
84	MG	O2	204	1/1	0.81	0.32	58,58,58,58	0
84	MG	6	1994	1/1	0.81	0.60	69,69,69,69	0
84	MG	O3	201	1/1	0.81	0.41	64,64,64,64	0
84	MG	5	3968	1/1	0.81	0.26	56,56,56,56	0
84	MG	1	3652	1/1	0.81	0.23	59,59,59,59	0
84	MG	5	3552	1/1	0.81	0.52	68,68,68,68	0
84	MG	5	3696	1/1	0.81	0.39	94,94,94,94	0
84	MG	1	3529	1/1	0.81	0.76	66,66,66,66	0
84	MG	5	3992	1/1	0.81	0.42	49,49,49,49	0
84	MG	2	2035	1/1	0.81	0.27	101,101,101,101	0
84	MG	n1	201	1/1	0.81	0.15	61,61,61,61	0
84	MG	6	2037	1/1	0.81	0.17	87,87,87,87	0
84	MG	3	210	1/1	0.81	0.22	65,65,65,65	0
84	MG	1	3494	1/1	0.82	0.40	81,81,81,81	0
84	MG	5	3565	1/1	0.82	0.39	57,57,57,57	0
84	MG	q2	503	1/1	0.82	0.35	52,52,52,52	0
84	MG	5	4015	1/1	0.82	0.41	59,59,59,59	0
84	MG	7	230	1/1	0.82	0.45	75,75,75,75	0
84	MG	1	3976	1/1	0.82	0.23	71,71,71,71	0
84	MG	1	3936	1/1	0.82	0.37	67,67,67,67	0
84	MG	N1	201	1/1	0.82	0.29	68,68,68,68	0
84	MG	5	3728	1/1	0.82	0.21	51,51,51,51	0
84	MG	1	3699	1/1	0.82	0.53	82,82,82,82	0
84	MG	5	3752	1/1	0.82	0.36	59,59,59,59	0
84	MG	1	3446	1/1	0.82	0.22	62,62,62,62	0
84	MG	8	212	1/1	0.82	0.34	66,66,66,66	0
84	MG	1	3509	1/1	0.82	0.54	60,60,60,60	0
84	MG	D3	205	1/1	0.82	0.23	86,86,86,86	0
84	MG	1	3477	1/1	0.82	0.38	51,51,51,51	0
84	MG	1	3575	1/1	0.82	0.18	61,61,61,61	0
84	MG	5	3927	1/1	0.82	0.40	55,55,55,55	1
84	MG	5	3616	1/1	0.82	0.17	82,82,82,82	0
84	MG	5	4060	1/1	0.82	0.32	68,68,68,68	0
84	MG	6	1950	1/1	0.82	0.28	72,72,72,72	0
84	MG	1	3418	1/1	0.82	0.57	65,65,65,65	0
84	MG	5	3786	1/1	0.82	0.38	43,43,43,43	0
84	MG	1	3505	1/1	0.82	0.37	67,67,67,67	0
84	MG	5	3943	1/1	0.82	0.69	75,75,75,75	0
84	MG	L8	301	1/1	0.82	0.18	103,103,103,103	0
84	MG	6	1976	1/1	0.82	0.22	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	4083	1/1	0.82	0.15	88,88,88,88	0
84	MG	6	1980	1/1	0.82	0.24	108,108,108,108	0
84	MG	2	2022	1/1	0.82	0.09	132,132,132,132	0
84	MG	5	3953	1/1	0.82	0.60	62,62,62,62	0
84	MG	2	1967	1/1	0.82	0.35	90,90,90,90	0
84	MG	5	3488	1/1	0.82	0.21	55,55,55,55	0
84	MG	2	1975	1/1	0.82	0.46	87,87,87,87	0
84	MG	O4	504	1/1	0.82	0.48	76,76,76,76	0
84	MG	s6	301	1/1	0.82	0.28	78,78,78,78	0
84	MG	2	2027	1/1	0.82	0.55	95,95,95,95	0
84	MG	5	3812	1/1	0.82	0.53	46,46,46,46	0
84	MG	2	2033	1/1	0.82	0.23	108,108,108,108	0
84	MG	5	3686	1/1	0.82	0.30	68,68,68,68	0
84	MG	1	3559	1/1	0.82	0.24	73,73,73,73	0
84	MG	5	3692	1/1	0.82	0.26	73,73,73,73	0
84	MG	6	2021	1/1	0.82	0.09	86,86,86,86	0
84	MG	5	3546	1/1	0.82	0.37	63,63,63,63	0
84	MG	5	3694	1/1	0.82	0.22	84,84,84,84	0
84	MG	1	3766	1/1	0.82	0.27	58,58,58,58	0
84	MG	1	3963	1/1	0.82	0.33	76,76,76,76	0
84	MG	M5	301	1/1	0.82	0.35	69,69,69,69	0
86	ZN	d7	101	1/1	0.82	0.15	272,272,272,272	0
84	MG	1	3914	1/1	0.83	0.27	59,59,59,59	0
84	MG	5	3566	1/1	0.83	0.27	60,60,60,60	0
84	MG	1	3629	1/1	0.83	0.14	136,136,136,136	0
84	MG	m9	201	1/1	0.83	0.24	74,74,74,74	0
84	MG	5	3839	1/1	0.83	0.25	68,68,68,68	0
84	MG	5	3708	1/1	0.83	0.30	75,75,75,75	0
84	MG	5	3980	1/1	0.83	0.39	52,52,52,52	0
84	MG	5	3841	1/1	0.83	0.25	61,61,61,61	0
84	MG	1	3922	1/1	0.83	0.25	61,61,61,61	0
84	MG	2	1991	1/1	0.83	0.15	103,103,103,103	0
84	MG	6	2065	1/1	0.83	0.20	104,104,104,104	0
84	MG	3	212	1/1	0.83	0.33	64,64,64,64	0
84	MG	5	3858	1/1	0.83	0.32	55,55,55,55	0
84	MG	2	1901	1/1	0.83	0.21	92,92,92,92	0
84	MG	5	3861	1/1	0.83	0.34	63,63,63,63	0
84	MG	D3	203	1/1	0.83	0.36	85,85,85,85	0
84	MG	M3	205	1/1	0.83	0.26	82,82,82,82	0
84	MG	5	3754	1/1	0.83	0.46	69,69,69,69	0
84	MG	5	4021	1/1	0.83	0.28	60,60,60,60	0
84	MG	1	3492	1/1	0.83	0.38	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	4027	1/1	0.83	0.54	50,50,50,50	0
84	MG	1	3957	1/1	0.83	0.21	71,71,71,71	0
84	MG	5	3423	1/1	0.83	0.29	54,54,54,54	1
84	MG	2	1919	1/1	0.83	0.28	84,84,84,84	0
84	MG	5	3897	1/1	0.83	0.42	76,76,76,76	0
84	MG	M7	205	1/1	0.83	0.30	59,59,59,59	0
84	MG	4	203	1/1	0.83	0.27	61,61,61,61	0
84	MG	1	3558	1/1	0.83	0.20	68,68,68,68	0
84	MG	8	220	1/1	0.83	0.35	94,94,94,94	0
84	MG	5	3922	1/1	0.83	0.30	56,56,56,56	0
84	MG	6	2130	1/1	0.83	0.16	95,95,95,95	0
84	MG	N0	203	1/1	0.83	0.09	80,80,80,80	0
84	MG	1	3929	1/1	0.83	0.54	63,63,63,63	0
84	MG	2	2018	1/1	0.83	0.10	135,135,135,135	0
84	MG	1	3807	1/1	0.83	0.46	77,77,77,77	0
84	MG	l3	411	1/1	0.83	0.16	53,53,53,53	0
84	MG	5	3939	1/1	0.83	0.24	76,76,76,76	0
84	MG	6	2150	1/1	0.83	0.21	81,81,81,81	0
84	MG	6	2153	1/1	0.83	0.19	68,68,68,68	0
84	MG	5	4072	1/1	0.83	0.09	109,109,109,109	0
84	MG	2	1960	1/1	0.83	0.20	94,94,94,94	0
84	MG	s0	301	1/1	0.83	0.16	103,103,103,103	0
84	MG	5	4074	1/1	0.83	0.08	105,105,105,105	0
84	MG	s3	301	1/1	0.83	0.29	84,84,84,84	0
84	MG	1	3972	1/1	0.83	0.20	65,65,65,65	0
84	MG	5	3944	1/1	0.83	0.67	61,61,61,61	0
84	MG	1	3824	1/1	0.83	0.37	62,62,62,62	0
84	MG	1	3935	1/1	0.83	0.26	68,68,68,68	0
84	MG	m3	203	1/1	0.83	0.48	81,81,81,81	0
84	MG	5	3691	1/1	0.83	0.43	74,74,74,74	0
84	MG	d3	202	1/1	0.83	0.35	69,69,69,69	0
84	MG	1	3445	1/1	0.83	0.41	64,64,64,64	0
84	MG	1	3695	1/1	0.83	0.64	67,67,67,67	0
84	MG	6	1998	1/1	0.83	0.26	78,78,78,78	0
84	MG	5	4101	1/1	0.83	0.21	75,75,75,75	0
84	MG	1	3941	1/1	0.83	0.17	66,66,66,66	0
85	LLL	5	4173	31/31	0.83	0.30	106,106,107,107	31
84	MG	m6	205	1/1	0.83	0.27	51,51,51,51	1
85	LLL	6	2174	31/31	0.83	0.29	81,81,81,81	31
84	MG	1	3837	1/1	0.83	0.48	58,58,58,58	0
84	MG	1	3502	1/1	0.83	0.37	64,64,64,64	0
84	MG	5	3709	1/1	0.84	0.17	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	3710	1/1	0.84	0.24	72,72,72,72	0
84	MG	2	1947	1/1	0.84	0.48	92,92,92,92	0
84	MG	6	2027	1/1	0.84	0.19	61,61,61,61	0
84	MG	5	3551	1/1	0.84	0.48	56,56,56,56	0
84	MG	2	1952	1/1	0.84	0.47	99,99,99,99	0
84	MG	1	3908	1/1	0.84	0.36	60,60,60,60	0
84	MG	1	3624	1/1	0.84	0.23	74,74,74,74	0
84	MG	1	3554	1/1	0.84	0.21	67,67,67,67	0
84	MG	2	2031	1/1	0.84	0.35	105,105,105,105	0
84	MG	2	1956	1/1	0.84	0.38	72,72,72,72	0
84	MG	6	2061	1/1	0.84	0.20	80,80,80,80	0
84	MG	5	3940	1/1	0.84	0.36	71,71,71,71	0
84	MG	5	3571	1/1	0.84	0.18	77,77,77,77	0
84	MG	1	3790	1/1	0.84	0.33	78,78,78,78	0
84	MG	1	3664	1/1	0.84	0.14	63,63,63,63	0
84	MG	1	3925	1/1	0.84	0.30	83,83,83,83	0
84	MG	1	3821	1/1	0.84	0.75	68,68,68,68	0
84	MG	2	2042	1/1	0.84	0.17	101,101,101,101	0
84	MG	6	2079	1/1	0.84	0.38	63,63,63,63	0
84	MG	1	3822	1/1	0.84	0.30	86,86,86,86	0
84	MG	6	2089	1/1	0.84	0.25	71,71,71,71	0
84	MG	5	4118	1/1	0.84	0.17	87,87,87,87	0
84	MG	6	2094	1/1	0.84	0.30	69,69,69,69	0
84	MG	1	3799	1/1	0.84	0.14	93,93,93,93	0
84	MG	n9	101	1/1	0.84	0.44	49,49,49,49	0
84	MG	5	4125	1/1	0.84	0.44	55,55,55,55	0
84	MG	5	4128	1/1	0.84	0.32	68,68,68,68	0
84	MG	5	3597	1/1	0.84	0.35	70,70,70,70	0
84	MG	5	3598	1/1	0.84	0.55	84,84,84,84	0
84	MG	5	4132	1/1	0.84	0.34	94,94,94,94	0
84	MG	1	3930	1/1	0.84	0.38	73,73,73,73	0
84	MG	5	3604	1/1	0.84	0.23	78,78,78,78	0
84	MG	6	1912	1/1	0.84	0.13	95,95,95,95	0
84	MG	5	4141	1/1	0.84	0.29	62,62,62,62	0
84	MG	6	2123	1/1	0.84	0.59	142,142,142,142	0
84	MG	6	1917	1/1	0.84	0.28	89,89,89,89	0
84	MG	6	2125	1/1	0.84	0.22	71,71,71,71	0
84	MG	6	2127	1/1	0.84	0.44	76,76,76,76	0
84	MG	5	3609	1/1	0.84	0.20	87,87,87,87	0
84	MG	1	3576	1/1	0.84	0.26	72,72,72,72	0
84	MG	7	216	1/1	0.84	0.09	74,74,74,74	1
84	MG	1	3984	1/1	0.84	0.32	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	7	222	1/1	0.84	0.13	66,66,66,66	0
84	MG	1	3718	1/1	0.84	0.26	60,60,60,60	0
84	MG	L9	201	1/1	0.84	0.27	59,59,59,59	0
84	MG	6	2144	1/1	0.84	0.15	76,76,76,76	0
84	MG	1	3884	1/1	0.84	0.22	80,80,80,80	0
84	MG	5	3823	1/1	0.84	0.20	57,57,57,57	1
84	MG	1	3666	1/1	0.84	0.27	72,72,72,72	0
84	MG	5	3414	1/1	0.84	0.51	54,54,54,54	0
84	MG	6	2154	1/1	0.84	0.15	78,78,78,78	0
84	MG	5	4004	1/1	0.84	0.32	80,80,80,80	0
84	MG	1	3834	1/1	0.84	0.70	70,70,70,70	0
84	MG	M3	204	1/1	0.84	0.29	69,69,69,69	0
84	MG	1	3543	1/1	0.84	0.64	51,51,51,51	0
84	MG	5	3660	1/1	0.84	0.17	96,96,96,96	0
84	MG	2	1908	1/1	0.84	0.37	104,104,104,104	0
84	MG	2	2003	1/1	0.84	0.28	118,118,118,118	0
84	MG	1	3896	1/1	0.84	0.19	73,73,73,73	0
84	MG	5	4023	1/1	0.84	0.17	58,58,58,58	1
84	MG	5	3688	1/1	0.84	0.39	73,73,73,73	0
84	MG	2	1914	1/1	0.84	0.50	83,83,83,83	0
84	MG	M5	302	1/1	0.84	0.32	58,58,58,58	0
84	MG	2	1923	1/1	0.84	0.41	87,87,87,87	0
84	MG	1	3730	1/1	0.84	0.38	65,65,65,65	0
84	MG	5	3509	1/1	0.84	0.48	65,65,65,65	0
84	MG	5	3512	1/1	0.84	0.36	56,56,56,56	0
84	MG	2	1930	1/1	0.84	0.71	81,81,81,81	0
85	LLL	1	4000	31/31	0.84	0.29	84,85,85,85	31
84	MG	1	3412	1/1	0.84	0.30	51,51,51,51	0
85	LLL	5	4176	31/31	0.84	0.27	74,74,74,74	31
84	MG	1	3623	1/1	0.84	0.35	68,68,68,68	0
85	LLL	7	233	31/31	0.84	0.23	82,82,82,82	31
84	MG	2	2020	1/1	0.84	0.21	111,111,111,111	0
84	MG	5	3891	1/1	0.84	0.70	75,75,75,75	0
84	MG	5	3543	1/1	0.84	0.32	52,52,52,52	1
84	MG	1	3965	1/1	0.85	0.32	67,67,67,67	1
84	MG	3	219	1/1	0.85	0.31	79,79,79,79	0
84	MG	1	3593	1/1	0.85	0.47	63,63,63,63	0
84	MG	6	2110	1/1	0.85	0.12	124,124,124,124	0
84	MG	1	3794	1/1	0.85	0.32	68,68,68,68	0
84	MG	1	3615	1/1	0.85	0.26	59,59,59,59	0
84	MG	1	3735	1/1	0.85	0.45	77,77,77,77	0
84	MG	6	2117	1/1	0.85	0.53	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	4136	1/1	0.85	0.25	70,70,70,70	0
84	MG	6	1971	1/1	0.85	0.36	73,73,73,73	0
