



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:58 PM BST

PDB ID : 5NDV
Title : Crystal structure of Paromomycin bound to the yeast 80S ribosome
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2017-03-09
Resolution : 3.30 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 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 : 2.13
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) : 2.13

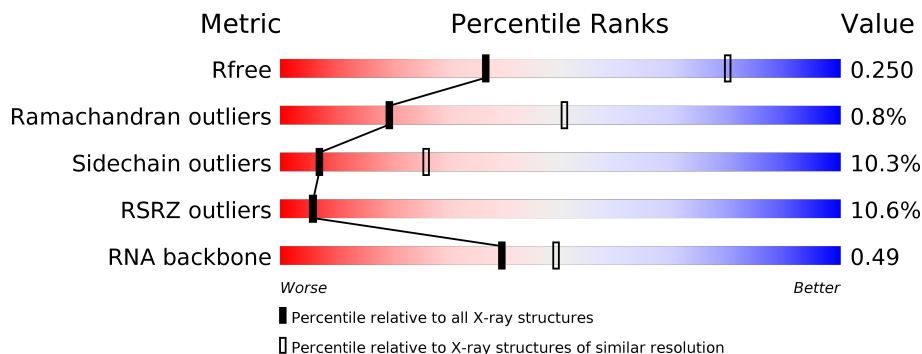
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



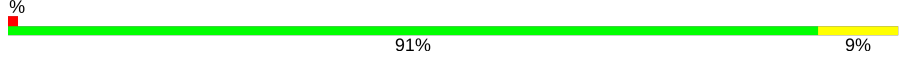
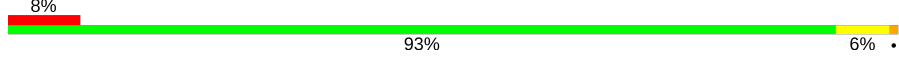
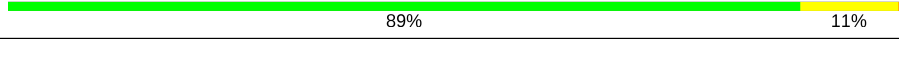
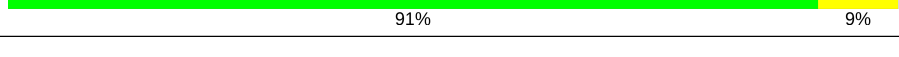
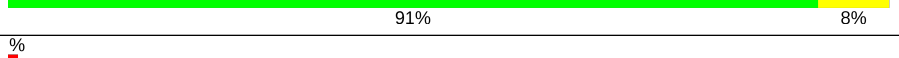
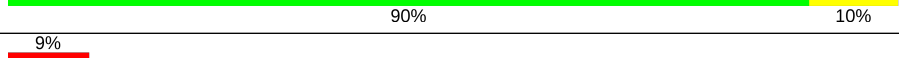
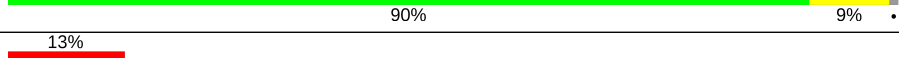
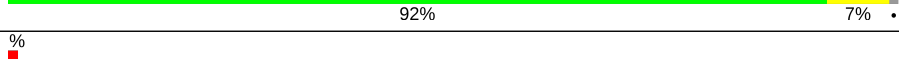
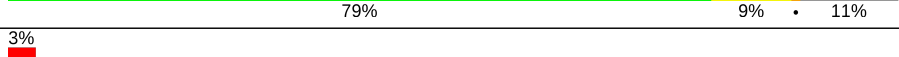

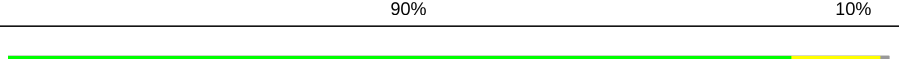
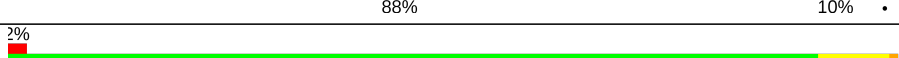
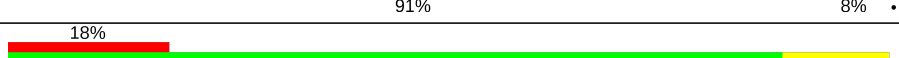






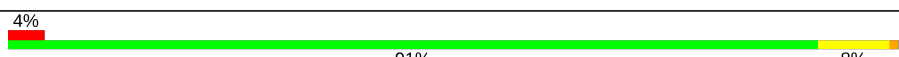
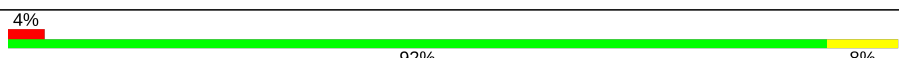
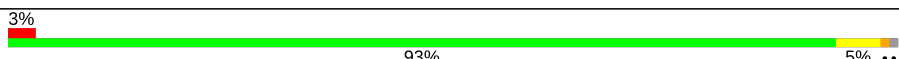
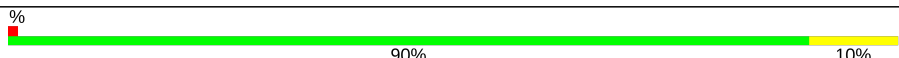
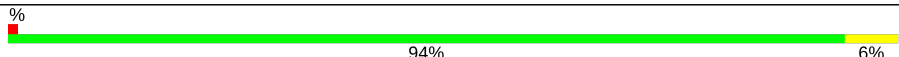

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	5	3396	
2	3	121	
2	7	121	
3	4	158	
3	8	158	

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Mol	Chain	Length	Quality of chain
4	L2	248	 91% 9%
4	l2	248	 93% 6% 8%
5	L3	386	 89% 11%
5	l3	386	 91% 9%
6	L4	361	 91% 8%
6	l4	361	 90% 10%
7	L5	296	 90% 9% 9%
7	l5	296	 92% 7% 13%
8	L6	176	 79% 9% 11%
8	l6	176	 82% 7% 3%
9	L7	226	 90% 10%
9	l7	226	 88% 10%
10	L8	231	 91% 8% 2%
10	l8	231	 87% 12% 18%
11	L9	191	 85% 13% 10%
11	l9	191	 85% 15% 2%
12	M0	221	 88% 10% 9%
12	m0	221	 88% 11% 6%
13	M1	169	 87% 12% 17%
13	m1	169	 86% 13% 17%
14	M3	194	 91% 8% 4%
14	m3	194	 92% 8% 4%
15	M4	137	 93% 5% 3%
15	m4	137	 90% 10%
16	M5	203	 94% 6%

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Mol	Chain	Length	Quality of chain
16	m5	203	7% 93% 7%
17	M6	197	% 93% 7%
17	m6	197	94% 6%
18	M7	184	7% 85% 10% 5%
18	m7	184	76% 8% 16%
19	M8	185	% 91% 9%
19	m8	185	5% 91% 9%
20	M9	188	88% 10% .
20	m9	188	8% 91% 9%
21	N0	172	4% 85% 14% .
21	n0	172	88% 12% .
22	N1	159	3% 86% 14%
22	n1	159	20% 92% 7% .
23	N2	99	3% 83% 17%
23	n2	99	8% 91% 8% .
24	N3	136	89% 8% .
24	n3	136	% 93% 7%
25	N4	155	% 40% 59%
25	n4	155	28% 81% 6% 13%
26	N5	120	% 84% 14% .
26	n5	120	13% 88% 10% .
27	N6	125	10% 94% 6%
27	n6	125	6% 92% 6% .
28	N7	135	7% 90% 10%
28	n7	135	37% 93% 7%

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Mol	Chain	Length	Quality of chain
29	N8	148	
29	n8	148	
30	N9	58	
30	n9	58	
31	O0	100	
31	o0	100	
32	O1	112	
32	o1	112	
33	O2	127	
33	o2	127	
34	O3	106	
34	o3	106	
35	O4	112	
35	o4	112	
36	O5	119	
36	o5	119	
37	O6	99	
37	o6	99	
38	O7	87	
38	o7	87	
39	O8	77	
39	o8	77	
40	O9	50	
40	o9	50	
41	Q0	52	

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Mol	Chain	Length	Quality of chain
41	q0	52	4% 87% 13%
42	Q1	25	84% 16%
42	q1	25	76% 24%
43	Q2	105	16% 89% 11%
43	q2	105	9% 90% 10%
44	Q3	91	88% 11%
44	q3	91	92% 8%
45	2	1800	2% 67% 27% 5%
45	6	1800	% 67% 26% 7%
46	S0	206	21% 90% 9%
46	s0	206	17% 91% 9%
47	S1	216	30% 79% 18% ..
47	s1	216	30% 90% 10%
48	S2	217	12% 90% 10%
48	s2	217	24% 94% 6%
49	S3	223	15% 86% 8% 6%
49	s3	223	34% 91% 8%
50	S4	260	34% 92% 7% .
50	s4	260	15% 92% 8%
51	S5	206	62% 91% 8% .
51	s5	206	32% 93% 7%
52	S6	236	18% 79% 6% 15%
53	S7	186	15% 87% 9% ..
53	s7	186	18% 89% 11% .
54	S8	200	14% 85% 8% 8%

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Mol	Chain	Length	Quality of chain
54	s8	200	10% 90% 5% 6%
55	S9	185	21% 88% 5% 6%
55	s9	185	24% 91% 9%
56	C0	105	10% 79% 6% 14%
56	c0	105	30% 79% 9% 9%
57	C1	146	10% 84% 10% 5%
57	c1	146	12% 90% 9%
58	C2	143	23% 59% 12% 29%
58	c2	143	38% 72% 14% 13%
59	C3	150	11% 93% 7%
59	c3	150	6% 91% 9%
60	C4	128	5% 87% 11% ..
60	c4	128	24% 89% 11%
61	C5	141	17% 79% 18%
61	c5	141	46% 82% 13% ..
62	C6	142	65% 85% 10% ..
62	c6	142	62% 93% 6%
63	C7	136	30% 74% 9% .. 15%
63	c7	136	13% 76% 9% 14%
64	C8	145	27% 87% 11% ..
64	c8	145	32% 89% 10%
65	C9	143	33% 86% 10%
65	c9	143	29% 92% 7%
66	D0	109	32% 83% 10% 6%
66	d0	109	24% 87% 12%

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Mol	Chain	Length	Quality of chain
67	D1	87	18% 90% 10%
67	d1	87	14% 86% 14%
68	D2	129	33% 88% 10%
68	d2	129	14% 90% 9%
69	D3	144	94% 6%
69	d3	144	5% 95% 5%
70	D4	134	22% 90% 10%
70	d4	134	17% 92% 7%
71	D5	70	61% 80% 20%
71	d5	70	43% 84% 14%
72	D6	97	3% 79% 16%
72	d6	97	13% 90% 8%
73	D7	81	17% 90% 10%
73	d7	81	15% 93% 7%
74	D8	63	40% 92% 8%
74	d8	63	57% 90% 8%
75	D9	53	30% 89% 11%
75	d9	53	11% 85% 13%
76	E0	62	29% 81% 16%
76	e0	62	24% 85% 15%
77	SR	318	58% 95% 5%
77	sR	318	54% 93% 7%
78	SM	272	11% 49% 6% 46%
78	sM	272	9% 33% 65%
79	s6	218	39% 90% 9%

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
80	PAR	5	3423	-	-	-	X
81	MG	1	3491	-	-	-	X
81	MG	1	3521	-	-	-	X
81	MG	1	3548	-	-	-	X
81	MG	1	3577	-	-	-	X
81	MG	1	3591	-	-	-	X
81	MG	1	3593	-	-	-	X
81	MG	1	3632	-	-	-	X
81	MG	1	3634	-	-	-	X
81	MG	1	3682	-	-	-	X
81	MG	1	3711	-	-	-	X
81	MG	1	3795	-	-	-	X
81	MG	1	3830	-	-	-	X
81	MG	1	3847	-	-	-	X
81	MG	1	3860	-	-	-	X
81	MG	1	3871	-	-	-	X
81	MG	1	3884	-	-	-	X
81	MG	1	3903	-	-	-	X
81	MG	1	3904	-	-	-	X
81	MG	1	3905	-	-	-	X
81	MG	1	3924	-	-	-	X
81	MG	1	3946	-	-	-	X
81	MG	1	3957	-	-	-	X
81	MG	1	3963	-	-	-	X
81	MG	1	3975	-	-	-	X
81	MG	1	3979	-	-	-	X
81	MG	1	3982	-	-	-	X
81	MG	1	3993	-	-	-	X
81	MG	1	3998	-	-	-	X
81	MG	1	4015	-	-	-	X
81	MG	1	4018	-	-	-	X
81	MG	1	4020	-	-	-	X
81	MG	1	4026	-	-	-	X
81	MG	1	4033	-	-	-	X
81	MG	1	4062	-	-	-	X
81	MG	1	4084	-	-	-	X
81	MG	1	4089	-	-	-	X
81	MG	1	4095	-	-	-	X
81	MG	1	4098	-	-	-	X
81	MG	1	4099	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	1	4100	-	-	-	X
81	MG	1	4102	-	-	-	X
81	MG	1	4107	-	-	-	X
81	MG	1	4108	-	-	-	X
81	MG	1	4109	-	-	-	X
81	MG	1	4118	-	-	-	X
81	MG	1	4121	-	-	-	X
81	MG	1	4136	-	-	-	X
81	MG	1	4139	-	-	-	X
81	MG	1	4155	-	-	-	X
81	MG	1	4173	-	-	-	X
81	MG	1	4175	-	-	-	X
81	MG	1	4180	-	-	-	X
81	MG	1	4184	-	-	-	X
81	MG	1	4186	-	-	-	X
81	MG	1	4198	-	-	-	X
81	MG	2	1923	-	-	-	X
81	MG	2	1932	-	-	-	X
81	MG	2	1937	-	-	-	X
81	MG	2	1940	-	-	-	X
81	MG	2	1982	-	-	-	X
81	MG	2	2003	-	-	-	X
81	MG	2	2010	-	-	-	X
81	MG	2	2011	-	-	-	X
81	MG	2	2019	-	-	-	X
81	MG	2	2025	-	-	-	X
81	MG	2	2026	-	-	-	X
81	MG	2	2044	-	-	-	X
81	MG	2	2048	-	-	-	X
81	MG	2	2059	-	-	-	X
81	MG	2	2061	-	-	-	X
81	MG	2	2094	-	-	-	X
81	MG	2	2103	-	-	-	X
81	MG	2	2111	-	-	-	X
81	MG	2	2113	-	-	-	X
81	MG	5	3529	-	-	-	X
81	MG	5	3535	-	-	-	X
81	MG	5	3536	-	-	-	X
81	MG	5	3537	-	-	-	X
81	MG	5	3561	-	-	-	X
81	MG	5	3658	-	-	-	X
81	MG	5	3677	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	5	3679	-	-	-	X
81	MG	5	3681	-	-	-	X
81	MG	5	3685	-	-	-	X
81	MG	5	3690	-	-	-	X
81	MG	5	3700	-	-	-	X
81	MG	5	3701	-	-	-	X
81	MG	5	3708	-	-	-	X
81	MG	5	3729	-	-	-	X
81	MG	5	3769	-	-	-	X
81	MG	5	3793	-	-	-	X
81	MG	5	3794	-	-	-	X
81	MG	5	3826	-	-	-	X
81	MG	5	3827	-	-	-	X
81	MG	5	3828	-	-	-	X
81	MG	5	3839	-	-	-	X
81	MG	5	3840	-	-	-	X
81	MG	5	3841	-	-	-	X
81	MG	5	3842	-	-	-	X
81	MG	5	3844	-	-	-	X
81	MG	5	3845	-	-	-	X
81	MG	5	3846	-	-	-	X
81	MG	5	3853	-	-	-	X
81	MG	5	3878	-	-	-	X
81	MG	5	3910	-	-	-	X
81	MG	5	3915	-	-	-	X
81	MG	5	3927	-	-	-	X
81	MG	5	3928	-	-	-	X
81	MG	5	3951	-	-	-	X
81	MG	5	3952	-	-	-	X
81	MG	5	3953	-	-	-	X
81	MG	5	3959	-	-	-	X
81	MG	5	3966	-	-	-	X
81	MG	5	3983	-	-	-	X
81	MG	5	3985	-	-	-	X
81	MG	5	3987	-	-	-	X
81	MG	5	3989	-	-	-	X
81	MG	5	3994	-	-	-	X
81	MG	5	3998	-	-	-	X
81	MG	5	3999	-	-	-	X
81	MG	5	4000	-	-	-	X
81	MG	5	4003	-	-	-	X
81	MG	5	4012	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	5	4013	-	-	-	X
81	MG	5	4019	-	-	-	X
81	MG	5	4025	-	-	-	X
81	MG	5	4038	-	-	-	X
81	MG	5	4057	-	-	-	X
81	MG	5	4058	-	-	-	X
81	MG	5	4059	-	-	-	X
81	MG	5	4062	-	-	-	X
81	MG	5	4066	-	-	-	X
81	MG	5	4067	-	-	-	X
81	MG	5	4068	-	-	-	X
81	MG	5	4079	-	-	-	X
81	MG	5	4082	-	-	-	X
81	MG	5	4085	-	-	-	X
81	MG	5	4090	-	-	-	X
81	MG	5	4091	-	-	-	X
81	MG	5	4098	-	-	-	X
81	MG	5	4099	-	-	-	X
81	MG	5	4100	-	-	-	X
81	MG	5	4105	-	-	-	X
81	MG	5	4111	-	-	-	X
81	MG	5	4115	-	-	-	X
81	MG	5	4116	-	-	-	X
81	MG	6	1921	-	-	-	X
81	MG	6	1922	-	-	-	X
81	MG	6	1937	-	-	-	X
81	MG	6	1966	-	-	-	X
81	MG	6	1986	-	-	-	X
81	MG	6	2011	-	-	-	X
81	MG	6	2013	-	-	-	X
81	MG	6	2020	-	-	-	X
81	MG	6	2058	-	-	-	X
81	MG	6	2060	-	-	-	X
81	MG	6	2064	-	-	-	X
81	MG	6	2065	-	-	-	X
81	MG	6	2067	-	-	-	X
81	MG	6	2070	-	-	-	X
81	MG	6	2071	-	-	-	X
81	MG	7	204	-	-	-	X
81	MG	7	211	-	-	-	X
81	MG	8	209	-	-	-	X
81	MG	8	212	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
81	MG	8	219	-	-	-	X
81	MG	8	220	-	-	-	X
81	MG	8	222	-	-	-	X
81	MG	8	223	-	-	-	X
81	MG	D3	202	-	-	-	X
81	MG	L3	402	-	-	-	X
81	MG	L7	302	-	-	-	X
81	MG	N8	203	-	-	-	X
81	MG	O2	202	-	-	-	X
81	MG	d3	204	-	-	-	X
81	MG	m9	204	-	-	-	X
81	MG	o2	204	-	-	-	X
81	MG	q3	502	-	-	-	X

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 397978 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	3078	Total	C	N	O	P	0	0	0
			65834	29406	11864	21486	3078			
1	5	3087	Total	C	N	O	P	0	0	0
			66030	29494	11905	21544	3087			

- 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	157	Total	C	N	O	P	0	0	0
			3333	1491	584	1101	157			
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	248	Total	C	N	O	S	0	0	0
			1884	1173	382	328	1			
4	12	248	Total	C	N	O	S	0	0	0
			1884	1173	382	328	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	14	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	293	Total	C	N	O	S	0	0	0
			2353	1489	409	453	2			
7	15	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	16	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	226	Total	C	N	O	S	0	0	0
			1818	1171	331	315	1			
9	17	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	231	Total	C	N	O	S	0	0	0
			1793	1145	321	324	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	18	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	189	Total 1502	C 953	N 272	O 273	S 4	0	0	0
11	19	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	217	Total 1759	C 1114	N 333	O 305	S 7	0	0	0
12	m0	219	Total 1773	C 1122	N 336	O 308	S 7	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	175	Total	C	N	O	0	0	0
			1378	856	273	249			
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	185	Total	C	N	O	0	0	0
			1499	923	323	253			
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	99	Total	C	N	O	0	0	0
			787	511	129	147			
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	132	Total	C	N	O	S	0	0	0
			981	617	184	173	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	63	Total	C	N	O	S	0	0	0
			521	336	102	82	1			
25	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	N5	118	Total	C	N	O	S	0	0	0
			946	608	166	170	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
27	N6	125	Total	C	N	O	0	0	0
			984	620	191	173			
27	n6	123	Total	C	N	O	0	0	0
			967	608	188	171			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	N9	56	Total	C	N	O	0	0	0
			444	277	96	71			
30	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	O1	106	Total 849	C 541	N 164	O 143	S 1	0	0	0
32	o1	109	Total 883	C 559	N 167	O 156	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	O2	125	Total 1007	C 638	N 203	O 165	S 1	0	0	0
33	o2	127	Total 1020	C 647	N 205	O 167	S 1	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	O6	97	Total	C	N	O	S	0	0	0
			750	469	149	130	2			
37	o6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	O7	84	Total	C	N	O	S	0	0	0
			665	405	145	110	5			
38	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	2	1712	Total	C	N	O	P	0	0	0
			36485	16312	6462	11999	1712			
45	6	1683	Total	C	N	O	P	0	0	0
			35865	16035	6355	11792	1683			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	S0	206	Total	C	N	O	S	0	0	0
			1581	1017	278	284	2			
46	s0	206	Total	C	N	O	S	0	0	0
			1581	1017	278	284	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	S1	211	Total	C	N	O	S	0	0	0
			1688	1071	305	308	4			
47	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- 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	209	Total 1621	C 1028	N 297	O 290	S 6	0	0	0
49	s3	223	Total 1734	C 1101	N 313	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	256	Total 2044	C 1300	N 385	O 356	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	200	Total 1593	C 997	N 313	O 280	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	179	Total 1442	C 926	N 259	O 257	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
53	s7	186	Total	C	N	O	0	0	0
			1492	957	267	268			

- 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	185	Total	C	N	O	S	0	0	0
			1466	910	293	261	2			
54	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- 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	174	Total	C	N	O	S	0	0	0
			1418	900	273	244	1			
55	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- 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	90	Total	C	N	O	S	0	0	0
			742	481	120	139	2			
56	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- 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	139	Total	C	N	O	S	0	0	0
			1127	724	214	186	3			
57	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
58	C2	102	Total	C	N	O	S	0	0	0
			764	485	132	145	2			
58	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- 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	116	Total	C	N	O	S	0	0	0
			918	583	171	157	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	136	Total	C	N	O	0	0	0
			1064	682	195	187			
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	115	Total	C	N	O	S	0	0	0
			901	562	172	165	2			
63	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	C8	143	Total	C	N	O	S	0	0	0
			1178	734	235	207	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	137	Total	C	N	O	S	0	0	0
			1072	669	202	199	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	102	Total	C	N	O	S	0	0	0
			818	519	148	150	1			
66	d0	109	Total	C	N	O	S	0	0	0
			873	549	159	164	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	134	1073	676	208	189	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 Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	SR	317	Total	C	N	O	S	0	0	0
			2432	1537	416	471	8			
77	sR	318	Total	C	N	O	S	0	0	0
			2437	1540	417	472	8			

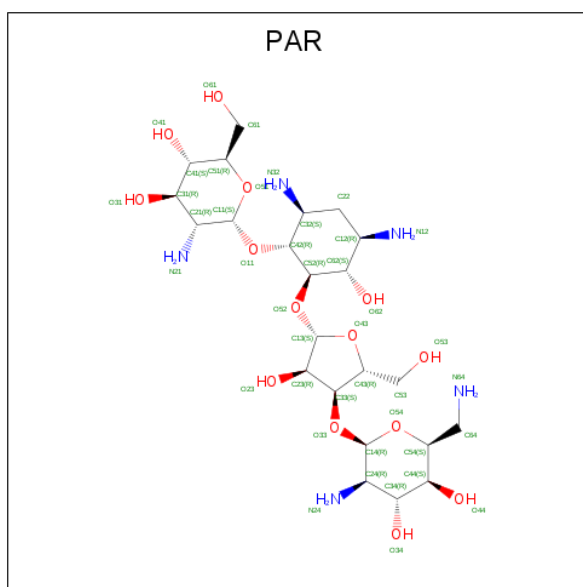
- Molecule 78 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
78	SM	147	Total	C	N	O	0	0	0
			1044	616	209	219			
78	sM	95	Total	C	N	O	0	0	0
			635	376	131	128			

- Molecule 79 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 80 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		
80	1	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
80	1	1	42	23	5	14	0	0
80	1	1	42	23	5	14	0	0
80	3	1	42	23	5	14	0	0
80	3	1	42	23	5	14	0	0
80	3	1	42	23	5	14	0	0
80	4	1	42	23	5	14	0	0
80	4	1	42	23	5	14	0	0
80	2	1	42	23	5	14	0	0
80	2	1	42	23	5	14	0	0
80	2	1	42	23	5	14	0	0
80	2	1	42	23	5	14	0	0
80	2	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0
80	5	1	42	23	5	14	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	5	1	Total	C	N	O	0	0
			42	23	5	14		
80	7	1	Total	C	N	O	0	0
			42	23	5	14		
80	7	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
80	8	1	42	23	5	14	0	0
80	8	1	42	23	5	14	0	0
80	n3	1	42	23	5	14	0	0
80	o2	1	42	23	5	14	0	0
80	6	1	42	23	5	14	0	0
80	6	1	42	23	5	14	0	0
80	6	1	42	23	5	14	0	0
80	6	1	42	23	5	14	0	0
80	6	1	42	23	5	14	0	0
80	6	1	42	23	5	14	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	n8	4	Total 4	Mg 4	0	0
81	N5	1	Total 1	Mg 1	0	0
81	d2	1	Total 1	Mg 1	0	0
81	n5	1	Total 1	Mg 1	0	0
81	S9	1	Total 1	Mg 1	0	0
81	M9	2	Total 2	Mg 2	0	0
81	q0	1	Total 1	Mg 1	0	0
81	c1	1	Total 1	Mg 1	0	0
81	o1	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	L4	3	Total 3	Mg 3	0	0
81	L5	3	Total 3	Mg 3	0	0
81	O2	3	Total 3	Mg 3	0	0
81	m9	5	Total 5	Mg 5	0	0
81	M3	1	Total 1	Mg 1	0	0
81	n2	1	Total 1	Mg 1	0	0
81	o2	3	Total 3	Mg 3	0	0
81	d4	1	Total 1	Mg 1	0	0
81	2	212	Total 212	Mg 212	0	0
81	M6	5	Total 5	Mg 5	0	0
81	S7	1	Total 1	Mg 1	0	0
81	n0	6	Total 6	Mg 6	0	0
81	m6	4	Total 4	Mg 4	0	0
81	n9	1	Total 1	Mg 1	0	0
81	M5	9	Total 9	Mg 9	0	0
81	S2	2	Total 2	Mg 2	0	0
81	N6	5	Total 5	Mg 5	0	0
81	Q3	2	Total 2	Mg 2	0	0
81	m5	2	Total 2	Mg 2	0	0
81	s4	1	Total 1	Mg 1	0	0
81	s2	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	n6	4	Total Mg 4 4	0	0
81	M8	2	Total Mg 2 2	0	0
81	q3	1	Total Mg 1 1	0	0
81	N3	4	Total Mg 4 4	0	0
81	4	35	Total Mg 35 35	0	0
81	L2	6	Total Mg 6 6	0	0
81	O1	3	Total Mg 3 3	0	0
81	s8	1	Total Mg 1 1	0	0
81	m8	1	Total Mg 1 1	0	0
81	n3	3	Total Mg 3 3	0	0
81	l2	3	Total Mg 3 3	0	0
81	N0	1	Total Mg 1 1	0	0
81	L7	2	Total Mg 2 2	0	0
81	D3	2	Total Mg 2 2	0	0
81	6	169	Total Mg 169 169	0	0
81	O4	3	Total Mg 3 3	0	0
81	D6	1	Total Mg 1 1	0	0
81	S6	1	Total Mg 1 1	0	0
81	c9	2	Total Mg 2 2	0	0
81	l7	6	Total Mg 6 6	0	0
81	L8	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	o4	1	Total Mg 1 1	0	0
81	O7	4	Total Mg 4 4	0	0
81	s6	2	Total Mg 2 2	0	0
81	M4	3	Total Mg 3 3	0	0
81	1	762	Total Mg 762 762	0	0
81	c4	3	Total Mg 3 3	0	0
81	l8	1	Total Mg 1 1	0	0
81	Q2	5	Total Mg 5 5	0	0
81	o7	2	Total Mg 2 2	0	0
81	d6	1	Total Mg 1 1	0	0
81	q2	1	Total Mg 1 1	0	0
81	Q1	1	Total Mg 1 1	0	0
81	L3	5	Total Mg 5 5	0	0
81	8	23	Total Mg 23 23	0	0
81	3	15	Total Mg 15 15	0	0
81	O0	1	Total Mg 1 1	0	0
81	l3	9	Total Mg 9 9	0	0
81	N1	3	Total Mg 3 3	0	0
81	C8	1	Total Mg 1 1	0	0
81	N7	2	Total Mg 2 2	0	0
81	o0	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	O3	2	Total Mg 2 2	0	0
81	M0	1	Total Mg 1 1	0	0
81	5	698	Total Mg 698 698	0	0
81	n1	2	Total Mg 2 2	0	0
81	l4	3	Total Mg 3 3	0	0
81	L9	4	Total Mg 4 4	0	0
81	d3	5	Total Mg 5 5	0	0
81	o3	1	Total Mg 1 1	0	0
81	O9	1	Total Mg 1 1	0	0
81	m0	3	Total Mg 3 3	0	0
81	O6	1	Total Mg 1 1	0	0
81	M7	6	Total Mg 6 6	0	0
81	N8	3	Total Mg 3 3	0	0
81	l9	1	Total Mg 1 1	0	0
81	C9	2	Total Mg 2 2	0	0
81	7	12	Total Mg 12 12	0	0
81	m7	9	Total Mg 9 9	0	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	o4	1	Total Zn 1 1	0	0
82	O7	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	q0	1	Total Zn 1 1	0	0
82	Q2	1	Total Zn 1 1	0	0
82	Q3	1	Total Zn 1 1	0	0
82	D9	1	Total Zn 1 1	0	0
82	q3	1	Total Zn 1 1	0	0
82	Q0	1	Total Zn 1 1	0	0
82	d7	1	Total Zn 1 1	0	0
82	O4	1	Total Zn 1 1	0	0
82	d9	1	Total Zn 1 1	0	0
82	D7	1	Total Zn 1 1	0	0
82	d6	1	Total Zn 1 1	0	0
82	o7	1	Total Zn 1 1	0	0
82	D6	1	Total Zn 1 1	0	0
82	q2	1	Total Zn 1 1	0	0

- Molecule 83 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	1	500	Total O 500 500	0	0
83	3	7	Total O 7 7	0	0
83	4	15	Total O 15 15	0	0
83	L2	5	Total O 5 5	0	0
83	L3	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	L4	2	Total O 2 2	0	0
83	L5	1	Total O 1 1	0	0
83	L7	1	Total O 1 1	0	0
83	M5	2	Total O 2 2	0	0
83	M6	2	Total O 2 2	0	0
83	M7	4	Total O 4 4	0	0
83	N0	2	Total O 2 2	0	0
83	N1	1	Total O 1 1	0	0
83	N3	3	Total O 3 3	0	0
83	N6	2	Total O 2 2	0	0
83	N7	2	Total O 2 2	0	0
83	N8	2	Total O 2 2	0	0
83	N9	2	Total O 2 2	0	0
83	O0	1	Total O 1 1	0	0
83	O2	2	Total O 2 2	0	0
83	O3	2	Total O 2 2	0	0
83	O4	1	Total O 1 1	0	0
83	O7	1	Total O 1 1	0	0
83	Q2	4	Total O 4 4	0	0
83	2	122	Total O 122 122	0	0
83	S1	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	S9	1	Total O 1 1	0	0
83	C3	1	Total O 1 1	0	0
83	C6	1	Total O 1 1	0	0
83	C7	1	Total O 1 1	0	0
83	C9	1	Total O 1 1	0	0
83	D3	4	Total O 4 4	0	0
83	5	477	Total O 477 477	0	0
83	7	12	Total O 12 12	0	0
83	8	7	Total O 7 7	0	0
83	12	5	Total O 5 5	0	0
83	13	2	Total O 2 2	0	0
83	15	1	Total O 1 1	0	0
83	17	1	Total O 1 1	0	0
83	19	1	Total O 1 1	0	0
83	m0	1	Total O 1 1	0	0
83	m6	1	Total O 1 1	0	0
83	m7	2	Total O 2 2	0	0
83	m9	1	Total O 1 1	0	0
83	n0	2	Total O 2 2	0	0
83	n1	2	Total O 2 2	0	0
83	n3	3	Total O 3 3	0	0

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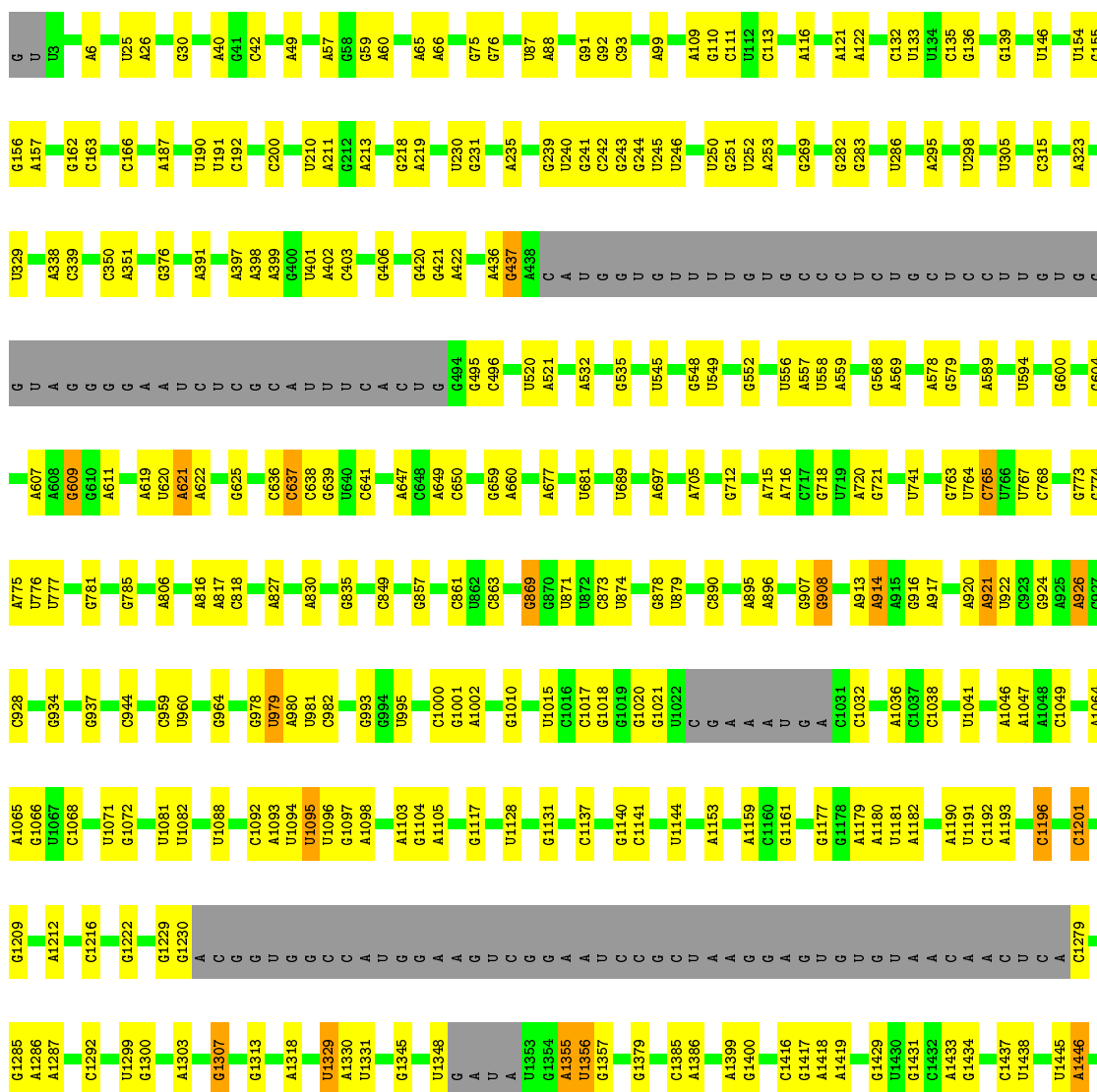
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	n6	1	Total 1	O 1	0	0
83	n7	1	Total 1	O 1	0	0
83	n8	3	Total 3	O 3	0	0
83	o2	3	Total 3	O 3	0	0
83	6	113	Total 113	O 113	0	0
83	c3	4	Total 4	O 4	0	0
83	c4	1	Total 1	O 1	0	0
83	c6	1	Total 1	O 1	0	0
83	c9	1	Total 1	O 1	0	0
83	d3	1	Total 1	O 1	0	0
83	d6	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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.

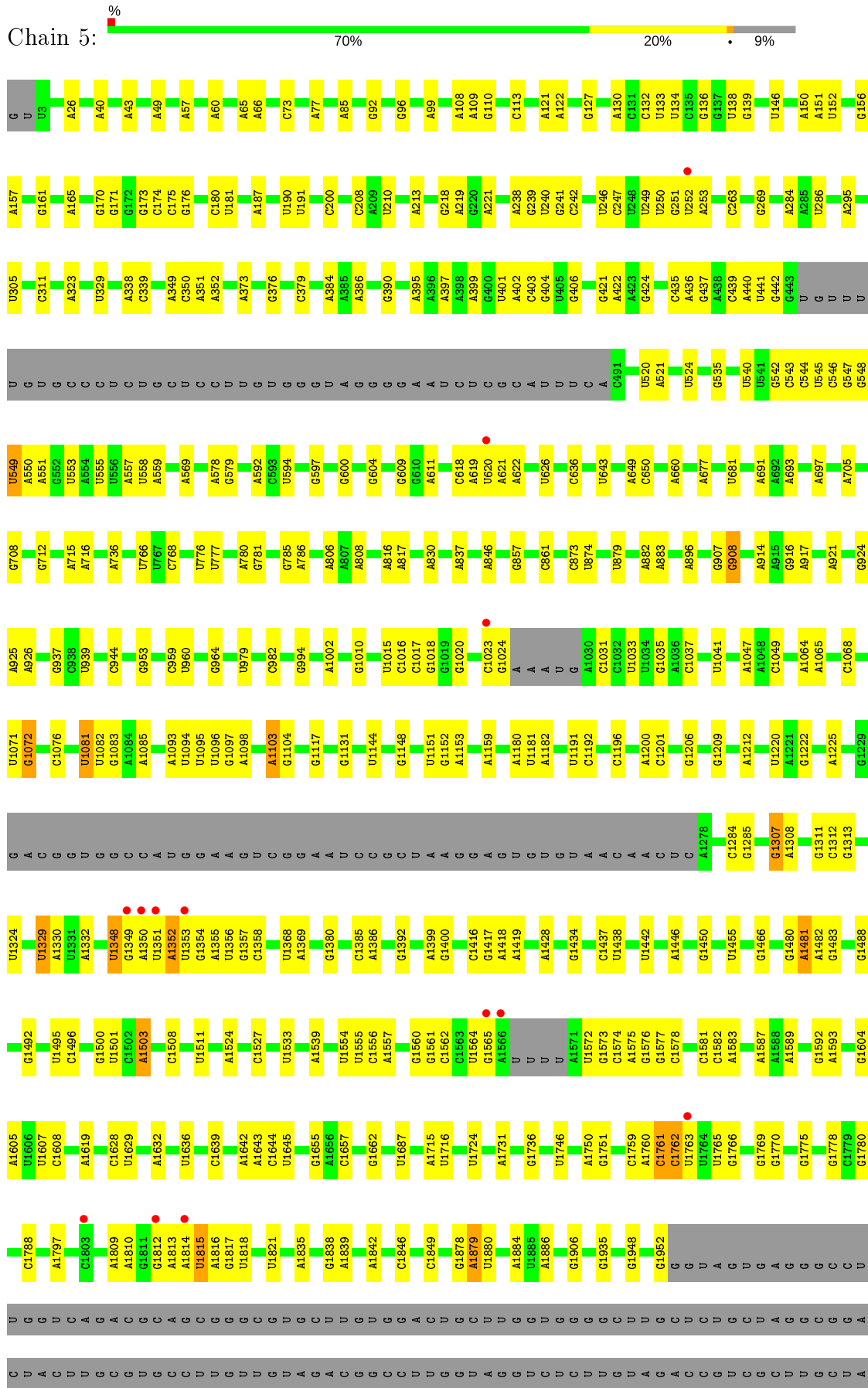
- Molecule 1: 25S ribosomal RNA

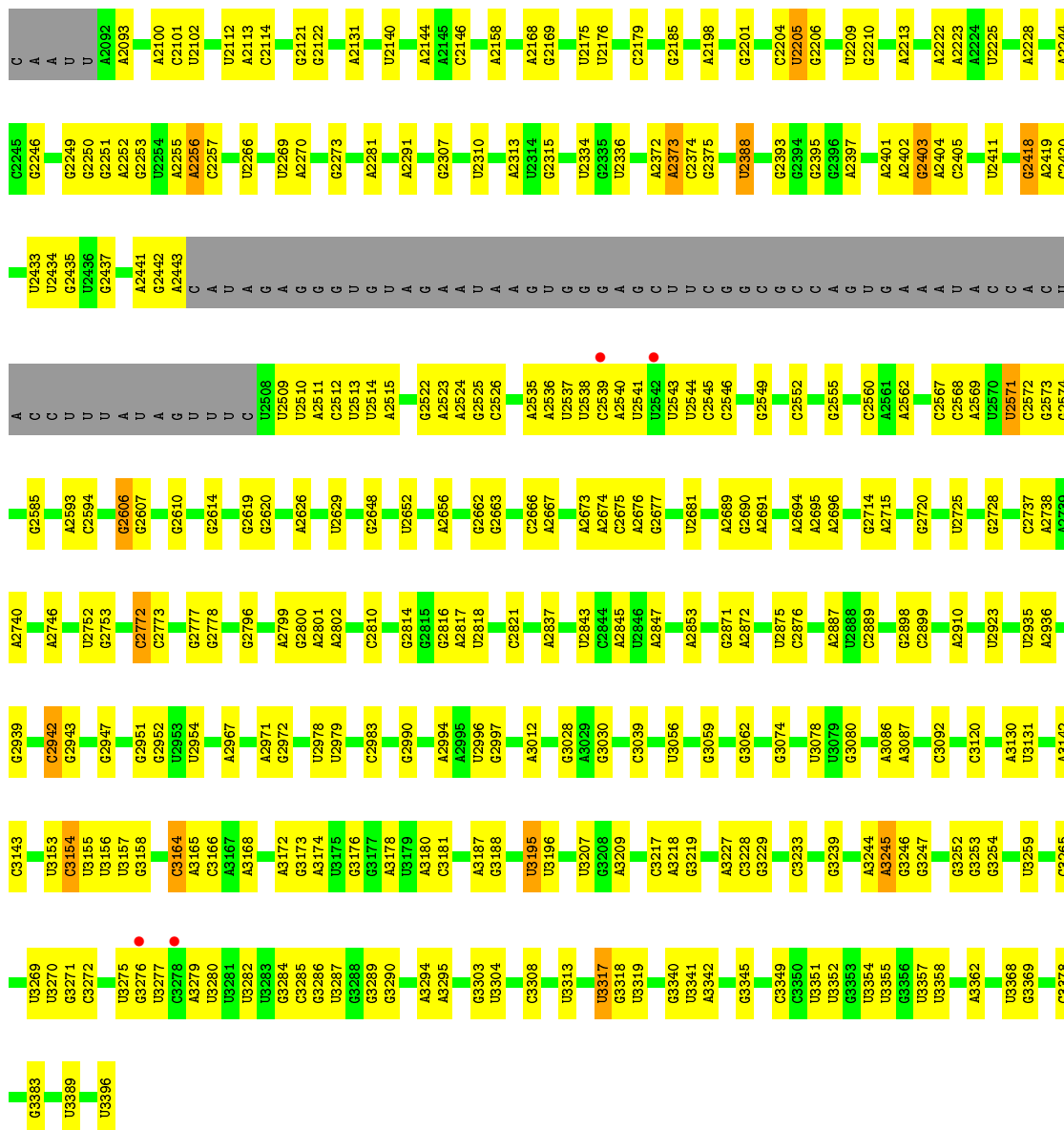
Chain 1: 



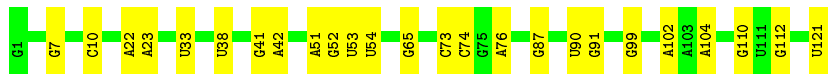
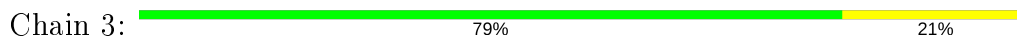
G3383	U3270	U3151	C2942	G2778	G2610	C2288	A2092	G1450
G3386	G3271	U3152	G2943	A2779	U2611	G2289	A2093	A1460
U3389	A3273	C	G2796	G2796	G2614	A2295	C2094	A1587
G3390	U3275	U	G2947	G2800	A2626	C2306	A2100	A1589
U3393	G3276	U	C2948	A2801	C2627	C2307	C2101	A1481
U3394	U3277	U	U2949	A2801	A2628	C2308	U2102	G1483
U3396	G3158	G3158	U2954	A2808	U2629	U2310	U2112	U1484
	A3163	A3163	A2967	C2810	A2637	A2313	C2114	G1485
	C3164	C3164	C2970	G2814	C2638	U2314	A1813	G1488
	A3165	A3165	A2971	G2815	U2639	G2315	U1814	U1495
	A3167	A3167	G2972	A2816	U2682	U2319	A1814	C1502
	U3168	U3168	G2977	A2817	A2656	A2320	U1819	C1508
	G3288	G3288	U2978	U2818	A2657	A2321	U1820	U1523
	G3289	G3289	U2978	U2827	G2663	U2334	U1821	G1640
	A3295	A3295	C2983	A2837	U2681	G2335	U1841	U1641
	U3304	U3304	G2990	A2837	A2674	U2336	A1842	C1527
	A3305	A3305	U2991	U2842	C2675	G2337	A1842	G1528
	U3306	U3306	U2992	A2845	A2677	G2355	C1643	A1529
	G3309	U3179	U2996	U2846	A2678	A2356	G1643	U1645
	A3316	A3180	G2997	A2847	A2679	A2357	A1846	U1533
	U3317	C3181	A3012	A2847	U2680	C2361	G1848	G1650
	G3318	G3174	G3030	U2853	U2681	C2362	C1849	C1657
	A3319	A3174	A3033	U2853	A2682	U2170	A1850	G1658
	A3320	U3185	U3056	U2853	A2683	A2188	U1539	U1540
	A3335	U3196	U3057	U2854	G2689	A2188	U1540	G1541
	U3341	G3202	U3058	U2854	A2691	U2205	U1877	U1553
	A3342	U3207	U3059	U2854	U2692	A2373	U1877	U1554
	G3343	U3207	U3078	U2854	A2693	C2374	G1878	U1555
	A3344	A3210	U3079	U2855	A2694	G2375	A1879	C1556
	G3345	G3218	A3086	U2855	A2695	G2376	U1688	A1557
	U3346	C3217	U3086	U2855	A2696	C2383	U1688	U1688
	A3347	A3218	U3079	U2855	U2705	A2384	U1716	U1716
	G3350	G3219	A3086	U2855	G2714	G2385	U1717	C1562
	U3351	C3228	C3092	U2855	U2723	U2388	G1953	C1563
	U3352	G3229	A3113	U2855	G2728	C2391	U1724	U1564
	G3353	U3244	U3121	U2855	U2728	C2392	C1725	U1565
	U3354	A3245	U3121	U2855	C2737	C2393	U1740	A1566
	U3355	G3246	A3122	U2855	U2750	G2394	U1741	U1567
	A3362	G3247	A3130	U2855	G2761	A2397	G1743	U1569
	C3367	G3253	U3130	U2855	U2752	A2402	A1750	A1571
	G3368	G3254	U3131	U2855	G2753	G2403	G1751	U1572
	G3369	U3254	U2923	U2855	A2762	A2404	G1751	G1574
	A3375	U3259	U2923	U2855	A2762	C2405	A1760	A1575
	G3378	G3263	U2935	U2855	C2764	C2406	U1763	G1576
	U3382	U3269	A3142	U2855	C2772	U2411	U1764	G1577
			C3143	U2855	G2772	G2412	U	C1578
			A3150	U2855	G2777	G2414	G1766	A1580
				U2855			U	C1581
				U2855			U	C1582

• Molecule 1: 25S ribosomal RNA

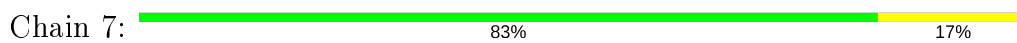




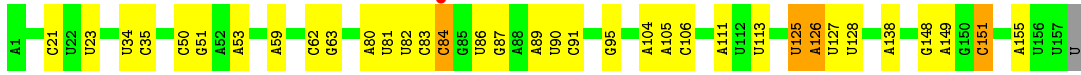
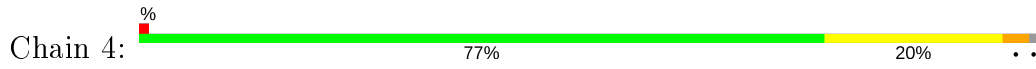
● Molecule 2: 5S ribosomal RNA



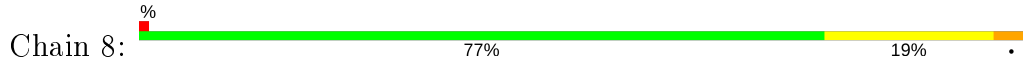
● Molecule 2: 5S ribosomal RNA



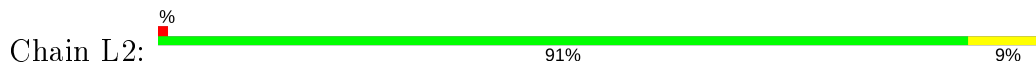
● Molecule 3: 5.8S ribosomal RNA



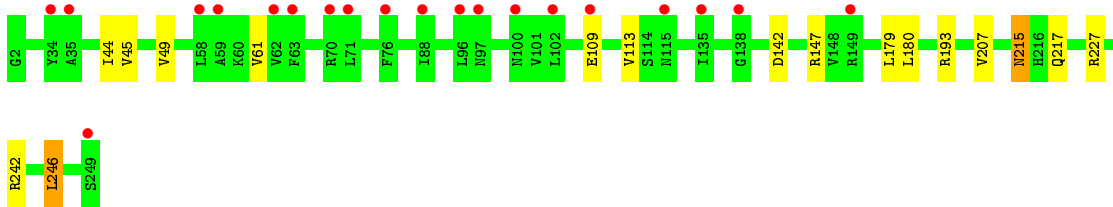
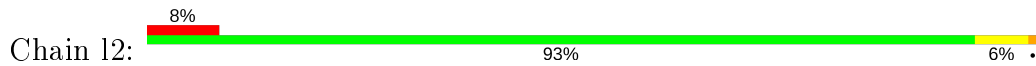
- Molecule 3: 5.8S ribosomal RNA



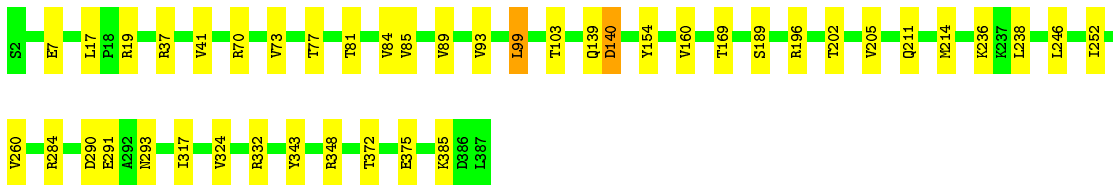
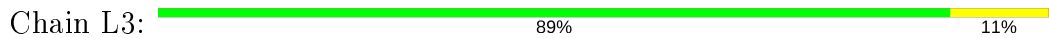
- Molecule 4: 60S ribosomal protein L2-A



- Molecule 4: 60S ribosomal protein L2-A



- Molecule 5: 60S ribosomal protein L3



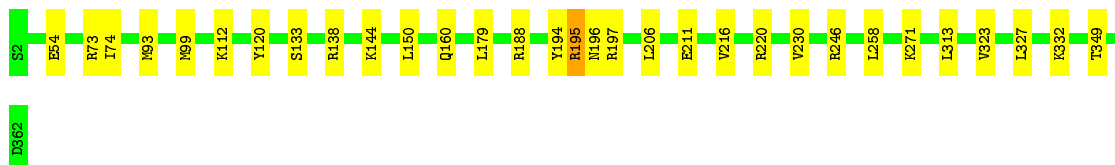
- Molecule 5: 60S ribosomal protein L3





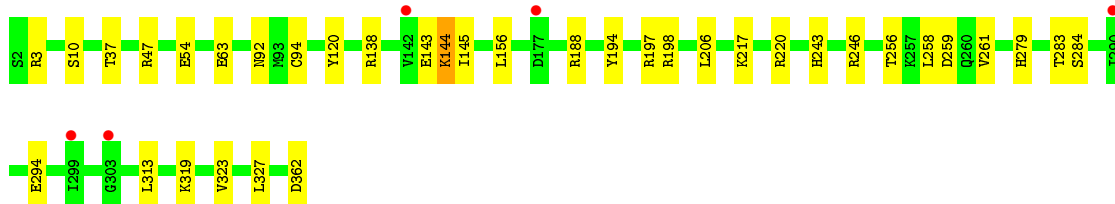
- Molecule 6: 60S ribosomal protein L4-A

Chain L4: 91% 8%



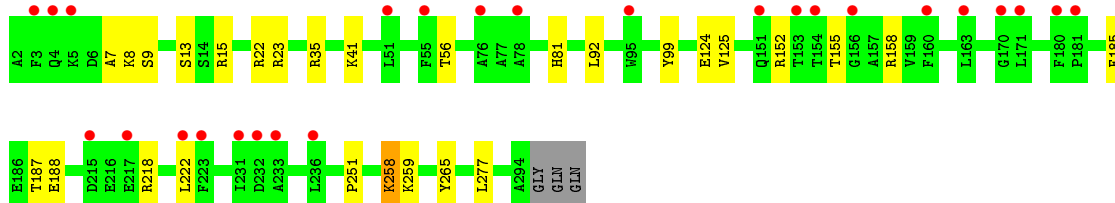
- Molecule 6: 60S ribosomal protein L4-A

Chain l4: 90% 10%



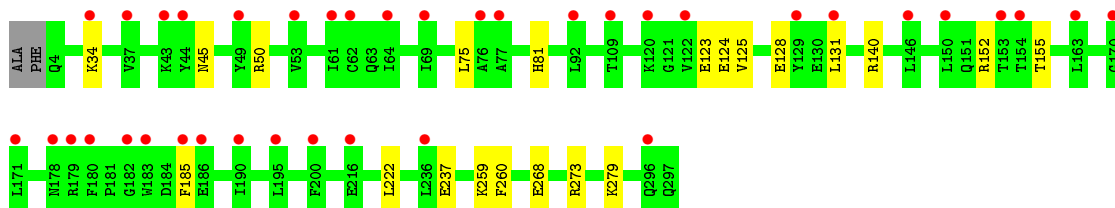
- Molecule 7: 60S ribosomal protein L5

Chain L5: 9% 90% 9%



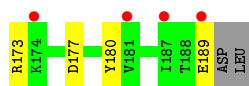
- Molecule 7: 60S ribosomal protein L5

Chain l5: 13% 92% 7%

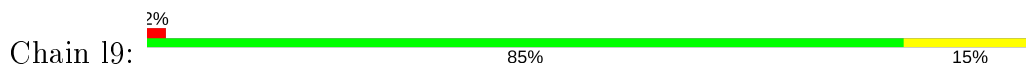


- Molecule 8: 60S ribosomal protein L6-A

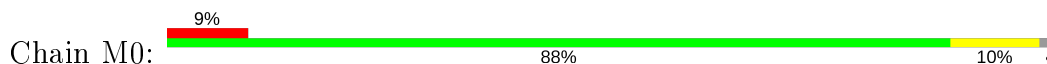
Chain L6: 79% 9% 11%



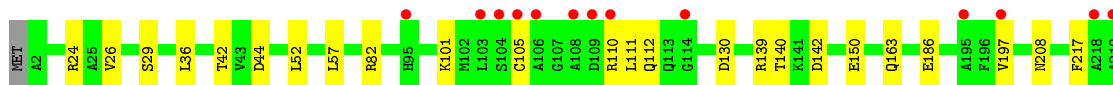
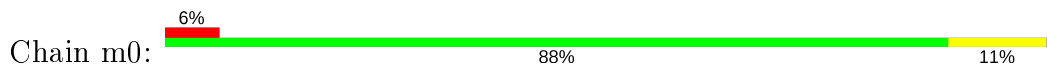
- Molecule 11: 60S ribosomal protein L9-A



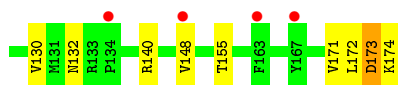
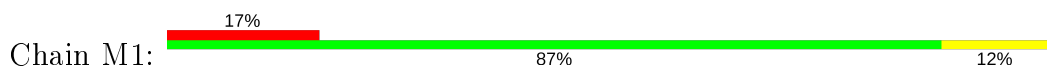
- Molecule 12: 60S ribosomal protein L10



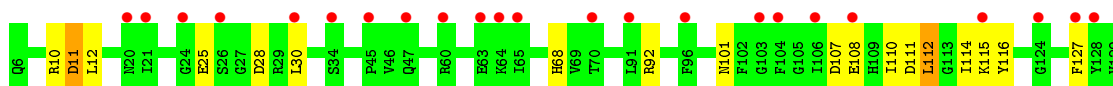
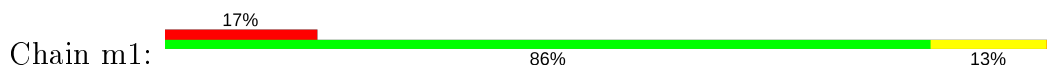
- Molecule 12: 60S ribosomal protein L10



- Molecule 13: 60S ribosomal protein L11-B



- Molecule 13: 60S ribosomal protein L11-B

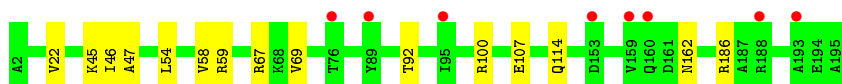




- Molecule 14: 60S ribosomal protein L13-A



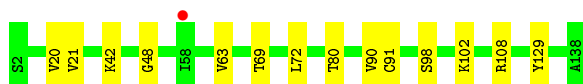
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 15: 60S ribosomal protein L14-A



- Molecule 15: 60S ribosomal protein L14-A



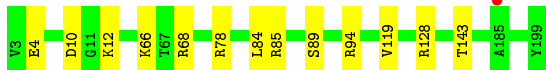
- Molecule 16: 60S ribosomal protein L15-A



- Molecule 16: 60S ribosomal protein L15-A



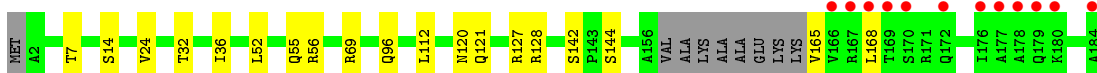
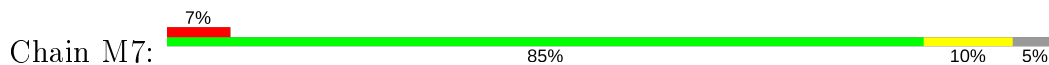
- Molecule 17: 60S ribosomal protein L16-A



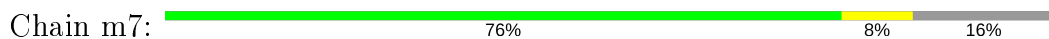
- Molecule 17: 60S ribosomal protein L16-A



- Molecule 18: 60S ribosomal protein L17-A



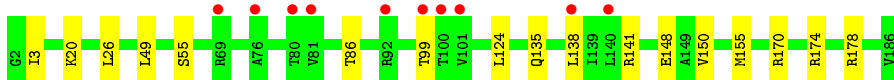
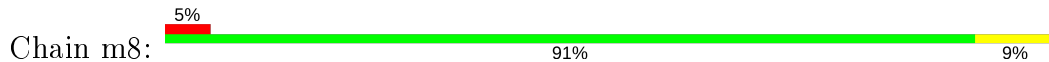
- Molecule 18: 60S ribosomal protein L17-A



- Molecule 19: 60S ribosomal protein L18-A



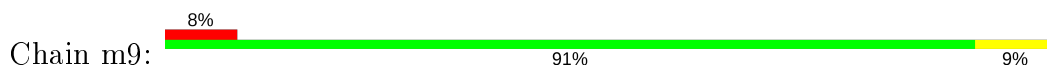
- Molecule 19: 60S ribosomal protein L18-A



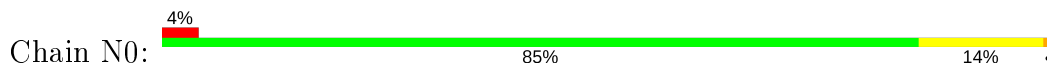
- Molecule 20: 60S ribosomal protein L19-A



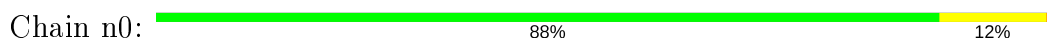
- Molecule 20: 60S ribosomal protein L19-A



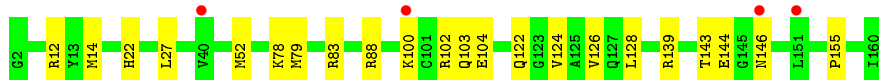
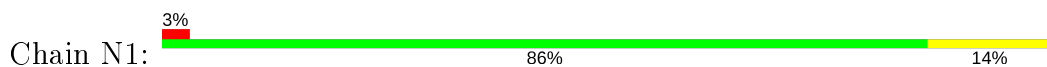
- Molecule 21: 60S ribosomal protein L20-A



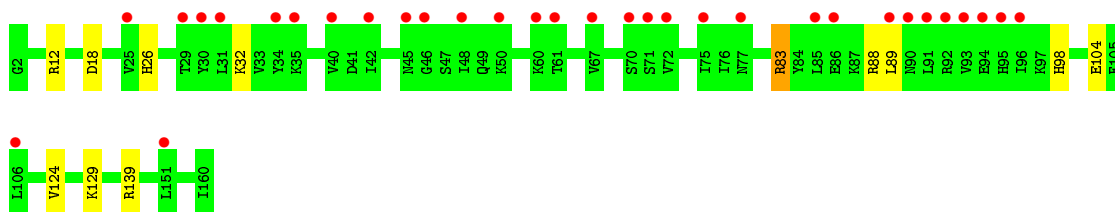
- Molecule 21: 60S ribosomal protein L20-A



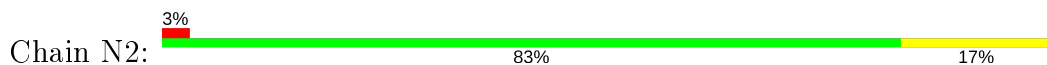
- Molecule 22: 60S ribosomal protein L21-A



- Molecule 22: 60S ribosomal protein L21-A

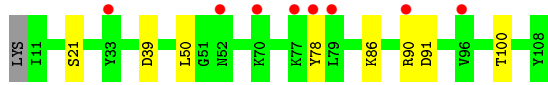


- Molecule 23: 60S ribosomal protein L22-A

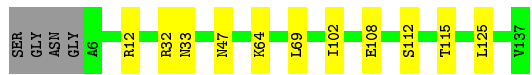
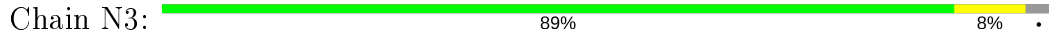


- Molecule 23: 60S ribosomal protein L22-A

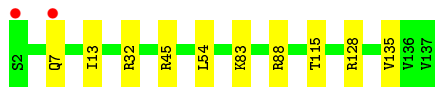




● Molecule 24: 60S ribosomal protein L23-A



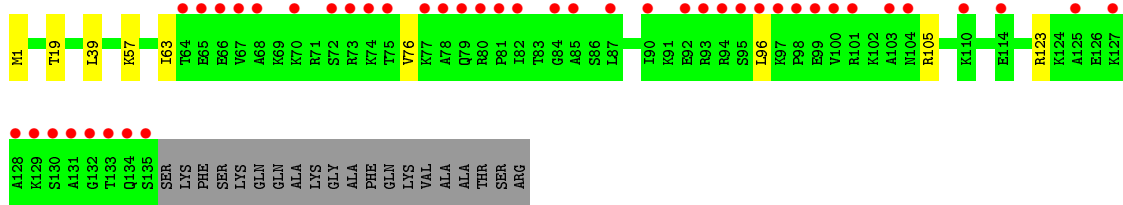
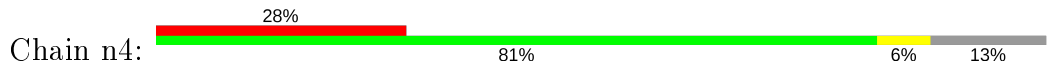
● Molecule 24: 60S ribosomal protein L23-A



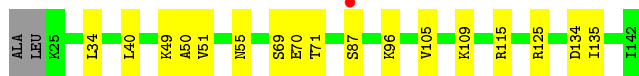
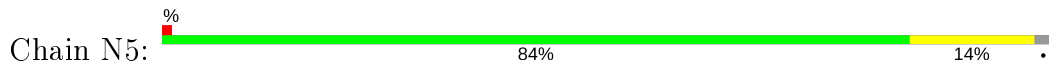
● Molecule 25: 60S ribosomal protein L24-A



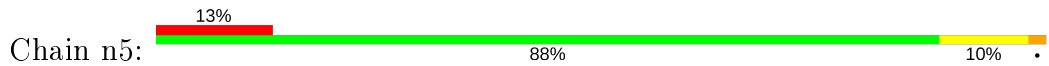
● Molecule 25: 60S ribosomal protein L24-A

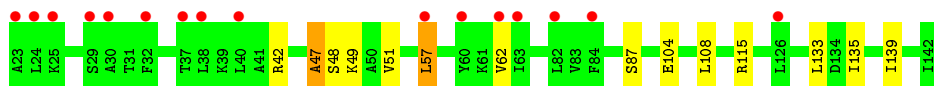


● Molecule 26: 60S ribosomal protein L25

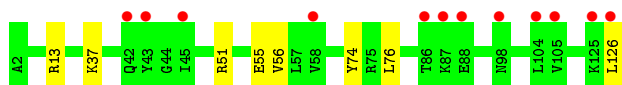


● Molecule 26: 60S ribosomal protein L25

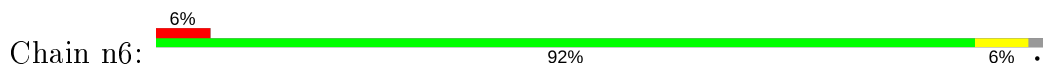




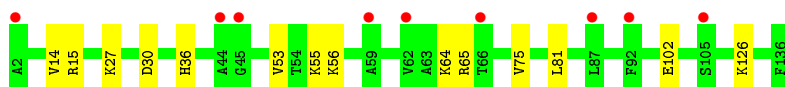
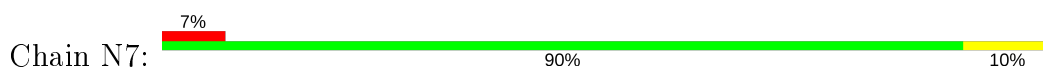
- Molecule 27: 60S ribosomal protein L26-A



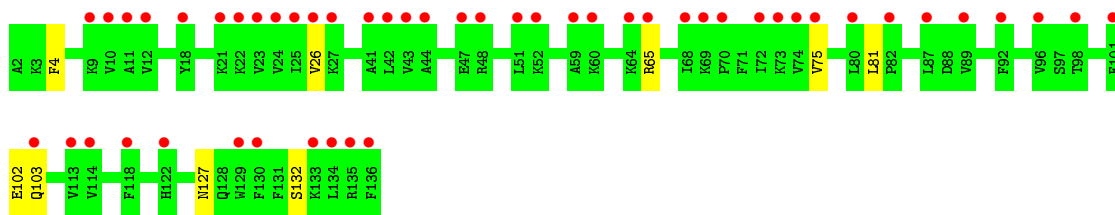
- Molecule 27: 60S ribosomal protein L26-A



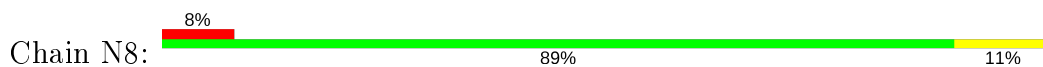
- Molecule 28: 60S ribosomal protein L27-A



- Molecule 28: 60S ribosomal protein L27-A

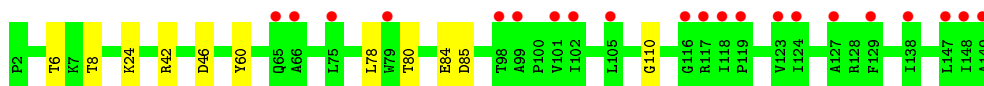


- Molecule 29: 60S ribosomal protein L28

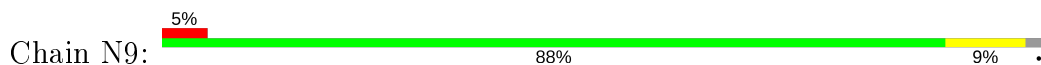


- Molecule 29: 60S ribosomal protein L28





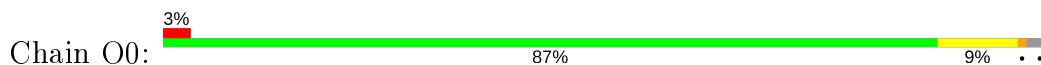
- Molecule 30: 60S ribosomal protein L29



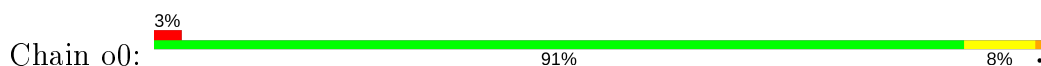
- Molecule 30: 60S ribosomal protein L29



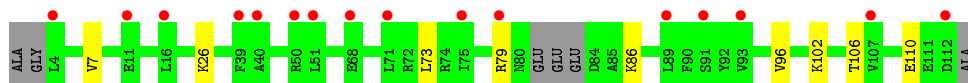
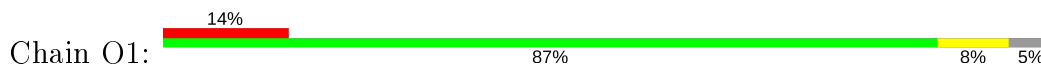
- Molecule 31: 60S ribosomal protein L30



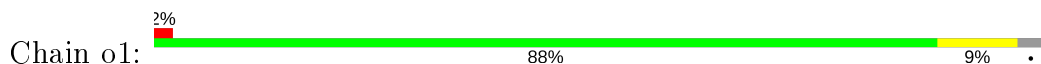
- Molecule 31: 60S ribosomal protein L30



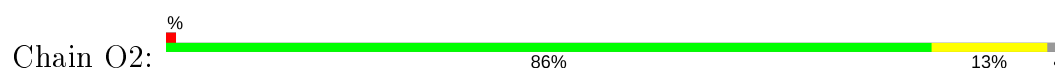
- Molecule 32: 60S ribosomal protein L31-A



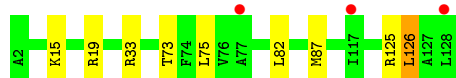
- Molecule 32: 60S ribosomal protein L31-A



- Molecule 33: 60S ribosomal protein L32



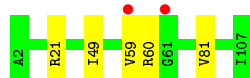
- Molecule 33: 60S ribosomal protein L32



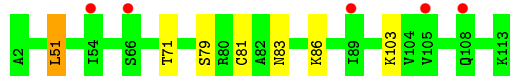
- Molecule 34: 60S ribosomal protein L33-A



- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-A



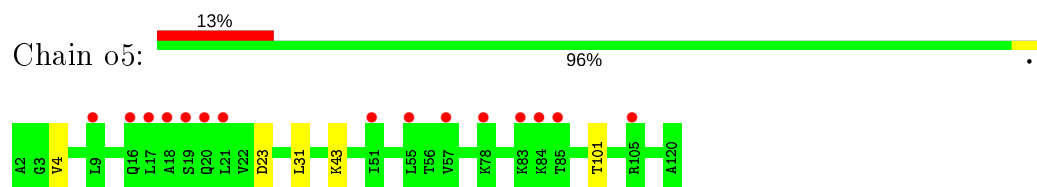
- Molecule 35: 60S ribosomal protein L34-A



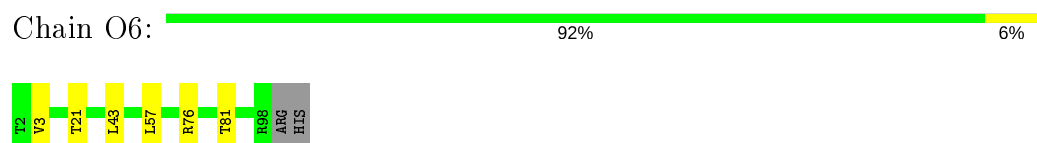
- Molecule 36: 60S ribosomal protein L35-A



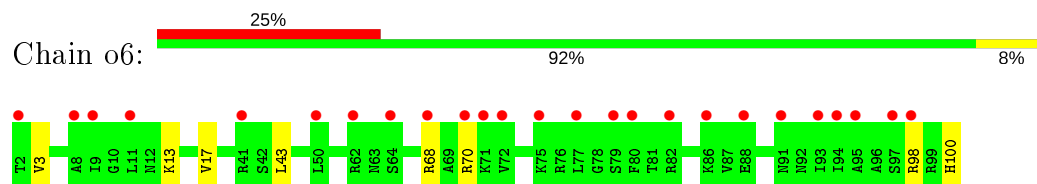
- Molecule 36: 60S ribosomal protein L35-A



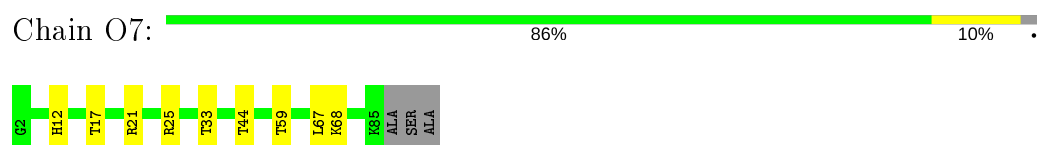
- Molecule 37: 60S ribosomal protein L36-A



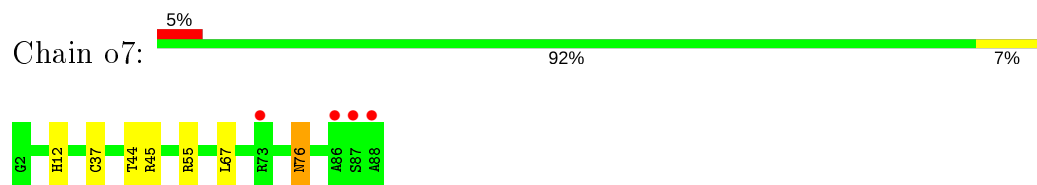
- Molecule 37: 60S ribosomal protein L36-A



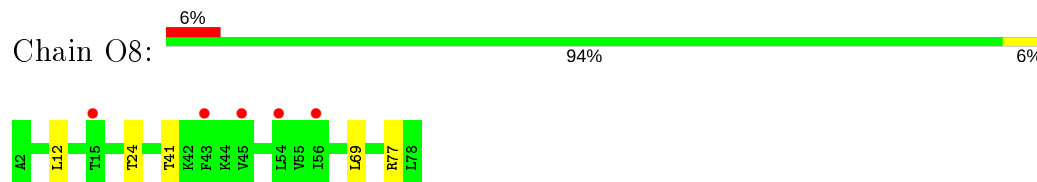
- Molecule 38: 60S ribosomal protein L37-A



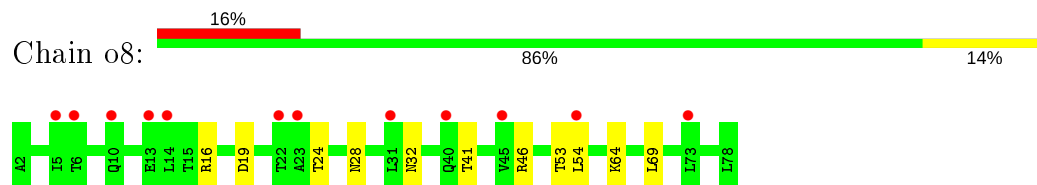
- Molecule 38: 60S ribosomal protein L37-A




- Molecule 39: 60S ribosomal protein L38



- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39

Chain O9:  88% 12%



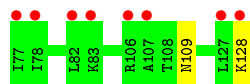
- Molecule 40: 60S ribosomal protein L39

Chain o9:  4% 96%




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Q0:  15% 96%




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain q0:  4% 87% 13%




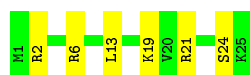
- Molecule 42: 60S ribosomal protein L41-B

Chain Q1:  84% 16%




- Molecule 42: 60S ribosomal protein L41-B

Chain q1:  76% 24%

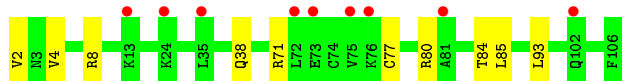
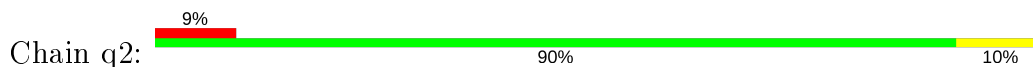


- Molecule 43: 60S ribosomal protein L42-A

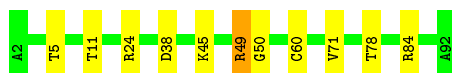
Chain Q2:  16% 89% 11%



• Molecule 43: 60S ribosomal protein L42-A



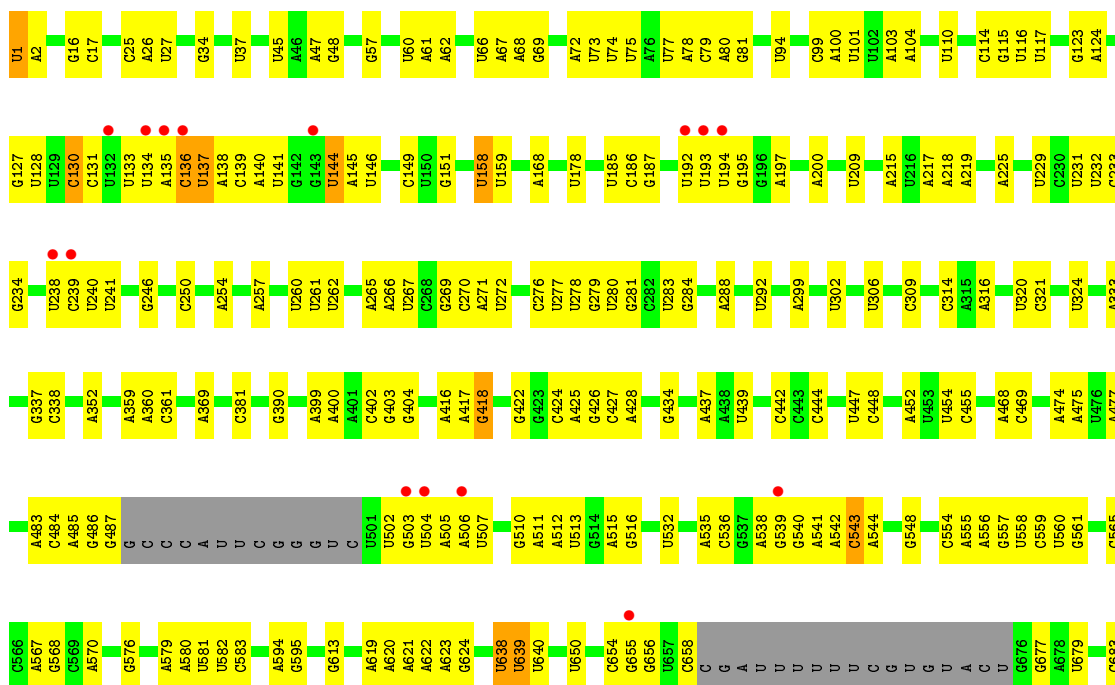
• Molecule 44: 60S ribosomal protein L43-A



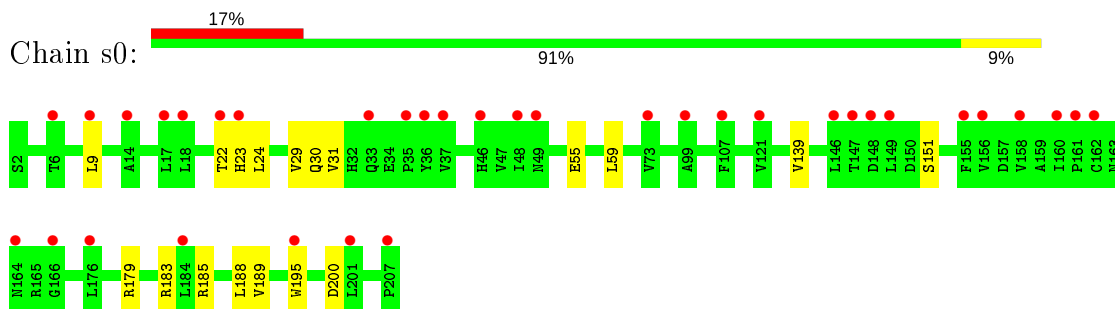
• Molecule 44: 60S ribosomal protein L43-A



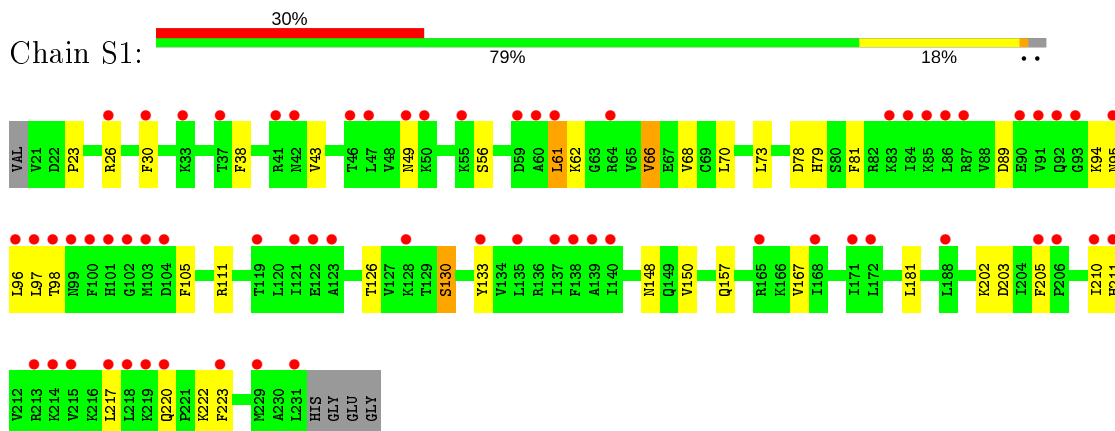
• Molecule 45: 18S ribosomal RNA



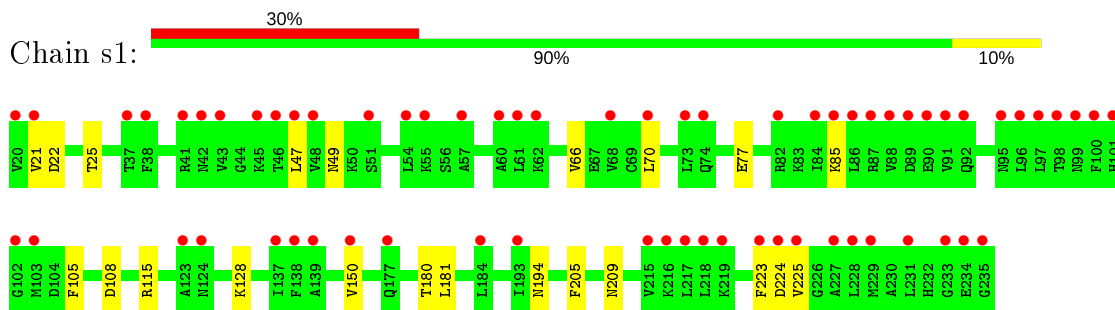
- Molecule 46: 40S ribosomal protein S0-A



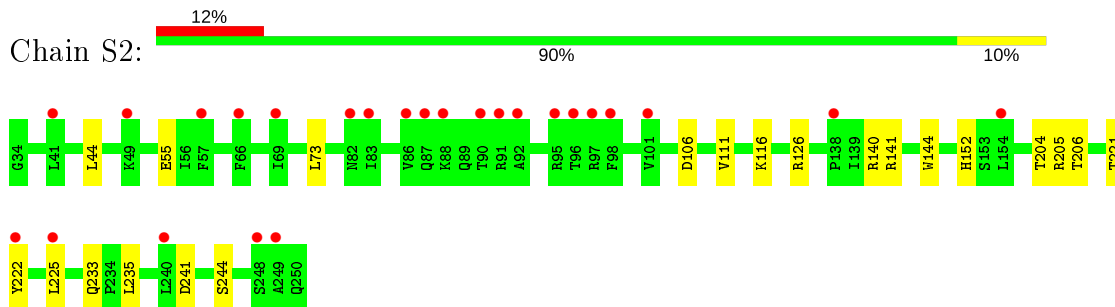
- Molecule 47: 40S ribosomal protein S1-A



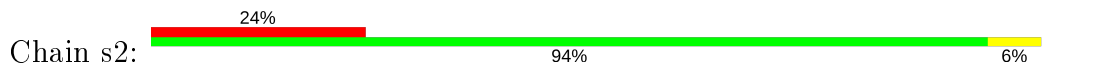
- Molecule 47: 40S ribosomal protein S1-A

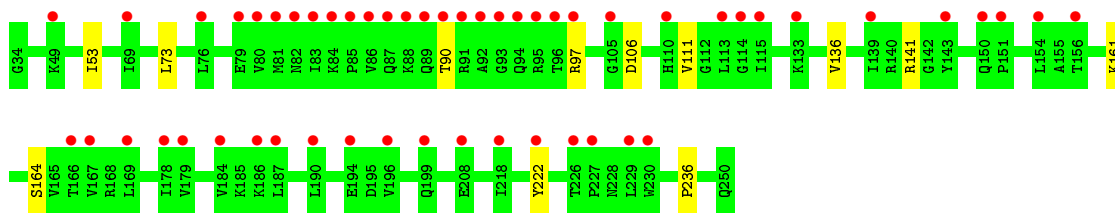


- Molecule 48: 40S ribosomal protein S2

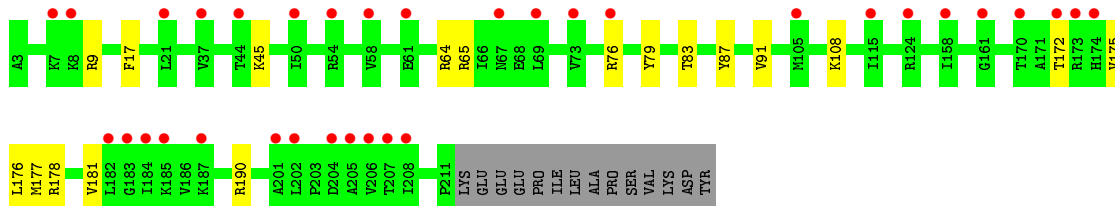
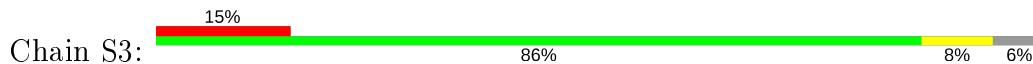