84	MG	5	4140	1/1	0.85	0.33	57,57,57,57	0
84	MG	6	1975	1/1	0.85	0.23	83,83,83,83	0
84	MG	m4	203	1/1	0.85	0.21	59,59,59,59	0
84	MG	1	3978	1/1	0.85	0.31	89,89,89,89	0
84	MG	5	4144	1/1	0.85	0.18	58,58,58,58	0
84	MG	5	4148	1/1	0.85	0.47	54,54,54,54	0
84	MG	1	3863	1/1	0.85	0.29	74,74,74,74	0
84	MG	5	3610	1/1	0.85	0.24	110,110,110,110	0
84	MG	1	3831	1/1	0.85	0.38	59,59,59,59	0
84	MG	1	3468	1/1	0.85	0.45	61,61,61,61	0
84	MG	1	3785	1/1	0.85	0.26	73,73,73,73	0
84	MG	m8	201	1/1	0.85	0.28	55,55,55,55	0
84	MG	5	3800	1/1	0.85	0.21	69,69,69,69	0
84	MG	1	3878	1/1	0.85	0.44	60,60,60,60	0
84	MG	6	2145	1/1	0.85	0.20	77,77,77,77	0
84	MG	5	3441	1/1	0.85	0.25	72,72,72,72	0
84	MG	7	229	1/1	0.85	0.27	72,72,72,72	0
84	MG	n0	206	1/1	0.85	0.44	48,48,48,48	0
84	MG	5	3969	1/1	0.85	0.49	70,70,70,70	0
84	MG	5	3881	1/1	0.85	0.43	63,63,63,63	0
84	MG	1	3905	1/1	0.85	0.22	76,76,76,76	0
84	MG	5	4077	1/1	0.85	0.26	70,70,70,70	0
84	MG	L3	402	1/1	0.85	0.58	60,60,60,60	0
84	MG	2	2009	1/1	0.85	0.19	117,117,117,117	0
84	MG	q2	504	1/1	0.85	0.56	60,60,60,60	0
84	MG	5	3650	1/1	0.85	0.51	80,80,80,80	0
84	MG	5	3477	1/1	0.85	0.42	60,60,60,60	0
84	MG	5	3822	1/1	0.85	0.16	60,60,60,60	0
84	MG	5	3653	1/1	0.85	0.26	76,76,76,76	0
84	MG	5	3919	1/1	0.85	0.30	51,51,51,51	0
84	MG	6	1906	1/1	0.85	0.29	76,76,76,76	0
84	MG	5	4099	1/1	0.85	0.27	105,105,105,105	0
84	MG	5	3732	1/1	0.85	0.32	70,70,70,70	0
84	MG	5	3923	1/1	0.85	0.90	67,67,67,67	0
84	MG	5	3924	1/1	0.85	0.30	56,56,56,56	0
84	MG	1	3700	1/1	0.85	0.91	52,52,52,52	0
84	MG	1	3961	1/1	0.85	0.18	80,80,80,80	0
84	MG	6	1929	1/1	0.85	0.38	69,69,69,69	0
85	LLL	1	4002	31/31	0.85	0.35	136,137,137,137	0
85	LLL	4	224	31/31	0.85	0.36	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	13	407	1/1	0.85	0.33	55,55,55,55	0
85	LLL	5	4175	31/31	0.85	0.29	60,60,60,60	31
84	MG	6	2083	1/1	0.85	0.29	78,78,78,78	0
84	MG	5	4116	1/1	0.85	0.13	82,82,82,82	0
84	MG	5	3935	1/1	0.85	0.28	52,52,52,52	0
84	MG	5	4020	1/1	0.85	0.34	72,72,72,72	0
85	LLL	6	2175	31/31	0.85	0.30	66,66,66,66	31
84	MG	1	3413	1/1	0.85	0.21	55,55,55,55	1
84	MG	5	3837	1/1	0.85	0.30	72,72,72,72	0
84	MG	1	3835	1/1	0.86	0.24	58,58,58,58	0
84	MG	6	2073	1/1	0.86	0.27	80,80,80,80	0
84	MG	5	3649	1/1	0.86	0.14	63,63,63,63	1
84	MG	1	3547	1/1	0.86	0.30	65,65,65,65	0
84	MG	5	4035	1/1	0.86	0.27	76,76,76,76	0
84	MG	1	3609	1/1	0.86	0.36	52,52,52,52	0
84	MG	5	3528	1/1	0.86	0.89	56,56,56,56	0
84	MG	5	4043	1/1	0.86	0.33	51,51,51,51	0
84	MG	6	1916	1/1	0.86	0.22	94,94,94,94	0
84	MG	3	205	1/1	0.86	0.21	61,61,61,61	1
84	MG	1	3841	1/1	0.86	0.45	92,92,92,92	0
84	MG	2	2038	1/1	0.86	0.12	117,117,117,117	0
84	MG	5	3806	1/1	0.86	0.39	73,73,73,73	0
84	MG	5	3674	1/1	0.86	0.45	65,65,65,65	0
84	MG	5	4059	1/1	0.86	0.37	66,66,66,66	0
84	MG	5	3550	1/1	0.86	0.39	59,59,59,59	0
84	MG	2	1989	1/1	0.86	0.10	114,114,114,114	0
84	MG	6	1938	1/1	0.86	0.36	59,59,59,59	0
84	MG	5	4067	1/1	0.86	0.24	76,76,76,76	0
84	MG	5	4069	1/1	0.86	0.12	110,110,110,110	0
84	MG	1	3813	1/1	0.86	0.29	80,80,80,80	0
84	MG	5	3557	1/1	0.86	0.24	62,62,62,62	1
84	MG	3	209	1/1	0.86	0.18	70,70,70,70	0
84	MG	6	1947	1/1	0.86	0.42	64,64,64,64	0
84	MG	1	3903	1/1	0.86	0.23	80,80,80,80	0
84	MG	13	403	1/1	0.86	0.45	43,43,43,43	0
84	MG	5	3950	1/1	0.86	0.66	61,61,61,61	0
84	MG	5	3951	1/1	0.86	0.92	68,68,68,68	0
84	MG	6	2133	1/1	0.86	0.20	84,84,84,84	0
84	MG	1	3774	1/1	0.86	0.30	61,61,61,61	0
84	MG	1	3569	1/1	0.86	0.16	75,75,75,75	0
84	MG	5	4084	1/1	0.86	0.19	96,96,96,96	0
84	MG	1	3622	1/1	0.86	0.38	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	M7	201	1/1	0.86	0.29	59,59,59,59	0
84	MG	5	3962	1/1	0.86	0.53	95,95,95,95	0
84	MG	1	3703	1/1	0.86	0.47	65,65,65,65	0
84	MG	5	3576	1/1	0.86	0.33	52,52,52,52	0
84	MG	1	3476	1/1	0.86	0.49	54,54,54,54	0
84	MG	5	3403	1/1	0.86	0.37	54,54,54,54	0
84	MG	1	3791	1/1	0.86	0.18	83,83,83,83	0
84	MG	6	1990	1/1	0.86	0.26	73,73,73,73	0
84	MG	2	1942	1/1	0.86	0.45	84,84,84,84	0
84	MG	5	3972	1/1	0.86	0.45	60,60,60,60	0
84	MG	1	3641	1/1	0.86	0.29	104,104,104,104	0
84	MG	1	3875	1/1	0.86	0.37	64,64,64,64	0
84	MG	1	3573	1/1	0.86	0.13	65,65,65,65	0
84	MG	5	3981	1/1	0.86	0.31	46,46,46,46	0
84	MG	1	3969	1/1	0.86	0.34	72,72,72,72	0
84	MG	c3	202	1/1	0.86	0.29	87,87,87,87	0
84	MG	1	3747	1/1	0.86	0.23	71,71,71,71	0
84	MG	5	3453	1/1	0.86	0.36	56,56,56,56	0
84	MG	2	2019	1/1	0.86	0.09	127,127,127,127	0
84	MG	6	2023	1/1	0.86	0.19	79,79,79,79	0
84	MG	d3	204	1/1	0.86	0.27	66,66,66,66	0
84	MG	m7	203	1/1	0.86	0.38	63,63,63,63	0
84	MG	1	3626	1/1	0.86	0.26	63,63,63,63	0
84	MG	1	3828	1/1	0.86	0.58	67,67,67,67	0
84	MG	5	3880	1/1	0.86	0.22	73,73,73,73	0
84	MG	1	3466	1/1	0.86	0.45	54,54,54,54	0
84	MG	1	3431	1/1	0.86	0.35	56,56,56,56	0
84	MG	1	3979	1/1	0.86	0.19	69,69,69,69	0
84	MG	5	3894	1/1	0.86	0.51	72,72,72,72	0
85	LLL	2	2044	31/31	0.86	0.28	116,116,116,116	0
85	LLL	2	2045	31/31	0.86	0.41	117,117,117,118	0
85	LLL	5	4156	31/31	0.86	0.28	83,84,84,84	31
84	MG	5	4146	1/1	0.86	0.22	63,63,63,63	0
84	MG	5	3494	1/1	0.86	0.23	59,59,59,59	0
84	MG	5	3627	1/1	0.86	0.32	53,53,53,53	1
85	LLL	5	4177	31/31	0.86	0.32	51,51,51,51	31
84	MG	5	4150	1/1	0.86	0.19	81,81,81,81	0
85	LLL	7	232	31/31	0.86	0.34	81,81,81,81	31
84	MG	q1	102	1/1	0.86	0.34	64,64,64,64	0
85	LLL	6	2173	31/31	0.86	0.35	102,102,103,103	31
84	MG	L4	401	1/1	0.86	0.32	69,69,69,69	0
84	MG	7	214	1/1	0.86	0.33	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	3781	1/1	0.86	0.21	56,56,56,56	0
84	MG	1	3592	1/1	0.86	0.35	62,62,62,62	1
84	MG	5	3744	1/1	0.87	0.40	65,65,65,65	0
84	MG	5	3749	1/1	0.87	0.39	77,77,77,77	0
84	MG	3	207	1/1	0.87	0.21	58,58,58,58	0
84	MG	5	3523	1/1	0.87	0.33	55,55,55,55	0
84	MG	5	3618	1/1	0.87	0.43	83,83,83,83	0
84	MG	5	3874	1/1	0.87	0.27	70,70,70,70	0
84	MG	1	3727	1/1	0.87	0.48	55,55,55,55	0
84	MG	15	306	1/1	0.87	0.13	70,70,70,70	0
84	MG	1	3687	1/1	0.87	0.36	51,51,51,51	0
84	MG	5	4115	1/1	0.87	0.44	59,59,59,59	0
84	MG	1	3691	1/1	0.87	0.26	59,59,59,59	0
84	MG	6	1961	1/1	0.87	0.29	75,75,75,75	0
84	MG	1	3488	1/1	0.87	0.26	73,73,73,73	0
84	MG	5	3887	1/1	0.87	0.12	84,84,84,84	0
84	MG	5	4006	1/1	0.87	0.44	64,64,64,64	0
84	MG	1	3819	1/1	0.87	0.30	80,80,80,80	0
84	MG	2	1968	1/1	0.87	0.29	95,95,95,95	0
84	MG	2	1917	1/1	0.87	0.22	88,88,88,88	0
84	MG	6	2131	1/1	0.87	0.16	89,89,89,89	0
84	MG	3	213	1/1	0.87	0.14	90,90,90,90	0
84	MG	m5	302	1/1	0.87	0.33	71,71,71,71	0
84	MG	1	3913	1/1	0.87	0.29	59,59,59,59	0
84	MG	6	1984	1/1	0.87	0.18	89,89,89,89	0
84	MG	1	3620	1/1	0.87	0.66	65,65,65,65	0
84	MG	5	3907	1/1	0.87	0.33	41,41,41,41	0
84	MG	1	3713	1/1	0.87	0.12	81,81,81,81	0
84	MG	1	3459	1/1	0.87	0.47	61,61,61,61	0
84	MG	2	2025	1/1	0.87	0.20	123,123,123,123	0
84	MG	4	204	1/1	0.87	0.30	69,69,69,69	0
84	MG	6	2152	1/1	0.87	0.19	68,68,68,68	0
84	MG	2	1941	1/1	0.87	0.36	60,60,60,60	0
84	MG	5	3925	1/1	0.87	0.31	53,53,53,53	0
84	MG	6	2160	1/1	0.87	0.29	88,88,88,88	0
84	MG	2	2028	1/1	0.87	0.21	117,117,117,117	0
84	MG	5	4034	1/1	0.87	0.24	68,68,68,68	0
84	MG	6	2163	1/1	0.87	0.43	66,66,66,66	1
84	MG	5	3446	1/1	0.87	0.33	53,53,53,53	0
84	MG	6	2010	1/1	0.87	0.33	68,68,68,68	0
84	MG	n0	201	1/1	0.87	0.15	68,68,68,68	0
84	MG	2	2029	1/1	0.87	0.18	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	3454	1/1	0.87	0.42	46,46,46,46	0
84	MG	5	3809	1/1	0.87	0.20	60,60,60,60	0
84	MG	5	3938	1/1	0.87	0.16	66,66,66,66	0
84	MG	5	3581	1/1	0.87	0.45	53,53,53,53	0
84	MG	5	4051	1/1	0.87	0.31	77,77,77,77	0
84	MG	o2	203	1/1	0.87	0.27	51,51,51,51	0
84	MG	o3	201	1/1	0.87	0.23	56,56,56,56	0
84	MG	1	3775	1/1	0.87	0.36	62,62,62,62	0
84	MG	7	228	1/1	0.87	0.27	73,73,73,73	0
84	MG	5	3466	1/1	0.87	0.34	50,50,50,50	0
84	MG	1	3582	1/1	0.87	0.28	65,65,65,65	0
84	MG	2	1951	1/1	0.87	0.70	95,95,95,95	0
84	MG	1	3784	1/1	0.87	0.51	72,72,72,72	0
84	MG	5	3947	1/1	0.87	0.48	57,57,57,57	0
84	MG	5	3698	1/1	0.87	0.32	81,81,81,81	0
84	MG	5	3596	1/1	0.87	0.34	82,82,82,82	0
84	MG	5	3484	1/1	0.87	0.47	74,74,74,74	0
84	MG	1	3549	1/1	0.87	0.27	67,67,67,67	0
85	LLL	5	4155	31/31	0.87	0.30	81,81,82,82	0
84	MG	5	3491	1/1	0.87	0.14	62,62,62,62	0
85	LLL	5	4169	31/31	0.87	0.31	51,51,51,51	31
85	LLL	5	4171	31/31	0.87	0.24	107,107,107,107	0
84	MG	6	1914	1/1	0.87	0.08	114,114,114,114	0
85	LLL	5	4174	31/31	0.87	0.33	47,47,47,47	31
84	MG	1	3625	1/1	0.87	0.17	71,71,71,71	0
84	MG	5	3605	1/1	0.87	0.12	76,76,76,76	0
84	MG	5	3608	1/1	0.87	0.13	95,95,95,95	0
84	MG	1	3869	1/1	0.87	0.39	62,62,62,62	0
84	MG	6	1921	1/1	0.87	0.22	76,76,76,76	0
84	MG	2	2005	1/1	0.87	0.16	83,83,83,83	0
84	MG	6	2091	1/1	0.87	0.49	68,68,68,68	0
84	MG	S1	301	1/1	0.87	0.27	94,94,94,94	0
84	MG	5	3741	1/1	0.87	0.45	58,58,58,58	0
84	MG	6	2101	1/1	0.87	0.34	82,82,82,82	0
84	MG	5	3743	1/1	0.87	0.44	61,61,61,61	0
84	MG	1	3692	1/1	0.88	0.39	64,64,64,64	0
84	MG	6	1954	1/1	0.88	0.27	80,80,80,80	0
84	MG	5	3932	1/1	0.88	0.25	52,52,52,52	0
84	MG	5	4133	1/1	0.88	0.28	114,114,114,114	0
84	MG	6	1966	1/1	0.88	0.18	73,73,73,73	0
84	MG	m4	205	1/1	0.88	0.15	58,58,58,58	0
84	MG	2	1935	1/1	0.88	0.44	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	m5	301	1/1	0.88	0.29	62,62,62,62	0
84	MG	4	218	1/1	0.88	0.23	60,60,60,60	0