- Molecule 48: 40S ribosomal protein S2

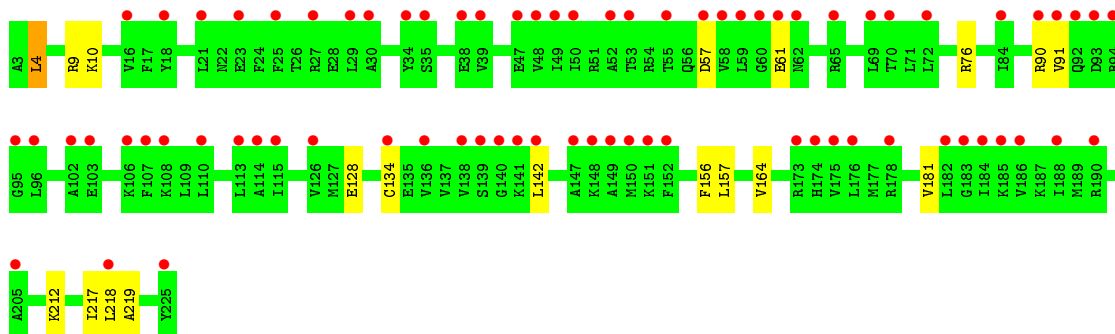
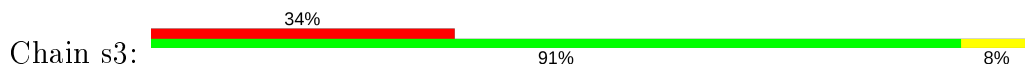




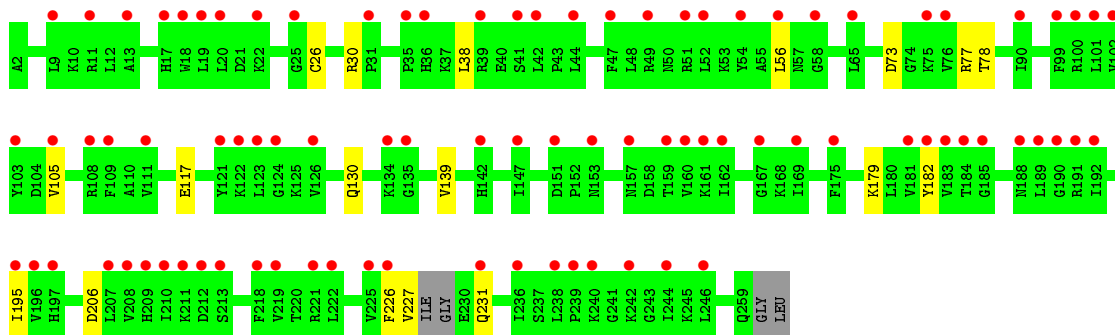
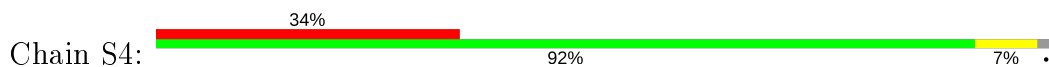
• Molecule 49: 40S ribosomal protein S3



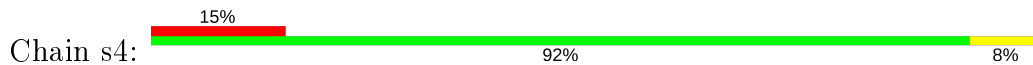
• Molecule 49: 40S ribosomal protein S3

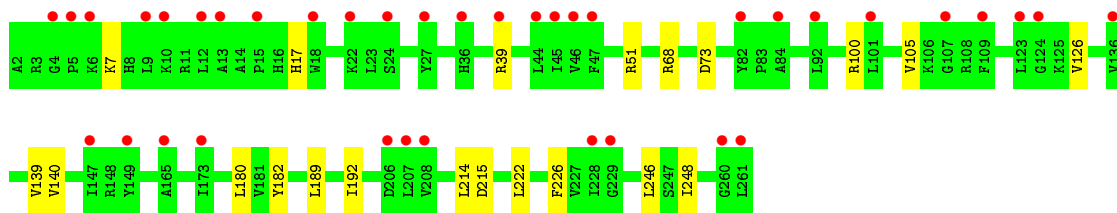


• Molecule 50: 40S ribosomal protein S4-A

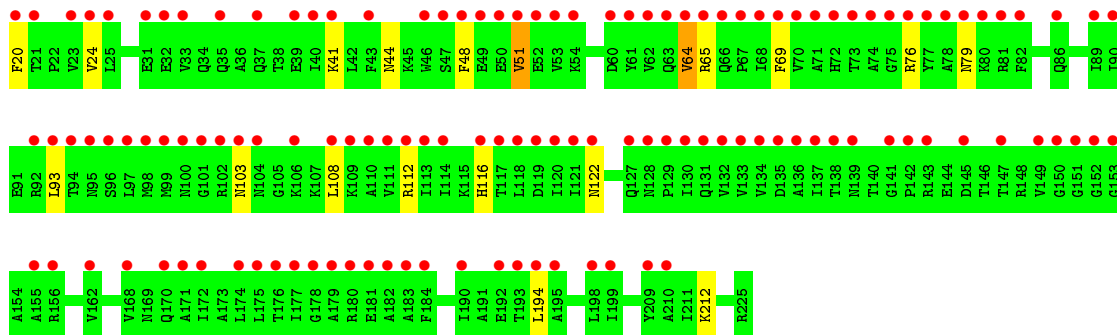


• Molecule 50: 40S ribosomal protein S4-A

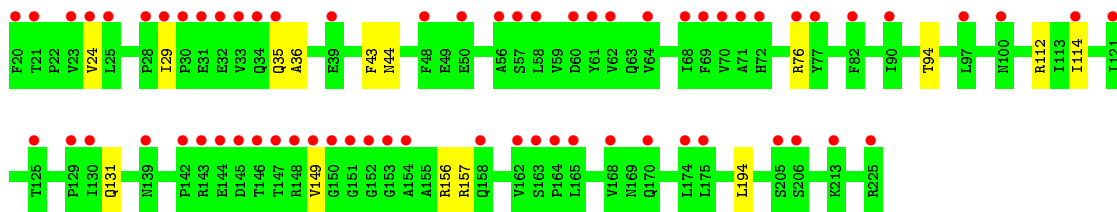
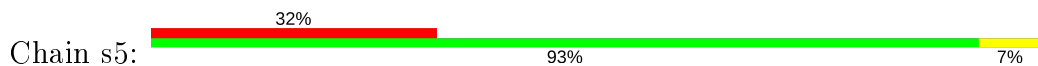




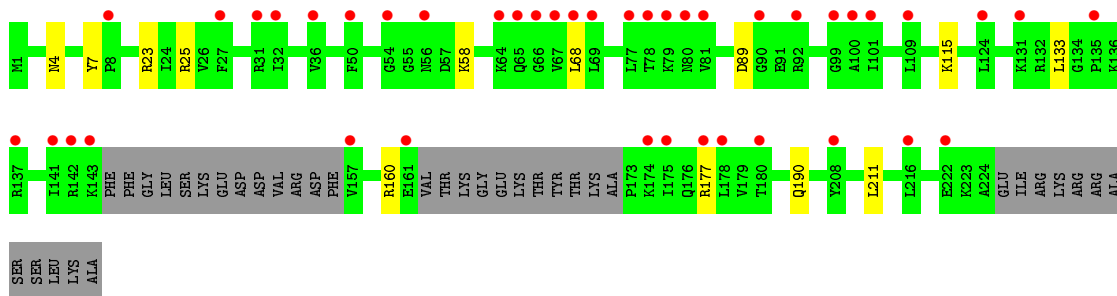
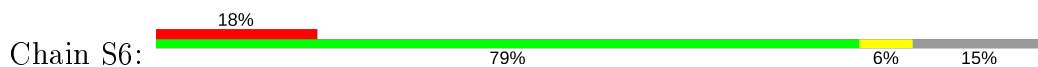
• Molecule 51: 40S ribosomal protein S5



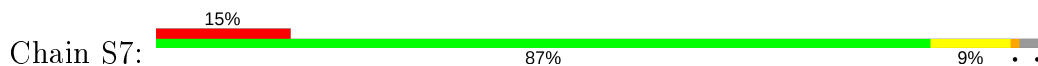
• Molecule 51: 40S ribosomal protein S5

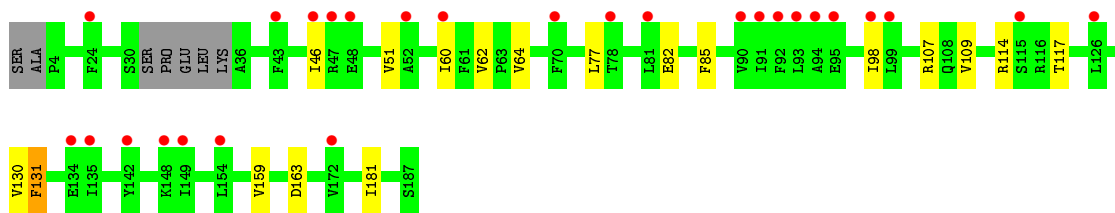


• Molecule 52: 40S ribosomal protein S6-A

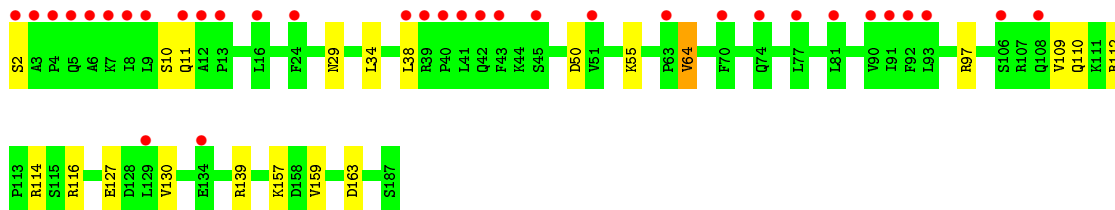
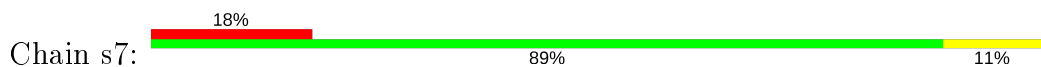


• Molecule 53: 40S ribosomal protein S7-A

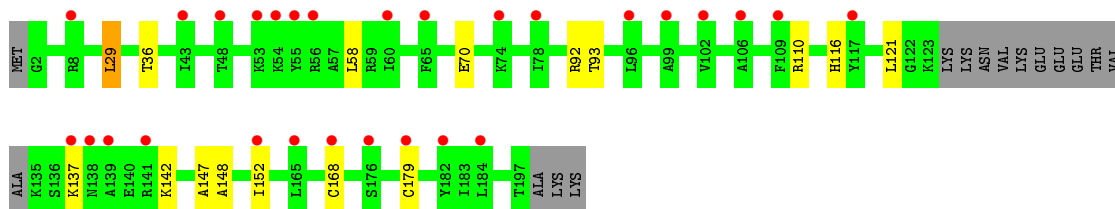
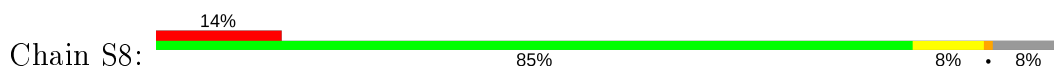




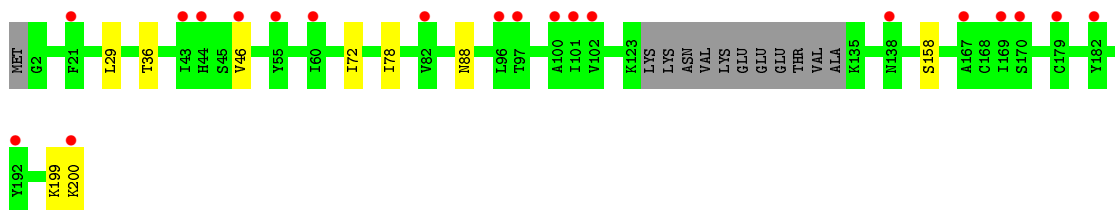
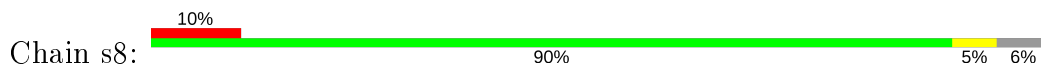
• Molecule 53: 40S ribosomal protein S7-A



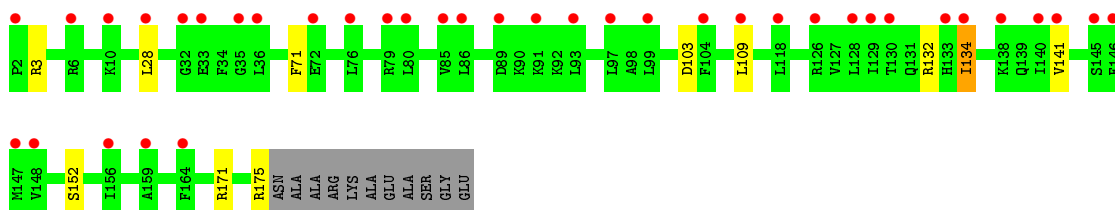
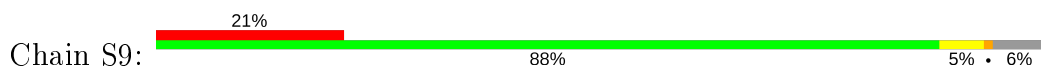
• Molecule 54: 40S ribosomal protein S8-A

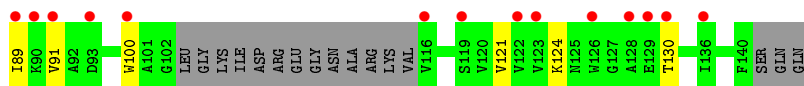


• Molecule 54: 40S ribosomal protein S8-A

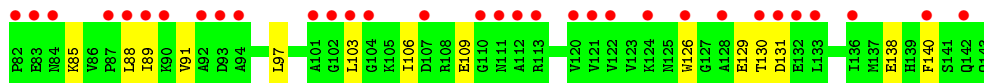
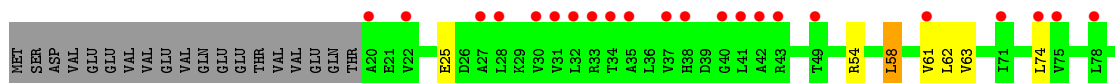
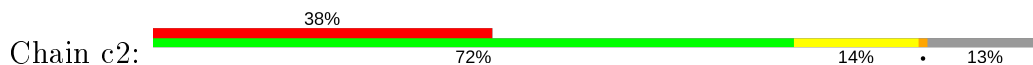


• Molecule 55: 40S ribosomal protein S9-A

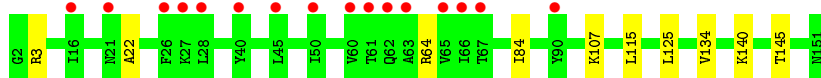




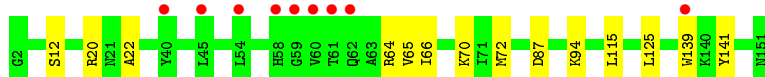
- Molecule 58: 40S ribosomal protein S12



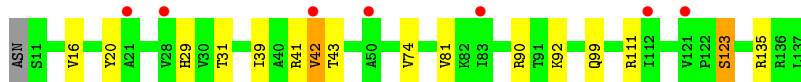
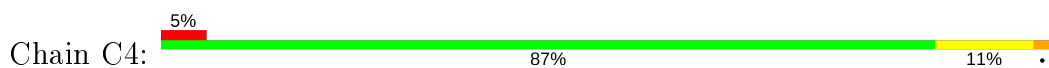
- Molecule 59: 40S ribosomal protein S13



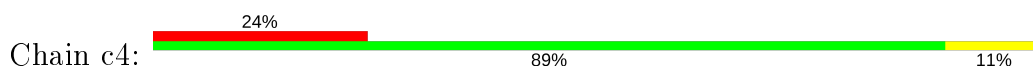
- Molecule 59: 40S ribosomal protein S13



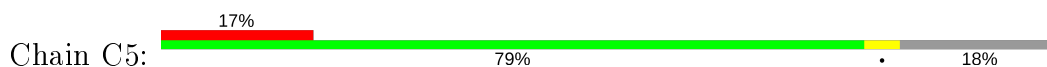
- Molecule 60: 40S ribosomal protein S14-B

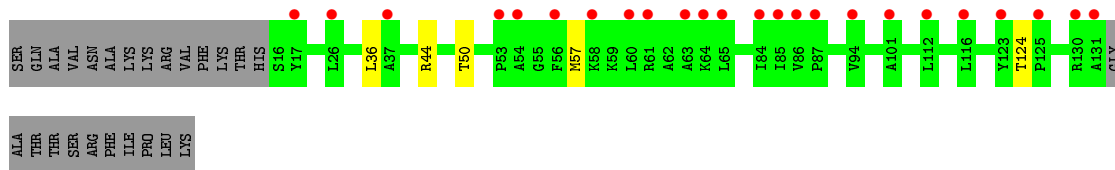


- Molecule 60: 40S ribosomal protein S14-B

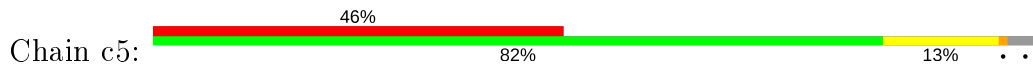


- Molecule 61: 40S ribosomal protein S15

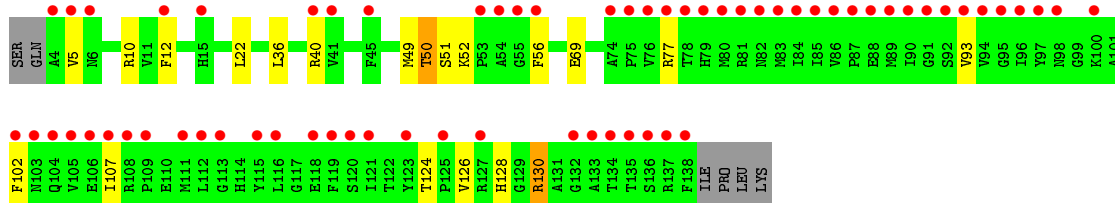




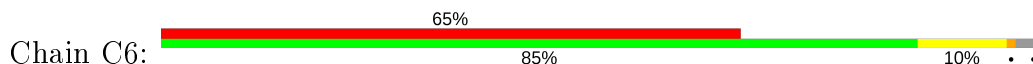
• Molecule 61: 40S ribosomal protein S15



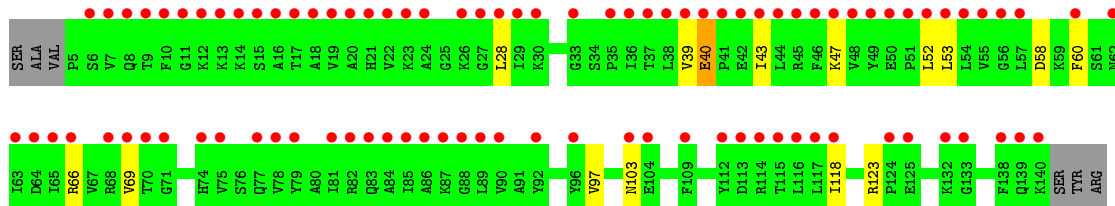
Chain c5:



• Molecule 62: 40S ribosomal protein S16-A



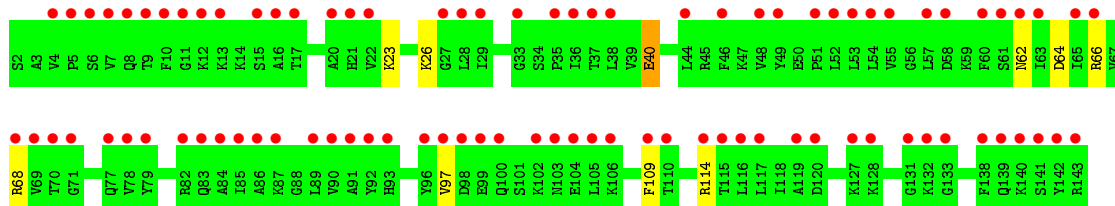
Chain C6:



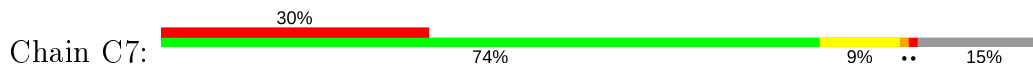
• Molecule 62: 40S ribosomal protein S16-A



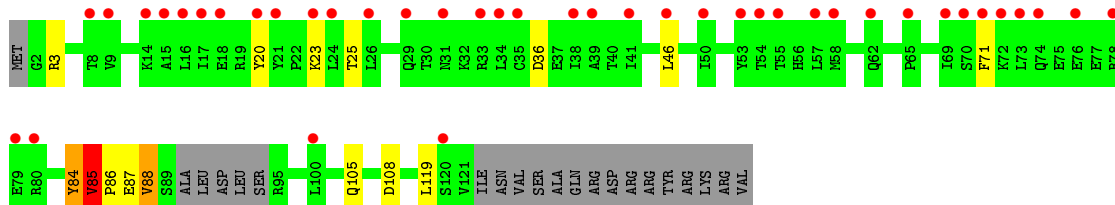
Chain c6:



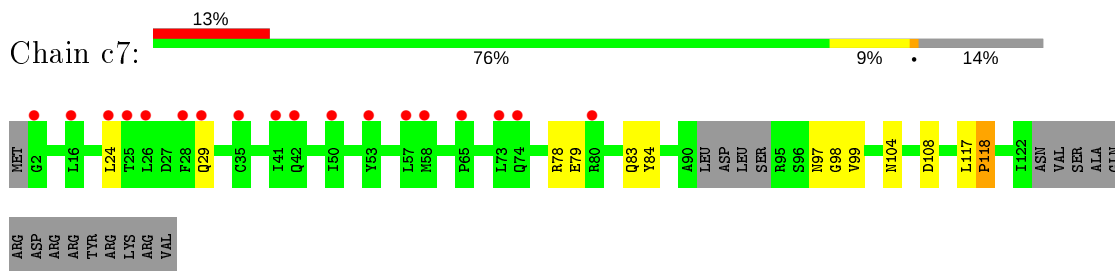
• Molecule 63: 40S ribosomal protein S17-A



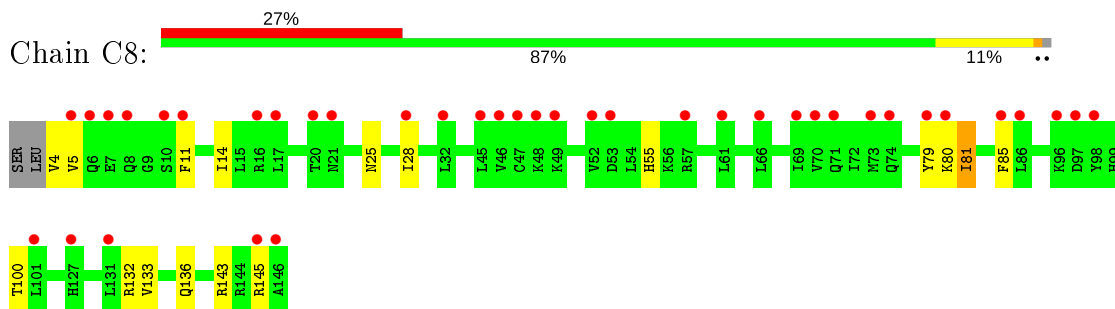
Chain C7:



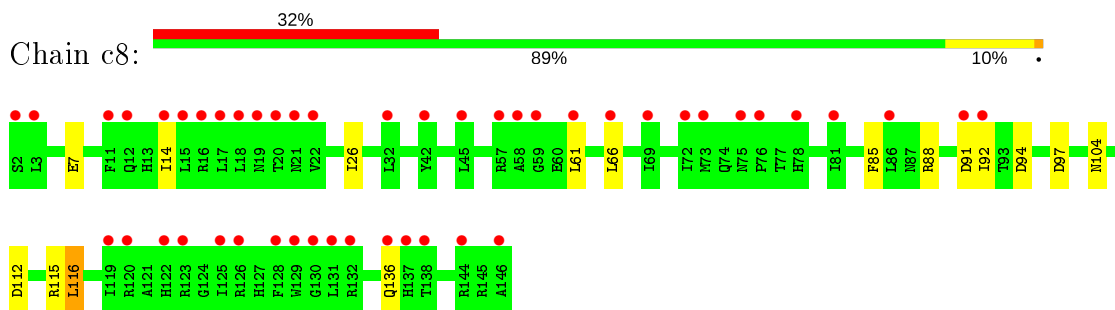
- Molecule 63: 40S ribosomal protein S17-A



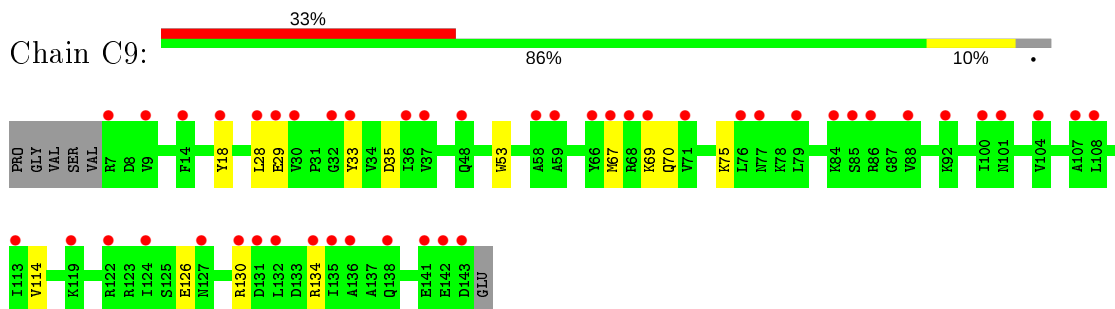
- Molecule 64: 40S ribosomal protein S18-A



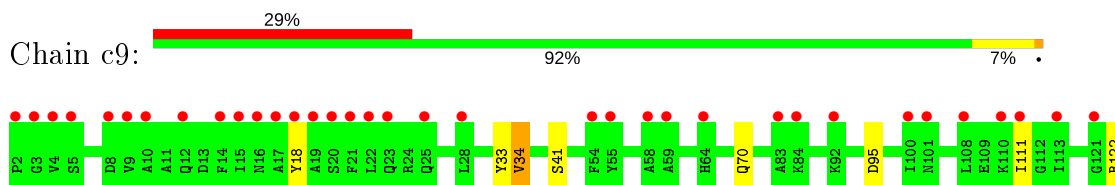
- Molecule 64: 40S ribosomal protein S18-A



- Molecule 65: 40S ribosomal protein S19-A

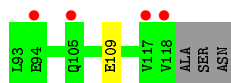
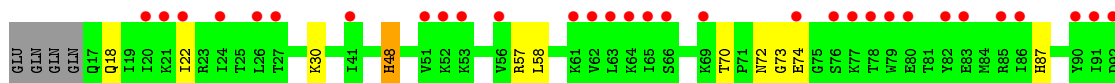
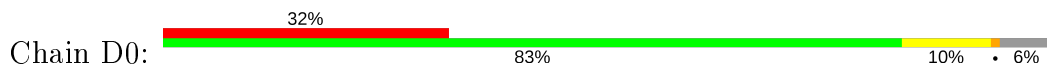


- Molecule 65: 40S ribosomal protein S19-A

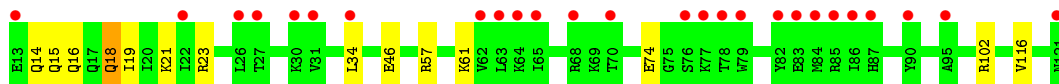
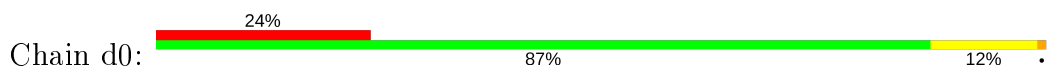




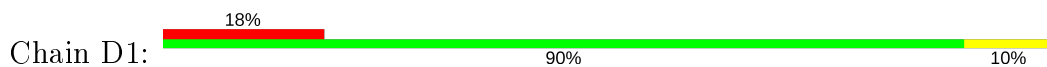
- Molecule 66: 40S ribosomal protein S20



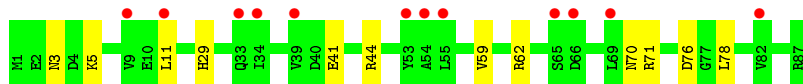
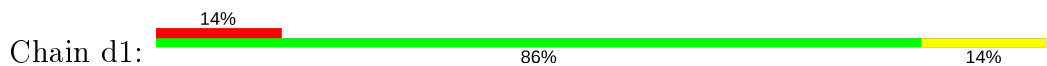
- Molecule 66: 40S ribosomal protein S20



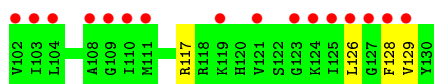
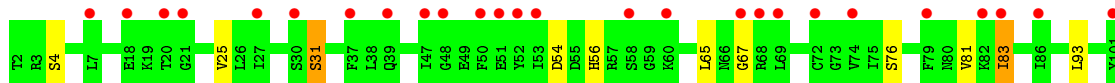
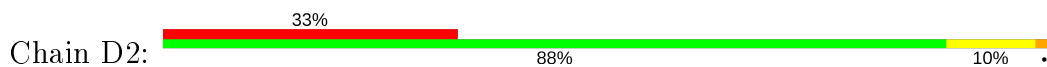
- Molecule 67: 40S ribosomal protein S21-A



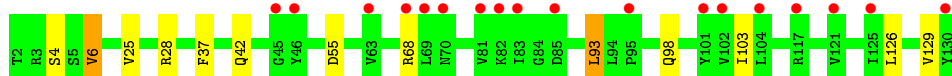
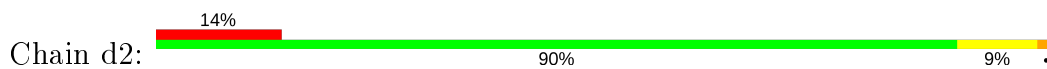
- Molecule 67: 40S ribosomal protein S21-A



- Molecule 68: 40S ribosomal protein S22-A



- Molecule 68: 40S ribosomal protein S22-A



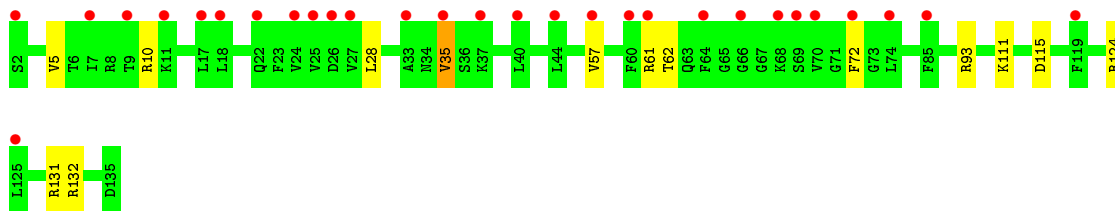
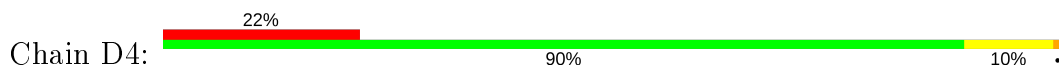
- Molecule 69: 40S ribosomal protein S23-A



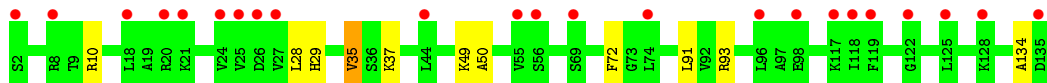
- Molecule 69: 40S ribosomal protein S23-A



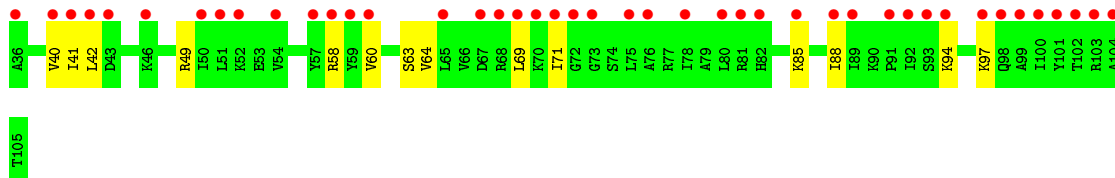
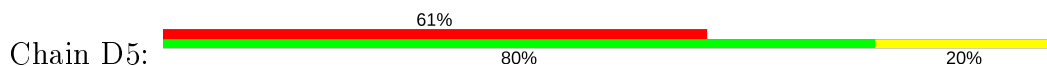
- Molecule 70: 40S ribosomal protein S24-A



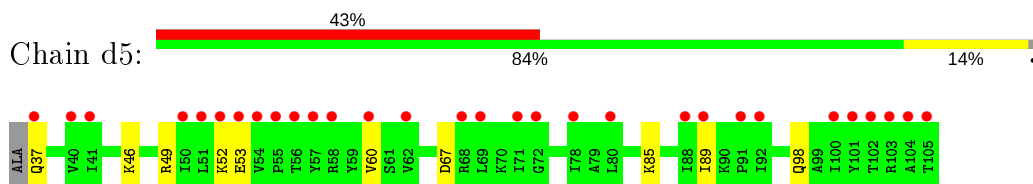
- Molecule 70: 40S ribosomal protein S24-A



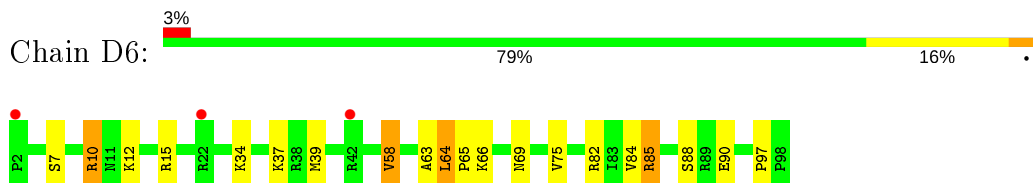
- Molecule 71: 40S ribosomal protein S25-A



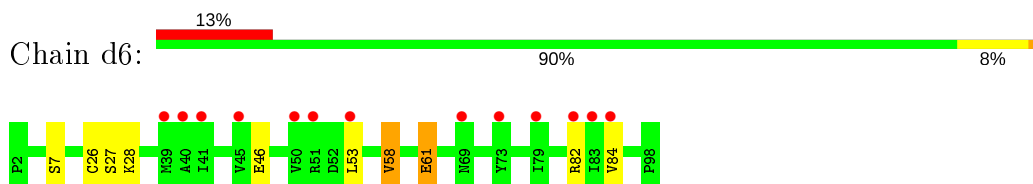
- Molecule 71: 40S ribosomal protein S25-A



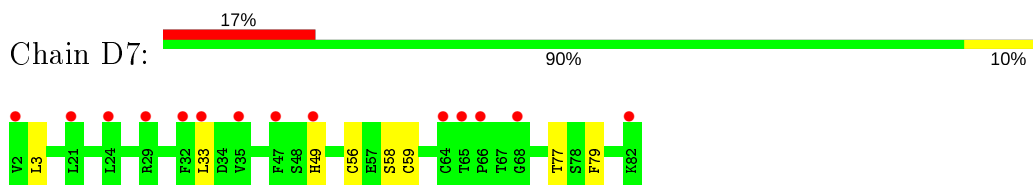
- Molecule 72: 40S ribosomal protein S26-B



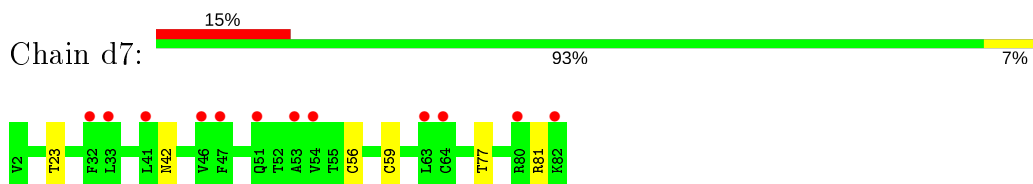
- Molecule 72: 40S ribosomal protein S26-B



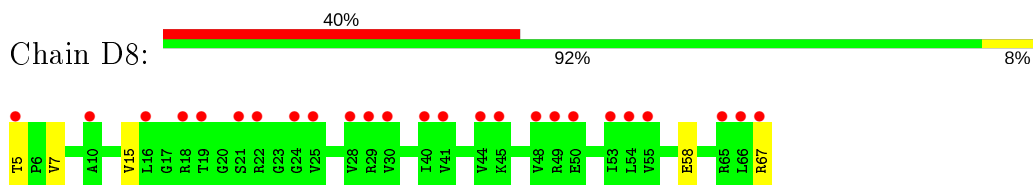
- Molecule 73: 40S ribosomal protein S27-A



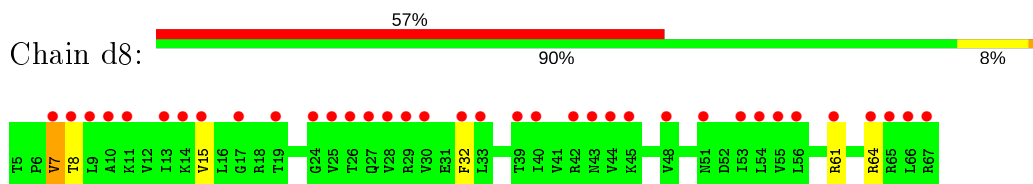
- Molecule 73: 40S ribosomal protein S27-A



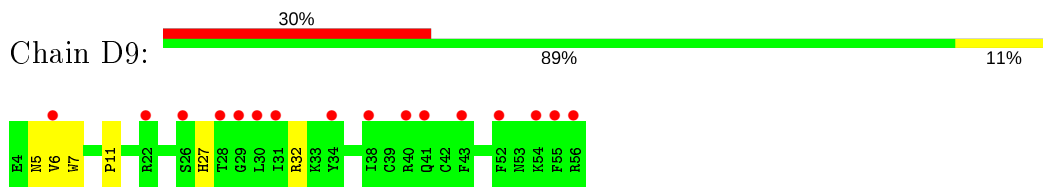
- Molecule 74: 40S ribosomal protein S28-A



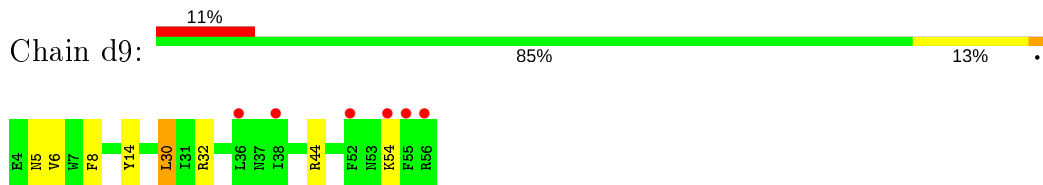
- Molecule 74: 40S ribosomal protein S28-A



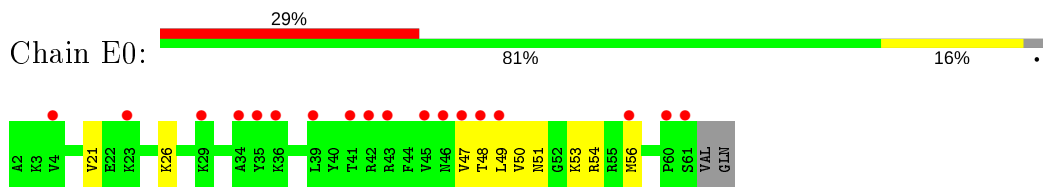
• Molecule 75: 40S ribosomal protein S29-A



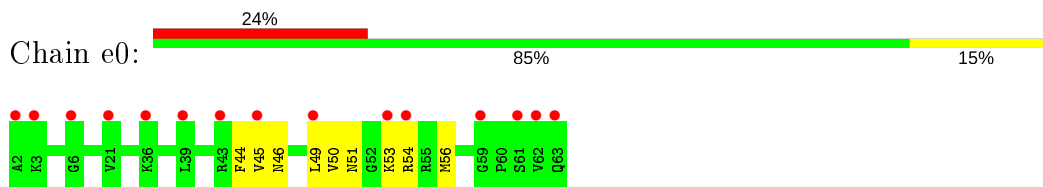
• Molecule 75: 40S ribosomal protein S29-A



• Molecule 76: 40S ribosomal protein S30-A



• Molecule 76: 40S ribosomal protein S30-A

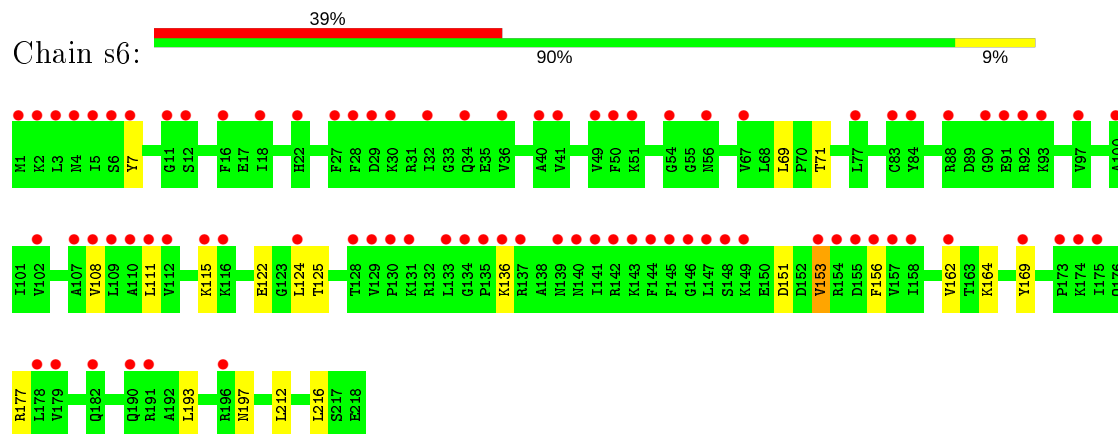


• Molecule 77: Guanine nucleotide-binding protein subunit beta-like protein



ARG ARG ARG GLY GLY ARG ARG ALA ARG LYS GLY ASN ASN THR THR SER ALA ASN VAL VAL SER ASN LEU PRO SER LEU ALA

• Molecule 79: 40S ribosomal protein S6-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	434.53Å 293.33Å 295.79Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	146.66 – 3.30 146.66 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (146.66-3.30) 91.8 (146.66-3.30)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 3.33Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.203 , 0.250 0.203 , 0.250	Depositor DCC
R_{free} test set	21969 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtrriage
Anisotropy	0.209	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.3	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	0.92	EDS
Total number of atoms	397978	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.67	4/73685 (0.0%)	1.11	189/114868 (0.2%)
1	5	0.55	2/73908 (0.0%)	1.02	101/115221 (0.1%)
2	3	0.51	0/2883	0.98	2/4491 (0.0%)
2	7	0.43	0/2883	0.89	0/4491
3	4	0.69	0/3724	1.14	14/5798 (0.2%)
3	8	0.51	0/3746	1.07	21/5832 (0.4%)
4	L2	0.46	0/1918	0.67	2/2577 (0.1%)
4	l2	0.35	0/1918	0.60	1/2577 (0.0%)
5	L3	0.42	0/3152	0.61	1/4239 (0.0%)
5	l3	0.43	1/3152 (0.0%)	0.59	0/4239
6	L4	0.45	0/2801	0.62	0/3792
6	l4	0.38	0/2801	0.59	0/3792
7	L5	0.35	0/2403	0.54	0/3242
7	l5	0.32	0/2408	0.50	0/3248
8	L6	0.38	0/1260	0.55	0/1694
8	l6	0.38	0/1269	0.56	0/1705
9	L7	0.40	0/1855	0.56	0/2496
9	l7	0.36	0/1828	0.57	0/2461
10	L8	0.40	0/1825	0.56	0/2466
10	l8	0.32	0/1795	0.55	1/2429 (0.0%)
11	L9	0.40	0/1523	0.60	0/2051
11	l9	0.38	0/1539	0.56	0/2073
12	M0	0.43	0/1796	0.61	0/2409
12	m0	0.40	0/1810	0.59	1/2428 (0.0%)
13	M1	0.34	0/1374	0.61	0/1842
13	m1	0.30	0/1374	0.53	1/1842 (0.1%)
14	M3	0.41	0/1568	0.59	1/2106 (0.0%)
14	m3	0.37	0/1573	0.58	0/2113
15	M4	0.36	0/1068	0.55	0/1438
15	m4	0.35	0/1074	0.55	0/1446
16	M5	0.45	0/1757	0.60	0/2354
16	m5	0.33	0/1757	0.53	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	M6	0.45	0/1585	0.56	0/2128
17	m6	0.46	0/1585	0.60	0/2128
18	M7	0.44	0/1400	0.62	0/1882
18	m7	0.42	0/1250	0.60	0/1683
19	M8	0.43	0/1465	0.61	0/1965
19	m8	0.34	0/1465	0.57	0/1965
20	M9	0.38	0/1516	0.56	2/2020 (0.1%)
20	m9	0.34	0/1538	0.49	0/2050
21	N0	0.41	0/1481	0.59	0/1990
21	n0	0.38	0/1481	0.53	0/1990
22	N1	0.41	0/1300	0.58	0/1743
22	n1	0.35	0/1300	0.54	0/1743
23	N2	0.35	0/803	0.61	0/1087
23	n2	0.32	0/794	0.55	0/1076
24	N3	0.45	0/996	0.62	0/1340
24	n3	0.43	0/1018	0.59	0/1369
25	N4	0.40	0/533	0.53	0/707
25	n4	0.33	0/1052	0.53	0/1398
26	N5	0.44	0/961	0.61	1/1296 (0.1%)
26	n5	0.34	0/974	0.59	1/1314 (0.1%)
27	N6	0.43	0/995	0.62	0/1329
27	n6	0.38	0/978	0.58	0/1307
28	N7	0.51	2/1118 (0.2%)	0.58	0/1497
28	n7	0.33	0/1118	0.52	0/1497
29	N8	0.40	0/1204	0.66	0/1612
29	n8	0.33	0/1204	0.59	0/1612
30	N9	0.40	0/455	0.54	0/607
30	n9	0.34	0/473	0.55	0/629
31	O0	0.38	0/751	0.54	0/1008
31	o0	0.31	0/775	0.54	0/1040
32	O1	0.39	0/862	0.56	0/1157
32	o1	0.42	0/897	0.57	0/1205
33	O2	0.45	0/1028	0.59	0/1376
33	o2	0.41	0/1041	0.66	1/1394 (0.1%)
34	O3	0.46	0/868	0.65	1/1168 (0.1%)
34	o3	0.41	0/868	0.56	0/1168
35	O4	0.41	0/891	0.63	1/1191 (0.1%)
35	o4	0.34	0/891	0.55	0/1191
36	O5	0.45	0/978	0.62	1/1301 (0.1%)
36	o5	0.32	0/974	0.51	0/1297
37	O6	0.41	0/756	0.58	0/1005
37	o6	0.31	0/778	0.51	0/1034
38	O7	0.51	0/680	0.70	0/901

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	o7	0.40	0/696	0.64	0/923
39	O8	0.36	0/618	0.54	0/826
39	o8	0.32	0/614	0.62	0/822
40	O9	0.49	0/443	0.67	0/588
40	o9	0.40	0/443	0.54	0/588
41	Q0	0.44	0/423	0.62	0/562
41	q0	0.46	0/423	0.63	0/562
42	Q1	0.36	0/234	0.45	0/300
42	q1	0.35	0/234	0.52	0/300
43	Q2	0.43	0/860	0.62	0/1136
43	q2	0.35	0/860	0.55	0/1136
44	Q3	0.48	0/701	0.70	2/934 (0.2%)
44	q3	0.35	0/701	0.58	0/934
45	2	0.42	0/40808	0.94	54/63582 (0.1%)
45	6	0.39	0/40116	0.91	42/62502 (0.1%)
46	S0	0.30	0/1621	0.54	1/2220 (0.0%)
46	s0	0.31	0/1621	0.54	1/2220 (0.0%)
47	S1	0.33	0/1713	0.64	1/2305 (0.0%)
47	s1	0.29	0/1748	0.54	0/2352
48	S2	0.32	0/1665	0.53	0/2263
48	s2	0.32	0/1665	0.58	0/2263
49	S3	0.31	0/1643	0.50	0/2210
49	s3	0.29	0/1759	0.55	1/2368 (0.0%)
50	S4	0.32	0/2084	0.57	0/2804
50	s4	0.32	0/2109	0.56	0/2839
51	S5	0.27	0/1629	0.56	0/2202
51	s5	0.29	0/1629	0.53	0/2202
52	S6	0.31	0/1611	0.52	0/2151
53	S7	0.30	0/1465	0.56	0/1971
53	s7	0.31	0/1517	0.58	0/2044
54	S8	0.34	0/1491	0.57	1/1992 (0.1%)
54	s8	0.32	0/1514	0.50	0/2021
55	S9	0.30	0/1443	0.54	0/1934
55	s9	0.30	0/1519	0.53	0/2035
56	C0	0.29	0/759	0.56	1/1025 (0.1%)
56	c0	0.29	0/776	0.73	4/1047 (0.4%)
57	C1	0.37	0/1153	0.57	0/1554
57	c1	0.34	0/1194	0.57	0/1610
58	C2	0.33	0/771	0.64	0/1044
58	c2	0.30	0/898	0.66	1/1220 (0.1%)
59	C3	0.32	0/1215	0.51	0/1638
59	c3	0.29	0/1215	0.50	0/1638
60	C4	0.31	0/901	0.60	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	c4	0.30	0/960	0.58	0/1290
61	C5	0.30	0/937	0.52	0/1258
61	c5	0.35	0/1060	0.64	0/1426
62	C6	0.29	0/1083	0.55	1/1452 (0.1%)
62	c6	0.29	0/1131	0.52	0/1518
63	C7	0.31	0/910	0.70	3/1219 (0.2%)
63	c7	0.30	0/914	0.64	1/1224 (0.1%)
64	C8	0.38	1/1197 (0.1%)	0.51	0/1609
64	c8	0.29	0/1211	0.58	1/1628 (0.1%)
65	C9	0.29	0/1089	0.50	0/1461
65	c9	0.29	0/1130	0.47	0/1517
66	D0	0.29	0/828	0.51	0/1119
66	d0	0.31	0/883	0.58	0/1193
67	D1	0.29	0/693	0.54	0/935
67	d1	0.30	0/693	0.59	0/935
68	D2	0.32	0/1038	0.56	0/1395
68	d2	0.31	0/1038	0.55	1/1395 (0.1%)
69	D3	0.40	0/1139	0.56	0/1518
69	d3	0.36	0/1139	0.54	0/1518
70	D4	0.31	0/1087	0.54	0/1449
70	d4	0.34	0/1087	0.57	1/1449 (0.1%)
71	D5	0.28	0/571	0.60	0/768
71	d5	0.26	0/566	0.45	0/761
72	D6	0.43	0/782	0.73	3/1047 (0.3%)
72	d6	0.32	0/782	0.59	0/1047
73	D7	0.30	0/620	0.58	0/838
73	d7	0.29	0/620	0.55	0/838
74	D8	0.29	0/499	0.57	0/670
74	d8	0.29	0/499	0.58	0/670
75	D9	0.40	0/453	0.62	0/602
75	d9	0.39	0/453	0.63	1/602 (0.2%)
76	E0	0.33	0/483	0.56	0/643
76	e0	0.34	0/499	0.61	0/665
77	SR	0.26	0/2485	0.51	0/3383
77	sR	0.27	0/2490	0.53	0/3390
78	SM	0.32	0/1053	0.57	1/1418 (0.1%)
78	sM	0.67	1/638 (0.2%)	0.51	0/860
79	s6	0.31	0/1779	0.51	0/2379
All	All	0.48	11/419528 (0.0%)	0.87	465/615687 (0.1%)

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
6	L4	0	1
7	L5	0	5
10	L8	0	3
10	l8	0	3
13	M1	0	1
13	m1	0	1
14	M3	0	1
15	m4	0	1
16	M5	0	1
20	M9	0	1
21	N0	0	3
21	n0	0	2
23	N2	0	2
26	n5	0	1
28	n7	0	1
29	n8	0	1
30	N9	0	1
30	n9	0	1
31	O0	0	1
33	O2	0	1
33	o2	0	1
35	o4	0	1
38	o7	0	1
43	Q2	0	1
47	S1	0	2
48	S2	0	1
48	s2	0	2
49	s3	0	1
51	S5	0	1
51	s5	0	1
53	S7	0	2
53	s7	0	5
54	S8	0	1
55	s9	0	4
57	c1	0	1
58	C2	0	1
58	c2	0	2
60	C4	0	3
61	c5	0	1
62	C6	0	1
62	c6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	C7	0	2
63	c7	0	1
65	C9	0	1
66	D0	0	2
68	D2	0	3
70	d4	0	3
71	D5	0	1
72	D6	0	3
73	D7	0	1
75	D9	0	2
75	d9	0	1
77	SR	0	2
77	sR	0	1
78	SM	0	1
78	sM	0	1
All	All	0	92

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	sM	51	ARG	C-N	14.96	1.62	1.34
28	N7	36	HIS	C-N	9.18	1.51	1.34
64	C8	81	ILE	C-N	-9.18	1.16	1.34
1	5	1152	G	N9-C4	-8.15	1.31	1.38
1	1	2606	G	N9-C4	-7.56	1.31	1.38
5	l3	168	LYS	C-N	-7.45	1.17	1.34
1	1	2971	A	N9-C4	7.10	1.42	1.37
1	5	1103	A	N9-C4	6.08	1.41	1.37
1	1	2971	A	N3-C4	5.63	1.38	1.34
28	N7	27	LYS	C-N	-5.44	1.24	1.34
1	1	2418	G	C6-N1	5.24	1.43	1.39

All (465) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1152	G	N3-C4-N9	-14.66	117.20	126.00
1	5	1152	G	N3-C4-C5	12.74	134.97	128.60
3	8	84	C	N1-C2-O2	12.54	126.42	118.90
1	1	2606	G	C5-N7-C8	-12.29	98.15	104.30
1	1	2606	G	N3-C4-C5	12.25	134.72	128.60
1	1	2606	G	N3-C4-N9	-10.16	119.91	126.00
3	8	84	C	C5-C6-N1	9.89	125.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2606	G	C4-C5-N7	9.69	114.68	110.80
1	1	2808	A	N1-C6-N6	9.40	124.24	118.60
1	1	1866	C	N1-C2-O2	9.38	124.53	118.90
3	8	84	C	C2-N1-C1'	9.22	128.94	118.80
1	1	1866	C	N3-C2-O2	-9.17	115.48	121.90
1	1	2606	G	N1-C6-O6	9.08	125.35	119.90
45	2	1274	C	N1-C2-O2	8.89	124.24	118.90
1	1	1866	C	C2-N1-C1'	8.79	128.47	118.80
3	8	84	C	C6-N1-C2	-8.62	116.85	120.30
3	4	126	A	O5'-P-OP1	-8.53	98.03	105.70
45	6	542	A	O4'-C1'-N9	8.43	114.95	108.20
1	1	2772	C	C6-N1-C1'	-8.26	110.89	120.80
1	1	1495	U	C5-C6-N1	-8.24	118.58	122.70
3	4	84	C	C2-N1-C1'	8.23	127.85	118.80
1	1	3217	C	N1-C2-O2	8.19	123.81	118.90
3	8	84	C	N3-C2-O2	-8.18	116.18	121.90
45	6	163	G	N3-C4-N9	-8.13	121.12	126.00
1	5	2205	U	N1-C2-O2	8.08	128.45	122.80
1	5	549	U	C2-N1-C1'	8.06	127.37	117.70
45	2	1274	C	C2-N1-C1'	8.05	127.65	118.80
1	5	437	G	N7-C8-N9	8.02	117.11	113.10
1	5	2256	A	O4'-C1'-N9	7.99	114.59	108.20
3	4	151	C	N3-C2-O2	-7.98	116.32	121.90
1	5	2205	U	N3-C2-O2	-7.96	116.63	122.20
3	4	84	C	C6-N1-C2	-7.93	117.13	120.30
45	2	1490	C	C2-N1-C1'	7.89	127.48	118.80
3	4	125	U	N1-C2-O2	7.86	128.30	122.80
1	1	2606	G	N7-C8-N9	7.86	117.03	113.10
44	Q3	49	ARG	C-N-CA	7.80	138.67	122.30
45	2	1490	C	N1-C2-O2	7.79	123.58	118.90
1	1	2772	C	C2-N1-C1'	7.73	127.30	118.80
1	1	2842	U	C2-N1-C1'	7.60	126.82	117.70
45	6	132	U	C2-N1-C1'	7.59	126.80	117.70
2	3	73	C	N1-C2-O2	7.57	123.44	118.90
3	8	84	C	C2-N3-C4	7.52	123.66	119.90
3	4	84	C	O5'-P-OP2	-7.47	98.97	105.70
1	1	895	A	N7-C8-N9	7.46	117.53	113.80
3	8	83	C	N1-C2-O2	7.42	123.35	118.90
3	8	83	C	N3-C2-O2	-7.41	116.71	121.90
1	5	1152	G	C5-N7-C8	-7.36	100.62	104.30
63	C7	85	VAL	C-N-CD	-7.36	104.41	120.60
1	1	895	A	C8-N9-C4	-7.33	102.87	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	934	C	C2-N1-C1'	7.32	126.85	118.80
1	1	2595	A	C5-N7-C8	-7.26	100.27	103.90
1	5	2205	U	C2-N1-C1'	7.26	126.41	117.70
1	1	1764	U	C2-N1-C1'	7.24	126.39	117.70
46	S0	9	LEU	CA-CB-CG	7.22	131.92	115.30
1	5	1200	A	N1-C6-N6	7.22	122.94	118.60
1	1	979	U	C5-C6-N1	7.21	126.31	122.70
1	5	1307	G	P-O3'-C3'	7.21	128.35	119.70
56	c0	88	PRO	N-CA-CB	7.20	111.94	103.30
1	1	2873	U	C5-C4-O4	7.17	130.20	125.90
45	2	137	U	C2-N1-C1'	7.15	126.28	117.70
1	1	1495	U	N1-C2-N3	7.15	119.19	114.90
1	5	3362	A	O4'-C1'-N9	7.09	113.88	108.20
1	1	895	A	C5-N7-C8	-7.05	100.38	103.90
1	1	3217	C	C2-N1-C1'	7.05	126.56	118.80
56	c0	97	PRO	N-CA-CB	7.03	111.73	103.30
3	4	151	C	N1-C2-O2	7.01	123.11	118.90
1	5	424	G	N1-C6-O6	7.01	124.11	119.90
3	4	84	C	N1-C2-O2	6.97	123.08	118.90
63	c7	118	PRO	N-CA-CB	6.96	111.66	103.30
45	2	137	U	N1-C2-O2	6.92	127.64	122.80
1	1	2971	A	C2-N3-C4	6.92	114.06	110.60
1	1	3341	U	N1-C2-O2	6.91	127.63	122.80
45	2	1274	C	N3-C2-O2	-6.89	117.08	121.90
1	5	1838	G	C8-N9-C4	6.89	109.16	106.40
1	5	3245	A	N7-C8-N9	6.88	117.24	113.80
45	2	934	C	N1-C2-O2	6.83	123.00	118.90
1	5	1072	G	N3-C4-N9	6.83	130.10	126.00
1	1	2870	C	N3-C4-C5	6.82	124.63	121.90
1	1	2606	G	C5-C6-O6	-6.81	124.51	128.60
45	2	830	U	N3-C2-O2	-6.80	117.44	122.20
1	1	895	A	C2-N3-C4	-6.79	107.20	110.60
1	1	2355	G	N1-C6-O6	6.73	123.94	119.90
45	6	163	G	N3-C4-C5	6.71	131.95	128.60
1	5	549	U	N1-C2-O2	6.70	127.49	122.80
3	4	125	U	C2-N1-C1'	6.68	125.72	117.70
1	5	2175	U	N1-C2-O2	-6.68	118.12	122.80
1	5	3245	A	C2-N3-C4	-6.67	107.26	110.60
1	1	2391	G	N1-C6-O6	-6.67	115.90	119.90
1	1	2772	C	N1-C2-O2	6.66	122.89	118.90
56	C0	88	PRO	N-CA-CB	6.66	111.29	103.30
1	1	3278	C	C2-N1-C1'	6.65	126.12	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	O3	21	ARG	NE-CZ-NH1	6.65	123.63	120.30
45	2	959	U	C2-N1-C1'	6.64	125.67	117.70
1	1	1495	U	C5-C4-O4	6.62	129.87	125.90
1	5	650	C	N1-C2-O2	-6.62	114.93	118.90
1	1	1604	G	C4-N9-C1'	6.60	135.08	126.50
1	1	3217	C	N3-C2-O2	-6.60	117.28	121.90
3	8	81	U	OP1-P-OP2	-6.59	109.72	119.60
45	6	1473	U	C2-N1-C1'	6.58	125.60	117.70
45	6	337	G	C4-C5-N7	6.56	113.42	110.80
45	2	959	U	N3-C2-O2	-6.56	117.61	122.20
45	6	1473	U	N1-C2-O2	6.55	127.39	122.80
1	1	765	C	N1-C2-O2	6.53	122.82	118.90
1	5	3308	C	C6-N1-C2	-6.53	117.69	120.30
1	1	2879	C	C6-N1-C2	6.52	122.91	120.30
3	8	81	U	OP2-P-O3'	6.52	119.55	105.20
45	6	1389	C	C2-N1-C1'	6.52	125.97	118.80
1	1	913	A	N1-C6-N6	-6.48	114.71	118.60
1	1	1741	A	O4'-C1'-N9	6.48	113.39	108.20
45	2	581	U	C2-N1-C1'	6.47	125.47	117.70
1	5	1879	A	C5-N7-C8	-6.46	100.67	103.90
1	1	2808	A	N9-C4-C5	-6.44	103.22	105.80
45	6	132	U	N1-C2-O2	6.42	127.29	122.80
1	1	2364	G	N1-C6-O6	-6.42	116.05	119.90
1	1	621	A	O4'-C1'-N9	6.42	113.33	108.20
3	4	151	C	C6-N1-C2	-6.42	117.73	120.30
1	1	621	A	C8-N9-C4	6.41	108.36	105.80
1	1	979	U	C2-N1-C1'	6.40	125.38	117.70
1	1	2873	U	N3-C4-O4	-6.38	114.93	119.40
54	S8	29	LEU	CA-CB-CG	6.38	129.98	115.30
1	1	621	A	C4-N9-C1'	-6.37	114.83	126.30
4	12	246	LEU	CA-CB-CG	6.35	129.90	115.30
3	4	125	U	N3-C2-O2	-6.34	117.76	122.20
45	2	959	U	N1-C2-O2	6.33	127.23	122.80
1	5	406	G	O4'-C1'-N9	6.33	113.26	108.20
1	5	1762	C	C2-N1-C1'	6.32	125.75	118.80
1	1	3278	C	N1-C2-O2	6.31	122.69	118.90
1	5	3362	A	N7-C8-N9	6.31	116.95	113.80
1	1	869	G	C2-N3-C4	-6.30	108.75	111.90
45	2	1082	C	C2-N1-C1'	6.30	125.73	118.80
1	1	2846	U	N3-C2-O2	-6.29	117.80	122.20
3	4	84	C	N3-C2-O2	-6.27	117.51	121.90
3	8	82	U	N3-C2-O2	-6.27	117.81	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	926	A	N1-C6-N6	6.26	122.36	118.60
1	1	2142	A	N1-C6-N6	-6.26	114.84	118.60
1	1	908	G	C4-N9-C1'	6.25	134.62	126.50
1	5	549	U	N3-C2-O2	-6.23	117.84	122.20
1	1	3382	U	N1-C2-O2	6.22	127.15	122.80
1	1	2943	G	N1-C6-O6	6.22	123.63	119.90
1	1	1604	G	N3-C4-C5	-6.21	125.50	128.60
1	5	1148	G	C8-N9-C4	6.19	108.88	106.40
47	S1	61	LEU	CA-CB-CG	6.19	129.53	115.30
64	c8	116	LEU	CA-CB-CG	6.19	129.53	115.30
1	1	1556	C	N1-C2-O2	6.18	122.61	118.90
1	1	1866	C	C6-N1-C1'	-6.18	113.39	120.80
1	5	1152	G	C8-N9-C1'	6.18	135.03	127.00
1	1	1495	U	N1-C2-O2	-6.17	118.48	122.80
45	2	144	U	N1-C2-O2	6.17	127.12	122.80
45	2	1274	C	C6-N1-C1'	-6.14	113.44	120.80
1	1	1495	U	C4-C5-C6	6.12	123.38	119.70
72	D6	85	ARG	N-CA-C	-6.11	94.50	111.00
1	5	1762	C	N1-C2-O2	6.10	122.56	118.90
1	5	2373	A	O5'-P-OP1	-6.10	100.21	105.70
1	1	2818	U	O5'-P-OP2	-6.09	100.22	105.70
45	2	830	U	N1-C2-O2	6.09	127.06	122.80
1	1	2320	A	N1-C2-N3	6.09	132.34	129.30
1	5	1152	G	N9-C4-C5	6.06	107.83	105.40
1	1	1848	G	C5-C6-O6	-6.06	124.97	128.60
1	1	765	C	C2-N1-C1'	6.04	125.44	118.80
1	5	1879	A	N7-C8-N9	6.04	116.82	113.80
1	1	1848	G	N1-C6-O6	6.03	123.52	119.90
1	5	437	G	C6-C5-N7	-6.03	126.78	130.40
45	2	137	U	N3-C2-O2	-6.02	117.98	122.20
1	5	2954	U	N1-C2-O2	6.01	127.01	122.80
45	2	1082	C	N1-C2-O2	6.01	122.51	118.90
5	L3	99	LEU	CA-CB-CG	6.01	129.12	115.30
45	6	1058	U	OP1-P-O3'	6.01	118.41	105.20
45	2	1456	C	C2-N1-C1'	6.00	125.39	118.80
1	1	2827	U	N1-C2-N3	5.99	118.49	114.90
1	5	3317	U	N3-C2-O2	-5.98	118.01	122.20
3	8	83	C	C6-N1-C2	-5.97	117.91	120.30
1	1	2816	G	C4-N9-C1'	-5.97	118.74	126.50
1	5	3245	A	N1-C6-N6	5.97	122.18	118.60
1	1	857	G	C8-N9-C4	5.96	108.79	106.40
45	6	1363	U	P-O3'-C3'	5.96	126.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	406	G	O4'-C1'-N9	5.96	112.97	108.20
1	1	3396	U	N1-C2-O2	5.96	126.97	122.80
1	1	2595	A	N1-C6-N6	5.95	122.17	118.60
13	m1	112	LEU	CA-CB-CG	5.94	128.97	115.30
1	1	3382	U	C2-N1-C1'	5.94	124.83	117.70
72	D6	64	LEU	CA-CB-CG	5.94	128.96	115.30
45	2	1490	C	N3-C2-O2	-5.94	117.74	121.90
45	6	163	G	N3-C2-N2	-5.94	115.75	119.90
45	6	1097	U	P-O3'-C3'	5.93	126.82	119.70
1	1	3344	A	O4'-C1'-N9	5.93	112.94	108.20
45	6	132	U	N3-C2-O2	-5.92	118.05	122.20
1	1	1279	C	N1-C2-O2	5.92	122.45	118.90
78	SM	166	PRO	N-CA-CB	5.92	110.40	103.30
1	5	1495	U	C2-N1-C1'	5.92	124.80	117.70
45	2	1761	U	C5-C4-O4	5.92	129.45	125.90
1	1	3341	U	N3-C2-O2	-5.92	118.06	122.20
45	6	158	U	P-O3'-C3'	5.91	126.80	119.70
1	5	437	G	C5-N7-C8	-5.91	101.34	104.30
1	5	424	G	C5-C6-O6	-5.90	125.06	128.60
1	1	2627	C	C4-C5-C6	5.89	120.35	117.40
1	1	2810	C	C6-N1-C2	5.89	122.66	120.30
45	2	442	C	C6-N1-C2	-5.89	117.94	120.30
1	5	1200	A	C5-C6-N6	-5.88	119.00	123.70
1	1	650	C	N1-C2-O2	-5.87	115.38	118.90
45	2	144	U	C2-N1-C1'	5.87	124.74	117.70
1	5	3245	A	C5-N7-C8	-5.87	100.97	103.90
1	1	922	U	C2-N1-C1'	5.86	124.74	117.70
1	5	3245	A	C6-C5-N7	-5.86	128.20	132.30
58	c2	58	LEU	CA-CB-CG	5.85	128.76	115.30
1	1	2967	A	C8-N9-C4	5.84	108.14	105.80
1	5	693	A	O5'-P-OP1	-5.84	100.44	105.70
1	1	1604	G	C8-N9-C1'	-5.84	119.41	127.00
1	5	1503	A	C8-N9-C4	5.84	108.14	105.80
36	O5	118	ILE	C-N-CA	5.82	136.25	121.70
1	5	1072	G	C8-N9-C1'	-5.82	119.44	127.00
1	1	2714	G	N3-C4-C5	5.80	131.50	128.60
1	1	2411	U	C6-N1-C2	5.80	124.48	121.00
1	1	3344	A	N7-C8-N9	5.78	116.69	113.80
1	1	3277	U	N3-C2-O2	-5.78	118.16	122.20
1	5	2571	U	C2-N1-C1'	5.77	124.63	117.70
1	5	2388	U	C5-C6-N1	-5.77	119.81	122.70
1	5	2821	C	N1-C2-O2	5.77	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	6	1473	U	N3-C2-O2	-5.76	118.17	122.20
1	1	1741	A	N7-C8-N9	5.76	116.68	113.80
1	1	2679	A	O4'-C1'-N9	5.74	112.79	108.20
1	5	1352	A	P-O3'-C3'	5.73	126.57	119.70
56	c0	83	PRO	N-CA-CB	5.73	110.17	103.30
1	1	895	A	N1-C2-N3	5.72	132.16	129.30
1	5	437	G	N1-C6-O6	5.72	123.33	119.90
45	2	934	C	C6-N1-C2	-5.72	118.01	120.30
45	2	1761	U	N3-C2-O2	-5.71	118.20	122.20
45	6	1000	C	C2-N1-C1'	5.71	125.08	118.80
1	5	1492	G	C8-N9-C4	5.71	108.68	106.40
45	6	337	G	C5-N7-C8	-5.71	101.45	104.30
1	1	2595	A	C4-C5-N7	5.70	113.55	110.70
1	1	2827	U	N3-C2-O2	-5.70	118.21	122.20
1	5	2291	A	N1-C6-N6	-5.70	115.18	118.60
45	6	542	A	C4-N9-C1'	5.70	136.56	126.30
1	5	3164	C	O4'-C1'-N1	5.69	112.75	108.20
1	5	424	G	C6-C5-N7	-5.69	126.98	130.40
1	1	2827	U	C5-C6-N1	-5.69	119.86	122.70
1	1	609	G	O5'-P-OP2	-5.69	100.58	105.70
1	1	3057	U	N3-C2-O2	-5.68	118.22	122.20
1	5	1592	G	C5-C6-N1	-5.68	108.66	111.50
1	1	2376	G	C5-C6-O6	-5.68	125.19	128.60
1	1	3196	U	O5'-P-OP2	-5.68	100.59	105.70
3	8	82	U	N1-C2-O2	5.68	126.78	122.80
1	1	2609	A	O5'-P-OP2	-5.68	100.59	105.70
1	1	1137	C	C6-N1-C2	5.67	122.57	120.30
1	1	2404	A	O4'-C1'-N9	-5.67	103.66	108.20
3	8	83	C	C2-N1-C1'	5.67	125.04	118.80
45	2	1560	U	N3-C2-O2	-5.67	118.23	122.20
1	1	2808	A	C4-C5-N7	5.65	113.53	110.70
45	2	1490	C	C6-N1-C2	-5.64	118.04	120.30
1	5	1072	G	N9-C4-C5	-5.64	103.14	105.40
1	5	1352	A	OP1-P-O3'	5.63	117.60	105.20
45	6	1560	U	C2-N1-C1'	5.63	124.46	117.70
3	4	84	C	C5-C6-N1	5.63	123.81	121.00
3	8	81	U	P-O3'-C3'	5.61	126.44	119.70
1	1	921	A	N1-C6-N6	-5.61	115.23	118.60
1	5	3362	A	C6-C5-N7	-5.60	128.38	132.30
45	2	1258	U	N3-C2-O2	-5.59	118.29	122.20
1	1	1502	C	N1-C2-O2	-5.58	115.55	118.90
45	2	1573	A	P-O3'-C3'	5.58	126.39	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	d4	134	ALA	CB-CA-C	5.58	118.46	110.10
1	1	1329	U	P-O3'-C3'	5.57	126.39	119.70
1	1	3362	A	C2-N3-C4	-5.57	107.81	110.60
1	1	1741	A	C8-N9-C4	-5.56	103.58	105.80
1	1	2842	U	N1-C2-O2	5.56	126.69	122.80
1	1	641	C	O4'-C1'-N1	5.56	112.64	108.20
1	1	1866	C	C6-N1-C2	-5.55	118.08	120.30
1	5	2978	U	C5-C6-N1	-5.55	119.92	122.70
1	5	3154	C	OP1-P-O3'	5.55	117.41	105.20
3	8	84	C	C6-N1-C1'	-5.55	114.14	120.80
3	4	151	C	C2-N1-C1'	5.55	124.90	118.80
1	1	2816	G	C5-C6-O6	-5.54	125.27	128.60
10	18	69	LEU	CA-CB-CG	5.54	128.04	115.30
1	5	1329	U	P-O3'-C3'	5.54	126.34	119.70
1	1	1433	A	N1-C2-N3	5.53	132.07	129.30
49	s3	4	LEU	CA-CB-CG	5.53	128.03	115.30
1	1	835	G	O4'-C1'-N9	5.53	112.62	108.20
1	1	2606	G	C2-N3-C4	-5.53	109.14	111.90
45	6	864	U	N3-C2-O2	-5.53	118.33	122.20
1	5	1604	G	C4-N9-C1'	5.53	133.69	126.50
3	8	11	C	C6-N1-C2	-5.52	118.09	120.30
1	1	1879	A	O4'-C1'-N9	5.51	112.61	108.20
45	2	1389	C	C2-N1-C1'	5.50	124.86	118.80
4	L2	180	LEU	CA-CB-CG	5.50	127.96	115.30
45	2	1039	A	O4'-C1'-N9	5.50	112.60	108.20
1	1	2939	G	C8-N9-C4	5.50	108.60	106.40
1	1	75	G	N1-C6-O6	5.50	123.20	119.90
1	1	3396	U	C2-N1-C1'	5.49	124.29	117.70
2	3	87	G	N9-C4-C5	-5.49	103.20	105.40
1	5	1081	U	P-O3'-C3'	5.49	126.28	119.70
1	1	283	G	O4'-C1'-N9	-5.48	103.82	108.20
45	2	418	G	C4-N9-C1'	5.48	133.62	126.50
1	1	437	G	C5-C6-O6	-5.48	125.31	128.60
45	2	934	C	N3-C2-O2	-5.47	118.07	121.90
45	2	1456	C	N1-C2-O2	5.47	122.18	118.90
1	1	1307	G	C4-N9-C1'	-5.46	119.40	126.50
12	m0	57	LEU	CA-CB-CG	5.46	127.86	115.30
1	1	2245	C	C6-N1-C2	-5.46	118.12	120.30
1	1	1299	U	C5-C6-N1	-5.45	119.97	122.70
1	1	1815	U	P-O3'-C3'	5.45	126.24	119.70
1	1	2816	G	C8-N9-C1'	5.44	134.07	127.00
1	1	2885	C	C6-N1-C2	5.44	122.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	1246	C	C2-N1-C1'	5.43	124.77	118.80
1	1	827	A	C8-N9-C4	5.41	107.97	105.80
1	5	424	G	C4-C5-N7	5.40	112.96	110.80
1	5	3362	A	C5-N7-C8	-5.40	101.20	103.90
1	1	1556	C	N3-C2-O2	-5.39	118.13	121.90
1	1	2983	C	C4-C5-C6	5.39	120.09	117.40
45	2	638	U	C2-N1-C1'	5.39	124.17	117.70
45	2	1773	C	C6-N1-C2	-5.39	118.14	120.30
1	5	2666	C	C2-N1-C1'	5.38	124.72	118.80
45	6	755	A	C3'-C2'-C1'	5.38	105.81	101.50
1	1	621	A	C4-C5-C6	-5.38	114.31	117.00
1	1	2970	C	P-O3'-C3'	5.38	126.16	119.70
45	2	1150	G	C2-N3-C4	-5.36	109.22	111.90
1	5	1496	C	C2-N1-C1'	5.36	124.70	118.80
1	1	91	G	C5-C6-O6	-5.36	125.38	128.60
45	6	934	C	N1-C2-O2	5.36	122.11	118.90
1	5	1152	G	C8-N9-C4	-5.35	104.26	106.40
1	1	2541	U	P-O3'-C3'	5.35	126.11	119.70
20	M9	24	LEU	CA-CB-CG	5.34	127.59	115.30
1	5	1481	A	C8-N9-C4	-5.34	103.66	105.80
1	1	2606	G	N1-C2-N2	5.34	121.00	116.20
45	2	1560	U	C2-N1-C1'	5.33	124.10	117.70
1	5	1072	G	N1-C6-O6	5.33	123.10	119.90
45	2	1490	C	C6-N1-C1'	-5.33	114.41	120.80
1	5	549	U	C5-C6-N1	5.33	125.36	122.70
1	1	2842	U	C6-N1-C1'	-5.32	113.75	121.20
33	o2	126	LEU	CA-CB-CG	5.32	127.53	115.30
1	1	914	A	N1-C6-N6	-5.32	115.41	118.60
46	s0	9	LEU	CA-CB-CG	5.32	127.53	115.30
45	6	1058	U	P-O3'-C3'	5.31	126.07	119.70
3	8	80	A	C8-N9-C4	5.31	107.92	105.80
45	6	864	U	C2-N1-C1'	5.31	124.07	117.70
56	c0	78	GLU	N-CA-C	-5.31	96.67	111.00
45	6	1773	C	N3-C4-C5	-5.30	119.78	121.90
1	5	1152	G	N1-C2-N2	5.30	120.97	116.20
1	1	2572	C	C2-N1-C1'	5.30	124.63	118.80
1	1	2595	A	N7-C8-N9	5.29	116.45	113.80
1	1	2663	G	N1-C6-O6	5.29	123.08	119.90
1	1	1141	C	C6-N1-C2	5.29	122.42	120.30
26	n5	57	LEU	CA-CB-CG	5.28	127.45	115.30
68	d2	93	LEU	CA-CB-CG	5.28	127.45	115.30
1	5	1815	U	P-O3'-C3'	5.28	126.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	437	G	C4-N9-C1'	5.28	133.36	126.50
1	5	1481	A	P-O3'-C3'	5.28	126.03	119.70
1	5	2978	U	O4'-C1'-N1	5.28	112.42	108.20
1	1	3218	A	P-O3'-C3'	5.27	126.02	119.70
45	2	1456	C	N3-C2-O2	-5.27	118.21	121.90
45	6	864	U	N1-C2-O2	5.27	126.49	122.80
72	D6	63	ALA	C-N-CA	5.26	134.86	121.70
45	6	272	U	P-O3'-C3'	5.26	126.02	119.70
1	1	2560	C	O4'-C1'-N1	5.26	112.41	108.20
1	5	1348	U	O4'-C1'-N1	5.26	112.41	108.20
45	6	756	A	C8-N9-C4	-5.25	103.70	105.80
45	6	781	U	N1-C2-O2	5.25	126.47	122.80
1	1	1092	C	N1-C2-O2	5.25	122.05	118.90
1	5	2725	U	O4'-C1'-N1	5.24	112.39	108.20
45	2	829	A	P-O3'-C3'	5.24	125.99	119.70
45	6	934	C	C2-N1-C1'	5.24	124.56	118.80
1	1	1196	C	N1-C2-O2	5.23	122.04	118.90
1	1	3278	C	C5-C6-N1	5.23	123.62	121.00
45	2	158	U	P-O3'-C3'	5.23	125.98	119.70
75	d9	30	LEU	CA-CB-CG	5.23	127.34	115.30
4	L2	191	LEU	CA-CB-CG	-5.23	103.28	115.30
1	5	2526	C	N1-C2-O2	5.23	122.04	118.90
1	1	155	G	C8-N9-C4	5.23	108.49	106.40
1	1	3137	C	C5-C6-N1	-5.22	118.39	121.00
1	5	2606	G	N3-C4-C5	-5.22	125.99	128.60
1	1	2357	A	N1-C6-N6	5.22	121.73	118.60
1	1	1095	U	P-O3'-C3'	5.21	125.95	119.70
1	5	2942	C	O5'-P-OP2	-5.21	101.01	105.70
1	1	3278	C	C6-N1-C2	-5.21	118.22	120.30
45	6	139	C	P-O3'-C3'	5.21	125.95	119.70
14	M3	85	LEU	CA-CB-CG	5.21	127.27	115.30
45	2	543	C	C2-N1-C1'	5.21	124.53	118.80
1	5	2939	G	C8-N9-C4	5.21	108.48	106.40
1	1	3362	A	C5-N7-C8	-5.21	101.30	103.90
1	5	908	G	O4'-C1'-N9	-5.20	104.04	108.20
1	1	1303	A	C8-N9-C4	5.20	107.88	105.80
1	1	113	C	N1-C2-O2	5.20	122.02	118.90
1	1	1379	G	N9-C4-C5	-5.20	103.32	105.40
1	5	2418	G	OP1-P-O3'	5.20	116.63	105.20
1	1	928	C	N3-C2-O2	-5.20	118.26	121.90
1	5	3195	U	N1-C2-O2	5.19	126.44	122.80
44	Q3	50	GLY	N-CA-C	-5.19	100.12	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	2	1	U	O4'-C1'-N1	5.19	112.35	108.20
1	1	1764	U	N1-C2-O2	5.19	126.43	122.80
1	1	1819	U	N3-C2-O2	-5.19	118.57	122.20
1	1	637	C	P-O3'-C3'	5.19	125.93	119.70
1	5	437	G	C5-C6-O6	-5.19	125.49	128.60
45	6	792	U	N1-C2-O2	5.19	126.43	122.80
45	6	1398	U	N1-C2-O2	5.18	126.43	122.80
1	5	1879	A	C4-C5-N7	5.18	113.29	110.70
1	1	2764	C	N1-C2-O2	-5.17	115.80	118.90
1	1	1356	U	C2-N1-C1'	-5.17	111.49	117.70
45	6	1600	A	OP1-P-O3'	5.17	116.58	105.20
26	N5	34	LEU	CA-CB-CG	5.16	127.18	115.30
45	2	1568	C	P-O3'-C3'	5.16	125.90	119.70
45	6	695	U	N3-C2-O2	-5.16	118.58	122.20
45	6	792	U	C2-N1-C1'	5.16	123.89	117.70
1	1	639	G	N1-C6-O6	5.16	122.99	119.90
3	8	79	A	C8-N9-C4	5.16	107.86	105.80
1	1	2611	U	N3-C4-O4	-5.15	115.79	119.40
3	8	80	A	O4'-C1'-N9	-5.14	104.08	108.20
1	1	1355	A	P-O3'-C3'	5.14	125.87	119.70
1	1	878	G	N1-C6-O6	-5.14	116.82	119.90
1	1	1446	A	C2-N3-C4	-5.14	108.03	110.60
45	6	1097	U	OP2-P-O3'	5.14	116.50	105.20
1	1	3306	U	N3-C2-O2	-5.13	118.61	122.20
1	1	1201	C	C6-N1-C2	-5.12	118.25	120.30
1	5	1442	U	C6-N1-C2	5.12	124.07	121.00
45	6	75	U	C2-N1-C1'	5.12	123.84	117.70
1	1	2169	G	C2-N3-C4	5.12	114.46	111.90
1	1	2978	U	O4'-C1'-N1	5.12	112.29	108.20
1	1	659	G	C8-N9-C4	5.11	108.44	106.40
3	8	83	C	OP2-P-O3'	5.11	116.44	105.20
1	5	3362	A	C8-N9-C4	-5.11	103.76	105.80
63	C7	86	PRO	N-CA-C	5.11	125.37	112.10
1	1	647	A	N1-C6-N6	5.10	121.66	118.60
1	1	1095	U	OP2-P-O3'	5.10	116.42	105.20
1	1	1650	G	N1-C6-O6	5.10	122.96	119.90
1	1	2938	G	C8-N9-C4	5.10	108.44	106.40
45	2	639	U	N1-C2-O2	5.10	126.37	122.80
1	1	1716	U	P-O3'-C3'	5.09	125.81	119.70
1	5	1761	C	C2-N1-C1'	5.09	124.40	118.80
45	6	695	U	N1-C2-O2	5.09	126.36	122.80
1	1	1141	C	N3-C4-C5	5.09	123.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3154	C	P-O3'-C3'	5.09	125.81	119.70
1	1	1137	C	C5-C6-N1	-5.08	118.46	121.00
1	1	2737	C	C6-N1-C2	-5.08	118.27	120.30
63	C7	85	VAL	C-N-CA	5.08	143.35	122.00
1	5	1480	G	C8-N9-C4	5.08	108.43	106.40
1	1	2363	A	N1-C6-N6	5.07	121.64	118.60
1	1	1495	U	C2-N1-C1'	-5.07	111.62	117.70
1	5	1152	G	C2-N3-C4	-5.07	109.37	111.90
1	5	208	C	N3-C2-O2	-5.07	118.35	121.90
45	6	1751	C	C6-N1-C2	5.06	122.33	120.30
20	M9	99	LEU	CA-CB-CG	5.05	126.92	115.30
45	2	831	U	C5-C6-N1	5.05	125.23	122.70
1	5	386	A	N1-C6-N6	5.05	121.63	118.60
35	O4	51	LEU	CA-CB-CG	5.05	126.91	115.30
45	2	130	C	C3'-C2'-C1'	5.05	105.54	101.50
62	C6	40	GLU	C-N-CD	-5.05	109.50	120.60
1	5	1481	A	C4-C5-C6	5.05	119.52	117.00
1	1	908	G	C8-N9-C1'	-5.05	120.44	127.00
45	2	1150	G	N3-C4-N9	-5.04	122.97	126.00
1	1	1429	G	C8-N9-C4	5.03	108.41	106.40
1	5	1072	G	C6-C5-N7	-5.03	127.38	130.40
1	5	1838	G	N7-C8-N9	-5.03	110.58	113.10
1	5	437	G	C8-N9-C4	-5.03	104.39	106.40
1	1	1604	G	N3-C4-N9	5.03	129.02	126.00
1	1	1445	U	N1-C2-O2	-5.03	119.28	122.80
45	6	1389	C	N1-C2-O2	5.03	121.92	118.90
1	1	1481	A	P-O3'-C3'	5.02	125.73	119.70
1	1	1650	G	C5-C6-O6	-5.02	125.59	128.60
1	5	2772	C	P-O3'-C3'	5.02	125.72	119.70
1	1	2608	G	N1-C6-O6	5.02	122.91	119.90
1	5	2403	G	N1-C6-O6	5.02	122.91	119.90
1	1	621	A	C8-N9-C1'	5.01	136.72	127.70
1	1	2750	U	C5-C6-N1	-5.01	120.19	122.70
45	2	136	C	P-O3'-C3'	5.01	125.71	119.70
1	1	869	G	C6-C5-N7	-5.01	127.40	130.40
1	1	2112	U	P-O3'-C3'	5.00	125.71	119.70
1	1	2595	A	C2-N3-C4	-5.00	108.10	110.60
45	2	1241	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (92) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	C2	39	ASP	Peptide
60	C4	123	SER	Peptide
60	C4	74	VAL	Peptide
60	C4	90	ARG	Peptide
62	C6	40	GLU	Peptide
63	C7	20	TYR	Peptide
63	C7	85	VAL	Peptide
65	C9	28	LEU	Peptide
66	D0	48	HIS	Peptide
66	D0	73	GLY	Peptide
68	D2	54	ASP	Peptide
68	D2	67	GLY	Peptide
68	D2	83	ILE	Peptide
71	D5	94	LYS	Peptide
72	D6	10	ARG	Peptide
72	D6	34	LYS	Peptide
72	D6	97	PRO	Peptide
73	D7	58	SER	Peptide
75	D9	5	ASN	Peptide
75	D9	6	VAL	Peptide
6	L4	196	ASN	Peptide
7	L5	124	GLU	Peptide
7	L5	251	PRO	Peptide
7	L5	258	LYS	Peptide
7	L5	7	ALA	Peptide
7	L5	8	LYS	Peptide
10	L8	24	ASN	Peptide
10	L8	30	THR	Peptide
10	L8	76	ALA	Peptide
13	M1	63	GLU	Peptide
14	M3	86	THR	Peptide
16	M5	74	PRO	Peptide
20	M9	131	ALA	Peptide
21	N0	166	LYS	Peptide
21	N0	22	PRO	Peptide
21	N0	69	PRO	Peptide
23	N2	26	GLY	Peptide
23	N2	90	ARG	Peptide
30	N9	20	GLY	Peptide
31	O0	36	GLN	Peptide
33	O2	122	PRO	Peptide
43	Q2	99	GLN	Peptide
47	S1	157	GLN	Peptide