84	MG	5	3718	1/1	0.88	0.34	68,68,68,68	0
84	MG	1	3910	1/1	0.88	0.64	56,56,56,56	0
84	MG	5	3723	1/1	0.88	0.26	74,74,74,74	0
84	MG	N3	203	1/1	0.88	0.25	75,75,75,75	0
84	MG	2	1946	1/1	0.88	0.55	80,80,80,80	0
84	MG	5	3941	1/1	0.88	0.62	78,78,78,78	0
84	MG	4	222	1/1	0.88	0.20	79,79,79,79	0
84	MG	1	3546	1/1	0.88	0.27	63,63,63,63	0
84	MG	1	3487	1/1	0.88	0.27	79,79,79,79	0
84	MG	7	205	1/1	0.88	0.38	55,55,55,55	0
84	MG	5	4047	1/1	0.88	0.33	52,52,52,52	0
84	MG	5	3850	1/1	0.88	0.24	58,58,58,58	0
84	MG	6	2147	1/1	0.88	0.18	78,78,78,78	0
84	MG	m9	202	1/1	0.88	0.62	90,90,90,90	0
84	MG	5	3629	1/1	0.88	0.33	60,60,60,60	0
84	MG	5	3632	1/1	0.88	0.38	49,49,49,49	0
84	MG	O2	202	1/1	0.88	0.32	55,55,55,55	0
84	MG	7	224	1/1	0.88	0.18	71,71,71,71	0
84	MG	L3	401	1/1	0.88	0.17	76,76,76,76	0
84	MG	1	3440	1/1	0.88	0.23	82,82,82,82	0
84	MG	1	3586	1/1	0.88	0.28	58,58,58,58	0
84	MG	5	3763	1/1	0.88	0.35	78,78,78,78	0
84	MG	5	4065	1/1	0.88	0.36	58,58,58,58	0
84	MG	5	3424	1/1	0.88	0.32	54,54,54,54	0
84	MG	1	3812	1/1	0.88	0.19	82,82,82,82	0
84	MG	1	3503	1/1	0.88	0.31	61,61,61,61	0
84	MG	5	3873	1/1	0.88	0.27	71,71,71,71	0
84	MG	1	3838	1/1	0.88	0.32	50,50,50,50	0
84	MG	1	3455	1/1	0.88	0.42	70,70,70,70	0
84	MG	1	3452	1/1	0.88	0.19	65,65,65,65	0
84	MG	6	2039	1/1	0.88	0.20	83,83,83,83	0
84	MG	1	3970	1/1	0.88	0.42	50,50,50,50	0
84	MG	6	2050	1/1	0.88	0.17	71,71,71,71	0
84	MG	M3	202	1/1	0.88	0.20	80,80,80,80	0
84	MG	5	3455	1/1	0.88	0.34	55,55,55,55	0
84	MG	5	3456	1/1	0.88	0.23	53,53,53,53	0
84	MG	5	3893	1/1	0.88	0.62	65,65,65,65	0
84	MG	3	217	1/1	0.88	0.13	100,100,100,100	0
84	MG	6	1915	1/1	0.88	0.13	74,74,74,74	0
84	MG	1	3786	1/1	0.88	0.78	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	LLL	1	3995	31/31	0.88	0.24	124,125,125,125	0
85	LLL	1	3996	31/31	0.88	0.28	107,107,108,108	31
85	LLL	1	3997	31/31	0.88	0.36	108,108,108,108	0
84	MG	1	3973	1/1	0.88	0.34	64,64,64,64	0
85	LLL	1	4001	31/31	0.88	0.22	121,121,121,121	0
84	MG	6	2067	1/1	0.88	0.24	92,92,92,92	0
84	MG	6	2068	1/1	0.88	0.14	83,83,83,83	0
84	MG	2	1912	1/1	0.88	0.55	86,86,86,86	0
84	MG	6	1919	1/1	0.88	0.11	80,80,80,80	0
84	MG	5	4001	1/1	0.88	0.25	59,59,59,59	0
84	MG	5	4002	1/1	0.88	0.22	64,64,64,64	0
84	MG	1	3570	1/1	0.88	0.34	71,71,71,71	0
84	MG	1	3654	1/1	0.88	0.34	53,53,53,53	0
84	MG	5	3909	1/1	0.88	0.27	48,48,48,48	1
84	MG	5	3910	1/1	0.88	0.27	52,52,52,52	0
84	MG	1	3710	1/1	0.88	0.28	90,90,90,90	0
84	MG	6	2093	1/1	0.88	0.25	75,75,75,75	0
84	MG	1	3683	1/1	0.88	0.29	64,64,64,64	0
84	MG	5	4014	1/1	0.88	0.32	62,62,62,62	0
85	LLL	7	231	31/31	0.88	0.20	81,82,82,82	31
84	MG	6	1941	1/1	0.88	0.45	66,66,66,66	1
84	MG	5	4119	1/1	0.88	0.09	142,142,142,142	0
84	MG	19	202	1/1	0.88	0.35	58,58,58,58	0
84	MG	1	3611	1/1	0.88	0.40	47,47,47,47	0
84	MG	1	3660	1/1	0.88	0.15	72,72,72,72	0
84	MG	1	3614	1/1	0.88	0.32	58,58,58,58	0
84	MG	5	3510	1/1	0.88	0.27	62,62,62,62	0
84	MG	1	3677	1/1	0.89	0.54	66,66,66,66	0
84	MG	5	3420	1/1	0.89	0.29	50,50,50,50	0
84	MG	8	204	1/1	0.89	0.30	70,70,70,70	0
84	MG	6	2102	1/1	0.89	0.29	80,80,80,80	0
84	MG	1	3462	1/1	0.89	0.21	54,54,54,54	1
84	MG	2	1958	1/1	0.89	0.15	108,108,108,108	0
84	MG	5	3657	1/1	0.89	0.27	73,73,73,73	0
84	MG	5	3431	1/1	0.89	0.33	53,53,53,53	0
84	MG	5	4053	1/1	0.89	0.15	94,94,94,94	0
84	MG	1	3661	1/1	0.89	0.26	78,78,78,78	0
84	MG	5	3435	1/1	0.89	0.20	50,50,50,50	0
84	MG	6	1936	1/1	0.89	0.79	65,65,65,65	0
84	MG	5	4058	1/1	0.89	0.13	95,95,95,95	0
84	MG	1	3451	1/1	0.89	0.11	69,69,69,69	0
84	MG	1	3887	1/1	0.89	0.35	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3524	1/1	0.89	0.40	71,71,71,71	0
84	MG	5	3567	1/1	0.89	0.19	62,62,62,62	0
84	MG	1	3931	1/1	0.89	0.25	79,79,79,79	0
84	MG	5	3448	1/1	0.89	0.35	49,49,49,49	0
84	MG	5	3449	1/1	0.89	0.42	50,50,50,50	0
84	MG	5	3821	1/1	0.89	0.27	53,53,53,53	0
84	MG	6	1949	1/1	0.89	0.18	74,74,74,74	0
84	MG	2	1911	1/1	0.89	0.16	91,91,91,91	0
84	MG	1	3489	1/1	0.89	0.24	79,79,79,79	0
84	MG	M7	203	1/1	0.89	0.22	59,59,59,59	0
84	MG	1	3806	1/1	0.89	0.24	65,65,65,65	0
84	MG	5	3829	1/1	0.89	0.20	57,57,57,57	0
84	MG	1	3898	1/1	0.89	0.09	99,99,99,99	0
84	MG	16	201	1/1	0.89	0.26	60,60,60,60	0
84	MG	5	3834	1/1	0.89	0.32	60,60,60,60	0
84	MG	5	3699	1/1	0.89	0.31	63,63,63,63	0
84	MG	5	3592	1/1	0.89	0.33	57,57,57,57	0
84	MG	19	204	1/1	0.89	0.21	57,57,57,57	0
84	MG	1	3899	1/1	0.89	0.11	82,82,82,82	0
84	MG	5	3964	1/1	0.89	0.59	82,82,82,82	0
84	MG	1	3402	1/1	0.89	0.24	60,60,60,60	0
84	MG	5	3474	1/1	0.89	0.18	67,67,67,67	0
84	MG	2	1924	1/1	0.89	0.24	90,90,90,90	0
84	MG	m3	204	1/1	0.89	0.35	59,59,59,59	0
84	MG	5	3845	1/1	0.89	0.24	48,48,48,48	1
84	MG	5	3846	1/1	0.89	0.21	55,55,55,55	0
84	MG	m4	204	1/1	0.89	0.38	57,57,57,57	0
84	MG	1	3901	1/1	0.89	0.20	74,74,74,74	0
84	MG	5	3971	1/1	0.89	0.84	72,72,72,72	0
84	MG	1	3988	1/1	0.89	0.23	53,53,53,53	0
84	MG	s5	301	1/1	0.89	0.38	74,74,74,74	0
84	MG	s5	302	1/1	0.89	0.31	76,76,76,76	0
84	MG	5	3486	1/1	0.89	0.31	52,52,52,52	0
84	MG	1	3864	1/1	0.89	0.21	61,61,61,61	0
84	MG	m6	201	1/1	0.89	0.25	52,52,52,52	0
84	MG	5	3977	1/1	0.89	0.27	67,67,67,67	0
84	MG	2	1993	1/1	0.89	0.21	99,99,99,99	0
84	MG	c3	205	1/1	0.89	0.28	84,84,84,84	0
84	MG	c4	201	1/1	0.89	0.20	87,87,87,87	0
84	MG	c8	202	1/1	0.89	0.19	75,75,75,75	0
84	MG	1	3808	1/1	0.89	0.24	71,71,71,71	0
84	MG	5	4126	1/1	0.89	0.48	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3729	1/1	0.89	0.36	57,57,57,57	0
84	MG	5	3990	1/1	0.89	0.34	47,47,47,47	0
84	MG	5	3862	1/1	0.89	0.34	67,67,67,67	0
84	MG	5	3730	1/1	0.89	0.30	74,74,74,74	0
84	MG	2	1939	1/1	0.89	0.26	80,80,80,80	0
84	MG	5	3736	1/1	0.89	0.43	59,59,59,59	0
84	MG	5	3495	1/1	0.89	0.26	58,58,58,58	0
84	MG	5	3496	1/1	0.89	0.24	56,56,56,56	0
84	MG	1	3867	1/1	0.89	0.33	59,59,59,59	0
84	MG	6	2038	1/1	0.89	0.30	85,85,85,85	0
85	LLL	1	3998	31/31	0.89	0.35	99,100,100,100	31
85	LLL	1	3999	31/31	0.89	0.29	85,86,86,86	31
84	MG	5	3746	1/1	0.89	0.41	40,40,40,40	0
84	MG	5	4143	1/1	0.89	0.17	72,72,72,72	0
84	MG	5	3748	1/1	0.89	0.33	46,46,46,46	0
84	MG	6	2053	1/1	0.89	0.16	74,74,74,74	0
84	MG	1	3443	1/1	0.89	0.26	58,58,58,58	0
84	MG	5	3620	1/1	0.89	0.13	65,65,65,65	0
84	MG	n8	202	1/1	0.89	0.20	73,73,73,73	0
84	MG	5	3621	1/1	0.89	0.15	77,77,77,77	0
85	LLL	5	4158	31/31	0.89	0.28	60,60,60,60	31
85	LLL	5	4166	31/31	0.89	0.26	77,78,78,78	31
84	MG	5	3888	1/1	0.89	0.32	62,62,62,62	0
84	MG	1	3512	1/1	0.89	0.50	66,66,66,66	0
84	MG	1	3753	1/1	0.89	0.46	64,64,64,64	0
84	MG	7	209	1/1	0.89	0.12	64,64,64,64	0
84	MG	7	212	1/1	0.89	0.25	65,65,65,65	0
84	MG	5	3762	1/1	0.89	0.38	65,65,65,65	0
84	MG	1	3653	1/1	0.89	0.26	59,59,59,59	0
84	MG	5	3628	1/1	0.89	0.40	60,60,60,60	0
84	MG	5	3765	1/1	0.89	0.24	64,64,64,64	0
84	MG	2	1949	1/1	0.89	0.32	102,102,102,102	0
84	MG	1	3877	1/1	0.89	0.31	68,68,68,68	0
84	MG	5	3769	1/1	0.89	0.23	79,79,79,79	0
84	MG	1	3441	1/1	0.89	0.33	62,62,62,62	0
84	MG	5	3530	1/1	0.89	0.37	47,47,47,47	1
84	MG	1	3915	1/1	0.89	0.16	78,78,78,78	0
84	MG	1	3632	1/1	0.89	0.10	72,72,72,72	0
84	MG	5	3631	1/1	0.90	0.21	55,55,55,55	0
84	MG	1	3916	1/1	0.90	0.15	70,70,70,70	0
84	MG	5	3978	1/1	0.90	0.37	51,51,51,51	0
84	MG	1	3702	1/1	0.90	0.63	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	17	303	1/1	0.90	0.20	56,56,56,56	0
84	MG	5	3756	1/1	0.90	0.38	61,61,61,61	0
84	MG	1	3572	1/1	0.90	0.17	70,70,70,70	0
84	MG	19	203	1/1	0.90	0.24	49,49,49,49	0
84	MG	5	3875	1/1	0.90	0.39	80,80,80,80	0
84	MG	5	3642	1/1	0.90	0.47	52,52,52,52	0
84	MG	5	3433	1/1	0.90	0.38	48,48,48,48	0
84	MG	5	3647	1/1	0.90	0.36	58,58,58,58	0
84	MG	4	213	1/1	0.90	0.42	80,80,80,80	0
84	MG	5	3554	1/1	0.90	0.22	60,60,60,60	0
84	MG	1	3924	1/1	0.90	0.35	65,65,65,65	0
84	MG	6	2136	1/1	0.90	0.16	85,85,85,85	0
84	MG	N8	202	1/1	0.90	0.72	73,73,73,73	0
84	MG	1	3825	1/1	0.90	0.74	77,77,77,77	0
84	MG	5	3779	1/1	0.90	0.38	67,67,67,67	0
84	MG	1	3680	1/1	0.90	0.35	59,59,59,59	0
84	MG	5	4013	1/1	0.90	0.31	58,58,58,58	0
84	MG	1	3550	1/1	0.90	0.24	69,69,69,69	0
84	MG	1	3798	1/1	0.90	0.36	60,60,60,60	0
84	MG	5	4138	1/1	0.90	0.24	48,48,48,48	0
84	MG	1	3708	1/1	0.90	0.38	66,66,66,66	0
84	MG	L2	305	1/1	0.90	0.31	60,60,60,60	0
84	MG	1	3709	1/1	0.90	0.27	60,60,60,60	0
84	MG	1	3551	1/1	0.90	0.22	68,68,68,68	0
84	MG	m6	206	1/1	0.90	0.36	51,51,51,51	0
84	MG	2	1962	1/1	0.90	0.19	100,100,100,100	0
84	MG	5	3801	1/1	0.90	0.17	61,61,61,61	0
84	MG	5	3921	1/1	0.90	0.19	52,52,52,52	0
84	MG	m7	205	1/1	0.90	0.21	53,53,53,53	0
84	MG	1	3757	1/1	0.90	0.56	62,62,62,62	0
84	MG	6	2008	1/1	0.90	0.25	67,67,67,67	0
84	MG	s4	301	1/1	0.90	0.23	103,103,103,103	0
84	MG	5	3460	1/1	0.90	0.20	49,49,49,49	0
84	MG	6	2012	1/1	0.90	0.21	61,61,61,61	0
84	MG	5	3804	1/1	0.90	0.06	73,73,73,73	1
84	MG	L4	404	1/1	0.90	0.58	59,59,59,59	0
84	MG	5	3590	1/1	0.90	0.35	59,59,59,59	0
84	MG	5	3467	1/1	0.90	0.25	48,48,48,48	0
84	MG	5	3933	1/1	0.90	0.34	55,55,55,55	0
84	MG	1	3564	1/1	0.90	0.14	71,71,71,71	0
84	MG	1	3552	1/1	0.90	0.14	84,84,84,84	0
84	MG	6	2028	1/1	0.90	0.12	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	2	1972	1/1	0.90	0.22	88,88,88,88	0
84	MG	n1	202	1/1	0.90	0.26	61,61,61,61	0