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Mol	Chain	Res	Type	Group
47	S1	23	PRO	Peptide
48	S2	106	ASP	Peptide
51	S5	44	ASN	Peptide
53	S7	107	ARG	Peptide
53	S7	131	PHE	Peptide
54	S8	147	ALA	Peptide
78	SM	50	ASN	Peptide
77	SR	163	ASP	Peptide
77	SR	193	ILE	Peptide
57	c1	120	GLY	Peptide
58	c2	109	GLU	Peptide
58	c2	130	THR	Peptide
61	c5	51	SER	Peptide
62	c6	40	GLU	Peptide
63	c7	83	GLN	Peptide
70	d4	29	HIS	Peptide
70	d4	35	VAL	Peptide
70	d4	50	ALA	Peptide
75	d9	6	VAL	Peptide
4	l2	215	ASN	Peptide
10	l8	222	PHE	Peptide
10	l8	24	ASN	Peptide
10	l8	25	PRO	Peptide
13	m1	151	SER	Peptide
15	m4	48	GLY	Peptide
21	n0	170	THR	Peptide
21	n0	3	HIS	Peptide
26	n5	47	ALA	Peptide
28	n7	132	SER	Peptide
29	n8	110	GLY	Peptide
30	n9	19	ASN	Peptide
33	o2	15	LYS	Peptide
35	o4	47	CYS	Peptide
38	o7	76	ASN	Peptide
48	s2	106	ASP	Peptide
48	s2	236	PRO	Peptide
49	s3	219	ALA	Peptide
51	s5	44	ASN	Peptide
53	s7	10	SER	Peptide
53	s7	11	GLN	Peptide
53	s7	130	VAL	Peptide
53	s7	29	ASN	Peptide

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Mol	Chain	Res	Type	Group
53	s7	64	VAL	Peptide
55	s9	132	ARG	Peptide
55	s9	133	HIS	Peptide
55	s9	134	ILE	Peptide
55	s9	89	ASP	Peptide
78	sM	64	LYS	Peptide
77	sR	146	GLY	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	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
4	l2	246/248 (99%)	229 (93%)	16 (6%)	1 (0%)	34	66
5	L3	384/386 (100%)	355 (92%)	27 (7%)	2 (0%)	29	61
5	l3	384/386 (100%)	359 (94%)	25 (6%)	0	100	100
6	L4	359/361 (99%)	334 (93%)	24 (7%)	1 (0%)	41	71
6	l4	359/361 (99%)	318 (89%)	39 (11%)	2 (1%)	25	57
7	L5	291/296 (98%)	260 (89%)	29 (10%)	2 (1%)	22	54
7	l5	292/296 (99%)	261 (89%)	30 (10%)	1 (0%)	41	71
8	L6	152/176 (86%)	142 (93%)	8 (5%)	2 (1%)	12	40
8	l6	153/176 (87%)	136 (89%)	16 (10%)	1 (1%)	22	54
9	L7	224/226 (99%)	206 (92%)	17 (8%)	1 (0%)	34	66
9	l7	221/226 (98%)	202 (91%)	18 (8%)	1 (0%)	29	61
10	L8	229/231 (99%)	199 (87%)	27 (12%)	3 (1%)	12	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	l8	229/231 (99%)	190 (83%)	35 (15%)	4 (2%)	9	35
11	L9	187/191 (98%)	167 (89%)	19 (10%)	1 (0%)	29	61
11	l9	189/191 (99%)	176 (93%)	11 (6%)	2 (1%)	14	45
12	M0	215/221 (97%)	196 (91%)	18 (8%)	1 (0%)	29	61
12	m0	217/221 (98%)	200 (92%)	17 (8%)	0	100	100
13	M1	167/169 (99%)	146 (87%)	18 (11%)	3 (2%)	8	35
13	m1	167/169 (99%)	140 (84%)	25 (15%)	2 (1%)	13	42
14	M3	191/194 (98%)	171 (90%)	19 (10%)	1 (0%)	29	61
14	m3	192/194 (99%)	157 (82%)	34 (18%)	1 (0%)	29	61
15	M4	134/137 (98%)	121 (90%)	12 (9%)	1 (1%)	22	54
15	m4	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
16	M5	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
16	m5	201/203 (99%)	184 (92%)	16 (8%)	1 (0%)	29	61
17	M6	195/197 (99%)	187 (96%)	8 (4%)	0	100	100
17	m6	195/197 (99%)	183 (94%)	11 (6%)	1 (0%)	29	61
18	M7	171/184 (93%)	164 (96%)	7 (4%)	0	100	100
18	m7	153/184 (83%)	142 (93%)	11 (7%)	0	100	100
19	M8	183/185 (99%)	169 (92%)	13 (7%)	1 (0%)	29	61
19	m8	183/185 (99%)	166 (91%)	15 (8%)	2 (1%)	14	45
20	M9	183/188 (97%)	162 (88%)	21 (12%)	0	100	100
20	m9	186/188 (99%)	173 (93%)	13 (7%)	0	100	100
21	N0	170/172 (99%)	151 (89%)	18 (11%)	1 (1%)	25	57
21	n0	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
22	N1	157/159 (99%)	139 (88%)	16 (10%)	2 (1%)	12	40
22	n1	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	57
23	N2	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	7	31
23	n2	96/99 (97%)	86 (90%)	10 (10%)	0	100	100
24	N3	130/136 (96%)	124 (95%)	6 (5%)	0	100	100
24	n3	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
25	N4	61/155 (39%)	56 (92%)	5 (8%)	0	100	100
25	n4	133/155 (86%)	121 (91%)	10 (8%)	2 (2%)	10	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	N5	116/120 (97%)	104 (90%)	11 (10%)	1 (1%)	17	48
26	n5	118/120 (98%)	105 (89%)	11 (9%)	2 (2%)	9	35
27	N6	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
27	n6	121/125 (97%)	114 (94%)	7 (6%)	0	100	100
28	N7	133/135 (98%)	118 (89%)	15 (11%)	0	100	100
28	n7	133/135 (98%)	117 (88%)	15 (11%)	1 (1%)	19	51
29	N8	146/148 (99%)	133 (91%)	12 (8%)	1 (1%)	22	54
29	n8	146/148 (99%)	128 (88%)	18 (12%)	0	100	100
30	N9	54/58 (93%)	46 (85%)	8 (15%)	0	100	100
30	n9	56/58 (97%)	47 (84%)	8 (14%)	1 (2%)	8	35
31	O0	95/100 (95%)	91 (96%)	3 (3%)	1 (1%)	14	45
31	o0	98/100 (98%)	86 (88%)	11 (11%)	1 (1%)	15	46
32	O1	102/112 (91%)	98 (96%)	3 (3%)	1 (1%)	15	46
32	o1	107/112 (96%)	96 (90%)	11 (10%)	0	100	100
33	O2	123/127 (97%)	114 (93%)	8 (6%)	1 (1%)	19	51
33	o2	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
34	O3	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
34	o3	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
35	O4	110/112 (98%)	101 (92%)	9 (8%)	0	100	100
35	o4	110/112 (98%)	99 (90%)	10 (9%)	1 (1%)	17	48
36	O5	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	17	48
36	o5	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
37	O6	95/99 (96%)	83 (87%)	11 (12%)	1 (1%)	14	45
37	o6	97/99 (98%)	83 (86%)	14 (14%)	0	100	100
38	O7	82/87 (94%)	78 (95%)	4 (5%)	0	100	100
38	o7	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
39	O8	75/77 (97%)	66 (88%)	9 (12%)	0	100	100
39	o8	75/77 (97%)	63 (84%)	12 (16%)	0	100	100
40	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
40	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
41	Q0	50/52 (96%)	45 (90%)	5 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	32
42	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
42	q1	23/25 (92%)	23 (100%)	0	0	100	100
43	Q2	103/105 (98%)	88 (85%)	15 (15%)	0	100	100
43	q2	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
44	Q3	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
44	q3	89/91 (98%)	80 (90%)	9 (10%)	0	100	100
46	S0	204/206 (99%)	179 (88%)	22 (11%)	3 (2%)	10	38
46	s0	204/206 (99%)	177 (87%)	26 (13%)	1 (0%)	29	61
47	S1	209/216 (97%)	161 (77%)	40 (19%)	8 (4%)	3	19
47	s1	214/216 (99%)	186 (87%)	26 (12%)	2 (1%)	17	48
48	S2	215/217 (99%)	194 (90%)	19 (9%)	2 (1%)	17	48
48	s2	215/217 (99%)	187 (87%)	28 (13%)	0	100	100
49	S3	207/223 (93%)	188 (91%)	19 (9%)	0	100	100
49	s3	221/223 (99%)	187 (85%)	33 (15%)	1 (0%)	29	61
50	S4	252/260 (97%)	219 (87%)	31 (12%)	2 (1%)	19	51
50	s4	258/260 (99%)	224 (87%)	34 (13%)	0	100	100
51	S5	204/206 (99%)	173 (85%)	29 (14%)	2 (1%)	15	46
51	s5	204/206 (99%)	177 (87%)	25 (12%)	2 (1%)	15	46
52	S6	194/236 (82%)	174 (90%)	20 (10%)	0	100	100
53	S7	175/186 (94%)	138 (79%)	35 (20%)	2 (1%)	14	45
53	s7	184/186 (99%)	155 (84%)	28 (15%)	1 (0%)	29	61
54	S8	181/200 (90%)	157 (87%)	22 (12%)	2 (1%)	14	45
54	s8	184/200 (92%)	162 (88%)	21 (11%)	1 (0%)	29	61
55	S9	172/185 (93%)	140 (81%)	31 (18%)	1 (1%)	25	57
55	s9	183/185 (99%)	165 (90%)	18 (10%)	0	100	100
56	C0	88/105 (84%)	73 (83%)	14 (16%)	1 (1%)	14	45
56	c0	92/105 (88%)	65 (71%)	19 (21%)	8 (9%)	1	5
57	C1	137/146 (94%)	126 (92%)	10 (7%)	1 (1%)	22	54
57	c1	144/146 (99%)	130 (90%)	12 (8%)	2 (1%)	11	38
58	C2	98/143 (68%)	70 (71%)	25 (26%)	3 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	c2	122/143 (85%)	91 (75%)	28 (23%)	3 (2%)	5	27
59	C3	148/150 (99%)	129 (87%)	18 (12%)	1 (1%)	22	54
59	c3	148/150 (99%)	130 (88%)	15 (10%)	3 (2%)	7	32
60	C4	125/128 (98%)	98 (78%)	25 (20%)	2 (2%)	9	36
60	c4	126/128 (98%)	108 (86%)	17 (14%)	1 (1%)	19	51
61	C5	114/141 (81%)	101 (89%)	13 (11%)	0	100	100
61	c5	133/141 (94%)	100 (75%)	29 (22%)	4 (3%)	4	24
62	C6	134/142 (94%)	114 (85%)	19 (14%)	1 (1%)	22	54
62	c6	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
63	C7	111/136 (82%)	94 (85%)	14 (13%)	3 (3%)	5	26
63	c7	113/136 (83%)	95 (84%)	12 (11%)	6 (5%)	2	12
64	C8	141/145 (97%)	111 (79%)	28 (20%)	2 (1%)	11	38
64	c8	143/145 (99%)	126 (88%)	15 (10%)	2 (1%)	11	38
65	C9	135/143 (94%)	120 (89%)	14 (10%)	1 (1%)	22	54
65	c9	141/143 (99%)	125 (89%)	15 (11%)	1 (1%)	22	54
66	D0	100/109 (92%)	90 (90%)	10 (10%)	0	100	100
66	d0	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	17	48
67	D1	85/87 (98%)	67 (79%)	15 (18%)	3 (4%)	3	21
67	d1	85/87 (98%)	74 (87%)	10 (12%)	1 (1%)	13	42
68	D2	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	9	36
68	d2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	19	51
69	D3	142/144 (99%)	120 (84%)	21 (15%)	1 (1%)	22	54
69	d3	142/144 (99%)	125 (88%)	17 (12%)	0	100	100
70	D4	132/134 (98%)	117 (89%)	13 (10%)	2 (2%)	10	38
70	d4	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
71	D5	68/70 (97%)	54 (79%)	11 (16%)	3 (4%)	2	16
71	d5	67/70 (96%)	56 (84%)	11 (16%)	0	100	100
72	D6	95/97 (98%)	69 (73%)	22 (23%)	4 (4%)	3	17
72	d6	95/97 (98%)	75 (79%)	18 (19%)	2 (2%)	7	31
73	D7	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
73	d7	79/81 (98%)	72 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	D8	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
74	d8	61/63 (97%)	48 (79%)	12 (20%)	1 (2%)	9	36
75	D9	51/53 (96%)	43 (84%)	7 (14%)	1 (2%)	7	32
75	d9	51/53 (96%)	43 (84%)	8 (16%)	0	100	100
76	E0	58/62 (94%)	50 (86%)	7 (12%)	1 (2%)	9	35
76	e0	60/62 (97%)	51 (85%)	7 (12%)	2 (3%)	4	22
77	SR	315/318 (99%)	274 (87%)	41 (13%)	0	100	100
77	sR	316/318 (99%)	278 (88%)	37 (12%)	1 (0%)	41	71
78	SM	143/272 (53%)	117 (82%)	25 (18%)	1 (1%)	22	54
78	sM	89/272 (33%)	73 (82%)	15 (17%)	1 (1%)	14	45
79	s6	216/218 (99%)	183 (85%)	30 (14%)	3 (1%)	11	38
All	All	21808/22972 (95%)	19331 (89%)	2311 (11%)	166 (1%)	19	51

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L6	98	VAL
10	L8	36	ILE
10	L8	116	VAL
11	L9	50	ASN
33	O2	123	LYS
51	S5	64	VAL
56	C0	88	PRO
57	C1	7	VAL
63	C7	85	VAL
68	D2	83	ILE
71	D5	88	ILE
8	l6	98	VAL
10	l8	203	VAL
19	m8	124	LEU
26	n5	47	ALA
30	n9	21	ILE
31	o0	100	ILE
56	c0	83	PRO
56	c0	88	PRO
56	c0	97	PRO
57	c1	7	VAL
59	c3	66	ILE

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Mol	Chain	Res	Type
63	c7	97	ASN
63	c7	99	VAL
65	c9	34	VAL
76	e0	45	VAL
5	L3	140	ASP
6	L4	195	ARG
13	M1	114	ILE
23	N2	11	ILE
23	N2	88	GLN
58	C2	89	ILE
60	C4	42	VAL
63	C7	84	TYR
71	D5	41	ILE
72	D6	75	VAL
25	n4	63	ILE
25	n4	76	VAL
35	o4	48	GLY
46	s0	189	VAL
51	s5	36	ALA
53	s7	109	VAL
56	c0	78	GLU
56	c0	82	LEU
56	c0	92	ILE
63	c7	117	LEU
63	c7	118	PRO
66	d0	18	GLN
68	d2	6	VAL
74	d8	7	VAL
12	M0	24	ARG
13	M1	56	THR
13	M1	173	ASP
31	O0	37	GLY
36	O5	98	SER
47	S1	49	ASN
47	S1	62	LYS
63	C7	88	VAL
67	D1	29	HIS
68	D2	31	SER
71	D5	71	ILE
72	D6	58	VAL
14	m3	47	ALA
49	s3	217	ILE

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Mol	Chain	Res	Type
56	c0	96	ASN
61	c5	12	PHE
61	c5	50	THR
67	d1	29	HIS
14	M3	47	ALA
15	M4	8	LYS
19	M8	99	THR
22	N1	22	HIS
22	N1	124	VAL
29	N8	48	TYR
46	S0	68	PRO
47	S1	130	SER
51	S5	51	VAL
54	S8	152	ILE
70	D4	5	VAL
9	l7	191	VAL
13	m1	11	ASP
16	m5	149	ASN
19	m8	99	THR
58	c2	91	VAL
58	c2	106	ILE
58	c2	131	ASP
63	c7	104	ASN
64	c8	92	ILE
72	d6	61	GLU
7	L5	9	SER
8	L6	97	ASN
26	N5	50	ALA
47	S1	56	SER
47	S1	94	LYS
48	S2	144	TRP
54	S8	148	ALA
58	C2	69	ALA
72	D6	64	LEU
10	l8	117	ALA
13	m1	114	ILE
22	n1	83	ARG
59	c3	22	ALA
59	c3	87	ASP
60	c4	133	ARG
61	c5	130	ARG
47	S1	68	VAL

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Mol	Chain	Res	Type
48	S2	126	ARG
50	S4	179	LYS
65	C9	53	TRP
72	D6	65	PRO
4	l2	49	VAL
6	l4	144	LYS
7	l5	125	VAL
10	l8	240	ASN
26	n5	62	VAL
28	n7	103	GLN
51	s5	35	GLN
76	e0	50	VAL
77	sR	308	ASN
78	sM	51	ARG
10	L8	157	VAL
46	S0	158	VAL
50	S4	195	ILE
58	C2	91	VAL
75	D9	11	PRO
6	l4	145	ILE
11	l9	144	ILE
21	N0	167	ARG
32	O1	7	VAL
37	O6	3	VAL
47	S1	66	VAL
67	D1	6	GLY
67	D1	32	VAL
47	s1	225	VAL
79	s6	69	LEU
56	c0	35	ILE
61	c5	5	VAL
9	L7	178	ILE
47	S1	210	ILE
53	S7	98	ILE
59	C3	22	ALA
64	C8	14	ILE
76	E0	47	VAL
10	l8	237	ILE
41	q0	78	ILE
47	s1	22	ASP
79	s6	153	VAL
54	s8	78	ILE

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Mol	Chain	Res	Type
57	c1	129	ARG
64	c8	14	ILE
5	L3	317	ILE
46	S0	103	THR
60	C4	39	ILE
62	C6	39	VAL
64	C8	5	VAL
69	D3	130	VAL
70	D4	35	VAL
78	SM	12	VAL
11	l9	167	VAL
79	s6	162	VAL
72	d6	58	VAL
7	L5	125	VAL
53	S7	181	ILE
55	S9	134	ILE
17	m6	4	GLU
63	c7	98	GLY

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	190/190 (100%)	169 (89%)	21 (11%)	6	23
4	l2	190/190 (100%)	174 (92%)	16 (8%)	11	35
5	L3	322/322 (100%)	280 (87%)	42 (13%)	4	17
5	l3	322/322 (100%)	287 (89%)	35 (11%)	6	24
6	L4	288/288 (100%)	258 (90%)	30 (10%)	7	25
6	l4	288/288 (100%)	253 (88%)	35 (12%)	5	20
7	L5	242/244 (99%)	220 (91%)	22 (9%)	9	31
7	l5	243/244 (100%)	223 (92%)	20 (8%)	11	36
8	L6	134/153 (88%)	118 (88%)	16 (12%)	5	21
8	l6	135/153 (88%)	123 (91%)	12 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	L7	190/190 (100%)	169 (89%)	21 (11%)	6	23
9	l7	187/190 (98%)	164 (88%)	23 (12%)	4	20
10	L8	186/190 (98%)	169 (91%)	17 (9%)	9	31
10	l8	177/190 (93%)	155 (88%)	22 (12%)	4	19
11	L9	169/171 (99%)	143 (85%)	26 (15%)	2	12
11	l9	171/171 (100%)	144 (84%)	27 (16%)	2	11
12	M0	185/187 (99%)	163 (88%)	22 (12%)	5	21
12	m0	186/187 (100%)	162 (87%)	24 (13%)	4	18
13	M1	147/147 (100%)	127 (86%)	20 (14%)	3	16
13	m1	147/147 (100%)	125 (85%)	22 (15%)	3	13
14	M3	154/154 (100%)	139 (90%)	15 (10%)	8	29
14	m3	154/154 (100%)	140 (91%)	14 (9%)	9	31
15	M4	107/108 (99%)	99 (92%)	8 (8%)	13	39
15	m4	108/108 (100%)	95 (88%)	13 (12%)	5	20
16	M5	175/175 (100%)	164 (94%)	11 (6%)	18	47
16	m5	175/175 (100%)	162 (93%)	13 (7%)	13	40
17	M6	160/160 (100%)	147 (92%)	13 (8%)	11	36
17	m6	160/160 (100%)	150 (94%)	10 (6%)	18	47
18	M7	139/146 (95%)	120 (86%)	19 (14%)	3	16
18	m7	125/146 (86%)	110 (88%)	15 (12%)	5	20
19	M8	150/150 (100%)	134 (89%)	16 (11%)	6	25
19	m8	150/150 (100%)	135 (90%)	15 (10%)	7	27
20	M9	151/153 (99%)	135 (89%)	16 (11%)	6	25
20	m9	153/153 (100%)	136 (89%)	17 (11%)	6	23
21	N0	156/156 (100%)	134 (86%)	22 (14%)	3	16
21	n0	156/156 (100%)	136 (87%)	20 (13%)	4	18
22	N1	136/136 (100%)	116 (85%)	20 (15%)	3	14
22	n1	136/136 (100%)	124 (91%)	12 (9%)	10	33
23	N2	86/86 (100%)	73 (85%)	13 (15%)	3	13
23	n2	85/86 (99%)	77 (91%)	8 (9%)	8	30
24	N3	102/104 (98%)	91 (89%)	11 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	n3	104/104 (100%)	94 (90%)	10 (10%)	8	29
25	N4	55/129 (43%)	54 (98%)	1 (2%)	59	78
25	n4	100/129 (78%)	93 (93%)	7 (7%)	15	43
26	N5	103/104 (99%)	88 (85%)	15 (15%)	3	14
26	n5	104/104 (100%)	92 (88%)	12 (12%)	5	22
27	N6	108/108 (100%)	100 (93%)	8 (7%)	13	40
27	n6	106/108 (98%)	98 (92%)	8 (8%)	13	39
28	N7	115/115 (100%)	103 (90%)	12 (10%)	7	25
28	n7	115/115 (100%)	108 (94%)	7 (6%)	18	48
29	N8	118/118 (100%)	102 (86%)	16 (14%)	3	16
29	n8	118/118 (100%)	108 (92%)	10 (8%)	10	35
30	N9	44/46 (96%)	40 (91%)	4 (9%)	9	31
30	n9	46/46 (100%)	41 (89%)	5 (11%)	6	24
31	O0	81/84 (96%)	72 (89%)	9 (11%)	6	23
31	o0	84/84 (100%)	75 (89%)	9 (11%)	6	25
32	O1	89/96 (93%)	81 (91%)	8 (9%)	9	32
32	o1	94/96 (98%)	84 (89%)	10 (11%)	6	25
33	O2	108/109 (99%)	94 (87%)	14 (13%)	4	17
33	o2	109/109 (100%)	101 (93%)	8 (7%)	14	41
34	O3	90/90 (100%)	83 (92%)	7 (8%)	12	38
34	o3	90/90 (100%)	85 (94%)	5 (6%)	21	52
35	O4	95/95 (100%)	88 (93%)	7 (7%)	13	40
35	o4	95/95 (100%)	88 (93%)	7 (7%)	13	40
36	O5	104/104 (100%)	96 (92%)	8 (8%)	13	38
36	o5	103/104 (99%)	98 (95%)	5 (5%)	25	56
37	O6	79/81 (98%)	74 (94%)	5 (6%)	18	47
37	o6	81/81 (100%)	73 (90%)	8 (10%)	8	28
38	O7	69/70 (99%)	60 (87%)	9 (13%)	4	17
38	o7	70/70 (100%)	63 (90%)	7 (10%)	7	27
39	O8	68/68 (100%)	63 (93%)	5 (7%)	13	40
39	o8	67/68 (98%)	56 (84%)	11 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	O9	45/45 (100%)	39 (87%)	6 (13%)	4	17
40	o9	45/45 (100%)	43 (96%)	2 (4%)	28	59
41	Q0	47/47 (100%)	45 (96%)	2 (4%)	29	59
41	q0	47/47 (100%)	41 (87%)	6 (13%)	4	18
42	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	8
42	q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
43	Q2	90/90 (100%)	79 (88%)	11 (12%)	5	20
43	q2	90/90 (100%)	80 (89%)	10 (11%)	6	23
44	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	16
44	q3	71/71 (100%)	64 (90%)	7 (10%)	8	28
46	S0	166/173 (96%)	149 (90%)	17 (10%)	7	27
46	s0	166/173 (96%)	150 (90%)	16 (10%)	8	29
47	S1	189/192 (98%)	156 (82%)	33 (18%)	2	8
47	s1	192/192 (100%)	172 (90%)	20 (10%)	7	25
48	S2	176/176 (100%)	158 (90%)	18 (10%)	7	27
48	s2	176/176 (100%)	166 (94%)	10 (6%)	20	51
49	S3	169/182 (93%)	151 (89%)	18 (11%)	6	25
49	s3	182/182 (100%)	165 (91%)	17 (9%)	9	30
50	S4	219/221 (99%)	203 (93%)	16 (7%)	14	41
50	s4	221/221 (100%)	200 (90%)	21 (10%)	8	29
51	S5	173/173 (100%)	155 (90%)	18 (10%)	7	25
51	s5	173/173 (100%)	161 (93%)	12 (7%)	15	44
52	S6	167/201 (83%)	154 (92%)	13 (8%)	12	38
53	S7	160/166 (96%)	145 (91%)	15 (9%)	8	30
53	s7	166/166 (100%)	150 (90%)	16 (10%)	8	29
54	S8	148/161 (92%)	135 (91%)	13 (9%)	10	33
54	s8	150/161 (93%)	142 (95%)	8 (5%)	22	53
55	S9	152/158 (96%)	141 (93%)	11 (7%)	14	41
55	s9	158/158 (100%)	146 (92%)	12 (8%)	13	39
56	C0	77/98 (79%)	71 (92%)	6 (8%)	12	38
56	c0	73/98 (74%)	68 (93%)	5 (7%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	C1	126/129 (98%)	110 (87%)	16 (13%)	4	19
57	c1	129/129 (100%)	117 (91%)	12 (9%)	9	30
58	C2	82/119 (69%)	69 (84%)	13 (16%)	2	11
58	c2	88/119 (74%)	72 (82%)	16 (18%)	1	7
59	C3	127/127 (100%)	118 (93%)	9 (7%)	14	42
59	c3	127/127 (100%)	116 (91%)	11 (9%)	10	34
60	C4	81/97 (84%)	68 (84%)	13 (16%)	2	11
60	c4	97/97 (100%)	84 (87%)	13 (13%)	4	16
61	C5	96/117 (82%)	91 (95%)	5 (5%)	23	54
61	c5	103/117 (88%)	86 (84%)	17 (16%)	2	10
62	C6	113/118 (96%)	100 (88%)	13 (12%)	5	22
62	c6	118/118 (100%)	108 (92%)	10 (8%)	10	35
63	C7	94/124 (76%)	81 (86%)	13 (14%)	3	16
63	c7	92/124 (74%)	86 (94%)	6 (6%)	17	46
64	C8	126/128 (98%)	111 (88%)	15 (12%)	5	21
64	c8	128/128 (100%)	114 (89%)	14 (11%)	6	24
65	C9	110/115 (96%)	98 (89%)	12 (11%)	6	24
65	c9	115/115 (100%)	104 (90%)	11 (10%)	8	29
66	D0	96/102 (94%)	85 (88%)	11 (12%)	5	22
66	d0	102/102 (100%)	88 (86%)	14 (14%)	3	16
67	D1	74/74 (100%)	68 (92%)	6 (8%)	11	36
67	d1	74/74 (100%)	63 (85%)	11 (15%)	3	13
68	D2	110/110 (100%)	98 (89%)	12 (11%)	6	24
68	d2	110/110 (100%)	97 (88%)	13 (12%)	5	21
69	D3	119/119 (100%)	111 (93%)	8 (7%)	16	45
69	d3	119/119 (100%)	112 (94%)	7 (6%)	19	49
70	D4	112/112 (100%)	99 (88%)	13 (12%)	5	22
70	d4	112/112 (100%)	104 (93%)	8 (7%)	14	42
71	D5	61/61 (100%)	51 (84%)	10 (16%)	2	10
71	d5	61/61 (100%)	51 (84%)	10 (16%)	2	10
72	D6	83/83 (100%)	69 (83%)	14 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	d6	83/83 (100%)	73 (88%)	10 (12%)	5	20
73	D7	70/70 (100%)	63 (90%)	7 (10%)	7	27
73	d7	70/70 (100%)	64 (91%)	6 (9%)	10	35
74	D8	56/56 (100%)	51 (91%)	5 (9%)	9	32
74	d8	56/56 (100%)	50 (89%)	6 (11%)	6	25
75	D9	47/47 (100%)	44 (94%)	3 (6%)	17	46
75	d9	47/47 (100%)	40 (85%)	7 (15%)	3	13
76	E0	51/53 (96%)	42 (82%)	9 (18%)	2	8
76	e0	53/53 (100%)	46 (87%)	7 (13%)	4	17
77	SR	259/261 (99%)	246 (95%)	13 (5%)	24	55
77	sR	259/261 (99%)	238 (92%)	21 (8%)	11	36
78	SM	97/227 (43%)	85 (88%)	12 (12%)	4	19
78	sM	54/227 (24%)	50 (93%)	4 (7%)	13	40
79	s6	187/187 (100%)	168 (90%)	19 (10%)	7	27
All	All	18408/19292 (95%)	16513 (90%)	1895 (10%)	7	26

All (1895) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L2	20	THR
4	L2	23	ARG
4	L2	32	LEU
4	L2	45	VAL
4	L2	62	VAL
4	L2	74	GLU
4	L2	93	LYS
4	L2	97	ASN
4	L2	113	VAL
4	L2	114	SER
4	L2	116	VAL
4	L2	142	ASP
4	L2	159	SER
4	L2	165	VAL
4	L2	179	LEU
4	L2	181	LYS
4	L2	195	SER
4	L2	204	MET

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Mol	Chain	Res	Type
4	L2	207	VAL
4	L2	227	ARG
4	L2	246	LEU
5	L3	7	GLU
5	L3	17	LEU
5	L3	19	ARG
5	L3	37	ARG
5	L3	41	VAL
5	L3	70	ARG
5	L3	73	VAL
5	L3	77	THR
5	L3	81	THR
5	L3	84	VAL
5	L3	85	VAL
5	L3	89	VAL
5	L3	93	VAL
5	L3	99	LEU
5	L3	103	THR
5	L3	139	GLN
5	L3	140	ASP
5	L3	154	TYR
5	L3	160	VAL
5	L3	169	THR
5	L3	189	SER
5	L3	196	ARG
5	L3	202	THR
5	L3	205	VAL
5	L3	211	GLN
5	L3	214	MET
5	L3	236	LYS
5	L3	238	LEU
5	L3	246	LEU
5	L3	252	ILE
5	L3	260	VAL
5	L3	284	ARG
5	L3	290	ASP
5	L3	291	GLU
5	L3	293	ASN
5	L3	324	VAL
5	L3	332	ARG
5	L3	343	TYR
5	L3	348	ARG

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Mol	Chain	Res	Type
5	L3	372	THR
5	L3	375	GLU
5	L3	385	LYS
6	L4	54	GLU
6	L4	73	ARG
6	L4	74	ILE
6	L4	93	MET
6	L4	99	MET
6	L4	112	LYS
6	L4	120	TYR
6	L4	133	SER
6	L4	138	ARG
6	L4	144	LYS
6	L4	150	LEU
6	L4	160	GLN
6	L4	179	LEU
6	L4	188	ARG
6	L4	194	TYR
6	L4	195	ARG
6	L4	197	ARG
6	L4	206	LEU
6	L4	211	GLU
6	L4	216	VAL
6	L4	220	ARG
6	L4	230	VAL
6	L4	246	ARG
6	L4	258	LEU
6	L4	271	LYS
6	L4	313	LEU
6	L4	323	VAL
6	L4	327	LEU
6	L4	332	LYS
6	L4	349	THR
7	L5	13	SER
7	L5	15	ARG
7	L5	22	ARG
7	L5	23	ARG
7	L5	35	ARG
7	L5	41	LYS
7	L5	56	THR
7	L5	81	HIS
7	L5	92	LEU

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Mol	Chain	Res	Type
7	L5	99	TYR
7	L5	152	ARG
7	L5	155	THR
7	L5	158	ARG
7	L5	185	PHE
7	L5	187	THR
7	L5	188	GLU
7	L5	218	ARG
7	L5	222	LEU
7	L5	258	LYS
7	L5	259	LYS
7	L5	265	TYR
7	L5	277	LEU
8	L6	15	VAL
8	L6	18	LEU
8	L6	21	THR
8	L6	30	LEU
8	L6	52	VAL
8	L6	64	LEU
8	L6	84	VAL
8	L6	89	THR
8	L6	93	VAL
8	L6	98	VAL
8	L6	99	GLU
8	L6	109	GLU
8	L6	152	THR
8	L6	154	LEU
8	L6	156	LYS
8	L6	175	LYS
9	L7	21	LYS
9	L7	30	ARG
9	L7	52	GLN
9	L7	59	GLU
9	L7	60	ARG
9	L7	80	GLN
9	L7	84	VAL
9	L7	87	VAL
9	L7	93	ASN
9	L7	98	LYS
9	L7	140	SER
9	L7	150	LYS
9	L7	151	ARG

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Mol	Chain	Res	Type
9	L7	157	ASN
9	L7	158	LYS
9	L7	173	LEU
9	L7	176	TYR
9	L7	179	LEU
9	L7	200	ASN
9	L7	234	GLU
9	L7	239	LEU
10	L8	27	THR
10	L8	36	ILE
10	L8	38	GLN
10	L8	74	THR
10	L8	79	GLN
10	L8	124	ASP
10	L8	136	LEU
10	L8	157	VAL
10	L8	169	LEU
10	L8	172	LYS
10	L8	180	VAL
10	L8	181	LYS
10	L8	185	ARG
10	L8	227	ASP
10	L8	230	LYS
10	L8	245	LYS
10	L8	249	ARG
11	L9	16	VAL
11	L9	18	VAL
11	L9	42	ASP
11	L9	44	THR
11	L9	50	ASN
11	L9	52	LEU
11	L9	62	ARG
11	L9	68	LEU
11	L9	69	ARG
11	L9	70	THR
11	L9	80	THR
11	L9	92	TYR
11	L9	93	VAL
11	L9	104	VAL
11	L9	118	LEU
11	L9	140	VAL
11	L9	146	LEU

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Mol	Chain	Res	Type
11	L9	151	VAL
11	L9	153	ASP
11	L9	157	ASN
11	L9	161	LEU
11	L9	168	ARG
11	L9	173	ARG
11	L9	177	ASP
11	L9	180	TYR
11	L9	189	GLU
12	M0	3	ARG
12	M0	21	ARG
12	M0	22	TYR
12	M0	24	ARG
12	M0	30	LYS
12	M0	32	ARG
12	M0	36	LEU
12	M0	52	LEU
12	M0	60	LEU
12	M0	87	LEU
12	M0	102	MET
12	M0	109	ASP
12	M0	110	ARG
12	M0	112	GLN
12	M0	142	ASP
12	M0	149	VAL
12	M0	177	ASP
12	M0	197	VAL
12	M0	206	LEU
12	M0	210	ILE
12	M0	212	GLU
12	M0	213	PHE
13	M1	11	ASP
13	M1	22	SER
13	M1	28	ASP
13	M1	44	THR
13	M1	64	LYS
13	M1	71	VAL
13	M1	80	LEU
13	M1	94	ARG
13	M1	95	ASN
13	M1	114	ILE
13	M1	125	MET

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Mol	Chain	Res	Type
13	M1	130	VAL
13	M1	132	ASN
13	M1	140	ARG
13	M1	148	VAL
13	M1	155	THR
13	M1	171	VAL
13	M1	172	LEU
13	M1	173	ASP
13	M1	174	LYS
14	M3	13	HIS
14	M3	15	ARG
14	M3	17	HIS
14	M3	37	ASN
14	M3	54	LEU
14	M3	55	ARG
14	M3	58	VAL
14	M3	85	LEU
14	M3	104	ARG
14	M3	114	GLN
14	M3	131	LYS
14	M3	164	GLU
14	M3	168	ARG
14	M3	176	GLU
14	M3	194	GLU
15	M4	6	ILE
15	M4	8	LYS
15	M4	50	LYS
15	M4	53	VAL
15	M4	69	THR
15	M4	72	LEU
15	M4	102	LYS
15	M4	107	GLU
16	M5	10	LEU
16	M5	19	LEU
16	M5	80	THR
16	M5	83	LYS
16	M5	109	ARG
16	M5	117	ASN
16	M5	133	ILE
16	M5	138	GLN
16	M5	151	ILE
16	M5	182	ASN

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Mol	Chain	Res	Type
16	M5	183	THR
17	M6	4	GLU
17	M6	10	ASP
17	M6	12	LYS
17	M6	66	LYS
17	M6	68	ARG
17	M6	78	ARG
17	M6	84	LEU
17	M6	85	ARG
17	M6	89	SER
17	M6	94	ARG
17	M6	119	VAL
17	M6	128	ARG
17	M6	143	THR
18	M7	7	THR
18	M7	14	SER
18	M7	24	VAL
18	M7	32	THR
18	M7	36	ILE
18	M7	52	LEU
18	M7	55	GLN
18	M7	56	ARG
18	M7	69	ARG
18	M7	96	GLN
18	M7	112	LEU
18	M7	120	ASN
18	M7	121	GLN
18	M7	127	ARG
18	M7	128	ARG
18	M7	142	SER
18	M7	144	SER
18	M7	165	VAL
18	M7	168	LEU
19	M8	7	SER
19	M8	13	SER
19	M8	26	LEU
19	M8	31	LYS
19	M8	32	LEU
19	M8	39	ARG
19	M8	46	LYS
19	M8	49	LEU
19	M8	82	VAL

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Mol	Chain	Res	Type
19	M8	86	THR
19	M8	135	GLN
19	M8	138	LEU
19	M8	168	THR
19	M8	170	ARG
19	M8	178	ARG
19	M8	180	ARG
20	M9	8	LYS
20	M9	22	VAL
20	M9	39	ASN
20	M9	46	LYS
20	M9	47	ASN
20	M9	60	LYS
20	M9	91	SER
20	M9	103	ARG
20	M9	108	LYS
20	M9	134	HIS
20	M9	138	LEU
20	M9	144	GLN
20	M9	152	GLU
20	M9	156	ASN
20	M9	163	ARG
20	M9	180	LYS
21	N0	1	MET
21	N0	3	HIS
21	N0	14	LEU
21	N0	18	SER
21	N0	23	LYS
21	N0	45	LEU
21	N0	47	LYS
21	N0	51	VAL
21	N0	80	ARG
21	N0	85	SER
21	N0	87	THR
21	N0	100	VAL
21	N0	117	ARG
21	N0	120	SER
21	N0	125	LYS
21	N0	132	THR
21	N0	136	LYS
21	N0	137	ARG
21	N0	155	ARG

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Mol	Chain	Res	Type
21	N0	156	VAL
21	N0	167	ARG
21	N0	172	TYR
22	N1	12	ARG
22	N1	14	MET
22	N1	27	LEU
22	N1	52	MET
22	N1	78	LYS
22	N1	79	MET
22	N1	83	ARG
22	N1	88	ARG
22	N1	100	LYS
22	N1	102	ARG
22	N1	103	GLN
22	N1	104	GLU
22	N1	122	GLN
22	N1	126	VAL
22	N1	128	LEU
22	N1	139	ARG
22	N1	143	THR
22	N1	144	GLU
22	N1	146	ASN
22	N1	155	PRO
23	N2	16	THR
23	N2	29	ASP
23	N2	39	ASP
23	N2	43	VAL
23	N2	44	GLU
23	N2	52	ASN
23	N2	70	LYS
23	N2	72	SER
23	N2	80	THR
23	N2	87	ASN
23	N2	95	PHE
23	N2	100	THR
23	N2	107	PHE
24	N3	12	ARG
24	N3	32	ARG
24	N3	33	ASN
24	N3	47	ASN
24	N3	64	LYS
24	N3	69	LEU

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Mol	Chain	Res	Type
24	N3	102	ILE
24	N3	108	GLU
24	N3	112	SER
24	N3	115	THR
24	N3	125	LEU
25	N4	32	GLN
26	N5	40	LEU
26	N5	49	LYS
26	N5	51	VAL
26	N5	55	ASN
26	N5	69	SER
26	N5	70	GLU
26	N5	71	THR
26	N5	87	SER
26	N5	96	LYS
26	N5	105	VAL
26	N5	109	LYS
26	N5	115	ARG
26	N5	125	ARG
26	N5	134	ASP
26	N5	135	ILE
27	N6	13	ARG
27	N6	37	LYS
27	N6	51	ARG
27	N6	55	GLU
27	N6	56	VAL
27	N6	74	TYR
27	N6	76	LEU
27	N6	126	LEU
28	N7	14	VAL
28	N7	15	ARG
28	N7	30	ASP
28	N7	53	VAL
28	N7	55	LYS
28	N7	56	LYS
28	N7	64	LYS
28	N7	65	ARG
28	N7	75	VAL
28	N7	81	LEU
28	N7	102	GLU
28	N7	126	LYS
29	N8	4	ARG

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Mol	Chain	Res	Type
29	N8	8	THR
29	N8	10	LYS
29	N8	16	SER
29	N8	25	HIS
29	N8	26	ARG
29	N8	46	ASP
29	N8	56	VAL
29	N8	60	TYR
29	N8	65	GLN
29	N8	72	VAL
29	N8	73	LEU
29	N8	76	ASP
29	N8	78	LEU
29	N8	85	ASP
29	N8	133	LEU
30	N9	18	ARG
30	N9	19	ASN
30	N9	28	LYS
30	N9	33	LYS
31	O0	16	LEU
31	O0	36	GLN
31	O0	41	LEU
31	O0	57	GLU
31	O0	61	MET
31	O0	83	LYS
31	O0	97	ASP
31	O0	99	ASP
31	O0	104	LEU
32	O1	26	LYS
32	O1	73	LEU
32	O1	79	ARG
32	O1	86	LYS
32	O1	96	VAL
32	O1	102	LYS
32	O1	106	THR
32	O1	110	GLU
33	O2	14	THR
33	O2	15	LYS
33	O2	24	ARG
33	O2	34	LYS
33	O2	35	GLN
33	O2	54	LYS

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Mol	Chain	Res	Type
33	O2	73	THR
33	O2	75	LEU
33	O2	87	MET
33	O2	88	HIS
33	O2	90	LYS
33	O2	109	LEU
33	O2	113	LYS
33	O2	120	THR
34	O3	4	SER
34	O3	15	SER
34	O3	21	ARG
34	O3	54	ARG
34	O3	73	ARG
34	O3	74	THR
34	O3	98	VAL
35	O4	51	LEU
35	O4	71	THR
35	O4	79	SER
35	O4	81	CYS
35	O4	83	ASN
35	O4	86	LYS
35	O4	103	LYS
36	O5	4	VAL
36	O5	28	LEU
36	O5	31	LEU
36	O5	74	LYS
36	O5	79	ASP
36	O5	89	ARG
36	O5	90	ARG
36	O5	119	LYS
37	O6	21	THR
37	O6	43	LEU
37	O6	57	LEU
37	O6	76	ARG
37	O6	81	THR
38	O7	12	HIS
38	O7	17	THR
38	O7	21	ARG
38	O7	25	ARG
38	O7	33	THR
38	O7	44	THR
38	O7	59	THR

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Mol	Chain	Res	Type
38	O7	67	LEU
38	O7	68	LYS
39	O8	12	LEU
39	O8	24	THR
39	O8	41	THR
39	O8	69	LEU
39	O8	77	ARG
40	O9	13	MET
40	O9	19	GLN
40	O9	21	ARG
40	O9	36	ARG
40	O9	45	ARG
40	O9	51	ILE
41	Q0	109	ASN
41	Q0	128	LYS
42	Q1	2	ARG
42	Q1	9	ARG
42	Q1	11	ARG
42	Q1	13	LEU
43	Q2	7	THR
43	Q2	16	THR
43	Q2	29	LYS
43	Q2	35	LEU
43	Q2	45	ARG
43	Q2	71	ARG
43	Q2	74	CYS
43	Q2	83	LEU
43	Q2	84	THR
43	Q2	105	GLN
43	Q2	106	PHE
44	Q3	5	THR
44	Q3	11	THR
44	Q3	24	ARG
44	Q3	38	ASP
44	Q3	45	LYS
44	Q3	49	ARG
44	Q3	60	CYS
44	Q3	71	VAL
44	Q3	78	THR
44	Q3	84	ARG
46	S0	2	SER
46	S0	6	THR

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Mol	Chain	Res	Type
46	S0	7	PHE
46	S0	9	LEU
46	S0	24	LEU
46	S0	33	GLN
46	S0	62	ARG
46	S0	87	LEU
46	S0	119	ARG
46	S0	139	VAL
46	S0	157	ASP
46	S0	162	CYS
46	S0	185	ARG
46	S0	188	LEU
46	S0	198	MET
46	S0	200	ASP
46	S0	203	PHE
47	S1	26	ARG
47	S1	30	PHE
47	S1	38	PHE
47	S1	43	VAL
47	S1	61	LEU
47	S1	66	VAL
47	S1	70	LEU
47	S1	73	LEU
47	S1	78	ASP
47	S1	79	HIS
47	S1	81	PHE
47	S1	89	ASP
47	S1	95	ASN
47	S1	96	LEU
47	S1	97	LEU
47	S1	98	THR
47	S1	105	PHE
47	S1	111	ARG
47	S1	126	THR
47	S1	130	SER
47	S1	133	TYR
47	S1	148	ASN
47	S1	150	VAL
47	S1	167	VAL
47	S1	181	LEU
47	S1	202	LYS
47	S1	203	ASP

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Mol	Chain	Res	Type
47	S1	205	PHE
47	S1	211	HIS
47	S1	217	LEU
47	S1	220	GLN
47	S1	222	LYS
47	S1	223	PHE
48	S2	44	LEU
48	S2	55	GLU
48	S2	73	LEU
48	S2	111	VAL
48	S2	116	LYS
48	S2	140	ARG
48	S2	141	ARG
48	S2	152	HIS
48	S2	204	THR
48	S2	205	ARG
48	S2	206	THR
48	S2	221	THR
48	S2	222	TYR
48	S2	225	LEU
48	S2	233	GLN
48	S2	235	LEU
48	S2	241	ASP
48	S2	244	SER
49	S3	9	ARG
49	S3	17	PHE
49	S3	45	LYS
49	S3	64	ARG
49	S3	65	ARG
49	S3	76	ARG
49	S3	79	TYR
49	S3	83	THR
49	S3	87	TYR
49	S3	91	VAL
49	S3	108	LYS
49	S3	172	THR
49	S3	175	VAL
49	S3	176	LEU
49	S3	177	MET
49	S3	178	ARG
49	S3	181	VAL
49	S3	190	ARG

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Mol	Chain	Res	Type
50	S4	26	CYS
50	S4	30	ARG
50	S4	38	LEU
50	S4	56	LEU
50	S4	73	ASP
50	S4	77	ARG
50	S4	78	THR
50	S4	105	VAL
50	S4	117	GLU
50	S4	130	GLN
50	S4	139	VAL
50	S4	182	TYR
50	S4	206	ASP
50	S4	226	PHE
50	S4	227	VAL
50	S4	231	GLN
51	S5	20	PHE
51	S5	24	VAL
51	S5	41	LYS
51	S5	48	PHE
51	S5	51	VAL
51	S5	64	VAL
51	S5	65	ARG
51	S5	69	PHE
51	S5	76	ARG
51	S5	79	ASN
51	S5	93	LEU
51	S5	103	ASN
51	S5	108	LEU
51	S5	112	ARG
51	S5	116	HIS
51	S5	122	ASN
51	S5	194	LEU
51	S5	212	LYS
52	S6	4	ASN
52	S6	7	TYR
52	S6	23	ARG
52	S6	25	ARG
52	S6	58	LYS
52	S6	68	LEU
52	S6	89	ASP
52	S6	115	LYS

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Mol	Chain	Res	Type
52	S6	133	LEU
52	S6	160	ARG
52	S6	177	ARG
52	S6	190	GLN
52	S6	211	LEU
53	S7	46	ILE
53	S7	51	VAL
53	S7	60	ILE
53	S7	62	VAL
53	S7	64	VAL
53	S7	77	LEU
53	S7	82	GLU
53	S7	85	PHE
53	S7	109	VAL
53	S7	114	ARG
53	S7	117	THR
53	S7	130	VAL
53	S7	131	PHE
53	S7	159	VAL
53	S7	163	ASP
54	S8	29	LEU
54	S8	36	THR
54	S8	58	LEU
54	S8	70	GLU
54	S8	92	ARG
54	S8	93	THR
54	S8	110	ARG
54	S8	116	HIS
54	S8	121	LEU
54	S8	137	LYS
54	S8	142	LYS
54	S8	168	CYS
54	S8	179	CYS
55	S9	3	ARG
55	S9	28	LEU
55	S9	71	PHE
55	S9	103	ASP
55	S9	109	LEU
55	S9	132	ARG
55	S9	134	ILE
55	S9	141	VAL
55	S9	152	SER

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Mol	Chain	Res	Type
55	S9	171	ARG
55	S9	175	ARG
56	C0	1	MET
56	C0	13	GLN
56	C0	22	VAL
56	C0	49	LEU
56	C0	51	SER
56	C0	56	LYS
57	C1	7	VAL
57	C1	8	GLN
57	C1	10	GLU
57	C1	15	LYS
57	C1	16	GLN
57	C1	20	PHE
57	C1	40	LEU
57	C1	63	LEU
57	C1	67	ARG
57	C1	69	LYS
57	C1	80	MET
57	C1	83	THR
57	C1	116	ARG
57	C1	125	VAL
57	C1	127	GLN
57	C1	129	ARG
58	C2	28	LEU
58	C2	29	LYS
58	C2	43	ARG
58	C2	52	LEU
58	C2	61	VAL
58	C2	62	LEU
58	C2	63	VAL
58	C2	66	VAL
58	C2	88	LEU
58	C2	100	TRP
58	C2	121	VAL
58	C2	124	LYS
58	C2	130	THR
59	C3	3	ARG
59	C3	64	ARG
59	C3	84	ILE
59	C3	107	LYS
59	C3	115	LEU

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Mol	Chain	Res	Type
59	C3	125	LEU
59	C3	134	VAL
59	C3	140	LYS
59	C3	145	THR
60	C4	16	VAL
60	C4	20	TYR
60	C4	29	HIS
60	C4	31	THR
60	C4	41	ARG
60	C4	42	VAL
60	C4	43	THR
60	C4	81	VAL
60	C4	92	LYS
60	C4	99	GLN
60	C4	111	ARG
60	C4	123	SER
60	C4	135	ARG
61	C5	36	LEU
61	C5	44	ARG
61	C5	50	THR
61	C5	57	MET
61	C5	124	THR
62	C6	28	LEU
62	C6	43	ILE
62	C6	47	LYS
62	C6	52	LEU
62	C6	53	LEU
62	C6	58	ASP
62	C6	60	PHE
62	C6	66	ARG
62	C6	69	VAL
62	C6	97	VAL
62	C6	103	ASN
62	C6	118	ILE
62	C6	123	ARG
63	C7	3	ARG
63	C7	23	LYS
63	C7	25	THR
63	C7	36	ASP
63	C7	46	LEU
63	C7	71	PHE
63	C7	84	TYR

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Mol	Chain	Res	Type
63	C7	85	VAL
63	C7	87	GLU
63	C7	88	VAL
63	C7	105	GLN
63	C7	108	ASP
63	C7	119	LEU
64	C8	4	VAL
64	C8	11	PHE
64	C8	25	ASN
64	C8	28	ILE
64	C8	55	HIS
64	C8	79	TYR
64	C8	80	LYS
64	C8	81	ILE
64	C8	85	PHE
64	C8	100	THR
64	C8	132	ARG
64	C8	133	VAL
64	C8	136	GLN
64	C8	143	ARG
64	C8	145	ARG
65	C9	18	TYR
65	C9	29	GLU
65	C9	33	TYR
65	C9	35	ASP
65	C9	67	MET
65	C9	69	LYS
65	C9	70	GLN
65	C9	75	LYS
65	C9	114	VAL
65	C9	126	GLU
65	C9	130	ARG
65	C9	134	ARG
66	D0	18	GLN
66	D0	22	ILE
66	D0	30	LYS
66	D0	48	HIS
66	D0	57	ARG
66	D0	58	LEU
66	D0	70	THR
66	D0	72	ASN
66	D0	74	GLU

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Mol	Chain	Res	Type
66	D0	87	HIS
66	D0	109	GLU
67	D1	1	MET
67	D1	60	ARG
67	D1	67	ASP
67	D1	80	LYS
67	D1	81	ASN
67	D1	86	SER
68	D2	4	SER
68	D2	25	VAL
68	D2	31	SER
68	D2	56	HIS
68	D2	65	LEU
68	D2	76	SER
68	D2	81	VAL
68	D2	93	LEU
68	D2	117	ARG
68	D2	126	LEU
68	D2	128	PHE
68	D2	129	VAL
69	D3	18	HIS
69	D3	19	ARG
69	D3	73	ARG
69	D3	75	GLN
69	D3	92	CYS
69	D3	107	PHE
69	D3	132	LEU
69	D3	135	LEU
70	D4	10	ARG
70	D4	28	LEU
70	D4	35	VAL
70	D4	57	VAL
70	D4	61	ARG
70	D4	62	THR
70	D4	72	PHE
70	D4	93	ARG
70	D4	111	LYS
70	D4	115	ASP
70	D4	124	ARG
70	D4	131	ARG
70	D4	132	ARG
71	D5	40	VAL

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Mol	Chain	Res	Type
71	D5	42	LEU
71	D5	49	ARG
71	D5	58	ARG
71	D5	60	VAL
71	D5	63	SER
71	D5	64	VAL
71	D5	69	LEU
71	D5	85	LYS
71	D5	97	LYS
72	D6	7	SER
72	D6	10	ARG
72	D6	12	LYS
72	D6	15	ARG
72	D6	37	LYS
72	D6	39	MET
72	D6	58	VAL
72	D6	66	LYS
72	D6	69	ASN
72	D6	82	ARG
72	D6	84	VAL
72	D6	85	ARG
72	D6	88	SER
72	D6	90	GLU
73	D7	3	LEU
73	D7	33	LEU
73	D7	49	HIS
73	D7	56	CYS
73	D7	59	CYS
73	D7	77	THR
73	D7	79	PHE
74	D8	5	THR
74	D8	7	VAL
74	D8	15	VAL
74	D8	58	GLU
74	D8	67	ARG
75	D9	7	TRP
75	D9	27	HIS
75	D9	32	ARG
76	E0	21	VAL
76	E0	26	LYS
76	E0	48	THR
76	E0	49	LEU

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Mol	Chain	Res	Type
76	E0	50	VAL
76	E0	51	ASN
76	E0	53	LYS
76	E0	54	ARG
76	E0	56	MET
77	SR	50	ASP
77	SR	52	GLN
77	SR	53	LYS
77	SR	64	HIS
77	SR	102	ARG
77	SR	121	MET
77	SR	141	LEU
77	SR	149	ASP
77	SR	156	VAL
77	SR	234	LEU
77	SR	248	ASN
77	SR	278	PHE
77	SR	290	VAL
78	SM	23	LYS
78	SM	24	GLU
78	SM	37	VAL
78	SM	49	LYS
78	SM	68	ARG
78	SM	69	ARG
78	SM	72	ARG
78	SM	73	SER
78	SM	84	LYS
78	SM	89	ARG
78	SM	102	THR
78	SM	134	ASP
4	12	44	ILE
4	12	45	VAL
4	12	61	VAL
4	12	109	GLU
4	12	113	VAL
4	12	142	ASP
4	12	147	ARG
4	12	179	LEU
4	12	180	LEU
4	12	193	ARG
4	12	207	VAL
4	12	215	ASN

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Mol	Chain	Res	Type
4	12	217	GLN
4	12	227	ARG
4	12	242	ARG
4	12	246	LEU
5	13	2	SER
5	13	3	HIS
5	13	4	ARG
5	13	10	ARG
5	13	24	SER
5	13	37	ARG
5	13	41	VAL
5	13	44	THR
5	13	84	VAL
5	13	85	VAL
5	13	99	LEU
5	13	103	THR
5	13	112	ASP
5	13	114	VAL
5	13	120	LYS
5	13	139	GLN
5	13	140	ASP
5	13	148	LEU
5	13	156	SER
5	13	169	THR
5	13	183	LEU
5	13	210	GLU
5	13	229	VAL
5	13	232	ARG
5	13	238	LEU
5	13	246	LEU
5	13	259	HIS
5	13	260	VAL
5	13	274	SER
5	13	284	ARG
5	13	328	ILE
5	13	332	ARG
5	13	338	LEU
5	13	348	ARG
5	13	369	ARG
6	14	3	ARG
6	14	10	SER
6	14	37	THR

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Mol	Chain	Res	Type
6	14	47	ARG
6	14	54	GLU
6	14	63	GLU
6	14	92	ASN
6	14	94	CYS
6	14	120	TYR
6	14	138	ARG
6	14	143	GLU
6	14	144	LYS
6	14	156	LEU
6	14	188	ARG
6	14	194	TYR
6	14	197	ARG
6	14	198	ARG
6	14	206	LEU
6	14	217	LYS
6	14	220	ARG
6	14	243	HIS
6	14	246	ARG
6	14	256	THR
6	14	258	LEU
6	14	259	ASP
6	14	261	VAL
6	14	279	HIS
6	14	283	THR
6	14	284	SER
6	14	294	GLU
6	14	313	LEU
6	14	319	LYS
6	14	323	VAL
6	14	327	LEU
6	14	362	ASP
7	15	34	LYS
7	15	45	ASN
7	15	50	ARG
7	15	75	LEU
7	15	81	HIS
7	15	123	GLU
7	15	124	GLU
7	15	128	GLU
7	15	131	LEU
7	15	140	ARG

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Mol	Chain	Res	Type
7	15	152	ARG
7	15	155	THR
7	15	185	PHE
7	15	222	LEU
7	15	237	GLU
7	15	259	LYS
7	15	260	PHE
7	15	268	GLU
7	15	273	ARG
7	15	279	LYS
8	16	21	THR
8	16	26	ARG
8	16	30	LEU
8	16	64	LEU
8	16	65	ILE
8	16	87	THR
8	16	90	LYS
8	16	93	VAL
8	16	134	ARG
8	16	152	THR
8	16	154	LEU
8	16	155	LEU
9	17	45	LEU
9	17	46	GLU
9	17	60	ARG
9	17	83	LEU
9	17	84	VAL
9	17	87	VAL
9	17	88	ARG
9	17	111	ILE
9	17	112	ASN
9	17	128	LYS
9	17	151	ARG
9	17	166	ASN
9	17	173	LEU
9	17	179	LEU
9	17	180	SER
9	17	182	ASP
9	17	184	LEU
9	17	190	THR
9	17	191	VAL
9	17	228	SER

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Mol	Chain	Res	Type
9	17	229	PHE
9	17	234	GLU
9	17	239	LEU
10	18	61	GLN
10	18	71	VAL
10	18	93	LEU
10	18	98	ARG
10	18	108	ARG
10	18	111	LYS
10	18	134	TYR
10	18	136	LEU
10	18	149	LYS
10	18	150	LEU
10	18	155	ASN
10	18	173	MET
10	18	180	VAL
10	18	183	LYS
10	18	200	LEU
10	18	202	GLU
10	18	204	ARG
10	18	213	LYS
10	18	222	PHE
10	18	226	TYR
10	18	228	GLU
10	18	238	LEU
11	19	3	TYR
11	19	5	GLN
11	19	6	THR
11	19	16	VAL
11	19	22	SER
11	19	33	THR
11	19	52	LEU
11	19	55	VAL
11	19	68	LEU
11	19	82	VAL
11	19	92	TYR
11	19	93	VAL
11	19	104	VAL
11	19	105	GLU
11	19	110	LYS
11	19	130	ASP
11	19	138	THR

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Mol	Chain	Res	Type
11	l9	140	VAL
11	l9	143	GLU
11	l9	146	LEU
11	l9	149	ASN
11	l9	151	VAL
11	l9	161	LEU
11	l9	165	CYS
11	l9	172	ILE
11	l9	177	ASP
11	l9	191	LEU
12	m0	24	ARG
12	m0	26	VAL
12	m0	29	SER
12	m0	36	LEU
12	m0	42	THR
12	m0	44	ASP
12	m0	52	LEU
12	m0	82	ARG
12	m0	101	LYS
12	m0	105	CYS
12	m0	110	ARG
12	m0	111	LEU
12	m0	112	GLN
12	m0	130	ASP
12	m0	139	ARG
12	m0	140	THR
12	m0	142	ASP
12	m0	150	GLU
12	m0	163	GLN
12	m0	186	GLU
12	m0	197	VAL
12	m0	208	ASN
12	m0	217	PHE
12	m0	220	GLN
13	m1	10	ARG
13	m1	11	ASP
13	m1	12	LEU
13	m1	25	GLU
13	m1	28	ASP
13	m1	30	LEU
13	m1	68	HIS
13	m1	92	ARG

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Mol	Chain	Res	Type
13	m1	101	ASN
13	m1	107	ASP
13	m1	108	GLU
13	m1	110	ILE
13	m1	111	ASP
13	m1	112	LEU
13	m1	115	LYS
13	m1	116	TYR
13	m1	127	PHE
13	m1	133	ARG
13	m1	152	HIS
13	m1	153	LYS
13	m1	155	THR
13	m1	174	LYS
14	m3	22	VAL
14	m3	45	LYS
14	m3	46	ILE
14	m3	54	LEU
14	m3	58	VAL
14	m3	59	ARG
14	m3	67	ARG
14	m3	69	VAL
14	m3	92	THR
14	m3	100	ARG
14	m3	107	GLU
14	m3	114	GLN
14	m3	162	ASN
14	m3	186	ARG
15	m4	20	VAL
15	m4	21	VAL
15	m4	42	LYS
15	m4	63	VAL
15	m4	69	THR
15	m4	72	LEU
15	m4	80	THR
15	m4	90	VAL
15	m4	91	CYS
15	m4	98	SER
15	m4	102	LYS
15	m4	108	ARG
15	m4	129	TYR
16	m5	10	LEU

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Mol	Chain	Res	Type
16	m5	13	LYS
16	m5	17	ASP
16	m5	24	ARG
16	m5	37	HIS
16	m5	49	ARG
16	m5	68	ARG
16	m5	75	VAL
16	m5	109	ARG
16	m5	116	LEU
16	m5	122	ASN
16	m5	190	THR
16	m5	201	ARG
17	m6	66	LYS
17	m6	67	THR
17	m6	68	ARG
17	m6	106	GLU
17	m6	108	ILE
17	m6	115	LYS
17	m6	119	VAL
17	m6	178	VAL
17	m6	182	ASN
17	m6	187	GLU
18	m7	23	ARG
18	m7	24	VAL
18	m7	31	GLU
18	m7	32	THR
18	m7	46	LYS
18	m7	53	ASP
18	m7	56	ARG
18	m7	64	ASN
18	m7	75	GLU
18	m7	96	GLN
18	m7	107	LEU
18	m7	116	HIS
18	m7	125	GLN
18	m7	126	ARG
18	m7	144	SER
19	m8	3	ILE
19	m8	20	LYS
19	m8	26	LEU
19	m8	49	LEU
19	m8	55	SER

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Mol	Chain	Res	Type
19	m8	86	THR
19	m8	135	GLN
19	m8	138	LEU
19	m8	141	ARG
19	m8	148	GLU
19	m8	150	VAL
19	m8	155	MET
19	m8	170	ARG
19	m8	174	ARG
19	m8	178	ARG
20	m9	7	GLN
20	m9	9	ARG
20	m9	10	LEU
20	m9	29	THR
20	m9	43	LYS
20	m9	70	LYS
20	m9	74	ARG
20	m9	99	LEU
20	m9	105	LEU
20	m9	128	LYS
20	m9	134	HIS
20	m9	144	GLN
20	m9	150	GLN
20	m9	164	LEU
20	m9	180	LYS
20	m9	184	LEU
20	m9	188	ASP
21	n0	1	MET
21	n0	3	HIS
21	n0	13	ARG
21	n0	40	ARG
21	n0	51	VAL
21	n0	80	ARG
21	n0	87	THR
21	n0	88	HIS
21	n0	113	ARG
21	n0	115	ARG
21	n0	120	SER
21	n0	131	LYS
21	n0	132	THR
21	n0	137	ARG
21	n0	155	ARG

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Mol	Chain	Res	Type
21	n0	160	THR
21	n0	162	THR
21	n0	164	SER
21	n0	167	ARG
21	n0	172	TYR
22	n1	12	ARG
22	n1	18	ASP
22	n1	26	HIS
22	n1	32	LYS
22	n1	83	ARG
22	n1	88	ARG
22	n1	89	LEU
22	n1	98	HIS
22	n1	104	GLU
22	n1	124	VAL
22	n1	129	LYS
22	n1	139	ARG
23	n2	21	SER
23	n2	39	ASP
23	n2	50	LEU
23	n2	78	TYR
23	n2	86	LYS
23	n2	90	ARG
23	n2	91	ASP
23	n2	100	THR
24	n3	7	GLN
24	n3	13	ILE
24	n3	32	ARG
24	n3	45	ARG
24	n3	54	LEU
24	n3	83	LYS
24	n3	88	ARG
24	n3	115	THR
24	n3	128	ARG
24	n3	135	VAL
25	n4	1	MET
25	n4	19	THR
25	n4	39	LEU
25	n4	57	LYS
25	n4	96	LEU
25	n4	105	ARG
25	n4	123	ARG

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Mol	Chain	Res	Type
26	n5	42	ARG
26	n5	48	SER
26	n5	49	LYS
26	n5	51	VAL
26	n5	57	LEU
26	n5	87	SER
26	n5	104	GLU
26	n5	108	LEU
26	n5	115	ARG
26	n5	133	LEU
26	n5	135	ILE
26	n5	139	ILE
27	n6	7	ASP
27	n6	8	VAL
27	n6	37	LYS
27	n6	56	VAL
27	n6	74	TYR
27	n6	89	LYS
27	n6	94	SER
27	n6	115	ARG
28	n7	4	PHE
28	n7	26	VAL
28	n7	65	ARG
28	n7	75	VAL
28	n7	81	LEU
28	n7	102	GLU
28	n7	127	ASN
29	n8	6	THR
29	n8	8	THR
29	n8	24	LYS
29	n8	42	ARG
29	n8	46	ASP
29	n8	60	TYR
29	n8	78	LEU
29	n8	80	THR
29	n8	84	GLU
29	n8	85	ASP
30	n9	18	ARG
30	n9	21	ILE
30	n9	23	LYS
30	n9	25	LYS
30	n9	27	TYR

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Mol	Chain	Res	Type
31	o0	10	ILE
31	o0	18	ILE
31	o0	41	LEU
31	o0	55	GLU
31	o0	61	MET
31	o0	64	LYS
31	o0	83	LYS
31	o0	86	ARG
31	o0	100	ILE
32	o1	16	LEU
32	o1	24	SER
32	o1	28	ARG
32	o1	31	ARG
32	o1	44	MET
32	o1	62	ARG
32	o1	64	VAL
32	o1	91	SER
32	o1	106	THR
32	o1	111	GLU
33	o2	19	ARG
33	o2	33	ARG
33	o2	73	THR
33	o2	75	LEU
33	o2	82	LEU
33	o2	87	MET
33	o2	125	ARG
33	o2	126	LEU
34	o3	21	ARG
34	o3	49	ILE
34	o3	59	VAL
34	o3	60	ARG
34	o3	81	VAL
35	o4	15	THR
35	o4	33	GLN
35	o4	44	CYS
35	o4	60	ARG
35	o4	71	THR
35	o4	80	ARG
35	o4	88	ARG
36	o5	4	VAL
36	o5	23	ASP
36	o5	31	LEU

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Mol	Chain	Res	Type
36	o5	43	LYS
36	o5	101	THR
37	o6	3	VAL
37	o6	13	LYS
37	o6	17	VAL
37	o6	43	LEU
37	o6	68	ARG
37	o6	70	ARG
37	o6	98	ARG
37	o6	100	HIS
38	o7	12	HIS
38	o7	37	CYS
38	o7	44	THR
38	o7	45	ARG
38	o7	55	ARG
38	o7	67	LEU
38	o7	76	ASN
39	o8	16	ARG
39	o8	19	ASP
39	o8	24	THR
39	o8	28	ASN
39	o8	32	ASN
39	o8	41	THR
39	o8	46	ARG
39	o8	53	THR
39	o8	54	LEU
39	o8	64	LYS
39	o8	69	LEU
40	o9	21	ARG
40	o9	23	LEU
41	q0	85	LEU
41	q0	92	ASP
41	q0	93	LYS
41	q0	99	CYS
41	q0	106	ARG
41	q0	127	LEU
42	q1	2	ARG
42	q1	6	ARG
42	q1	13	LEU
42	q1	19	LYS
42	q1	21	ARG
42	q1	24	SER

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Mol	Chain	Res	Type
43	q2	2	VAL
43	q2	4	VAL
43	q2	8	ARG
43	q2	38	GLN
43	q2	71	ARG
43	q2	77	CYS
43	q2	80	ARG
43	q2	84	THR
43	q2	85	LEU
43	q2	93	LEU
44	q3	4	ARG
44	q3	6	LYS
44	q3	16	VAL
44	q3	20	SER
44	q3	59	CYS
44	q3	62	LYS
44	q3	90	VAL
46	s0	22	THR
46	s0	23	HIS
46	s0	24	LEU
46	s0	29	VAL
46	s0	30	GLN
46	s0	31	VAL
46	s0	55	GLU
46	s0	59	LEU
46	s0	139	VAL
46	s0	151	SER
46	s0	179	ARG
46	s0	183	ARG
46	s0	185	ARG
46	s0	188	LEU
46	s0	195	TRP
46	s0	200	ASP
47	s1	21	VAL
47	s1	25	THR
47	s1	47	LEU
47	s1	49	ASN
47	s1	66	VAL
47	s1	70	LEU
47	s1	77	GLU
47	s1	85	LYS
47	s1	105	PHE

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Mol	Chain	Res	Type
47	s1	108	ASP
47	s1	115	ARG
47	s1	128	LYS
47	s1	150	VAL
47	s1	180	THR
47	s1	181	LEU
47	s1	194	ASN
47	s1	205	PHE
47	s1	209	ASN
47	s1	223	PHE
47	s1	224	ASP
48	s2	53	ILE
48	s2	73	LEU
48	s2	90	THR
48	s2	97	ARG
48	s2	111	VAL
48	s2	136	VAL
48	s2	141	ARG
48	s2	161	LYS
48	s2	164	SER
48	s2	222	TYR
49	s3	4	LEU
49	s3	9	ARG
49	s3	10	LYS
49	s3	57	ASP
49	s3	61	GLU
49	s3	76	ARG
49	s3	90	ARG
49	s3	91	VAL
49	s3	128	GLU
49	s3	134	CYS
49	s3	142	LEU
49	s3	156	PHE
49	s3	157	LEU
49	s3	164	VAL
49	s3	181	VAL
49	s3	212	LYS
49	s3	218	LEU
50	s4	7	LYS
50	s4	17	HIS
50	s4	39	ARG
50	s4	51	ARG

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Mol	Chain	Res	Type
50	s4	68	ARG
50	s4	73	ASP
50	s4	100	ARG
50	s4	105	VAL
50	s4	126	VAL
50	s4	139	VAL
50	s4	140	VAL
50	s4	180	LEU
50	s4	182	TYR
50	s4	189	LEU
50	s4	192	ILE
50	s4	214	LEU
50	s4	215	ASP
50	s4	222	LEU
50	s4	226	PHE
50	s4	246	LEU
50	s4	248	ILE
51	s5	24	VAL
51	s5	29	ILE
51	s5	43	PHE
51	s5	76	ARG
51	s5	94	THR
51	s5	112	ARG
51	s5	114	ILE
51	s5	131	GLN
51	s5	149	VAL
51	s5	156	ARG
51	s5	157	ARG
51	s5	194	LEU
79	s6	7	TYR
79	s6	71	THR
79	s6	108	VAL
79	s6	111	LEU
79	s6	115	LYS
79	s6	122	GLU
79	s6	124	LEU
79	s6	125	THR
79	s6	136	LYS
79	s6	151	ASP
79	s6	153	VAL
79	s6	156	PHE
79	s6	164	LYS

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Mol	Chain	Res	Type
79	s6	169	TYR
79	s6	177	ARG
79	s6	193	LEU
79	s6	197	ASN
79	s6	212	LEU
79	s6	216	LEU
53	s7	2	SER
53	s7	34	LEU
53	s7	38	LEU
53	s7	50	ASP
53	s7	55	LYS
53	s7	64	VAL
53	s7	97	ARG
53	s7	110	GLN
53	s7	112	ARG
53	s7	114	ARG
53	s7	116	ARG
53	s7	127	GLU
53	s7	139	ARG
53	s7	157	LYS
53	s7	159	VAL
53	s7	163	ASP
54	s8	29	LEU
54	s8	36	THR
54	s8	46	VAL
54	s8	72	ILE
54	s8	88	ASN
54	s8	158	SER
54	s8	199	LYS
54	s8	200	LYS
55	s9	13	SER
55	s9	14	THR
55	s9	17	ARG
55	s9	28	LEU
55	s9	39	LYS
55	s9	59	LEU
55	s9	78	ARG
55	s9	105	LEU
55	s9	130	THR
55	s9	141	VAL
55	s9	149	ARG
55	s9	154	LYS

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Mol	Chain	Res	Type
56	c0	3	MET
56	c0	15	LEU
56	c0	28	ASN
56	c0	41	TYR
56	c0	55	VAL
57	c1	5	LEU
57	c1	16	GLN
57	c1	28	SER
57	c1	33	ARG
57	c1	60	PHE
57	c1	67	ARG
57	c1	82	ARG
57	c1	102	LYS
57	c1	116	ARG
57	c1	121	ASP
57	c1	129	ARG
57	c1	138	ASN
58	c2	25	GLU
58	c2	54	ARG
58	c2	58	LEU
58	c2	61	VAL
58	c2	62	LEU
58	c2	63	VAL
58	c2	74	LEU
58	c2	85	LYS
58	c2	88	LEU
58	c2	89	ILE
58	c2	97	LEU
58	c2	103	LEU
58	c2	126	TRP
58	c2	129	GLU
58	c2	138	GLU
58	c2	140	PHE
59	c3	12	SER
59	c3	20	ARG
59	c3	64	ARG
59	c3	65	VAL
59	c3	70	LYS
59	c3	72	MET
59	c3	94	LYS
59	c3	115	LEU
59	c3	125	LEU

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Mol	Chain	Res	Type
59	c3	139	TRP
59	c3	141	TYR
60	c4	10	ASN
60	c4	14	PHE
60	c4	16	VAL
60	c4	20	TYR
60	c4	58	TYR
60	c4	66	ASP
60	c4	102	LEU
60	c4	110	LEU
60	c4	116	GLU
60	c4	118	VAL
60	c4	124	ASP
60	c4	136	ARG
60	c4	137	LEU
61	c5	10	ARG
61	c5	22	LEU
61	c5	36	LEU
61	c5	40	ARG
61	c5	49	MET
61	c5	50	THR
61	c5	52	LYS
61	c5	56	PHE
61	c5	69	GLU
61	c5	77	ARG
61	c5	93	VAL
61	c5	102	PHE
61	c5	107	ILE
61	c5	124	THR
61	c5	126	VAL
61	c5	128	HIS
61	c5	130	ARG
62	c6	23	LYS
62	c6	26	LYS
62	c6	40	GLU
62	c6	62	ASN
62	c6	64	ASP
62	c6	66	ARG
62	c6	68	ARG
62	c6	97	VAL
62	c6	109	PHE
62	c6	114	ARG

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Mol	Chain	Res	Type
63	c7	24	LEU
63	c7	29	GLN
63	c7	78	ARG
63	c7	79	GLU
63	c7	84	TYR
63	c7	108	ASP
64	c8	7	GLU
64	c8	26	ILE
64	c8	61	LEU
64	c8	66	LEU
64	c8	85	PHE
64	c8	88	ARG
64	c8	91	ASP
64	c8	94	ASP
64	c8	97	ASP
64	c8	104	ASN
64	c8	112	ASP
64	c8	115	ARG
64	c8	116	LEU
64	c8	136	GLN
65	c9	18	TYR
65	c9	33	TYR
65	c9	34	VAL
65	c9	41	SER
65	c9	70	GLN
65	c9	95	ASP
65	c9	111	ILE
65	c9	122	ARG
65	c9	123	ARG
65	c9	133	ASP
65	c9	141	GLU
66	d0	14	GLN
66	d0	15	GLN
66	d0	16	GLN
66	d0	18	GLN
66	d0	19	ILE
66	d0	21	LYS
66	d0	23	ARG
66	d0	34	LEU
66	d0	46	GLU
66	d0	57	ARG
66	d0	61	LYS

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Mol	Chain	Res	Type
66	d0	74	GLU
66	d0	102	ARG
66	d0	116	VAL
67	d1	3	ASN
67	d1	5	LYS
67	d1	11	LEU
67	d1	41	GLU
67	d1	44	ARG
67	d1	59	VAL
67	d1	62	ARG
67	d1	70	ASN
67	d1	71	ARG
67	d1	76	ASP
67	d1	78	LEU
68	d2	4	SER
68	d2	6	VAL
68	d2	25	VAL
68	d2	28	ARG
68	d2	37	PHE
68	d2	42	GLN
68	d2	55	ASP
68	d2	68	ARG
68	d2	93	LEU
68	d2	98	GLN
68	d2	103	ILE
68	d2	126	LEU
68	d2	129	VAL
69	d3	9	LEU
69	d3	19	ARG
69	d3	99	ASN
69	d3	107	PHE
69	d3	131	SER
69	d3	132	LEU
69	d3	144	ARG
70	d4	10	ARG
70	d4	28	LEU
70	d4	35	VAL
70	d4	37	LYS
70	d4	49	LYS
70	d4	72	PHE
70	d4	91	LEU
70	d4	93	ARG

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Mol	Chain	Res	Type
71	d5	37	GLN
71	d5	46	LYS
71	d5	49	ARG
71	d5	52	LYS
71	d5	53	GLU
71	d5	60	VAL
71	d5	67	ASP
71	d5	85	LYS
71	d5	89	ILE
71	d5	98	GLN
72	d6	7	SER
72	d6	26	CYS
72	d6	27	SER
72	d6	28	LYS
72	d6	46	GLU
72	d6	53	LEU
72	d6	58	VAL
72	d6	61	GLU
72	d6	82	ARG
72	d6	84	VAL
73	d7	23	THR
73	d7	42	ASN
73	d7	56	CYS
73	d7	59	CYS
73	d7	77	THR
73	d7	81	ARG
74	d8	7	VAL
74	d8	8	THR
74	d8	15	VAL
74	d8	32	PHE
74	d8	61	ARG
74	d8	64	ARG
75	d9	5	ASN
75	d9	8	PHE
75	d9	14	TYR
75	d9	30	LEU
75	d9	32	ARG
75	d9	44	ARG
75	d9	54	LYS
76	e0	44	PHE
76	e0	46	ASN
76	e0	49	LEU

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Mol	Chain	Res	Type
76	e0	51	ASN
76	e0	53	LYS
76	e0	54	ARG
76	e0	56	MET
77	sR	4	ASN
77	sR	5	GLU
77	sR	9	LEU
77	sR	16	HIS
77	sR	29	GLN
77	sR	38	ARG
77	sR	60	SER
77	sR	106	HIS
77	sR	127	ARG
77	sR	139	GLN
77	sR	140	CYS
77	sR	145	LEU
77	sR	163	ASP
77	sR	167	VAL
77	sR	185	GLN
77	sR	207	ASP
77	sR	248	ASN
77	sR	250	TYR
77	sR	251	TRP
77	sR	290	VAL
77	sR	316	MET
78	sM	30	THR
78	sM	53	ARG
78	sM	63	ASP
78	sM	83	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
4	L2	209	HIS
4	L2	216	HIS
7	L5	40	HIS
10	L8	79	GLN
12	M0	112	GLN
13	M1	109	HIS
14	M3	99	HIS
16	M5	194	GLN
18	M7	10	ASN

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Mol	Chain	Res	Type
21	N0	62	ASN
22	N1	77	ASN
24	N3	33	ASN
46	S0	23	HIS
46	S0	30	GLN
47	S1	149	GLN
50	S4	130	GLN
51	S5	44	ASN
52	S6	13	GLN
52	S6	176	GLN
55	S9	48	GLN
56	C0	39	ASN
60	C4	29	HIS
67	D1	3	ASN
68	D2	56	HIS
69	D3	48	HIS
70	D4	29	HIS
72	D6	25	ASN
4	l2	50	HIS
6	l4	316	ASN
12	m0	112	GLN
21	n0	8	GLN
24	n3	33	ASN
24	n3	47	ASN
25	n4	32	GLN
28	n7	57	HIS
28	n7	78	ASN
51	s5	63	GLN
51	s5	122	ASN
79	s6	201	GLN
53	s7	86	GLN
53	s7	180	GLN
56	c0	12	HIS
56	c0	32	HIS
56	c0	47	GLN
57	c1	104	HIS
64	c8	99	HIS
66	d0	16	GLN
66	d0	72	ASN
74	d8	27	GLN
77	sR	182	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3069/3396 (90%)	618 (20%)	56 (1%)
1	5	3080/3396 (90%)	657 (21%)	53 (1%)
2	3	120/121 (99%)	22 (18%)	1 (0%)
2	7	120/121 (99%)	20 (16%)	0
3	4	156/158 (98%)	35 (22%)	4 (2%)
3	8	157/158 (99%)	35 (22%)	7 (4%)
45	2	1708/1800 (94%)	485 (28%)	33 (1%)
45	6	1678/1800 (93%)	453 (26%)	39 (2%)
All	All	10088/10950 (92%)	2325 (23%)	193 (1%)

All (2325) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	6	A
1	1	25	U
1	1	26	A
1	1	30	G
1	1	40	A
1	1	42	C
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	76	G
1	1	87	U
1	1	88	A
1	1	92	G
1	1	93	C
1	1	99	A
1	1	109	A
1	1	110	G
1	1	111	C
1	1	116	A
1	1	121	A
1	1	122	A
1	1	132	C
1	1	133	U
1	1	135	C
1	1	136	G

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Mol	Chain	Res	Type
1	1	139	G
1	1	146	U
1	1	154	U
1	1	156	G
1	1	157	A
1	1	162	G
1	1	163	C
1	1	166	C
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	213	A
1	1	218	G
1	1	219	A
1	1	230	U
1	1	231	G
1	1	235	A
1	1	240	U
1	1	241	G
1	1	242	C
1	1	243	G
1	1	244	G
1	1	245	U
1	1	246	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	253	A
1	1	269	G
1	1	282	G
1	1	286	U
1	1	295	A
1	1	298	U
1	1	305	U
1	1	315	C
1	1	323	A
1	1	329	U
1	1	338	A

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Mol	Chain	Res	Type
1	1	339	C
1	1	350	C
1	1	351	A
1	1	376	G
1	1	391	A
1	1	397	A
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	420	G
1	1	421	G
1	1	422	A
1	1	436	A
1	1	437	G
1	1	495	G
1	1	496	C
1	1	520	U
1	1	521	A
1	1	532	A
1	1	535	G
1	1	545	U
1	1	548	G
1	1	549	U
1	1	552	G
1	1	556	U
1	1	557	A
1	1	558	U
1	1	559	A
1	1	568	G
1	1	569	A
1	1	578	A
1	1	579	G
1	1	589	A
1	1	594	U
1	1	600	G
1	1	604	G
1	1	607	A
1	1	609	G
1	1	611	A
1	1	619	A

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Mol	Chain	Res	Type
1	1	620	U
1	1	621	A
1	1	622	A
1	1	625	G
1	1	636	C
1	1	637	C
1	1	638	C
1	1	649	A
1	1	660	A
1	1	677	A
1	1	681	U
1	1	689	U
1	1	697	A
1	1	705	A
1	1	712	G
1	1	715	A
1	1	716	A
1	1	718	G
1	1	720	A
1	1	721	G
1	1	741	U
1	1	764	U
1	1	765	C
1	1	767	U
1	1	768	C
1	1	773	G
1	1	774	G
1	1	775	A
1	1	776	U
1	1	777	U
1	1	781	G
1	1	785	G
1	1	806	A
1	1	817	A
1	1	818	C
1	1	830	A
1	1	849	C
1	1	861	C
1	1	863	C
1	1	869	G
1	1	871	U
1	1	874	U

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Mol	Chain	Res	Type
1	1	879	U
1	1	890	C
1	1	896	A
1	1	907	G
1	1	908	G
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	926	A
1	1	934	G
1	1	937	G
1	1	944	C
1	1	959	C
1	1	960	U
1	1	964	G
1	1	979	U
1	1	980	A
1	1	982	C
1	1	995	U
1	1	1000	C
1	1	1001	G
1	1	1002	A
1	1	1010	G
1	1	1015	U
1	1	1017	C
1	1	1018	G
1	1	1020	G
1	1	1021	G
1	1	1032	C
1	1	1036	A
1	1	1038	C
1	1	1041	U
1	1	1046	A
1	1	1047	A
1	1	1049	C
1	1	1064	A
1	1	1065	A
1	1	1066	G
1	1	1068	C

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Mol	Chain	Res	Type
1	1	1071	U
1	1	1072	G
1	1	1081	U
1	1	1082	U
1	1	1088	U
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	1105	A
1	1	1117	G
1	1	1128	U
1	1	1131	G
1	1	1140	G
1	1	1144	U
1	1	1153	A
1	1	1159	A
1	1	1161	G
1	1	1177	G
1	1	1179	A
1	1	1180	A
1	1	1181	U
1	1	1182	A
1	1	1191	U
1	1	1192	C
1	1	1193	A
1	1	1196	C
1	1	1201	C
1	1	1209	G
1	1	1212	A
1	1	1216	C
1	1	1222	G
1	1	1229	G
1	1	1230	G
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1292	C

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Mol	Chain	Res	Type
1	1	1300	G
1	1	1307	G
1	1	1313	G
1	1	1318	A
1	1	1330	A
1	1	1345	G
1	1	1348	U
1	1	1356	U
1	1	1357	G
1	1	1385	C
1	1	1386	A
1	1	1399	A
1	1	1400	G
1	1	1416	C
1	1	1417	G
1	1	1418	A
1	1	1419	A
1	1	1431	G
1	1	1434	G
1	1	1437	C
1	1	1438	U
1	1	1446	A
1	1	1450	G
1	1	1460	A
1	1	1481	A
1	1	1482	A
1	1	1483	G
1	1	1485	G
1	1	1488	G
1	1	1502	C
1	1	1508	C
1	1	1523	U
1	1	1527	C
1	1	1528	G
1	1	1529	A
1	1	1533	U
1	1	1536	G
1	1	1539	A
1	1	1541	G
1	1	1553	U
1	1	1554	U
1	1	1555	U

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Mol	Chain	Res	Type
1	1	1556	C
1	1	1557	A
1	1	1561	G
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	1571	A
1	1	1572	U
1	1	1573	G
1	1	1574	C
1	1	1575	A
1	1	1576	G
1	1	1578	C
1	1	1579	C
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	1605	A
1	1	1607	U
1	1	1620	U
1	1	1629	U
1	1	1632	A
1	1	1639	C
1	1	1641	U
1	1	1642	A
1	1	1643	A
1	1	1644	C
1	1	1645	U
1	1	1657	C
1	1	1658	G
1	1	1673	G
1	1	1675	G
1	1	1683	A
1	1	1688	U

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Mol	Chain	Res	Type
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1740	U
1	1	1743	G
1	1	1750	A
1	1	1751	G
1	1	1760	A
1	1	1763	U
1	1	1764	U
1	1	1770	G
1	1	1780	G
1	1	1787	A
1	1	1790	G
1	1	1797	A
1	1	1808	G
1	1	1813	A
1	1	1816	A
1	1	1821	U
1	1	1841	A
1	1	1842	A
1	1	1846	C
1	1	1847	A
1	1	1850	A
1	1	1866	C
1	1	1867	A
1	1	1877	U
1	1	1879	A
1	1	1886	A
1	1	1906	G
1	1	1952	G
1	1	2093	A
1	1	2094	C
1	1	2100	A
1	1	2101	C
1	1	2102	U
1	1	2113	A
1	1	2114	C
1	1	2121	G
1	1	2122	G
1	1	2130	G

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Mol	Chain	Res	Type
1	1	2131	A
1	1	2140	U
1	1	2144	A
1	1	2158	A
1	1	2169	G
1	1	2170	U
1	1	2188	A
1	1	2205	U
1	1	2206	G
1	1	2207	A
1	1	2209	U
1	1	2210	G
1	1	2223	A
1	1	2246	G
1	1	2248	C
1	1	2249	G
1	1	2250	G
1	1	2251	G
1	1	2252	A
1	1	2256	A
1	1	2257	C
1	1	2272	G
1	1	2273	G
1	1	2276	G
1	1	2280	A
1	1	2281	A
1	1	2282	U
1	1	2288	G
1	1	2295	A
1	1	2306	C
1	1	2307	G
1	1	2308	C
1	1	2309	A
1	1	2310	U
1	1	2313	A
1	1	2314	U
1	1	2315	G
1	1	2319	U
1	1	2334	U
1	1	2336	U
1	1	2361	A
1	1	2372	A

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Mol	Chain	Res	Type
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2383	C
1	1	2385	G
1	1	2388	U
1	1	2393	G
1	1	2394	G
1	1	2397	A
1	1	2402	A
1	1	2403	G
1	1	2404	A
1	1	2406	C
1	1	2411	U
1	1	2413	A
1	1	2414	G
1	1	2418	G
1	1	2419	A
1	1	2435	G
1	1	2441	A
1	1	2442	G
1	1	2507	C
1	1	2510	U
1	1	2511	A
1	1	2514	U
1	1	2515	A
1	1	2522	G
1	1	2533	G
1	1	2536	A
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	2544	U
1	1	2545	C
1	1	2546	C
1	1	2549	G
1	1	2552	C
1	1	2554	A

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Mol	Chain	Res	Type
1	1	2555	G
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2585	G
1	1	2593	A
1	1	2594	C
1	1	2606	G
1	1	2607	G
1	1	2614	G
1	1	2626	A
1	1	2629	U
1	1	2637	A
1	1	2638	C
1	1	2652	U
1	1	2656	A
1	1	2657	A
1	1	2674	A
1	1	2676	A
1	1	2677	G
1	1	2678	A
1	1	2681	U
1	1	2688	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	2723	U
1	1	2728	G
1	1	2737	C
1	1	2752	U
1	1	2753	G
1	1	2762	A
1	1	2772	C
1	1	2777	G
1	1	2778	G
1	1	2779	A
1	1	2796	G

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Mol	Chain	Res	Type
1	1	2800	G
1	1	2801	A
1	1	2810	C
1	1	2814	G
1	1	2817	A
1	1	2818	U
1	1	2837	A
1	1	2842	U
1	1	2845	A
1	1	2847	A
1	1	2853	A
1	1	2861	U
1	1	2871	G
1	1	2872	A
1	1	2873	U
1	1	2876	C
1	1	2887	A
1	1	2889	C
1	1	2899	C
1	1	2904	U
1	1	2910	A
1	1	2923	U
1	1	2935	U
1	1	2936	A
1	1	2938	G
1	1	2942	C
1	1	2947	G
1	1	2949	U
1	1	2954	U
1	1	2971	A
1	1	2972	G
1	1	2977	G
1	1	2983	C
1	1	2990	G
1	1	2992	U
1	1	2996	U
1	1	2997	G
1	1	3012	A
1	1	3030	G
1	1	3033	A
1	1	3056	U
1	1	3058	U

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Mol	Chain	Res	Type
1	1	3059	G
1	1	3078	U
1	1	3079	U
1	1	3086	A
1	1	3092	C
1	1	3113	A
1	1	3122	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3150	A
1	1	3151	U
1	1	3152	U
1	1	3163	A
1	1	3164	C
1	1	3165	A
1	1	3167	A
1	1	3168	A
1	1	3169	U
1	1	3170	A
1	1	3171	U
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3187	A
1	1	3194	C
1	1	3196	U
1	1	3202	G
1	1	3207	U
1	1	3210	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3228	C
1	1	3229	G
1	1	3244	A
1	1	3245	A
1	1	3247	G

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Mol	Chain	Res	Type
1	1	3253	G
1	1	3254	G
1	1	3259	U
1	1	3263	G
1	1	3270	U
1	1	3271	G
1	1	3273	A
1	1	3275	U
1	1	3276	G
1	1	3279	A
1	1	3281	U
1	1	3286	G
1	1	3287	U
1	1	3288	G
1	1	3289	G
1	1	3295	A
1	1	3304	U
1	1	3309	G
1	1	3316	A
1	1	3317	U
1	1	3318	G
1	1	3319	U
1	1	3320	A
1	1	3335	A
1	1	3341	U
1	1	3342	A
1	1	3345	G
1	1	3347	A
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3354	U
1	1	3355	U
1	1	3367	C
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3383	G
1	1	3386	G
1	1	3389	U
1	1	3390	G

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Mol	Chain	Res	Type
1	1	3394	U
1	1	3396	U
2	3	7	G
2	3	10	C
2	3	22	A
2	3	23	A
2	3	33	U
2	3	38	U
2	3	41	G
2	3	42	A
2	3	51	A
2	3	53	U
2	3	54	U
2	3	65	G
2	3	74	C
2	3	76	A
2	3	90	U
2	3	91	G
2	3	99	G
2	3	102	A
2	3	104	A
2	3	110	G
2	3	112	G
2	3	121	U
3	4	21	C
3	4	23	U
3	4	34	U
3	4	35	C
3	4	50	C
3	4	51	G
3	4	53	A
3	4	59	A
3	4	62	C
3	4	63	G
3	4	80	A
3	4	81	U
3	4	82	U
3	4	83	C
3	4	84	C
3	4	86	U
3	4	87	G
3	4	89	A

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Mol	Chain	Res	Type
3	4	90	U
3	4	91	C
3	4	95	G
3	4	104	A
3	4	105	A
3	4	106	C
3	4	111	A
3	4	113	U
3	4	125	U
3	4	126	A
3	4	127	U
3	4	128	U
3	4	138	A
3	4	148	G
3	4	149	A
3	4	151	C
3	4	155	A
45	2	2	A
45	2	16	G
45	2	17	C
45	2	25	C
45	2	26	A
45	2	27	U
45	2	34	G
45	2	37	U
45	2	45	U
45	2	47	A
45	2	48	G
45	2	57	G
45	2	60	U
45	2	61	A
45	2	62	A
45	2	66	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	77	U
45	2	78	A

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Mol	Chain	Res	Type
45	2	79	C
45	2	80	A
45	2	81	G
45	2	94	U
45	2	99	C
45	2	100	A
45	2	101	U
45	2	103	A
45	2	104	A
45	2	110	U
45	2	114	C
45	2	115	G
45	2	116	U
45	2	117	U
45	2	123	G
45	2	124	A
45	2	127	G
45	2	128	U
45	2	130	C
45	2	131	C
45	2	133	U
45	2	134	U
45	2	135	A
45	2	136	C
45	2	137	U
45	2	138	A
45	2	140	A
45	2	141	U
45	2	144	U
45	2	145	A
45	2	146	U
45	2	149	C
45	2	151	G
45	2	158	U
45	2	159	U
45	2	168	A
45	2	178	U
45	2	185	U
45	2	186	C
45	2	187	G
45	2	192	U
45	2	193	U

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Mol	Chain	Res	Type
45	2	194	U
45	2	195	G
45	2	197	A
45	2	200	A
45	2	209	U
45	2	215	A
45	2	217	A
45	2	218	A
45	2	219	A
45	2	225	A
45	2	229	U
45	2	231	U
45	2	232	U
45	2	233	C
45	2	234	G
45	2	238	U
45	2	239	C
45	2	240	U
45	2	241	U
45	2	246	G
45	2	250	C
45	2	254	A
45	2	257	A
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	269	G
45	2	270	C
45	2	271	A
45	2	272	U
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	283	U
45	2	284	G
45	2	288	A

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Mol	Chain	Res	Type
45	2	292	U
45	2	299	A
45	2	302	U
45	2	306	U
45	2	309	C
45	2	314	C
45	2	316	A
45	2	320	U
45	2	321	C
45	2	324	U
45	2	333	A
45	2	337	G
45	2	338	C
45	2	352	A
45	2	359	A
45	2	360	A
45	2	361	C
45	2	369	A
45	2	381	C
45	2	390	G
45	2	399	A
45	2	400	A
45	2	402	C
45	2	403	G
45	2	404	G
45	2	416	A
45	2	417	A
45	2	418	G
45	2	422	G
45	2	424	C
45	2	425	A
45	2	426	G
45	2	427	C
45	2	428	A
45	2	434	G
45	2	437	A
45	2	439	U
45	2	444	C
45	2	447	U
45	2	448	C
45	2	452	A
45	2	454	U

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Mol	Chain	Res	Type
45	2	455	C
45	2	468	A
45	2	469	C
45	2	474	A
45	2	475	A
45	2	477	A
45	2	483	A
45	2	484	C
45	2	485	A
45	2	486	G
45	2	487	G
45	2	502	U
45	2	504	U
45	2	505	A
45	2	506	A
45	2	507	U
45	2	510	G
45	2	511	A
45	2	512	A
45	2	513	U
45	2	515	A
45	2	516	G
45	2	532	U
45	2	535	A
45	2	536	C
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	548	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	560	U
45	2	561	G
45	2	565	C

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Mol	Chain	Res	Type
45	2	567	A
45	2	568	G
45	2	570	A
45	2	576	G
45	2	579	A
45	2	580	A
45	2	582	U
45	2	583	C
45	2	594	A
45	2	595	G
45	2	613	G
45	2	619	A
45	2	620	A
45	2	621	A
45	2	622	A
45	2	623	A
45	2	624	G
45	2	638	U
45	2	639	U
45	2	640	U
45	2	650	U
45	2	654	C
45	2	655	G
45	2	656	G
45	2	658	C
45	2	677	G
45	2	679	U
45	2	683	C
45	2	684	A
45	2	686	C
45	2	694	U
45	2	695	U
45	2	696	C
45	2	697	C
45	2	699	U
45	2	702	G
45	2	703	G
45	2	704	C
45	2	735	C
45	2	737	A
45	2	738	G
45	2	739	G

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Mol	Chain	Res	Type
45	2	741	C
45	2	742	U
45	2	743	U
45	2	754	A
45	2	755	A
45	2	756	A
45	2	762	A
45	2	765	G
45	2	766	U
45	2	770	A
45	2	771	A
45	2	774	A
45	2	775	G
45	2	777	C
45	2	778	G
45	2	779	U
45	2	780	A
45	2	781	U
45	2	782	U
45	2	783	G
45	2	784	C
45	2	789	A
45	2	793	A
45	2	794	U
45	2	795	U
45	2	812	A
45	2	814	A
45	2	815	G
45	2	816	G
45	2	818	C
45	2	820	U
45	2	821	U
45	2	824	G
45	2	827	C
45	2	829	A
45	2	830	U
45	2	831	U
45	2	833	U
45	2	839	U
45	2	840	U
45	2	846	G
45	2	847	A

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Mol	Chain	Res	Type
45	2	855	A
45	2	856	A
45	2	860	U
45	2	863	A
45	2	864	U
45	2	865	A
45	2	873	U
45	2	886	U
45	2	894	U
45	2	895	G
45	2	898	A
45	2	906	A
45	2	911	U
45	2	912	U
45	2	913	G
45	2	914	G
45	2	916	U
45	2	921	U
45	2	927	C
45	2	933	A
45	2	935	U
45	2	942	G
45	2	944	A
45	2	954	G
45	2	960	U
45	2	966	A
45	2	992	A
45	2	993	A
45	2	1003	A
45	2	1004	U
45	2	1005	A
45	2	1021	C
45	2	1026	A
45	2	1028	C
45	2	1039	A
45	2	1040	G
45	2	1042	G
45	2	1052	U
45	2	1056	U
45	2	1057	U
45	2	1059	U
45	2	1060	U

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Mol	Chain	Res	Type
45	2	1061	A
45	2	1063	U
45	2	1072	C
45	2	1075	C
45	2	1076	A
45	2	1079	U
45	2	1081	A
45	2	1083	G
45	2	1091	A
45	2	1092	A
45	2	1096	C
45	2	1097	U
45	2	1100	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	1166	A
45	2	1167	G
45	2	1185	U
45	2	1194	A
45	2	1196	A
45	2	1197	C
45	2	1199	G
45	2	1200	G
45	2	1202	A
45	2	1207	C
45	2	1208	A
45	2	1217	A
45	2	1218	G
45	2	1227	A
45	2	1228	G
45	2	1229	G
45	2	1230	A
45	2	1235	C
45	2	1244	A

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Mol	Chain	Res	Type
45	2	1245	G
45	2	1246	C
45	2	1255	G
45	2	1256	A
45	2	1258	U
45	2	1260	U
45	2	1261	G
45	2	1263	G
45	2	1276	U
45	2	1287	A
45	2	1290	U
45	2	1301	U
45	2	1314	U
45	2	1315	U
45	2	1321	A
45	2	1325	A
45	2	1335	U
45	2	1337	A
45	2	1339	C
45	2	1340	U
45	2	1341	A
45	2	1343	U
45	2	1344	A
45	2	1345	A
45	2	1346	A
45	2	1348	A
45	2	1349	G
45	2	1361	U
45	2	1362	U
45	2	1364	G
45	2	1369	U
45	2	1370	U
45	2	1371	A
45	2	1372	U
45	2	1381	U
45	2	1383	G
45	2	1385	G
45	2	1388	A
45	2	1390	U
45	2	1398	U
45	2	1399	C
45	2	1400	A

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Mol	Chain	Res	Type
45	2	1412	G
45	2	1413	U
45	2	1414	U
45	2	1415	U
45	2	1427	A
45	2	1428	G
45	2	1432	U
45	2	1445	G
45	2	1446	A
45	2	1447	C
45	2	1456	C
45	2	1457	C
45	2	1458	G
45	2	1459	C
45	2	1460	A
45	2	1461	C
45	2	1471	A
45	2	1473	U
45	2	1474	G
45	2	1482	C
45	2	1483	A
45	2	1485	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	1499	G
45	2	1503	A
45	2	1506	G
45	2	1514	U
45	2	1515	A
45	2	1516	A
45	2	1518	C
45	2	1520	U
45	2	1521	G
45	2	1523	G
45	2	1524	A
45	2	1535	U
45	2	1536	G
45	2	1537	C

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Mol	Chain	Res	Type
45	2	1538	U
45	2	1542	G
45	2	1557	U
45	2	1559	A
45	2	1569	A
45	2	1574	G
45	2	1575	G
45	2	1584	G
45	2	1590	G
45	2	1601	G
45	2	1614	A
45	2	1616	G
45	2	1619	C
45	2	1625	C
45	2	1631	A
45	2	1634	C
45	2	1635	A
45	2	1657	U
45	2	1658	G
45	2	1663	G
45	2	1681	A
45	2	1682	U
45	2	1683	C
45	2	1684	U
45	2	1715	G
45	2	1716	C
45	2	1717	G
45	2	1755	A
45	2	1760	G
45	2	1762	A
45	2	1766	A
45	2	1769	U
45	2	1770	U
45	2	1780	G
45	2	1782	A
45	2	1783	C
45	2	1792	G
45	2	1793	G
45	2	1794	A
45	2	1796	C
1	5	26	A
1	5	40	A

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Mol	Chain	Res	Type
1	5	43	A
1	5	49	A
1	5	57	A
1	5	60	A
1	5	65	A
1	5	66	A
1	5	73	C
1	5	77	A
1	5	85	A
1	5	92	G
1	5	96	G
1	5	99	A
1	5	108	A
1	5	109	A
1	5	110	G
1	5	113	C
1	5	121	A
1	5	122	A
1	5	127	G
1	5	130	A
1	5	132	C
1	5	133	U
1	5	134	U
1	5	136	G
1	5	138	U
1	5	139	G
1	5	146	U
1	5	150	A
1	5	152	U
1	5	156	G
1	5	157	A
1	5	161	G
1	5	165	A
1	5	170	G
1	5	171	G
1	5	173	G
1	5	174	C
1	5	175	C
1	5	176	G
1	5	180	C
1	5	181	U
1	5	187	A

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Mol	Chain	Res	Type
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	221	A
1	5	238	A
1	5	239	G
1	5	240	U
1	5	241	G
1	5	242	C
1	5	246	U
1	5	247	C
1	5	249	U
1	5	250	U
1	5	251	G
1	5	252	U
1	5	253	A
1	5	263	C
1	5	269	G
1	5	284	A
1	5	286	U
1	5	295	A
1	5	305	U
1	5	311	C
1	5	323	A
1	5	329	U
1	5	338	A
1	5	339	C
1	5	349	A
1	5	350	C
1	5	351	A
1	5	352	A
1	5	373	A
1	5	376	G
1	5	379	C
1	5	384	A
1	5	390	G
1	5	395	A
1	5	397	A

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Mol	Chain	Res	Type
1	5	399	A
1	5	401	U
1	5	402	A
1	5	403	C
1	5	404	G
1	5	421	G
1	5	422	A
1	5	435	C
1	5	436	A
1	5	439	C
1	5	440	A
1	5	441	U
1	5	442	G
1	5	520	U
1	5	521	A
1	5	524	U
1	5	535	G
1	5	540	U
1	5	542	G
1	5	543	C
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	550	A
1	5	551	A
1	5	553	U
1	5	555	U
1	5	557	A
1	5	559	A
1	5	569	A
1	5	578	A
1	5	579	G
1	5	592	A
1	5	594	U
1	5	597	G
1	5	600	G
1	5	604	G
1	5	609	G
1	5	611	A

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Mol	Chain	Res	Type
1	5	618	C
1	5	619	A
1	5	620	U
1	5	621	A
1	5	622	A
1	5	626	U
1	5	636	C
1	5	643	U
1	5	649	A
1	5	660	A
1	5	677	A
1	5	681	U
1	5	691	A
1	5	697	A
1	5	705	A
1	5	708	G
1	5	712	G
1	5	715	A
1	5	716	A
1	5	736	A
1	5	766	U
1	5	768	C
1	5	776	U
1	5	777	U
1	5	780	A
1	5	781	G
1	5	785	G
1	5	786	A
1	5	806	A
1	5	808	A
1	5	816	A
1	5	817	A
1	5	830	A
1	5	837	A
1	5	846	A
1	5	857	G
1	5	861	C
1	5	874	U
1	5	879	U
1	5	882	A
1	5	883	A
1	5	896	A

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Mol	Chain	Res	Type
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	926	A
1	5	937	G
1	5	939	U
1	5	944	C
1	5	953	G
1	5	959	C
1	5	960	U
1	5	964	G
1	5	979	U
1	5	982	C
1	5	994	G
1	5	1002	A
1	5	1010	G
1	5	1015	U
1	5	1016	C
1	5	1017	C
1	5	1018	G
1	5	1020	G
1	5	1023	C
1	5	1024	G
1	5	1031	C
1	5	1033	U
1	5	1035	G
1	5	1037	C
1	5	1041	U
1	5	1047	A
1	5	1049	C
1	5	1064	A
1	5	1065	A
1	5	1068	C
1	5	1071	U
1	5	1072	G
1	5	1076	C
1	5	1081	U

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Mol	Chain	Res	Type
1	5	1082	U
1	5	1083	G
1	5	1085	A
1	5	1093	A
1	5	1094	U
1	5	1095	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	1144	U
1	5	1151	U
1	5	1153	A
1	5	1159	A
1	5	1180	A
1	5	1181	U
1	5	1182	A
1	5	1191	U
1	5	1192	C
1	5	1196	C
1	5	1201	C
1	5	1206	G
1	5	1209	G
1	5	1212	A
1	5	1220	U
1	5	1222	G
1	5	1225	A
1	5	1285	G
1	5	1308	A
1	5	1311	G
1	5	1312	C
1	5	1313	G
1	5	1324	U
1	5	1330	A
1	5	1332	A
1	5	1348	U
1	5	1349	G
1	5	1350	A
1	5	1351	U
1	5	1352	A

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Mol	Chain	Res	Type
1	5	1353	U
1	5	1354	G
1	5	1356	U
1	5	1357	G
1	5	1358	C
1	5	1369	A
1	5	1380	G
1	5	1385	C
1	5	1386	A
1	5	1392	G
1	5	1399	A
1	5	1400	G
1	5	1416	C
1	5	1417	G
1	5	1418	A
1	5	1419	A
1	5	1428	A
1	5	1434	G
1	5	1437	C
1	5	1438	U
1	5	1446	A
1	5	1450	G
1	5	1455	U
1	5	1466	G
1	5	1481	A
1	5	1482	A
1	5	1483	G
1	5	1488	G
1	5	1500	G
1	5	1501	U
1	5	1503	A
1	5	1508	C
1	5	1511	U
1	5	1524	A
1	5	1527	C
1	5	1533	U
1	5	1539	A
1	5	1554	U
1	5	1555	U
1	5	1556	C
1	5	1557	A
1	5	1560	G

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Mol	Chain	Res	Type
1	5	1561	G
1	5	1562	C
1	5	1564	U
1	5	1565	G
1	5	1572	U
1	5	1573	G
1	5	1574	C
1	5	1575	A
1	5	1576	G
1	5	1577	G
1	5	1578	C
1	5	1581	C
1	5	1582	C
1	5	1583	A
1	5	1587	A
1	5	1589	A
1	5	1593	A
1	5	1605	A
1	5	1607	U
1	5	1608	C
1	5	1619	A
1	5	1628	C
1	5	1629	U
1	5	1632	A
1	5	1636	U
1	5	1639	C
1	5	1642	A
1	5	1643	A
1	5	1644	C
1	5	1645	U
1	5	1655	G
1	5	1657	C
1	5	1662	G
1	5	1687	U
1	5	1715	A
1	5	1716	U
1	5	1724	U
1	5	1731	A
1	5	1736	G
1	5	1746	U
1	5	1750	A
1	5	1751	G

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Mol	Chain	Res	Type
1	5	1759	C
1	5	1760	A
1	5	1761	C
1	5	1762	C
1	5	1763	U
1	5	1765	U
1	5	1766	G
1	5	1769	G
1	5	1770	G
1	5	1775	G
1	5	1778	G
1	5	1780	G
1	5	1788	C
1	5	1797	A
1	5	1809	A
1	5	1810	A
1	5	1812	G
1	5	1813	A
1	5	1814	A
1	5	1815	U
1	5	1816	A
1	5	1817	G
1	5	1818	U
1	5	1821	U
1	5	1835	A
1	5	1839	A
1	5	1842	A
1	5	1846	C
1	5	1849	C
1	5	1878	G
1	5	1879	A
1	5	1880	U
1	5	1884	A
1	5	1886	A
1	5	1906	G
1	5	1935	G
1	5	1948	G
1	5	1952	G
1	5	2093	A
1	5	2100	A
1	5	2101	C
1	5	2102	U

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Mol	Chain	Res	Type
1	5	2112	U
1	5	2113	A
1	5	2114	C
1	5	2121	G
1	5	2122	G
1	5	2131	A
1	5	2140	U
1	5	2146	C
1	5	2158	A
1	5	2168	A
1	5	2169	G
1	5	2176	U
1	5	2179	C
1	5	2185	G
1	5	2198	A
1	5	2201	G
1	5	2205	U
1	5	2206	G
1	5	2210	G
1	5	2213	A
1	5	2222	A
1	5	2223	A
1	5	2225	U
1	5	2228	A
1	5	2244	A
1	5	2246	G
1	5	2250	G
1	5	2251	G
1	5	2252	A
1	5	2253	G
1	5	2255	A
1	5	2256	A
1	5	2257	C
1	5	2266	U
1	5	2269	U
1	5	2270	A
1	5	2273	G
1	5	2281	A
1	5	2307	G
1	5	2310	U
1	5	2313	A
1	5	2315	G

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Mol	Chain	Res	Type
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	2388	U
1	5	2393	G
1	5	2395	G
1	5	2397	A
1	5	2401	A
1	5	2402	A
1	5	2403	G
1	5	2404	A
1	5	2405	C
1	5	2411	U
1	5	2418	G
1	5	2419	A
1	5	2420	C
1	5	2433	U
1	5	2434	U
1	5	2435	G
1	5	2437	G
1	5	2441	A
1	5	2442	G
1	5	2443	A
1	5	2509	U
1	5	2510	U
1	5	2511	A
1	5	2512	C
1	5	2514	U
1	5	2515	A
1	5	2522	G
1	5	2523	A
1	5	2524	A
1	5	2525	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

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Mol	Chain	Res	Type
1	5	2541	U
1	5	2543	U
1	5	2544	U
1	5	2545	C
1	5	2546	C
1	5	2549	G
1	5	2552	C
1	5	2555	G
1	5	2560	C
1	5	2562	A
1	5	2567	C
1	5	2568	C
1	5	2569	A
1	5	2571	U
1	5	2572	C
1	5	2573	G
1	5	2574	G
1	5	2585	G
1	5	2593	A
1	5	2594	C
1	5	2606	G
1	5	2607	G
1	5	2610	G
1	5	2614	G
1	5	2619	G
1	5	2620	G
1	5	2626	A
1	5	2629	U
1	5	2648	G
1	5	2652	U
1	5	2656	A
1	5	2663	G
1	5	2667	A
1	5	2673	A
1	5	2674	A
1	5	2675	C
1	5	2676	A
1	5	2677	G
1	5	2681	U
1	5	2689	A
1	5	2690	G
1	5	2691	A

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Mol	Chain	Res	Type
1	5	2694	A
1	5	2695	A
1	5	2696	A
1	5	2714	G
1	5	2715	A
1	5	2720	G
1	5	2728	G
1	5	2737	C
1	5	2738	A
1	5	2740	A
1	5	2746	A
1	5	2752	U
1	5	2753	G
1	5	2773	C
1	5	2777	G
1	5	2778	G
1	5	2796	G
1	5	2799	A
1	5	2800	G
1	5	2801	A
1	5	2802	A
1	5	2810	C
1	5	2814	G
1	5	2816	G
1	5	2817	A
1	5	2818	U
1	5	2837	A
1	5	2843	U
1	5	2845	A
1	5	2847	A
1	5	2853	A
1	5	2871	G
1	5	2872	A
1	5	2875	U
1	5	2876	C
1	5	2887	A
1	5	2889	C
1	5	2898	G
1	5	2899	C
1	5	2910	A
1	5	2923	U
1	5	2935	U

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Mol	Chain	Res	Type
1	5	2936	A
1	5	2942	C
1	5	2943	G
1	5	2947	G
1	5	2951	G
1	5	2952	G
1	5	2967	A
1	5	2971	A
1	5	2972	G
1	5	2979	U
1	5	2983	C
1	5	2990	G
1	5	2994	A
1	5	2996	U
1	5	2997	G
1	5	3012	A
1	5	3028	G
1	5	3030	G
1	5	3039	C
1	5	3056	U
1	5	3059	G
1	5	3062	G
1	5	3074	G
1	5	3078	U
1	5	3080	G
1	5	3086	A
1	5	3087	A
1	5	3092	C
1	5	3120	C
1	5	3130	A
1	5	3131	U
1	5	3142	A
1	5	3143	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	3164	C
1	5	3165	A
1	5	3166	C

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Mol	Chain	Res	Type
1	5	3168	A
1	5	3172	A
1	5	3173	G
1	5	3174	A
1	5	3176	G
1	5	3178	A
1	5	3180	A
1	5	3181	C
1	5	3187	A
1	5	3188	G
1	5	3195	U
1	5	3196	U
1	5	3207	U
1	5	3209	A
1	5	3217	C
1	5	3218	A
1	5	3219	G
1	5	3227	A
1	5	3229	G
1	5	3233	C
1	5	3239	G
1	5	3244	A
1	5	3245	A
1	5	3246	G
1	5	3247	G
1	5	3252	G
1	5	3253	G
1	5	3254	G
1	5	3259	U
1	5	3265	C
1	5	3270	U
1	5	3271	G
1	5	3272	C
1	5	3275	U
1	5	3276	G
1	5	3277	U
1	5	3279	A
1	5	3280	U
1	5	3282	U
1	5	3284	G
1	5	3285	C
1	5	3286	G

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Mol	Chain	Res	Type
1	5	3287	U
1	5	3289	G
1	5	3290	G
1	5	3294	A
1	5	3295	A
1	5	3304	U
1	5	3313	U
1	5	3317	U
1	5	3318	G
1	5	3319	U
1	5	3341	U
1	5	3342	A
1	5	3345	G
1	5	3349	C
1	5	3351	U
1	5	3352	U
1	5	3354	U
1	5	3355	U
1	5	3358	U
1	5	3368	U
1	5	3369	G
1	5	3378	C
1	5	3383	G
1	5	3389	U
1	5	3396	U
2	7	5	G
2	7	7	G
2	7	21	G
2	7	22	A
2	7	26	C
2	7	27	A
2	7	41	G
2	7	42	A
2	7	52	G
2	7	54	U
2	7	55	A
2	7	65	G
2	7	73	C
2	7	74	C
2	7	76	A
2	7	91	G
2	7	93	C

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Mol	Chain	Res	Type
2	7	102	A
2	7	112	G
2	7	121	U
3	8	18	U
3	8	30	C
3	8	34	U
3	8	35	C
3	8	39	G
3	8	50	C
3	8	52	A
3	8	58	G
3	8	59	A
3	8	62	C
3	8	63	G
3	8	79	A
3	8	80	A
3	8	81	U
3	8	82	U
3	8	83	C
3	8	84	C
3	8	85	G
3	8	86	U
3	8	87	G
3	8	90	U
3	8	95	G
3	8	104	A
3	8	106	C
3	8	109	A
3	8	111	A
3	8	113	U
3	8	125	U
3	8	126	A
3	8	127	U
3	8	128	U
3	8	138	A
3	8	155	A
3	8	157	U
3	8	158	U
45	6	2	A
45	6	17	C
45	6	25	C
45	6	26	A

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Mol	Chain	Res	Type
45	6	27	U
45	6	34	G
45	6	42	G
45	6	45	U
45	6	46	A
45	6	47	A
45	6	50	C
45	6	57	G
45	6	60	U
45	6	63	G
45	6	67	A
45	6	68	A
45	6	69	G
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	104	A
45	6	114	C
45	6	116	U
45	6	121	U
45	6	130	C
45	6	131	C
45	6	138	A
45	6	139	C
45	6	140	A
45	6	141	U
45	6	144	U
45	6	153	G
45	6	158	U
45	6	159	U
45	6	166	C
45	6	170	U
45	6	178	U
45	6	179	A
45	6	185	U
45	6	191	C
45	6	192	U
45	6	193	U

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Mol	Chain	Res	Type
45	6	195	G
45	6	197	A
45	6	198	A
45	6	199	G
45	6	200	A
45	6	201	G
45	6	215	A
45	6	218	A
45	6	222	A
45	6	224	C
45	6	226	A
45	6	227	U
45	6	228	G
45	6	229	U
45	6	231	U
45	6	232	U
45	6	233	C
45	6	234	G
45	6	235	G
45	6	240	U
45	6	241	U
45	6	242	U
45	6	243	G
45	6	249	U
45	6	250	C
45	6	261	U
45	6	262	U
45	6	265	A
45	6	266	A
45	6	267	U
45	6	268	C
45	6	271	A
45	6	272	U
45	6	273	G
45	6	276	C
45	6	277	U
45	6	278	U
45	6	279	G
45	6	280	U
45	6	285	G
45	6	287	G
45	6	299	A

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Mol	Chain	Res	Type
45	6	302	U
45	6	314	C
45	6	316	A
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	352	A
45	6	359	A
45	6	360	A
45	6	361	C
45	6	369	A
45	6	370	A
45	6	379	U
45	6	380	U
45	6	393	C
45	6	400	A
45	6	401	A
45	6	402	C
45	6	403	G
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
45	6	434	G
45	6	437	A
45	6	439	U
45	6	444	C
45	6	448	C
45	6	449	C
45	6	452	A
45	6	454	U
45	6	455	C
45	6	468	A
45	6	474	A
45	6	475	A

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Mol	Chain	Res	Type
45	6	480	G
45	6	485	A
45	6	486	G
45	6	487	G
45	6	488	G
45	6	500	C
45	6	501	U
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	519	C
45	6	527	A
45	6	534	A
45	6	538	A
45	6	539	G
45	6	540	G
45	6	541	A
45	6	542	A
45	6	543	C
45	6	544	A
45	6	554	C
45	6	555	A
45	6	556	A
45	6	557	G
45	6	558	U
45	6	564	G
45	6	565	C
45	6	566	C
45	6	570	A
45	6	574	G
45	6	579	A
45	6	580	A
45	6	582	U
45	6	583	C
45	6	585	A

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Mol	Chain	Res	Type
45	6	594	A
45	6	595	G
45	6	596	C
45	6	606	A
45	6	610	G
45	6	611	U
45	6	619	A
45	6	620	A
45	6	622	A
45	6	623	A
45	6	624	G
45	6	639	U
45	6	647	G
45	6	648	G
45	6	649	U
45	6	650	U
45	6	685	A
45	6	745	U
45	6	746	A
45	6	754	A
45	6	755	A
45	6	756	A
45	6	758	U
45	6	765	G
45	6	766	U
45	6	774	A
45	6	775	G
45	6	778	G
45	6	780	A
45	6	781	U
45	6	782	U
45	6	783	G
45	6	789	A
45	6	793	A
45	6	794	U
45	6	803	A
45	6	811	A
45	6	812	A
45	6	813	U
45	6	815	G
45	6	819	G
45	6	820	U

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Mol	Chain	Res	Type
45	6	821	U
45	6	823	G
45	6	825	U
45	6	826	U
45	6	829	A
45	6	830	U
45	6	831	U
45	6	832	U
45	6	834	G
45	6	835	U
45	6	839	U
45	6	842	C
45	6	843	U
45	6	845	G
45	6	849	C
45	6	856	A
45	6	863	A
45	6	864	U
45	6	876	G
45	6	877	G
45	6	886	U
45	6	898	A
45	6	906	A
45	6	913	G
45	6	914	G
45	6	916	U
45	6	926	A
45	6	929	A
45	6	933	A
45	6	935	U
45	6	942	G
45	6	944	A
45	6	945	U
45	6	951	A
45	6	957	G
45	6	959	U
45	6	960	U
45	6	966	A
45	6	969	C
45	6	971	A
45	6	984	G
45	6	992	A

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Mol	Chain	Res	Type
45	6	993	A
45	6	995	A
45	6	996	U
45	6	997	G
45	6	1003	A
45	6	1004	U
45	6	1005	A
45	6	1024	U
45	6	1025	A
45	6	1026	A
45	6	1028	C
45	6	1030	A
45	6	1039	A
45	6	1040	G
45	6	1042	G
45	6	1043	A
45	6	1051	G
45	6	1052	U
45	6	1053	G
45	6	1058	U
45	6	1059	U
45	6	1060	U
45	6	1061	A
45	6	1062	A
45	6	1063	U
45	6	1071	U
45	6	1076	A
45	6	1081	A
45	6	1082	C
45	6	1083	G
45	6	1092	A
45	6	1096	C
45	6	1097	U
45	6	1098	U
45	6	1100	G
45	6	1109	G
45	6	1112	G
45	6	1138	A
45	6	1140	G
45	6	1150	G
45	6	1155	G
45	6	1158	C

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Mol	Chain	Res	Type
45	6	1160	A
45	6	1163	A
45	6	1167	G
45	6	1185	U
45	6	1186	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	1212	G
45	6	1217	A
45	6	1218	G
45	6	1225	U
45	6	1226	A
45	6	1228	G
45	6	1229	G
45	6	1230	A
45	6	1235	C
45	6	1240	U
45	6	1243	G
45	6	1244	A
45	6	1245	G
45	6	1249	U
45	6	1252	C
45	6	1254	U
45	6	1256	A
45	6	1257	U
45	6	1258	U
45	6	1261	G
45	6	1263	G
45	6	1285	U
45	6	1312	A
45	6	1314	U
45	6	1315	U
45	6	1316	G
45	6	1321	A
45	6	1337	A
45	6	1341	A
45	6	1344	A
45	6	1345	A

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Mol	Chain	Res	Type
45	6	1346	A
45	6	1347	U
45	6	1349	G
45	6	1354	G
45	6	1356	U
45	6	1357	A
45	6	1360	A
45	6	1361	U
45	6	1362	U
45	6	1363	U
45	6	1364	G
45	6	1366	U
45	6	1371	A
45	6	1372	U
45	6	1385	G
45	6	1388	A
45	6	1390	U
45	6	1398	U
45	6	1399	C
45	6	1400	A
45	6	1402	G
45	6	1406	A
45	6	1413	U
45	6	1414	U
45	6	1415	U
45	6	1427	A
45	6	1428	G
45	6	1433	G
45	6	1435	G
45	6	1437	U
45	6	1445	G
45	6	1446	A
45	6	1447	C
45	6	1459	C
45	6	1460	A
45	6	1461	C
45	6	1469	A
45	6	1471	A
45	6	1477	G
45	6	1481	C
45	6	1482	C
45	6	1486	G

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Mol	Chain	Res	Type
45	6	1489	U
45	6	1490	C
45	6	1491	U
45	6	1492	A
45	6	1493	A
45	6	1506	G
45	6	1510	U
45	6	1511	U
45	6	1514	U
45	6	1516	A
45	6	1518	C
45	6	1520	U
45	6	1521	G
45	6	1523	G
45	6	1524	A
45	6	1533	C
45	6	1535	U
45	6	1536	G
45	6	1537	C
45	6	1538	U
45	6	1542	G
45	6	1554	U
45	6	1557	U
45	6	1559	A
45	6	1569	A
45	6	1571	C
45	6	1574	G
45	6	1575	G
45	6	1584	G
45	6	1590	G
45	6	1597	A
45	6	1600	A
45	6	1601	G
45	6	1610	G
45	6	1616	G
45	6	1625	C
45	6	1629	G
45	6	1637	C
45	6	1638	G
45	6	1656	U
45	6	1657	U
45	6	1658	G

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Mol	Chain	Res	Type
45	6	1678	A
45	6	1680	G
45	6	1683	C
45	6	1685	G
45	6	1713	G
45	6	1715	G
45	6	1716	C
45	6	1717	G
45	6	1736	G
45	6	1750	A
45	6	1755	A
45	6	1756	A
45	6	1760	G
45	6	1762	A
45	6	1763	A
45	6	1766	A
45	6	1767	G
45	6	1769	U
45	6	1780	G
45	6	1782	A
45	6	1783	C
45	6	1789	G
45	6	1791	A
45	6	1792	G
45	6	1793	G
45	6	1794	A
45	6	1795	U
45	6	1796	C
45	6	1799	U

All (193) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	25	U
1	1	239	G
1	1	594	U
1	1	637	C
1	1	763	G
1	1	816	A
1	1	873	C
1	1	916	G
1	1	978	G

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Mol	Chain	Res	Type
1	1	981	U
1	1	993	G
1	1	1064	A
1	1	1095	U
1	1	1097	G
1	1	1103	A
1	1	1190	A
1	1	1329	U
1	1	1331	U
1	1	1355	A
1	1	1399	A
1	1	1481	A
1	1	1482	A
1	1	1484	U
1	1	1556	C
1	1	1563	C
1	1	1580	A
1	1	1716	U
1	1	1815	U
1	1	2101	C
1	1	2112	U
1	1	2205	U
1	1	2209	U
1	1	2249	G
1	1	2372	A
1	1	2405	C
1	1	2418	G
1	1	2537	U
1	1	2540	A
1	1	2541	U
1	1	2571	U
1	1	2585	G
1	1	2656	A
1	1	2728	G
1	1	2801	A
1	1	2817	A
1	1	2818	U
1	1	2872	A
1	1	2970	C
1	1	3121	U
1	1	3169	U
1	1	3195	U

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Mol	Chain	Res	Type
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3350	C
1	1	3393	U
2	3	52	G
3	4	80	A
3	4	82	U
3	4	89	A
3	4	125	U
45	2	1	U
45	2	68	A
45	2	77	U
45	2	103	A
45	2	130	C
45	2	136	C
45	2	139	C
45	2	158	U
45	2	218	A
45	2	232	U
45	2	278	U
45	2	280	U
45	2	320	U
45	2	417	A
45	2	503	G
45	2	512	A
45	2	555	A
45	2	558	U
45	2	685	A
45	2	782	U
45	2	829	A
45	2	1150	G
45	2	1157	A
45	2	1196	A
45	2	1244	A
45	2	1344	A
45	2	1369	U
45	2	1370	U
45	2	1481	C
45	2	1568	C
45	2	1573	A
45	2	1615	C

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Mol	Chain	Res	Type
45	2	1761	U
1	5	65	A
1	5	151	A
1	5	252	U
1	5	441	U
1	5	558	U
1	5	618	C
1	5	873	C
1	5	916	G
1	5	979	U
1	5	1081	U
1	5	1093	A
1	5	1096	U
1	5	1284	C
1	5	1307	G
1	5	1329	U
1	5	1348	U
1	5	1352	A
1	5	1355	A
1	5	1368	U
1	5	1481	A
1	5	1560	G
1	5	1573	G
1	5	1589	A
1	5	1715	A
1	5	1814	A
1	5	1815	U
1	5	1816	A
1	5	2101	C
1	5	2112	U
1	5	2144	A
1	5	2204	C
1	5	2205	U
1	5	2209	U
1	5	2249	G
1	5	2255	A
1	5	2281	A
1	5	2372	A
1	5	2404	A
1	5	2513	U
1	5	2662	G
1	5	2772	C

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Mol	Chain	Res	Type
1	5	2801	A
1	5	2818	U
1	5	2971	A
1	5	3154	C
1	5	3218	A
1	5	3228	C
1	5	3269	U
1	5	3289	G
1	5	3303	G
1	5	3317	U
1	5	3340	G
1	5	3357	U
3	8	79	A
3	8	80	A
3	8	81	U
3	8	82	U
3	8	83	C
3	8	84	C
3	8	126	A
45	6	25	C
45	6	76	A
45	6	103	A
45	6	114	C
45	6	139	C
45	6	158	U
45	6	217	A
45	6	233	C
45	6	272	U
45	6	321	C
45	6	417	A
45	6	487	G
45	6	506	A
45	6	512	A
45	6	540	G
45	6	542	A
45	6	555	A
45	6	744	U
45	6	745	U
45	6	755	A
45	6	841	U
45	6	968	U
45	6	1051	G

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Mol	Chain	Res	Type
45	6	1058	U
45	6	1097	U
45	6	1207	C
45	6	1244	A
45	6	1255	G
45	6	1344	A
45	6	1346	A
45	6	1363	U
45	6	1413	U
45	6	1481	C
45	6	1535	U
45	6	1568	C
45	6	1573	A
45	6	1600	A
45	6	1615	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 2242 ligands modelled in this entry, 2155 are monoatomic - leaving 87 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	$\# Z > 2$
80	PAR	1	3421	-	45,45,45	0.21	0	64,67,67	0.93	2 (3%)
80	PAR	5	3413	-	45,45,45	0.21	0	64,67,67	1.40	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	PAR	1	3433	-	45,45,45	0.27	0	64,67,67	1.24	6 (9%)
80	PAR	5	3419	-	45,45,45	0.33	0	64,67,67	1.27	8 (12%)
80	PAR	3	201	-	45,45,45	0.26	0	64,67,67	1.46	5 (7%)
80	PAR	1	3431	-	45,45,45	0.19	0	64,67,67	1.13	3 (4%)
80	PAR	1	3405	-	45,45,45	0.24	0	64,67,67	0.89	2 (3%)
80	PAR	5	3408	-	45,45,45	0.22	0	64,67,67	0.91	3 (4%)
80	PAR	1	3406	-	45,45,45	0.21	0	64,67,67	0.89	4 (6%)
80	PAR	7	201	-	45,45,45	0.17	0	64,67,67	0.75	2 (3%)
80	PAR	1	3434	-	45,45,45	0.20	0	64,67,67	0.89	5 (7%)
80	PAR	2	1904	-	45,45,45	0.21	0	64,67,67	1.42	4 (6%)
80	PAR	5	3425	-	45,45,45	0.22	0	64,67,67	0.98	4 (6%)
80	PAR	2	1902	-	45,45,45	0.24	0	64,67,67	1.34	5 (7%)
80	PAR	1	3414	-	45,45,45	0.21	0	64,67,67	1.05	4 (6%)
80	PAR	1	3422	-	45,45,45	0.22	0	64,67,67	1.05	3 (4%)
80	PAR	n3	201	-	45,45,45	0.24	0	64,67,67	1.07	4 (6%)
80	PAR	5	3423	-	45,45,45	0.21	0	64,67,67	0.96	4 (6%)
80	PAR	6	1905	-	45,45,45	0.20	0	64,67,67	1.05	4 (6%)
80	PAR	6	1906	-	45,45,45	0.20	0	64,67,67	0.75	2 (3%)
80	PAR	5	3410	-	45,45,45	0.17	0	64,67,67	0.87	2 (3%)
80	PAR	1	3427	-	45,45,45	0.21	0	64,67,67	0.83	3 (4%)
80	PAR	3	203	-	45,45,45	0.21	0	64,67,67	0.99	3 (4%)
80	PAR	5	3416	-	45,45,45	0.22	0	64,67,67	0.91	3 (4%)
80	PAR	1	3408	-	45,45,45	0.22	0	64,67,67	1.07	5 (7%)
80	PAR	1	3403	81	45,45,45	0.22	0	64,67,67	0.92	1 (1%)
80	PAR	1	3426	-	45,45,45	0.25	0	64,67,67	1.02	3 (4%)
80	PAR	1	3432	-	45,45,45	0.25	0	64,67,67	1.11	2 (3%)
80	PAR	5	3426	-	45,45,45	0.23	0	64,67,67	0.89	1 (1%)
80	PAR	5	3404	-	45,45,45	0.24	0	64,67,67	1.22	4 (6%)
80	PAR	1	3418	-	45,45,45	0.26	0	64,67,67	0.87	2 (3%)
80	PAR	1	3424	-	45,45,45	0.16	0	64,67,67	0.71	2 (3%)
80	PAR	2	1901	-	45,45,45	0.19	0	64,67,67	0.74	2 (3%)
80	PAR	6	1902	-	45,45,45	0.24	0	64,67,67	0.98	3 (4%)
80	PAR	5	3402	-	45,45,45	0.20	0	64,67,67	1.05	2 (3%)
80	PAR	8	202	-	45,45,45	0.22	0	64,67,67	0.88	1 (1%)
80	PAR	5	3428	81	45,45,45	0.39	0	64,67,67	1.21	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	PAR	1	3417	-	45,45,45	0.17	0	64,67,67	0.88	2 (3%)
80	PAR	1	3412	-	45,45,45	0.21	0	64,67,67	1.23	8 (12%)
80	PAR	1	3411	-	45,45,45	0.32	0	64,67,67	1.68	5 (7%)
80	PAR	5	3421	-	45,45,45	0.20	0	64,67,67	1.25	2 (3%)
80	PAR	2	1903	-	45,45,45	0.22	0	64,67,67	0.84	3 (4%)
80	PAR	1	3401	-	45,45,45	0.18	0	64,67,67	1.22	2 (3%)
80	PAR	6	1904	-	45,45,45	0.21	0	64,67,67	0.90	3 (4%)
80	PAR	5	3415	-	45,45,45	0.26	0	64,67,67	1.01	2 (3%)
80	PAR	5	3409	-	45,45,45	0.22	0	64,67,67	0.98	4 (6%)
80	PAR	1	3425	-	45,45,45	0.28	0	64,67,67	1.17	5 (7%)
80	PAR	1	3410	-	45,45,45	0.36	0	64,67,67	1.38	8 (12%)
80	PAR	5	3427	-	45,45,45	0.22	0	64,67,67	1.05	3 (4%)
80	PAR	2	1905	-	45,45,45	0.20	0	64,67,67	0.79	4 (6%)
80	PAR	5	3417	-	45,45,45	0.16	0	64,67,67	0.78	2 (3%)
80	PAR	1	3429	-	45,45,45	0.23	0	64,67,67	1.26	4 (6%)
80	PAR	5	3420	-	45,45,45	0.23	0	64,67,67	1.30	7 (10%)
80	PAR	4	201	-	45,45,45	0.29	0	64,67,67	1.21	5 (7%)
80	PAR	5	3407	-	45,45,45	0.20	0	64,67,67	0.81	3 (4%)
80	PAR	1	3419	-	45,45,45	0.22	0	64,67,67	1.15	5 (7%)
80	PAR	5	3418	-	45,45,45	0.24	0	64,67,67	1.08	3 (4%)
80	PAR	1	3420	-	45,45,45	0.20	0	64,67,67	0.99	3 (4%)
80	PAR	6	1901	-	45,45,45	0.25	0	64,67,67	0.92	2 (3%)
80	PAR	5	3401	-	45,45,45	0.27	0	64,67,67	1.01	2 (3%)
80	PAR	1	3415	-	45,45,45	0.25	0	64,67,67	0.88	3 (4%)
80	PAR	1	3407	-	45,45,45	0.21	0	64,67,67	0.95	3 (4%)
80	PAR	1	3435	-	45,45,45	0.38	0	64,67,67	1.31	4 (6%)
80	PAR	8	201	-	45,45,45	0.24	0	64,67,67	1.01	5 (7%)
80	PAR	7	202	-	45,45,45	0.18	0	64,67,67	0.87	3 (4%)
80	PAR	1	3409	-	45,45,45	0.29	0	64,67,67	1.45	4 (6%)
80	PAR	5	3403	-	45,45,45	0.25	0	64,67,67	1.02	3 (4%)
80	PAR	1	3430	-	45,45,45	0.24	0	64,67,67	0.95	3 (4%)
80	PAR	5	3422	-	45,45,45	0.20	0	64,67,67	0.91	4 (6%)
80	PAR	1	3413	-	45,45,45	0.20	0	64,67,67	0.66	1 (1%)
80	PAR	1	3437	1	45,45,45	0.19	0	64,67,67	0.73	2 (3%)
80	PAR	1	3402	-	45,45,45	0.21	0	64,67,67	0.78	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
80	PAR	3	202	81	45,45,45	0.21	0	64,67,67	1.06	3 (4%)
80	PAR	4	202	-	45,45,45	0.26	0	64,67,67	1.06	4 (6%)
80	PAR	5	3424	-	45,45,45	0.23	0	64,67,67	1.02	3 (4%)
80	PAR	5	3405	-	45,45,45	0.22	0	64,67,67	0.80	2 (3%)
80	PAR	o2	201	-	45,45,45	0.28	0	64,67,67	1.17	4 (6%)
80	PAR	5	3406	81	45,45,45	0.27	0	64,67,67	0.95	5 (7%)
80	PAR	5	3414	-	45,45,45	0.19	0	64,67,67	0.80	4 (6%)
80	PAR	1	3423	-	45,45,45	0.20	0	64,67,67	0.75	1 (1%)
80	PAR	1	3416	-	45,45,45	0.28	0	64,67,67	1.13	5 (7%)
80	PAR	1	3404	-	45,45,45	0.22	0	64,67,67	0.92	2 (3%)
80	PAR	1	3436	-	45,45,45	0.23	0	64,67,67	1.01	3 (4%)
80	PAR	6	1903	-	45,45,45	0.18	0	64,67,67	0.88	1 (1%)
80	PAR	1	3428	81	45,45,45	0.22	0	64,67,67	0.99	2 (3%)
80	PAR	5	3412	-	45,45,45	0.21	0	64,67,67	0.89	2 (3%)
80	PAR	5	3411	-	45,45,45	0.24	0	64,67,67	1.13	5 (7%)

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
80	PAR	1	3421	-	-	3/18/94/94	0/4/4/4
80	PAR	5	3413	-	-	2/18/94/94	0/4/4/4
80	PAR	1	3433	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3419	-	-	7/18/94/94	0/4/4/4
80	PAR	3	201	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3431	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3405	-	-	11/18/94/94	0/4/4/4
80	PAR	5	3408	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3406	-	-	2/18/94/94	0/4/4/4
80	PAR	7	201	-	-	3/18/94/94	0/4/4/4
80	PAR	1	3434	-	-	6/18/94/94	0/4/4/4
80	PAR	2	1904	-	-	4/18/94/94	0/4/4/4
80	PAR	5	3425	-	-	5/18/94/94	0/4/4/4
80	PAR	2	1902	-	-	3/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	PAR	1	3414	-	-	3/18/94/94	0/4/4/4
80	PAR	1	3422	-	-	8/18/94/94	0/4/4/4
80	PAR	n3	201	-	-	8/18/94/94	0/4/4/4
80	PAR	5	3423	-	-	5/18/94/94	0/4/4/4
80	PAR	6	1905	-	-	7/18/94/94	0/4/4/4
80	PAR	6	1906	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3410	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3427	-	-	5/18/94/94	0/4/4/4
80	PAR	3	203	-	-	4/18/94/94	1/4/4/4
80	PAR	5	3416	-	-	2/18/94/94	0/4/4/4
80	PAR	1	3408	-	-	3/18/94/94	0/4/4/4
80	PAR	1	3403	81	-	5/18/94/94	0/4/4/4
80	PAR	1	3426	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3432	-	-	3/18/94/94	1/4/4/4
80	PAR	5	3426	-	-	4/18/94/94	1/4/4/4
80	PAR	5	3404	-	-	8/18/94/94	0/4/4/4
80	PAR	1	3418	-	-	7/18/94/94	1/4/4/4
80	PAR	1	3424	-	-	4/18/94/94	0/4/4/4
80	PAR	2	1901	-	-	1/18/94/94	0/4/4/4
80	PAR	6	1902	-	-	9/18/94/94	0/4/4/4
80	PAR	5	3402	-	-	8/18/94/94	0/4/4/4
80	PAR	8	202	-	-	5/18/94/94	0/4/4/4
80	PAR	5	3428	81	-	7/18/94/94	0/4/4/4
80	PAR	1	3417	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3412	-	-	4/18/94/94	0/4/4/4
80	PAR	1	3411	-	-	8/18/94/94	0/4/4/4
80	PAR	5	3421	-	-	7/18/94/94	0/4/4/4
80	PAR	2	1903	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3401	-	-	5/18/94/94	0/4/4/4
80	PAR	6	1904	-	-	6/18/94/94	0/4/4/4
80	PAR	5	3415	-	-	7/18/94/94	0/4/4/4
80	PAR	5	3409	-	-	9/18/94/94	0/4/4/4
80	PAR	1	3425	-	-	10/18/94/94	0/4/4/4
80	PAR	1	3410	-	-	6/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	PAR	5	3427	-	-	3/18/94/94	1/4/4/4
80	PAR	2	1905	-	-	4/18/94/94	0/4/4/4
80	PAR	5	3417	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3429	-	-	3/18/94/94	0/4/4/4
80	PAR	5	3420	-	-	3/18/94/94	1/4/4/4
80	PAR	4	201	-	-	6/18/94/94	1/4/4/4
80	PAR	5	3407	-	-	9/18/94/94	0/4/4/4
80	PAR	1	3419	-	-	7/18/94/94	1/4/4/4
80	PAR	5	3418	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3420	-	-	1/18/94/94	0/4/4/4
80	PAR	6	1901	-	-	2/18/94/94	0/4/4/4
80	PAR	5	3401	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3415	-	-	4/18/94/94	0/4/4/4
80	PAR	1	3407	-	-	7/18/94/94	0/4/4/4
80	PAR	1	3435	-	-	11/18/94/94	0/4/4/4
80	PAR	8	201	-	-	1/18/94/94	0/4/4/4
80	PAR	7	202	-	-	8/18/94/94	0/4/4/4
80	PAR	1	3409	-	-	9/18/94/94	1/4/4/4
80	PAR	5	3403	-	-	6/18/94/94	0/4/4/4
80	PAR	1	3430	-	-	7/18/94/94	0/4/4/4
80	PAR	5	3422	-	-	4/18/94/94	0/4/4/4
80	PAR	1	3413	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3437	1	-	5/18/94/94	0/4/4/4
80	PAR	1	3402	-	-	7/18/94/94	0/4/4/4
80	PAR	3	202	81	-	8/18/94/94	0/4/4/4
80	PAR	4	202	-	-	3/18/94/94	0/4/4/4
80	PAR	5	3424	-	-	4/18/94/94	0/4/4/4
80	PAR	5	3405	-	-	7/18/94/94	0/4/4/4
80	PAR	o2	201	-	-	10/18/94/94	0/4/4/4
80	PAR	5	3406	81	-	5/18/94/94	0/4/4/4
80	PAR	5	3414	-	-	1/18/94/94	1/4/4/4
80	PAR	1	3423	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3416	-	-	3/18/94/94	0/4/4/4
80	PAR	1	3404	-	-	3/18/94/94	0/4/4/4
80	PAR	1	3436	-	-	9/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	PAR	6	1903	-	-	5/18/94/94	0/4/4/4
80	PAR	1	3428	81	-	3/18/94/94	0/4/4/4
80	PAR	5	3412	-	-	6/18/94/94	0/4/4/4
80	PAR	5	3411	-	-	7/18/94/94	0/4/4/4

There are no bond length outliers.

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	1	3409	PAR	O11-C11-C21	8.93	123.60	108.22
80	5	3421	PAR	O52-C13-O43	-8.23	102.52	111.43
80	2	1904	PAR	O52-C13-O43	-7.82	102.97	111.43
80	1	3431	PAR	O52-C13-O43	-7.17	103.67	111.43
80	5	3413	PAR	O11-C11-C21	6.84	120.00	108.22
80	1	3411	PAR	O33-C14-C24	6.81	119.95	108.22
80	1	3435	PAR	O52-C13-O43	-6.78	104.09	111.43
80	1	3411	PAR	C14-C24-N24	6.69	122.25	110.20
80	1	3411	PAR	O52-C13-O43	-6.59	104.29	111.43
80	3	201	PAR	O52-C13-O43	-6.41	104.49	111.43
80	5	3402	PAR	O52-C13-O43	-6.30	104.61	111.43
80	1	3401	PAR	O33-C14-C24	6.29	119.05	108.22
80	1	3429	PAR	O52-C13-O43	-6.00	104.93	111.43
80	5	3404	PAR	O11-C11-C21	5.93	118.43	108.22
80	1	3425	PAR	O11-C11-C21	5.85	118.29	108.22
80	5	3425	PAR	O52-C13-O43	-5.81	105.15	111.43
80	o2	201	PAR	O52-C13-O43	-5.74	105.22	111.43
80	4	202	PAR	O52-C13-O43	-5.57	105.41	111.43
80	5	3410	PAR	O52-C13-O43	-5.53	105.44	111.43
80	4	201	PAR	O11-C11-C21	5.45	117.61	108.22
80	1	3421	PAR	O52-C13-O43	-5.44	105.54	111.43
80	5	3401	PAR	O52-C13-O43	-5.42	105.56	111.43
80	6	1901	PAR	O52-C13-O43	-5.40	105.58	111.43
80	3	201	PAR	O11-C11-C21	5.40	117.52	108.22
80	6	1903	PAR	O52-C13-O43	-5.37	105.62	111.43
80	1	3422	PAR	O52-C13-O43	-5.29	105.70	111.43
80	5	3428	PAR	O11-C11-C21	5.28	117.31	108.22
80	5	3427	PAR	O11-C11-C21	5.26	117.28	108.22
80	6	1905	PAR	O52-C13-O43	-5.24	105.75	111.43
80	1	3432	PAR	O11-C11-C21	5.16	117.10	108.22
80	5	3416	PAR	O52-C13-O43	-5.15	105.85	111.43
80	3	202	PAR	O52-C13-O43	-5.12	105.89	111.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	5	3420	PAR	O52-C13-O43	-5.09	105.92	111.43
80	2	1902	PAR	O52-C52-C62	5.09	120.81	107.28
80	5	3403	PAR	O52-C13-O43	-5.08	105.93	111.43
80	5	3415	PAR	O52-C13-O43	-5.08	105.93	111.43
80	5	3418	PAR	O52-C13-O43	-5.06	105.95	111.43
80	1	3420	PAR	O52-C13-O43	-5.04	105.98	111.43
80	2	1902	PAR	O33-C33-C23	5.03	127.48	111.32
80	6	1902	PAR	O52-C13-O43	-5.01	106.00	111.43
80	1	3436	PAR	O52-C13-O43	-4.89	106.13	111.43
80	8	202	PAR	O52-C13-O43	-4.86	106.17	111.43
80	1	3401	PAR	O52-C13-O43	-4.85	106.19	111.43
80	5	3412	PAR	O52-C13-O43	-4.72	106.32	111.43
80	1	3432	PAR	O52-C13-O43	-4.66	106.39	111.43
80	2	1904	PAR	O11-C11-C21	4.61	116.15	108.22
80	5	3413	PAR	O52-C13-O43	-4.59	106.46	111.43
80	n3	201	PAR	O52-C13-O43	-4.59	106.46	111.43
80	1	3412	PAR	C13-C23-C33	-4.50	96.69	102.10
80	1	3408	PAR	O52-C13-O43	-4.47	106.59	111.43
80	1	3433	PAR	C14-C24-N24	4.46	118.25	110.20
80	1	3412	PAR	O33-C14-C24	-4.45	100.55	108.22
80	5	3417	PAR	O52-C13-O43	-4.43	106.64	111.43
80	1	3414	PAR	O52-C52-C62	4.40	118.98	107.28
80	3	203	PAR	O33-C14-C24	4.40	115.79	108.22
80	1	3417	PAR	O52-C13-O43	-4.39	106.68	111.43
80	1	3416	PAR	O52-C52-C62	4.39	118.95	107.28
80	5	3411	PAR	O11-C42-C32	-4.33	98.85	109.18
80	1	3403	PAR	O11-C11-C21	4.32	115.65	108.22
80	5	3424	PAR	O52-C13-O43	-4.32	106.76	111.43
80	1	3419	PAR	O11-C42-C32	-4.31	98.89	109.18
80	7	202	PAR	O52-C13-O43	-4.28	106.80	111.43
80	5	3426	PAR	O52-C13-O43	-4.25	106.83	111.43
80	1	3433	PAR	O33-C14-C24	4.24	115.53	108.22
80	n3	201	PAR	O11-C11-C21	4.24	115.52	108.22
80	5	3409	PAR	O52-C13-O43	-4.21	106.87	111.43
80	1	3410	PAR	O52-C52-C62	4.19	118.42	107.28
80	8	201	PAR	O52-C13-O43	-4.15	106.94	111.43
80	1	3405	PAR	O33-C14-C24	4.14	115.35	108.22
80	6	1905	PAR	O11-C11-C21	4.11	115.30	108.22
80	5	3427	PAR	O52-C13-O43	-4.11	106.98	111.43
80	1	3430	PAR	O52-C13-O43	-4.11	106.98	111.43
80	1	3404	PAR	O52-C13-O43	-4.08	107.02	111.43
80	5	3428	PAR	C13-C23-C33	-4.07	97.21	102.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	5	3418	PAR	O11-C11-C21	4.06	115.21	108.22
80	1	3426	PAR	O11-C11-C21	4.01	115.12	108.22
80	5	3420	PAR	O33-C14-C24	4.00	115.10	108.22
80	5	3419	PAR	O52-C52-C62	3.98	117.87	107.28
80	1	3410	PAR	O11-C11-C21	3.96	115.03	108.22
80	1	3422	PAR	O33-C14-C24	-3.91	101.47	108.22
80	5	3413	PAR	O33-C14-C24	-3.88	101.53	108.22
80	5	3423	PAR	C13-C23-C33	-3.87	97.45	102.10
80	1	3424	PAR	O52-C13-O43	-3.87	107.25	111.43
80	1	3415	PAR	O11-C11-C21	3.82	114.80	108.22
80	1	3433	PAR	O52-C13-O43	-3.82	107.29	111.43
80	1	3429	PAR	O33-C14-C24	3.81	114.78	108.22
80	6	1902	PAR	O11-C11-C21	3.80	114.77	108.22
80	1	3407	PAR	O52-C13-O43	-3.80	107.32	111.43
80	1	3428	PAR	O33-C14-C24	-3.78	101.70	108.22
80	2	1904	PAR	O33-C14-C24	-3.77	101.72	108.22
80	5	3420	PAR	O52-C13-C23	3.77	115.77	107.96
80	1	3416	PAR	C13-C23-C33	-3.76	97.58	102.10
80	5	3422	PAR	O52-C13-O43	-3.75	107.37	111.43
80	1	3406	PAR	O52-C13-O43	-3.75	107.37	111.43
80	5	3421	PAR	O11-C11-C21	3.73	114.65	108.22
80	5	3419	PAR	C32-C22-C12	3.73	118.85	111.18
80	5	3409	PAR	O11-C11-C21	3.70	114.59	108.22
80	1	3429	PAR	C13-C23-C33	-3.68	97.67	102.10
80	1	3425	PAR	C14-C24-N24	3.68	116.83	110.20
80	1	3410	PAR	O11-C42-C32	3.62	117.81	109.18
80	1	3419	PAR	O52-C13-O43	-3.62	107.52	111.43
80	3	202	PAR	O52-C52-C62	3.62	116.90	107.28
80	1	3404	PAR	O52-C52-C62	3.58	116.79	107.28
80	1	3410	PAR	O52-C13-O43	-3.56	107.57	111.43
80	1	3423	PAR	O52-C13-O43	-3.48	107.66	111.43
80	2	1903	PAR	O33-C14-C24	-3.47	102.23	108.22
80	1	3413	PAR	O52-C13-O43	-3.44	107.71	111.43
80	5	3411	PAR	O52-C13-O43	-3.43	107.72	111.43
80	5	3424	PAR	O11-C11-C21	3.41	114.09	108.22
80	5	3408	PAR	O11-C11-C21	3.41	114.08	108.22
80	1	3434	PAR	O52-C13-O43	-3.40	107.75	111.43
80	7	201	PAR	O52-C13-O43	-3.37	107.78	111.43
80	1	3427	PAR	O52-C13-O43	-3.36	107.80	111.43
80	1	3420	PAR	O33-C14-C24	-3.35	102.44	108.22
80	5	3413	PAR	O11-C42-C32	3.34	117.15	109.18
80	1	3426	PAR	O33-C33-C23	-3.31	100.66	111.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	2	1902	PAR	O33-C14-C24	-3.30	102.53	108.22
80	1	3431	PAR	O11-C11-C21	3.29	113.89	108.22
80	3	201	PAR	O33-C33-C23	3.28	121.87	111.32
80	1	3427	PAR	O11-C11-C21	3.27	113.85	108.22
80	1	3436	PAR	O11-C11-C21	3.24	113.80	108.22
80	5	3422	PAR	O33-C33-C23	3.23	121.70	111.32
80	5	3411	PAR	O33-C33-C23	3.22	121.66	111.32
80	5	3415	PAR	O11-C42-C52	3.20	115.61	107.48
80	5	3419	PAR	O33-C14-C24	-3.19	102.72	108.22
80	1	3419	PAR	O33-C14-C24	-3.18	102.75	108.22
80	8	201	PAR	O11-C42-C32	-3.15	101.65	109.18
80	1	3422	PAR	O11-C11-C21	3.12	113.59	108.22
80	1	3428	PAR	O11-C11-C21	3.12	113.59	108.22
80	1	3406	PAR	O33-C14-C24	-3.11	102.85	108.22
80	5	3416	PAR	O11-C11-C21	3.11	113.58	108.22
80	1	3426	PAR	C13-C23-C33	-3.11	98.36	102.10
80	3	201	PAR	O33-C14-C24	-3.10	102.88	108.22
80	5	3408	PAR	O33-C14-C24	3.09	113.55	108.22
80	5	3404	PAR	O52-C52-C62	3.08	115.46	107.28
80	5	3420	PAR	O11-C11-C21	3.06	113.49	108.22
80	5	3405	PAR	O11-C11-C21	3.06	113.49	108.22
80	1	3433	PAR	O11-C42-C32	-3.05	101.90	109.18
80	7	202	PAR	O11-C11-C21	3.05	113.47	108.22
80	5	3407	PAR	O52-C13-O43	-3.03	108.15	111.43
80	2	1902	PAR	O23-C23-C33	3.03	119.76	111.17
80	5	3428	PAR	C11-C21-N21	3.02	115.64	110.20
80	4	202	PAR	O33-C14-C24	-3.01	103.02	108.22
80	5	3428	PAR	O33-C33-C23	-3.01	101.63	111.32
80	5	3414	PAR	O52-C13-O43	-2.96	108.22	111.43
80	1	3410	PAR	C32-C22-C12	2.96	117.25	111.18
80	5	3408	PAR	O52-C13-O43	-2.94	108.25	111.43
80	5	3406	PAR	C13-C23-C33	-2.91	98.60	102.10
80	4	201	PAR	O52-C13-C23	2.91	113.99	107.96
80	1	3425	PAR	C11-C21-N21	2.91	115.44	110.20
80	1	3402	PAR	O11-C42-C32	-2.90	102.26	109.18
80	5	3419	PAR	O11-C11-C21	2.89	113.20	108.22
80	1	3408	PAR	C11-C21-N21	-2.87	105.03	110.20
80	1	3410	PAR	C62-C52-C42	-2.86	105.12	111.66
80	8	201	PAR	C32-C22-C12	-2.86	105.31	111.18
80	n3	201	PAR	O11-C42-C32	2.83	115.94	109.18
80	6	1904	PAR	O11-C42-C32	-2.82	102.44	109.18
80	3	203	PAR	O11-C11-C21	2.80	113.04	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	1	3429	PAR	C14-C24-N24	2.79	115.23	110.20
80	5	3406	PAR	C14-O54-C54	2.76	119.11	113.69
80	7	201	PAR	O11-C11-C21	2.76	112.97	108.22
80	2	1901	PAR	O11-C11-C21	2.76	112.97	108.22
80	1	3409	PAR	O33-C14-C24	-2.73	103.51	108.22
80	1	3434	PAR	C13-C23-C33	2.71	105.36	102.10
80	1	3412	PAR	O52-C13-C23	2.70	113.57	107.96
80	1	3411	PAR	O11-C42-C32	-2.70	102.75	109.18
80	2	1905	PAR	O11-C42-C32	-2.69	102.75	109.18
80	5	3420	PAR	C14-C24-N24	2.69	115.05	110.20
80	1	3437	PAR	O52-C13-O43	-2.69	108.52	111.43
80	5	3409	PAR	C11-C21-N21	2.64	114.97	110.20
80	2	1903	PAR	O11-C11-C21	2.64	112.77	108.22
80	1	3412	PAR	O33-C33-C23	-2.63	102.84	111.32
80	5	3420	PAR	O33-C33-C23	2.63	119.78	111.32
80	1	3436	PAR	C13-C23-C33	-2.63	98.94	102.10
80	5	3417	PAR	O11-C11-C21	2.62	112.72	108.22
80	5	3409	PAR	O33-C14-C24	-2.61	103.71	108.22
80	5	3406	PAR	O52-C13-O43	-2.61	108.60	111.43
80	1	3416	PAR	O33-C33-C23	-2.59	102.98	111.32
80	6	1906	PAR	O11-C11-C21	2.59	112.67	108.22
80	1	3434	PAR	O52-C52-C62	2.59	114.16	107.28
80	4	201	PAR	O11-C42-C32	2.58	115.34	109.18
80	2	1905	PAR	O52-C13-O43	-2.58	108.63	111.43
80	o2	201	PAR	C32-C22-C12	-2.57	105.90	111.18
80	1	3407	PAR	O11-C11-C21	2.53	112.58	108.22
80	1	3417	PAR	O11-C11-C21	2.53	112.58	108.22
80	5	3404	PAR	O11-C42-C32	2.53	115.22	109.18
80	1	3409	PAR	O11-C11-O51	2.52	117.72	110.67
80	6	1902	PAR	C13-C23-C33	2.51	105.12	102.10
80	5	3411	PAR	C14-C24-N24	2.48	114.68	110.20
80	1	3414	PAR	O52-C13-O43	-2.48	108.75	111.43
80	5	3422	PAR	O23-C23-C33	2.48	118.20	111.17
80	5	3407	PAR	C13-C23-C33	-2.47	99.13	102.10
80	5	3414	PAR	O33-C14-C24	-2.47	103.97	108.22
80	2	1905	PAR	O11-C11-C21	2.47	112.46	108.22
80	3	202	PAR	C13-C23-C33	2.46	105.06	102.10
80	5	3419	PAR	C14-C24-N24	2.45	114.63	110.20
80	1	3434	PAR	O33-C33-C23	2.45	119.19	111.32
80	1	3416	PAR	O52-C13-O43	-2.45	108.78	111.43
80	1	3427	PAR	O33-C14-C24	2.45	112.43	108.22
80	5	3422	PAR	O11-C11-C21	2.42	112.39	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	1	3421	PAR	O33-C14-C24	-2.42	104.04	108.22
80	1	3416	PAR	O43-C13-C23	-2.41	101.87	104.98
80	1	3430	PAR	O11-C11-C21	2.38	112.32	108.22
80	5	3401	PAR	O33-C14-C24	-2.38	104.11	108.22
80	1	3406	PAR	O11-C11-C21	2.38	112.32	108.22
80	5	3425	PAR	O33-C14-C24	-2.38	104.12	108.22
80	5	3413	PAR	C11-C21-N21	2.37	114.47	110.20
80	2	1901	PAR	O52-C13-O43	-2.37	108.87	111.43
80	1	3410	PAR	O33-C14-C24	2.37	112.29	108.22
80	5	3425	PAR	O11-C11-C21	2.35	112.27	108.22
80	o2	201	PAR	O33-C33-C23	2.35	118.88	111.32
80	1	3437	PAR	O11-C11-C21	2.35	112.26	108.22
80	1	3405	PAR	O52-C52-C62	2.35	113.52	107.28
80	5	3419	PAR	C62-C52-C42	-2.34	106.31	111.66
80	4	201	PAR	O33-C14-C24	2.34	112.25	108.22
80	1	3420	PAR	O11-C42-C32	-2.33	103.61	109.18
80	5	3423	PAR	O52-C13-O43	-2.33	108.91	111.43
80	4	201	PAR	C13-C23-C33	2.33	104.90	102.10
80	1	3418	PAR	C13-C23-C33	-2.33	99.30	102.10
80	1	3412	PAR	O52-C13-O43	-2.31	108.93	111.43
80	5	3403	PAR	O11-C11-C21	-2.31	104.24	108.22
80	5	3405	PAR	C32-C22-C12	-2.29	106.48	111.18
80	8	201	PAR	C52-C42-C32	2.28	115.42	111.16
80	5	3414	PAR	C32-C22-C12	2.27	115.85	111.18
80	5	3419	PAR	C22-C12-C62	2.26	113.46	110.04
80	1	3425	PAR	O52-C13-O43	-2.26	108.98	111.43
80	2	1902	PAR	O11-C11-C21	2.26	112.11	108.22
80	o2	201	PAR	O23-C23-C33	2.23	117.51	111.17
80	7	202	PAR	O11-C42-C32	-2.23	103.87	109.18
80	2	1905	PAR	O33-C14-C24	-2.22	104.39	108.22
80	1	3415	PAR	C13-C23-C33	-2.21	99.44	102.10
80	6	1905	PAR	O33-C14-C24	2.21	112.02	108.22
80	8	201	PAR	O33-C14-C24	-2.21	104.41	108.22
80	1	3433	PAR	C52-C42-C32	2.20	115.28	111.16
80	1	3414	PAR	O11-C42-C32	-2.20	103.92	109.18
80	1	3411	PAR	O54-C54-C64	2.20	110.11	106.01
80	2	1903	PAR	C13-O43-C43	-2.20	97.98	106.13
80	5	3412	PAR	O11-C11-C21	2.20	112.00	108.22
80	5	3425	PAR	C13-C23-C33	2.20	104.74	102.10
80	1	3414	PAR	C13-C23-C33	-2.19	99.46	102.10
80	1	3419	PAR	O52-C52-C42	2.19	113.03	107.48
80	2	1904	PAR	C14-O54-C54	2.17	117.96	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	5	3423	PAR	O11-C11-C21	2.17	111.96	108.22
80	1	3408	PAR	O11-C11-C21	2.16	111.94	108.22
80	1	3412	PAR	C23-C33-C43	-2.16	99.40	103.22
80	5	3424	PAR	C13-O43-C43	-2.16	98.13	106.13
80	6	1904	PAR	O52-C13-O43	-2.15	109.10	111.43
80	1	3412	PAR	O11-C42-C32	-2.15	104.04	109.18
80	5	3407	PAR	O33-C14-C24	2.15	111.91	108.22
80	5	3406	PAR	O54-C54-C64	2.14	110.00	106.01
80	1	3425	PAR	O33-C33-C23	-2.14	104.43	111.32
80	4	202	PAR	O33-C33-C23	-2.14	104.45	111.32
80	3	203	PAR	C32-C22-C12	2.13	115.57	111.18
80	5	3406	PAR	O52-C13-C23	2.13	112.38	107.96
80	5	3404	PAR	C62-C52-C42	-2.13	106.81	111.66
80	1	3433	PAR	O54-C54-C64	2.12	109.96	106.01
80	1	3402	PAR	O52-C13-O43	-2.12	109.13	111.43
80	5	3423	PAR	O52-C52-C42	-2.11	102.11	107.48
80	5	3414	PAR	O11-C11-C21	2.11	111.85	108.22
80	6	1906	PAR	C11-C21-N21	2.11	114.01	110.20
80	1	3435	PAR	C41-C31-C21	-2.11	107.44	111.07
80	1	3408	PAR	O51-C11-C21	2.11	114.80	110.06
80	6	1901	PAR	O33-C14-C24	-2.11	104.58	108.22
80	1	3406	PAR	O11-C42-C32	-2.09	104.18	109.18
80	3	201	PAR	O23-C23-C33	2.09	117.10	111.17
80	1	3418	PAR	C23-C33-C43	-2.09	99.52	103.22
80	1	3407	PAR	C14-O54-C54	2.09	117.78	113.69
80	1	3434	PAR	O33-C14-C24	-2.08	104.63	108.22
80	5	3402	PAR	O11-C42-C32	-2.08	104.22	109.18
80	1	3424	PAR	O11-C11-C21	2.08	111.80	108.22
80	1	3419	PAR	O11-C11-C21	2.07	111.79	108.22
80	n3	201	PAR	O11-C42-C52	-2.07	102.21	107.48
80	1	3408	PAR	O33-C33-C23	2.07	117.97	111.32
80	5	3411	PAR	O52-C52-C62	2.07	112.78	107.28
80	5	3419	PAR	O43-C43-C33	-2.07	100.44	104.87
80	5	3413	PAR	C62-C52-C42	-2.07	106.94	111.66
80	4	202	PAR	O11-C42-C32	-2.06	104.26	109.18
80	1	3430	PAR	O33-C14-C24	2.06	111.76	108.22
80	1	3431	PAR	O52-C52-C62	2.06	112.76	107.28
80	5	3428	PAR	O52-C13-O43	-2.06	109.20	111.43
80	5	3420	PAR	C13-C23-C33	-2.06	99.63	102.10
80	1	3409	PAR	C62-C52-C42	-2.05	106.98	111.66
80	5	3416	PAR	C11-C21-N21	2.05	113.89	110.20
80	1	3435	PAR	O23-C23-C33	-2.05	105.36	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	1	3415	PAR	O33-C14-C24	2.04	111.73	108.22
80	1	3412	PAR	C14-O33-C33	2.04	123.02	117.96
80	5	3427	PAR	C13-C23-C33	2.04	104.55	102.10
80	6	1904	PAR	C52-C42-C32	2.04	114.96	111.16
80	6	1905	PAR	C14-C24-N24	2.03	113.87	110.20
80	5	3403	PAR	O52-C52-C62	2.03	112.67	107.28
80	5	3418	PAR	C13-C23-C33	-2.02	99.67	102.10
80	5	3410	PAR	O11-C11-C21	2.02	111.70	108.22
80	1	3435	PAR	O33-C14-C24	-2.01	104.76	108.22
80	1	3410	PAR	O62-C62-C52	2.00	115.25	109.94

There are no chirality outliers.