84	MG	1	3714	1/1	0.90	0.16	90,90,90,90	0
84	MG	5	3700	1/1	0.90	0.32	65,65,65,65	0
84	MG	7	226	1/1	0.90	0.14	72,72,72,72	0
84	MG	d6	103	1/1	0.90	0.24	77,77,77,77	0
84	MG	n8	203	1/1	0.90	0.20	70,70,70,70	0
84	MG	1	3939	1/1	0.90	0.30	61,61,61,61	0
84	MG	2	1907	1/1	0.90	0.17	95,95,95,95	0
84	MG	1	3536	1/1	0.90	0.31	64,64,64,64	0
84	MG	5	3602	1/1	0.90	0.26	81,81,81,81	0
84	MG	1	3642	1/1	0.90	0.25	71,71,71,71	0
84	MG	1	3767	1/1	0.90	0.56	57,57,57,57	0
84	MG	5	3714	1/1	0.90	0.23	71,71,71,71	0
84	MG	5	3606	1/1	0.90	0.10	84,84,84,84	0
84	MG	1	3768	1/1	0.90	0.44	67,67,67,67	0
84	MG	1	3645	1/1	0.90	0.55	55,55,55,55	0
84	MG	1	3724	1/1	0.90	0.15	63,63,63,63	0
85	LLL	1	4004	31/31	0.90	0.23	100,101,101,101	31
84	MG	6	1902	1/1	0.90	0.34	51,51,51,51	0
84	MG	1	3538	1/1	0.90	0.35	64,64,64,64	0
84	MG	8	211	1/1	0.90	0.58	63,63,63,63	0
84	MG	1	3424	1/1	0.90	0.38	61,61,61,61	0
84	MG	5	3844	1/1	0.90	0.28	52,52,52,52	0
84	MG	1	3500	1/1	0.90	0.51	68,68,68,68	0
85	LLL	5	4162	31/31	0.90	0.16	117,118,118,118	0
84	MG	1	3618	1/1	0.90	0.61	58,58,58,58	1
85	LLL	5	4167	31/31	0.90	0.17	125,126,126,126	0
84	MG	8	218	1/1	0.90	0.32	84,84,84,84	0
84	MG	5	3619	1/1	0.90	0.18	86,86,86,86	0
84	MG	5	3854	1/1	0.90	0.23	60,60,60,60	0
84	MG	5	4082	1/1	0.90	0.13	71,71,71,71	0
84	MG	1	3911	1/1	0.90	0.40	56,56,56,56	0
84	MG	2	2002	1/1	0.90	0.47	117,117,117,117	0
84	MG	5	3525	1/1	0.90	0.17	51,51,51,51	1
84	MG	6	1927	1/1	0.90	0.28	78,78,78,78	0
84	MG	1	3737	1/1	0.90	0.33	73,73,73,73	0
84	MG	5	3747	1/1	0.90	0.24	46,46,46,46	0
84	MG	13	409	1/1	0.90	0.22	70,70,70,70	0
85	LLL	8	221	31/31	0.90	0.22	100,100,100,100	31
85	LLL	8	222	31/31	0.90	0.36	102,102,102,102	31
85	LLL	6	2168	31/31	0.90	0.24	86,86,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	LLL	6	2172	31/31	0.90	0.26	103,104,104,104	0
84	MG	4	205	1/1	0.90	0.20	87,87,87,87	0
84	MG	1	3874	1/1	0.90	0.21	66,66,66,66	0
84	MG	14	1101	1/1	0.90	0.29	65,65,65,65	0
84	MG	14	1102	1/1	0.90	0.27	57,57,57,57	0
84	MG	1	3672	1/1	0.90	0.31	52,52,52,52	0
84	MG	5	3529	1/1	0.91	0.35	47,47,47,47	0
84	MG	m7	204	1/1	0.91	0.30	62,62,62,62	0
84	MG	5	4062	1/1	0.91	0.16	86,86,86,86	0
84	MG	6	2126	1/1	0.91	0.33	92,92,92,92	0
84	MG	6	1978	1/1	0.91	0.13	93,93,93,93	0
84	MG	5	3703	1/1	0.91	0.20	70,70,70,70	0
84	MG	5	3876	1/1	0.91	0.14	66,66,66,66	0
84	MG	5	3614	1/1	0.91	0.21	81,81,81,81	0
84	MG	5	4068	1/1	0.91	0.12	112,112,112,112	0
84	MG	6	2132	1/1	0.91	0.13	83,83,83,83	0
84	MG	1	3649	1/1	0.91	0.19	61,61,61,61	0
84	MG	1	3933	1/1	0.91	0.71	84,84,84,84	0
84	MG	1	3749	1/1	0.91	0.37	60,60,60,60	0
84	MG	1	3862	1/1	0.91	0.20	63,63,63,63	0
84	MG	6	2140	1/1	0.91	0.33	65,65,65,65	0
84	MG	2	1938	1/1	0.91	0.51	76,76,76,76	0
84	MG	5	3889	1/1	0.91	0.21	55,55,55,55	0
84	MG	1	3751	1/1	0.91	0.80	72,72,72,72	0
84	MG	5	4079	1/1	0.91	0.14	70,70,70,70	0
84	MG	5	3892	1/1	0.91	0.80	68,68,68,68	0
84	MG	1	3912	1/1	0.91	0.17	58,58,58,58	0
84	MG	5	3553	1/1	0.91	0.39	59,59,59,59	0
84	MG	5	3895	1/1	0.91	0.32	57,57,57,57	0
84	MG	6	2011	1/1	0.91	0.29	68,68,68,68	0
84	MG	1	3773	1/1	0.91	0.33	62,62,62,62	0
84	MG	1	3449	1/1	0.91	0.26	56,56,56,56	0
84	MG	6	2158	1/1	0.91	0.22	77,77,77,77	0
84	MG	6	2016	1/1	0.91	0.17	79,79,79,79	0
84	MG	6	2017	1/1	0.91	0.12	81,81,81,81	0
84	MG	5	4089	1/1	0.91	0.70	62,62,62,62	0
84	MG	2	1944	1/1	0.91	0.72	87,87,87,87	0
84	MG	5	3991	1/1	0.91	0.59	57,57,57,57	0
84	MG	1	3755	1/1	0.91	0.72	60,60,60,60	0
84	MG	6	2025	1/1	0.91	0.18	81,81,81,81	1
84	MG	1	3781	1/1	0.91	0.33	69,69,69,69	1
84	MG	5	4102	1/1	0.91	0.33	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	q2	508	1/1	0.91	0.17	62,62,62,62	0
84	MG	1	3872	1/1	0.91	0.31	73,73,73,73	0
84	MG	6	2032	1/1	0.91	0.06	77,77,77,77	0
84	MG	1	3987	1/1	0.91	0.20	60,60,60,60	0
84	MG	5	4107	1/1	0.91	0.27	59,59,59,59	0
84	MG	c3	203	1/1	0.91	0.10	108,108,108,108	0
84	MG	5	4111	1/1	0.91	0.43	46,46,46,46	0
84	MG	5	3476	1/1	0.91	0.19	53,53,53,53	0
84	MG	c3	206	1/1	0.91	0.24	80,80,80,80	0
84	MG	6	1909	1/1	0.91	0.28	67,67,67,67	0
84	MG	6	2041	1/1	0.91	0.16	73,73,73,73	0
84	MG	6	2042	1/1	0.91	0.15	77,77,77,77	0
84	MG	6	2046	1/1	0.91	0.11	72,72,72,72	0
84	MG	6	2048	1/1	0.91	0.40	68,68,68,68	0
84	MG	5	3917	1/1	0.91	0.31	62,62,62,62	0
84	MG	Q2	505	1/1	0.91	0.35	59,59,59,59	0
84	MG	1	3594	1/1	0.91	0.18	53,53,53,53	0
84	MG	2	1904	1/1	0.91	0.27	91,91,91,91	0
84	MG	5	4010	1/1	0.91	0.33	53,53,53,53	0
84	MG	15	303	1/1	0.91	0.19	74,74,74,74	0
84	MG	5	3485	1/1	0.91	0.29	57,57,57,57	0
84	MG	1	3923	1/1	0.91	0.47	72,72,72,72	0
84	MG	2	2012	1/1	0.91	0.11	127,127,127,127	0
84	MG	1	3633	1/1	0.91	0.29	79,79,79,79	0
84	MG	5	3928	1/1	0.91	0.22	46,46,46,46	0
84	MG	4	219	1/1	0.91	0.26	68,68,68,68	0
84	MG	5	3753	1/1	0.91	0.47	85,85,85,85	0
84	MG	4	220	1/1	0.91	0.25	71,71,71,71	0
84	MG	2	1910	1/1	0.91	0.79	80,80,80,80	0
84	MG	1	3956	1/1	0.91	0.25	71,71,71,71	0
85	LLL	3	220	31/31	0.91	0.24	98,98,99,99	0
84	MG	6	2075	1/1	0.91	0.28	61,61,61,61	0
84	MG	5	3503	1/1	0.91	0.31	42,42,42,42	0
84	MG	6	2080	1/1	0.91	0.31	62,62,62,62	0
85	LLL	5	4153	31/31	0.91	0.28	64,64,65,65	0
84	MG	5	3505	1/1	0.91	0.19	50,50,50,50	0
84	MG	5	4137	1/1	0.91	0.31	58,58,58,58	0
84	MG	1	3563	1/1	0.91	0.13	76,76,76,76	0
84	MG	1	3926	1/1	0.91	0.33	54,54,54,54	0
85	LLL	5	4164	31/31	0.91	0.23	62,62,62,62	31
84	MG	5	3430	1/1	0.91	0.33	49,49,49,49	0
84	MG	6	2092	1/1	0.91	0.21	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	1	3643	1/1	0.91	0.17	67,67,67,67	0
84	MG	5	3603	1/1	0.91	0.15	80,80,80,80	0
85	LLL	5	4172	31/31	0.91	0.18	77,77,77,77	31
84	MG	6	2096	1/1	0.91	0.40	65,65,65,65	0
84	MG	6	1946	1/1	0.91	0.14	70,70,70,70	0
84	MG	2	1915	1/1	0.91	0.25	95,95,95,95	0
84	MG	5	3945	1/1	0.91	0.45	59,59,59,59	0
84	MG	6	2103	1/1	0.91	0.13	94,94,94,94	0
84	MG	5	3773	1/1	0.91	0.10	139,139,139,139	0
84	MG	1	3531	1/1	0.91	0.30	68,68,68,68	0
84	MG	6	1953	1/1	0.91	0.18	83,83,83,83	0
84	MG	1	3849	1/1	0.91	0.22	58,58,58,58	0
84	MG	1	3733	1/1	0.91	0.61	80,80,80,80	0
84	MG	6	2112	1/1	0.91	0.27	81,81,81,81	0
85	LLL	6	2164	31/31	0.91	0.27	73,74,74,74	0
85	LLL	6	2167	31/31	0.91	0.35	97,98,98,98	0
84	MG	5	3527	1/1	0.91	0.59	53,53,53,53	0
84	MG	5	3785	1/1	0.91	0.38	51,51,51,51	0
84	MG	1	3906	1/1	0.91	0.19	67,67,67,67	0
84	MG	5	3871	1/1	0.91	0.24	71,71,71,71	0
84	MG	5	3787	1/1	0.91	0.24	48,48,48,48	1
85	LLL	6	2176	31/31	0.91	0.24	80,80,80,80	31
84	MG	6	1973	1/1	0.91	0.38	65,65,65,65	0
84	MG	5	3961	1/1	0.91	0.33	53,53,53,53	0
84	MG	1	3801	1/1	0.92	0.19	69,69,69,69	0
84	MG	5	4113	1/1	0.92	0.18	72,72,72,72	0
84	MG	5	3504	1/1	0.92	0.18	54,54,54,54	0
84	MG	5	3409	1/1	0.92	0.18	45,45,45,45	0
84	MG	5	3996	1/1	0.92	0.26	44,44,44,44	0
84	MG	5	3998	1/1	0.92	0.23	54,54,54,54	0
84	MG	1	3845	1/1	0.92	0.17	53,53,53,53	0
84	MG	5	3796	1/1	0.92	0.10	67,67,67,67	0
84	MG	2	2008	1/1	0.92	0.16	117,117,117,117	0
84	MG	5	4121	1/1	0.92	0.14	84,84,84,84	0
84	MG	1	3535	1/1	0.92	0.48	62,62,62,62	0
84	MG	1	3754	1/1	0.92	0.68	68,68,68,68	0
84	MG	1	3651	1/1	0.92	0.26	59,59,59,59	0
84	MG	5	3429	1/1	0.92	0.36	48,48,48,48	0
84	MG	1	3962	1/1	0.92	0.28	78,78,78,78	0
84	MG	6	1982	1/1	0.92	0.21	104,104,104,104	0
84	MG	5	3613	1/1	0.92	0.31	79,79,79,79	0
84	MG	5	3712	1/1	0.92	0.13	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	6	1986	1/1	0.92	0.28	82,82,82,82	0
84	MG	1	3605	1/1	0.92	0.72	46,46,46,46	0
84	MG	5	3912	1/1	0.92	0.28	45,45,45,45	0
84	MG	m6	204	1/1	0.92	0.35	48,48,48,48	0
84	MG	1	3712	1/1	0.92	0.17	82,82,82,82	0
84	MG	6	2146	1/1	0.92	0.12	87,87,87,87	0
84	MG	5	4016	1/1	0.92	0.25	62,62,62,62	0
84	MG	1	3968	1/1	0.92	0.11	74,74,74,74	0
84	MG	5	3918	1/1	0.92	0.31	58,58,58,58	0
84	MG	5	3815	1/1	0.92	0.35	55,55,55,55	0
84	MG	6	1995	1/1	0.92	0.11	117,117,117,117	0
84	MG	5	3817	1/1	0.92	0.25	41,41,41,41	0
84	MG	2	1963	1/1	0.92	0.14	117,117,117,117	0
84	MG	6	2156	1/1	0.92	0.42	77,77,77,77	0
84	MG	6	2157	1/1	0.92	0.24	63,63,63,63	0
84	MG	2	1964	1/1	0.92	0.20	90,90,90,90	0
84	MG	6	2001	1/1	0.92	0.36	79,79,79,79	0
84	MG	6	2006	1/1	0.92	0.39	63,63,63,63	0
84	MG	5	4147	1/1	0.92	0.17	61,61,61,61	0
84	MG	5	3534	1/1	0.92	0.39	50,50,50,50	0
84	MG	1	3585	1/1	0.92	0.29	52,52,52,52	0
84	MG	s2	301	1/1	0.92	0.34	69,69,69,69	0
84	MG	L3	403	1/1	0.92	0.27	62,62,62,62	0
84	MG	5	3827	1/1	0.92	0.16	51,51,51,51	1
84	MG	5	3929	1/1	0.92	0.27	43,43,43,43	0
84	MG	5	3443	1/1	0.92	0.33	49,49,49,49	0
84	MG	n0	205	1/1	0.92	0.16	47,47,47,47	0
84	MG	6	2020	1/1	0.92	0.13	85,85,85,85	0
84	MG	5	4037	1/1	0.92	0.17	77,77,77,77	0
84	MG	6	2022	1/1	0.92	0.26	88,88,88,88	0
84	MG	5	4039	1/1	0.92	0.22	77,77,77,77	0
84	MG	5	3734	1/1	0.92	0.17	67,67,67,67	0
84	MG	5	3549	1/1	0.92	0.40	63,63,63,63	0
84	MG	1	3685	1/1	0.92	0.40	56,56,56,56	0
84	MG	2	1920	1/1	0.92	0.28	88,88,88,88	0
84	MG	L4	403	1/1	0.92	0.22	55,55,55,55	0
84	MG	1	3811	1/1	0.92	0.20	80,80,80,80	0
84	MG	o1	201	1/1	0.92	0.18	79,79,79,79	0
84	MG	d2	201	1/1	0.92	0.22	80,80,80,80	0
84	MG	o2	202	1/1	0.92	0.43	55,55,55,55	0
84	MG	1	3890	1/1	0.92	0.39	50,50,50,50	0
84	MG	L4	406	1/1	0.92	0.29	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	d3	205	1/1	0.92	0.29	98,98,98,98	0
84	MG	o3	202	1/1	0.92	0.22	70,70,70,70	0