All (474) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	5	3413	PAR	C23-C13-O52-C52
80	1	3431	PAR	C43-C33-O33-C14
80	1	3414	PAR	C24-C14-O33-C33
80	5	3418	PAR	C23-C13-O52-C52
80	5	3418	PAR	C24-C14-O33-C33
80	1	3406	PAR	C23-C13-O52-C52
80	o2	201	PAR	C23-C33-O33-C14
80	2	1902	PAR	C23-C33-O33-C14
80	5	3404	PAR	C21-C11-O11-C42
80	5	3404	PAR	C24-C14-O33-C33
80	7	202	PAR	C23-C13-O52-C52
80	7	202	PAR	O43-C13-O52-C52
80	7	202	PAR	C24-C14-O33-C33
80	3	202	PAR	C23-C13-O52-C52
80	3	202	PAR	C44-C54-C64-N64
80	3	202	PAR	O54-C54-C64-N64
80	1	3422	PAR	C21-C11-O11-C42
80	1	3422	PAR	C23-C13-O52-C52
80	1	3422	PAR	C44-C54-C64-N64
80	1	3422	PAR	O54-C54-C64-N64
80	6	1905	PAR	C23-C13-O52-C52
80	6	1905	PAR	O43-C13-O52-C52
80	6	1905	PAR	C24-C14-O33-C33
80	1	3432	PAR	C44-C54-C64-N64
80	1	3432	PAR	O54-C54-C64-N64
80	1	3435	PAR	C21-C11-O11-C42
80	1	3435	PAR	O54-C54-C64-N64

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Mol	Chain	Res	Type	Atoms
80	1	3436	PAR	C23-C13-O52-C52
80	1	3436	PAR	O43-C13-O52-C52
80	5	3423	PAR	C21-C11-O11-C42
80	5	3423	PAR	C23-C13-O52-C52
80	5	3423	PAR	O43-C13-O52-C52
80	5	3421	PAR	C24-C14-O33-C33
80	5	3407	PAR	C23-C13-O52-C52
80	5	3407	PAR	O43-C13-O52-C52
80	5	3407	PAR	C24-C14-O33-C33
80	5	3407	PAR	O54-C54-C64-N64
80	6	1901	PAR	C23-C13-O52-C52
80	1	3407	PAR	C23-C13-O52-C52
80	1	3407	PAR	O43-C13-O52-C52
80	1	3407	PAR	C23-C33-O33-C14
80	6	1904	PAR	C23-C13-O52-C52
80	6	1904	PAR	C24-C14-O33-C33
80	6	1904	PAR	O54-C54-C64-N64
80	1	3402	PAR	C23-C13-O52-C52
80	5	3419	PAR	C23-C13-O52-C52
80	5	3409	PAR	C23-C13-O52-C52
80	5	3409	PAR	C44-C54-C64-N64
80	5	3409	PAR	O54-C54-C64-N64
80	5	3403	PAR	C23-C13-O52-C52
80	5	3403	PAR	O43-C13-O52-C52
80	5	3403	PAR	O54-C54-C64-N64
80	3	201	PAR	C23-C13-O52-C52
80	3	201	PAR	C23-C33-O33-C14
80	6	1906	PAR	C21-C11-O11-C42
80	5	3410	PAR	C23-C13-O52-C52
80	5	3410	PAR	O43-C13-O52-C52
80	1	3417	PAR	C24-C14-O33-C33
80	1	3410	PAR	C23-C13-O52-C52
80	1	3410	PAR	O43-C13-O52-C52
80	1	3410	PAR	C24-C14-O33-C33
80	1	3410	PAR	O54-C54-C64-N64
80	5	3420	PAR	C23-C33-O33-C14
80	5	3420	PAR	C24-C14-O33-C33
80	5	3405	PAR	C23-C13-O52-C52
80	5	3405	PAR	O43-C13-O52-C52
80	5	3405	PAR	C43-C33-O33-C14
80	5	3405	PAR	C24-C14-O33-C33
80	6	1903	PAR	C23-C13-O52-C52

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Mol	Chain	Res	Type	Atoms
80	5	3425	PAR	C23-C13-O52-C52
80	1	3403	PAR	C21-C11-O11-C42
80	1	3403	PAR	C23-C13-O52-C52
80	1	3403	PAR	O43-C13-O52-C52
80	8	202	PAR	C23-C13-O52-C52
80	8	202	PAR	O43-C13-O52-C52
80	1	3411	PAR	C23-C13-O52-C52
80	1	3411	PAR	O43-C13-O52-C52
80	1	3411	PAR	C43-C33-O33-C14
80	1	3411	PAR	C24-C14-O33-C33
80	1	3411	PAR	O54-C54-C64-N64
80	1	3437	PAR	C23-C13-O52-C52
80	1	3437	PAR	O43-C13-O52-C52
80	1	3437	PAR	C43-C33-O33-C14
80	1	3437	PAR	C44-C54-C64-N64
80	1	3437	PAR	O54-C54-C64-N64
80	1	3433	PAR	C23-C13-O52-C52
80	1	3433	PAR	C24-C14-O33-C33
80	3	203	PAR	C24-C14-O33-C33
80	6	1902	PAR	C21-C11-O11-C42
80	6	1902	PAR	C43-C33-O33-C14
80	6	1902	PAR	C24-C14-O33-C33
80	5	3428	PAR	C23-C13-O52-C52
80	5	3428	PAR	O43-C13-O52-C52
80	1	3401	PAR	C23-C13-O52-C52
80	1	3401	PAR	C24-C14-O33-C33
80	5	3412	PAR	C23-C13-O52-C52
80	5	3412	PAR	O43-C13-O52-C52
80	5	3401	PAR	C23-C13-O52-C52
80	5	3401	PAR	O43-C13-O52-C52
80	5	3424	PAR	C24-C14-O33-C33
80	1	3427	PAR	C23-C13-O52-C52
80	1	3427	PAR	C44-C54-C64-N64
80	1	3427	PAR	O54-C54-C64-N64
80	5	3417	PAR	C23-C13-O52-C52
80	5	3417	PAR	O43-C13-O52-C52
80	1	3426	PAR	C23-C13-O52-C52
80	1	3426	PAR	O43-C13-O52-C52
80	1	3426	PAR	C24-C14-O33-C33
80	1	3425	PAR	C23-C13-O52-C52
80	1	3425	PAR	O43-C13-O52-C52
80	1	3425	PAR	C43-C33-O33-C14

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Mol	Chain	Res	Type	Atoms
80	1	3425	PAR	C24-C14-O33-C33
80	5	3422	PAR	C62-C52-O52-C13
80	5	3422	PAR	C23-C33-O33-C14
80	1	3421	PAR	C23-C13-O52-C52
80	1	3421	PAR	O43-C13-O52-C52
80	1	3405	PAR	C21-C11-O11-C42
80	1	3405	PAR	O51-C11-O11-C42
80	1	3405	PAR	C23-C13-O52-C52
80	1	3405	PAR	O43-C13-O52-C52
80	1	3405	PAR	C43-C33-O33-C14
80	1	3405	PAR	C24-C14-O33-C33
80	5	3408	PAR	C23-C13-O52-C52
80	5	3408	PAR	O43-C13-O52-C52
80	5	3408	PAR	C24-C14-O33-C33
80	n3	201	PAR	C21-C11-O11-C42
80	n3	201	PAR	C32-C42-O11-C11
80	n3	201	PAR	C23-C13-O52-C52
80	n3	201	PAR	O43-C13-O52-C52
80	1	3418	PAR	C23-C13-O52-C52
80	1	3418	PAR	C23-C33-O33-C14
80	2	1903	PAR	C23-C13-O52-C52
80	2	1903	PAR	O43-C13-O52-C52
80	1	3415	PAR	C24-C14-O33-C33
80	5	3411	PAR	C43-C33-O33-C14
80	1	3424	PAR	C43-C33-O33-C14
80	5	3427	PAR	C23-C13-O52-C52
80	5	3427	PAR	O43-C13-O52-C52
80	4	201	PAR	C23-C13-O52-C52
80	4	201	PAR	C24-C14-O33-C33
80	1	3409	PAR	C21-C11-O11-C42
80	1	3409	PAR	C23-C13-O52-C52
80	1	3409	PAR	O43-C13-O52-C52
80	1	3416	PAR	O54-C14-O33-C33
80	1	3408	PAR	C23-C13-O52-C52
80	1	3429	PAR	C23-C13-O52-C52
80	1	3429	PAR	O43-C13-O52-C52
80	1	3430	PAR	C23-C13-O52-C52
80	1	3430	PAR	O43-C13-O52-C52
80	1	3430	PAR	C24-C14-O33-C33
80	1	3413	PAR	C24-C14-O33-C33
80	1	3414	PAR	C62-C52-O52-C13
80	1	3434	PAR	C62-C52-O52-C13

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Mol	Chain	Res	Type	Atoms
80	5	3411	PAR	C62-C52-O52-C13
80	5	3415	PAR	C52-C42-O11-C11
80	6	1904	PAR	O54-C14-O33-C33
80	5	3403	PAR	O54-C14-O33-C33
80	5	3405	PAR	O54-C14-O33-C33
80	1	3433	PAR	O54-C14-O33-C33
80	5	3424	PAR	O54-C14-O33-C33
80	1	3415	PAR	O54-C14-O33-C33
80	3	201	PAR	C62-C52-O52-C13
80	5	3401	PAR	C62-C52-O52-C13
80	1	3416	PAR	C62-C52-O52-C13
80	5	3409	PAR	O54-C14-O33-C33
80	5	3420	PAR	O51-C11-O11-C42
80	5	3401	PAR	O54-C14-O33-C33
80	1	3412	PAR	O51-C11-O11-C42
80	1	3413	PAR	O54-C14-O33-C33
80	1	3431	PAR	C62-C52-O52-C13
80	2	1902	PAR	C62-C52-O52-C13
80	3	202	PAR	C62-C52-O52-C13
80	3	203	PAR	C42-C52-O52-C13
80	7	202	PAR	O54-C14-O33-C33
80	1	3435	PAR	O54-C14-O33-C33
80	5	3406	PAR	O51-C11-O11-C42
80	2	1905	PAR	O54-C14-O33-C33
80	5	3403	PAR	O51-C11-O11-C42
80	1	3410	PAR	O54-C14-O33-C33
80	2	1904	PAR	O54-C14-O33-C33
80	1	3403	PAR	O51-C11-O11-C42
80	8	202	PAR	O54-C14-O33-C33
80	1	3426	PAR	O54-C14-O33-C33
80	n3	201	PAR	O54-C14-O33-C33
80	5	3415	PAR	O54-C14-O33-C33
80	1	3414	PAR	O54-C14-O33-C33
80	2	1901	PAR	O51-C11-O11-C42
80	6	1902	PAR	O54-C14-O33-C33
80	5	3426	PAR	O51-C11-O11-C42
80	1	3425	PAR	C52-C42-O11-C11
80	5	3404	PAR	O54-C14-O33-C33
80	6	1905	PAR	O54-C14-O33-C33
80	1	3411	PAR	O54-C14-O33-C33
80	1	3412	PAR	O54-C14-O33-C33
80	1	3404	PAR	C62-C52-O52-C13

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Mol	Chain	Res	Type	Atoms
80	5	3415	PAR	C42-C52-O52-C13
80	1	3402	PAR	O54-C14-O33-C33
80	n3	201	PAR	O51-C11-O11-C42
80	5	3401	PAR	O43-C43-C53-O53
80	5	3427	PAR	O51-C11-O11-C42
80	6	1906	PAR	C52-C42-O11-C11
80	6	1902	PAR	C62-C52-O52-C13
80	5	3402	PAR	C62-C52-O52-C13
80	1	3417	PAR	O54-C14-O33-C33
80	1	3405	PAR	O43-C43-C53-O53
80	3	202	PAR	O51-C51-C61-O61
80	1	3419	PAR	C52-C42-O11-C11
80	5	3401	PAR	C33-C43-C53-O53
80	1	3419	PAR	C42-C52-O52-C13
80	1	3422	PAR	O51-C51-C61-O61
80	1	3436	PAR	O51-C51-C61-O61
80	1	3419	PAR	O54-C14-O33-C33
80	1	3419	PAR	O43-C43-C53-O53
80	5	3423	PAR	C42-C52-O52-C13
80	5	3404	PAR	O51-C11-O11-C42
80	1	3425	PAR	O54-C14-O33-C33
80	1	3435	PAR	C41-C51-C61-O61
80	1	3425	PAR	O43-C43-C53-O53
80	1	3430	PAR	O51-C51-C61-O61
80	5	3417	PAR	O54-C14-O33-C33
80	1	3405	PAR	C33-C43-C53-O53
80	5	3408	PAR	O54-C14-O33-C33
80	1	3402	PAR	O51-C51-C61-O61
80	1	3419	PAR	C33-C43-C53-O53
80	5	3409	PAR	C33-C43-C53-O53
80	5	3410	PAR	C41-C51-C61-O61
80	1	3430	PAR	O51-C11-O11-C42
80	3	202	PAR	C41-C51-C61-O61
80	1	3402	PAR	C41-C51-C61-O61
80	5	3423	PAR	C62-C52-O52-C13
80	1	3425	PAR	O51-C51-C61-O61
80	5	3405	PAR	O51-C11-O11-C42
80	1	3420	PAR	O54-C14-O33-C33
80	5	3422	PAR	O54-C14-O33-C33
80	5	3409	PAR	O43-C43-C53-O53
80	6	1903	PAR	C33-C43-C53-O53
80	1	3401	PAR	C42-C52-O52-C13

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Mol	Chain	Res	Type	Atoms
80	1	3435	PAR	O51-C51-C61-O61
80	5	3411	PAR	C52-C42-O11-C11
80	5	3419	PAR	O54-C14-O33-C33
80	1	3401	PAR	C62-C52-O52-C13
80	5	3408	PAR	O51-C11-O11-C42
80	o2	201	PAR	C52-C42-O11-C11
80	5	3428	PAR	O43-C43-C53-O53
80	1	3422	PAR	C41-C51-C61-O61
80	o2	201	PAR	O54-C14-O33-C33
80	7	201	PAR	O51-C11-O11-C42
80	1	3417	PAR	O51-C11-O11-C42
80	7	202	PAR	O51-C51-C61-O61
80	5	3412	PAR	O51-C11-O11-C42
80	1	3405	PAR	C62-C52-O52-C13
80	5	3413	PAR	O43-C13-O52-C52
80	1	3431	PAR	O43-C13-O52-C52
80	5	3418	PAR	O43-C13-O52-C52
80	1	3406	PAR	O43-C13-O52-C52
80	o2	201	PAR	O43-C13-O52-C52
80	3	202	PAR	O43-C13-O52-C52
80	1	3422	PAR	O43-C13-O52-C52
80	1	3435	PAR	O43-C13-O52-C52
80	6	1901	PAR	O43-C13-O52-C52
80	1	3402	PAR	O43-C13-O52-C52
80	1	3423	PAR	O43-C13-O52-C52
80	5	3409	PAR	O43-C13-O52-C52
80	3	201	PAR	O43-C13-O52-C52
80	6	1903	PAR	O43-C13-O52-C52
80	5	3425	PAR	O43-C13-O52-C52
80	1	3433	PAR	O43-C13-O52-C52
80	1	3401	PAR	O43-C13-O52-C52
80	4	202	PAR	O43-C13-O52-C52
80	1	3427	PAR	O43-C13-O52-C52
80	1	3418	PAR	O43-C13-O52-C52
80	1	3424	PAR	O43-C13-O52-C52
80	1	3408	PAR	O43-C13-O52-C52
80	5	3415	PAR	O43-C13-O52-C52
80	5	3410	PAR	O51-C51-C61-O61
80	8	201	PAR	O51-C51-C61-O61
80	5	3406	PAR	O51-C51-C61-O61
80	5	3411	PAR	O51-C51-C61-O61
80	1	3436	PAR	O51-C11-O11-C42

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Mol	Chain	Res	Type	Atoms
80	6	1906	PAR	C42-C52-O52-C13
80	o2	201	PAR	C62-C52-O52-C13
80	1	3409	PAR	O51-C51-C61-O61
80	1	3419	PAR	C62-C52-O52-C13
80	1	3434	PAR	O51-C51-C61-O61
80	6	1906	PAR	C62-C52-O52-C13
80	1	3418	PAR	C42-C52-O52-C13
80	1	3405	PAR	C42-C52-O52-C13
80	1	3404	PAR	O54-C14-O33-C33
80	2	1905	PAR	C44-C54-C64-N64
80	3	201	PAR	C44-C54-C64-N64
80	1	3434	PAR	C23-C33-O33-C14
80	2	1903	PAR	C44-C54-C64-N64
80	1	3430	PAR	C43-C33-O33-C14
80	6	1903	PAR	O43-C43-C53-O53
80	1	3425	PAR	C21-C11-O11-C42
80	1	3418	PAR	C62-C52-O52-C13
80	1	3411	PAR	C42-C52-O52-C13
80	n3	201	PAR	C52-C42-O11-C11
80	1	3424	PAR	O51-C11-O11-C42
80	7	202	PAR	O51-C11-O11-C42
80	1	3436	PAR	C41-C51-C61-O61
80	1	3425	PAR	C33-C43-C53-O53
80	o2	201	PAR	C42-C52-O52-C13
80	5	3425	PAR	C41-C51-C61-O61
80	5	3402	PAR	C42-C52-O52-C13
80	1	3423	PAR	C52-C42-O11-C11
80	1	3409	PAR	C42-C52-O52-C13
80	5	3404	PAR	O43-C43-C53-O53
80	5	3407	PAR	O54-C14-O33-C33
80	7	201	PAR	O43-C13-O52-C52
80	5	3421	PAR	O43-C13-O52-C52
80	5	3419	PAR	O43-C13-O52-C52
80	1	3417	PAR	O43-C13-O52-C52
80	5	3424	PAR	O43-C13-O52-C52
80	1	3411	PAR	C62-C52-O52-C13
80	6	1902	PAR	C52-C42-O11-C11
80	1	3428	PAR	O51-C11-O11-C42
80	1	3417	PAR	C23-C13-O52-C52
80	4	202	PAR	C23-C13-O52-C52
80	1	3424	PAR	C23-C13-O52-C52
80	5	3416	PAR	O51-C11-O11-C42

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Mol	Chain	Res	Type	Atoms
80	5	3402	PAR	O54-C14-O33-C33
80	5	3425	PAR	O51-C51-C61-O61
80	5	3411	PAR	C32-C42-O11-C11
80	1	3409	PAR	C62-C52-O52-C13
80	5	3415	PAR	C62-C52-O52-C13
80	o2	201	PAR	O54-C54-C64-N64
80	2	1902	PAR	O54-C54-C64-N64
80	6	1905	PAR	O54-C54-C64-N64
80	5	3402	PAR	O54-C54-C64-N64
80	1	3436	PAR	O54-C54-C64-N64
80	5	3421	PAR	O54-C54-C64-N64
80	5	3419	PAR	O54-C54-C64-N64
80	5	3410	PAR	O54-C54-C64-N64
80	2	1904	PAR	O54-C54-C64-N64
80	1	3434	PAR	O54-C54-C64-N64
80	5	3412	PAR	O54-C54-C64-N64
80	1	3404	PAR	O54-C54-C64-N64
80	5	3417	PAR	O54-C54-C64-N64
80	5	3422	PAR	O54-C54-C64-N64
80	1	3418	PAR	O54-C54-C64-N64
80	2	1903	PAR	O54-C54-C64-N64
80	1	3415	PAR	O54-C54-C64-N64
80	5	3416	PAR	O54-C54-C64-N64
80	1	3412	PAR	O54-C54-C64-N64
80	4	201	PAR	O54-C54-C64-N64
80	5	3426	PAR	O54-C54-C64-N64
80	1	3428	PAR	C52-C42-O11-C11
80	4	201	PAR	O54-C14-O33-C33
80	5	3421	PAR	O51-C11-O11-C42
80	6	1902	PAR	C42-C52-O52-C13
80	6	1904	PAR	O51-C11-O11-C42
80	5	3418	PAR	O54-C14-O33-C33
80	1	3435	PAR	C42-C52-O52-C13
80	1	3409	PAR	C52-C42-O11-C11
80	2	1904	PAR	C52-C42-O11-C11
80	1	3426	PAR	C42-C52-O52-C13
80	5	3408	PAR	C41-C51-C61-O61
80	5	3428	PAR	C42-C52-O52-C13
80	o2	201	PAR	O43-C43-C53-O53
80	3	202	PAR	C43-C33-O33-C14
80	1	3432	PAR	C23-C33-O33-C14
80	5	3402	PAR	C23-C33-O33-C14

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Mol	Chain	Res	Type	Atoms
80	5	3406	PAR	C44-C54-C64-N64
80	1	3436	PAR	C43-C33-O33-C14
80	5	3419	PAR	C44-C54-C64-N64
80	8	202	PAR	C43-C33-O33-C14
80	3	203	PAR	C23-C33-O33-C14
80	1	3405	PAR	C23-C33-O33-C14
80	5	3415	PAR	C43-C33-O33-C14
80	1	3413	PAR	C43-C33-O33-C14
80	1	3422	PAR	C24-C14-O33-C33
80	1	3418	PAR	C24-C14-O33-C33
80	5	3411	PAR	C24-C14-O33-C33
80	1	3416	PAR	C24-C14-O33-C33
80	1	3429	PAR	C24-C14-O33-C33
80	1	3407	PAR	C62-C52-O52-C13
80	1	3409	PAR	O54-C14-O33-C33
80	5	3428	PAR	O51-C51-C61-O61
80	2	1905	PAR	C52-C42-O11-C11
80	1	3407	PAR	C42-C52-O52-C13
80	4	202	PAR	O43-C43-C53-O53
80	1	3435	PAR	C62-C52-O52-C13
80	1	3419	PAR	O51-C11-O11-C42
80	5	3412	PAR	O54-C14-O33-C33
80	5	3407	PAR	O43-C43-C53-O53
80	1	3433	PAR	C52-C42-O11-C11
80	5	3407	PAR	C42-C52-O52-C13
80	5	3409	PAR	C41-C51-C61-O61
80	1	3402	PAR	C52-C42-O11-C11
80	1	3426	PAR	C62-C52-O52-C13
80	7	202	PAR	C52-C42-O11-C11
80	5	3428	PAR	C62-C52-O52-C13
80	5	3408	PAR	O51-C51-C61-O61
80	1	3407	PAR	C52-C42-O11-C11
80	5	3419	PAR	O51-C51-C61-O61
80	5	3407	PAR	C62-C52-O52-C13
80	3	201	PAR	O54-C14-O33-C33
80	1	3410	PAR	O51-C11-O11-C42
80	5	3414	PAR	C52-C42-O11-C11
80	4	201	PAR	O51-C51-C61-O61
80	2	1904	PAR	C62-C52-O52-C13
80	2	1903	PAR	C52-C42-O11-C11
80	1	3431	PAR	C23-C13-O52-C52
80	7	201	PAR	C23-C13-O52-C52

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Mol	Chain	Res	Type	Atoms
80	o2	201	PAR	C23-C13-O52-C52
80	5	3402	PAR	C23-C13-O52-C52
80	1	3435	PAR	C23-C13-O52-C52
80	5	3421	PAR	C23-C13-O52-C52
80	1	3423	PAR	C23-C13-O52-C52
80	5	3424	PAR	C23-C13-O52-C52
80	5	3415	PAR	C23-C13-O52-C52
80	o2	201	PAR	C32-C42-O11-C11
80	1	3427	PAR	O51-C11-O11-C42
80	5	3421	PAR	O54-C14-O33-C33
80	5	3426	PAR	C52-C42-O11-C11
80	1	3430	PAR	C52-C42-O11-C11
80	1	3436	PAR	O43-C43-C53-O53
80	1	3408	PAR	C42-C52-O52-C13
80	2	1905	PAR	C42-C52-O52-C13
80	5	3418	PAR	C23-C33-O33-C14
80	5	3418	PAR	C44-C54-C64-N64
80	1	3428	PAR	C23-C33-O33-C14
80	5	3404	PAR	C23-C33-O33-C14
80	5	3404	PAR	C43-C33-O33-C14
80	7	202	PAR	C23-C33-O33-C14
80	6	1905	PAR	C23-C33-O33-C14
80	6	1905	PAR	C44-C54-C64-N64
80	5	3402	PAR	C43-C33-O33-C14
80	1	3435	PAR	C44-C54-C64-N64
80	5	3406	PAR	C23-C33-O33-C14
80	5	3406	PAR	C43-C33-O33-C14
80	1	3436	PAR	C23-C33-O33-C14
80	5	3421	PAR	C43-C33-O33-C14
80	5	3407	PAR	C43-C33-O33-C14
80	1	3407	PAR	C44-C54-C64-N64
80	6	1904	PAR	C23-C33-O33-C14
80	1	3402	PAR	C23-C33-O33-C14
80	1	3423	PAR	C23-C33-O33-C14
80	1	3423	PAR	C43-C33-O33-C14
80	5	3419	PAR	C23-C33-O33-C14
80	6	1906	PAR	C44-C54-C64-N64
80	5	3410	PAR	C23-C33-O33-C14
80	1	3417	PAR	C43-C33-O33-C14
80	6	1903	PAR	C44-C54-C64-N64
80	5	3425	PAR	C23-C33-O33-C14
80	1	3403	PAR	C23-C33-O33-C14

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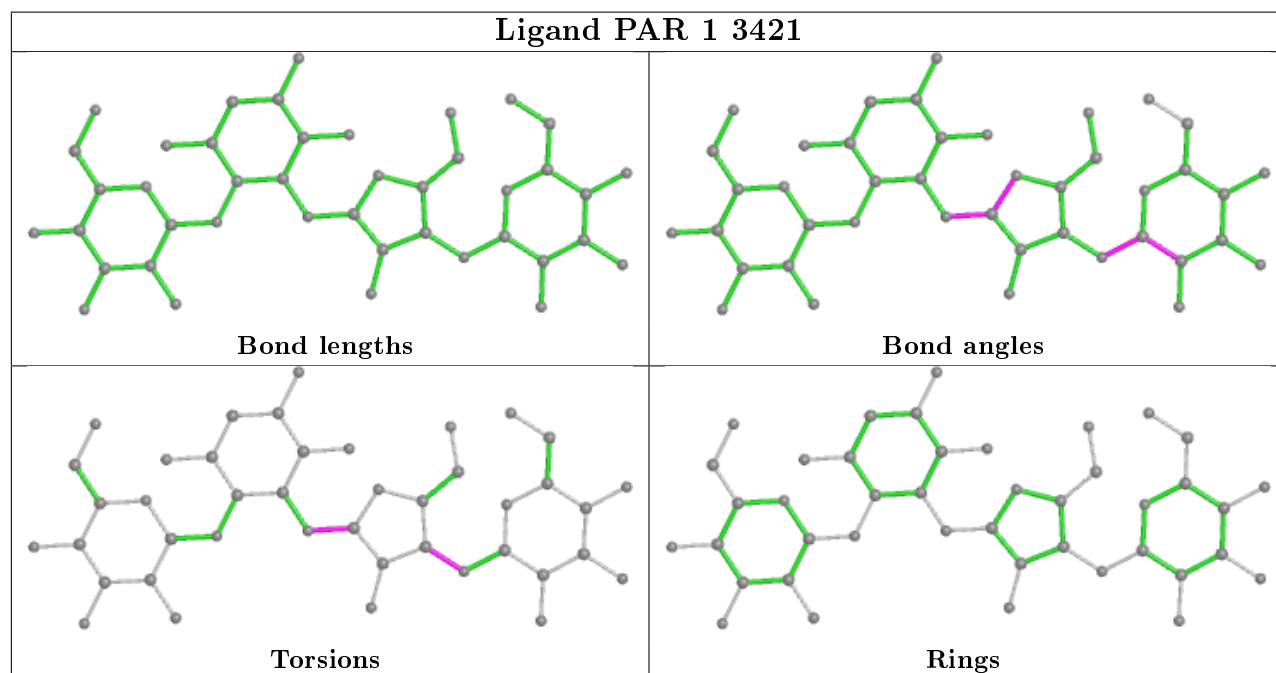
Mol	Chain	Res	Type	Atoms
80	8	202	PAR	C23-C33-O33-C14
80	1	3434	PAR	C43-C33-O33-C14
80	3	203	PAR	C43-C33-O33-C14
80	6	1902	PAR	C23-C33-O33-C14
80	6	1902	PAR	C44-C54-C64-N64
80	5	3412	PAR	C44-C54-C64-N64
80	5	3417	PAR	C43-C33-O33-C14
80	1	3421	PAR	C43-C33-O33-C14
80	n3	201	PAR	C43-C33-O33-C14
80	1	3415	PAR	C44-C54-C64-N64
80	1	3412	PAR	C43-C33-O33-C14
80	4	201	PAR	C44-C54-C64-N64
80	1	3409	PAR	C44-C54-C64-N64
80	5	3426	PAR	C44-C54-C64-N64
80	1	3413	PAR	C23-C33-O33-C14
80	1	3431	PAR	C24-C14-O33-C33
80	5	3403	PAR	C24-C14-O33-C33
80	1	3434	PAR	C21-C11-O11-C42
80	5	3428	PAR	C21-C11-O11-C42
80	5	3411	PAR	C21-C11-O11-C42
80	1	3413	PAR	C21-C11-O11-C42
80	5	3410	PAR	O54-C14-O33-C33
80	1	3435	PAR	O51-C11-O11-C42
80	5	3402	PAR	C52-C42-O11-C11
80	5	3404	PAR	C41-C51-C61-O61
80	5	3405	PAR	C42-C52-O52-C13
80	5	3409	PAR	O51-C51-C61-O61

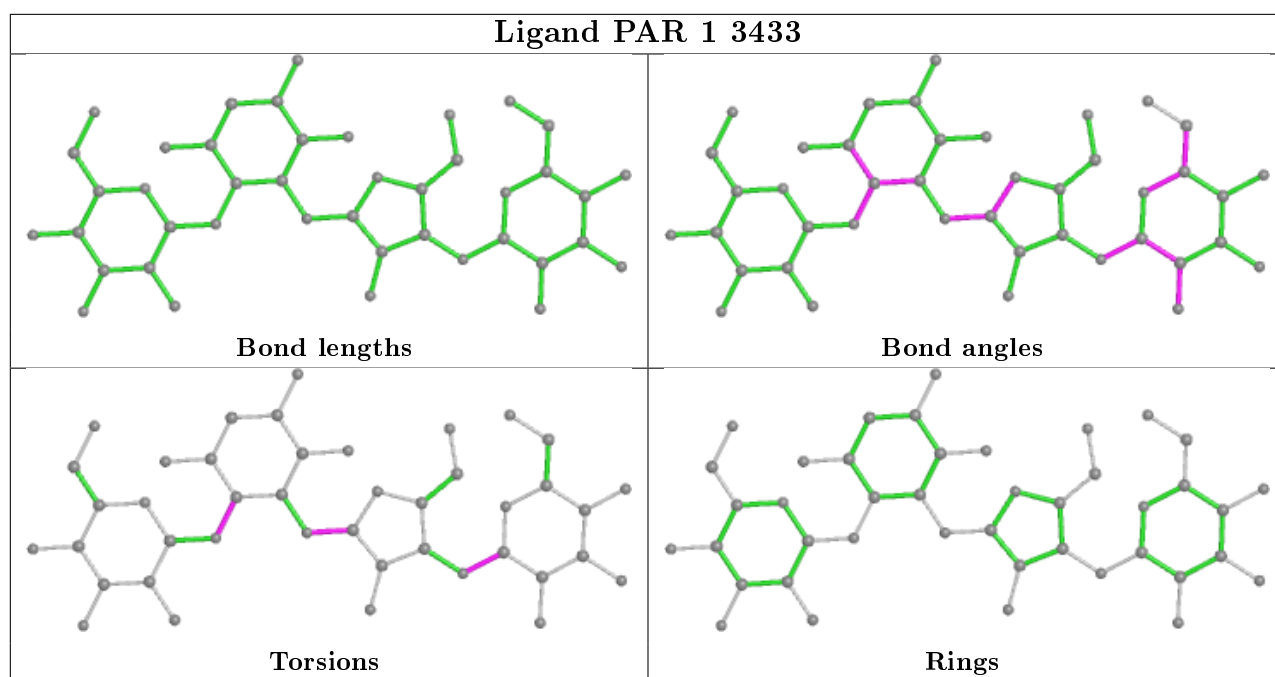
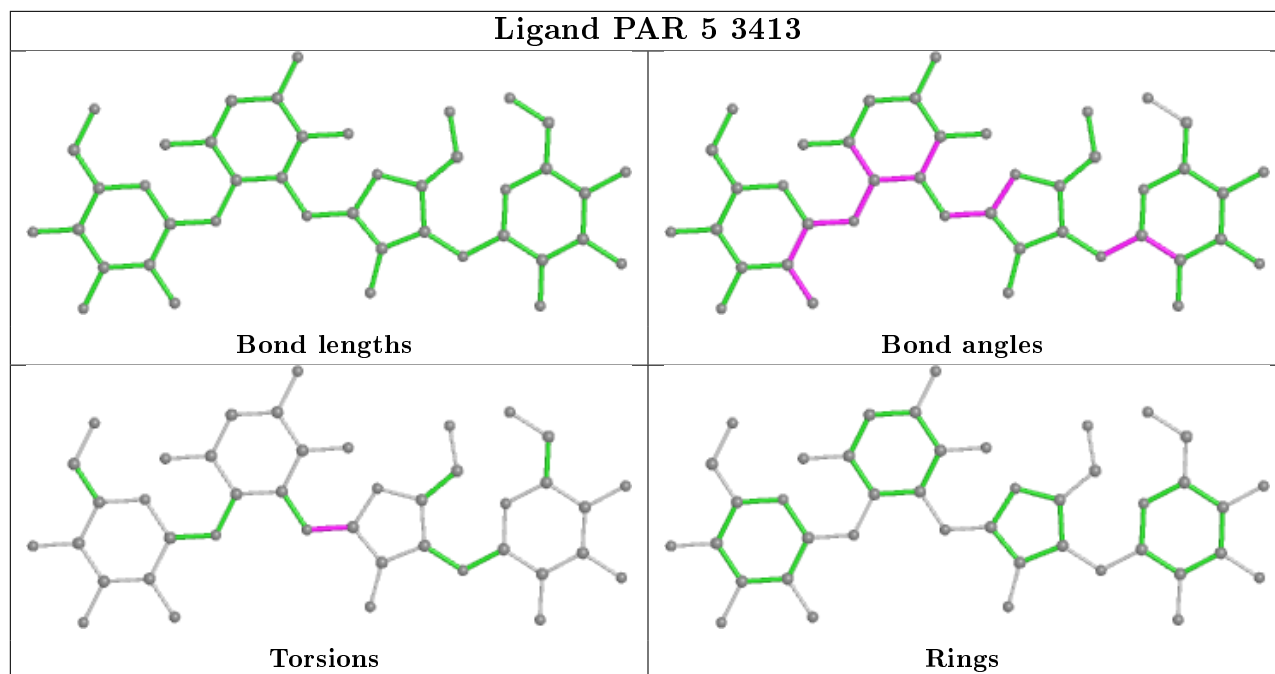
All (10) ring outliers are listed below:

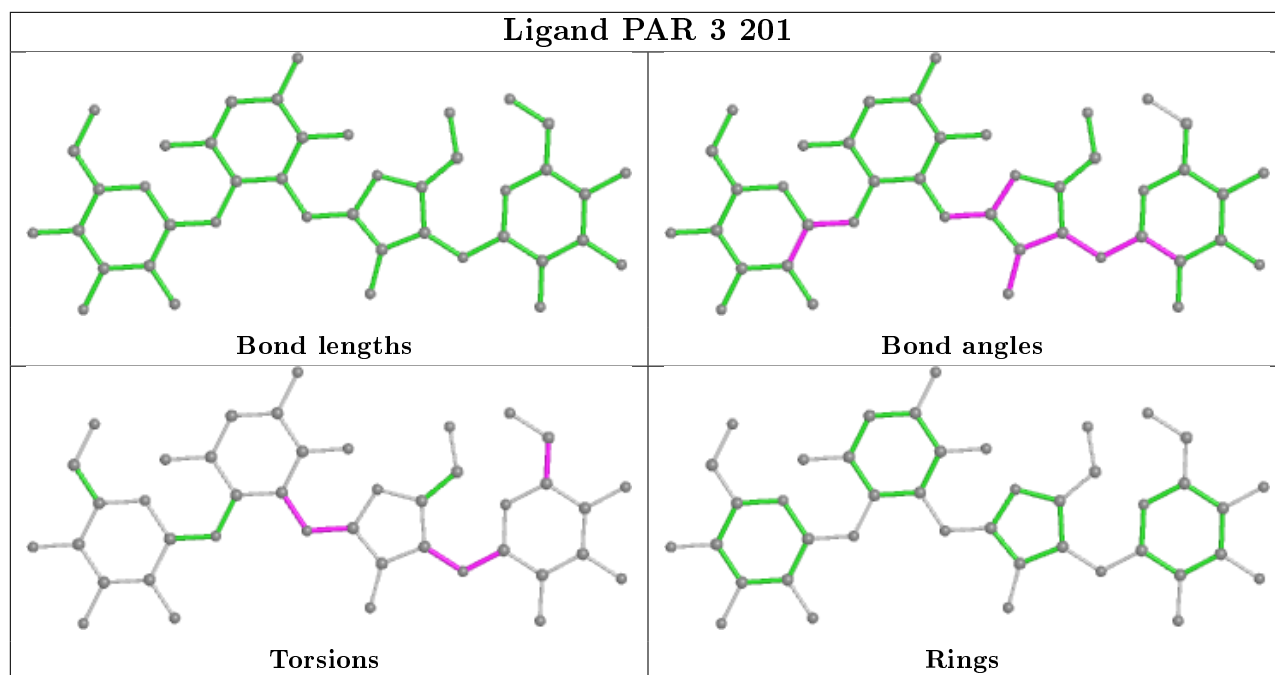
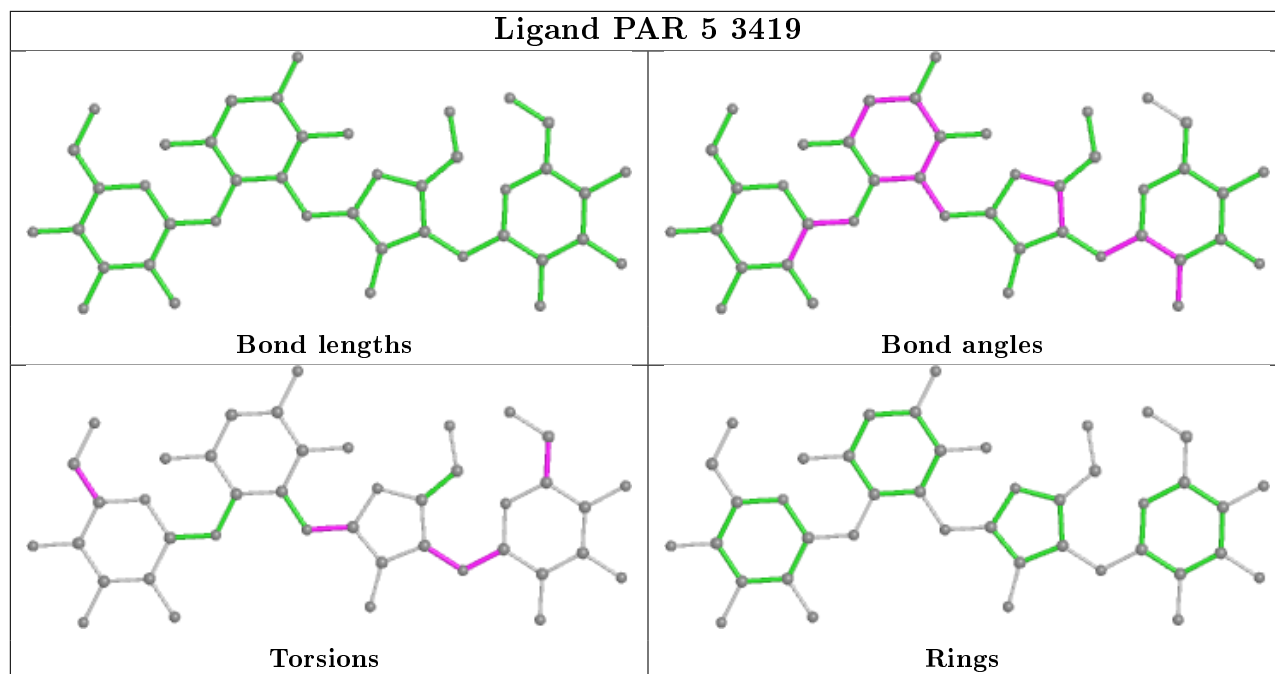
Mol	Chain	Res	Type	Atoms
80	1	3409	PAR	C12-C22-C32-C42-C52-C62
80	5	3414	PAR	C12-C22-C32-C42-C52-C62
80	4	201	PAR	C12-C22-C32-C42-C52-C62
80	3	203	PAR	C12-C22-C32-C42-C52-C62
80	1	3418	PAR	C14-C24-C34-C44-C54-O54
80	1	3432	PAR	C12-C22-C32-C42-C52-C62
80	5	3426	PAR	C14-C24-C34-C44-C54-O54
80	1	3419	PAR	C14-C24-C34-C44-C54-O54
80	5	3427	PAR	C12-C22-C32-C42-C52-C62
80	5	3420	PAR	C12-C22-C32-C42-C52-C62

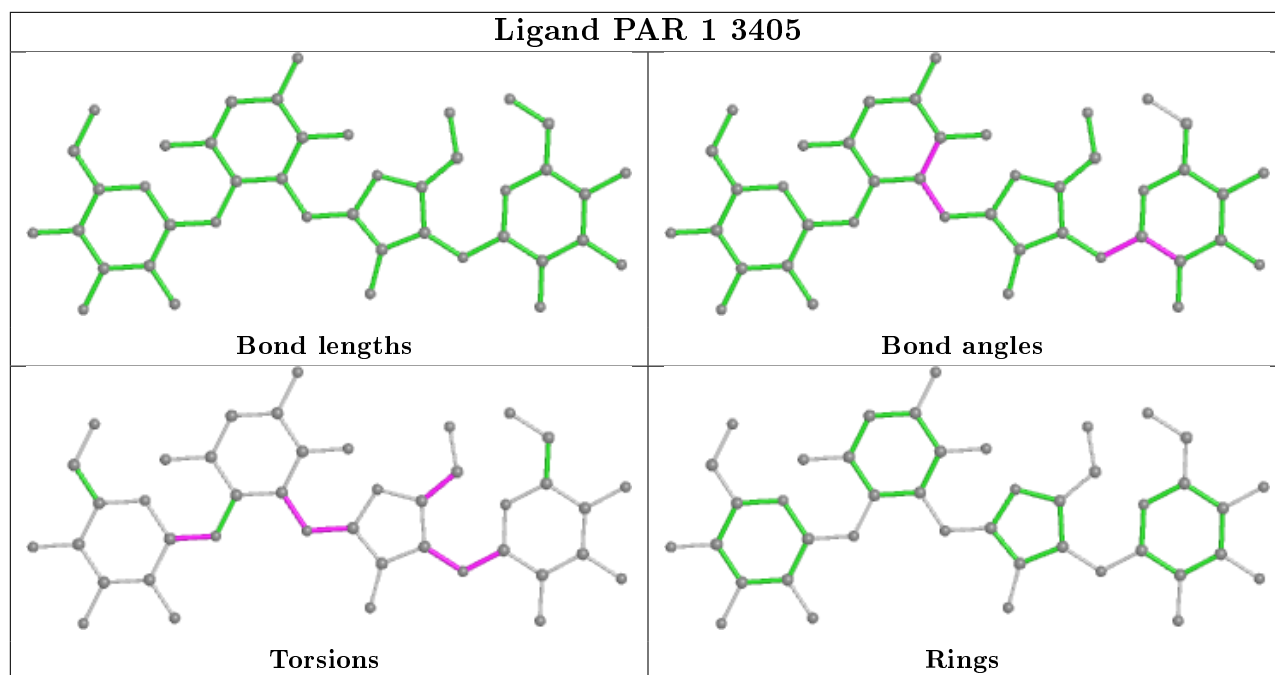
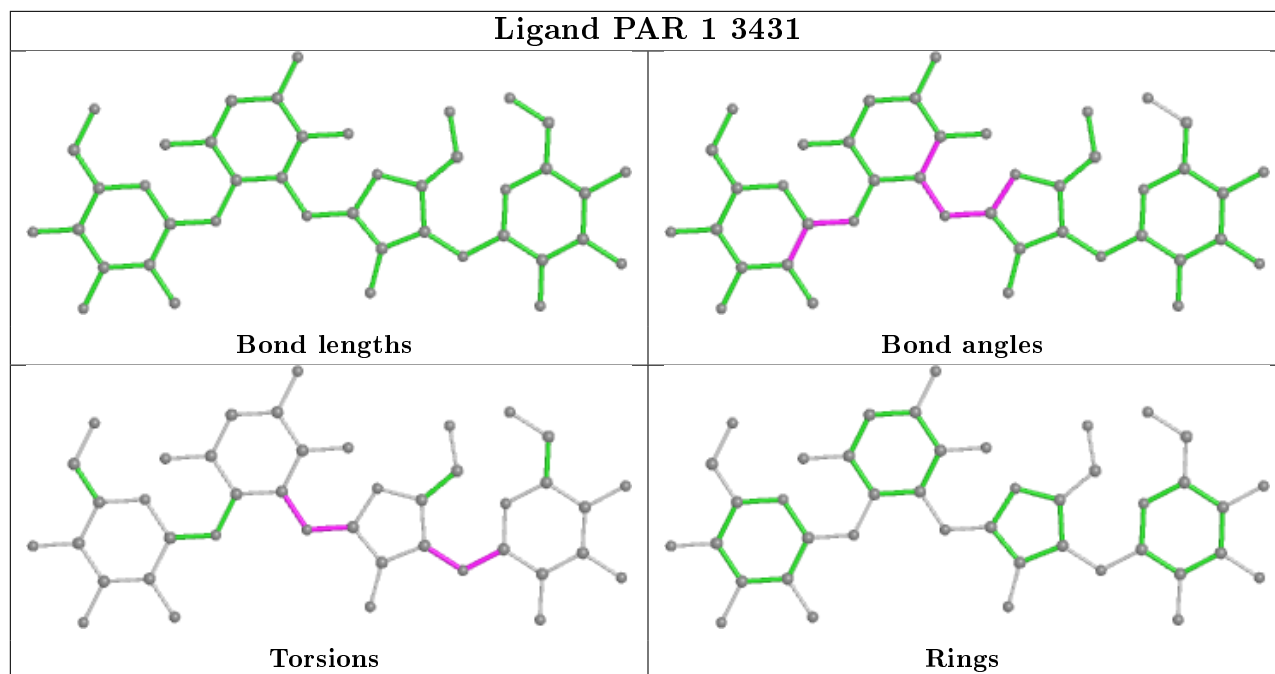
No monomer is involved in short contacts.

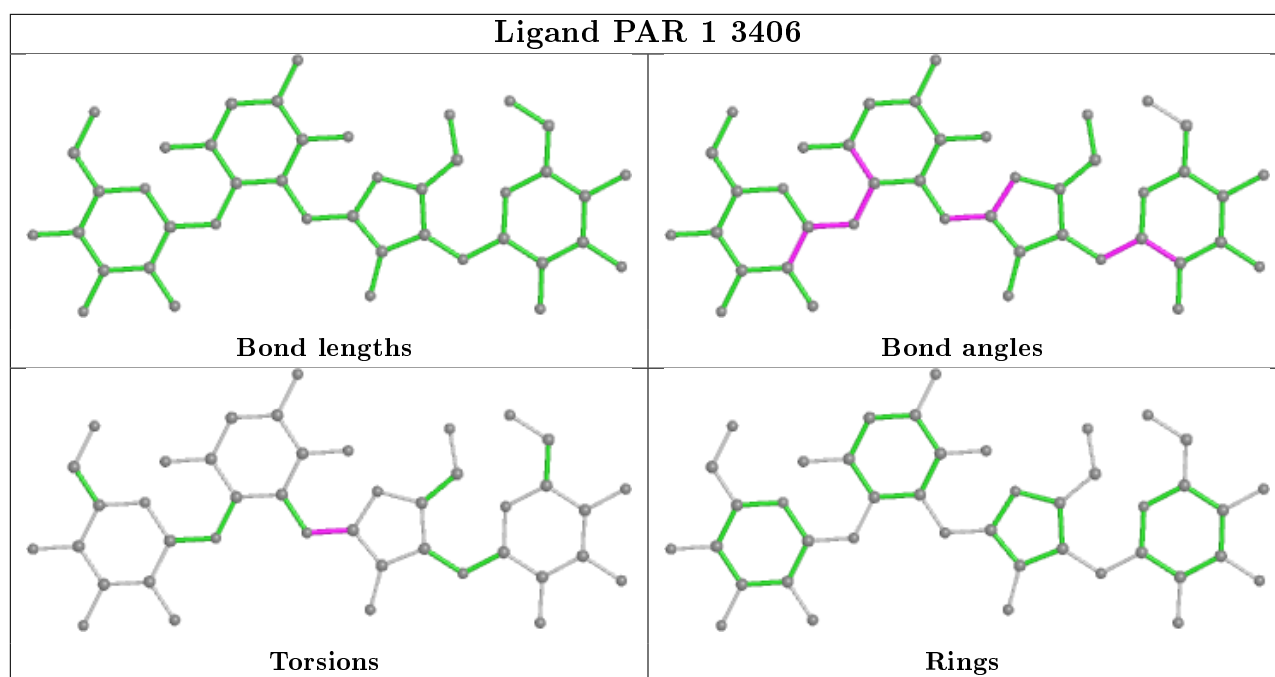
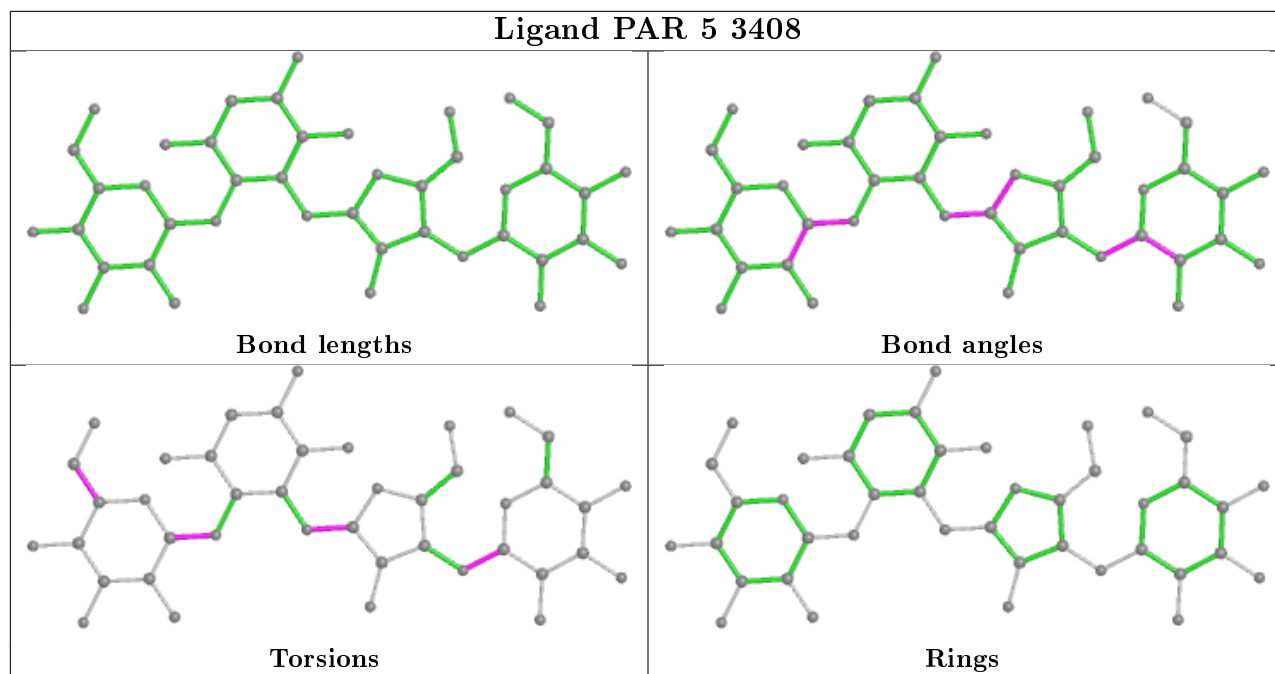
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

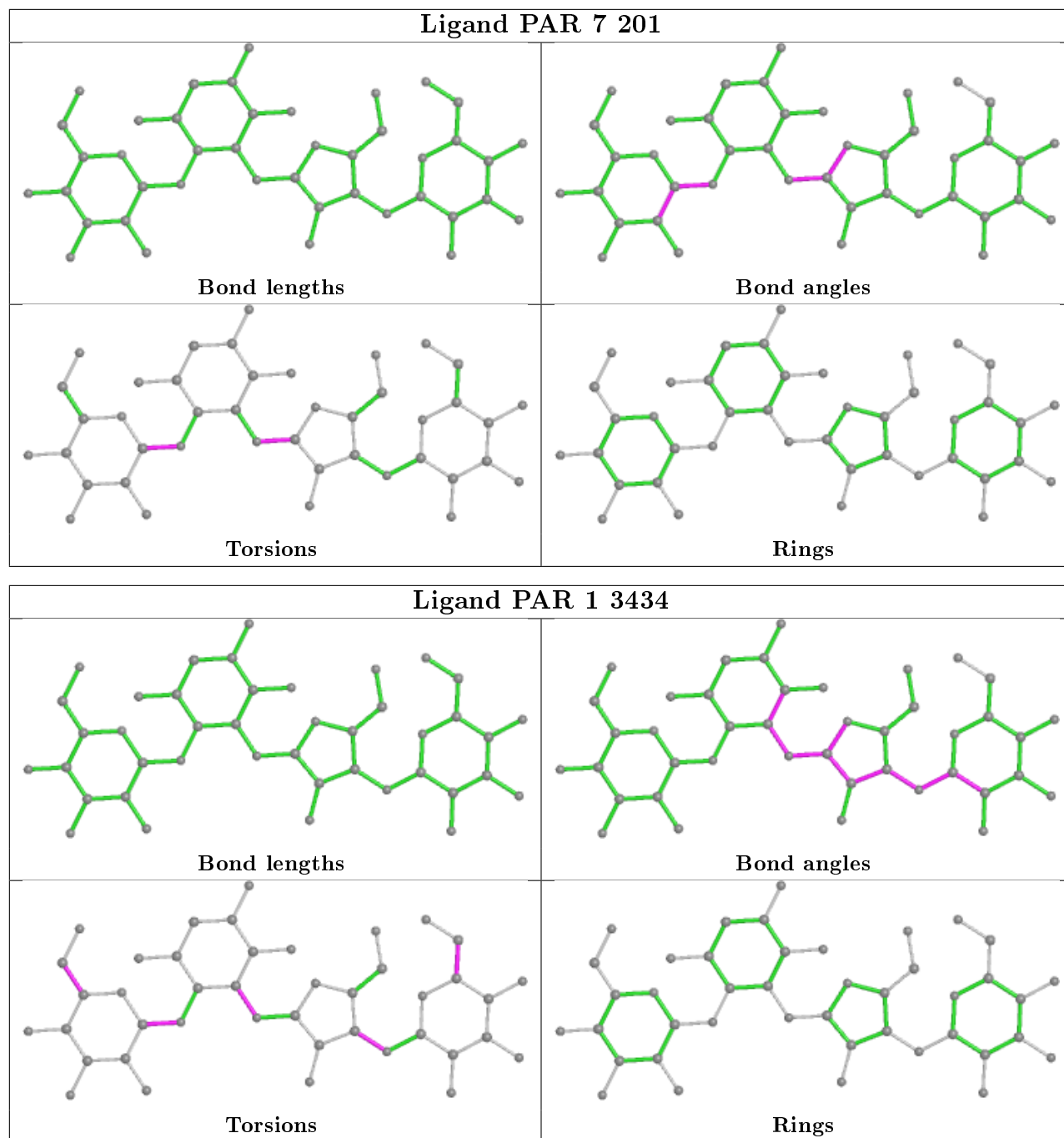


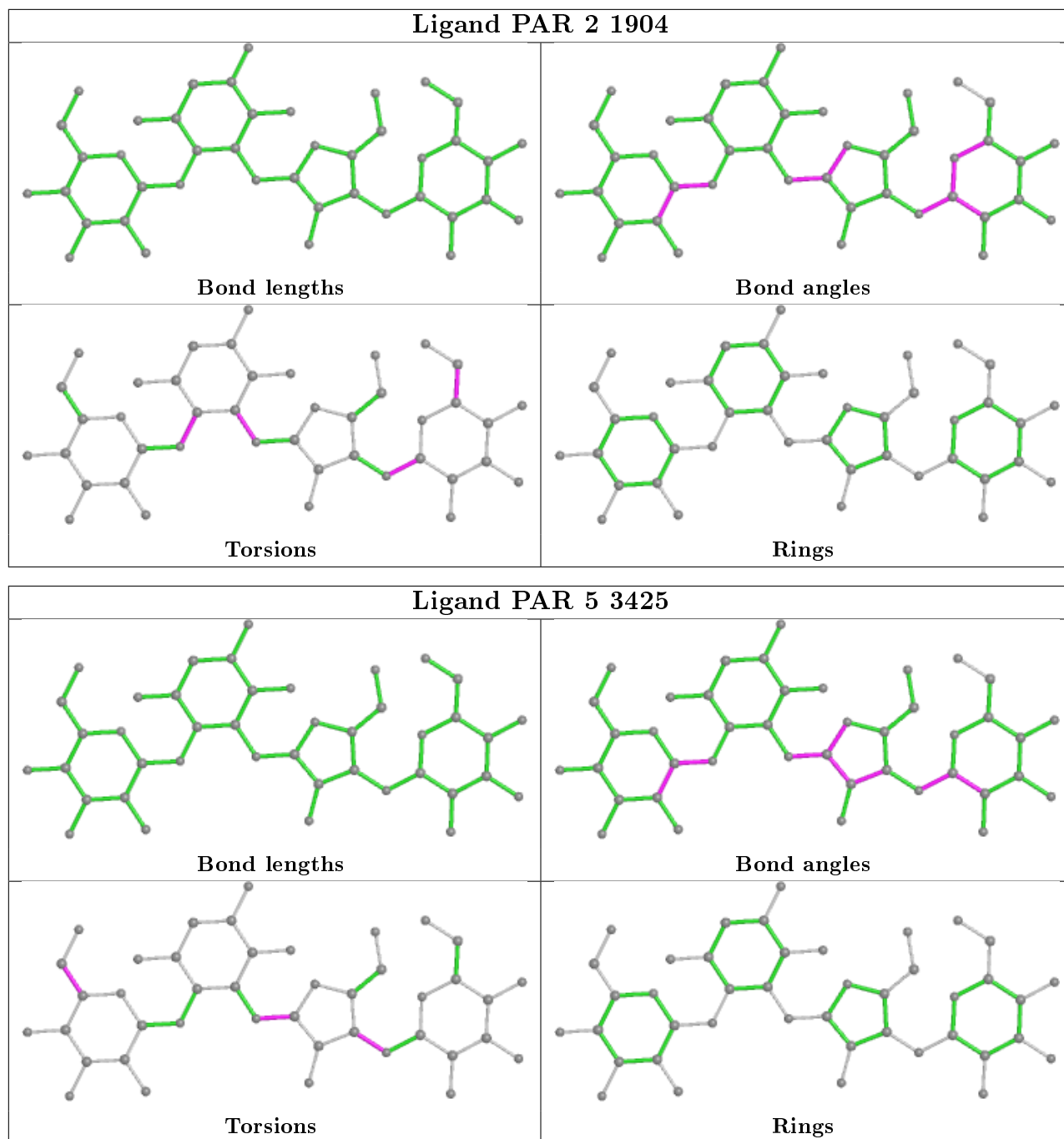


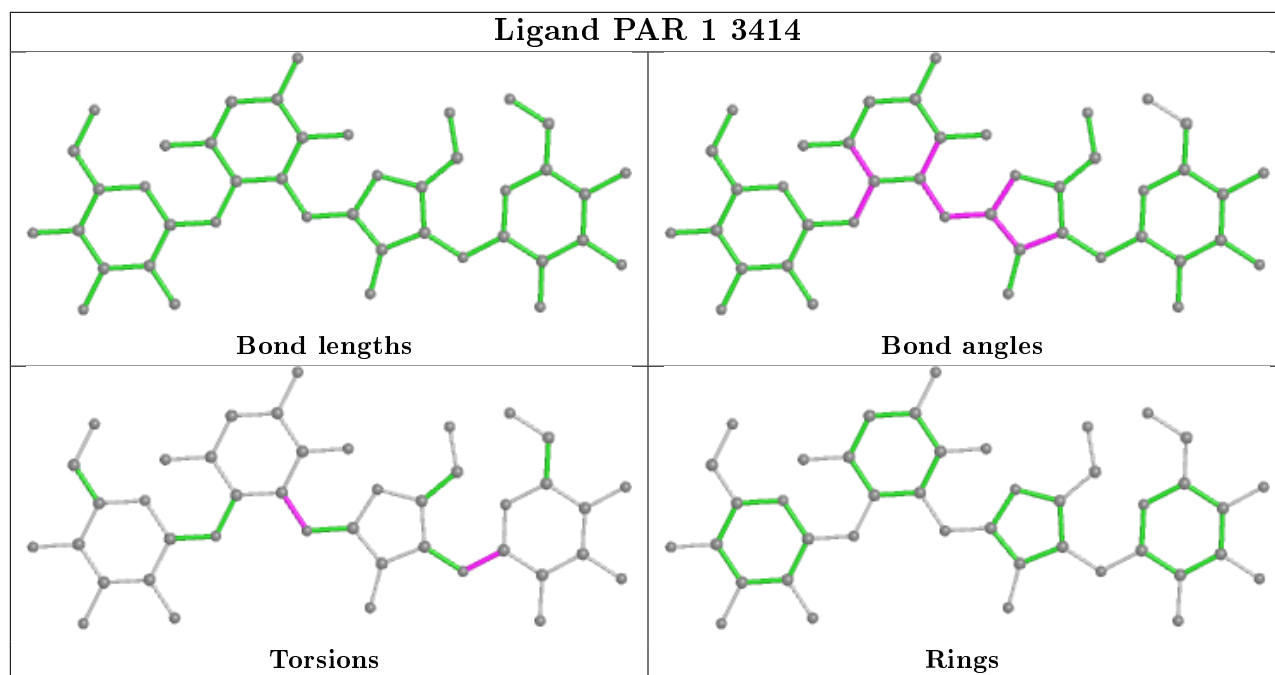
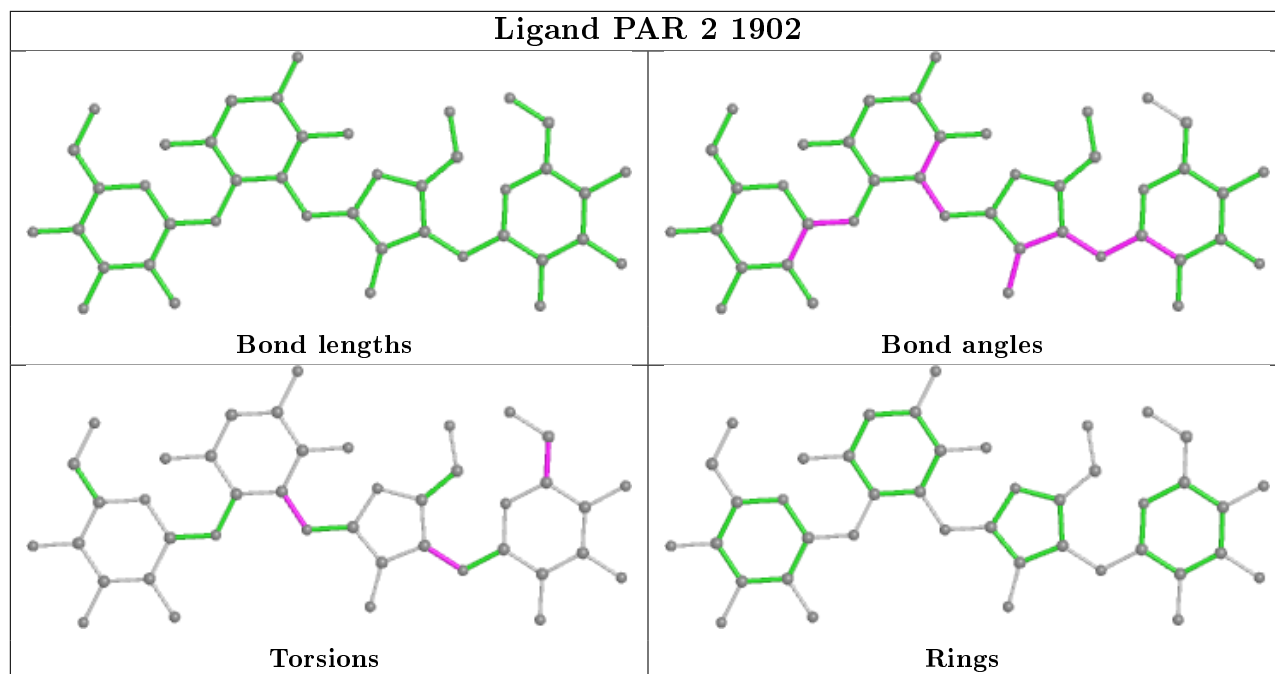


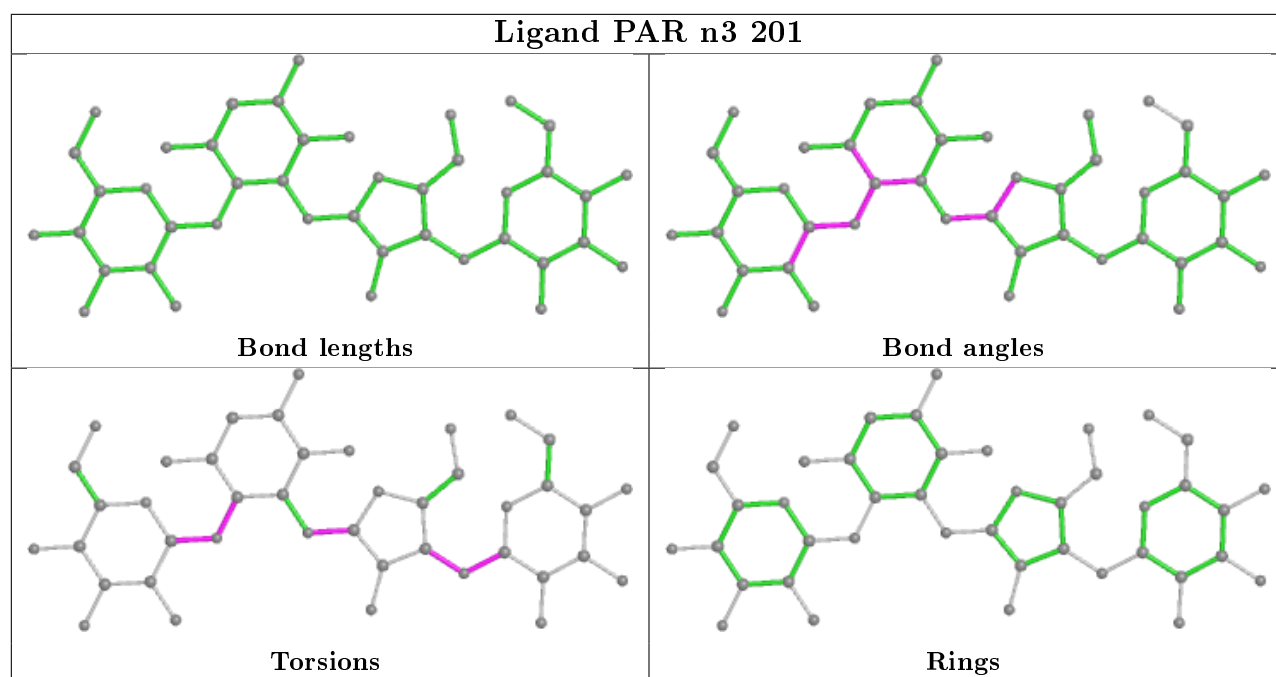
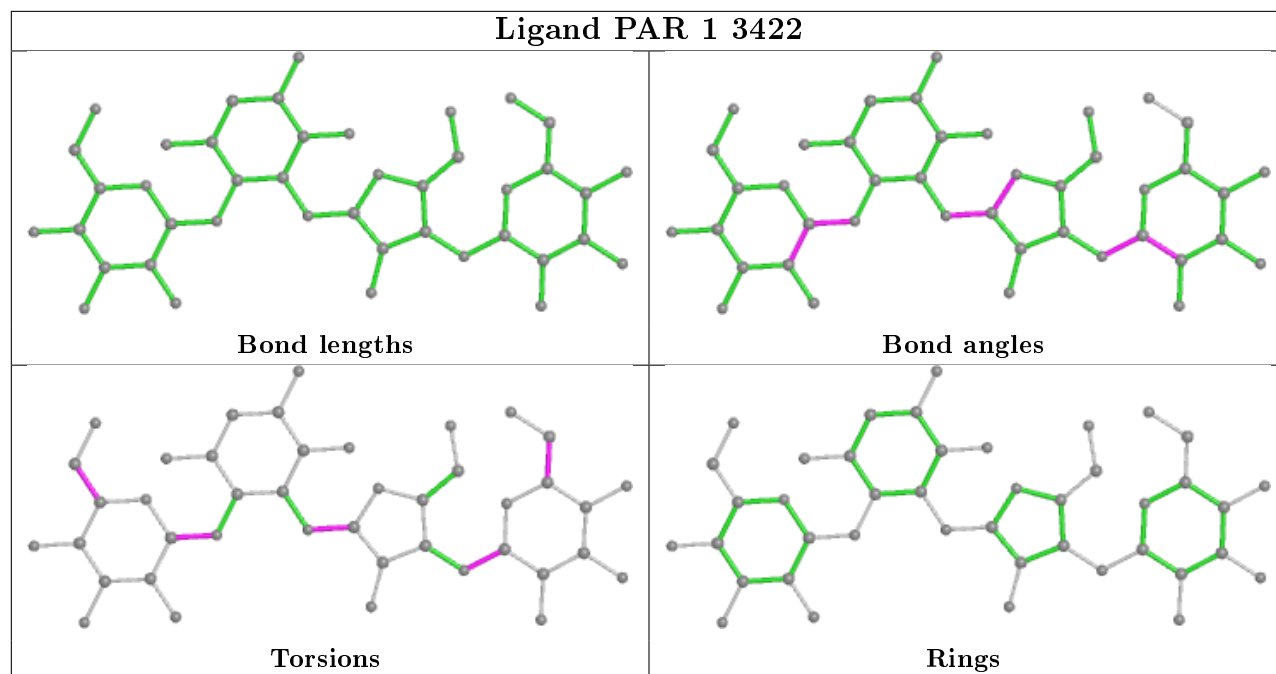


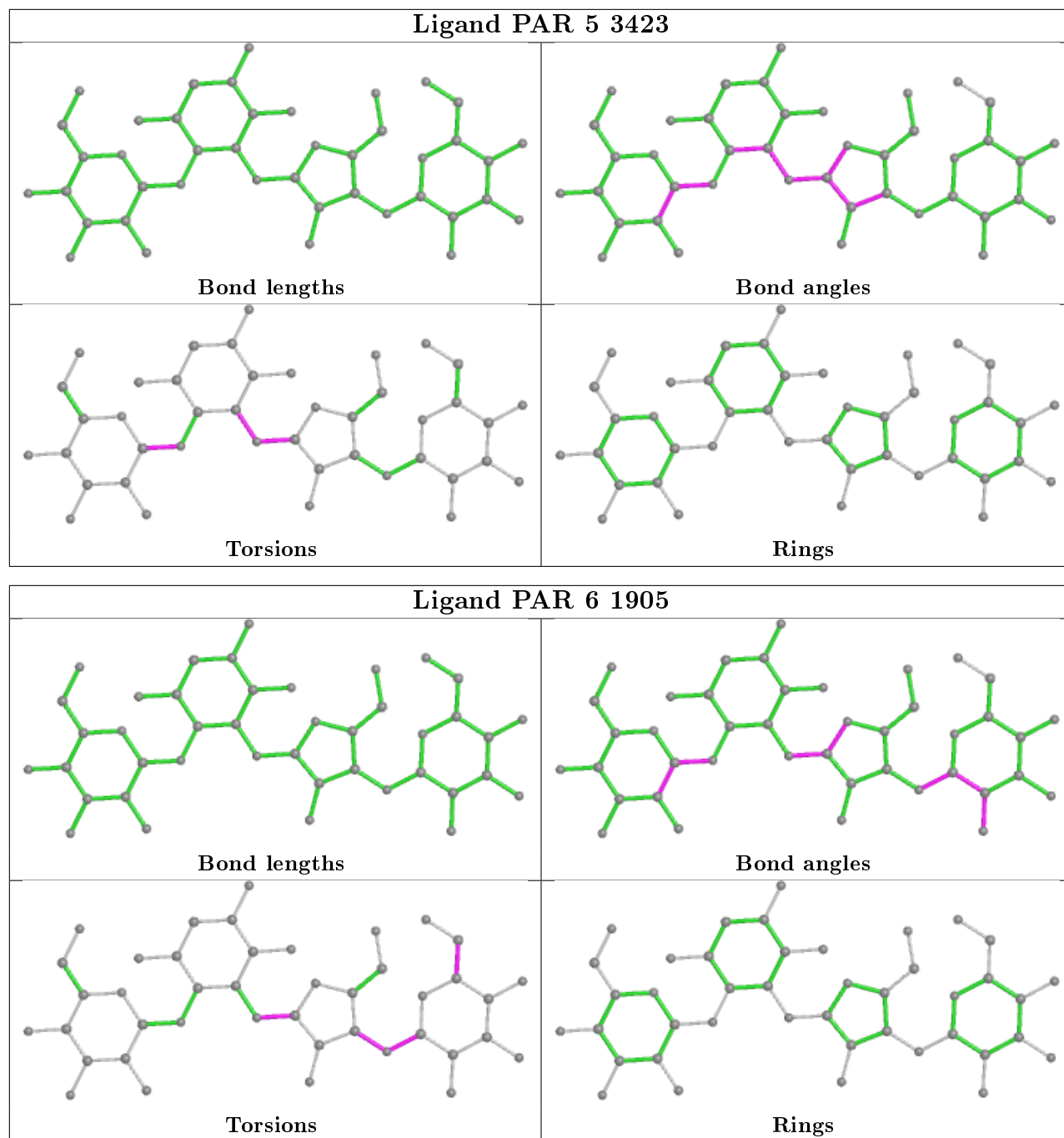


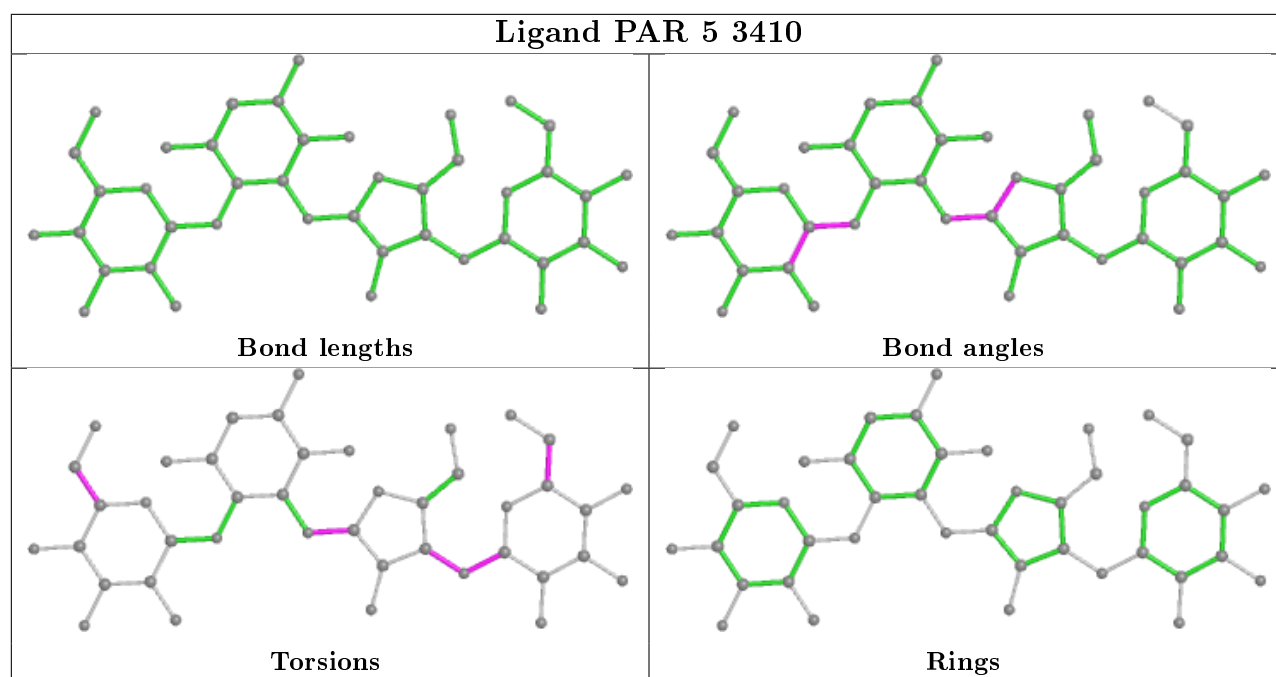
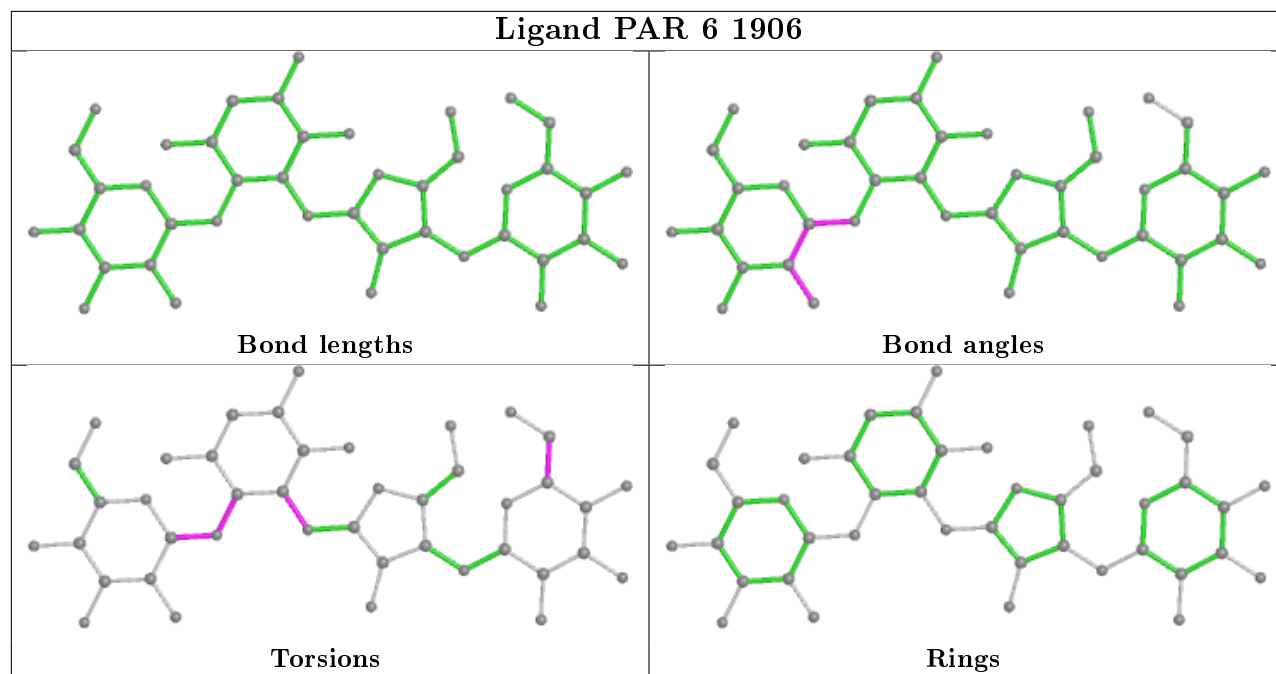


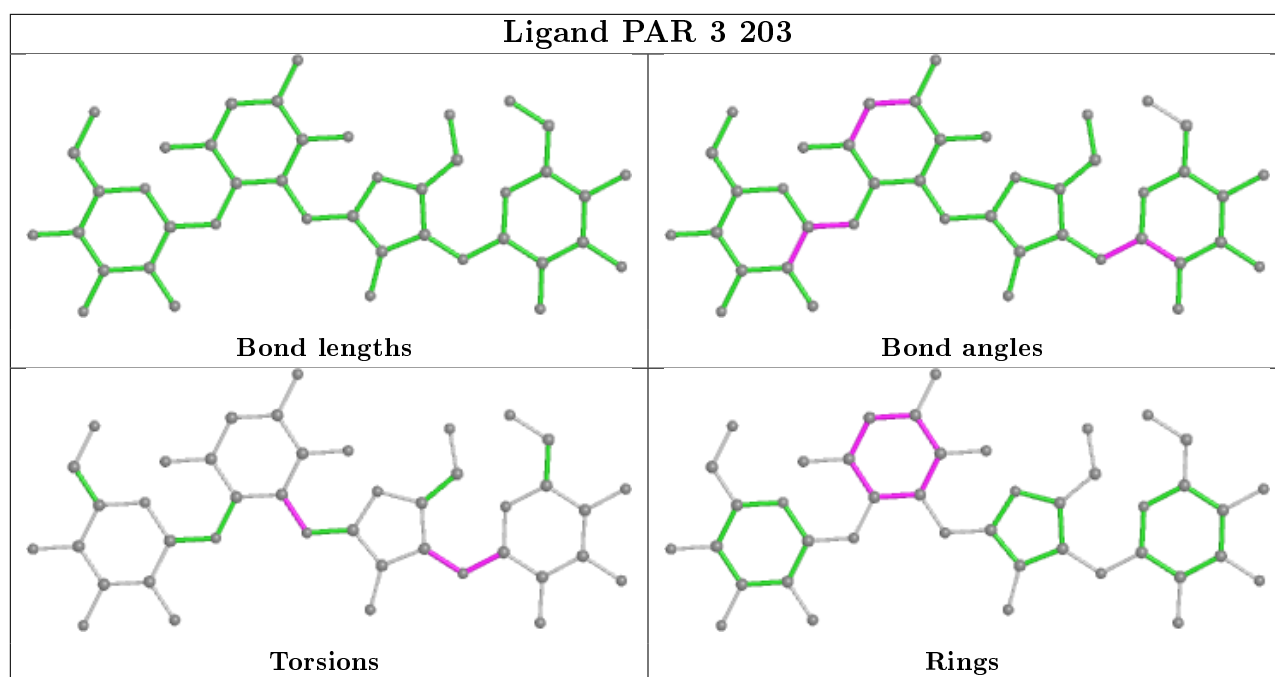
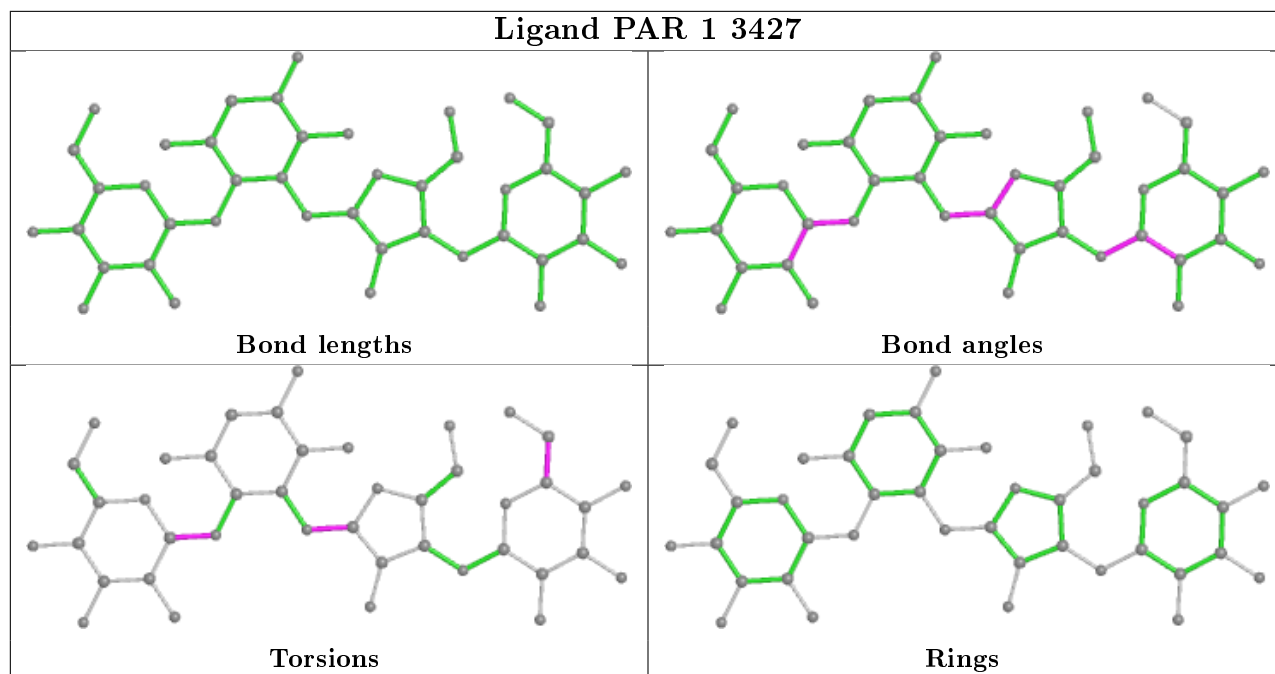


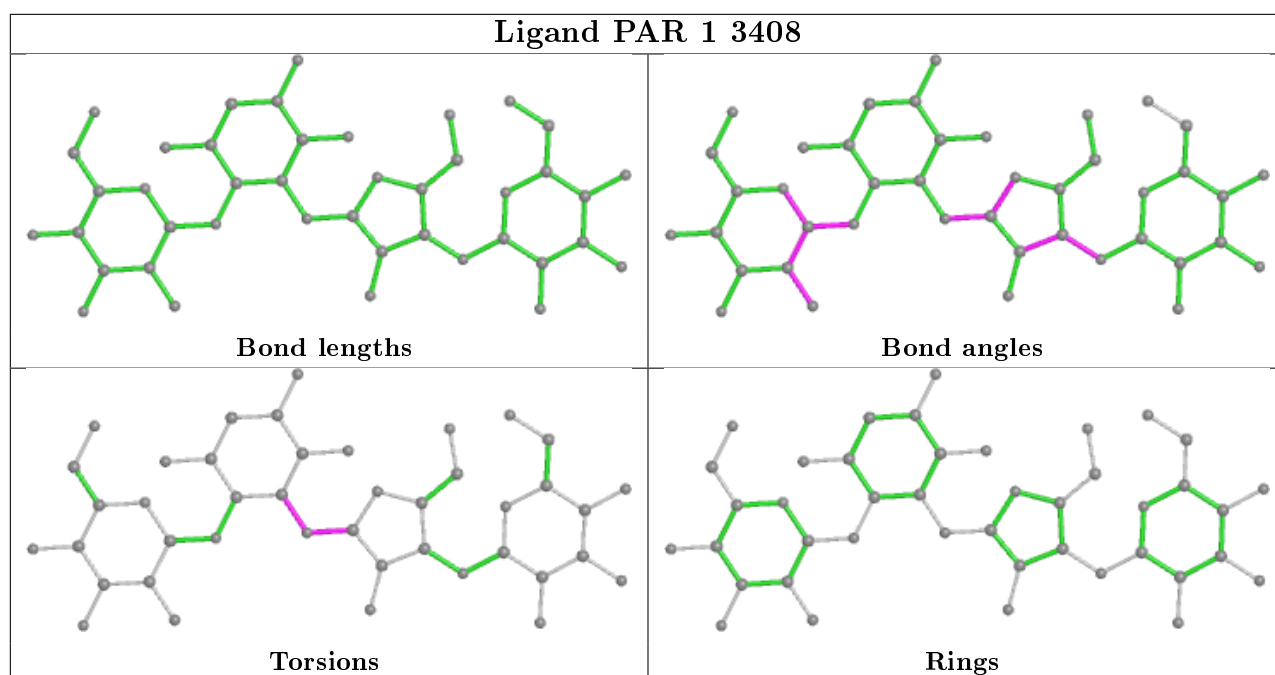
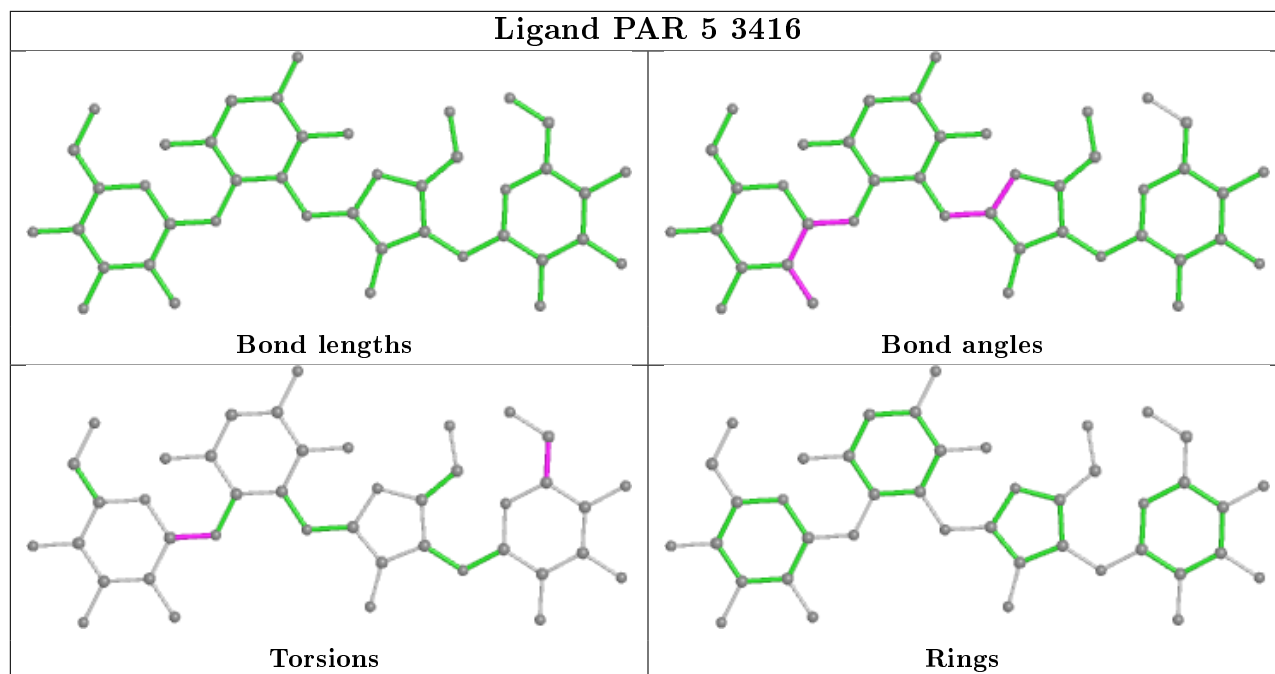


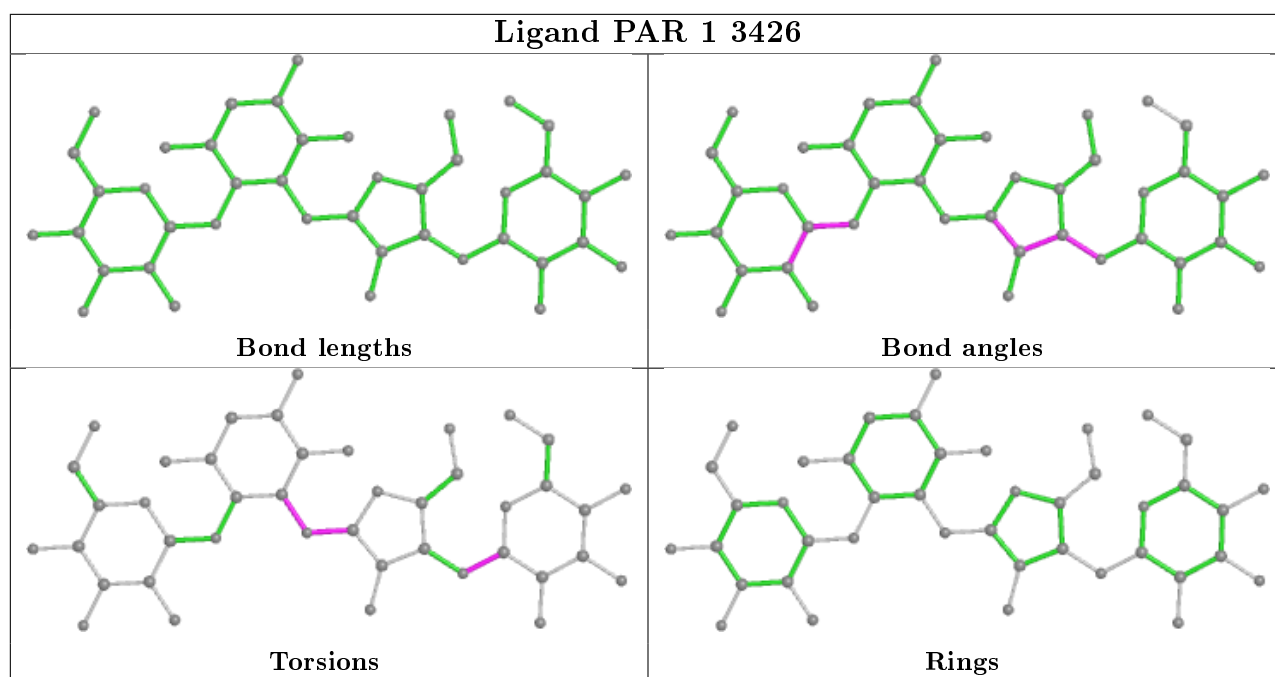
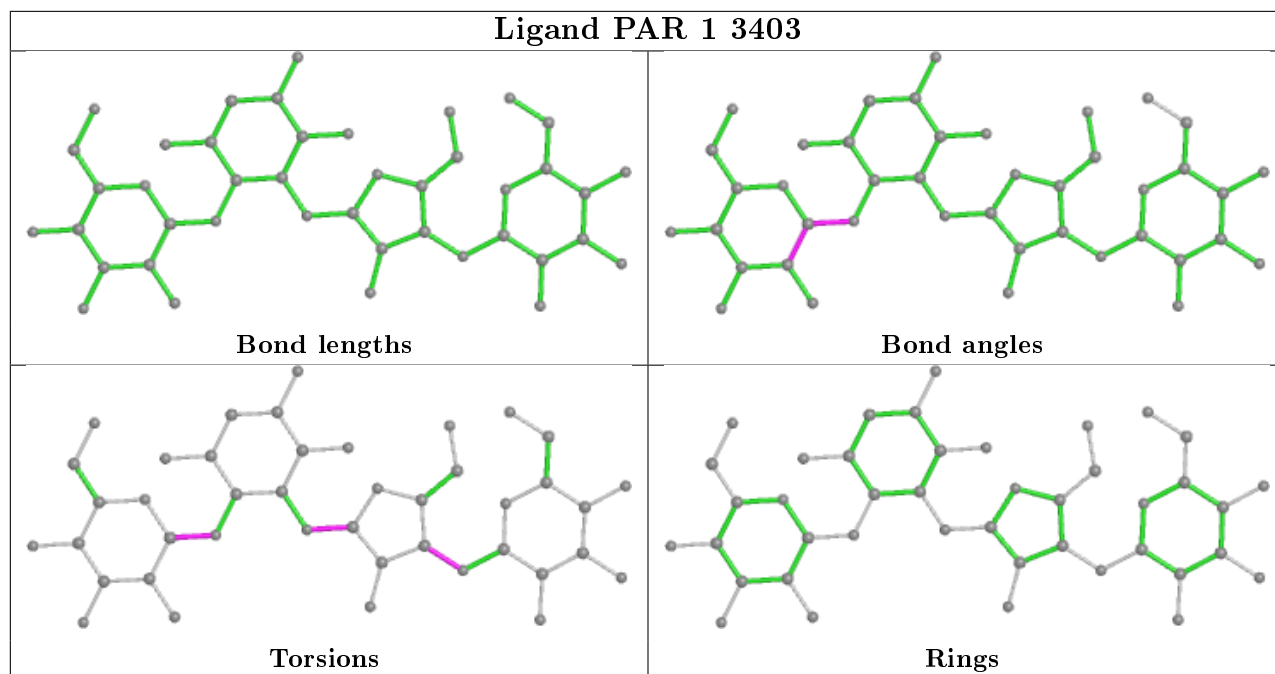