84	MG	1	3527	1/1	0.92	0.45	70,70,70,70	0
84	MG	5	4054	1/1	0.92	0.12	97,97,97,97	0
84	MG	5	3644	1/1	0.92	0.25	64,64,64,64	0
84	MG	1	3568	1/1	0.92	0.14	83,83,83,83	0
84	MG	q2	505	1/1	0.92	0.26	63,63,63,63	0
84	MG	2	1981	1/1	0.92	0.61	58,58,58,58	0
84	MG	8	203	1/1	0.92	0.18	83,83,83,83	1
84	MG	1	3722	1/1	0.92	0.10	68,68,68,68	0
84	MG	q3	502	1/1	0.92	0.38	68,68,68,68	0
84	MG	2	1986	1/1	0.92	0.13	117,117,117,117	0
84	MG	5	3468	1/1	0.92	0.14	55,55,55,55	0
84	MG	5	3760	1/1	0.92	0.29	59,59,59,59	0
84	MG	1	3945	1/1	0.92	0.28	54,54,54,54	0
84	MG	5	3470	1/1	0.92	0.35	54,54,54,54	0
84	MG	1	3920	1/1	0.92	0.29	53,53,53,53	0
84	MG	6	1910	1/1	0.92	0.29	60,60,60,60	0
85	LLL	L3	404	31/31	0.92	0.22	82,82,82,82	0
84	MG	5	3860	1/1	0.92	0.18	56,56,56,56	0
84	MG	5	3955	1/1	0.92	0.32	52,52,52,52	0
85	LLL	5	4152	31/31	0.92	0.27	79,79,79,79	31
84	MG	6	2069	1/1	0.92	0.12	86,86,86,86	0
84	MG	1	3921	1/1	0.92	0.18	72,72,72,72	0
84	MG	O7	103	1/1	0.92	0.18	59,59,59,59	0
84	MG	5	3767	1/1	0.92	0.34	60,60,60,60	0
84	MG	6	2074	1/1	0.92	0.15	64,64,64,64	0
85	LLL	5	4163	31/31	0.92	0.17	112,112,112,112	0
84	MG	5	4076	1/1	0.92	0.29	77,77,77,77	0
84	MG	5	3866	1/1	0.92	0.27	51,51,51,51	1
84	MG	12	301	1/1	0.92	0.30	59,59,59,59	0
84	MG	1	3983	1/1	0.92	0.20	61,61,61,61	0
84	MG	5	3586	1/1	0.92	0.42	55,55,55,55	0
84	MG	12	305	1/1	0.92	0.27	50,50,50,50	0
84	MG	2	1994	1/1	0.92	0.14	109,109,109,109	0
84	MG	5	3870	1/1	0.92	0.37	54,54,54,54	0
84	MG	2	1996	1/1	0.92	0.15	111,111,111,111	0
84	MG	1	3437	1/1	0.92	0.19	51,51,51,51	0
84	MG	5	3777	1/1	0.92	0.35	70,70,70,70	0
84	MG	5	3778	1/1	0.92	0.24	92,92,92,92	0
84	MG	5	4087	1/1	0.92	0.28	52,52,52,52	0
84	MG	6	1939	1/1	0.92	0.40	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	2	1999	1/1	0.92	0.63	73,73,73,73	0
84	MG	5	4092	1/1	0.92	0.43	71,71,71,71	0
84	MG	1	3705	1/1	0.92	0.25	59,59,59,59	0
84	MG	5	3879	1/1	0.92	0.31	64,64,64,64	0
85	LLL	6	2165	31/31	0.92	0.22	76,77,77,77	31
84	MG	5	3976	1/1	0.92	0.20	68,68,68,68	0
84	MG	6	2109	1/1	0.92	0.11	91,91,91,91	0
85	LLL	6	2170	31/31	0.92	0.19	82,82,83,83	0
84	MG	2	1948	1/1	0.92	0.47	82,82,82,82	0
84	MG	1	3648	1/1	0.92	0.29	57,57,57,57	0
84	MG	5	3882	1/1	0.92	0.28	67,67,67,67	0
84	MG	6	2113	1/1	0.92	0.17	67,67,67,67	0
84	MG	2	1950	1/1	0.92	0.34	94,94,94,94	0
84	MG	1	3464	1/1	0.92	0.32	51,51,51,51	0
84	MG	5	3987	1/1	0.92	0.35	48,48,48,48	0
86	ZN	e1	501	1/1	0.92	0.10	150,150,150,150	0
84	MG	1	3760	1/1	0.93	0.34	69,69,69,69	0
84	MG	15	304	1/1	0.93	0.07	80,80,80,80	0
84	MG	5	3638	1/1	0.93	0.23	51,51,51,51	0
84	MG	5	3865	1/1	0.93	0.37	56,56,56,56	0
84	MG	6	1952	1/1	0.93	0.14	68,68,68,68	0
84	MG	5	3451	1/1	0.93	0.44	45,45,45,45	0
84	MG	5	4096	1/1	0.93	0.34	54,54,54,54	0
84	MG	2	1976	1/1	0.93	0.35	92,92,92,92	0
84	MG	4	217	1/1	0.93	0.25	79,79,79,79	0
84	MG	19	201	1/1	0.93	0.18	53,53,53,53	0
84	MG	2	1921	1/1	0.93	0.20	91,91,91,91	0
84	MG	5	3648	1/1	0.93	0.17	65,65,65,65	0
84	MG	6	1970	1/1	0.93	0.35	63,63,63,63	0
84	MG	2	2030	1/1	0.93	0.08	122,122,122,122	0
84	MG	19	205	1/1	0.93	0.13	72,72,72,72	0
84	MG	5	4103	1/1	0.93	0.20	50,50,50,50	0
84	MG	1	3583	1/1	0.93	0.19	63,63,63,63	0
84	MG	1	3607	1/1	0.93	0.59	58,58,58,58	0
84	MG	5	3465	1/1	0.93	0.29	41,41,41,41	0
84	MG	1	3548	1/1	0.93	0.33	70,70,70,70	0
84	MG	5	3983	1/1	0.93	0.21	50,50,50,50	0
84	MG	6	1981	1/1	0.93	0.13	97,97,97,97	0
84	MG	1	3463	1/1	0.93	0.28	52,52,52,52	0
84	MG	1	3613	1/1	0.93	0.43	48,48,48,48	0
84	MG	5	3661	1/1	0.93	0.34	61,61,61,61	0
84	MG	6	1985	1/1	0.93	0.14	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3570	1/1	0.93	0.24	67,67,67,67	0
84	MG	5	3672	1/1	0.93	0.46	67,67,67,67	0
84	MG	5	3993	1/1	0.93	0.44	56,56,56,56	0
84	MG	5	3883	1/1	0.93	0.23	67,67,67,67	0
84	MG	2	1987	1/1	0.93	0.17	110,110,110,110	0
84	MG	1	3830	1/1	0.93	0.51	72,72,72,72	0
84	MG	5	3685	1/1	0.93	0.31	66,66,66,66	0
84	MG	6	2155	1/1	0.93	0.11	84,84,84,84	0
84	MG	N8	201	1/1	0.93	0.24	75,75,75,75	0
84	MG	5	3687	1/1	0.93	0.40	69,69,69,69	0
84	MG	5	3791	1/1	0.93	0.33	54,54,54,54	0
84	MG	L2	302	1/1	0.93	0.46	43,43,43,43	0
84	MG	1	3458	1/1	0.93	0.39	64,64,64,64	0
84	MG	5	3482	1/1	0.93	0.19	46,46,46,46	0
84	MG	m7	202	1/1	0.93	0.38	49,49,49,49	0
84	MG	1	3486	1/1	0.93	0.33	62,62,62,62	0
84	MG	6	2007	1/1	0.93	0.35	61,61,61,61	0
84	MG	1	3616	1/1	0.93	0.21	54,54,54,54	0
84	MG	5	3797	1/1	0.93	0.24	57,57,57,57	0
84	MG	5	3799	1/1	0.93	0.25	64,64,64,64	0
84	MG	1	3617	1/1	0.93	0.60	70,70,70,70	0
84	MG	5	4139	1/1	0.93	0.29	66,66,66,66	0
84	MG	6	2015	1/1	0.93	0.37	68,68,68,68	0
84	MG	1	3777	1/1	0.93	0.61	62,62,62,62	0
84	MG	1	3779	1/1	0.93	0.35	58,58,58,58	0
84	MG	5	3911	1/1	0.93	0.32	43,43,43,43	0
84	MG	1	3748	1/1	0.93	0.37	61,61,61,61	0
84	MG	5	3913	1/1	0.93	0.31	57,57,57,57	0
84	MG	5	3914	1/1	0.93	0.24	56,56,56,56	0
84	MG	1	3532	1/1	0.93	0.66	68,68,68,68	0
84	MG	5	4025	1/1	0.93	0.18	55,55,55,55	0
84	MG	5	4026	1/1	0.93	0.26	66,66,66,66	0
84	MG	c8	203	1/1	0.93	0.11	74,74,74,74	0
84	MG	5	3595	1/1	0.93	0.17	74,74,74,74	0
84	MG	1	3814	1/1	0.93	0.16	103,103,103,103	0
84	MG	5	3701	1/1	0.93	0.18	66,66,66,66	0
84	MG	7	210	1/1	0.93	0.14	67,67,67,67	0
84	MG	5	4032	1/1	0.93	0.06	69,69,69,69	1
84	MG	5	3920	1/1	0.93	0.35	55,55,55,55	0
84	MG	1	3448	1/1	0.93	0.52	68,68,68,68	0
84	MG	6	2036	1/1	0.93	0.09	83,83,83,83	0
84	MG	7	217	1/1	0.93	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3810	1/1	0.93	0.33	59,59,59,59	0
84	MG	7	220	1/1	0.93	0.21	66,66,66,66	0
84	MG	o4	503	1/1	0.93	0.11	94,94,94,94	0
85	LLL	1	3992	31/31	0.93	0.32	78,79,79,79	31
85	LLL	1	3994	31/31	0.93	0.23	68,69,69,69	0
84	MG	7	221	1/1	0.93	0.09	75,75,75,75	0
84	MG	1	3889	1/1	0.93	0.31	54,54,54,54	0
84	MG	5	3705	1/1	0.93	0.32	81,81,81,81	0
84	MG	5	3600	1/1	0.93	0.21	92,92,92,92	0
84	MG	5	3501	1/1	0.93	0.19	54,54,54,54	0
84	MG	L7	301	1/1	0.93	0.34	58,58,58,58	0
84	MG	1	3752	1/1	0.93	0.28	62,62,62,62	0
84	MG	1	3964	1/1	0.93	0.60	87,87,87,87	0
85	LLL	1	4003	31/31	0.93	0.23	79,80,80,80	31
84	MG	6	2060	1/1	0.93	0.13	86,86,86,86	0
84	MG	5	4048	1/1	0.93	0.56	64,64,64,64	0
84	MG	5	3506	1/1	0.93	0.32	49,49,49,49	0
84	MG	5	3421	1/1	0.93	0.20	51,51,51,51	0
84	MG	1	3621	1/1	0.93	0.48	68,68,68,68	0
84	MG	1	3967	1/1	0.93	0.20	72,72,72,72	0
84	MG	6	1904	1/1	0.93	0.29	65,65,65,65	0
84	MG	5	3519	1/1	0.93	0.33	42,42,42,42	0
84	MG	5	3832	1/1	0.93	0.24	50,50,50,50	0
84	MG	5	3427	1/1	0.93	0.30	45,45,45,45	0
84	MG	6	1911	1/1	0.93	0.21	71,71,71,71	0
85	LLL	5	4159	31/31	0.93	0.23	59,59,60,60	0
84	MG	6	2071	1/1	0.93	0.14	76,76,76,76	1
84	MG	1	3894	1/1	0.93	0.35	60,60,60,60	0
84	MG	1	3676	1/1	0.93	0.52	53,53,53,53	0
85	LLL	5	4165	31/31	0.93	0.21	84,84,84,84	0
84	MG	5	3615	1/1	0.93	0.21	89,89,89,89	0
84	MG	5	3731	1/1	0.93	0.11	69,69,69,69	0
85	LLL	5	4168	31/31	0.93	0.27	76,76,76,76	0
84	MG	6	2077	1/1	0.93	0.32	65,65,65,65	0
85	LLL	5	4170	31/31	0.93	0.21	61,61,61,61	31
84	MG	1	3855	1/1	0.93	0.28	55,55,55,55	1
84	MG	5	4064	1/1	0.93	0.36	44,44,44,44	0
84	MG	1	3971	1/1	0.93	0.40	56,56,56,56	0
84	MG	5	3735	1/1	0.93	0.13	64,64,64,64	0
84	MG	6	2088	1/1	0.93	0.38	83,83,83,83	0
84	MG	1	3657	1/1	0.93	0.26	50,50,50,50	0
84	MG	1	3860	1/1	0.93	0.19	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	6	1922	1/1	0.93	0.17	74,74,74,74	0
84	MG	6	1923	1/1	0.93	0.17	71,71,71,71	0
84	MG	5	4070	1/1	0.93	0.11	99,99,99,99	0
84	MG	1	3504	1/1	0.93	0.28	66,66,66,66	0
84	MG	6	2095	1/1	0.93	0.33	65,65,65,65	0
84	MG	5	3849	1/1	0.93	0.27	50,50,50,50	0
84	MG	5	3438	1/1	0.93	0.16	64,64,64,64	1
84	MG	5	3852	1/1	0.93	0.31	57,57,57,57	0
84	MG	13	401	1/1	0.93	0.28	57,57,57,57	0
84	MG	5	3532	1/1	0.93	0.18	43,43,43,43	0
85	LLL	6	2169	31/31	0.93	0.20	89,89,90,90	0
84	MG	1	3659	1/1	0.93	0.15	69,69,69,69	0
85	LLL	6	2171	31/31	0.93	0.21	87,88,88,88	0
84	MG	5	3959	1/1	0.93	0.36	51,51,51,51	0
84	MG	5	3535	1/1	0.93	0.44	57,57,57,57	0
84	MG	5	3541	1/1	0.93	0.31	52,52,52,52	0
84	MG	5	4081	1/1	0.93	0.08	79,79,79,79	0
84	MG	1	3706	1/1	0.93	0.26	51,51,51,51	0
84	MG	2	1969	1/1	0.93	0.22	100,100,100,100	0
84	MG	4	214	1/1	0.93	0.36	63,63,63,63	0
84	MG	2	1974	1/1	0.93	0.27	96,96,96,96	0
84	MG	5	4123	1/1	0.94	0.28	53,53,53,53	0
84	MG	5	3665	1/1	0.94	0.54	56,56,56,56	0
84	MG	1	3743	1/1	0.94	0.63	72,72,72,72	0
84	MG	1	3982	1/1	0.94	0.12	90,90,90,90	0
84	MG	5	3462	1/1	0.94	0.21	53,53,53,53	0
84	MG	5	3680	1/1	0.94	0.15	73,73,73,73	0
84	MG	5	3684	1/1	0.94	0.12	79,79,79,79	0
84	MG	6	2135	1/1	0.94	0.25	77,77,77,77	0
84	MG	5	3463	1/1	0.94	0.28	49,49,49,49	0
84	MG	6	2137	1/1	0.94	0.29	76,76,76,76	0
84	MG	1	3883	1/1	0.94	0.11	75,75,75,75	0
84	MG	5	3905	1/1	0.94	0.45	44,44,44,44	0
84	MG	1	3640	1/1	0.94	0.19	100,100,100,100	0
84	MG	2	1918	1/1	0.94	0.22	91,91,91,91	0
84	MG	6	2143	1/1	0.94	0.26	104,104,104,104	0
84	MG	2	2032	1/1	0.94	0.10	111,111,111,111	0
84	MG	1	3852	1/1	0.94	0.51	65,65,65,65	0
84	MG	1	3526	1/1	0.94	0.57	65,65,65,65	0
84	MG	5	4022	1/1	0.94	0.28	50,50,50,50	0
84	MG	m7	206	1/1	0.94	0.36	55,55,55,55	0
84	MG	1	3470	1/1	0.94	0.38	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3597	1/1	0.94	0.37	46,46,46,46	0
84	MG	5	4145	1/1	0.94	0.13	54,54,54,54	0