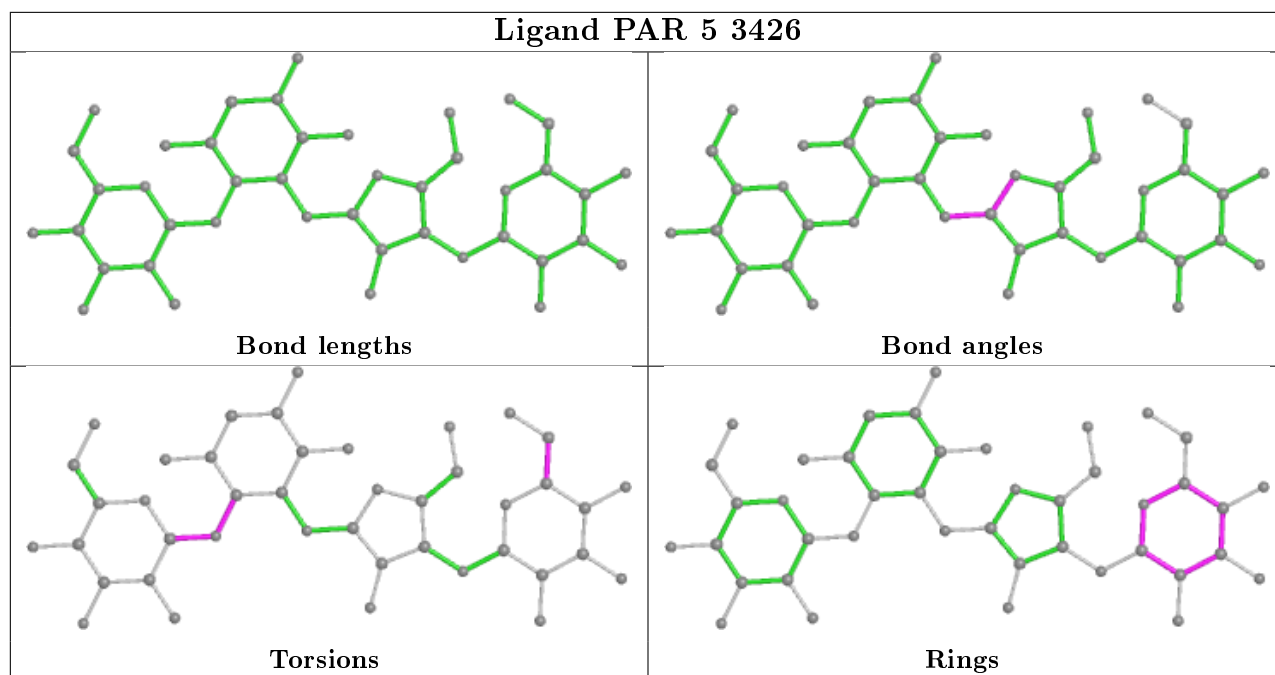
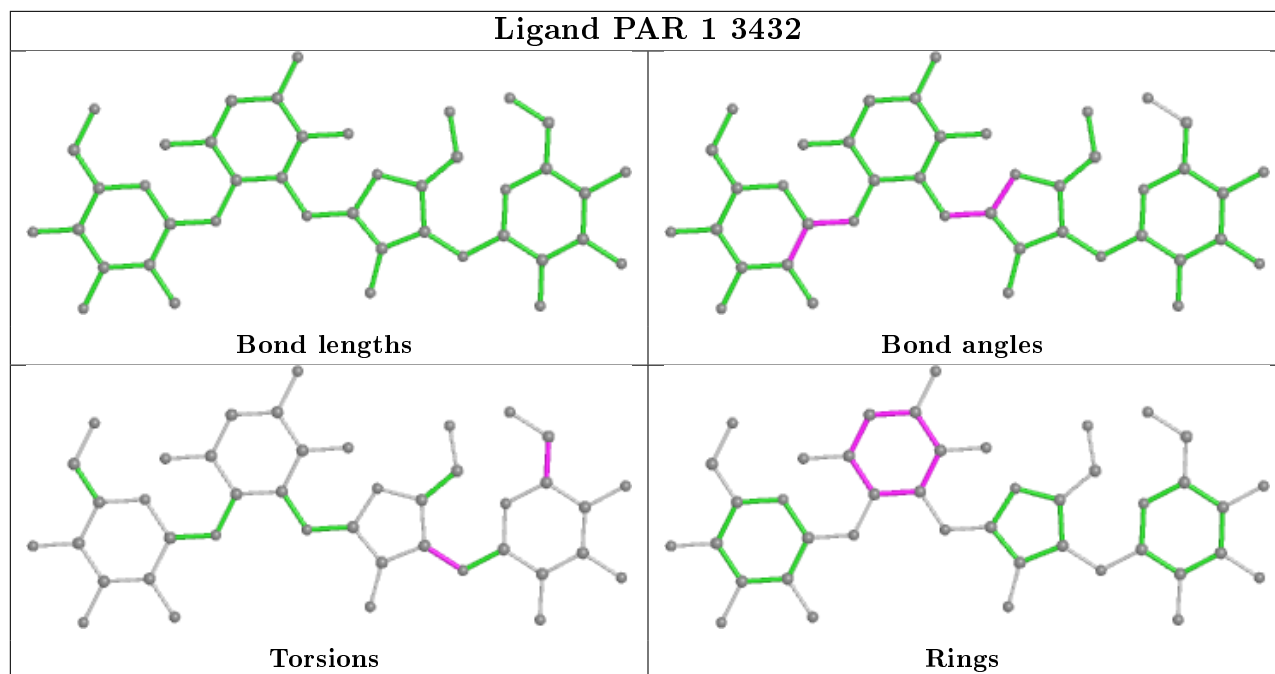


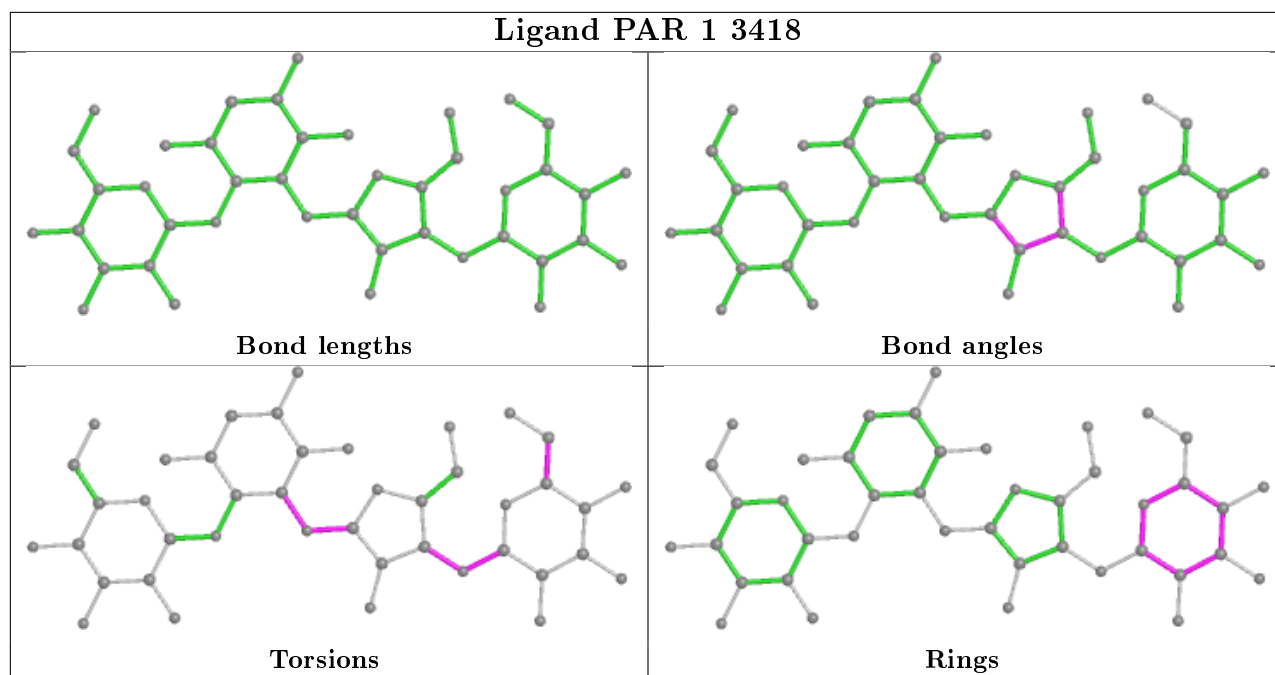
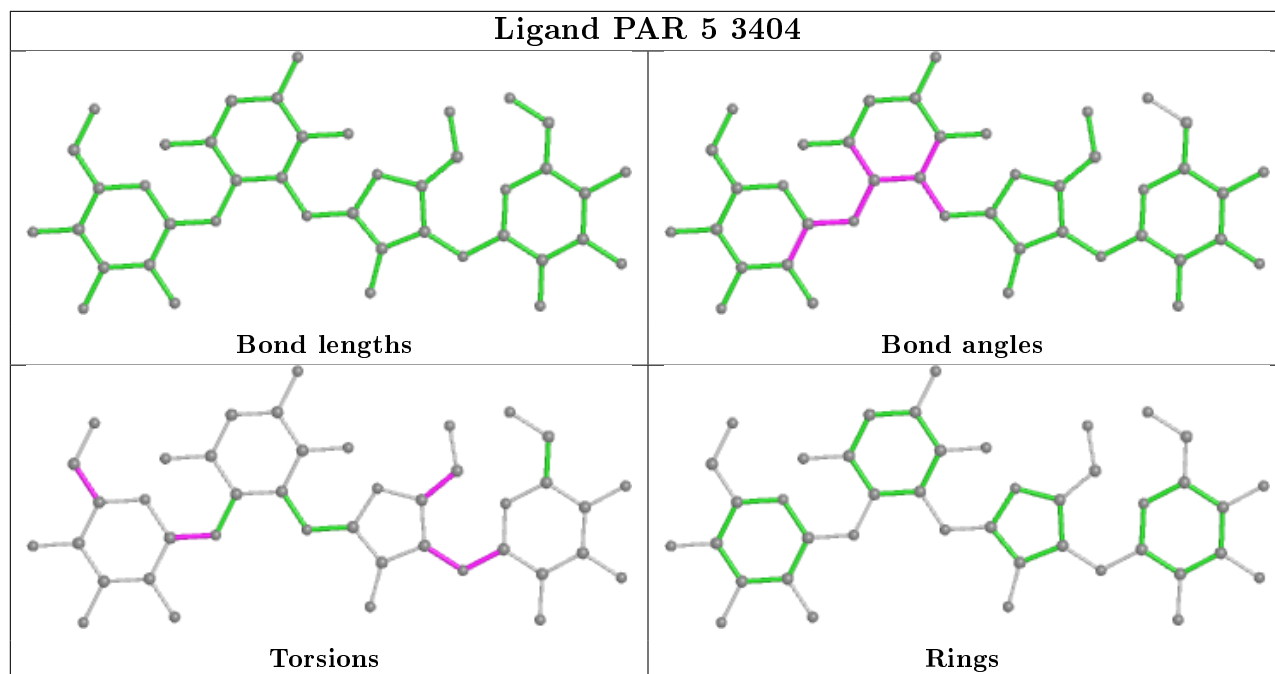


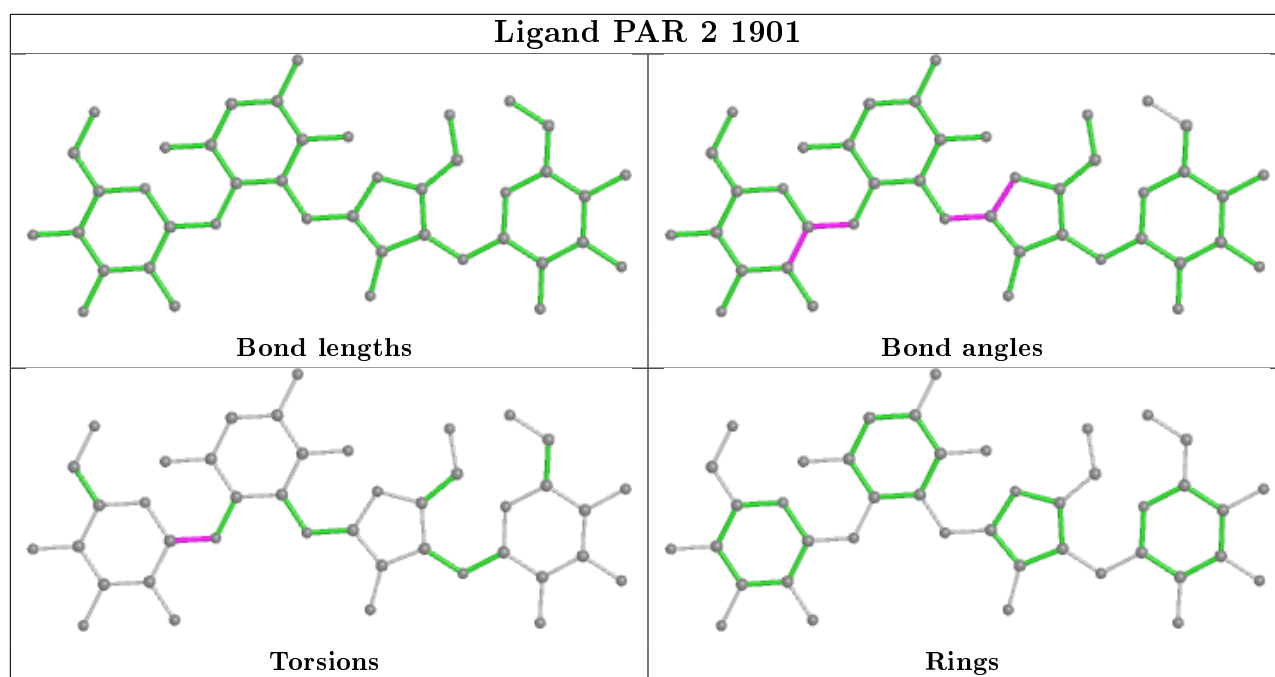
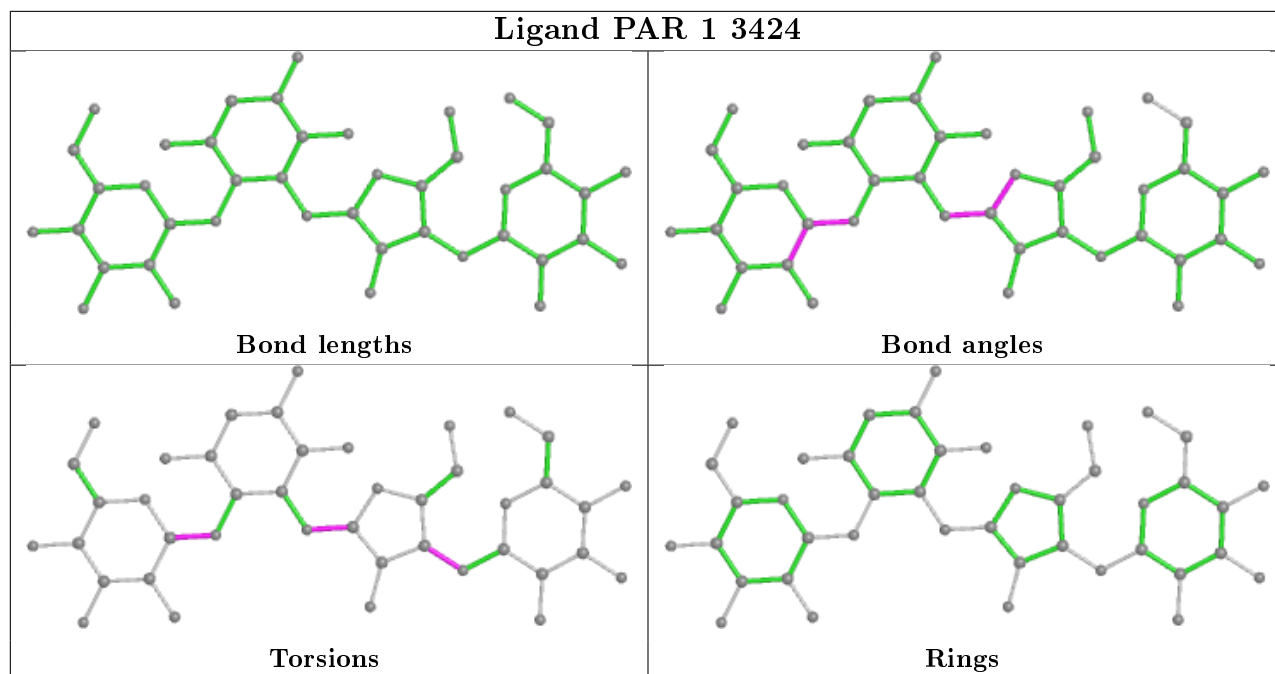


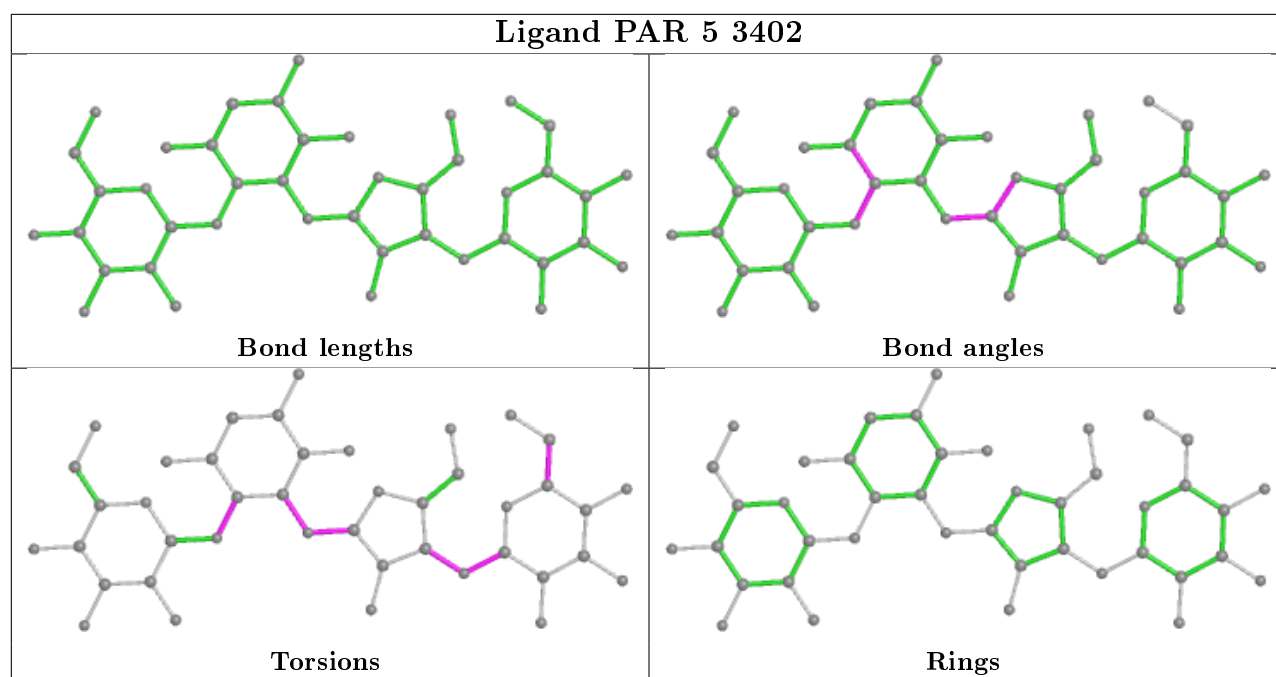
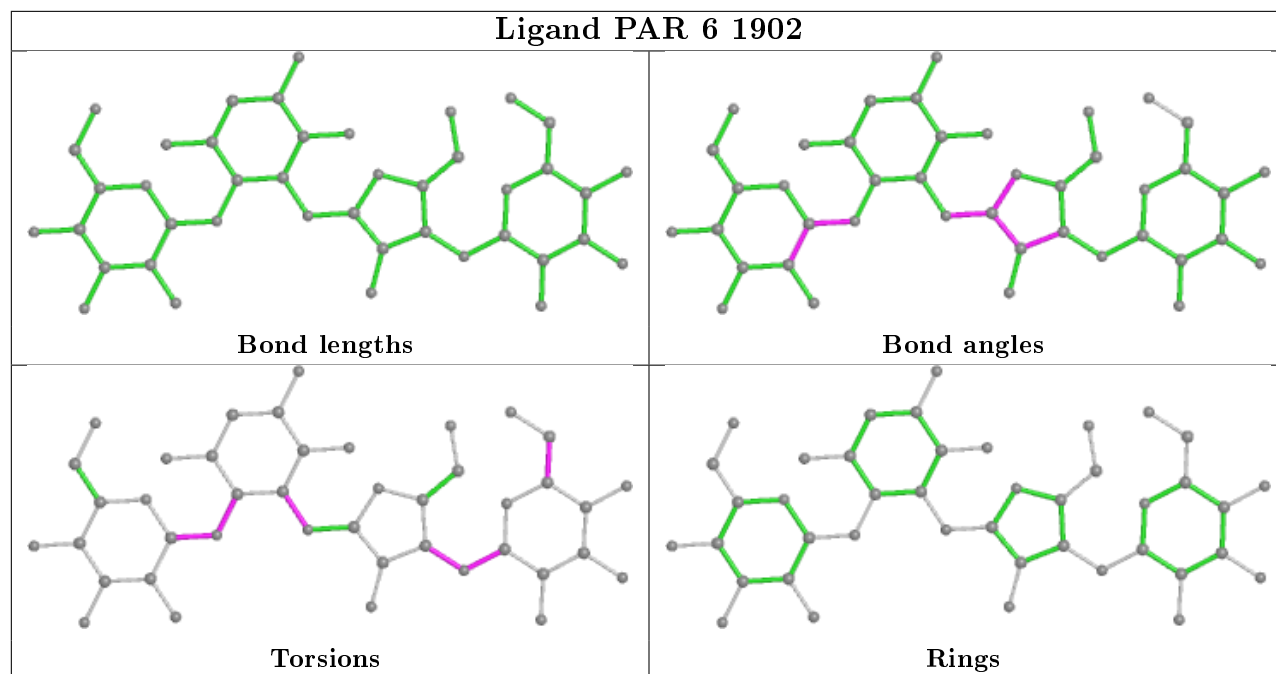


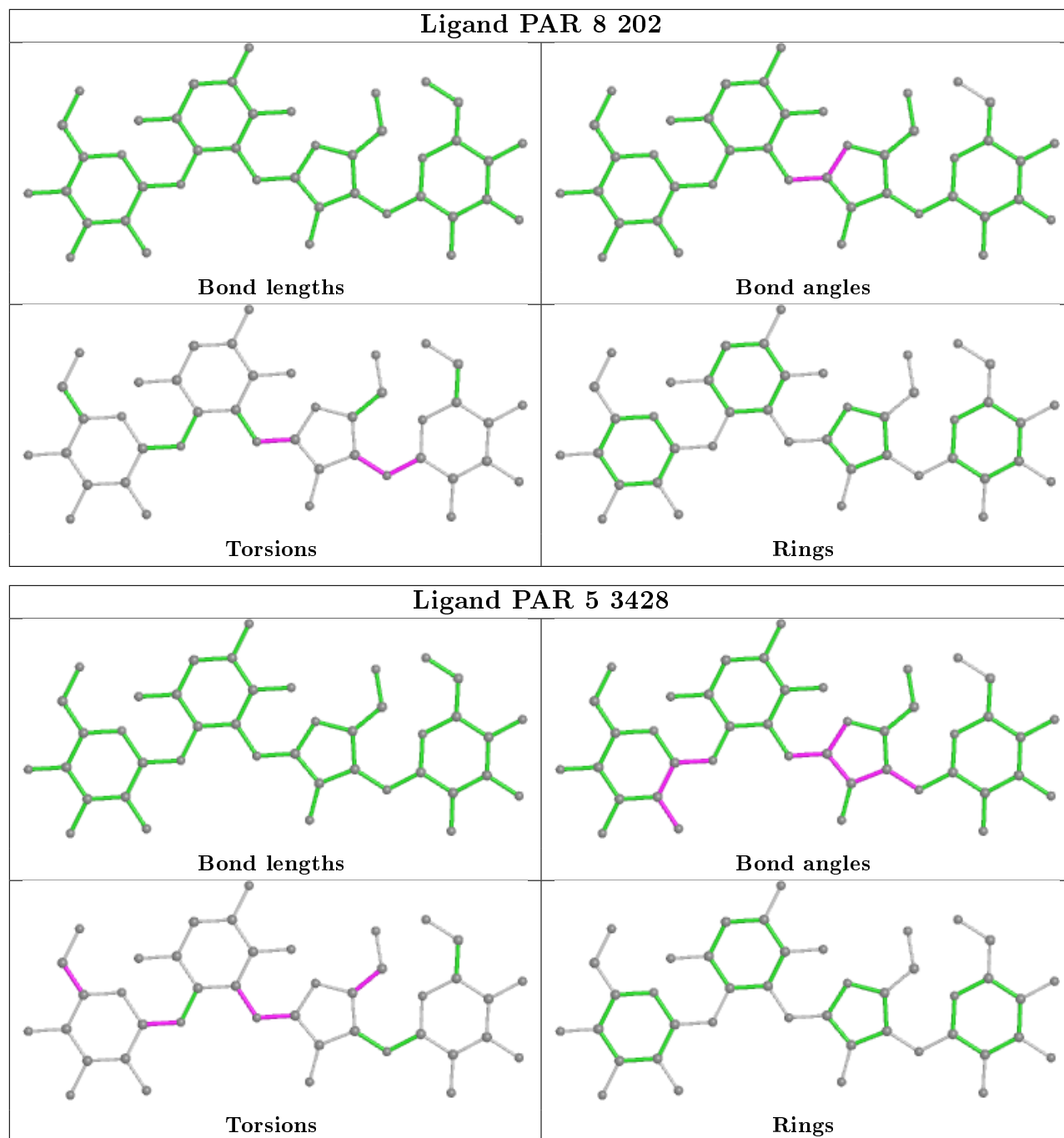


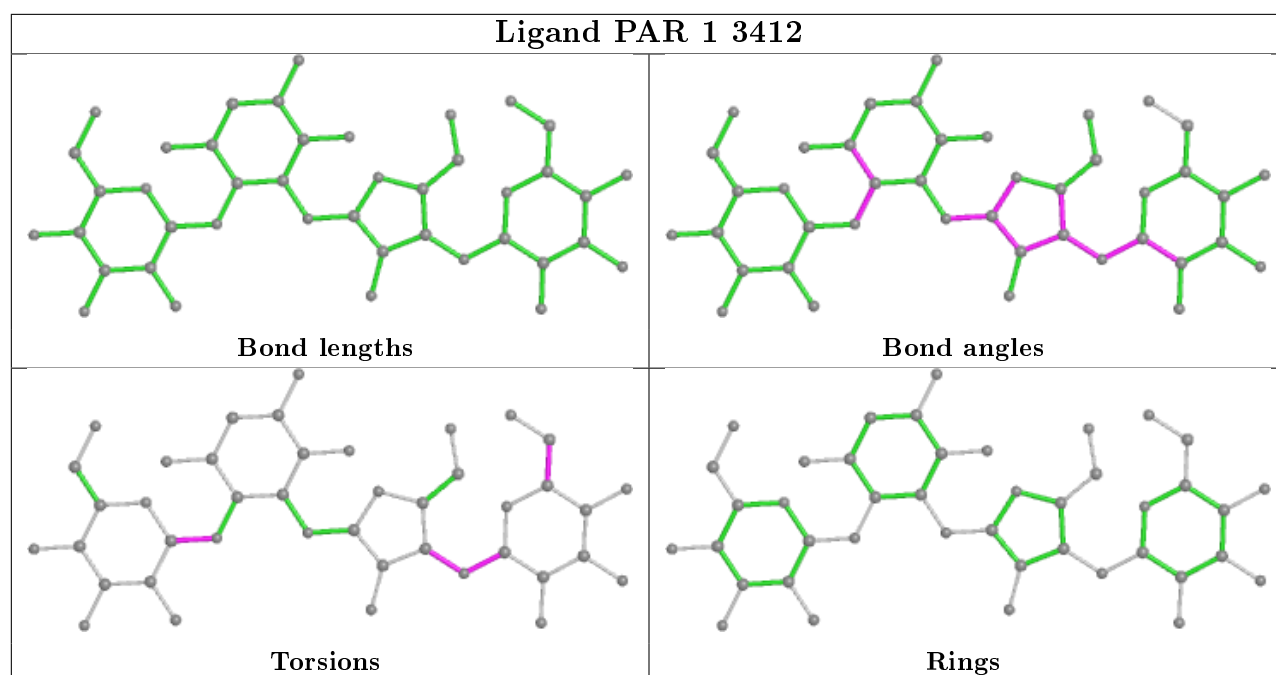
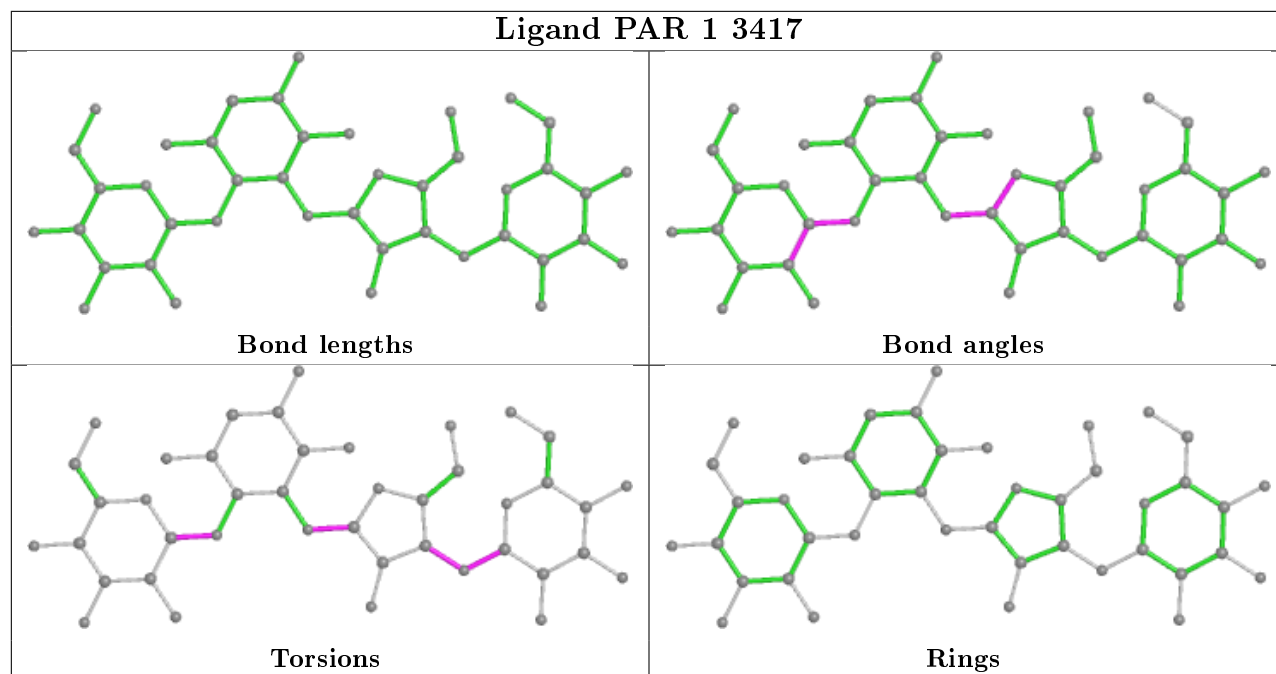


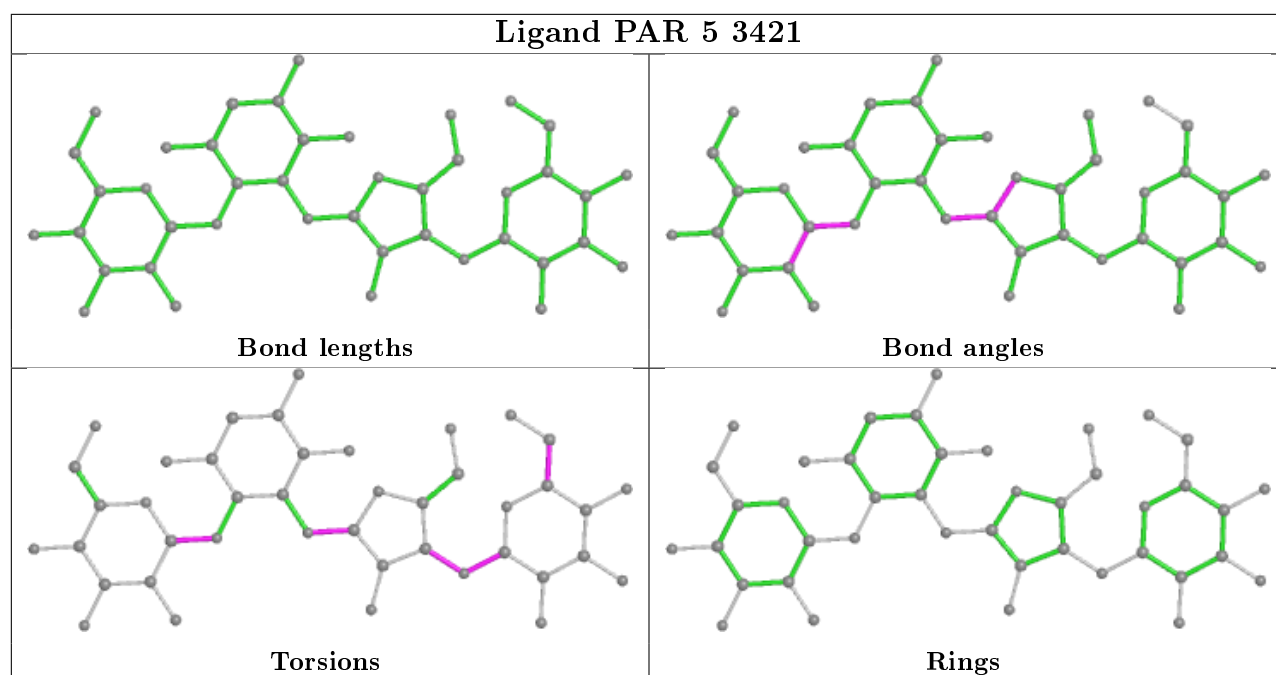
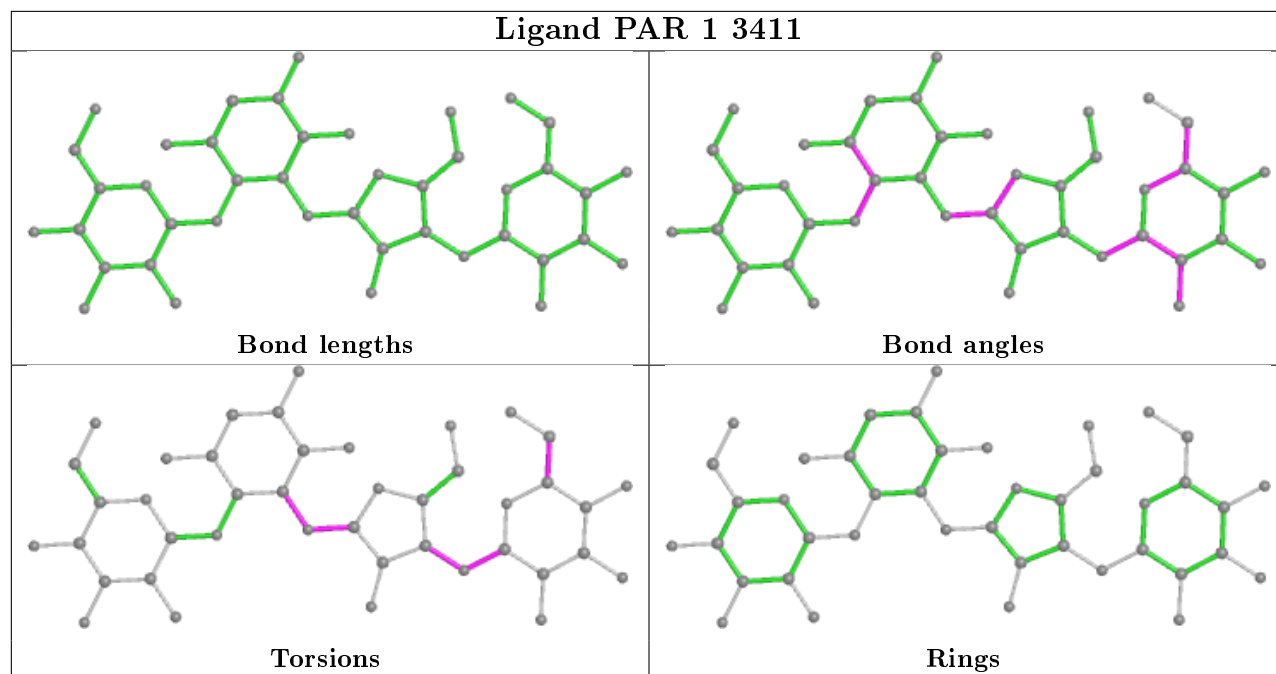


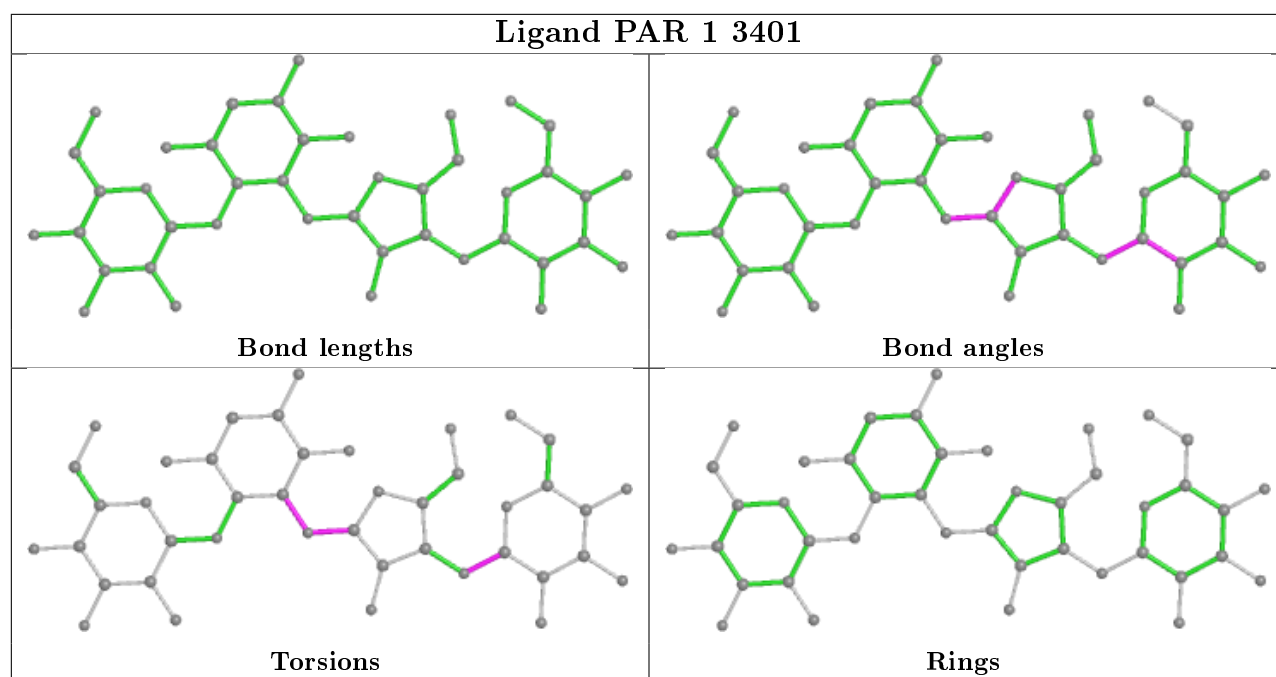
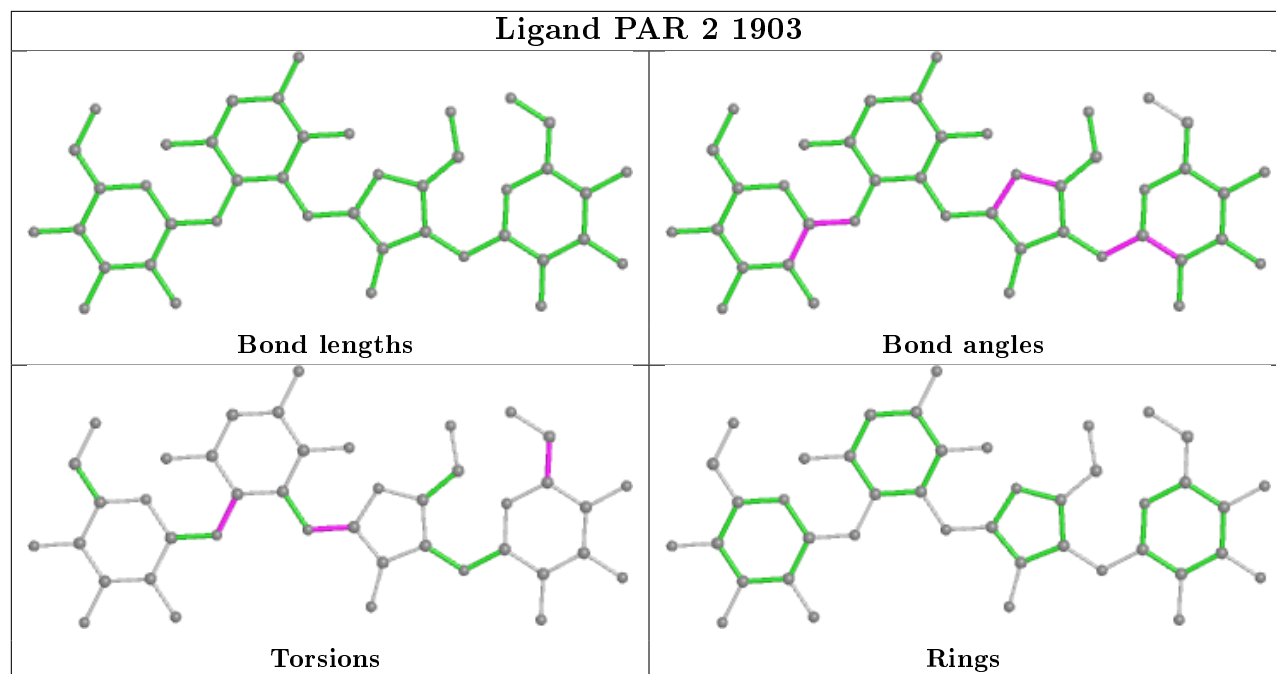


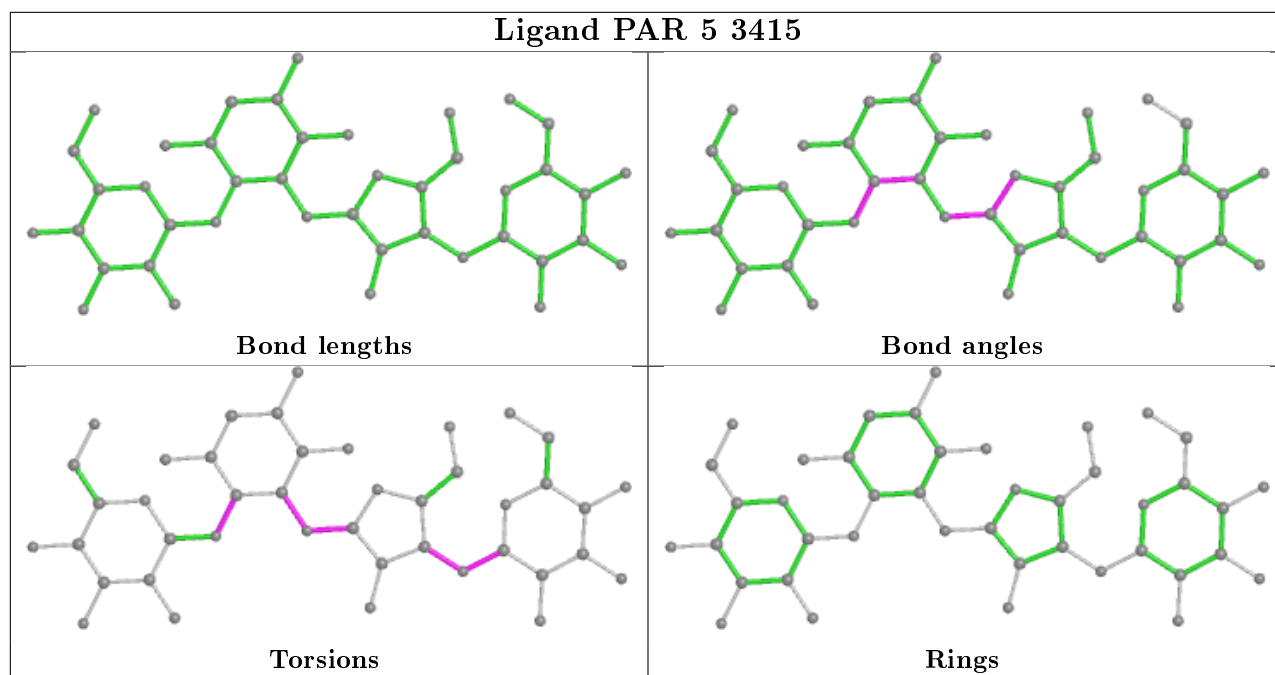
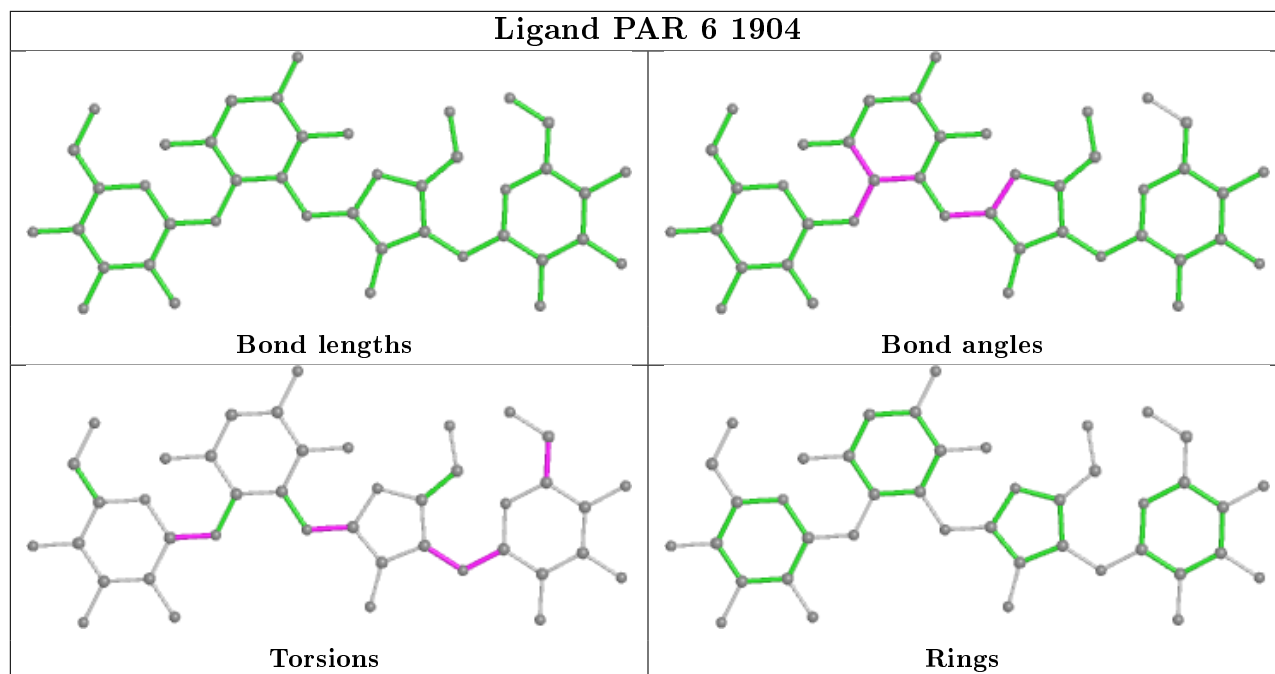


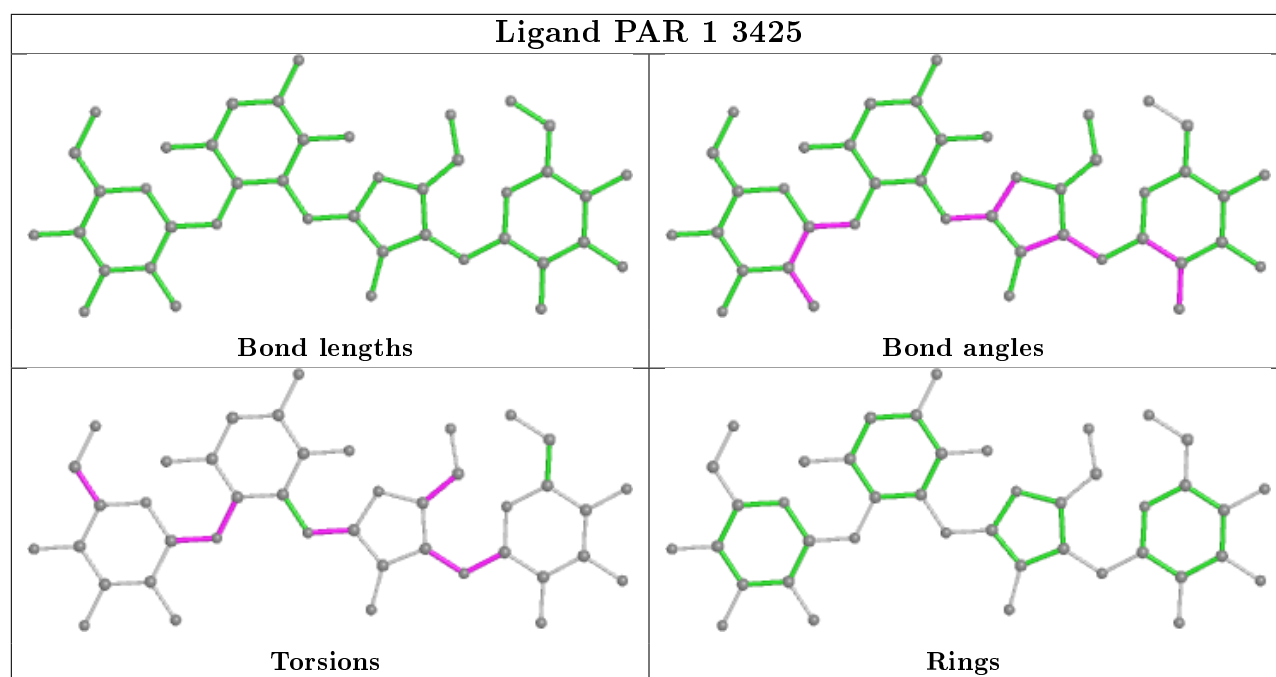
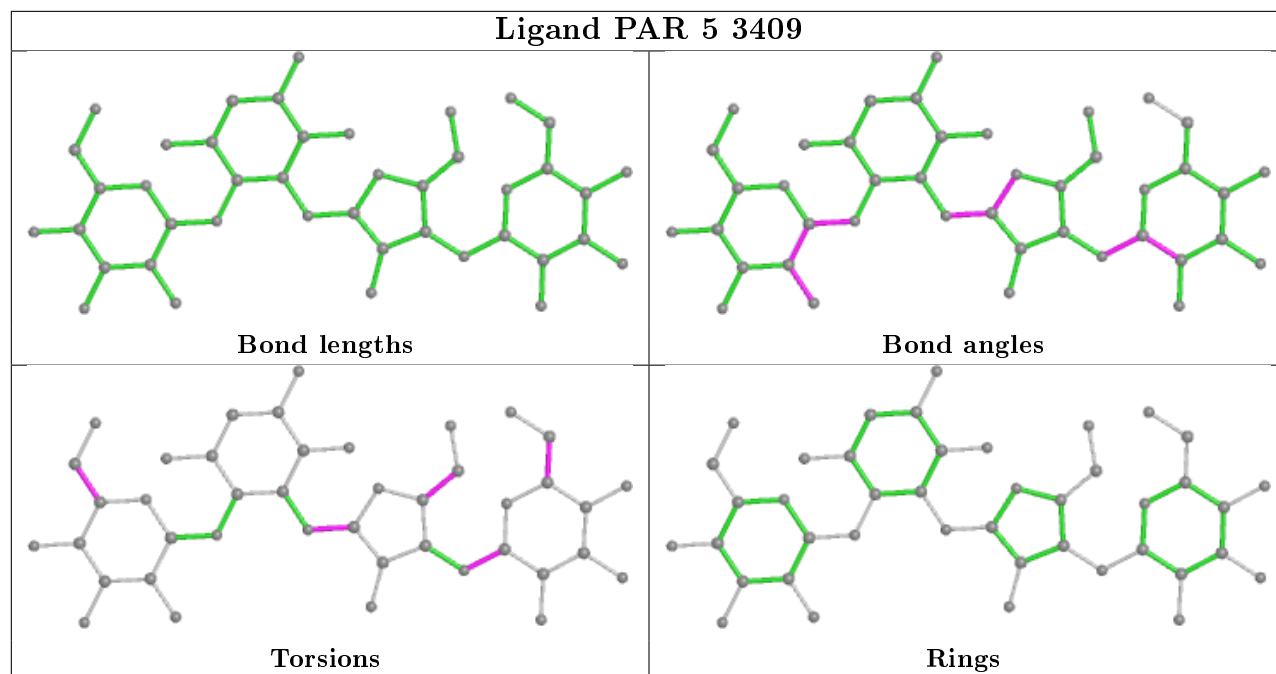


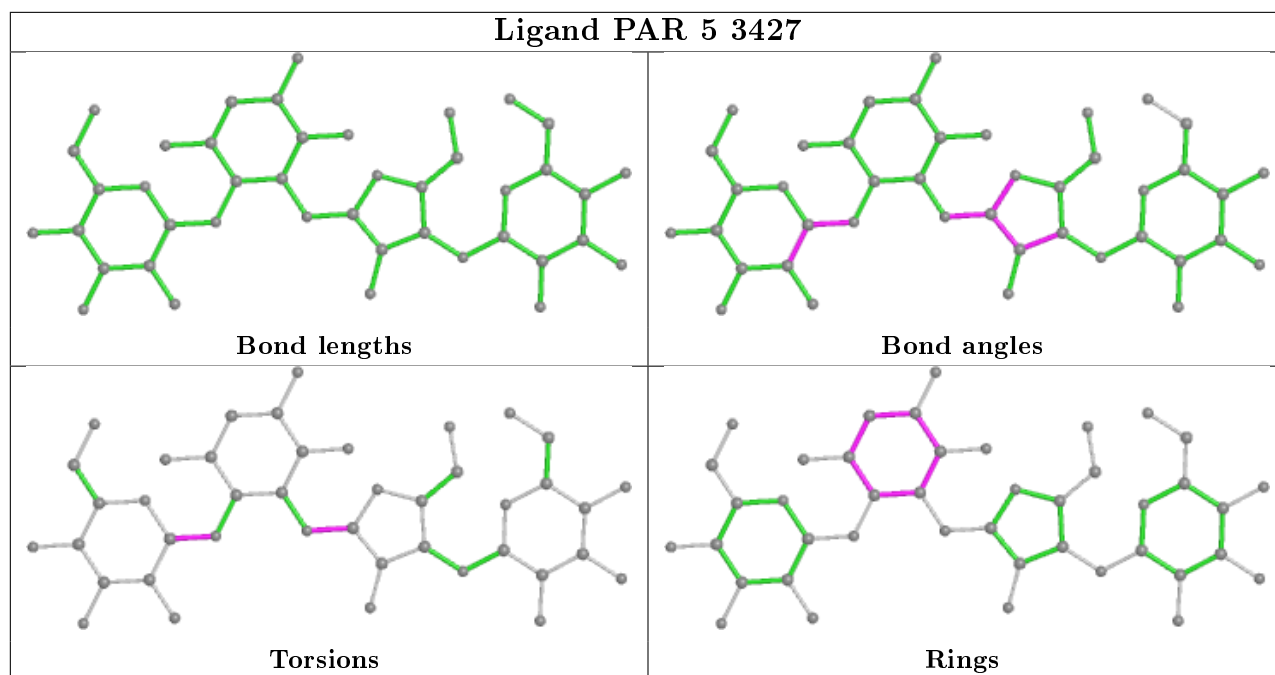
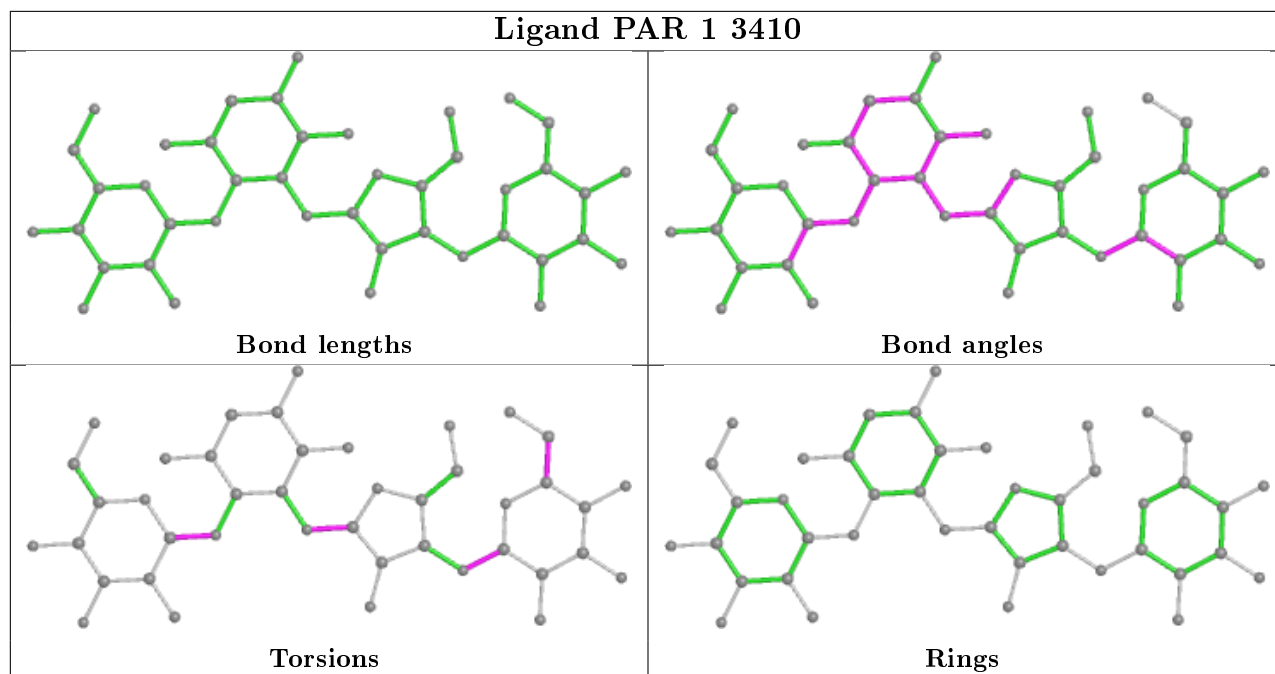


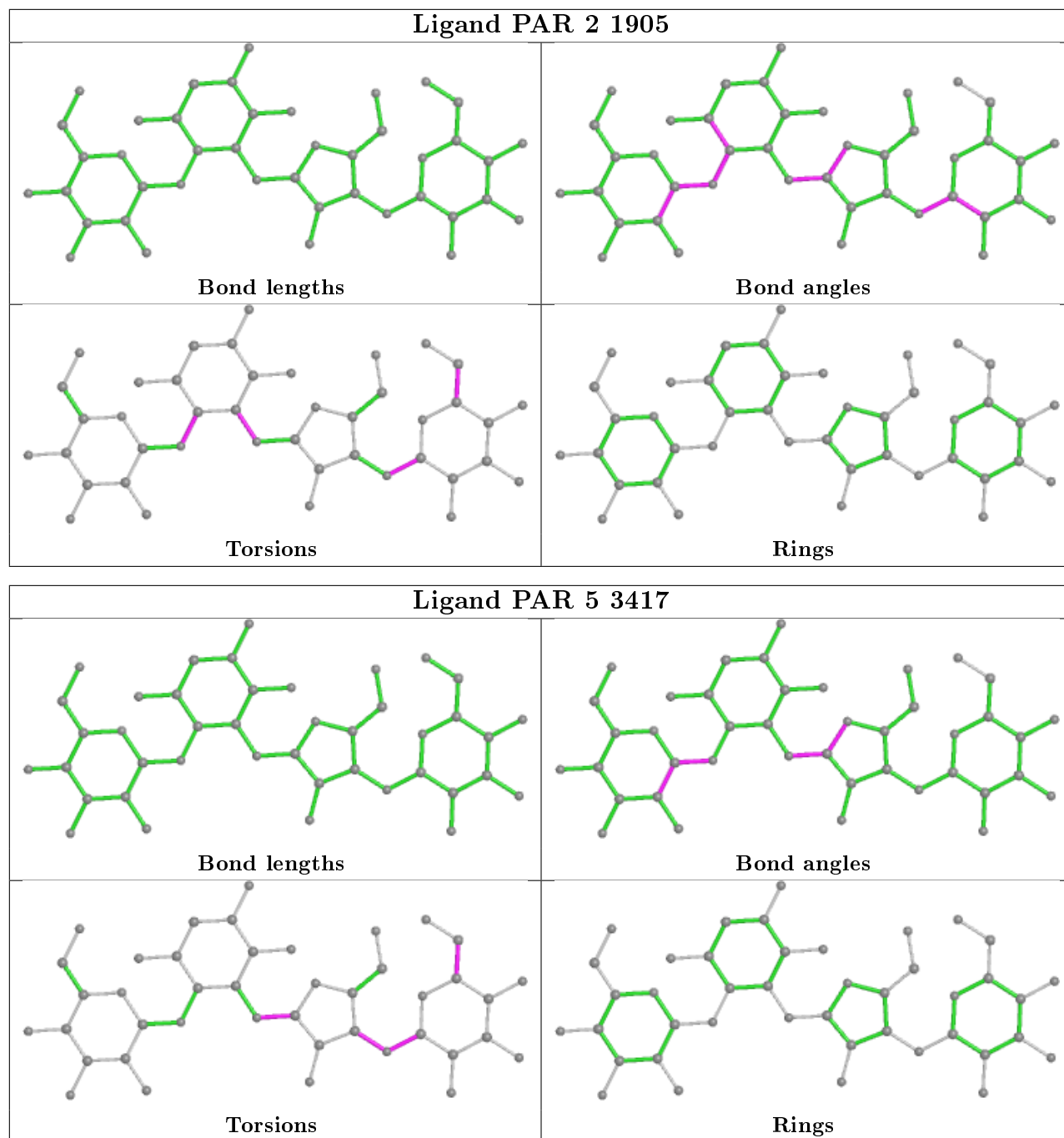


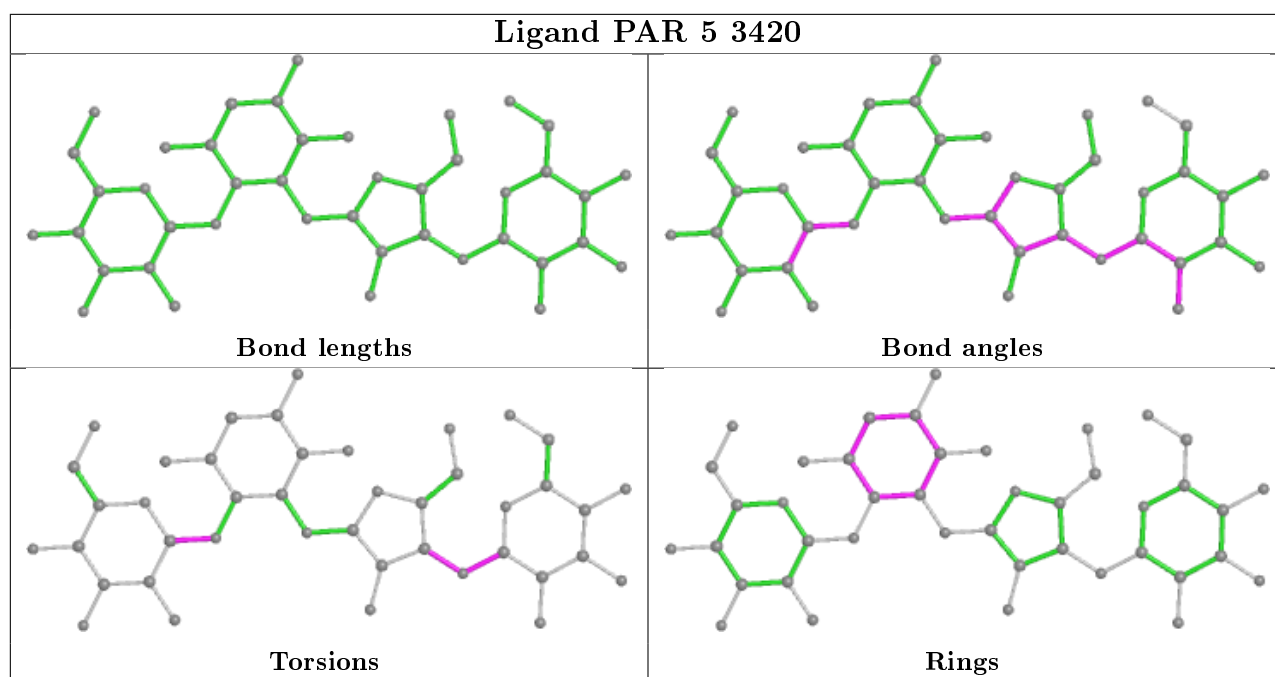
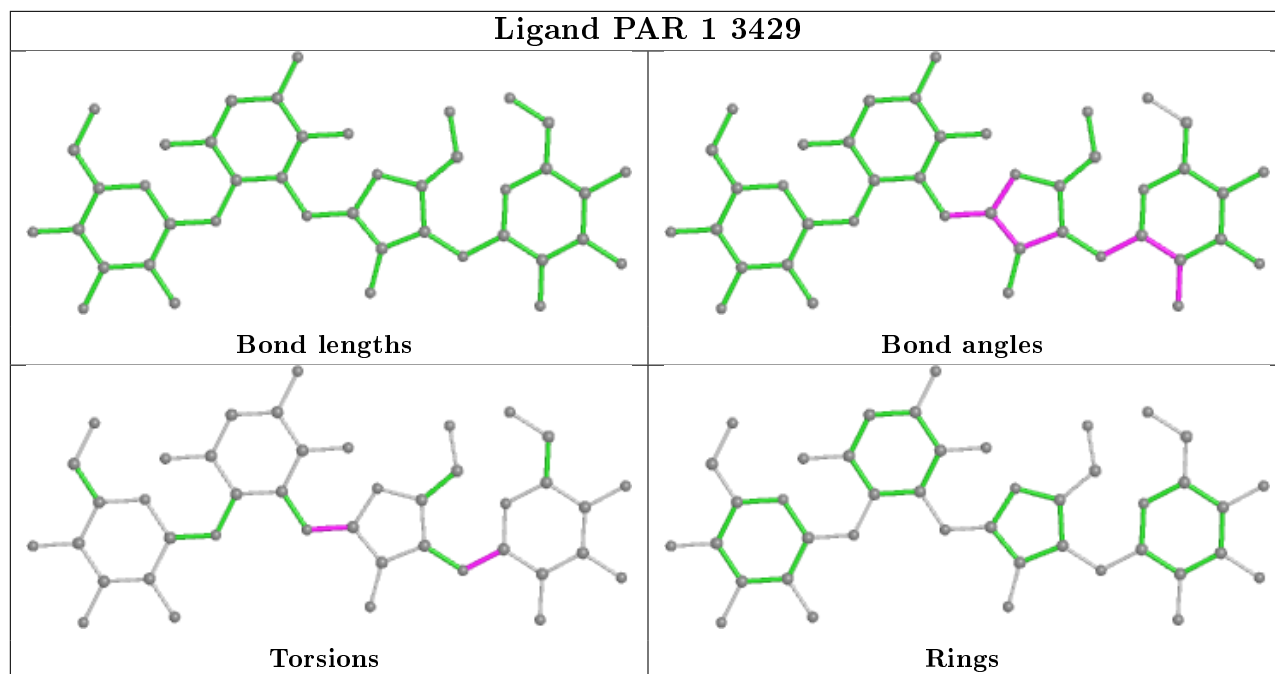


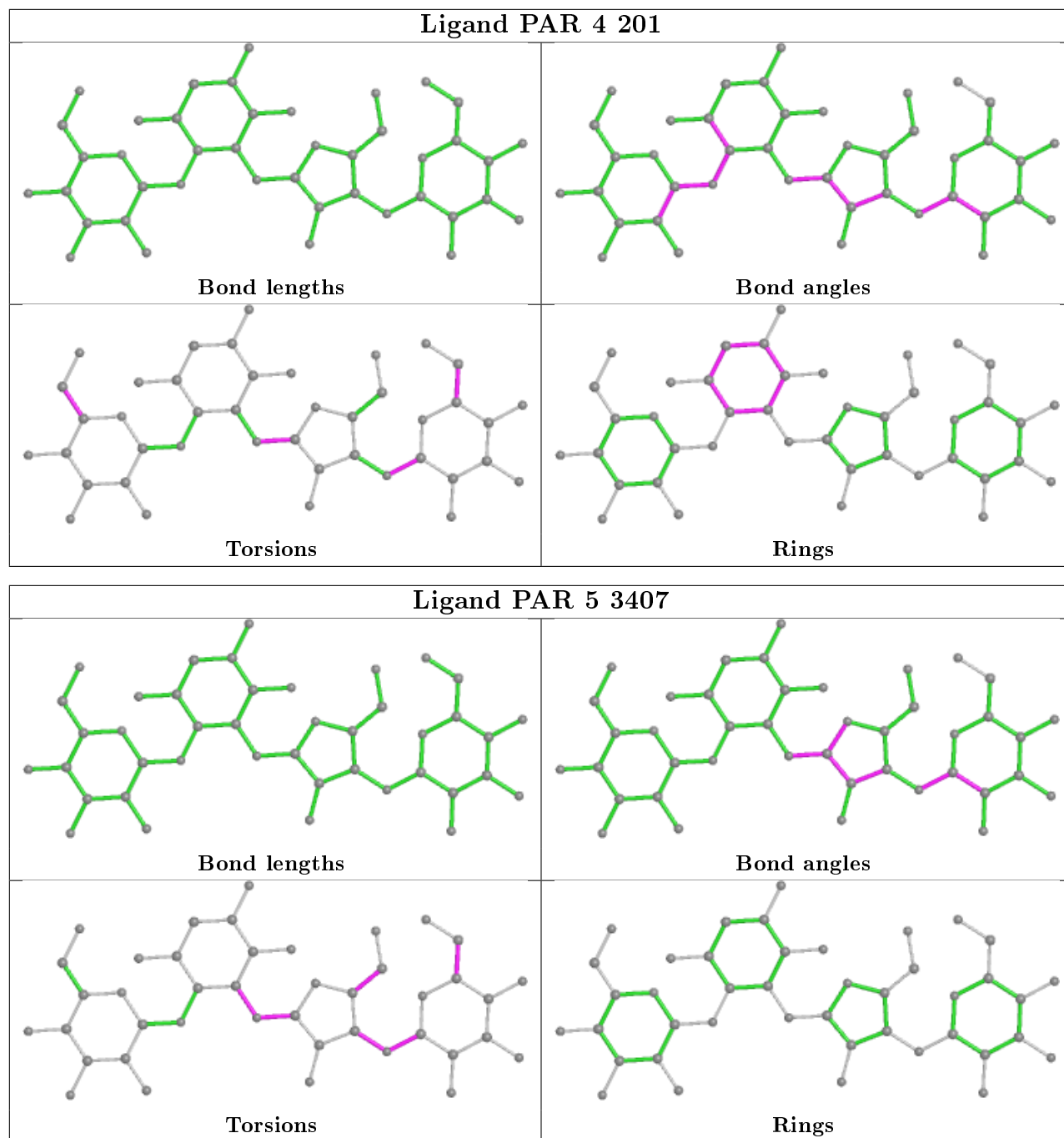


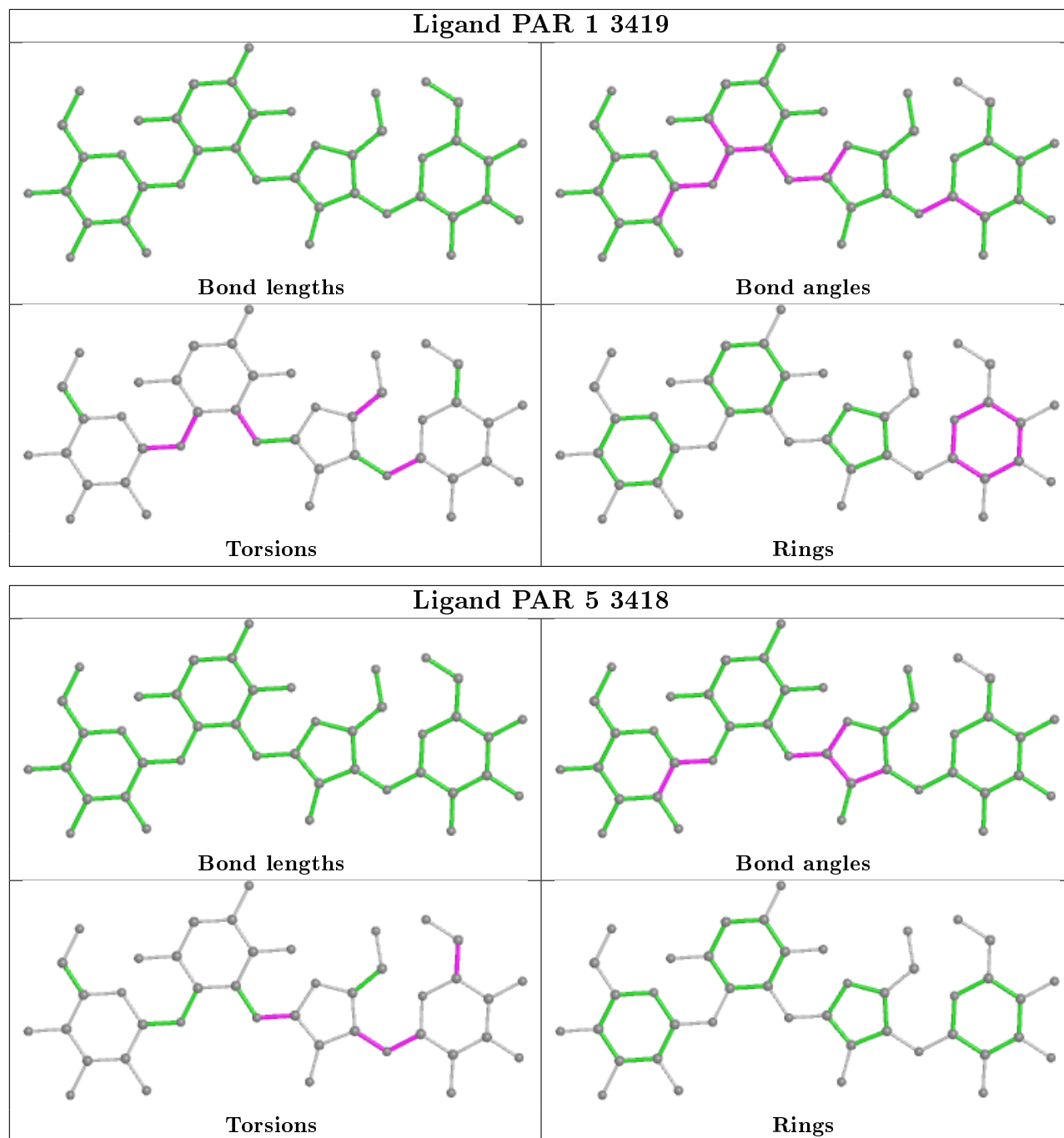


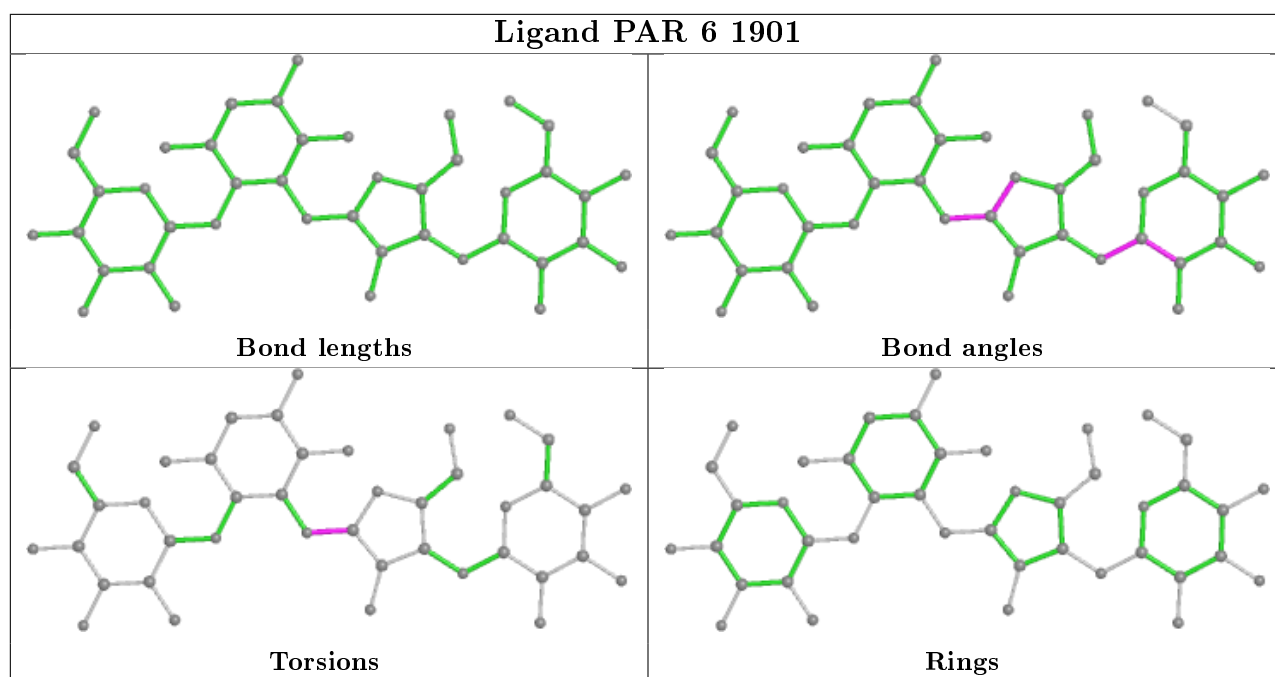
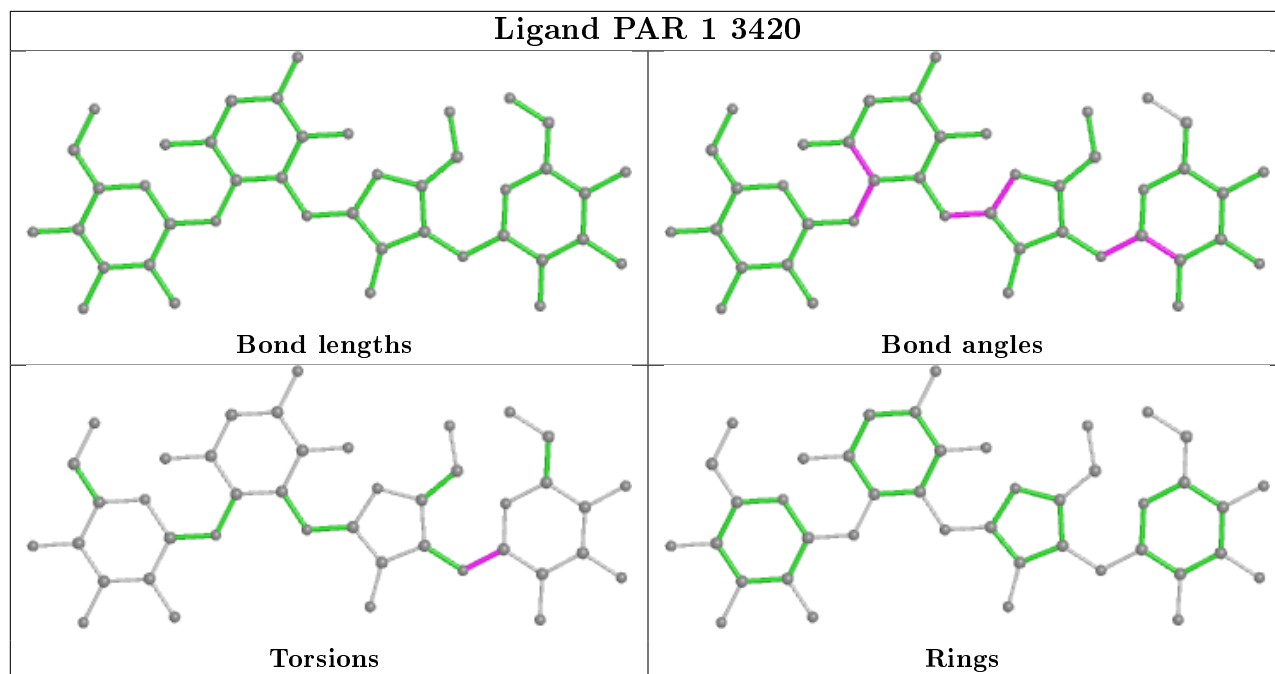


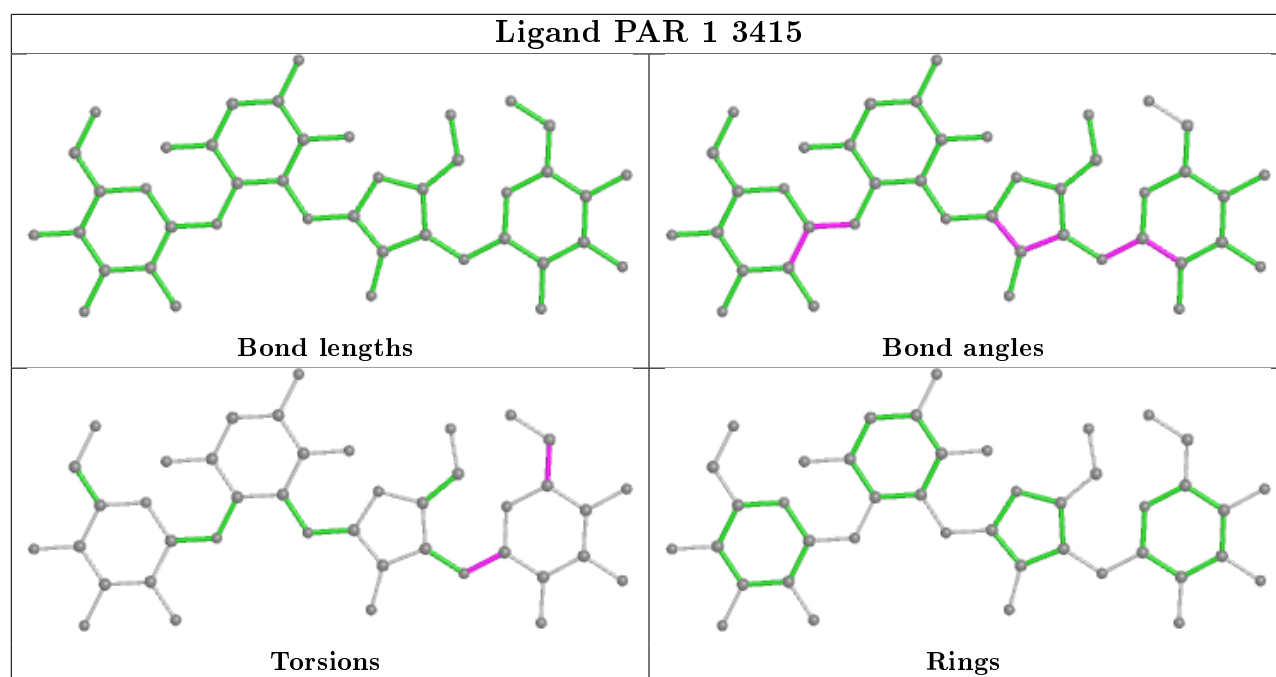
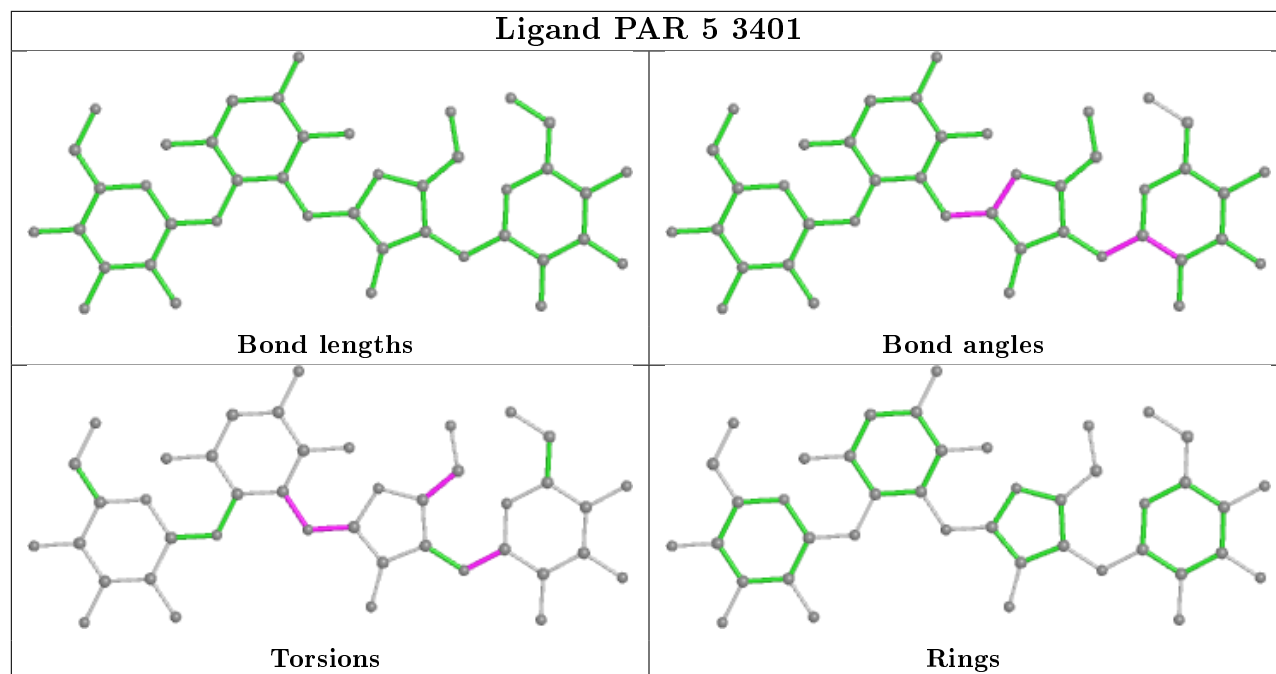


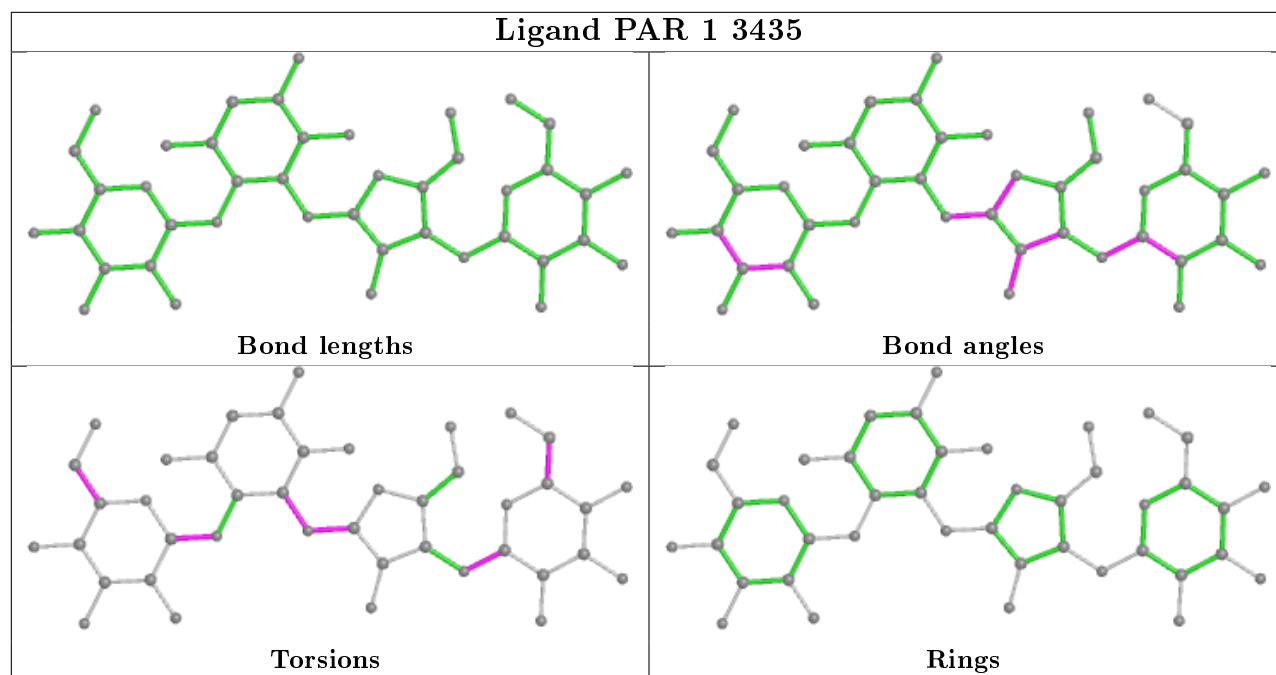
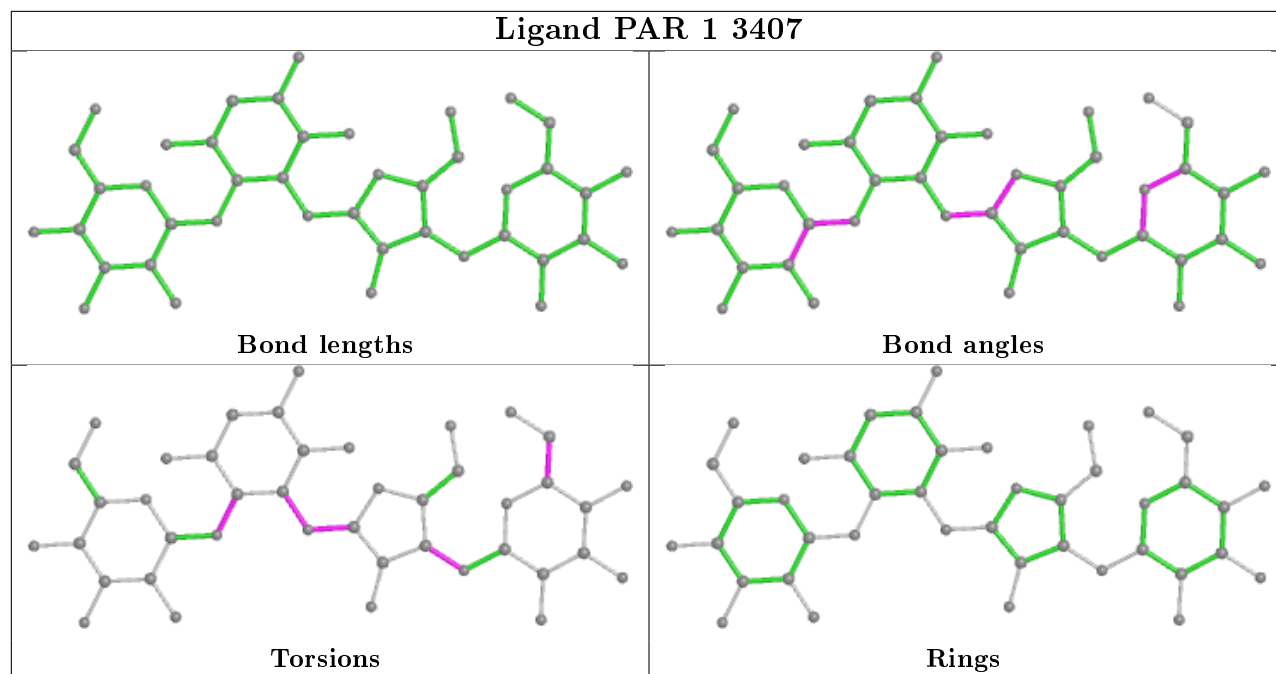


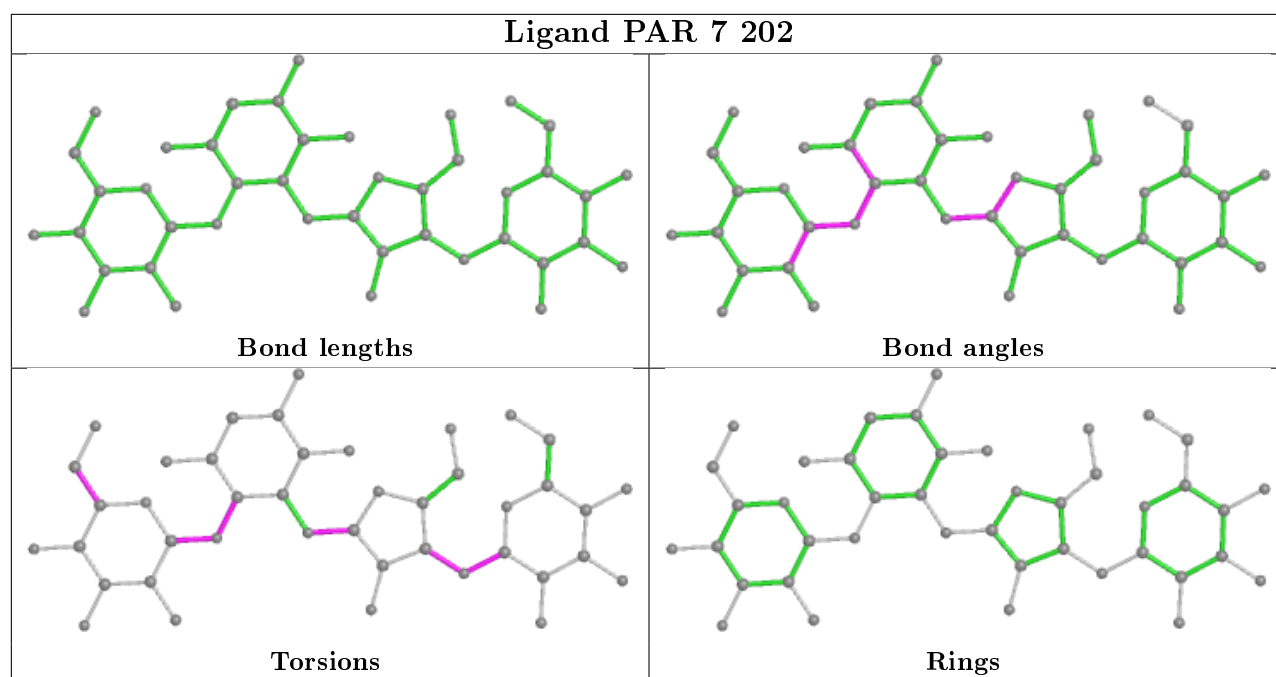
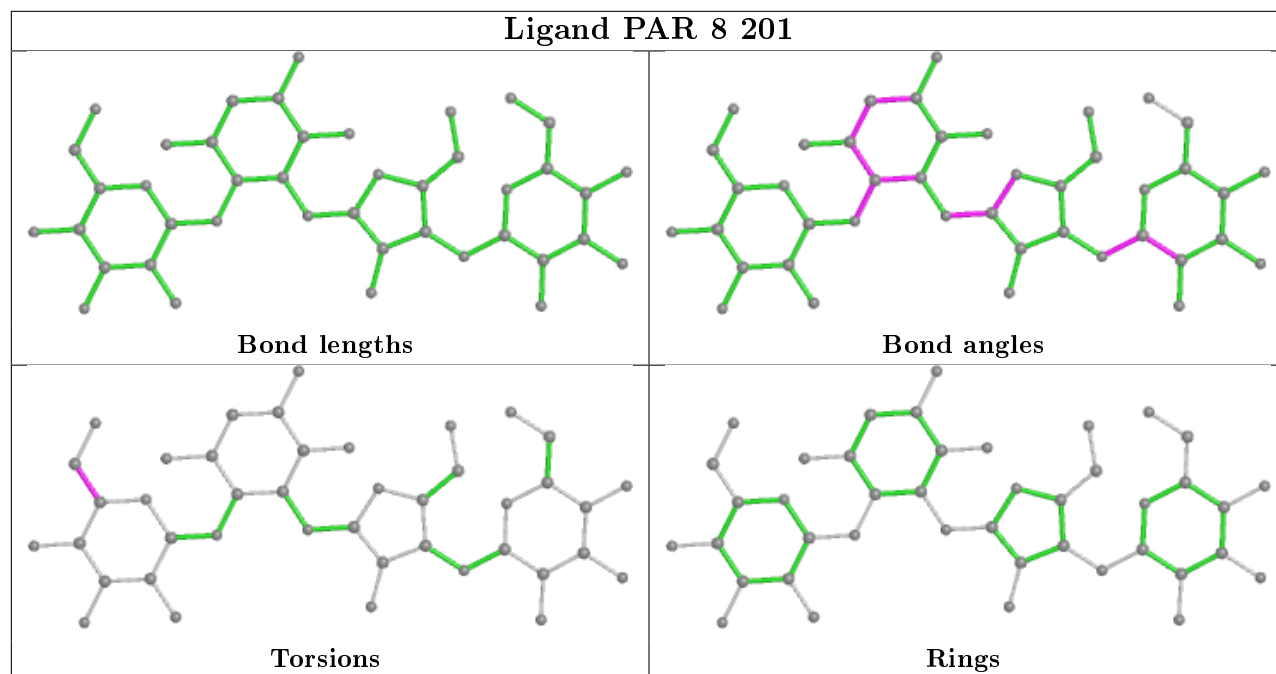


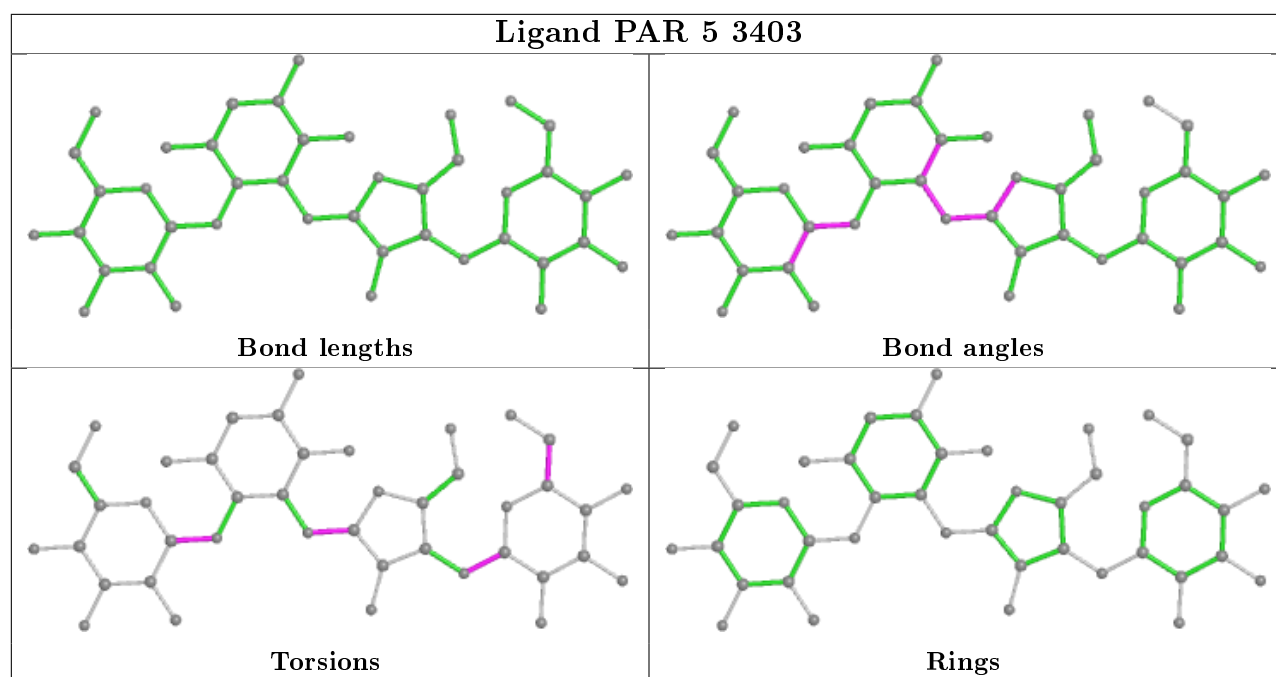
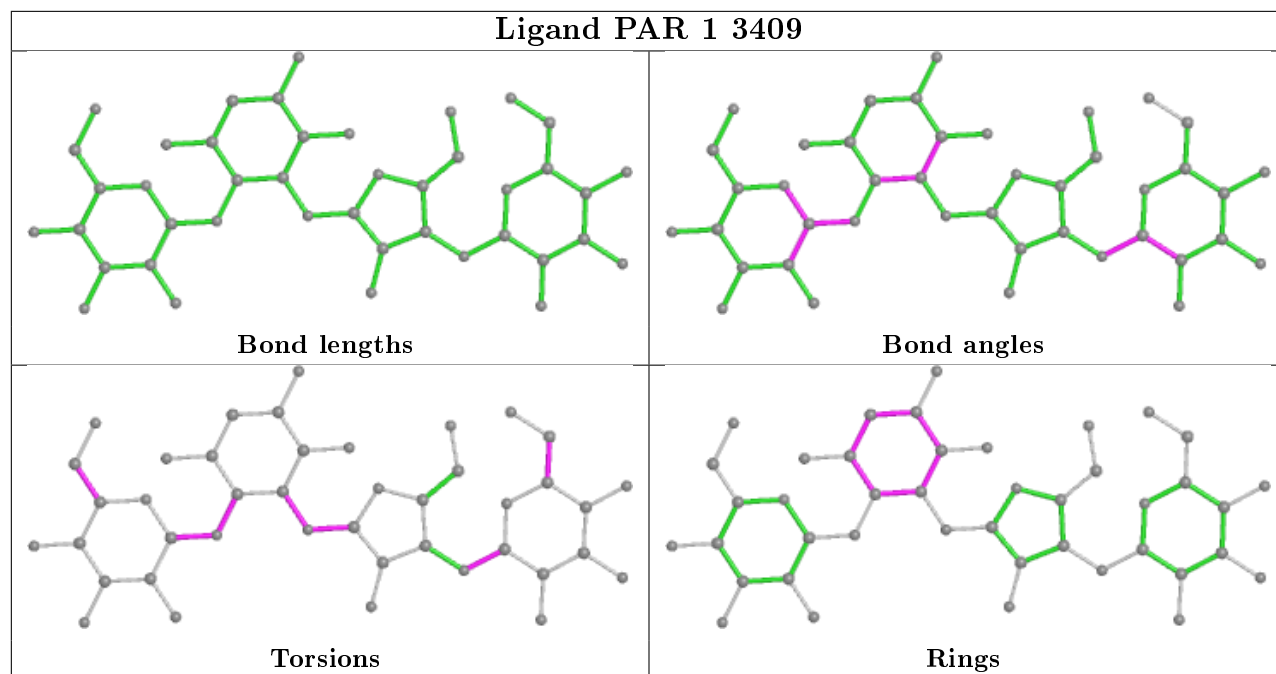


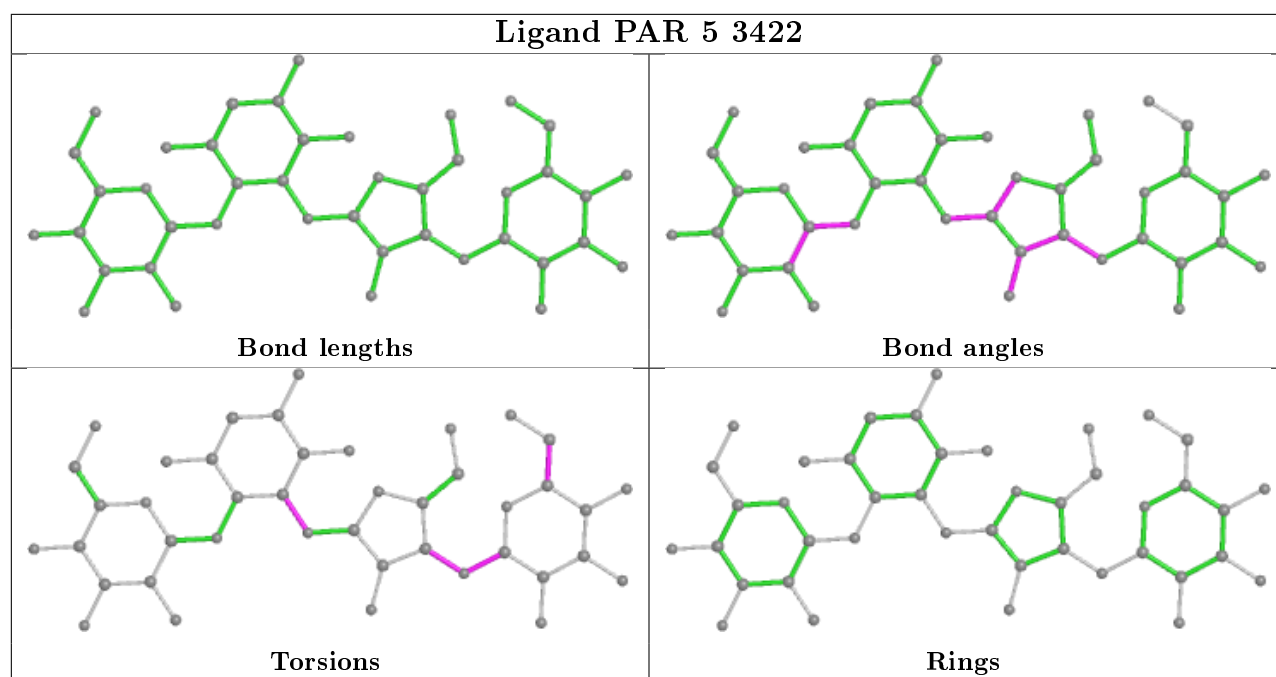
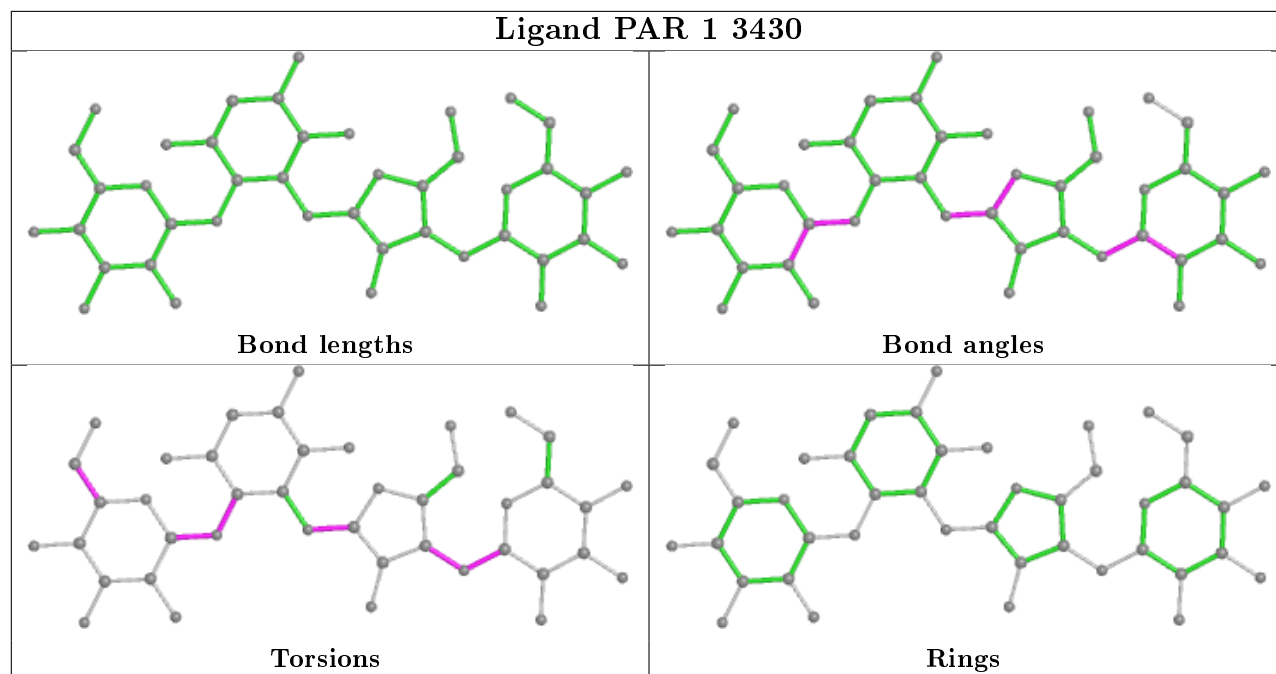


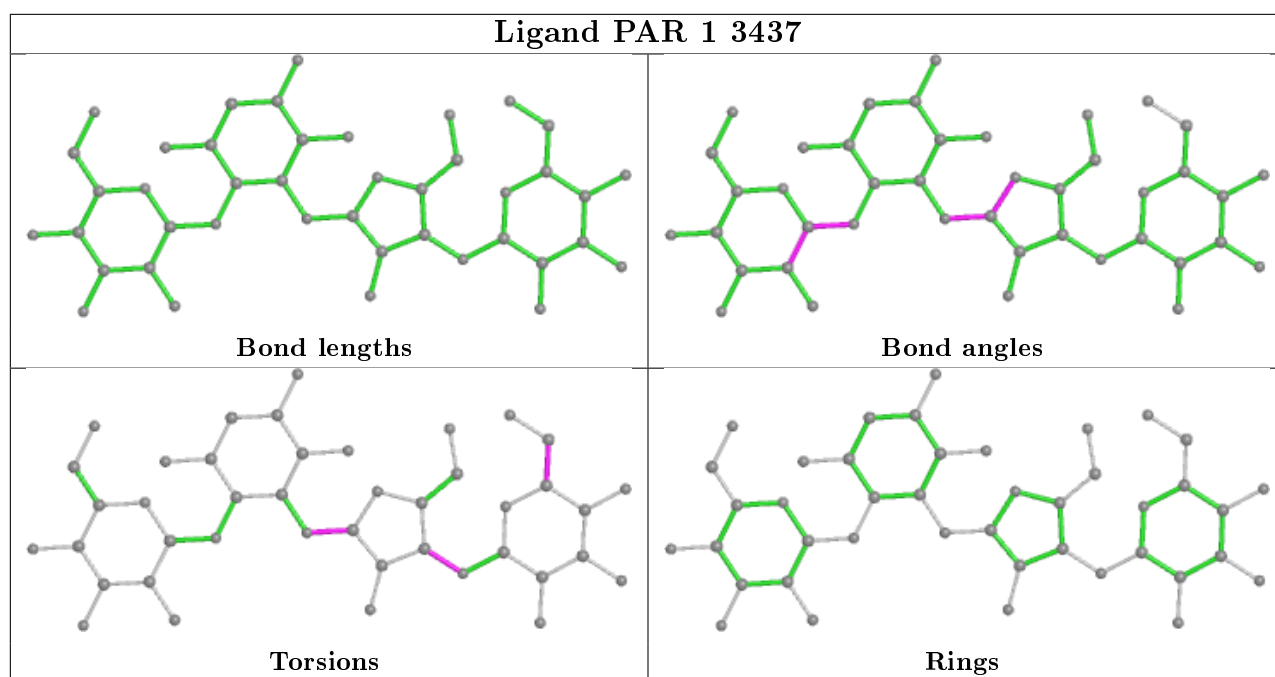
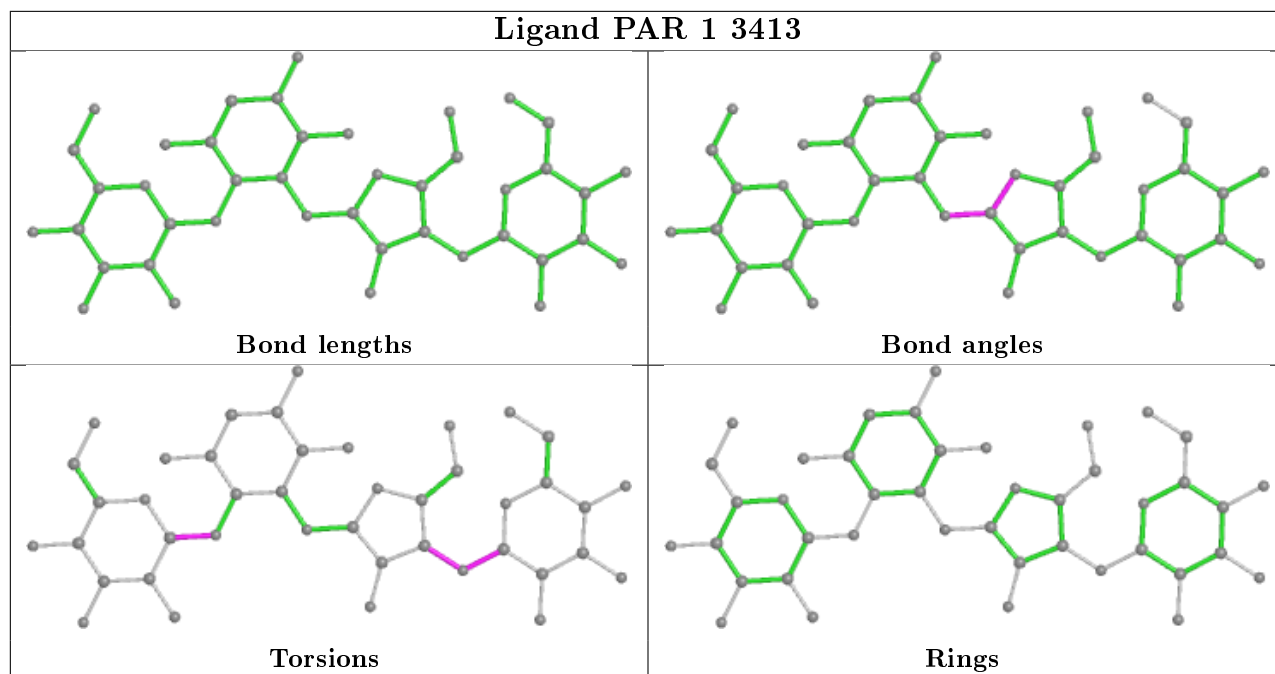


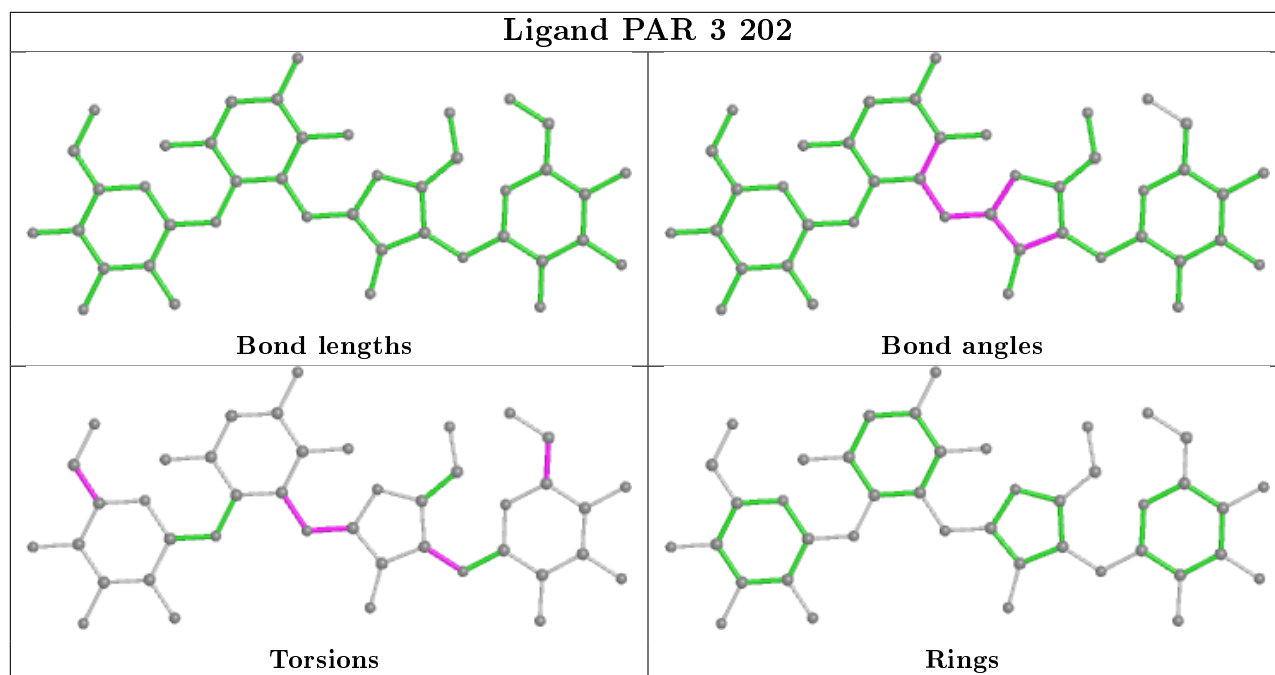
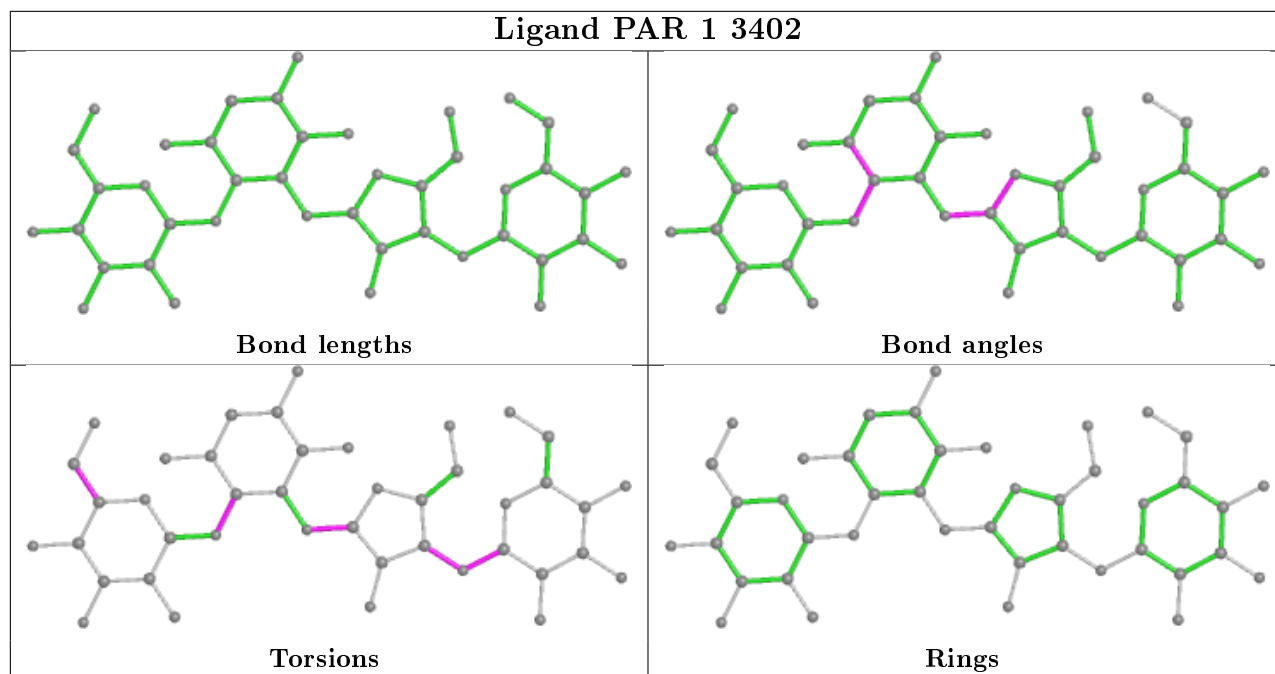


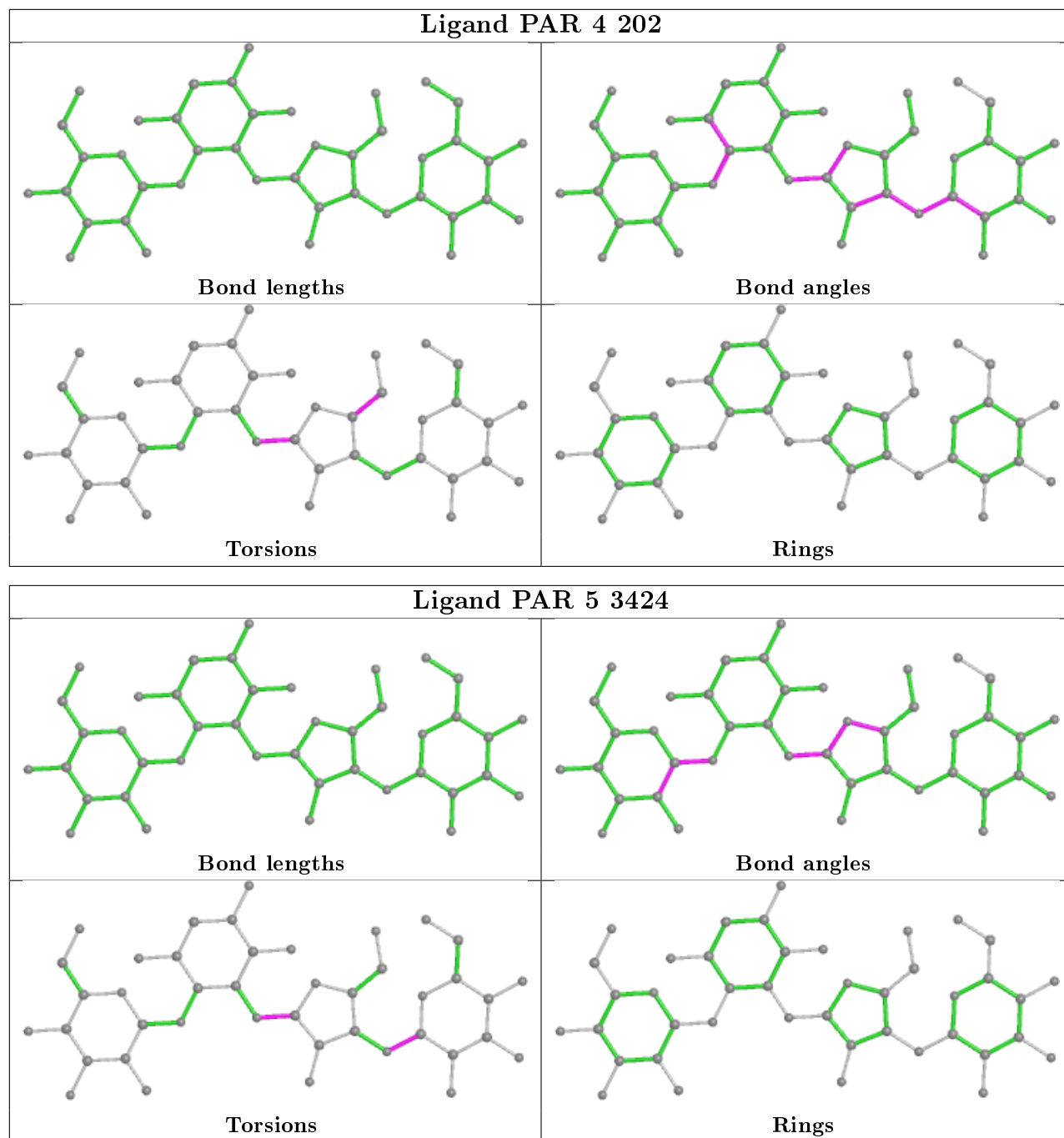


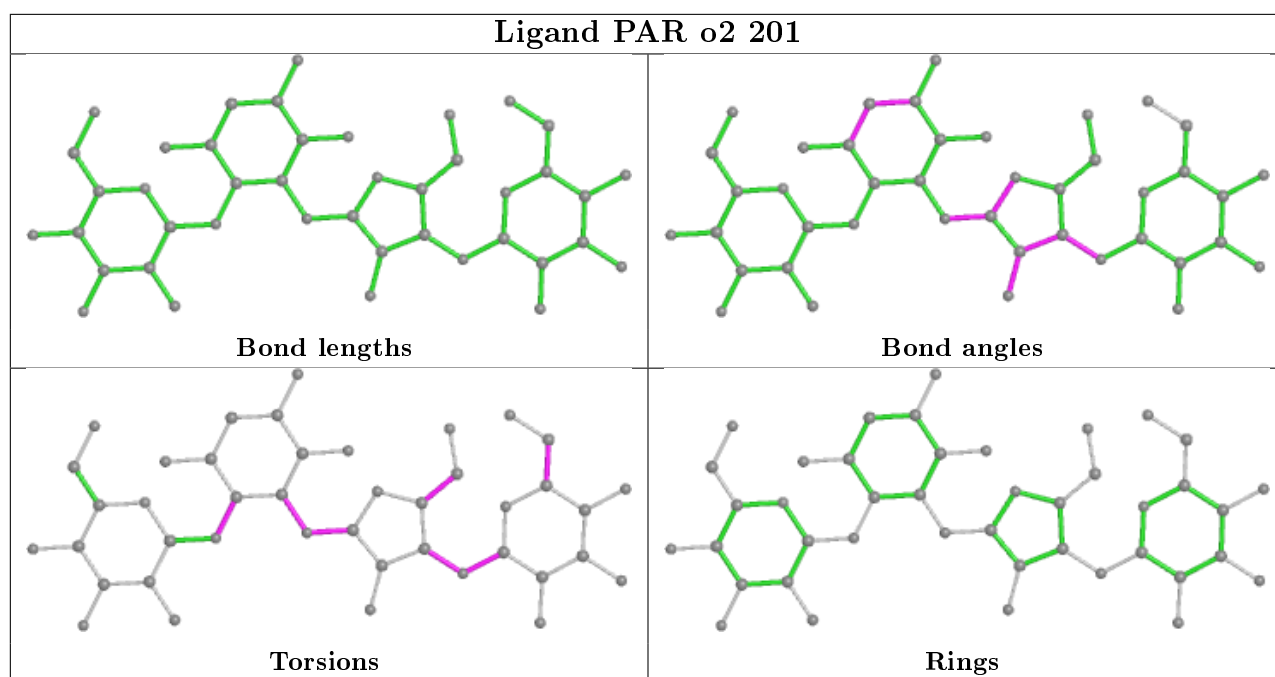
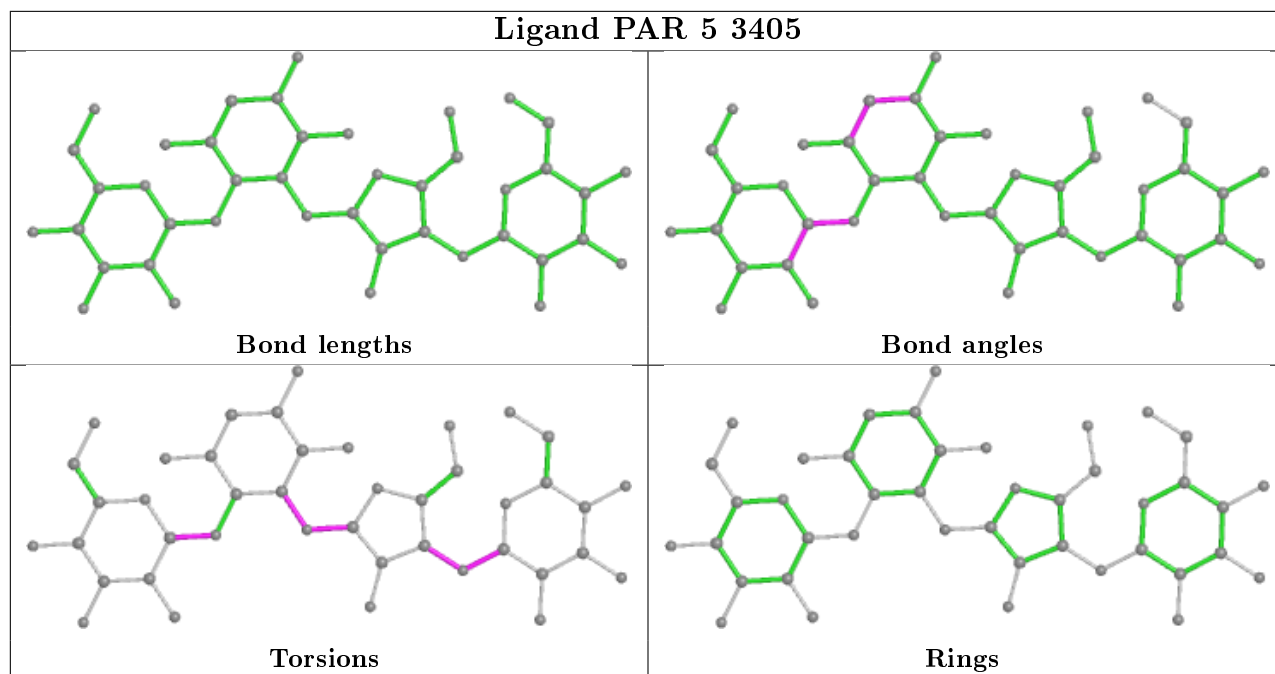


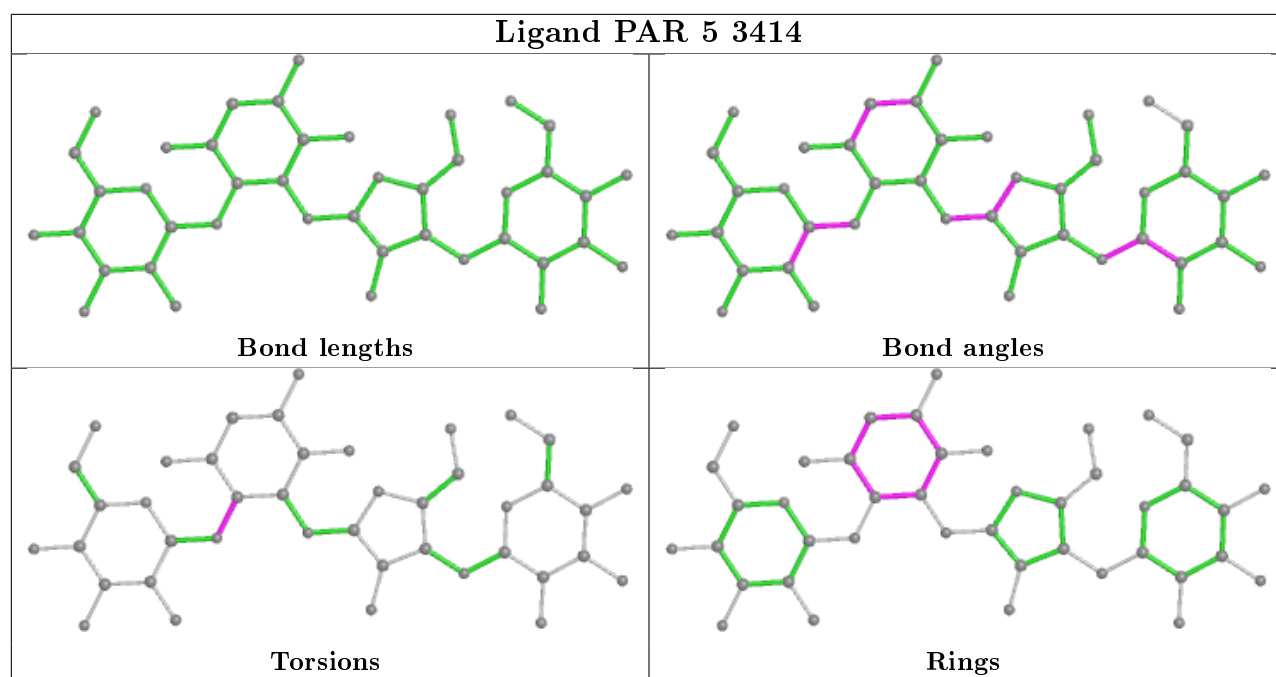
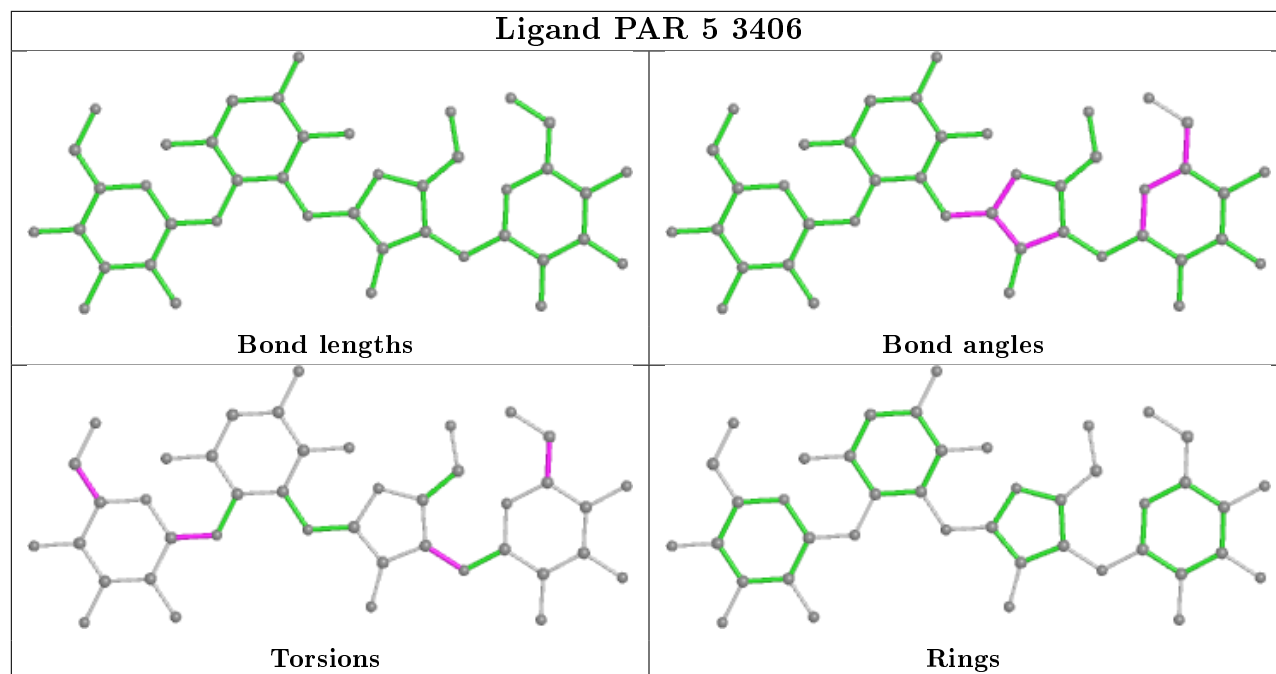


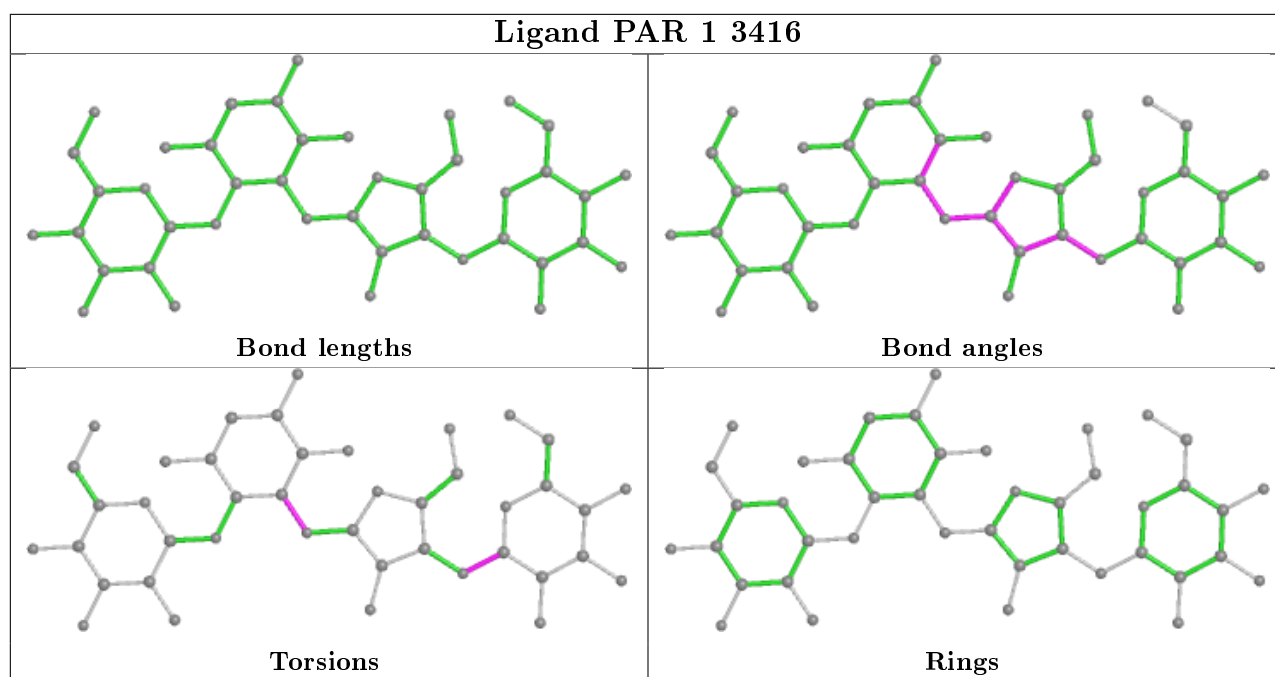
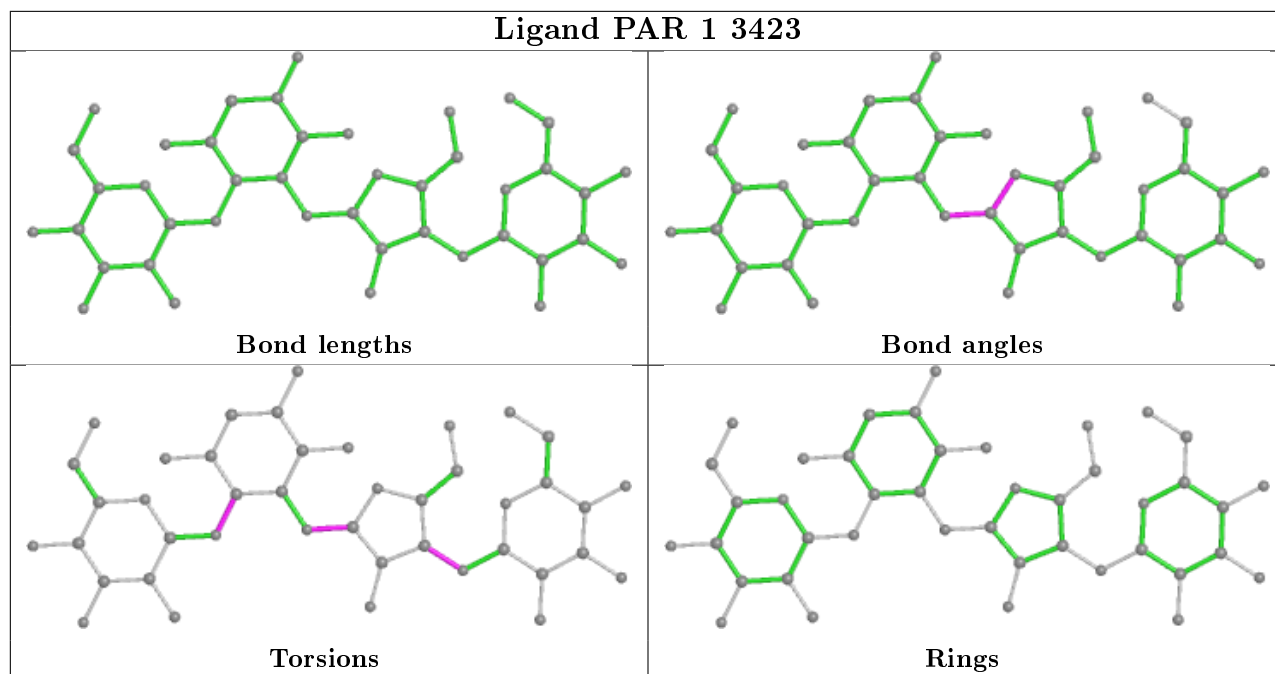


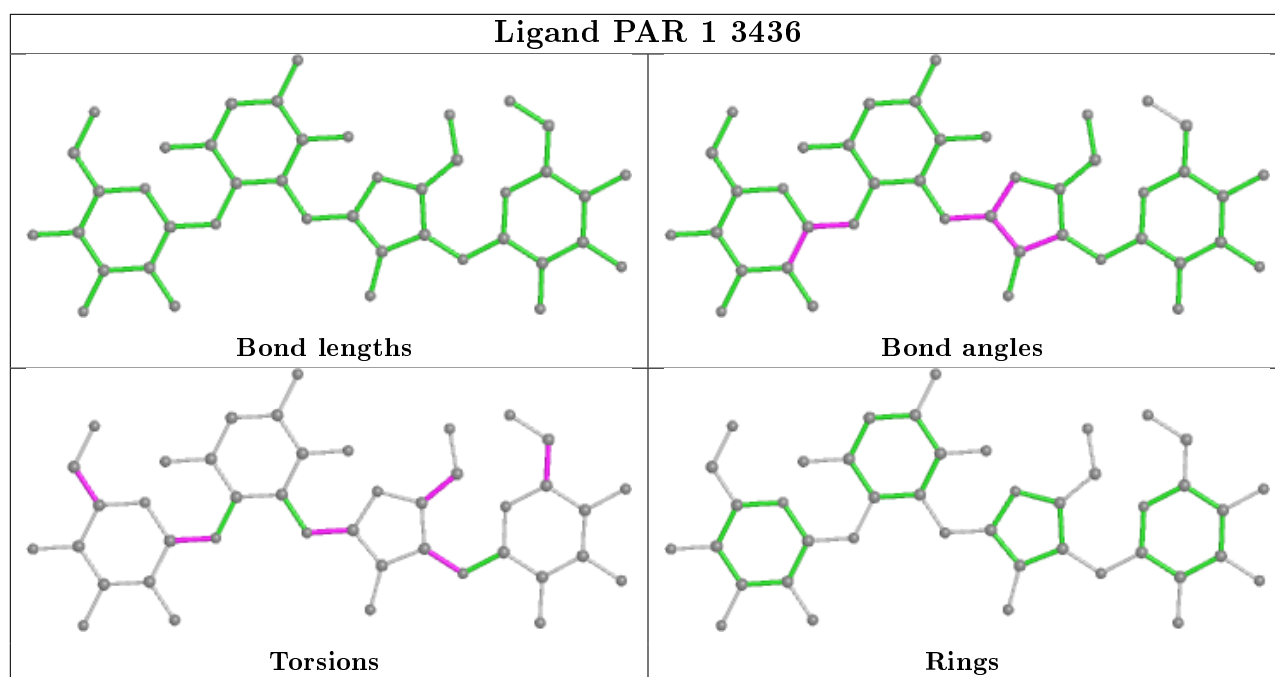
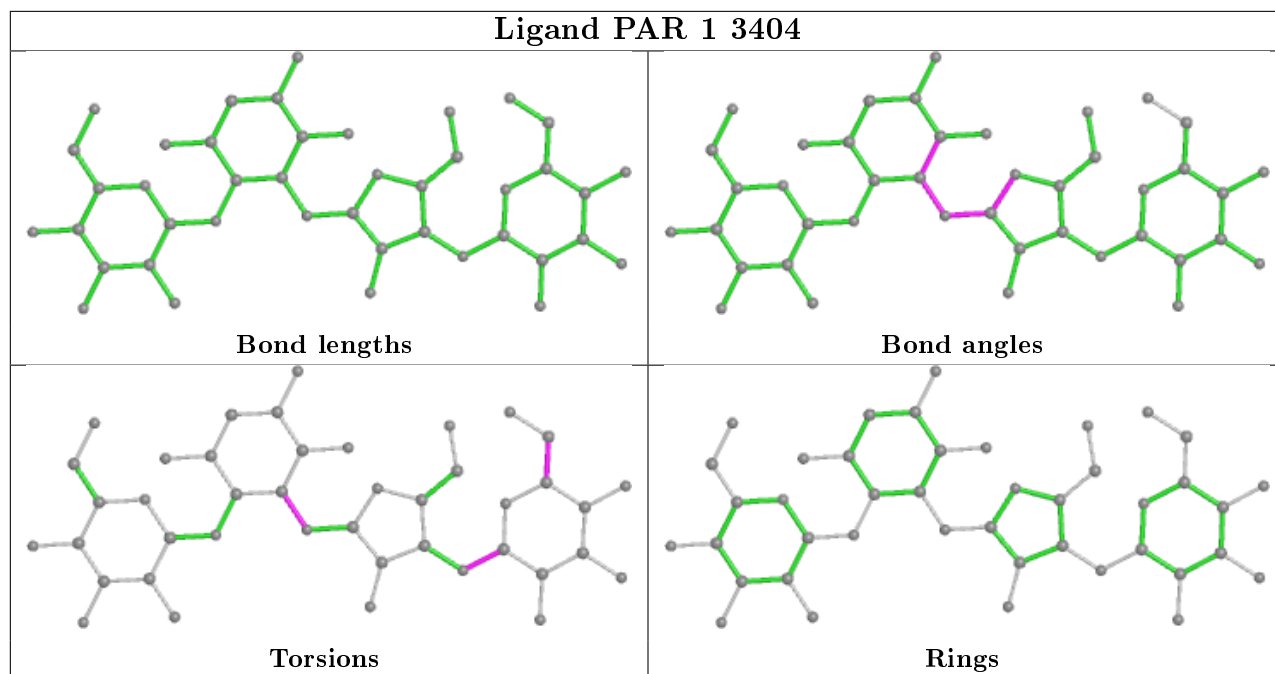


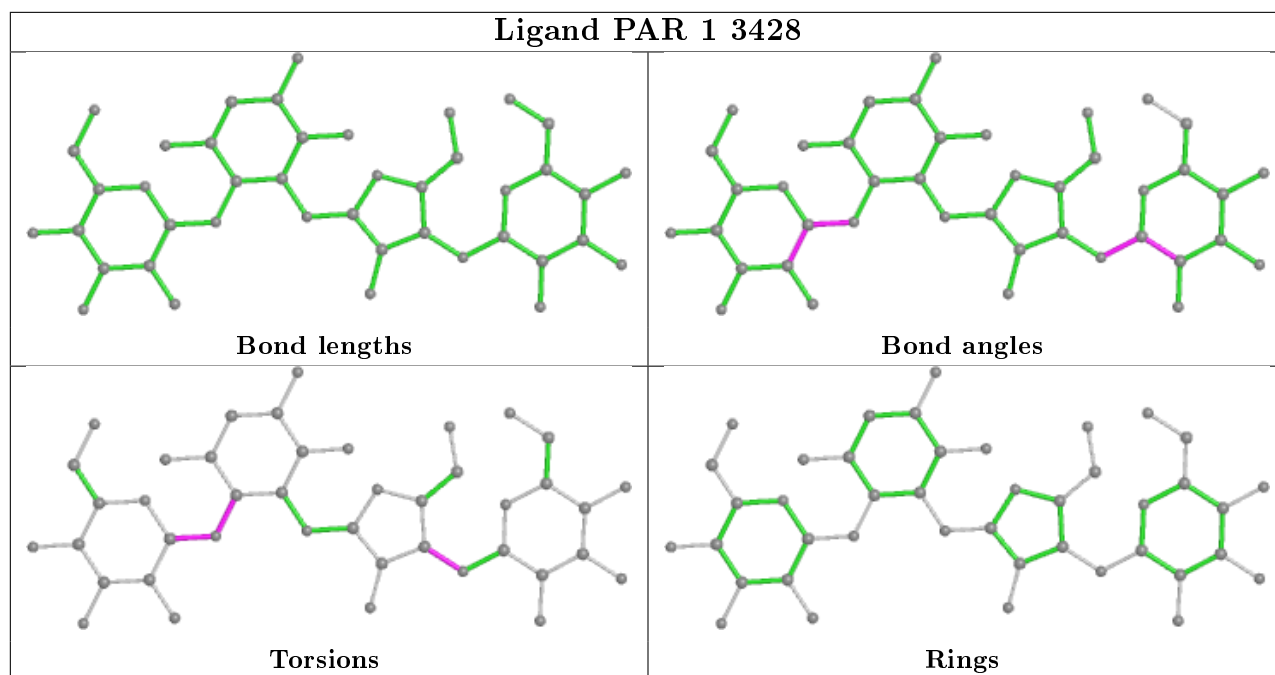
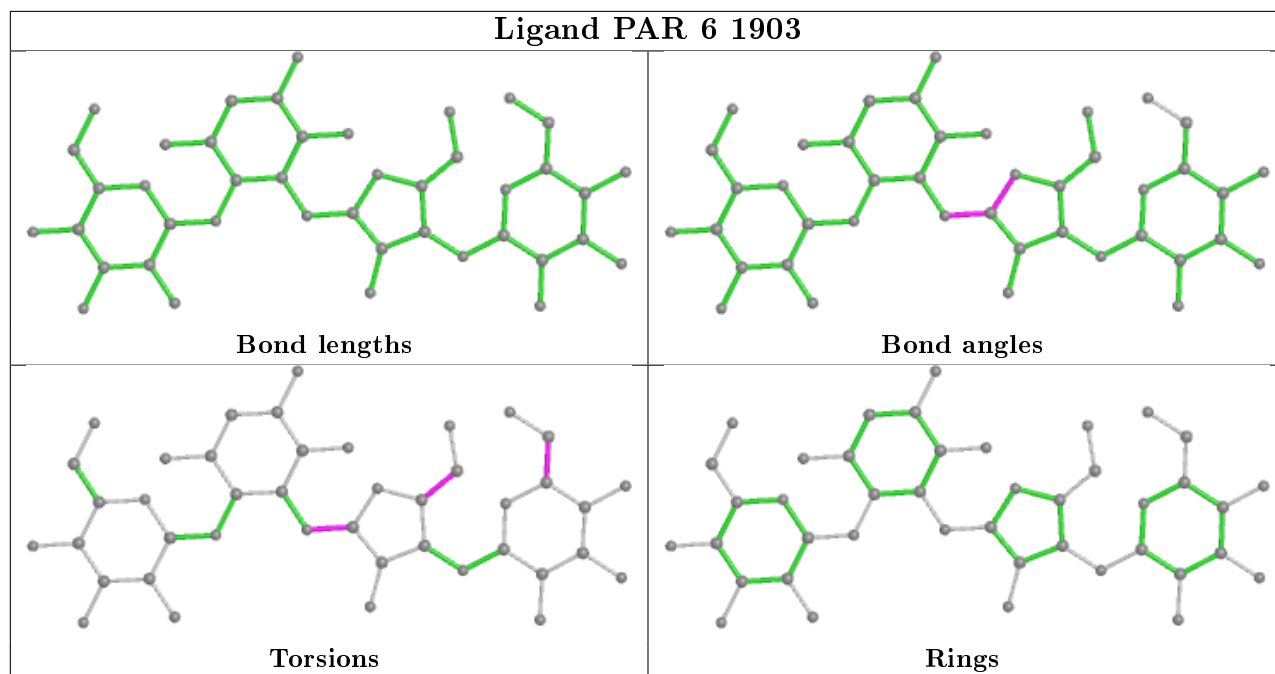


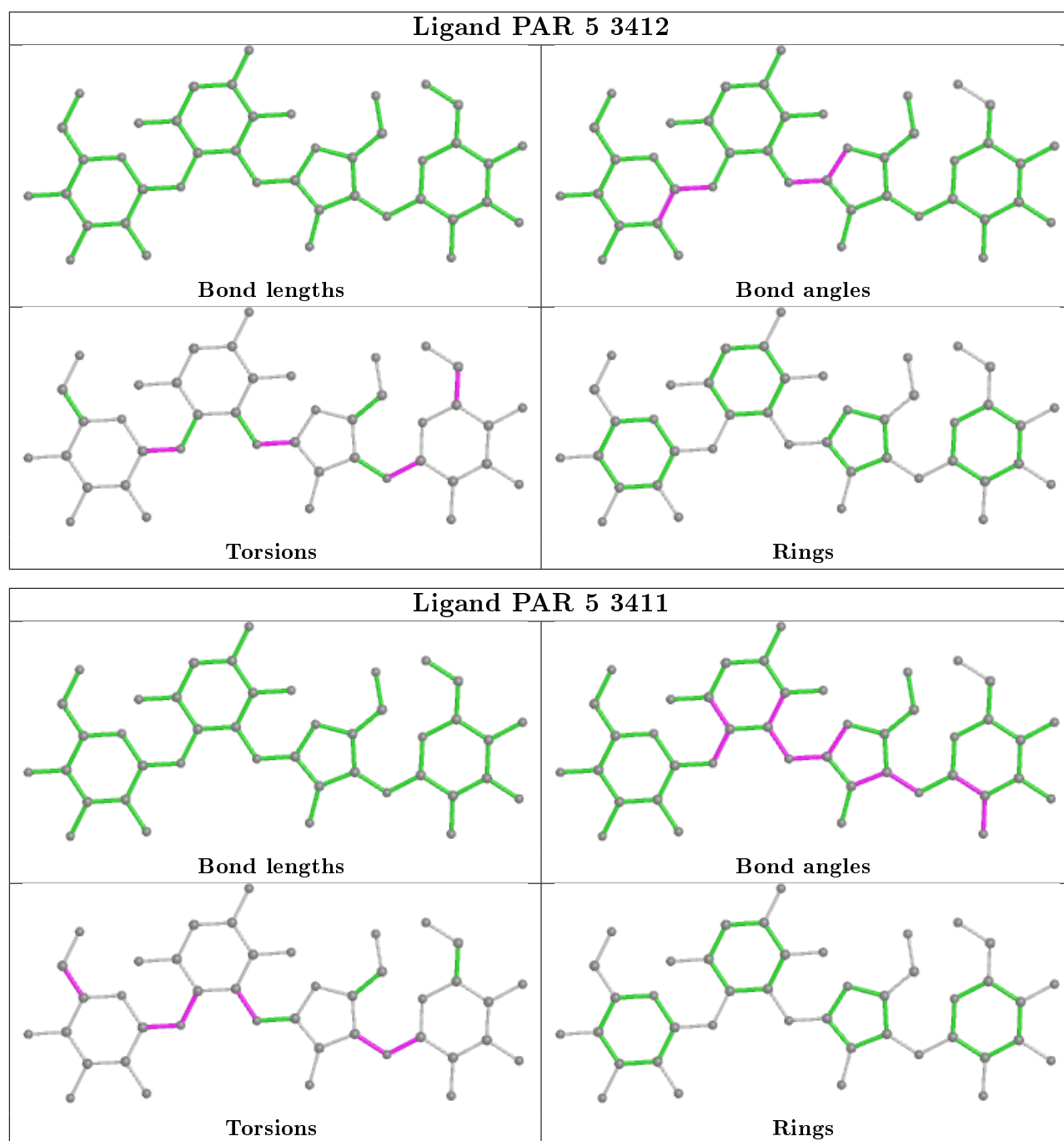












5.7 Other polymers [i](#)

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
78	sM	1
64	C8	1
5	l3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	51:ARG	C	52:PRO	N	1.62
1	C8	81:ILE	C	82:PRO	N	1.16
1	l3	168:LYS	C	169:THR	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	3078/3396 (90%)	0.18	9 (0%) 94 94	29, 61, 151, 275	0
1	5	3087/3396 (90%)	0.20	17 (0%) 89 90	36, 77, 179, 287	0
2	3	121/121 (100%)	0.00	0 100 100	49, 98, 117, 142	0
2	7	121/121 (100%)	-0.12	0 100 100	51, 115, 151, 169	0
3	4	157/158 (99%)	0.19	1 (0%) 89 90	36, 58, 138, 255	0
3	8	158/158 (100%)	0.17	2 (1%) 77 77	48, 90, 161, 264	0
4	L2	248/248 (100%)	0.33	2 (0%) 86 86	22, 47, 66, 101	0
4	12	248/248 (100%)	0.76	20 (8%) 12 11	49, 86, 120, 160	0
5	L3	386/386 (100%)	0.18	0 100 100	28, 69, 100, 156	0
5	13	386/386 (100%)	0.02	1 (0%) 94 94	26, 64, 92, 160	0
6	L4	361/361 (100%)	0.12	0 100 100	23, 65, 101, 156	0
6	14	361/361 (100%)	0.21	5 (1%) 75 75	32, 84, 121, 155	0
7	L5	293/296 (98%)	0.75	26 (8%) 9 10	72, 111, 149, 179	0
7	15	294/296 (99%)	0.89	38 (12%) 3 3	81, 139, 182, 214	0
8	L6	156/176 (88%)	0.05	1 (0%) 89 90	47, 76, 109, 146	0
8	16	157/176 (89%)	0.35	5 (3%) 47 46	55, 81, 127, 162	0
9	L7	226/226 (100%)	0.07	0 100 100	37, 63, 117, 200	0
9	17	223/226 (98%)	0.11	0 100 100	43, 70, 123, 195	0
10	L8	231/231 (100%)	0.60	5 (2%) 62 60	48, 83, 139, 171	0
10	18	231/231 (100%)	0.92	41 (17%) 1 1	93, 143, 197, 244	0
11	L9	189/191 (98%)	0.80	19 (10%) 7 6	56, 87, 120, 156	0
11	19	191/191 (100%)	0.38	3 (1%) 72 70	52, 77, 100, 189	0
12	M0	217/221 (98%)	0.67	19 (8%) 10 10	47, 83, 141, 196	0
12	m0	219/221 (99%)	0.67	14 (6%) 19 19	49, 76, 148, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M1	169/169 (100%)	1.02	29 (17%) 1 1	86, 113, 147, 170	0
13	m1	169/169 (100%)	1.01	28 (16%) 1 2	101, 142, 176, 196	0
14	M3	193/194 (99%)	0.38	7 (3%) 42 40	33, 75, 134, 214	0
14	m3	194/194 (100%)	0.44	8 (4%) 37 35	61, 120, 172, 211	0
15	M4	136/137 (99%)	0.33	4 (2%) 51 50	52, 78, 107, 152	0
15	m4	137/137 (100%)	0.14	1 (0%) 87 88	51, 77, 124, 152	0
16	M5	203/203 (100%)	0.37	3 (1%) 73 72	26, 50, 67, 80	0
16	m5	203/203 (100%)	0.85	14 (6%) 16 16	62, 96, 123, 139	0
17	M6	197/197 (100%)	0.33	1 (0%) 91 91	36, 57, 97, 118	0
17	m6	197/197 (100%)	-0.01	0 100 100	35, 54, 107, 138	0
18	M7	175/184 (95%)	0.43	12 (6%) 16 16	30, 52, 139, 184	0
18	m7	155/184 (84%)	0.12	0 100 100	39, 55, 86, 143	0
19	M8	185/185 (100%)	0.26	2 (1%) 80 81	43, 65, 91, 111	0
19	m8	185/185 (100%)	0.48	10 (5%) 25 24	53, 93, 121, 143	0
20	M9	185/188 (98%)	0.26	0 100 100	45, 72, 158, 199	0
20	m9	188/188 (100%)	0.54	15 (7%) 12 11	50, 83, 212, 255	0
21	N0	172/172 (100%)	0.68	7 (4%) 37 35	51, 72, 105, 144	0
21	n0	172/172 (100%)	0.40	0 100 100	45, 71, 101, 139	0
22	N1	159/159 (100%)	0.54	4 (2%) 57 54	45, 74, 130, 198	0
22	n1	159/159 (100%)	1.10	32 (20%) 1 1	62, 90, 155, 204	0
23	N2	99/99 (100%)	0.32	3 (3%) 50 49	77, 110, 147, 168	0
23	n2	98/99 (98%)	0.76	8 (8%) 11 11	85, 120, 146, 169	0
24	N3	132/136 (97%)	0.20	0 100 100	38, 66, 93, 155	0
24	n3	136/136 (100%)	0.28	2 (1%) 73 72	33, 58, 98, 150	0
25	N4	63/155 (40%)	0.55	1 (1%) 72 70	52, 74, 98, 121	0
25	n4	135/155 (87%)	1.53	44 (32%) 0 0	44, 140, 224, 256	0
26	N5	118/120 (98%)	0.40	1 (0%) 86 86	42, 62, 91, 116	0
26	n5	120/120 (100%)	1.01	16 (13%) 3 3	59, 95, 135, 176	0
27	N6	125/125 (100%)	0.73	12 (9%) 8 8	34, 71, 101, 131	0
27	n6	123/125 (98%)	0.50	7 (5%) 23 23	55, 85, 123, 139	0
28	N7	135/135 (100%)	0.82	9 (6%) 17 17	57, 84, 115, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	n7	135/135 (100%)	1.80	50 (37%) 0 0	99, 133, 175, 194	0
29	N8	148/148 (100%)	0.64	12 (8%) 12 11	27, 63, 117, 156	0
29	n8	148/148 (100%)	0.83	21 (14%) 2 2	34, 104, 145, 167	0
30	N9	56/58 (96%)	0.57	3 (5%) 25 24	34, 81, 137, 171	0
30	n9	58/58 (100%)	0.75	6 (10%) 6 6	53, 112, 157, 189	0
31	O0	97/100 (97%)	0.70	3 (3%) 49 48	51, 76, 110, 145	0
31	o0	100/100 (100%)	0.16	3 (3%) 50 49	82, 117, 167, 201	0
32	O1	106/112 (94%)	1.14	16 (15%) 2 2	50, 77, 130, 149	0
32	o1	109/112 (97%)	0.53	2 (1%) 68 67	43, 75, 137, 178	0
33	O2	125/127 (98%)	0.23	1 (0%) 86 86	29, 55, 78, 114	0
33	o2	127/127 (100%)	0.32	3 (2%) 59 56	35, 65, 92, 147	0
34	O3	106/106 (100%)	0.18	1 (0%) 84 84	37, 55, 95, 133	0
34	o3	106/106 (100%)	0.31	2 (1%) 66 65	37, 59, 106, 127	0
35	O4	112/112 (100%)	0.66	5 (4%) 33 32	41, 61, 123, 175	0
35	o4	112/112 (100%)	0.97	16 (14%) 2 2	60, 96, 167, 193	0
36	O5	119/119 (100%)	0.41	2 (1%) 70 68	42, 75, 107, 130	0
36	o5	119/119 (100%)	0.81	15 (12%) 3 3	78, 108, 138, 167	0
37	O6	97/99 (97%)	0.26	0 100 100	51, 75, 108, 125	0
37	o6	99/99 (100%)	1.37	25 (25%) 0 0	95, 131, 170, 205	0
38	O7	84/87 (96%)	0.10	0 100 100	29, 43, 76, 102	0
38	o7	87/87 (100%)	0.54	4 (4%) 32 30	37, 71, 122, 180	0
39	O8	77/77 (100%)	0.55	5 (6%) 18 18	63, 94, 148, 185	0
39	o8	77/77 (100%)	1.09	12 (15%) 2 2	87, 121, 154, 182	0
40	O9	50/50 (100%)	0.41	0 100 100	37, 54, 77, 83	0
40	o9	50/50 (100%)	0.40	2 (4%) 38 36	57, 72, 95, 108	0
41	Q0	52/52 (100%)	1.14	8 (15%) 2 2	57, 76, 122, 133	0
41	q0	52/52 (100%)	0.46	2 (3%) 40 37	48, 62, 91, 122	0
42	Q1	25/25 (100%)	0.30	0 100 100	52, 66, 82, 94	0
42	q1	25/25 (100%)	0.19	0 100 100	61, 74, 90, 92	0
43	Q2	105/105 (100%)	0.90	17 (16%) 1 2	31, 66, 119, 192	0
43	q2	105/105 (100%)	0.73	9 (8%) 10 10	59, 102, 140, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	Q3	91/91 (100%)	0.09	0 100 100	33, 53, 85, 98	0
44	q3	91/91 (100%)	0.14	0 100 100	44, 83, 118, 135	0
45	2	1712/1800 (95%)	0.24	27 (1%) 72 70	55, 121, 223, 318	0
45	6	1683/1800 (93%)	0.20	23 (1%) 75 75	57, 119, 222, 300	0
46	S0	206/206 (100%)	1.14	44 (21%) 0 1	92, 133, 170, 223	0
46	s0	206/206 (100%)	1.00	35 (16%) 1 1	98, 140, 187, 229	0
47	S1	211/216 (97%)	1.47	64 (30%) 0 0	89, 142, 196, 244	0
47	s1	216/216 (100%)	1.55	65 (30%) 0 0	94, 145, 190, 236	0
48	S2	217/217 (100%)	0.72	25 (11%) 4 4	76, 119, 159, 170	0
48	s2	217/217 (100%)	1.31	53 (24%) 0 0	74, 120, 156, 179	0
49	S3	209/223 (93%)	1.00	34 (16%) 1 2	87, 131, 176, 214	0
49	s3	223/223 (100%)	1.67	75 (33%) 0 0	97, 140, 196, 224	0
50	S4	256/260 (98%)	1.67	89 (34%) 0 0	92, 137, 169, 240	0
50	s4	260/260 (100%)	0.99	38 (14%) 2 2	80, 125, 157, 209	0
51	S5	206/206 (100%)	2.79	127 (61%) 0 0	107, 158, 207, 239	0
51	s5	206/206 (100%)	1.56	66 (32%) 0 0	108, 156, 202, 234	0
52	S6	200/236 (84%)	1.03	42 (21%) 1 1	77, 138, 206, 301	0
53	S7	179/186 (96%)	0.86	27 (15%) 2 2	97, 147, 192, 216	0
53	s7	186/186 (100%)	1.00	34 (18%) 1 1	101, 162, 213, 267	0
54	S8	185/200 (92%)	1.03	28 (15%) 2 2	63, 106, 162, 218	0
54	s8	188/200 (94%)	0.85	20 (10%) 6 6	65, 104, 156, 206	0
55	S9	174/185 (94%)	1.31	38 (21%) 0 1	98, 145, 187, 217	0
55	s9	185/185 (100%)	1.23	45 (24%) 0 0	93, 130, 177, 209	0
56	C0	90/105 (85%)	0.64	10 (11%) 5 5	120, 153, 193, 210	0
56	c0	96/105 (91%)	1.33	31 (32%) 0 0	119, 171, 207, 261	0
57	C1	139/146 (95%)	1.01	14 (10%) 7 6	68, 98, 146, 171	0
57	c1	146/146 (100%)	0.88	17 (11%) 4 4	70, 96, 165, 231	0
58	C2	102/143 (71%)	1.90	33 (32%) 0 0	147, 210, 256, 296	0
58	c2	124/143 (86%)	1.85	54 (43%) 0 0	170, 230, 275, 291	0
59	C3	150/150 (100%)	0.77	16 (10%) 6 5	65, 107, 140, 180	0
59	c3	150/150 (100%)	0.32	9 (6%) 21 21	78, 127, 170, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	C4	127/128 (99%)	0.34	7 (5%) 25 23	71, 133, 184, 207	0
60	c4	128/128 (100%)	1.19	31 (24%) 0 0	77, 138, 177, 239	0
61	C5	116/141 (82%)	1.15	24 (20%) 1 1	97, 149, 199, 225	0
61	c5	135/141 (95%)	2.29	65 (48%) 0 0	111, 152, 206, 244	0
62	C6	136/142 (95%)	2.90	92 (67%) 0 0	88, 160, 201, 253	0
62	c6	142/142 (100%)	2.64	88 (61%) 0 0	98, 160, 210, 264	0
63	C7	115/136 (84%)	1.68	41 (35%) 0 0	109, 149, 191, 223	0
63	c7	117/136 (86%)	1.02	18 (15%) 2 2	104, 152, 200, 226	0
64	C8	143/145 (98%)	1.40	39 (27%) 0 0	104, 163, 211, 244	0
64	c8	145/145 (100%)	1.48	47 (32%) 0 0	103, 149, 197, 217	0
65	C9	137/143 (95%)	1.76	47 (34%) 0 0	104, 168, 206, 231	0
65	c9	143/143 (100%)	1.48	41 (28%) 0 0	117, 170, 215, 240	0
66	D0	102/109 (93%)	1.57	35 (34%) 0 0	92, 163, 218, 276	0
66	d0	109/109 (100%)	1.20	26 (23%) 0 0	91, 159, 218, 265	0
67	D1	87/87 (100%)	0.99	16 (18%) 1 1	101, 130, 167, 213	0
67	d1	87/87 (100%)	0.88	12 (13%) 2 2	101, 131, 176, 206	0
68	D2	129/129 (100%)	1.47	42 (32%) 0 0	73, 110, 134, 165	0
68	d2	129/129 (100%)	0.92	18 (13%) 2 2	85, 111, 133, 175	0
69	D3	144/144 (100%)	0.52	1 (0%) 87 88	63, 86, 109, 154	0
69	d3	144/144 (100%)	0.53	7 (4%) 29 27	61, 86, 107, 141	0
70	D4	134/134 (100%)	1.06	29 (21%) 0 1	106, 155, 191, 221	0
70	d4	134/134 (100%)	1.05	23 (17%) 1 1	100, 140, 175, 195	0
71	D5	70/70 (100%)	2.78	43 (61%) 0 0	137, 193, 229, 237	0
71	d5	69/70 (98%)	1.95	30 (43%) 0 0	131, 174, 211, 238	0
72	D6	97/97 (100%)	0.48	3 (3%) 49 48	67, 105, 176, 218	0
72	d6	97/97 (100%)	1.05	13 (13%) 3 3	79, 111, 173, 203	0
73	D7	81/81 (100%)	1.08	14 (17%) 1 1	84, 127, 181, 205	0
73	d7	81/81 (100%)	0.69	12 (14%) 2 2	96, 147, 202, 227	0
74	D8	63/63 (100%)	1.76	25 (39%) 0 0	114, 146, 173, 198	0
74	d8	63/63 (100%)	2.64	36 (57%) 0 0	110, 163, 192, 218	0
75	D9	53/53 (100%)	1.41	16 (30%) 0 0	101, 121, 151, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	d9	53/53 (100%)	0.68	6 (11%) 5 5	106, 127, 150, 180	0
76	E0	60/62 (96%)	1.47	18 (30%) 0 0	76, 140, 183, 197	0
76	e0	62/62 (100%)	1.52	15 (24%) 0 0	74, 133, 181, 208	0
77	SR	317/318 (99%)	2.50	184 (58%) 0 0	137, 198, 248, 295	0
77	sR	318/318 (100%)	2.42	171 (53%) 0 0	136, 194, 243, 296	0
78	SM	147/272 (54%)	1.18	30 (20%) 1 1	74, 137, 205, 240	0
78	sM	95/272 (34%)	1.29	24 (25%) 0 0	99, 146, 191, 217	0
79	s6	218/218 (100%)	1.82	84 (38%) 0 0	75, 136, 176, 211	0
All	All	32255/33922 (95%)	0.67	3409 (10%) 6 6	22, 100, 194, 318	0

All (3409) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
76	e0	63	GLN	14.3
51	S5	152	GLY	13.9
51	S5	71	ALA	13.9
51	S5	151	GLY	12.3
51	S5	70	VAL	11.1
77	SR	79	TYR	10.9
78	SM	141	ALA	10.8
77	SR	244	ALA	10.2
12	m0	104	SER	9.9
62	c6	6	SER	9.9
62	c6	60	PHE	9.7
53	s7	3	ALA	9.6
77	sR	50	ASP	9.3
78	SM	16	ASP	9.3
77	SR	121	MET	9.2
61	c5	134	THR	9.1
12	m0	105	CYS	9.1
48	s2	93	GLY	9.1
77	SR	81	LEU	8.7
48	s2	92	ALA	8.7
58	c2	110	GLY	8.6
58	c2	111	ASN	8.5
58	C2	63	VAL	8.4
25	n4	131	ALA	8.4
65	c9	3	GLY	8.4
37	o6	98	ARG	8.4

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Mol	Chain	Res	Type	RSRZ
58	C2	82	PRO	8.3
45	2	134	U	8.2
77	sR	158	PRO	8.2
45	2	135	A	8.1
77	sR	51	ASP	8.1
57	c1	2	SER	8.0
77	SR	80	ALA	8.0
76	E0	61	SER	7.9
47	s1	92	GLN	7.9
77	sR	214	ALA	7.9
47	S1	91	VAL	7.8
65	c9	2	PRO	7.7
47	s1	100	PHE	7.7
47	s1	84	ILE	7.6
77	sR	16	HIS	7.6
77	sR	157	VAL	7.6
77	sR	311	ARG	7.6
77	SR	253	ALA	7.6
61	c5	135	THR	7.5
77	SR	211	ILE	7.4
50	S4	47	PHE	7.4
25	n4	132	GLY	7.3
77	SR	73	LEU	7.2
61	c5	136	SER	7.2
53	s7	2	SER	7.1
62	c6	51	PRO	7.1
38	o7	87	SER	7.1
77	sR	5	GLU	7.0
79	s6	158	ILE	7.0
51	S5	20	PHE	7.0
60	c4	14	PHE	6.9
55	S9	147	MET	6.9
74	d8	54	LEU	6.9
62	C6	41	PRO	6.9
51	S5	119	ASP	6.9
77	sR	55	GLY	6.9
76	e0	62	VAL	6.8
61	c5	119	PHE	6.8
50	s4	261	LEU	6.8
70	D4	7	ILE	6.8
74	d8	55	VAL	6.8
25	n4	135	SER	6.8

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Mol	Chain	Res	Type	RSRZ
61	c5	138	PHE	6.8
65	c9	4	VAL	6.8
58	C2	61	VAL	6.7
77	sR	253	ALA	6.7
76	E0	48	THR	6.7
62	c6	83	GLN	6.7
47	S1	92	GLN	6.7
58	c2	112	ALA	6.6
62	c6	7	VAL	6.6
70	D4	2	SER	6.5
77	SR	122	ILE	6.5
62	C6	65	ILE	6.5
74	d8	65	ARG	6.5
77	SR	115	ILE	6.4
62	C6	66	ARG	6.4
53	s7	7	LYS	6.4
77	sR	34	LEU	6.4
51	S5	54	LYS	6.4
18	M7	177	ALA	6.4
51	S5	32	GLU	6.4
62	C6	52	LEU	6.3
77	SR	72	THR	6.3
62	c6	12	LYS	6.3
61	c5	133	ALA	6.3
66	d0	84	MET	6.3
79	s6	156	PHE	6.3
47	S1	217	LEU	6.3
77	SR	225	LEU	6.2
61	c5	112	LEU	6.2
47	s1	139	ALA	6.2
77	sR	15	GLY	6.2
41	Q0	77	ILE	6.2
56	c0	96	ASN	6.2
77	SR	210	LEU	6.2
62	C6	29	ILE	6.2
51	S5	170	GLN	6.2
58	C2	62	LEU	6.2
79	s6	157	VAL	6.2
49	s3	184	ILE	6.1
76	e0	2	ALA	6.1
53	s7	5	GLN	6.1
74	d8	53	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
47	s1	235	GLY	6.1
25	n4	64	THR	6.1
65	c9	18	TYR	6.1
78	SM	17	VAL	6.1
53	s7	63	PRO	6.1
21	N0	1	MET	6.1
58	C2	60	VAL	6.0
77	SR	119	ALA	6.0
77	sR	167	VAL	6.0
77	sR	204	ALA	6.0
62	C6	40	GLU	6.0
77	sR	244	ALA	6.0
77	sR	252	LEU	6.0
77	sR	168	THR	6.0
77	sR	295	SER	6.0
62	c6	66	ARG	6.0
77	sR	293	ALA	5.9
77	sR	300	THR	5.9
64	C8	47	CYS	5.9
7	l5	185	PHE	5.9
78	sM	53	ARG	5.9
51	S5	184	PHE	5.9
50	s4	229	GLY	5.9
61	c5	105	VAL	5.9
78	sM	52	PRO	5.9
78	SM	18	VAL	5.8
77	sR	24	ALA	5.8
70	d4	135	ASP	5.8
71	D5	91	PRO	5.8
18	M7	169	THR	5.8
72	d6	40	ALA	5.8
77	SR	284	ALA	5.8
78	SM	88	ARG	5.8
61	c5	137	ARG	5.8
7	L5	154	THR	5.7
55	s9	2	PRO	5.7
29	n8	79	TRP	5.7
51	S5	78	ALA	5.7
61	c5	104	GLN	5.7
46	s0	36	TYR	5.7
77	SR	74	THR	5.6
7	L5	4	GLN	5.6