84	MG	6	2000	1/1	0.94	0.17	84,84,84,84	0
84	MG	3	204	1/1	0.94	0.15	85,85,85,85	0
84	MG	6	2005	1/1	0.94	0.19	83,83,83,83	0
84	MG	5	3916	1/1	0.94	0.19	51,51,51,51	0
84	MG	5	3478	1/1	0.94	0.42	50,50,50,50	0
84	MG	5	4028	1/1	0.94	0.10	59,59,59,59	0
84	MG	5	3807	1/1	0.94	0.27	71,71,71,71	0
84	MG	2	1925	1/1	0.94	0.28	90,90,90,90	0
84	MG	2	2040	1/1	0.94	0.34	95,95,95,95	0
84	MG	N3	201	1/1	0.94	0.30	67,67,67,67	0
84	MG	2	1985	1/1	0.94	0.28	122,122,122,122	0
84	MG	1	3601	1/1	0.94	0.35	53,53,53,53	0
84	MG	7	213	1/1	0.94	0.17	71,71,71,71	0
84	MG	1	3959	1/1	0.94	0.34	61,61,61,61	0
84	MG	7	215	1/1	0.94	0.28	63,63,63,63	0
84	MG	2	1933	1/1	0.94	0.16	88,88,88,88	0
84	MG	5	3926	1/1	0.94	0.21	55,55,55,55	1
84	MG	7	218	1/1	0.94	0.09	68,68,68,68	0
84	MG	2	1934	1/1	0.94	0.29	87,87,87,87	0
84	MG	5	3599	1/1	0.94	0.24	92,92,92,92	0
84	MG	C8	201	1/1	0.94	0.05	138,138,138,138	0
84	MG	5	3931	1/1	0.94	0.51	44,44,44,44	0
84	MG	q1	101	1/1	0.94	0.39	67,67,67,67	0
84	MG	6	2029	1/1	0.94	0.27	75,75,75,75	0
84	MG	1	3750	1/1	0.94	0.57	70,70,70,70	0
84	MG	2	1936	1/1	0.94	0.35	86,86,86,86	0
84	MG	c8	201	1/1	0.94	0.18	75,75,75,75	0
84	MG	5	3826	1/1	0.94	0.21	56,56,56,56	0
84	MG	5	3498	1/1	0.94	0.15	52,52,52,52	0
84	MG	2	1937	1/1	0.94	0.23	80,80,80,80	0
84	MG	5	3502	1/1	0.94	0.18	50,50,50,50	0
84	MG	N5	201	1/1	0.94	0.15	95,95,95,95	0
84	MG	5	3721	1/1	0.94	0.21	65,65,65,65	0
84	MG	5	3607	1/1	0.94	0.21	83,83,83,83	0
84	MG	5	3835	1/1	0.94	0.30	62,62,62,62	0
84	MG	d5	201	1/1	0.94	0.17	90,90,90,90	0
84	MG	L2	304	1/1	0.94	0.32	73,73,73,73	0
84	MG	1	3861	1/1	0.94	0.30	58,58,58,58	0
84	MG	5	3726	1/1	0.94	0.45	52,52,52,52	0
84	MG	2	1998	1/1	0.94	0.10	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	6	2051	1/1	0.94	0.16	69,69,69,69	0
84	MG	5	3410	1/1	0.94	0.52	46,46,46,46	0
85	LLL	1	3990	31/31	0.94	0.20	75,75,75,75	0
84	MG	6	2056	1/1	0.94	0.24	83,83,83,83	0
84	MG	6	1907	1/1	0.94	0.21	69,69,69,69	0
84	MG	5	4066	1/1	0.94	0.12	84,84,84,84	0
84	MG	5	3612	1/1	0.94	0.20	80,80,80,80	0
84	MG	8	210	1/1	0.94	0.18	96,96,96,96	0
84	MG	5	3842	1/1	0.94	0.24	46,46,46,46	0
84	MG	1	3602	1/1	0.94	0.43	49,49,49,49	0
84	MG	5	3415	1/1	0.94	0.24	48,48,48,48	1
84	MG	5	3517	1/1	0.94	0.60	49,49,49,49	0
84	MG	1	3776	1/1	0.94	0.27	68,68,68,68	1
84	MG	2	1943	1/1	0.94	0.27	95,95,95,95	0
84	MG	1	3604	1/1	0.94	0.26	52,52,52,52	0
84	MG	5	3742	1/1	0.94	0.27	67,67,67,67	0
84	MG	1	3410	1/1	0.94	0.55	56,56,56,56	0
84	MG	1	3966	1/1	0.94	0.17	68,68,68,68	0
85	LLL	2	2043	31/31	0.94	0.31	101,101,101,101	0
84	MG	3	214	1/1	0.94	0.07	86,86,86,86	0
84	MG	1	3780	1/1	0.94	0.34	64,64,64,64	0
84	MG	1	3809	1/1	0.94	0.14	59,59,59,59	0
84	MG	13	402	1/1	0.94	0.35	51,51,51,51	0
85	LLL	5	4154	31/31	0.94	0.25	67,67,67,67	0
84	MG	3	218	1/1	0.94	0.13	97,97,97,97	0
84	MG	1	3871	1/1	0.94	0.14	73,73,73,73	0
84	MG	5	3531	1/1	0.94	0.35	43,43,43,43	0
84	MG	2	2011	1/1	0.94	0.19	102,102,102,102	0
84	MG	1	3540	1/1	0.94	0.27	54,54,54,54	0
84	MG	5	3436	1/1	0.94	0.22	66,66,66,66	0
84	MG	5	3539	1/1	0.94	0.49	54,54,54,54	0
84	MG	5	3973	1/1	0.94	0.33	69,69,69,69	0
84	MG	5	4094	1/1	0.94	0.14	63,63,63,63	0
84	MG	5	3759	1/1	0.94	0.32	67,67,67,67	0
84	MG	5	3636	1/1	0.94	0.41	53,53,53,53	0
84	MG	5	3540	1/1	0.94	0.32	49,49,49,49	0
84	MG	Q2	502	1/1	0.94	0.14	65,65,65,65	0
84	MG	5	4100	1/1	0.94	0.45	90,90,90,90	0
84	MG	6	2098	1/1	0.94	0.32	63,63,63,63	0
84	MG	5	3872	1/1	0.94	0.14	76,76,76,76	0
84	MG	2	2014	1/1	0.94	0.24	88,88,88,88	0
84	MG	1	3635	1/1	0.94	0.09	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3646	1/1	0.94	0.17	65,65,65,65	0
84	MG	6	2105	1/1	0.94	0.25	67,67,67,67	0
84	MG	M0	301	1/1	0.94	0.23	51,51,51,51	0
84	MG	5	3985	1/1	0.94	0.25	56,56,56,56	0
84	MG	5	4108	1/1	0.94	0.19	59,59,59,59	0
84	MG	6	1958	1/1	0.94	0.26	66,66,66,66	0
84	MG	6	1959	1/1	0.94	0.22	68,68,68,68	0
84	MG	5	4110	1/1	0.94	0.17	47,47,47,47	0
85	LLL	13	412	31/31	0.94	0.20	69,69,70,70	0
84	MG	1	3836	1/1	0.94	0.21	58,58,58,58	0
84	MG	6	1962	1/1	0.94	0.20	69,69,69,69	0
85	LLL	6	2166	31/31	0.94	0.26	77,77,77,77	31
84	MG	1	3693	1/1	0.94	0.26	64,64,64,64	0
84	MG	1	3496	1/1	0.94	0.58	73,73,73,73	0
84	MG	6	2116	1/1	0.94	0.24	71,71,71,71	0
84	MG	1	3497	1/1	0.94	0.22	73,73,73,73	0
84	MG	6	1969	1/1	0.94	0.15	69,69,69,69	1
84	MG	4	209	1/1	0.94	0.50	59,59,59,59	0
84	MG	1	3656	1/1	0.94	0.24	52,52,52,52	0
84	MG	6	1972	1/1	0.94	0.42	70,70,70,70	0
84	MG	1	3761	1/1	0.94	0.17	73,73,73,73	1
84	MG	5	3659	1/1	0.94	0.13	98,98,98,98	0
84	MG	1	3581	1/1	0.94	0.15	64,64,64,64	0
84	MG	5	3562	1/1	0.94	0.41	57,57,57,57	0
84	MG	M5	303	1/1	0.94	0.19	65,65,65,65	0
84	MG	1	3479	1/1	0.95	0.41	59,59,59,59	0
84	MG	5	3404	1/1	0.95	0.22	55,55,55,55	0
84	MG	1	3882	1/1	0.95	0.24	71,71,71,71	0
84	MG	7	208	1/1	0.95	0.11	65,65,65,65	0
84	MG	5	3497	1/1	0.95	0.17	49,49,49,49	0
84	MG	6	2003	1/1	0.95	0.16	64,64,64,64	0
84	MG	n0	207	1/1	0.95	0.23	56,56,56,56	0
84	MG	1	3603	1/1	0.95	0.35	45,45,45,45	0
84	MG	5	3814	1/1	0.95	0.13	48,48,48,48	0
84	MG	n3	202	1/1	0.95	0.51	62,62,62,62	1
84	MG	5	4042	1/1	0.95	0.27	46,46,46,46	0
84	MG	6	2151	1/1	0.95	0.20	67,67,67,67	0
84	MG	1	3919	1/1	0.95	0.25	69,69,69,69	0
84	MG	5	4045	1/1	0.95	0.21	71,71,71,71	0
84	MG	1	3793	1/1	0.95	0.16	85,85,85,85	0
84	MG	5	3818	1/1	0.95	0.18	54,54,54,54	0
84	MG	5	3416	1/1	0.95	0.31	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	3707	1/1	0.95	0.18	73,73,73,73	0
84	MG	1	3885	1/1	0.95	0.19	80,80,80,80	0
84	MG	2	2006	1/1	0.95	0.28	106,106,106,106	0
84	MG	1	3414	1/1	0.95	0.21	56,56,56,56	0
84	MG	3	216	1/1	0.95	0.08	74,74,74,74	0
84	MG	q0	202	1/1	0.95	0.18	51,51,51,51	0
84	MG	Q2	503	1/1	0.95	0.27	67,67,67,67	0
84	MG	5	3425	1/1	0.95	0.17	46,46,46,46	0
84	MG	5	3716	1/1	0.95	0.57	62,62,62,62	0
84	MG	5	3514	1/1	0.95	0.26	65,65,65,65	0
84	MG	5	3516	1/1	0.95	0.18	49,49,49,49	0
84	MG	1	3797	1/1	0.95	0.54	56,56,56,56	0
84	MG	5	3518	1/1	0.95	0.44	53,53,53,53	0
84	MG	1	3533	1/1	0.95	0.56	75,75,75,75	0
84	MG	1	3517	1/1	0.95	0.43	54,54,54,54	0
84	MG	2	1902	1/1	0.95	0.09	95,95,95,95	0
84	MG	5	3432	1/1	0.95	0.19	54,54,54,54	0
84	MG	2	1957	1/1	0.95	0.13	95,95,95,95	0
84	MG	1	3608	1/1	0.95	0.19	57,57,57,57	0
84	MG	M3	201	1/1	0.95	0.16	65,65,65,65	0
84	MG	5	3843	1/1	0.95	0.11	50,50,50,50	0
84	MG	1	3892	1/1	0.95	0.23	64,64,64,64	0
84	MG	1	3518	1/1	0.95	0.28	64,64,64,64	0
84	MG	6	2047	1/1	0.95	0.12	79,79,79,79	0
84	MG	1	3802	1/1	0.95	0.20	98,98,98,98	0
84	MG	5	4075	1/1	0.95	0.12	97,97,97,97	0
84	MG	d1	102	1/1	0.95	0.10	106,106,106,106	0
84	MG	5	3739	1/1	0.95	0.33	52,52,52,52	0
84	MG	5	3740	1/1	0.95	0.28	56,56,56,56	0
84	MG	6	2052	1/1	0.95	0.11	73,73,73,73	0
84	MG	5	3439	1/1	0.95	0.25	54,54,54,54	0
84	MG	8	217	1/1	0.95	0.22	64,64,64,64	0
84	MG	5	3853	1/1	0.95	0.15	58,58,58,58	0
84	MG	5	3440	1/1	0.95	0.16	56,56,56,56	0
84	MG	2	1909	1/1	0.95	0.45	94,94,94,94	0
84	MG	1	3719	1/1	0.95	0.25	55,55,55,55	0
84	MG	5	3745	1/1	0.95	0.34	52,52,52,52	0
84	MG	5	3538	1/1	0.95	0.28	52,52,52,52	0
84	MG	1	3720	1/1	0.95	0.47	59,59,59,59	0
85	LLL	1	3989	31/31	0.95	0.21	69,69,69,69	0
84	MG	5	3445	1/1	0.95	0.21	50,50,50,50	0
84	MG	1	3519	1/1	0.95	0.35	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	4088	1/1	0.95	0.22	69,69,69,69	0
84	MG	6	1925	1/1	0.95	0.28	68,68,68,68	0
84	MG	6	1926	1/1	0.95	0.24	75,75,75,75	0
84	MG	13	405	1/1	0.95	0.30	43,43,43,43	0
84	MG	1	3482	1/1	0.95	0.25	72,72,72,72	0
84	MG	5	4090	1/1	0.95	0.39	60,60,60,60	0
84	MG	5	3637	1/1	0.95	0.30	48,48,48,48	0
84	MG	6	1935	1/1	0.95	0.24	73,73,73,73	0
84	MG	M5	304	1/1	0.95	0.26	67,67,67,67	0
84	MG	5	3641	1/1	0.95	0.24	51,51,51,51	0
84	MG	1	3421	1/1	0.95	0.25	50,50,50,50	0
84	MG	5	3547	1/1	0.95	0.49	54,54,54,54	0
84	MG	6	2082	1/1	0.95	0.26	67,67,67,67	0
84	MG	5	3757	1/1	0.95	0.09	64,64,64,64	0
84	MG	2	1973	1/1	0.95	0.20	96,96,96,96	0
84	MG	6	2087	1/1	0.95	0.22	82,82,82,82	0
84	MG	M6	201	1/1	0.95	0.43	60,60,60,60	0
84	MG	5	3982	1/1	0.95	0.15	50,50,50,50	0
84	MG	1	3868	1/1	0.95	0.21	61,61,61,61	0
84	MG	1	3833	1/1	0.95	0.27	64,64,64,64	0
84	MG	M7	204	1/1	0.95	0.25	60,60,60,60	0
84	MG	1	3484	1/1	0.95	0.31	60,60,60,60	0
84	MG	17	302	1/1	0.95	0.30	55,55,55,55	0
84	MG	5	3555	1/1	0.95	0.21	62,62,62,62	1
85	LLL	5	4160	31/31	0.95	0.28	49,50,50,50	31
85	LLL	5	4161	31/31	0.95	0.22	69,70,70,70	0
84	MG	5	3652	1/1	0.95	0.19	76,76,76,76	0
84	MG	5	3556	1/1	0.95	0.49	57,57,57,57	0
84	MG	2	1922	1/1	0.95	0.28	84,84,84,84	0
84	MG	1	3574	1/1	0.95	0.12	67,67,67,67	0
84	MG	6	1957	1/1	0.95	0.17	66,66,66,66	0
84	MG	5	3658	1/1	0.95	0.17	71,71,71,71	0
84	MG	1	3728	1/1	0.95	0.13	83,83,83,83	0
84	MG	5	4000	1/1	0.95	0.27	45,45,45,45	0
84	MG	5	3884	1/1	0.95	0.09	69,69,69,69	0
84	MG	1	3944	1/1	0.95	0.20	67,67,67,67	0
84	MG	1	3907	1/1	0.95	0.31	62,62,62,62	0
84	MG	1	3427	1/1	0.95	0.27	51,51,51,51	0
84	MG	2	2041	1/1	0.95	0.08	94,94,94,94	0
84	MG	5	4122	1/1	0.95	0.18	89,89,89,89	0
84	MG	5	3667	1/1	0.95	0.56	49,49,49,49	0
84	MG	5	3784	1/1	0.95	0.37	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	5	3668	1/1	0.95	0.44	49,49,49,49	0
84	MG	5	3671	1/1	0.95	0.37	63,63,63,63	0
84	MG	1	3986	1/1	0.95	0.41	68,68,68,68	0
84	MG	5	3790	1/1	0.95	0.32	47,47,47,47	0
84	MG	5	4131	1/1	0.95	0.30	70,70,70,70	0
84	MG	5	3569	1/1	0.95	0.43	64,64,64,64	0
84	MG	1	3423	1/1	0.95	0.30	51,51,51,51	0
84	MG	1	3561	1/1	0.95	0.15	79,79,79,79	0
84	MG	L2	301	1/1	0.95	0.20	55,55,55,55	0
84	MG	1	3951	1/1	0.95	0.06	82,82,82,82	0
84	MG	3	203	1/1	0.95	0.12	103,103,103,103	0
84	MG	1	3598	1/1	0.95	0.42	52,52,52,52	0
84	MG	5	3798	1/1	0.95	0.39	58,58,58,58	0
84	MG	2	1995	1/1	0.95	0.40	100,100,100,100	0
84	MG	5	3584	1/1	0.95	0.48	51,51,51,51	0
84	MG	5	4142	1/1	0.95	0.33	69,69,69,69	0
84	MG	1	3530	1/1	0.95	0.28	67,67,67,67	0
84	MG	1	3954	1/1	0.95	0.14	71,71,71,71	0
84	MG	5	3487	1/1	0.95	0.16	61,61,61,61	0
84	MG	1	3843	1/1	0.95	0.28	58,58,58,58	0
84	MG	5	3490	1/1	0.95	0.24	58,58,58,58	0
84	MG	1	3844	1/1	0.95	0.22	56,56,56,56	0
84	MG	5	3401	1/1	0.95	0.36	49,49,49,49	0
84	MG	1	3772	1/1	0.96	0.23	59,59,59,59	1
84	MG	5	3903	1/1	0.96	1.06	61,61,61,61	0
84	MG	1	3674	1/1	0.96	0.25	63,63,63,63	0
84	MG	5	3663	1/1	0.96	0.31	46,46,46,46	0
84	MG	5	3986	1/1	0.96	0.34	45,45,45,45	1
84	MG	1	3675	1/1	0.96	0.11	62,62,62,62	0
84	MG	5	3457	1/1	0.96	0.14	51,51,51,51	0
84	MG	4	207	1/1	0.96	0.24	59,59,59,59	0
84	MG	6	1956	1/1	0.96	0.33	69,69,69,69	0
84	MG	1	3610	1/1	0.96	0.29	52,52,52,52	0
84	MG	5	3461	1/1	0.96	0.24	50,50,50,50	0
84	MG	5	3750	1/1	0.96	0.26	52,52,52,52	0
84	MG	5	3997	1/1	0.96	0.16	50,50,50,50	0
84	MG	1	3851	1/1	0.96	0.20	57,57,57,57	0
84	MG	m8	204	1/1	0.96	0.50	63,63,63,63	0
84	MG	1	3891	1/1	0.96	0.21	60,60,60,60	0
84	MG	1	3974	1/1	0.96	0.19	79,79,79,79	0
84	MG	1	3450	1/1	0.96	0.35	62,62,62,62	0
84	MG	n0	203	1/1	0.96	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3682	1/1	0.96	0.17	73,73,73,73	0
84	MG	6	2078	1/1	0.96	0.28	65,65,65,65	0
84	MG	1	3631	1/1	0.96	0.12	76,76,76,76	0
84	MG	1	3778	1/1	0.96	0.39	61,61,61,61	0
84	MG	5	4091	1/1	0.96	0.41	68,68,68,68	0
84	MG	1	3655	1/1	0.96	0.31	50,50,50,50	0
84	MG	6	2084	1/1	0.96	0.27	67,67,67,67	0
84	MG	1	3858	1/1	0.96	0.37	46,46,46,46	0
84	MG	n3	201	1/1	0.96	0.25	43,43,43,43	0
84	MG	5	3473	1/1	0.96	0.22	63,63,63,63	0
84	MG	5	4009	1/1	0.96	0.38	53,53,53,53	0
84	MG	6	1979	1/1	0.96	0.09	100,100,100,100	0
84	MG	5	3689	1/1	0.96	0.14	78,78,78,78	0
84	MG	n8	201	1/1	0.96	0.30	54,54,54,54	0
84	MG	5	4011	1/1	0.96	0.16	45,45,45,45	0
84	MG	1	3612	1/1	0.96	0.37	55,55,55,55	0
85	LLL	1	3991	31/31	0.96	0.21	67,67,67,67	0
84	MG	5	3475	1/1	0.96	0.17	64,64,64,64	0
85	LLL	1	3993	31/31	0.96	0.22	61,61,61,61	0
84	MG	1	3981	1/1	0.96	0.39	63,63,63,63	0
84	MG	6	2097	1/1	0.96	0.35	63,63,63,63	0
84	MG	1	3417	1/1	0.96	0.28	52,52,52,52	0
84	MG	8	215	1/1	0.96	0.44	58,58,58,58	0
84	MG	1	3408	1/1	0.96	0.27	51,51,51,51	0
84	MG	5	4017	1/1	0.96	0.19	63,63,63,63	0
84	MG	5	3480	1/1	0.96	0.25	49,49,49,49	0
84	MG	6	2104	1/1	0.96	0.11	89,89,89,89	0
84	MG	5	3770	1/1	0.96	0.12	79,79,79,79	0
84	MG	5	3771	1/1	0.96	0.14	77,77,77,77	0
84	MG	1	3940	1/1	0.96	0.13	64,64,64,64	0
84	MG	1	3453	1/1	0.96	0.09	70,70,70,70	0
84	MG	5	3774	1/1	0.96	0.29	116,116,116,116	0
84	MG	1	3942	1/1	0.96	0.27	49,49,49,49	0
84	MG	5	3776	1/1	0.96	0.12	65,65,65,65	0
84	MG	2	2021	1/1	0.96	0.40	90,90,90,90	0
84	MG	1	3689	1/1	0.96	0.26	58,58,58,58	0
85	LLL	5	4151	31/31	0.96	0.22	48,48,49,49	0
84	MG	1	3596	1/1	0.96	0.36	55,55,55,55	0
84	MG	1	3787	1/1	0.96	0.85	67,67,67,67	0
84	MG	5	3623	1/1	0.96	0.30	62,62,62,62	0
84	MG	5	3782	1/1	0.96	0.16	67,67,67,67	0
84	MG	5	3783	1/1	0.96	0.31	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	LLL	5	4157	31/31	0.96	0.25	49,49,49,49	0
84	MG	1	3432	1/1	0.96	0.43	46,46,46,46	0
84	MG	1	3789	1/1	0.96	0.27	80,80,80,80	0
84	MG	5	4036	1/1	0.96	0.30	56,56,56,56	0
84	MG	5	4127	1/1	0.96	0.22	62,62,62,62	0
84	MG	1	3425	1/1	0.96	0.26	57,57,57,57	0
84	MG	5	3561	1/1	0.96	0.29	57,57,57,57	0
84	MG	5	3789	1/1	0.96	0.35	48,48,48,48	0
84	MG	5	3493	1/1	0.96	0.18	57,57,57,57	0
84	MG	2	1983	1/1	0.96	0.22	112,112,112,112	0
84	MG	6	2019	1/1	0.96	0.18	81,81,81,81	0
84	MG	1	3721	1/1	0.96	0.26	59,59,59,59	0
84	MG	5	3957	1/1	0.96	0.31	57,57,57,57	0
84	MG	1	3600	1/1	0.96	0.34	54,54,54,54	0
84	MG	5	3713	1/1	0.96	0.21	78,78,78,78	0
84	MG	1	3438	1/1	0.96	0.30	51,51,51,51	0
84	MG	1	3553	1/1	0.96	0.20	71,71,71,71	0
84	MG	1	3439	1/1	0.96	0.27	49,49,49,49	0
84	MG	5	3963	1/1	0.96	0.12	102,102,102,102	0
84	MG	6	2138	1/1	0.96	0.13	84,84,84,84	0
84	MG	5	3719	1/1	0.96	0.24	66,66,66,66	0
84	MG	1	3419	1/1	0.96	0.22	55,55,55,55	0
84	MG	1	3528	1/1	0.96	0.41	63,63,63,63	0
84	MG	6	2031	1/1	0.96	0.18	73,73,73,73	0
84	MG	1	3701	1/1	0.96	0.29	59,59,59,59	0
84	MG	1	3732	1/1	0.96	0.35	75,75,75,75	0
84	MG	1	3918	1/1	0.96	0.16	59,59,59,59	0
84	MG	5	3580	1/1	0.96	0.43	48,48,48,48	0
84	MG	5	4061	1/1	0.96	0.37	68,68,68,68	0
84	MG	5	3507	1/1	0.96	0.20	55,55,55,55	0
84	MG	1	3765	1/1	0.96	0.29	61,61,61,61	0
84	MG	1	3557	1/1	0.96	0.18	71,71,71,71	0
84	MG	1	3405	1/1	0.96	0.35	53,53,53,53	0
84	MG	6	2043	1/1	0.96	0.21	96,96,96,96	0
84	MG	6	2045	1/1	0.96	0.12	68,68,68,68	0
84	MG	7	207	1/1	0.96	0.16	62,62,62,62	0
84	MG	5	3587	1/1	0.96	0.35	55,55,55,55	0
84	MG	1	3736	1/1	0.96	0.15	82,82,82,82	0
84	MG	5	3515	1/1	0.96	0.21	43,43,43,43	0
84	MG	7	211	1/1	0.96	0.14	67,67,67,67	0
84	MG	5	3450	1/1	0.96	0.34	42,42,42,42	0
84	MG	1	3589	1/1	0.96	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	ZN	E1	501	1/1	0.96	0.09	182,182,182,182	0
84	MG	1	3770	1/1	0.96	0.36	55,55,55,55	0
84	MG	6	2054	1/1	0.96	0.14	76,76,76,76	0
84	MG	6	1999	1/1	0.97	0.24	87,87,87,87	0
84	MG	1	3857	1/1	0.97	0.44	47,47,47,47	0
84	MG	5	3568	1/1	0.97	0.20	67,67,67,67	0
84	MG	6	2002	1/1	0.97	0.12	68,68,68,68	0
84	MG	1	3895	1/1	0.97	0.18	66,66,66,66	0
84	MG	1	3587	1/1	0.97	0.32	58,58,58,58	0
84	MG	2	1959	1/1	0.97	0.15	110,110,110,110	0
84	MG	n5	203	1/1	0.97	0.06	89,89,89,89	0
84	MG	1	3897	1/1	0.97	0.14	104,104,104,104	0
84	MG	6	2009	1/1	0.97	0.12	73,73,73,73	0
84	MG	5	4055	1/1	0.97	0.24	103,103,103,103	0
84	MG	5	3575	1/1	0.97	0.21	51,51,51,51	0
84	MG	5	3428	1/1	0.97	0.14	47,47,47,47	0
84	MG	6	2013	1/1	0.97	0.26	76,76,76,76	0
84	MG	1	3638	1/1	0.97	0.17	90,90,90,90	0
84	MG	o2	201	1/1	0.97	0.30	55,55,55,55	0
84	MG	5	3949	1/1	0.97	0.36	56,56,56,56	0
84	MG	5	3579	1/1	0.97	0.45	45,45,45,45	0
84	MG	5	3847	1/1	0.97	0.31	45,45,45,45	0
84	MG	5	3952	1/1	0.97	0.19	58,58,58,58	0
84	MG	o4	502	1/1	0.97	0.42	87,87,87,87	0
84	MG	5	3848	1/1	0.97	0.26	44,44,44,44	0
84	MG	1	3734	1/1	0.97	0.17	77,77,77,77	0
84	MG	6	2159	1/1	0.97	0.15	81,81,81,81	0
84	MG	1	3938	1/1	0.97	0.30	62,62,62,62	0
84	MG	5	3582	1/1	0.97	0.30	54,54,54,54	0
84	MG	1	3606	1/1	0.97	0.29	52,52,52,52	0
84	MG	M7	202	1/1	0.97	0.36	48,48,48,48	0
84	MG	5	3585	1/1	0.97	0.38	48,48,48,48	0
84	MG	1	3429	1/1	0.97	0.34	50,50,50,50	0
84	MG	5	3666	1/1	0.97	0.14	55,55,55,55	0
84	MG	1	3795	1/1	0.97	0.41	56,56,56,56	0
84	MG	1	3826	1/1	0.97	0.41	65,65,65,65	0
84	MG	5	3589	1/1	0.97	0.35	58,58,58,58	0
84	MG	6	2033	1/1	0.97	0.18	74,74,74,74	0
84	MG	s5	303	1/1	0.97	0.33	77,77,77,77	0
84	MG	1	3796	1/1	0.97	0.18	60,60,60,60	0
84	MG	5	3508	1/1	0.97	0.10	53,53,53,53	0
84	MG	2	1971	1/1	0.97	0.27	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3864	1/1	0.97	0.34	68,68,68,68	0
84	MG	5	3678	1/1	0.97	0.25	68,68,68,68	0
84	MG	5	3679	1/1	0.97	0.23	66,66,66,66	0
84	MG	1	3866	1/1	0.97	0.28	55,55,55,55	0
84	MG	6	1908	1/1	0.97	0.18	70,70,70,70	0
84	MG	5	3681	1/1	0.97	0.29	66,66,66,66	0
84	MG	6	2044	1/1	0.97	0.15	71,71,71,71	0
84	MG	1	3474	1/1	0.97	0.29	59,59,59,59	0
84	MG	N0	204	1/1	0.97	0.13	68,68,68,68	0
84	MG	1	3404	1/1	0.97	0.34	53,53,53,53	0
84	MG	1	3534	1/1	0.97	0.46	63,63,63,63	0
84	MG	1	3740	1/1	0.97	0.17	74,74,74,74	0
84	MG	5	3979	1/1	0.97	0.37	46,46,46,46	0
84	MG	N3	202	1/1	0.97	0.32	55,55,55,55	0
84	MG	1	3690	1/1	0.97	0.40	58,58,58,58	0
84	MG	2	1926	1/1	0.97	0.52	89,89,89,89	0
84	MG	5	3877	1/1	0.97	0.17	89,89,89,89	0
84	MG	6	2055	1/1	0.97	0.17	77,77,77,77	0
84	MG	5	4093	1/1	0.97	0.15	73,73,73,73	0
84	MG	2	1928	1/1	0.97	0.47	67,67,67,67	0
84	MG	1	3771	1/1	0.97	0.23	59,59,59,59	0
84	MG	1	3644	1/1	0.97	0.32	49,49,49,49	0
84	MG	1	3403	1/1	0.97	0.35	58,58,58,58	0
84	MG	5	3988	1/1	0.97	0.36	45,45,45,45	0
84	MG	5	3989	1/1	0.97	0.28	47,47,47,47	0
84	MG	2	2039	1/1	0.97	0.20	95,95,95,95	0
84	MG	2	1932	1/1	0.97	0.25	91,91,91,91	0
84	MG	6	1932	1/1	0.97	0.34	62,62,62,62	0
84	MG	1	3647	1/1	0.97	0.13	55,55,55,55	0
84	MG	15	301	1/1	0.97	0.15	56,56,56,56	0
84	MG	1	3745	1/1	0.97	0.11	73,73,73,73	0
84	MG	5	4105	1/1	0.97	0.32	56,56,56,56	0
84	MG	5	3459	1/1	0.97	0.14	52,52,52,52	1
84	MG	1	3478	1/1	0.97	0.31	58,58,58,58	0
84	MG	1	3537	1/1	0.97	0.30	60,60,60,60	0
84	MG	5	3890	1/1	0.97	0.19	62,62,62,62	0
84	MG	5	3702	1/1	0.97	0.11	85,85,85,85	0
84	MG	6	2076	1/1	0.97	0.21	64,64,64,64	0
84	MG	S3	301	1/1	0.97	0.14	100,100,100,100	0
84	MG	1	3407	1/1	0.97	0.28	59,59,59,59	0
84	MG	5	3464	1/1	0.97	0.29	52,52,52,52	0
84	MG	1	3697	1/1	0.97	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	6	2081	1/1	0.97	0.20	69,69,69,69	0
84	MG	5	4005	1/1	0.97	0.21	58,58,58,58	0
84	MG	1	3480	1/1	0.97	0.31	62,62,62,62	0
84	MG	6	1948	1/1	0.97	0.27	66,66,66,66	0
84	MG	O4	502	1/1	0.97	0.10	106,106,106,106	0
84	MG	6	2086	1/1	0.97	0.09	83,83,83,83	0
84	MG	1	3420	1/1	0.97	0.18	53,53,53,53	0
84	MG	5	3901	1/1	0.97	0.74	55,55,55,55	0
84	MG	19	207	1/1	0.97	0.11	52,52,52,52	0
84	MG	1	3846	1/1	0.97	0.26	53,53,53,53	0
84	MG	1	3415	1/1	0.97	0.39	55,55,55,55	0
84	MG	6	1955	1/1	0.97	0.16	77,77,77,77	0
84	MG	5	3471	1/1	0.97	0.40	56,56,56,56	0
84	MG	1	3848	1/1	0.97	0.15	57,57,57,57	0
84	MG	2	1945	1/1	0.97	0.31	87,87,87,87	0
84	MG	5	3625	1/1	0.97	0.27	54,54,54,54	0
84	MG	5	3717	1/1	0.97	0.31	52,52,52,52	0
84	MG	5	3626	1/1	0.97	0.28	52,52,52,52	0
84	MG	6	2099	1/1	0.97	0.31	57,57,57,57	0
84	MG	1	3544	1/1	0.97	0.38	54,54,54,54	0
84	MG	6	1965	1/1	0.97	0.13	72,72,72,72	0
84	MG	5	3720	1/1	0.97	0.08	71,71,71,71	0
84	MG	1	3619	1/1	0.97	0.32	59,59,59,59	0
84	MG	Q1	101	1/1	0.97	0.25	83,83,83,83	0
84	MG	5	3630	1/1	0.97	0.20	50,50,50,50	0
84	MG	5	3724	1/1	0.97	0.17	60,60,60,60	1
84	MG	1	3516	1/1	0.97	0.34	54,54,54,54	0
84	MG	M0	304	1/1	0.97	0.13	62,62,62,62	0
84	MG	5	3633	1/1	0.97	0.30	45,45,45,45	0
84	MG	5	3820	1/1	0.97	0.13	52,52,52,52	0
84	MG	5	3411	1/1	0.97	0.38	46,46,46,46	0
84	MG	5	4029	1/1	0.97	0.27	52,52,52,52	0
84	MG	5	3413	1/1	0.97	0.30	46,46,46,46	0
84	MG	m7	201	1/1	0.97	0.25	57,57,57,57	0
84	MG	5	3560	1/1	0.97	0.24	51,51,51,51	0
84	MG	5	3824	1/1	0.97	0.15	58,58,58,58	0
84	MG	1	3729	1/1	0.97	0.21	72,72,72,72	0
84	MG	5	3733	1/1	0.97	0.14	65,65,65,65	0
84	MG	1	3678	1/1	0.97	0.28	69,69,69,69	0
84	MG	5	3930	1/1	0.97	0.20	45,45,45,45	0
84	MG	5	3639	1/1	0.97	0.30	42,42,42,42	0
84	MG	5	4038	1/1	0.97	0.10	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	7	202	1/1	0.97	0.23	52,52,52,52	0
84	MG	5	3640	1/1	0.97	0.42	41,41,41,41	0
84	MG	7	204	1/1	0.97	0.28	54,54,54,54	0
84	MG	5	3830	1/1	0.97	0.07	49,49,49,49	1
84	MG	7	206	1/1	0.97	0.12	62,62,62,62	0
84	MG	n0	202	1/1	0.97	0.26	52,52,52,52	0
84	MG	5	3831	1/1	0.97	0.26	44,44,44,44	0
84	MG	5	3737	1/1	0.97	0.27	49,49,49,49	0
86	ZN	O4	501	1/1	0.97	0.08	141,141,141,141	0
86	ZN	Q3	501	1/1	0.97	0.12	108,108,108,108	0
84	MG	1	3731	1/1	0.97	0.15	80,80,80,80	0
84	MG	5	3417	1/1	0.97	0.38	43,43,43,43	0
84	MG	1	3856	1/1	0.97	0.26	55,55,55,55	0
84	MG	2	1903	1/1	0.97	0.33	90,90,90,90	0
84	MG	2	1927	1/1	0.98	0.26	95,95,95,95	0
84	MG	1	3850	1/1	0.98	0.29	57,57,57,57	0
84	MG	1	3433	1/1	0.98	0.30	49,49,49,49	0
84	MG	5	3788	1/1	0.98	0.22	50,50,50,50	0
84	MG	5	3572	1/1	0.98	0.23	67,67,67,67	0
84	MG	5	3573	1/1	0.98	0.31	61,61,61,61	0
84	MG	2	1970	1/1	0.98	0.18	105,105,105,105	0
84	MG	1	3947	1/1	0.98	0.48	79,79,79,79	0
84	MG	5	3956	1/1	0.98	0.29	55,55,55,55	0
84	MG	5	3511	1/1	0.98	0.18	47,47,47,47	0
84	MG	1	3591	1/1	0.98	0.41	46,46,46,46	0
84	MG	5	4044	1/1	0.98	0.40	72,72,72,72	0
84	MG	5	3578	1/1	0.98	0.17	48,48,48,48	1
84	MG	d3	203	1/1	0.98	0.11	68,68,68,68	0
84	MG	5	3643	1/1	0.98	0.26	55,55,55,55	0
84	MG	q3	504	1/1	0.98	0.23	74,74,74,74	0
84	MG	5	3513	1/1	0.98	0.22	48,48,48,48	0
84	MG	5	3405	1/1	0.98	0.42	47,47,47,47	0
84	MG	5	3407	1/1	0.98	0.37	43,43,43,43	0
84	MG	5	3408	1/1	0.98	0.26	45,45,45,45	0
84	MG	6	1905	1/1	0.98	0.26	64,64,64,64	0
84	MG	17	301	1/1	0.98	0.24	45,45,45,45	0
84	MG	1	3511	1/1	0.98	0.39	59,59,59,59	0
84	MG	1	3688	1/1	0.98	0.26	61,61,61,61	0
84	MG	1	3498	1/1	0.98	0.19	62,62,62,62	0
84	MG	5	3412	1/1	0.98	0.27	47,47,47,47	0
84	MG	5	3522	1/1	0.98	0.22	42,42,42,42	0
84	MG	5	3885	1/1	0.98	0.20	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3513	1/1	0.98	0.34	55,55,55,55	0
84	MG	1	3595	1/1	0.98	0.27	54,54,54,54	0
84	MG	5	3655	1/1	0.98	0.17	78,78,78,78	0
84	MG	5	3656	1/1	0.98	0.19	78,78,78,78	0
84	MG	1	3434	1/1	0.98	0.24	53,53,53,53	0
84	MG	m0	302	1/1	0.98	0.21	53,53,53,53	0
84	MG	5	3811	1/1	0.98	0.30	44,44,44,44	0
84	MG	7	201	1/1	0.98	0.27	45,45,45,45	0
84	MG	4	216	1/1	0.98	0.12	69,69,69,69	0
84	MG	1	3401	1/1	0.98	0.31	56,56,56,56	0
84	MG	5	3418	1/1	0.98	0.29	44,44,44,44	0
84	MG	m4	202	1/1	0.98	0.19	52,52,52,52	0
84	MG	3	201	1/1	0.98	0.13	81,81,81,81	0
84	MG	5	3662	1/1	0.98	0.22	50,50,50,50	0
84	MG	5	3472	1/1	0.98	0.17	57,57,57,57	0
84	MG	5	3898	1/1	0.98	0.20	56,56,56,56	0
84	MG	6	2122	1/1	0.98	0.30	96,96,96,96	0
84	MG	6	1930	1/1	0.98	0.22	70,70,70,70	0
84	MG	6	1931	1/1	0.98	0.31	67,67,67,67	0
84	MG	1	3411	1/1	0.98	0.39	53,53,53,53	0
84	MG	1	3422	1/1	0.98	0.25	50,50,50,50	0
84	MG	5	3533	1/1	0.98	0.27	45,45,45,45	0
84	MG	5	3422	1/1	0.98	0.27	49,49,49,49	0
84	MG	1	3832	1/1	0.98	0.21	58,58,58,58	0
84	MG	5	3906	1/1	0.98	0.22	50,50,50,50	0
84	MG	5	3669	1/1	0.98	0.23	63,63,63,63	0
84	MG	5	3908	1/1	0.98	0.33	48,48,48,48	0
84	MG	5	3670	1/1	0.98	0.30	63,63,63,63	0
84	MG	5	3536	1/1	0.98	0.43	56,56,56,56	0
84	MG	5	3537	1/1	0.98	0.49	48,48,48,48	0
84	MG	1	3491	1/1	0.98	0.34	79,79,79,79	0
84	MG	6	2040	1/1	0.98	0.16	78,78,78,78	0
84	MG	1	3471	1/1	0.98	0.20	63,63,63,63	0
84	MG	5	3676	1/1	0.98	0.10	65,65,65,65	0
84	MG	5	3677	1/1	0.98	0.22	59,59,59,59	0
84	MG	5	3479	1/1	0.98	0.32	48,48,48,48	0
84	MG	2	1988	1/1	0.98	0.14	112,112,112,112	0
84	MG	5	3481	1/1	0.98	0.31	49,49,49,49	0
84	MG	1	3725	1/1	0.98	0.26	62,62,62,62	0
84	MG	5	3758	1/1	0.98	0.25	65,65,65,65	0
84	MG	5	3544	1/1	0.98	0.30	61,61,61,61	0
84	MG	5	3683	1/1	0.98	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3761	1/1	0.98	0.34	69,69,69,69	0
84	MG	5	3545	1/1	0.98	0.23	49,49,49,49	0
84	MG	5	4095	1/1	0.98	0.12	68,68,68,68	0
84	MG	1	3539	1/1	0.98	0.24	52,52,52,52	0
84	MG	1	3472	1/1	0.98	0.32	57,57,57,57	0
84	MG	5	3548	1/1	0.98	0.33	60,60,60,60	0
84	MG	6	2057	1/1	0.98	0.24	81,81,81,81	0
84	MG	N0	202	1/1	0.98	0.12	49,49,49,49	0
84	MG	1	3673	1/1	0.98	0.12	66,66,66,66	0
84	MG	1	3839	1/1	0.98	0.34	57,57,57,57	0
84	MG	6	1964	1/1	0.98	0.40	73,73,73,73	0
84	MG	1	3870	1/1	0.98	0.21	58,58,58,58	0
84	MG	5	3489	1/1	0.98	0.16	55,55,55,55	0
84	MG	1	3523	1/1	0.98	0.18	70,70,70,70	0
84	MG	1	3542	1/1	0.98	0.26	52,52,52,52	0
84	MG	5	3851	1/1	0.98	0.20	54,54,54,54	0
84	MG	1	3416	1/1	0.98	0.17	56,56,56,56	0
84	MG	2	1916	1/1	0.98	0.16	90,90,90,90	0
84	MG	L4	402	1/1	0.98	0.08	65,65,65,65	0
84	MG	1	3525	1/1	0.98	0.23	69,69,69,69	0
84	MG	1	3507	1/1	0.98	0.35	60,60,60,60	0
84	MG	1	3679	1/1	0.98	0.18	68,68,68,68	0
84	MG	1	3762	1/1	0.98	0.26	70,70,70,70	0
86	ZN	Q2	501	1/1	0.98	0.08	102,102,102,102	0
84	MG	4	201	1/1	0.98	0.34	55,55,55,55	0
84	MG	1	3475	1/1	0.98	0.29	60,60,60,60	0
86	ZN	D9	101	1/1	0.98	0.11	121,121,121,121	0
84	MG	1	3567	1/1	0.98	0.16	66,66,66,66	0
86	ZN	o4	501	1/1	0.98	0.17	127,127,127,127	0
84	MG	1	3485	1/1	0.98	0.21	70,70,70,70	0
84	MG	1	3943	1/1	0.98	0.30	60,60,60,60	0
84	MG	6	1928	1/1	0.99	0.31	68,68,68,68	0
84	MG	1	3562	1/1	0.99	0.10	80,80,80,80	0
84	MG	1	3684	1/1	0.99	0.25	58,58,58,58	0
84	MG	12	302	1/1	0.99	0.29	53,53,53,53	0
84	MG	5	3499	1/1	0.99	0.15	53,53,53,53	0
84	MG	5	3500	1/1	0.99	0.19	51,51,51,51	0
84	MG	5	3727	1/1	0.99	0.25	46,46,46,46	0
84	MG	2	1982	1/1	0.99	0.13	97,97,97,97	0
84	MG	5	3444	1/1	0.99	0.24	45,45,45,45	0
84	MG	1	3646	1/1	0.99	0.22	52,52,52,52	0
84	MG	13	404	1/1	0.99	0.27	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	5	3994	1/1	0.99	0.21	48,48,48,48	0
84	MG	5	3995	1/1	0.99	0.22	47,47,47,47	0
84	MG	1	3716	1/1	0.99	0.32	66,66,66,66	0
84	MG	5	3447	1/1	0.99	0.34	49,49,49,49	0
84	MG	5	4124	1/1	0.99	0.22	50,50,50,50	0
84	MG	1	3717	1/1	0.99	0.64	56,56,56,56	0
84	MG	1	3671	1/1	0.99	0.35	55,55,55,55	0
84	MG	1	3522	1/1	0.99	0.34	63,63,63,63	0
84	MG	1	3473	1/1	0.99	0.37	59,59,59,59	0
84	MG	5	3452	1/1	0.99	0.16	48,48,48,48	0
84	MG	5	3738	1/1	0.99	0.30	50,50,50,50	0
84	MG	1	3428	1/1	0.99	0.22	54,54,54,54	0
84	MG	5	3426	1/1	0.99	0.21	48,48,48,48	0
84	MG	5	3402	1/1	0.99	0.22	47,47,47,47	0
84	MG	5	3673	1/1	0.99	0.33	55,55,55,55	0
84	MG	O2	201	1/1	0.99	0.11	60,60,60,60	0
84	MG	6	2004	1/1	0.99	0.22	67,67,67,67	0
84	MG	5	4050	1/1	0.99	0.10	80,80,80,80	0
84	MG	5	3816	1/1	0.99	0.17	43,43,43,43	0
84	MG	1	3756	1/1	0.99	0.24	62,62,62,62	0
84	MG	1	3946	1/1	0.99	0.27	54,54,54,54	0
84	MG	5	3406	1/1	0.99	0.27	44,44,44,44	0
84	MG	1	3435	1/1	0.99	0.23	53,53,53,53	0
84	MG	1	3460	1/1	0.99	0.27	58,58,58,58	0
84	MG	1	3436	1/1	0.99	0.28	49,49,49,49	0
84	MG	6	1963	1/1	0.99	0.32	68,68,68,68	0
84	MG	5	3521	1/1	0.99	0.19	50,50,50,50	0
84	MG	5	3715	1/1	0.99	0.15	54,54,54,54	0
84	MG	1	3520	1/1	0.99	0.22	69,69,69,69	0
84	MG	5	3900	1/1	0.99	0.41	51,51,51,51	0
84	MG	1	3588	1/1	0.99	0.26	58,58,58,58	0
86	ZN	Q0	500	1/1	0.99	0.17	72,72,72,72	0
84	MG	m0	301	1/1	0.99	0.26	49,49,49,49	1
84	MG	5	3902	1/1	0.99	0.42	55,55,55,55	0
86	ZN	D6	500	1/1	0.99	0.13	101,101,101,101	0
84	MG	1	3599	1/1	0.99	0.28	52,52,52,52	0
84	MG	1	3406	1/1	0.99	0.11	58,58,58,58	0
84	MG	1	3682	1/1	0.99	0.09	65,65,65,65	0
84	MG	5	4109	1/1	0.99	0.22	42,42,42,42	0
86	ZN	o7	501	1/1	0.99	0.19	80,80,80,80	0
86	ZN	q2	501	1/1	0.99	0.10	94,94,94,94	0
86	ZN	q3	501	1/1	0.99	0.14	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	ZN	d6	101	1/1	0.99	0.16	82,82,82,82	0
84	MG	1	3783	1/1	0.99	0.21	61,61,61,61	0
86	ZN	d9	101	1/1	0.99	0.12	89,89,89,89	0
84	MG	5	3559	1/1	0.99	0.11	56,56,56,56	1
86	ZN	O7	101	1/1	1.00	0.14	77,77,77,77	0
86	ZN	q0	201	1/1	1.00	0.15	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.