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Mol	Chain	Res	Type	RSRZ
62	C6	117	LEU	5.6
77	sR	301	LEU	5.6
74	d8	48	VAL	5.6
47	s1	102	GLY	5.6
51	S5	72	HIS	5.6
77	sR	299	GLN	5.6
77	SR	134	TRP	5.6
71	D5	60	VAL	5.6
50	S4	103	TYR	5.6
45	2	194	U	5.6
52	S6	80	ASN	5.6
51	S5	51	VAL	5.6
74	d8	28	VAL	5.6
71	D5	36	ALA	5.6
62	C6	28	LEU	5.6
50	S4	54	TYR	5.5
74	d8	27	GLN	5.5
56	c0	97	PRO	5.5
62	C6	10	PHE	5.5
65	C9	143	ASP	5.5
70	D4	72	PHE	5.5
77	sR	3	SER	5.5
62	C6	21	HIS	5.5
78	sM	61	ILE	5.5
56	c0	98	THR	5.5
61	c5	75	PRO	5.5
10	l8	49	TYR	5.5
46	S0	201	LEU	5.5
51	S5	90	ILE	5.5
71	D5	41	ILE	5.5
71	D5	80	LEU	5.5
77	sR	183	LEU	5.5
78	sM	60	ALA	5.5
62	c6	22	VAL	5.4
62	c6	29	ILE	5.4
64	c8	22	VAL	5.4
28	n7	136	PHE	5.4
51	s5	71	ALA	5.4
45	2	1361	U	5.4
58	c2	102	GLY	5.4
51	s5	31	GLU	5.4
77	sR	319	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
77	sR	33	LEU	5.4
25	n4	97	LYS	5.4
50	S4	190	GLY	5.4
64	C8	53	ASP	5.4
74	d8	67	ARG	5.4
56	c0	20	VAL	5.4
79	s6	169	TYR	5.4
48	s2	95	ARG	5.4
71	D5	102	THR	5.4
55	S9	148	VAL	5.3
77	SR	120	SER	5.3
58	c2	31	VAL	5.3
48	s2	89	GLN	5.3
49	s3	48	VAL	5.3
64	c8	146	ALA	5.3
61	c5	93	VAL	5.3
77	SR	181	TRP	5.3
77	sR	159	ASN	5.3
25	n4	134	GLN	5.3
77	sR	6	VAL	5.3
79	s6	147	LEU	5.3
79	s6	145	PHE	5.2
38	o7	88	ALA	5.2
49	s3	186	VAL	5.2
77	sR	315	VAL	5.2
51	S5	21	THR	5.2
71	D5	59	TYR	5.2
49	s3	188	ILE	5.2
65	c9	10	ALA	5.2
62	C6	12	LYS	5.2
31	o0	7	GLN	5.2
47	s1	223	PHE	5.2
71	D5	71	ILE	5.2
62	c6	89	LEU	5.2
58	C2	59	LEU	5.2
51	S5	190	ILE	5.2
4	l2	249	SER	5.2
64	c8	73	MET	5.2
55	S9	6	ARG	5.2
74	d8	26	THR	5.2
77	SR	252	LEU	5.2
47	s1	90	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
51	S5	153	GLY	5.2
77	SR	26	SER	5.1
62	C6	22	VAL	5.1
61	C5	87	PRO	5.1
62	C6	26	LYS	5.1
64	c8	131	LEU	5.1
11	l9	190	ASP	5.1
77	sR	245	PHE	5.1
47	s1	103	MET	5.1
49	s3	150	MET	5.1
77	SR	168	THR	5.1
60	c4	15	GLY	5.1
62	C6	7	VAL	5.1
53	s7	6	ALA	5.1
71	d5	101	TYR	5.1
10	l8	200	LEU	5.1
49	s3	30	ALA	5.1
62	C6	138	PHE	5.1
51	S5	25	LEU	5.1
53	s7	70	PHE	5.1
74	d8	29	ARG	5.1
51	S5	93	LEU	5.1
36	O5	120	ALA	5.1
62	C6	11	GLY	5.1
58	C2	93	ASP	5.0
77	SR	83	ALA	5.0
49	S3	170	THR	5.0
62	C6	42	GLU	5.0
71	D5	97	LYS	5.0
43	Q2	104	LEU	5.0
51	s5	152	GLY	5.0
77	sR	7	LEU	5.0
77	sR	211	ILE	5.0
78	SM	19	VAL	5.0
20	m9	185	LEU	5.0
77	SR	116	ASP	5.0
53	s7	8	ILE	5.0
61	c5	78	THR	5.0
79	s6	22	HIS	5.0
61	c5	121	ILE	5.0
50	S4	123	LEU	5.0
47	s1	101	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
65	C9	108	LEU	5.0
46	S0	20	ALA	5.0
64	c8	21	ASN	5.0
79	s6	141	ILE	5.0
63	C7	70	SER	5.0
63	C7	71	PHE	5.0
70	d4	25	VAL	5.0
60	c4	98	GLY	5.0
51	S5	62	VAL	5.0
51	s5	70	VAL	5.0
62	C6	36	ILE	5.0
47	s1	227	ALA	4.9
55	s9	80	LEU	4.9
62	c6	127	LYS	4.9
62	C6	20	ALA	4.9
58	c2	32	LEU	4.9
1	5	1350	A	4.9
63	C7	21	TYR	4.9
58	C2	28	LEU	4.9
37	o6	97	SER	4.9
51	S5	24	VAL	4.9
66	D0	21	LYS	4.9
66	D0	91	ILE	4.9
79	s6	1	MET	4.9
62	c6	27	GLY	4.9
47	s1	48	VAL	4.9
70	d4	119	PHE	4.9
77	SR	302	PHE	4.9
53	S7	47	ARG	4.9
77	SR	141	LEU	4.9
78	sM	57	ASN	4.9
37	o6	79	SER	4.9
71	D5	104	ALA	4.9
72	d6	39	MET	4.9
48	s2	90	THR	4.9
77	SR	183	LEU	4.9
58	C2	42	ALA	4.9
77	sR	4	ASN	4.9
65	c9	55	TYR	4.9
77	SR	32	LEU	4.8
70	d4	74	LEU	4.8
77	SR	314	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
13	m1	104	PHE	4.8
61	c5	103	ASN	4.8
77	sR	294	TRP	4.8
68	D2	108	ALA	4.8
64	c8	15	LEU	4.8
61	c5	132	GLY	4.8
47	S1	87	ARG	4.8
58	c2	33	ARG	4.8
77	sR	62	LYS	4.8
12	m0	106	ALA	4.8
14	M3	135	ALA	4.8
50	S4	188	ASN	4.8
77	SR	227	ALA	4.8
74	d8	66	LEU	4.8
47	S1	101	HIS	4.8
51	s5	100	ASN	4.8
51	S5	77	TYR	4.8
47	S1	61	LEU	4.8
74	D8	67	ARG	4.7
77	SR	124	SER	4.7
50	S4	100	ARG	4.7
51	S5	33	VAL	4.7
77	sR	121	MET	4.7
78	SM	84	LYS	4.7
71	D5	101	TYR	4.7
61	c5	102	PHE	4.7
45	2	1360	A	4.7
71	D5	103	ARG	4.7
57	c1	3	THR	4.7
47	S1	96	LEU	4.7
77	sR	52	GLN	4.7
78	SM	86	ASN	4.7
79	s6	131	LYS	4.7
77	sR	144	LEU	4.7
62	c6	141	SER	4.7
28	n7	92	PHE	4.7
47	s1	91	VAL	4.7
49	S3	184	ILE	4.7
65	c9	9	VAL	4.7
20	m9	187	GLU	4.7
55	s9	134	ILE	4.7
65	c9	14	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
75	D9	54	LYS	4.7
46	S0	28	ASN	4.7
58	c2	84	ASN	4.7
64	C8	32	LEU	4.7
25	n4	98	PRO	4.7
62	C6	87	LYS	4.7
1	5	1349	G	4.7
62	C6	57	LEU	4.7
56	c0	25	LYS	4.7
65	C9	124	ILE	4.6
61	c5	116	LEU	4.6
52	S6	36	VAL	4.6
71	d5	54	VAL	4.6
29	n8	102	ILE	4.6
25	n4	67	VAL	4.6
63	c7	2	GLY	4.6
51	S5	48	PHE	4.6
77	sR	220	ILE	4.6
49	s3	178	ARG	4.6
71	D5	69	LEU	4.6
71	D5	100	ILE	4.6
51	S5	37	GLN	4.6
77	sR	302	PHE	4.6
77	sR	292	LEU	4.6
45	6	226	A	4.6
77	SR	185	GLN	4.6
47	s1	73	LEU	4.6
49	s3	53	THR	4.6
62	c6	9	THR	4.6
74	D8	24	GLY	4.6
51	S5	199	ILE	4.6
62	C6	24	ALA	4.6
47	S1	97	LEU	4.6
25	n4	100	VAL	4.6
77	SR	123	ILE	4.5
77	sR	71	CYS	4.5
25	n4	65	GLU	4.5
64	c8	129	TRP	4.5
77	sR	56	VAL	4.5
37	o6	2	THR	4.5
62	c6	28	LEU	4.5
68	D2	69	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
77	SR	172	ALA	4.5
77	SR	254	ALA	4.5
79	s6	155	ASP	4.5
58	c2	88	LEU	4.5
71	D5	93	SER	4.5
51	S5	69	PHE	4.5
77	sR	191	ASP	4.5
62	c6	116	LEU	4.5
79	s6	108	VAL	4.5
78	SM	15	ALA	4.5
63	C7	55	THR	4.5
1	5	1353	U	4.5
45	6	238	U	4.5
79	s6	142	ARG	4.5
77	SR	25	THR	4.5
76	E0	45	VAL	4.5
77	sR	257	ALA	4.5
53	S7	48	GLU	4.5
46	s0	33	GLN	4.5
61	c5	111	MET	4.5
62	c6	114	ARG	4.4
64	c8	16	ARG	4.4
70	d4	26	ASP	4.4
62	C6	85	ILE	4.4
77	sR	63	GLY	4.4
50	S4	219	VAL	4.4
77	SR	62	LYS	4.4
77	SR	118	LYS	4.4
58	c2	37	VAL	4.4
74	d8	14	LYS	4.4
51	S5	47	SER	4.4
51	S5	118	LEU	4.4
46	S0	107	PHE	4.4
56	c0	65	TYR	4.4
71	d5	41	ILE	4.4
55	S9	133	HIS	4.4
53	s7	43	PHE	4.4
64	C8	98	TYR	4.4
78	sM	62	ARG	4.4
77	SR	91	LEU	4.4
77	SR	226	ALA	4.4
79	s6	143	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
58	C2	91	VAL	4.4
51	S5	50	GLU	4.4
51	S5	100	ASN	4.4
55	s9	156	ILE	4.4
7	L5	5	LYS	4.4
71	D5	42	LEU	4.3
50	S4	191	ARG	4.3
79	s6	144	PHE	4.3
25	n4	81	PRO	4.3
49	s3	183	GLY	4.3
46	s0	107	PHE	4.3
54	S8	179	CYS	4.3
72	d6	41	ILE	4.3
78	sM	69	ARG	4.3
61	c5	79	HIS	4.3
49	s3	35	SER	4.3
77	SR	3	SER	4.3
65	C9	71	VAL	4.3
70	d4	18	LEU	4.3
49	s3	218	LEU	4.3
51	S5	108	LEU	4.3
70	d4	69	SER	4.3
7	L5	3	PHE	4.3
62	c6	93	HIS	4.3
20	m9	186	LYS	4.3
43	Q2	2	VAL	4.3
61	c5	95	GLY	4.3
62	C6	55	VAL	4.3
31	O0	105	ALA	4.3
77	SR	13	LEU	4.3
55	s9	148	VAL	4.3
49	s3	34	TYR	4.3
77	SR	313	TRP	4.3
29	N8	92	LYS	4.3
76	E0	36	LYS	4.3
70	d4	2	SER	4.3
71	d5	57	TYR	4.3
51	S5	175	LEU	4.3
47	S1	213	ARG	4.3
62	c6	86	ALA	4.3
65	C9	59	ALA	4.3
62	C6	79	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
77	sR	313	TRP	4.3
47	S1	60	ALA	4.3
52	S6	78	THR	4.2
62	c6	92	TYR	4.2
46	S0	57	LEU	4.2
62	C6	116	LEU	4.2
22	n1	67	VAL	4.2
71	d5	60	VAL	4.2
74	d8	44	VAL	4.2
62	c6	54	LEU	4.2
70	D4	22	GLN	4.2
62	c6	36	ILE	4.2
70	d4	27	VAL	4.2
28	n7	10	VAL	4.2
65	C9	88	VAL	4.2
77	sR	316	MET	4.2
48	s2	88	LYS	4.2
51	S5	155	ALA	4.2
48	s2	150	GLN	4.2
51	S5	130	ILE	4.2
51	S5	147	THR	4.2
77	sR	20	VAL	4.2
77	sR	251	TRP	4.2
48	s2	82	ASN	4.2
61	c5	77	ARG	4.2
79	s6	153	VAL	4.2
62	c6	85	ILE	4.2
77	SR	136	ILE	4.2
56	c0	57	THR	4.2
53	S7	142	TYR	4.2
49	s3	52	ALA	4.2
58	c2	41	LEU	4.2
61	c5	56	PHE	4.2
62	C6	39	VAL	4.2
58	c2	136	ILE	4.2
61	C5	85	ILE	4.2
56	c0	75	TYR	4.2
78	sM	55	SER	4.2
62	C6	81	ILE	4.2
71	D5	88	ILE	4.2
77	sR	262	VAL	4.2
62	C6	51	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
25	n4	75	THR	4.2
48	s2	94	GLN	4.1
70	d4	98	GLU	4.1
68	d2	101	TYR	4.1
66	D0	52	LYS	4.1
47	S1	98	THR	4.1
77	SR	7	LEU	4.1
50	s4	260	GLY	4.1
62	C6	49	TYR	4.1
62	C6	43	ILE	4.1
77	sR	263	PHE	4.1
46	s0	158	VAL	4.1
56	c0	21	VAL	4.1
77	SR	63	GLY	4.1
51	s5	68	ILE	4.1
10	l8	34	PHE	4.1
51	S5	179	ALA	4.1
77	SR	212	ALA	4.1
10	l8	118	GLU	4.1
56	c0	95	ARG	4.1
62	C6	60	PHE	4.1
79	s6	27	PHE	4.1
71	D5	40	VAL	4.1
13	m1	65	ILE	4.1
77	SR	82	SER	4.1
50	S4	65	LEU	4.1
61	c5	86	VAL	4.1
79	s6	91	GLU	4.1
45	2	136	C	4.1
46	S0	177	LEU	4.1
62	c6	35	PRO	4.1
60	c4	21	ALA	4.1
71	D5	99	ALA	4.1
61	c5	5	VAL	4.1
78	SM	61	ILE	4.1
49	s3	142	LEU	4.1
50	S4	101	LEU	4.1
51	S5	174	LEU	4.1
79	s6	178	LEU	4.1
68	d2	85	ASP	4.1
61	C5	61	ARG	4.1
47	s1	38	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
47	S1	211	HIS	4.1
25	n4	78	ALA	4.0
62	c6	132	LYS	4.0
66	D0	80	GLU	4.0
74	D8	19	THR	4.0
79	s6	34	GLN	4.0
65	C9	76	LEU	4.0
25	n4	133	THR	4.0
45	2	1362	U	4.0
77	sR	156	VAL	4.0
77	SR	165	ASP	4.0
77	SR	251	TRP	4.0
64	C8	6	GLN	4.0
77	SR	235	SER	4.0
49	s3	148	LYS	4.0
51	s5	20	PHE	4.0
50	S4	181	VAL	4.0
51	S5	181	GLU	4.0
62	C6	50	GLU	4.0
51	s5	150	GLY	4.0
65	c9	132	LEU	4.0
66	D0	64	LYS	4.0
47	S1	135	LEU	4.0
47	s1	55	LYS	4.0
73	d7	33	LEU	4.0
62	C6	92	TYR	4.0
66	d0	82	TYR	4.0
77	SR	186	PHE	4.0
49	S3	206	VAL	4.0
79	s6	90	GLY	4.0
1	5	1565	G	4.0
46	S0	50	VAL	4.0
60	c4	13	VAL	4.0
77	sR	280	GLY	4.0
51	s5	58	LEU	4.0
29	n8	124	ILE	4.0
62	C6	23	LYS	4.0
10	l8	117	ALA	4.0
64	c8	17	LEU	4.0
53	s7	92	PHE	4.0
25	n4	130	SER	4.0
18	M7	167	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
51	S5	156	ARG	4.0
48	s2	87	GLN	4.0
46	S0	54	TRP	4.0
51	S5	133	VAL	4.0
65	c9	58	ALA	4.0
64	C8	46	VAL	3.9
50	S4	124	GLY	3.9
66	d0	63	LEU	3.9
47	s1	229	MET	3.9
70	D4	68	LYS	3.9
47	s1	123	ALA	3.9
61	c5	54	ALA	3.9
74	d8	13	ILE	3.9
77	sR	291	SER	3.9
45	2	132	U	3.9
70	D4	70	VAL	3.9
73	D7	68	GLY	3.9
53	s7	11	GLN	3.9
55	S9	128	LEU	3.9
7	L5	231	ILE	3.9
13	m1	106	ILE	3.9
55	S9	134	ILE	3.9
61	c5	125	PRO	3.9
65	C9	135	ILE	3.9
66	D0	65	ILE	3.9
77	sR	279	ALA	3.9
51	S5	145	ASP	3.9
66	D0	53	LYS	3.9
55	S9	156	ILE	3.9
61	C5	130	ARG	3.9
62	C6	54	LEU	3.9
48	S2	97	ARG	3.9
55	S9	85	VAL	3.9
61	C5	86	VAL	3.9
66	d0	87	HIS	3.9
79	s6	109	LEU	3.9
62	C6	16	ALA	3.9
55	S9	130	THR	3.9
62	C6	132	LYS	3.9
68	D2	110	ILE	3.9
77	sR	303	ALA	3.9
62	C6	19	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
3	8	80	A	3.9
46	S0	22	THR	3.9
62	c6	37	THR	3.9
46	s0	149	LEU	3.9
62	c6	38	LEU	3.9
64	C8	5	VAL	3.9
28	n7	22	LYS	3.9
65	c9	92	LYS	3.9
64	c8	138	THR	3.9
39	o8	14	LEU	3.9
50	S4	25	GLY	3.9
46	s0	48	ILE	3.9
28	n7	23	VAL	3.9
53	S7	93	LEU	3.9
60	c4	102	LEU	3.9
62	c6	87	LYS	3.9
74	D8	66	LEU	3.9
46	s0	161	PRO	3.9
63	C7	35	CYS	3.9
56	c0	66	TYR	3.8
61	c5	97	TYR	3.8
10	l8	254	ASP	3.8
77	SR	41	THR	3.8
77	SR	52	GLN	3.8
46	s0	23	HIS	3.8
78	SM	87	THR	3.8
79	s6	135	PRO	3.8
29	N8	94	ALA	3.8
77	sR	73	LEU	3.8
49	S3	208	ILE	3.8
51	S5	138	THR	3.8
55	S9	86	LEU	3.8
68	D2	102	VAL	3.8
77	sR	162	ALA	3.8
62	c6	104	GLU	3.8
62	c6	61	SER	3.8
51	s5	130	ILE	3.8
71	D5	92	ILE	3.8
47	S1	231	LEU	3.8
28	n7	41	ALA	3.8
51	s5	153	GLY	3.8
61	c5	92	SER	3.8

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Mol	Chain	Res	Type	RSRZ
71	d5	103	ARG	3.8
75	D9	29	GLY	3.8
49	s3	174	HIS	3.8
51	S5	52	GLU	3.8
46	S0	21	ASN	3.8
62	C6	89	LEU	3.8
65	C9	28	LEU	3.8
47	S1	206	PRO	3.8
47	s1	98	THR	3.8
63	C7	8	THR	3.8
7	l5	236	LEU	3.8
53	s7	129	LEU	3.8
49	S3	173	ARG	3.8
11	L9	95	ALA	3.8
18	M7	184	ALA	3.8
62	c6	84	ALA	3.8
65	c9	59	ALA	3.8
71	d5	72	GLY	3.8
63	C7	54	THR	3.8
71	d5	102	THR	3.8
57	c1	28	SER	3.8
27	N6	126	LEU	3.8
47	s1	137	ILE	3.8
61	c5	107	ILE	3.8
50	S4	183	VAL	3.8
1	5	1566	A	3.8
65	c9	54	PHE	3.8
62	C6	84	ALA	3.8
47	s1	219	LYS	3.8
49	s3	113	LEU	3.8
59	C3	66	ILE	3.8
26	n5	23	ALA	3.8
28	n7	47	GLU	3.8
77	SR	106	HIS	3.8
77	SR	178	VAL	3.8
13	M1	90	GLN	3.7
75	d9	56	ARG	3.7
58	C2	136	ILE	3.7
61	c5	84	ILE	3.7
47	S1	139	ALA	3.7
52	S6	178	LEU	3.7
53	s7	4	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
75	D9	30	LEU	3.7
77	SR	54	PHE	3.7
24	n3	2	SER	3.7
71	d5	56	THR	3.7
77	SR	55	GLY	3.7
78	SM	69	ARG	3.7
48	s2	199	GLN	3.7
50	S4	182	TYR	3.7
57	C1	35	TYR	3.7
58	c2	28	LEU	3.7
64	C8	17	LEU	3.7
79	s6	77	LEU	3.7
50	s4	109	PHE	3.7
76	E0	47	VAL	3.7
20	m9	181	ARG	3.7
25	n4	93	ARG	3.7
57	c1	145	ALA	3.7
48	s2	229	LEU	3.7
59	C3	62	GLN	3.7
49	s3	115	ILE	3.7
77	SR	243	LEU	3.7
77	SR	292	LEU	3.7
46	s0	156	VAL	3.7
51	s5	62	VAL	3.7
10	L8	252	ASN	3.7
25	n4	99	GLU	3.7
77	sR	53	LYS	3.7
65	C9	18	TYR	3.7
4	l2	63	PHE	3.7
65	C9	30	VAL	3.7
73	d7	32	PHE	3.7
54	s8	179	CYS	3.7
61	c5	89	MET	3.7
47	s1	97	LEU	3.7
77	sR	243	LEU	3.7
22	n1	70	SER	3.7
61	c5	96	ILE	3.7
49	s3	91	VAL	3.7
61	c5	76	VAL	3.7
54	s8	200	LYS	3.7
78	sM	83	LYS	3.7
49	s3	49	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
56	C0	65	TYR	3.7
68	d2	83	ILE	3.7
25	n4	72	SER	3.7
49	s3	139	SER	3.7
12	m0	218	ALA	3.7
50	s4	165	ALA	3.7
51	S5	194	LEU	3.7
51	s5	225	ARG	3.7
58	C2	41	LEU	3.7
65	C9	132	LEU	3.7
76	E0	46	ASN	3.7
56	c0	64	TYR	3.7
49	s3	106	LYS	3.7
50	s4	10	LYS	3.7
51	S5	53	VAL	3.7
77	sR	186	PHE	3.7
62	C6	35	PRO	3.7
64	C8	7	GLU	3.7
78	SM	140	ASP	3.7
51	S5	137	ILE	3.7
58	C2	122	VAL	3.7
51	S5	96	SER	3.7
70	D4	61	ARG	3.7
32	O1	71	LEU	3.7
28	N7	92	PHE	3.7
63	C7	69	ILE	3.7
28	n7	43	VAL	3.7
47	S1	95	ASN	3.7
77	SR	315	VAL	3.7
47	s1	177	GLN	3.7
62	C6	104	GLU	3.7
47	S1	102	GLY	3.7
59	c3	59	GLY	3.7
79	s6	196	ARG	3.7
37	o6	50	LEU	3.7
50	S4	246	LEU	3.7
51	s5	30	PRO	3.7
62	C6	38	LEU	3.7
77	SR	267	PRO	3.7
77	sR	45	TRP	3.7
22	n1	34	TYR	3.7
77	sR	304	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
18	M7	168	LEU	3.6
53	S7	99	LEU	3.6
62	C6	18	ALA	3.6
79	s6	148	SER	3.6
62	C6	68	ARG	3.6
37	o6	94	ILE	3.6
62	C6	45	ARG	3.6
47	S1	210	ILE	3.6
47	s1	60	ALA	3.6
70	d4	118	ILE	3.6
10	l8	152	LEU	3.6
25	n4	79	GLN	3.6
62	c6	52	LEU	3.6
76	E0	43	ARG	3.6
25	n4	68	ALA	3.6
75	D9	38	ILE	3.6
77	sR	296	ALA	3.6
61	c5	87	PRO	3.6
10	l8	150	LEU	3.6
28	n7	60	LYS	3.6
49	s3	27	ARG	3.6
51	s5	28	PRO	3.6
49	s3	185	LYS	3.6
62	c6	13	LYS	3.6
26	n5	30	ALA	3.6
12	M0	109	ASP	3.6
62	C6	139	GLN	3.6
71	d5	37	GLN	3.6
77	sR	72	THR	3.6
37	o6	68	ARG	3.6
51	S5	134	VAL	3.6
63	C7	78	ARG	3.6
64	C8	52	VAL	3.6
43	q2	13	LYS	3.6
47	s1	184	LEU	3.6
55	S9	80	LEU	3.6
77	SR	148	ASN	3.6
77	sR	192	PHE	3.6
49	S3	207	THR	3.6
51	S5	120	ILE	3.6
70	D4	69	SER	3.6
60	c4	72	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
77	SR	236	ALA	3.6
62	C6	77	GLN	3.6
78	SM	68	ARG	3.6
29	n8	66	ALA	3.6
47	s1	89	ASP	3.6
77	sR	203	THR	3.6
56	c0	59	PHE	3.6
62	c6	10	PHE	3.6
77	sR	57	PRO	3.6
66	D0	83	GLU	3.6
77	SR	139	GLN	3.6
79	s6	36	VAL	3.6
12	m0	109	ASP	3.6
25	n4	95	SER	3.6
36	o5	18	ALA	3.6
47	s1	46	THR	3.6
62	c6	115	THR	3.6
13	m1	127	PHE	3.5
77	sR	118	LYS	3.5
56	c0	28	ASN	3.5
28	n7	59	ALA	3.5
71	d5	80	LEU	3.5
61	c5	120	SER	3.5
22	n1	72	VAL	3.5
48	s2	151	PRO	3.5
49	s3	138	VAL	3.5
53	s7	13	PRO	3.5
64	C8	70	VAL	3.5
69	d3	60	GLU	3.5
65	c9	15	ILE	3.5
71	d5	92	ILE	3.5
47	S1	26	ARG	3.5
77	sR	230	ALA	3.5
48	s2	166	THR	3.5
58	C2	75	VAL	3.5
77	sR	247	PRO	3.5
25	n4	96	LEU	3.5
77	sR	206	PRO	3.5
12	m0	103	LEU	3.5
51	S5	75	GLY	3.5
58	C2	55	GLY	3.5
61	c5	55	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
77	SR	40	LYS	3.5
62	c6	63	ILE	3.5
65	C9	85	SER	3.5
74	D8	25	VAL	3.5
51	s5	34	GLN	3.5
61	c5	53	PRO	3.5
62	c6	140	LYS	3.5
63	C7	72	LYS	3.5
65	C9	48	GLN	3.5
76	E0	49	LEU	3.5
77	SR	223	TRP	3.5
47	S1	205	PHE	3.5
57	c1	105	LYS	3.5
76	e0	53	LYS	3.5
77	sR	170	ILE	3.5
62	c6	20	ALA	3.5
7	l5	178	ASN	3.5
45	6	75	U	3.5
55	s9	136	VAL	3.5
46	s0	148	ASP	3.5
77	SR	220	ILE	3.5
62	c6	117	LEU	3.5
71	d5	51	LEU	3.5
77	SR	34	LEU	3.5
46	s0	195	TRP	3.5
77	sR	212	ALA	3.5
63	C7	53	TYR	3.5
52	S6	143	LYS	3.5
20	m9	182	ASP	3.5
25	n4	101	ARG	3.5
37	o6	80	PHE	3.5
57	c1	20	PHE	3.5
65	C9	84	LYS	3.5
66	D0	94	GLU	3.5
19	m8	81	VAL	3.5
58	c2	121	VAL	3.5
62	c6	65	ILE	3.5
64	C8	66	LEU	3.5
67	d1	11	LEU	3.5
51	s5	139	ASN	3.5
75	D9	22	ARG	3.5
18	M7	178	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
62	C6	17	THR	3.5
66	D0	78	THR	3.5
68	d2	46	TYR	3.5
16	m5	121	VAL	3.5
65	C9	113	ILE	3.5
22	n1	46	GLY	3.5
49	S3	205	ALA	3.5
20	m9	177	VAL	3.5
73	d7	80	ARG	3.5
50	S4	58	GLY	3.5
51	S5	150	GLY	3.5
62	C6	46	PHE	3.5
61	c5	6	ASN	3.4
79	s6	139	ASN	3.4
77	SR	100	TYR	3.4
62	C6	48	VAL	3.4
41	Q0	83	LYS	3.4
52	S6	77	LEU	3.4
51	S5	101	GLY	3.4
28	n7	75	VAL	3.4
35	o4	62	TYR	3.4
48	s2	222	TYR	3.4
62	c6	79	TYR	3.4
50	s4	228	ILE	3.4
55	S9	97	LEU	3.4
67	d1	34	ILE	3.4
77	SR	46	LYS	3.4
47	S1	133	TYR	3.4
77	sR	314	GLN	3.4
49	s3	175	VAL	3.4
60	c4	33	LEU	3.4
60	c4	74	VAL	3.4
7	L5	95	TRP	3.4
1	1	1580	A	3.4
71	D5	58	ARG	3.4
65	C9	37	VAL	3.4
77	SR	184	ASN	3.4
62	C6	56	GLY	3.4
51	S5	180	ARG	3.4
65	C9	29	GLU	3.4
68	d2	82	LYS	3.4
25	n4	85	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
40	o9	4	GLN	3.4
68	D2	52	TYR	3.4
71	D5	50	ILE	3.4
77	SR	192	PHE	3.4
50	S4	51	ARG	3.4
55	s9	3	ARG	3.4
78	SM	41	SER	3.4
48	S2	92	ALA	3.4
64	C8	146	ALA	3.4
77	sR	8	VAL	3.4
51	S5	172	ILE	3.4
64	c8	119	ILE	3.4
28	n7	135	ARG	3.4
12	M0	171	TRP	3.4
22	n1	91	LEU	3.4
28	n7	114	VAL	3.4
73	d7	82	LYS	3.4
47	S1	122	GLU	3.4
51	S5	98	MET	3.4
12	M0	87	LEU	3.4
18	M7	170	SER	3.4
26	n5	29	SER	3.4
62	C6	44	LEU	3.4
72	d6	53	LEU	3.4
77	SR	309	VAL	3.4
49	S3	174	HIS	3.4
50	S4	109	PHE	3.4
62	C6	30	LYS	3.4
62	C6	83	GLN	3.4
62	C6	118	ILE	3.4
47	s1	217	LEU	3.4
61	C5	101	ALA	3.4
79	s6	102	VAL	3.4
51	s5	61	TYR	3.4
47	s1	74	GLN	3.4
62	C6	9	THR	3.4
75	d9	55	PHE	3.4
1	5	620	U	3.4
10	l8	198	ALA	3.4
51	S5	182	ALA	3.4
51	s5	23	VAL	3.4
54	S8	141	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
55	s9	118	LEU	3.4
64	c8	86	LEU	3.4
71	D5	65	LEU	3.4
76	E0	39	LEU	3.4
77	sR	234	LEU	3.4
68	D2	53	ILE	3.4
50	s4	24	SER	3.4
53	s7	45	SER	3.4
58	c2	38	HIS	3.4
47	s1	45	LYS	3.4
50	S4	49	ARG	3.4
68	d2	102	VAL	3.4
47	S1	104	ASP	3.4
78	SM	43	ASP	3.4
50	S4	121	TYR	3.4
62	c6	15	SER	3.4
70	d4	24	VAL	3.3
77	SR	47	LEU	3.3
77	sR	145	LEU	3.3
77	sR	270	LEU	3.3
49	s3	147	ALA	3.3
77	SR	75	ALA	3.3
28	n7	72	ILE	3.3
65	c9	124	ILE	3.3
51	S5	193	THR	3.3
51	s5	25	LEU	3.3
62	C6	75	VAL	3.3
61	c5	12	PHE	3.3
25	n4	82	ILE	3.3
43	Q2	11	TYR	3.3
50	s4	27	TYR	3.3
64	c8	14	ILE	3.3
72	d6	73	TYR	3.3
58	c2	113	ARG	3.3
66	d0	85	ARG	3.3
74	d8	17	GLY	3.3
28	n7	26	VAL	3.3
78	SM	85	SER	3.3
67	d1	54	ALA	3.3
47	s1	224	ASP	3.3
68	D2	109	GLY	3.3
53	s7	74	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
47	s1	47	LEU	3.3
48	s2	86	VAL	3.3
47	S1	33	LYS	3.3
75	D9	43	PHE	3.3
77	sR	36	ALA	3.3
71	D5	67	ASP	3.3
50	S4	52	LEU	3.3
77	sR	9	LEU	3.3
48	S2	98	PHE	3.3
32	O1	91	SER	3.3
43	Q2	92	GLU	3.3
61	C5	125	PRO	3.3
65	C9	142	GLU	3.3
77	SR	260	ILE	3.3
78	SM	81	THR	3.3
51	S5	142	PRO	3.3
70	D4	26	ASP	3.3
46	S0	160	ILE	3.3
49	s3	114	ALA	3.3
8	l6	67	GLY	3.3
62	c6	71	GLY	3.3
77	sR	258	THR	3.3
49	s3	96	LEU	3.3
51	S5	127	GLN	3.3
53	s7	93	LEU	3.3
63	C7	26	LEU	3.3
58	c2	131	ASP	3.3
62	c6	78	VAL	3.3
65	C9	130	ARG	3.3
20	m9	179	GLU	3.3
46	S0	49	ASN	3.3
55	s9	72	GLU	3.3
10	l8	253	SER	3.3
74	D8	65	ARG	3.3
51	S5	79	ASN	3.3
61	c5	113	GLY	3.3
74	d8	43	ASN	3.3
26	n5	24	LEU	3.3
50	s4	9	LEU	3.3
53	S7	126	LEU	3.3
55	s9	5	PRO	3.3
63	C7	46	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
64	c8	18	LEU	3.3
77	sR	222	LEU	3.3
77	SR	300	THR	3.3
13	M1	65	ILE	3.3
51	S5	135	ASP	3.3
51	S5	177	ILE	3.3
78	sM	68	ARG	3.3
50	s4	207	LEU	3.3
53	s7	41	LEU	3.3
62	c6	62	ASN	3.3
62	c6	105	LEU	3.3
52	S6	67	VAL	3.3
78	SM	22	PRO	3.3
77	SR	99	THR	3.3
50	S4	240	LYS	3.3
65	C9	67	MET	3.3
78	SM	46	LYS	3.3
52	S6	137	ARG	3.3
62	c6	58	ASP	3.3
73	d7	63	LEU	3.3
77	sR	47	LEU	3.3
50	S4	111	VAL	3.3
66	d0	121	ASN	3.3
74	d8	45	LYS	3.3
28	n7	11	ALA	3.3
49	s3	95	GLY	3.3
51	S5	97	LEU	3.3
63	C7	73	LEU	3.3
50	S4	225	VAL	3.3
46	s0	207	PRO	3.2
52	S6	65	GLN	3.2
61	c5	80	MET	3.2
64	c8	57	ARG	3.2
62	C6	63	ILE	3.2
65	c9	83	ALA	3.2
62	C6	64	ASP	3.2
4	l2	76	PHE	3.2
47	s1	68	VAL	3.2
61	c5	94	VAL	3.2
65	C9	9	VAL	3.2
71	D5	70	LYS	3.2
55	s9	144	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
58	C2	84	ASN	3.2
50	S4	18	TRP	3.2
50	S4	222	LEU	3.2
75	D9	28	THR	3.2
51	s5	162	VAL	3.2
55	S9	104	PHE	3.2
76	e0	43	ARG	3.2
55	s9	33	GLU	3.2
51	s5	151	GLY	3.2
62	C6	27	GLY	3.2
29	n8	149	ALA	3.2
43	Q2	83	LEU	3.2
48	s2	186	LYS	3.2
51	S5	183	ALA	3.2
74	D8	21	SER	3.2
77	SR	283	LYS	3.2
51	S5	117	THR	3.2
46	S0	156	VAL	3.2
50	s4	47	PHE	3.2
54	S8	109	PHE	3.2
51	S5	39	GLU	3.2
10	l8	67	ILE	3.2
25	n4	90	ILE	3.2
25	n4	127	LYS	3.2
32	O1	75	ILE	3.2
77	sR	177	MET	3.2
26	n5	82	LEU	3.2
28	n7	51	LEU	3.2
58	c2	133	LEU	3.2
64	c8	3	LEU	3.2
77	sR	49	GLY	3.2
51	S5	110	ALA	3.2
76	E0	34	ALA	3.2
77	sR	2	ALA	3.2
68	D2	101	TYR	3.2
28	n7	52	LYS	3.2
47	S1	85	LYS	3.2
4	l2	138	GLY	3.2
46	S0	185	ARG	3.2
46	s0	162	CYS	3.2
77	SR	89	LEU	3.2
28	n7	129	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
56	C0	22	VAL	3.2
64	C8	79	TYR	3.2
65	C9	104	VAL	3.2
41	Q0	128	LYS	3.2
48	s2	84	LYS	3.2
70	D4	9	THR	3.2
28	n7	25	ILE	3.2
36	o5	9	LEU	3.2
48	S2	83	ILE	3.2
58	C2	89	ILE	3.2
58	c2	40	GLY	3.2
66	D0	20	ILE	3.2
12	M0	105	CYS	3.2
20	m9	178	ALA	3.2
74	D8	48	VAL	3.2
64	c8	45	LEU	3.2
77	sR	23	LEU	3.2
71	d5	91	PRO	3.2
77	sR	119	ALA	3.2
29	N8	79	TRP	3.2
47	s1	95	ASN	3.2
65	c9	101	ASN	3.2
77	SR	14	GLU	3.2
13	m1	70	THR	3.2
60	c4	105	LEU	3.2
77	sR	48	THR	3.2
79	s6	133	LEU	3.2
51	S5	116	HIS	3.2
62	C6	86	ALA	3.2
50	S4	105	VAL	3.2
58	C2	123	VAL	3.2
62	C6	78	VAL	3.2
51	S5	92	ARG	3.2
63	C7	33	ARG	3.2
23	n2	52	ASN	3.2
46	S0	133	ILE	3.2
47	s1	86	LEU	3.2
50	S4	19	LEU	3.2
58	c2	89	ILE	3.2
79	s6	124	LEU	3.2
76	e0	3	LYS	3.2
28	n7	74	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
58	C2	56	GLU	3.2
58	C2	129	GLU	3.2
65	C9	86	ARG	3.2
37	o6	77	LEU	3.2
46	s0	18	LEU	3.2
52	S6	54	GLY	3.2
71	d5	88	ILE	3.2
68	D2	111	MET	3.2
49	s3	90	ARG	3.2
60	C4	50	ALA	3.2
61	C5	17	TYR	3.2
79	s6	130	PRO	3.2
45	6	1052	U	3.2
66	d0	79	TRP	3.2
65	C9	32	GLY	3.2
74	D8	53	ILE	3.2
73	D7	29	ARG	3.2
7	l5	296	GLN	3.2
19	m8	80	THR	3.2
62	c6	97	VAL	3.2
61	c5	118	GLU	3.2
77	sR	254	ALA	3.2
13	M1	91	LEU	3.1
37	o6	93	ILE	3.1
47	S1	93	GLY	3.1
50	S4	90	ILE	3.1
64	C8	101	LEU	3.1
51	S5	43	PHE	3.1
43	q2	102	GLN	3.1
47	S1	90	GLU	3.1
49	s3	58	VAL	3.1
67	D1	10	GLU	3.1
79	s6	179	VAL	3.1
32	O1	112	ASP	3.1
55	s9	61	THR	3.1
74	D8	45	LYS	3.1
54	S8	152	ILE	3.1
3	4	84	C	3.1
52	S6	161	GLU	3.1
67	D1	54	ALA	3.1
78	SM	42	ALA	3.1
54	S8	55	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
25	n4	87	LEU	3.1
77	sR	10	ARG	3.1
68	D2	83	ILE	3.1
61	c5	4	ALA	3.1
61	c5	106	GLU	3.1
79	s6	107	ALA	3.1
46	s0	46	HIS	3.1
47	s1	228	LEU	3.1
71	D5	51	LEU	3.1
51	S5	40	ILE	3.1
51	s5	147	THR	3.1
59	c3	61	THR	3.1
65	c9	113	ILE	3.1
73	d7	46	VAL	3.1
65	C9	107	ALA	3.1
78	sM	66	ALA	3.1
52	S6	208	TYR	3.1
53	s7	9	LEU	3.1
58	C2	88	LEU	3.1
22	n1	96	ILE	3.1
47	s1	138	PHE	3.1
48	s2	227	PRO	3.1
47	S1	41	ARG	3.1
77	SR	180	ALA	3.1
50	s4	12	LEU	3.1
56	c0	62	GLN	3.1
63	C7	34	LEU	3.1
27	n6	46	LYS	3.1
28	n7	130	PHE	3.1
45	2	1363	U	3.1
51	S5	41	LYS	3.1
57	c1	73	GLY	3.1
64	C8	85	PHE	3.1
77	sR	115	ILE	3.1
77	sR	108	SER	3.1
47	s1	57	ALA	3.1
58	C2	128	ALA	3.1
77	sR	261	LYS	3.1
61	c5	85	ILE	3.1
62	c6	11	GLY	3.1
77	SR	131	ILE	3.1
47	S1	103	MET	3.1

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Mol	Chain	Res	Type	RSRZ
61	c5	81	ARG	3.1
67	d1	82	VAL	3.1
77	sR	17	ASN	3.1
66	d0	34	LEU	3.1
63	c7	74	GLN	3.1
66	d0	22	ILE	3.1
26	n5	62	VAL	3.1
45	2	193	U	3.1
50	S4	197	HIS	3.1
47	s1	54	LEU	3.1
48	S2	41	LEU	3.1
50	S4	44	LEU	3.1
55	S9	109	LEU	3.1
77	SR	27	ALA	3.1
16	m5	142	ILE	3.1
50	S4	192	ILE	3.1
70	D4	66	GLY	3.1
77	SR	61	PHE	3.1
77	sR	122	ILE	3.1
48	s2	80	VAL	3.1
68	d2	81	VAL	3.1
63	c7	35	CYS	3.1
76	E0	60	PRO	3.1
77	SR	145	LEU	3.1
56	c0	61	TRP	3.1
7	L5	160	PHE	3.1
62	c6	68	ARG	3.1
57	C1	70	ILE	3.1
12	M0	138	VAL	3.1
48	S2	86	VAL	3.1
11	L9	161	LEU	3.1
47	S1	123	ALA	3.1
55	s9	135	ALA	3.1
77	SR	301	LEU	3.1
55	s9	54	ARG	3.1
78	SM	21	PRO	3.1
62	c6	120	ASP	3.1
67	D1	34	ILE	3.1
74	d8	32	PHE	3.1
22	n1	40	VAL	3.1
52	S6	124	LEU	3.1
63	c7	57	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
77	sR	81	LEU	3.1
49	s3	107	PHE	3.0
50	S4	175	PHE	3.0
48	S2	69	ILE	3.0
51	S5	128	ASN	3.0
64	c8	125	ILE	3.0
68	d2	45	GLY	3.0
77	SR	92	TRP	3.0
51	S5	168	VAL	3.0
79	s6	112	VAL	3.0
50	S4	9	LEU	3.0
78	sM	51	ARG	3.0
67	D1	26	ALA	3.0
8	l6	128	LYS	3.0
37	o6	71	LYS	3.0
62	C6	112	TYR	3.0
63	c7	53	TYR	3.0
54	S8	176	SER	3.0
55	s9	142	ASN	3.0
77	SR	242	SER	3.0
77	sR	181	TRP	3.0
28	n7	98	THR	3.0
74	d8	33	LEU	3.0
50	S4	242	LYS	3.0
52	S6	27	PHE	3.0
47	S1	121	ILE	3.0
55	s9	143	ILE	3.0
68	D2	47	ILE	3.0
12	m0	110	ARG	3.0
36	o5	19	SER	3.0
53	s7	39	ARG	3.0
74	d8	25	VAL	3.0
77	sR	205	SER	3.0
53	S7	43	PHE	3.0
79	s6	175	ILE	3.0
13	m1	47	GLN	3.0
29	n8	123	VAL	3.0
51	S5	149	VAL	3.0
51	s5	158	GLN	3.0
54	s8	46	VAL	3.0
49	S3	182	LEU	3.0
50	S4	213	SER	3.0

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Mol	Chain	Res	Type	RSRZ
57	c1	29	LYS	3.0
51	s5	48	PHE	3.0
63	c7	28	PHE	3.0
77	sR	130	THR	3.0
51	s5	154	ALA	3.0
53	s7	12	ALA	3.0
74	D8	49	ARG	3.0
47	s1	20	VAL	3.0
72	d6	45	VAL	3.0
46	S0	149	LEU	3.0
56	c0	29	GLN	3.0
62	c6	103	ASN	3.0
51	S5	76	ARG	3.0
48	s2	179	VAL	3.0
70	d4	44	LEU	3.0
77	SR	265	LEU	3.0
28	n7	48	ARG	3.0
58	c2	107	ASP	3.0
62	C6	114	ARG	3.0
7	L5	217	GLU	3.0
36	O5	2	ALA	3.0
77	sR	305	TYR	3.0
79	s6	84	TYR	3.0
28	n7	96	VAL	3.0
28	n7	87	LEU	3.0
55	S9	2	PRO	3.0
77	SR	16	HIS	3.0
51	S5	143	ARG	3.0
7	l5	190	ILE	3.0
43	Q2	3	ASN	3.0
51	S5	31	GLU	3.0
68	D2	18	GLU	3.0
77	sR	169	ILE	3.0
29	n8	147	LEU	3.0
7	L5	181	PRO	3.0
22	n1	95	HIS	3.0
64	C8	45	LEU	3.0
66	D0	85	ARG	3.0
71	D5	82	HIS	3.0
66	D0	79	TRP	3.0
52	S6	66	GLY	3.0
35	o4	29	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
22	n1	93	VAL	3.0
77	SR	58	VAL	3.0
77	SR	157	VAL	3.0
65	c9	22	LEU	3.0
29	n8	129	PHE	3.0
50	S4	195	ILE	3.0
50	s4	13	ALA	3.0
61	C5	131	ALA	3.0
10	L8	150	LEU	3.0
13	M1	102	PHE	3.0
65	C9	69	LYS	3.0
73	D7	47	PHE	3.0
74	D8	5	THR	3.0
36	o5	16	GLN	3.0
77	SR	101	GLN	3.0
79	s6	146	GLY	3.0
1	5	252	U	3.0
58	c2	30	VAL	3.0
64	c8	58	ALA	3.0
10	l8	186	LEU	3.0
64	C8	97	ASP	3.0
13	m1	174	LYS	3.0
63	C7	14	LYS	3.0
68	D2	124	LYS	3.0
52	S6	50	PHE	3.0
64	c8	11	PHE	3.0
46	s0	147	THR	3.0
49	s3	140	GLY	2.9
51	S5	113	ILE	2.9
62	C6	82	ARG	2.9
67	D1	23	ILE	2.9
50	S4	161	LYS	2.9
50	s4	101	LEU	2.9
59	c3	40	TYR	2.9
61	C5	60	LEU	2.9
61	C5	94	VAL	2.9
32	O1	79	ARG	2.9
55	s9	130	THR	2.9
76	e0	6	GLY	2.9
77	SR	98	GLU	2.9
41	Q0	78	ILE	2.9
47	S1	84	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
68	D2	72	CYS	2.9
68	d2	125	ILE	2.9
71	d5	71	ILE	2.9
71	d5	78	ILE	2.9
13	M1	12	LEU	2.9
13	m1	115	LYS	2.9
18	M7	166	VAL	2.9
67	d1	55	LEU	2.9
68	d2	69	LEU	2.9
77	SR	156	VAL	2.9
77	SR	261	LYS	2.9
57	C1	60	PHE	2.9
79	s6	50	PHE	2.9
10	l8	179	ILE	2.9
47	s1	231	LEU	2.9
51	S5	64	VAL	2.9
51	s5	64	VAL	2.9
69	d3	118	PRO	2.9
7	l5	62	CYS	2.9
71	D5	57	TYR	2.9
49	s3	173	ARG	2.9
51	S5	112	ARG	2.9
7	l5	34	LYS	2.9
13	m1	64	LYS	2.9
62	C6	125	GLU	2.9
64	c8	59	GLY	2.9
77	SR	117	LYS	2.9
47	S1	215	VAL	2.9
54	S8	43	ILE	2.9
49	S3	201	ALA	2.9
49	s3	39	VAL	2.9
64	C8	69	ILE	2.9
49	s3	72	LEU	2.9
63	c7	26	LEU	2.9
73	D7	33	LEU	2.9
66	D0	82	TYR	2.9
77	SR	135	THR	2.9
58	C2	100	TRP	2.9
49	s3	134	CYS	2.9
50	S4	221	ARG	2.9
66	d0	83	GLU	2.9
62	C6	71	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
50	S4	56	LEU	2.9
61	C5	53	PRO	2.9
62	c6	21	HIS	2.9
67	D1	55	LEU	2.9
70	D4	18	LEU	2.9
74	D8	54	LEU	2.9
77	SR	23	LEU	2.9
77	sR	26	SER	2.9
52	S6	100	ALA	2.9
62	c6	142	TYR	2.9
64	c8	42	TYR	2.9
77	sR	317	THR	2.9
74	D8	50	GLU	2.9
77	sR	146	GLY	2.9
18	M7	176	ILE	2.9
19	m8	138	LEU	2.9
50	S4	160	VAL	2.9
63	C7	9	VAL	2.9
62	c6	16	ALA	2.9
65	C9	134	ARG	2.9
13	M1	163	PHE	2.9
48	S2	96	THR	2.9
71	d5	105	THR	2.9
57	c1	4	GLU	2.9
28	n7	42	LEU	2.9
28	n7	134	LEU	2.9
52	S6	92	ARG	2.9
65	c9	8	ASP	2.9
68	d2	121	VAL	2.9
13	m1	96	PHE	2.9
43	Q2	81	ALA	2.9
58	C2	85	LYS	2.9
65	C9	66	TYR	2.9
65	c9	19	ALA	2.9
46	s0	35	PRO	2.9
16	m5	120	TRP	2.9
58	C2	126	TRP	2.9
49	S3	183	GLY	2.9
29	n8	75	LEU	2.9
48	s2	76	LEU	2.9
49	s3	94	ARG	2.9
55	s9	141	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
64	c8	81	ILE	2.9
67	d1	9	VAL	2.9
70	D4	17	LEU	2.9
65	C9	101	ASN	2.9
22	n1	29	THR	2.9
54	S8	48	THR	2.9
56	c0	67	THR	2.9
68	d2	68	ARG	2.9
77	sR	256	THR	2.9
10	l8	43	LYS	2.9
62	C6	69	VAL	2.9
68	D2	60	LYS	2.9
70	D4	44	LEU	2.9
12	m0	220	GLN	2.9
20	m9	188	ASP	2.9
55	S9	164	PHE	2.9
58	C2	69	ALA	2.9
64	c8	136	GLN	2.9
62	c6	49	TYR	2.9
56	C0	25	LYS	2.9
76	e0	36	LYS	2.9
77	sR	19	TRP	2.9
6	l4	290	ILE	2.9
22	n1	75	ILE	2.9
48	s2	81	MET	2.9
55	s9	113	VAL	2.9
68	D2	128	PHE	2.9
63	C7	65	PRO	2.9
79	s6	173	PRO	2.9
10	l8	252	ASN	2.9
73	D7	24	LEU	2.9
19	m8	99	THR	2.9
57	c1	27	THR	2.9
62	C6	37	THR	2.9
73	D7	65	THR	2.9
68	D2	51	GLU	2.9
66	D0	61	LYS	2.9
71	d5	52	LYS	2.9
13	m1	45	PRO	2.9
16	M5	58	GLY	2.9
48	s2	154	LEU	2.9
59	C3	28	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
77	SR	270	LEU	2.9
52	S6	32	ILE	2.8
62	C6	15	SER	2.8
65	C9	100	ILE	2.8
67	d1	39	VAL	2.8
75	D9	55	PHE	2.8
79	s6	4	ASN	2.8
4	l2	59	ALA	2.8
20	m9	11	ALA	2.8
49	s3	61	GLU	2.8
62	C6	140	LYS	2.8
78	sM	123	ALA	2.8
7	l5	171	LEU	2.8
43	Q2	93	LEU	2.8
45	2	754	A	2.8
47	S1	171	ILE	2.8
52	S6	141	ILE	2.8
52	S6	175	ILE	2.8
66	d0	65	ILE	2.8
75	D9	31	ILE	2.8
13	M1	41	SER	2.8
79	s6	92	ARG	2.8
47	S1	50	LYS	2.8
1	5	3278	C	2.8
36	o5	85	THR	2.8
51	S5	61	TYR	2.8
54	s8	97	THR	2.8
46	s0	9	LEU	2.8
71	D5	73	GLY	2.8
10	l8	50	VAL	2.8
47	S1	140	ILE	2.8
50	S4	102	VAL	2.8
53	S7	172	VAL	2.8
62	c6	69	VAL	2.8
28	n7	65	ARG	2.8
68	D2	103	ILE	2.8
45	2	506	A	2.8
49	S3	8	LYS	2.8
66	d0	64	LYS	2.8
13	m1	20	ASN	2.8
79	s6	140	ASN	2.8
77	sR	25	THR	2.8

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Mol	Chain	Res	Type	RSRZ
52	S6	99	GLY	2.8
27	N6	125	LYS	2.8
37	o6	41	ARG	2.8
50	S4	210	ILE	2.8
77	sR	154	VAL	2.8
79	s6	162	VAL	2.8
51	S5	129	PRO	2.8
77	SR	57	PRO	2.8
28	n7	44	ALA	2.8
63	C7	62	GLN	2.8
7	L5	153	THR	2.8
37	o6	11	LEU	2.8
47	S1	86	LEU	2.8
65	c9	108	LEU	2.8
60	c4	92	LYS	2.8
77	SR	203	THR	2.8
3	8	82	U	2.8
12	m0	197	VAL	2.8
50	S4	76	VAL	2.8
62	c6	5	PRO	2.8
63	C7	58	MET	2.8
75	d9	52	PHE	2.8
46	S0	158	VAL	2.8
65	C9	36	ILE	2.8
50	S4	35	PRO	2.8
73	D7	66	PRO	2.8
25	n4	128	ALA	2.8
7	L5	163	LEU	2.8
12	M0	103	LEU	2.8
23	n2	70	LYS	2.8
56	c0	15	LEU	2.8
68	d2	104	LEU	2.8
68	d2	130	TYR	2.8
70	D4	40	LEU	2.8
10	L8	195	SER	2.8
62	c6	4	VAL	2.8
68	D2	125	ILE	2.8
47	s1	37	THR	2.8
58	c2	34	THR	2.8
76	E0	56	MET	2.8
48	S2	95	ARG	2.8
48	s2	97	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
51	s5	164	PRO	2.8
52	S6	135	PRO	2.8
62	C6	124	PRO	2.8
64	c8	76	PRO	2.8
78	SM	40	PRO	2.8
22	n1	151	LEU	2.8
43	q2	72	LEU	2.8
58	C2	57	ALA	2.8
58	c2	74	LEU	2.8
60	c4	20	TYR	2.8
51	S5	68	ILE	2.8
53	S7	90	VAL	2.8
53	S7	92	PHE	2.8
71	d5	89	ILE	2.8
74	d8	15	VAL	2.8
77	SR	213	SER	2.8
77	sR	312	VAL	2.8
51	S5	95	ASN	2.8
77	SR	200	ASN	2.8
47	s1	234	GLU	2.8
28	n7	82	PRO	2.8
22	n1	30	TYR	2.8
32	O1	51	LEU	2.8
55	s9	93	LEU	2.8
62	c6	44	LEU	2.8
68	D2	126	LEU	2.8
77	SR	208	GLY	2.8
77	sR	32	LEU	2.8
43	Q2	91	PHE	2.8
72	d6	50	VAL	2.8
77	SR	104	VAL	2.8
49	S3	158	ILE	2.8
8	l6	129	GLU	2.8
29	N8	95	SER	2.8
51	S5	104	ASN	2.8
60	c4	43	THR	2.8
50	S4	207	LEU	2.8
64	c8	32	LEU	2.8
71	d5	55	PRO	2.8
77	SR	222	LEU	2.8
47	S1	100	PHE	2.8
51	S5	162	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
51	s5	24	VAL	2.8
66	D0	105	GLN	2.8
10	l8	143	ILE	2.8
60	c4	83	ILE	2.8
77	SR	263	PHE	2.8
71	D5	94	LYS	2.8
77	sR	43	ILE	2.8
14	M3	134	GLU	2.8
68	D2	30	SER	2.8
7	l5	129	TYR	2.8
37	o6	95	ALA	2.8
49	s3	69	LEU	2.8
49	s3	149	ALA	2.8
53	s7	38	LEU	2.8
55	S9	28	LEU	2.8
51	S5	178	GLY	2.8
59	C3	63	ALA	2.8
12	M0	50	VAL	2.8
12	M0	85	PHE	2.8
64	C8	71	GLN	2.8
77	sR	109	ASP	2.8
13	M1	114	ILE	2.8
52	S6	79	LYS	2.8
74	D8	18	ARG	2.8
79	s6	136	LYS	2.8
45	6	194	U	2.8
77	sR	189	GLU	2.8
75	d9	36	LEU	2.8
25	n4	94	ARG	2.8
54	S8	182	TYR	2.8
77	SR	78	ALA	2.8
73	D7	2	VAL	2.8
76	E0	29	LYS	2.8
77	SR	167	VAL	2.8
77	sR	54	PHE	2.8
75	d9	38	ILE	2.7
45	6	648	G	2.7
41	Q0	82	LEU	2.7
49	S3	69	LEU	2.7
51	s5	97	LEU	2.7
55	s9	36	LEU	2.7
7	l5	179	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
45	6	793	A	2.7
51	S5	74	ALA	2.7
65	C9	119	LYS	2.7
67	D1	84	SER	2.7
78	sM	85	SER	2.7
29	N8	121	VAL	2.7
51	S5	82	PHE	2.7
78	sM	119	ALA	2.7
7	l5	109	THR	2.7
13	M1	134	PRO	2.7
66	D0	117	VAL	2.7
50	S4	184	THR	2.7
53	S7	149	ILE	2.7
77	SR	30	PRO	2.7
47	S1	188	LEU	2.7
50	s4	107	GLY	2.7
49	s3	16	VAL	2.7
64	c8	2	SER	2.7
74	D8	28	VAL	2.7
76	e0	61	SER	2.7
77	sR	240	VAL	2.7
11	L9	30	PRO	2.7
66	D0	41	ILE	2.7
26	n5	37	THR	2.7
65	c9	131	ASP	2.7
7	l5	150	LEU	2.7
52	S6	216	LEU	2.7
55	s9	174	ARG	2.7
62	C6	14	LYS	2.7
25	n4	103	ALA	2.7
37	o6	8	ALA	2.7
71	D5	76	ALA	2.7
53	S7	134	GLU	2.7
77	SR	209	THR	2.7
50	S4	189	LEU	2.7
4	l2	62	VAL	2.7
7	l5	200	PHE	2.7
68	D2	21	GLY	2.7
62	c6	96	TYR	2.7
73	D7	35	VAL	2.7
78	sM	42	ALA	2.7
74	d8	40	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
64	C8	48	LYS	2.7
65	C9	7	ARG	2.7
65	c9	110	LYS	2.7
68	d2	95	PRO	2.7
71	D5	98	GLN	2.7
79	s6	93	LYS	2.7
32	O1	89	LEU	2.7
46	s0	164	ASN	2.7
47	s1	42	ASN	2.7
47	s1	99	ASN	2.7
50	s4	18	TRP	2.7
55	S9	146	PHE	2.7
56	c0	19	GLY	2.7
70	D4	64	PHE	2.7
49	S3	37	VAL	2.7
66	D0	56	VAL	2.7
77	sR	318	ALA	2.7
41	q0	77	ILE	2.7
60	c4	36	LYS	2.7
68	d2	117	ARG	2.7
71	D5	89	ILE	2.7
79	s6	32	ILE	2.7
45	2	504	U	2.7
45	6	239	C	2.7
63	C7	74	GLN	2.7
65	c9	12	GLN	2.7
68	D2	104	LEU	2.7
73	d7	41	LEU	2.7
76	e0	49	LEU	2.7
79	s6	12	SER	2.7
77	SR	182	ASN	2.7
7	l5	180	PHE	2.7
68	D2	67	GLY	2.7
50	s4	84	ALA	2.7
50	s4	149	TYR	2.7
51	s5	32	GLU	2.7
55	s9	4	ALA	2.7
65	C9	122	ARG	2.7
70	d4	20	ARG	2.7
61	c5	109	PRO	2.7
62	C6	53	LEU	2.7
13	M1	96	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
28	n7	27	LYS	2.7
47	S1	223	PHE	2.7
77	SR	125	GLY	2.7
52	S6	81	VAL	2.7
60	c4	103	ARG	2.7
67	D1	32	VAL	2.7
51	S5	49	GLU	2.7
39	o8	31	LEU	2.7
47	S1	47	LEU	2.7
61	C5	112	LEU	2.7
7	L5	223	PHE	2.7
25	n4	70	LYS	2.7
46	S0	162	CYS	2.7
49	S3	7	LYS	2.7
62	C6	47	LYS	2.7
78	sM	54	PRO	2.7
36	o5	57	VAL	2.7
65	C9	68	ARG	2.7
62	C6	103	ASN	2.7
68	D2	74	VAL	2.7
71	D5	81	ARG	2.7
77	sR	309	VAL	2.7
1	5	2539	C	2.7
51	S5	94	THR	2.7
77	SR	149	ASP	2.7
49	S3	202	LEU	2.7
53	S7	81	LEU	2.7
66	d0	26	LEU	2.7
35	o4	59	PRO	2.7
54	S8	65	PHE	2.7
77	SR	237	GLN	2.7
19	m8	101	VAL	2.7
48	s2	208	GLU	2.7
49	s3	47	GLU	2.7
55	S9	145	SER	2.7
59	C3	21	ASN	2.7
71	d5	104	ALA	2.7
64	c8	91	ASP	2.7
77	SR	114	ASP	2.7
25	n4	129	LYS	2.7
46	s0	201	LEU	2.7
49	s3	29	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
67	D1	8	LEU	2.7
49	S3	105	MET	2.7
64	C8	74	GLN	2.7
25	n4	66	GLU	2.7
50	s4	5	PRO	2.7
77	SR	77	GLY	2.7
7	l5	44	TYR	2.7
7	l5	61	ILE	2.7
37	o6	9	ILE	2.7
61	c5	90	ILE	2.7
77	SR	24	ALA	2.7
77	SR	170	ILE	2.7
45	2	1573	A	2.7
48	S2	225	LEU	2.7
58	c2	43	ARG	2.7
61	C5	65	LEU	2.7
66	d0	27	THR	2.7
74	D8	16	LEU	2.7
16	m5	130	PHE	2.7
45	2	655	G	2.7
47	s1	225	VAL	2.7
50	S4	208	VAL	2.7
54	S8	102	VAL	2.7
50	s4	147	ILE	2.7
54	s8	192	TYR	2.6
60	c4	115	ILE	2.7
48	s2	113	LEU	2.6
51	S5	198	LEU	2.6
77	sR	210	LEU	2.6
55	s9	157	ASP	2.6
7	L5	180	PHE	2.6
74	d8	39	THR	2.6
77	sR	103	PHE	2.6
37	o6	72	VAL	2.6
60	C4	42	VAL	2.6
79	s6	11	GLY	2.6
11	L9	2	LYS	2.6
50	s4	22	LYS	2.6
55	s9	37	LYS	2.6
20	m9	173	ARG	2.6
20	m9	183	ALA	2.6
50	s4	92	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
51	S5	81	ARG	2.6
54	S8	184	LEU	2.6
63	C7	24	LEU	2.6
75	D9	40	ARG	2.6
77	SR	171	SER	2.6
50	S4	157	ASN	2.6
35	o4	72	VAL	2.6
49	S3	44	THR	2.6
50	S4	134	LYS	2.6
50	S4	211	LYS	2.6
51	S5	23	VAL	2.6
56	c0	58	GLN	2.6
60	c4	88	GLY	2.6
62	C6	33	GLY	2.6
64	C8	20	THR	2.6
71	D5	52	LYS	2.6
78	sM	64	LYS	2.6
14	m3	89	TYR	2.6
26	n5	38	LEU	2.6
50	S4	147	ILE	2.6
66	d0	95	ALA	2.6
61	c5	45	PHE	2.6
51	S5	99	MET	2.6
55	S9	91	LYS	2.6
60	c4	10	ASN	2.6
68	D2	123	GLY	2.6
78	sM	23	LYS	2.6
48	S2	91	ARG	2.6
62	c6	100	GLN	2.6
45	6	1688	U	2.6
10	l8	199	ALA	2.6
51	S5	114	ILE	2.6
53	S7	135	ILE	2.6
55	S9	129	ILE	2.6
77	SR	234	LEU	2.6
79	s6	5	ILE	2.6
53	S7	24	PHE	2.6
77	sR	61	PHE	2.6
68	D2	58	SER	2.6
77	sR	120	SER	2.6
43	q2	75	VAL	2.6
48	s2	167	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
66	D0	92	ASP	2.6
72	D6	42	ARG	2.6
72	d6	84	VAL	2.6
77	SR	113	VAL	2.6
26	n5	57	LEU	2.6
51	S5	121	ILE	2.6
51	S5	136	ALA	2.6
55	S9	36	LEU	2.6
55	S9	76	LEU	2.6
66	D0	22	ILE	2.6
77	SR	169	ILE	2.6
77	sR	310	ILE	2.6
29	n8	119	PRO	2.6
51	S5	46	TRP	2.6
58	c2	120	VAL	2.6
65	c9	134	ARG	2.6
67	d1	65	SER	2.6
29	n8	65	GLN	2.6
51	s5	35	GLN	2.6
59	C3	16	ILE	2.6
16	m5	43	THR	2.6
55	s9	183	ALA	2.6
64	c8	132	ARG	2.6
65	c9	21	PHE	2.6
77	SR	103	PHE	2.6
79	s6	149	LYS	2.6
29	N8	117	ARG	2.6
77	sR	155	ARG	2.6
71	d5	53	GLU	2.6
79	s6	134	GLY	2.6
29	n8	118	ILE	2.6
31	O0	101	LEU	2.6
58	c2	142	GLN	2.6
59	C3	50	ILE	2.6
60	c4	19	ILE	2.6
65	C9	79	LEU	2.6
66	D0	86	ILE	2.6
74	d8	56	LEU	2.6
77	SR	299	GLN	2.6
12	m0	108	ALA	2.6
13	M1	20	ASN	2.6
35	o4	92	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
58	c2	92	ALA	2.6
59	C3	40	TYR	2.6
65	C9	77	ASN	2.6
67	D1	22	ARG	2.6
77	sR	178	VAL	2.6
61	c5	83	MET	2.6
64	C8	73	MET	2.6
53	s7	77	LEU	2.6
64	c8	66	LEU	2.6
66	D0	24	ILE	2.6
79	s6	190	GLN	2.6
4	l2	70	ARG	2.6
11	L9	92	TYR	2.6
47	s1	41	ARG	2.6
1	1	2971	A	2.6
79	s6	56	ASN	2.6
57	C1	61	THR	2.6
7	L5	156	GLY	2.6
28	n7	89	VAL	2.6
48	s2	105	GLY	2.6
50	S4	36	HIS	2.6
71	D5	54	VAL	2.6
79	s6	97	VAL	2.6
22	n1	31	LEU	2.6
36	o5	55	LEU	2.6
58	c2	126	TRP	2.6
49	S3	54	ARG	2.6
53	S7	60	ILE	2.6
70	d4	125	LEU	2.6
62	c6	139	GLN	2.6
13	M1	167	TYR	2.6
73	d7	64	CYS	2.6
62	c6	98	ASP	2.6
22	n1	50	LYS	2.6
28	n7	69	LYS	2.6
51	s5	149	VAL	2.6
55	S9	35	GLY	2.6
58	c2	75	VAL	2.6
60	C4	28	VAL	2.6
65	C9	92	LYS	2.6
77	sR	233	THR	2.6
1	5	1351	U	2.6

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Mol	Chain	Res	Type	RSRZ
15	M4	38	ILE	2.6
63	C7	16	LEU	2.6
14	m3	160	GLN	2.6
12	M0	108	ALA	2.6
25	n4	125	ALA	2.6
6	l4	177	ASP	2.6
77	SR	152	SER	2.6
7	l5	43	LYS	2.6
39	o8	13	GLU	2.6
47	s1	150	VAL	2.6
48	S2	49	LYS	2.6
66	d0	30	LYS	2.6
77	SR	238	ASP	2.6
49	s3	62	ASN	2.6
55	S9	141	VAL	2.6
48	s2	91	ARG	2.6
30	n9	48	HIS	2.6
53	s7	81	LEU	2.6
64	C8	61	LEU	2.6
48	s2	218	ILE	2.6
49	s3	50	ILE	2.6
51	S5	89	ILE	2.6
55	S9	140	ILE	2.6
1	5	3276	G	2.6
4	l2	34	TYR	2.6
12	M0	106	ALA	2.6
30	N9	56	ALA	2.6
51	S5	86	GLN	2.6
61	C5	56	PHE	2.6
60	c4	60	ALA	2.6
61	c5	74	ALA	2.6
50	S4	185	GLY	2.6
51	s5	39	GLU	2.6
62	C6	13	LYS	2.6
77	SR	20	VAL	2.6
77	SR	138	GLY	2.6
77	SR	286	GLU	2.6
50	S4	196	VAL	2.6
51	s5	145	ASP	2.6
58	c2	122	VAL	2.6
79	s6	6	SER	2.6
79	s6	67	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
11	L9	112	ILE	2.6
28	N7	66	THR	2.6
46	s0	6	THR	2.6
50	S4	244	ILE	2.6
51	s5	90	ILE	2.6
72	d6	83	ILE	2.6
77	SR	231	MET	2.6
62	c6	109	PHE	2.5
12	m0	219	ALA	2.5
23	N2	10	LYS	2.5
54	S8	74	LYS	2.5
65	c9	17	ALA	2.5
7	l5	216	GLU	2.5
58	c2	83	GLU	2.5
75	D9	34	TYR	2.5
45	6	230	C	2.5
70	D4	27	VAL	2.5
77	SR	68	VAL	2.5
74	d8	9	LEU	2.5
4	l2	97	ASN	2.5
11	L9	4	ILE	2.5
26	n5	63	ILE	2.5
54	S8	60	ILE	2.5
50	S4	75	LYS	2.5
50	S4	218	PHE	2.5
59	C3	26	PHE	2.5
67	D1	21	ASN	2.5
71	d5	50	ILE	2.5
51	S5	176	THR	2.5
68	D2	119	LYS	2.5
75	d9	54	LYS	2.5
28	N7	2	ALA	2.5
13	m1	124	GLY	2.5
58	c2	104	GLY	2.5
74	d8	24	GLY	2.5
41	q0	82	LEU	2.5
45	6	558	U	2.5
45	6	1687	U	2.5
46	s0	146	LEU	2.5
22	n1	48	ILE	2.5
36	o5	78	LYS	2.5
45	6	237	C	2.5

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Mol	Chain	Res	Type	RSRZ
65	c9	5	SER	2.5
47	S1	83	LYS	2.5
70	D4	11	LYS	2.5
78	sM	84	LYS	2.5
45	6	228	G	2.5
47	S1	99	ASN	2.5
50	S4	153	ASN	2.5
29	n8	98	THR	2.5
51	S5	66	GLN	2.5
56	C0	66	TYR	2.5
62	c6	143	ARG	2.5
66	D0	90	TYR	2.5
77	sR	139	GLN	2.5
79	s6	110	ALA	2.5
6	l4	303	GLY	2.5
54	s8	102	VAL	2.5
13	M1	40	LEU	2.5
57	c1	69	LYS	2.5
59	c3	45	LEU	2.5
27	n6	45	ILE	2.5
29	N8	118	ILE	2.5
39	O8	56	ILE	2.5
58	c2	71	ILE	2.5
73	d7	47	PHE	2.5
79	s6	29	ASP	2.5
4	l2	149	ARG	2.5
10	l8	44	ARG	2.5
32	o1	31	ARG	2.5
47	S1	46	THR	2.5
50	S4	231	GLN	2.5
60	C4	21	ALA	2.5
60	c4	80	HIS	2.5
62	C6	88	GLY	2.5
67	D1	33	GLN	2.5
70	d4	55	VAL	2.5
77	SR	201	THR	2.5
7	L5	236	LEU	2.5
49	s3	59	LEU	2.5
55	S9	10	LYS	2.5
57	C1	40	LEU	2.5
50	S4	236	ILE	2.5
52	S6	101	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
12	M0	47	PRO	2.5
12	M0	104	SER	2.5
22	n1	86	GLU	2.5
45	2	238	U	2.5
58	C2	119	SER	2.5
65	c9	126	GLU	2.5
10	l8	39	ALA	2.5
13	M1	70	THR	2.5
22	n1	25	VAL	2.5
47	s1	21	VAL	2.5
50	S4	126	VAL	2.5
51	S5	35	GLN	2.5
56	C0	12	HIS	2.5
60	c4	42	VAL	2.5
60	c4	81	VAL	2.5
77	SR	133	VAL	2.5
13	m1	60	ARG	2.5
29	N8	124	ILE	2.5
46	S0	170	ILE	2.5
13	m1	26	SER	2.5
27	n6	53	ASP	2.5
56	c0	60	SER	2.5
7	l5	122	VAL	2.5
10	l8	114	ALA	2.5
11	L9	93	VAL	2.5
58	c2	42	ALA	2.5
60	c4	47	LYS	2.5
55	s9	112	GLN	2.5
61	C5	116	LEU	2.5
7	l5	153	THR	2.5
72	d6	51	ARG	2.5
77	SR	233	THR	2.5
54	s8	60	ILE	2.5
28	n7	9	LYS	2.5
51	s5	213	LYS	2.5
52	S6	222	GLU	2.5
62	C6	113	ASP	2.5
79	s6	51	LYS	2.5
11	L9	3	TYR	2.5
16	m5	6	TYR	2.5
46	S0	36	TYR	2.5
63	c7	65	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
73	d7	54	VAL	2.5
28	n7	103	GLN	2.5
34	O3	60	ARG	2.5
47	S1	218	LEU	2.5
50	S4	238	LEU	2.5
54	s8	44	HIS	2.5
74	d8	61	ARG	2.5
4	l2	100	ASN	2.5
46	S0	173	ILE	2.5
49	s3	152	PHE	2.5
55	s9	146	PHE	2.5
57	C1	20	PHE	2.5
58	c2	140	PHE	2.5
77	SR	224	ASN	2.5
77	sR	182	ASN	2.5
53	S7	98	ILE	2.5
62	c6	17	THR	2.5
11	L9	189	GLU	2.5
62	c6	99	GLU	2.5
70	D4	37	LYS	2.5
10	L8	189	LEU	2.5
28	N7	44	ALA	2.5
28	N7	62	VAL	2.5
48	s2	196	VAL	2.5
51	s5	56	ALA	2.5
52	S6	177	ARG	2.5
58	c2	20	ALA	2.5
77	sR	83	ALA	2.5
27	N6	42	GLN	2.5
56	c0	12	HIS	2.5
64	c8	122	HIS	2.5
16	m5	122	ASN	2.5
43	q2	24	LYS	2.5
62	c6	70	THR	2.5
77	sR	46	LYS	2.5
35	o4	110	GLU	2.5
13	m1	128	TYR	2.5
14	M3	119	TYR	2.5
29	n8	127	ALA	2.5
43	q2	35	LEU	2.5
49	S3	73	VAL	2.5
49	s3	60	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
63	c7	80	ARG	2.5
55	s9	128	LEU	2.5
66	d0	31	VAL	2.5
71	d5	62	VAL	2.5
76	E0	42	ARG	2.5
48	S2	138	PRO	2.5
52	S6	8	PRO	2.5
10	l8	121	SER	2.5
54	s8	170	SER	2.5
65	c9	25	GLN	2.5
68	D2	37	PHE	2.5
77	sR	87	LYS	2.5
11	l9	59	ASN	2.5
13	m1	63	GLU	2.5
35	o4	60	ARG	2.5
61	c5	108	ARG	2.5
64	c8	19	ASN	2.5
7	L5	51	LEU	2.5
28	n7	113	VAL	2.5
29	N8	130	VAL	2.5
61	C5	63	ALA	2.5
63	c7	73	LEU	2.5
79	s6	129	VAL	2.5
47	S1	128	LYS	2.5
57	C1	16	GLN	2.5
77	SR	247	PRO	2.5
4	l2	135	ILE	2.5
13	M1	14	ILE	2.5
28	N7	105	SER	2.5
30	n9	21	ILE	2.5
48	s2	139	ILE	2.5
7	l5	154	THR	2.5
27	N6	104	LEU	2.5
56	c0	68	LEU	2.5
76	E0	4	VAL	2.5
49	s3	141	LYS	2.5
54	s8	182	TYR	2.5
59	C3	27	LYS	2.5
62	c6	8	GLN	2.5
48	s2	110	HIS	2.5
61	c5	40	ARG	2.5
63	c7	41	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
7	L5	171	LEU	2.4
47	s1	124	ASN	2.4
51	s5	165	LEU	2.4
58	c2	103	LEU	2.4
62	C6	90	VAL	2.4
66	D0	63	LEU	2.4
51	S5	210	ALA	2.4
60	c4	26	THR	2.4
62	c6	46	PHE	2.4
46	s0	160	ILE	2.4
49	s3	84	ILE	2.4
51	s5	121	ILE	2.4
64	c8	69	ILE	2.4
74	d8	64	ARG	2.4
77	SR	266	ASP	2.4
27	N6	105	VAL	2.4
28	n7	21	LYS	2.4
35	O4	66	SER	2.4
46	s0	176	LEU	2.4
50	S4	42	LEU	2.4
50	s4	6	LYS	2.4
52	S6	109	LEU	2.4
58	C2	58	LEU	2.4
62	c6	57	LEU	2.4
64	c8	130	GLY	2.4
66	D0	51	VAL	2.4
71	D5	72	GLY	2.4
25	n4	104	ASN	2.4
39	O8	15	THR	2.4
47	S1	42	ASN	2.4
50	S4	99	PHE	2.4
76	E0	35	TYR	2.4
10	l8	153	ILE	2.4
13	m1	21	ILE	2.4
51	s5	144	GLU	2.4
55	S9	138	LYS	2.4
20	m9	18	GLY	2.4
49	s3	136	VAL	2.4
51	s5	205	SER	2.4
58	C2	116	VAL	2.4
58	c2	78	LEU	2.4
68	D2	7	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
70	d4	56	SER	2.4
51	s5	82	PHE	2.4
58	c2	101	ALA	2.4
67	d1	53	TYR	2.4
70	D4	60	PHE	2.4
62	C6	62	ASN	2.4
13	m1	108	GLU	2.4
22	N1	100	LYS	2.4
25	n4	77	LYS	2.4
45	2	1060	U	2.4
49	S3	115	ILE	2.4
62	c6	106	LYS	2.4
63	c7	29	GLN	2.4
65	c9	84	LYS	2.4
68	D2	86	ILE	2.4
10	l8	203	VAL	2.4
11	L9	85	GLY	2.4
12	M0	48	LEU	2.4
30	n9	45	HIS	2.4
55	s9	85	VAL	2.4
62	c6	33	GLY	2.4
77	sR	68	VAL	2.4
79	s6	88	ARG	2.4
30	n9	27	TYR	2.4
65	C9	33	TYR	2.4
22	n1	42	ILE	2.4
49	S3	185	LYS	2.4
54	S8	137	LYS	2.4
77	SR	277	GLU	2.4
46	S0	147	THR	2.4
60	c4	89	THR	2.4
21	N0	76	GLY	2.4
46	s0	166	GLY	2.4
47	s1	61	LEU	2.4
50	s4	46	VAL	2.4
50	s4	136	VAL	2.4
56	c0	76	LEU	2.4
59	C3	60	VAL	2.4
65	c9	121	GLY	2.4
71	d5	69	LEU	2.4
76	e0	54	ARG	2.4
79	s6	54	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
31	o0	105	ALA	2.4
49	s3	92	GLN	2.4
10	l8	197	VAL	2.4
51	S5	102	ARG	2.4
51	s5	125	THR	2.4
52	S6	68	LEU	2.4
62	c6	90	VAL	2.4
62	c6	110	THR	2.4
63	c7	16	LEU	2.4
76	E0	41	THR	2.4
77	SR	194	GLY	2.4
45	2	192	U	2.4
79	s6	28	PHE	2.4
7	l5	183	TRP	2.4
21	N0	2	ALA	2.4
36	o5	51	ILE	2.4
51	s5	57	SER	2.4
22	n1	89	LEU	2.4
24	n3	7	GLN	2.4
22	n1	61	THR	2.4
49	s3	55	THR	2.4
50	S4	135	GLY	2.4
51	S5	67	PRO	2.4
59	C3	67	THR	2.4
64	c8	75	ASN	2.4
62	c6	102	LYS	2.4
62	c6	133	GLY	2.4
74	D8	30	VAL	2.4
78	SM	50	ASN	2.4
79	s6	41	VAL	2.4
54	S8	53	LYS	2.4
23	n2	33	TYR	2.4
8	l6	130	ILE	2.4
13	M1	79	ILE	2.4
19	m8	69	ARG	2.4
29	N8	82	ILE	2.4
56	c0	77	ARG	2.4
29	n8	105	LEU	2.4
46	S0	73	VAL	2.4
70	d4	96	LEU	2.4
79	s6	3	LEU	2.4
14	m3	76	THR	2.4

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Mol	Chain	Res	Type	RSRZ
21	N0	4	PHE	2.4
46	S0	39	ASN	2.4
68	D2	48	GLY	2.4
49	s3	25	PHE	2.4
49	s3	70	THR	2.4
55	s9	169	PRO	2.4
13	M1	66	ALA	2.4
4	l2	88	ILE	2.4
13	M1	59	ILE	2.4
50	S4	212	ASP	2.4
73	d7	53	ALA	2.4
45	6	1491	U	2.4
63	C7	50	ILE	2.4
29	n8	101	VAL	2.4
56	c0	44	LYS	2.4
68	D2	39	GLN	2.4
77	SR	71	CYS	2.4
35	o4	93	PHE	2.4
55	S9	32	GLY	2.4
27	N6	43	TYR	2.4
46	S0	53	THR	2.4
51	S5	73	THR	2.4
74	D8	22	ARG	2.4
45	6	503	G	2.4
53	S7	91	ILE	2.4
53	s7	91	ILE	2.4
58	c2	93	ASP	2.4
64	C8	28	ILE	2.4
64	C8	80	LYS	2.4
66	d0	77	LYS	2.4
71	D5	43	ASP	2.4
55	S9	99	LEU	2.4
13	m1	34	SER	2.4
43	Q2	106	PHE	2.4
63	c7	42	GLN	2.4
37	o6	62	ARG	2.4
36	o5	84	LYS	2.4
38	o7	86	ALA	2.4
57	c1	146	ALA	2.4
61	c5	88	GLU	2.4
65	C9	127	ASN	2.4
71	d5	100	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
77	sR	41	THR	2.4
13	M1	17	LEU	2.4
65	c9	28	LEU	2.4
4	L2	248	GLY	2.4
22	N1	40	VAL	2.4
68	D2	129	VAL	2.4
10	l8	94	PHE	2.4
26	n5	32	PHE	2.4
50	S4	41	SER	2.4
77	SR	166	SER	2.4
10	l8	245	LYS	2.4
48	s2	85	PRO	2.4
65	C9	136	ALA	2.4
71	D5	85	LYS	2.4
77	SR	53	LYS	2.4
78	sM	49	LYS	2.4
19	m8	100	THR	2.4
29	N8	102	ILE	2.4
35	O4	54	ILE	2.4
51	S5	103	ASN	2.4
53	S7	46	ILE	2.4
41	Q0	127	LEU	2.4
46	S0	172	LEU	2.4
53	S7	154	LEU	2.4
12	M0	114	GLY	2.3
75	D9	52	PHE	2.3
58	c2	132	GLU	2.3
66	D0	66	SER	2.3
77	SR	132	LYS	2.3
1	1	2522	G	2.3
7	l5	92	LEU	2.3
47	S1	168	ILE	2.3
74	d8	10	ALA	2.3
77	sR	255	ALA	2.3
79	s6	100	ALA	2.3
1	1	2539	C	2.3
13	m1	130	VAL	2.3
22	n1	45	ASN	2.3
48	s2	184	VAL	2.3
50	S4	11	ARG	2.3
57	C1	135	VAL	2.3
64	c8	120	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
73	D7	49	HIS	2.3
74	d8	30	VAL	2.3
74	d8	51	ASN	2.3
26	n5	84	PHE	2.3
39	O8	43	PHE	2.3
77	SR	19	TRP	2.3
77	SR	294	TRP	2.3
12	M0	76	MET	2.3
77	SR	87	LYS	2.3
1	5	1763	U	2.3
4	l2	96	LEU	2.3
10	l8	237	ILE	2.3
15	m4	58	ILE	2.3
25	n4	80	ARG	2.3
50	S4	239	PRO	2.3
55	s9	140	ILE	2.3
63	C7	38	ILE	2.3
61	c5	127	ARG	2.3
64	c8	126	ARG	2.3
67	d1	69	LEU	2.3
30	N9	52	LYS	2.3
51	S5	80	LYS	2.3
54	S8	138	ASN	2.3
61	c5	100	LYS	2.3
63	C7	31	ASN	2.3
65	C9	14	PHE	2.3
66	d0	70	THR	2.3
74	d8	8	THR	2.3
18	M7	179	GLN	2.3
51	s5	50	GLU	2.3
1	5	1814	A	2.3
7	l5	77	ALA	2.3
47	S1	172	LEU	2.3
48	s2	143	TYR	2.3
48	s2	169	LEU	2.3
50	S4	169	ILE	2.3
51	s5	29	ILE	2.3
54	s8	43	ILE	2.3
62	C6	96	TYR	2.3
77	SR	295	SER	2.3
45	2	1682	U	2.3
23	N2	28	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
48	S2	88	LYS	2.3
49	S3	161	GLY	2.3
50	s4	208	VAL	2.3
77	sR	283	LYS	2.3
78	SM	67	GLY	2.3
14	M3	92	THR	2.3
47	S1	229	MET	2.3
43	Q2	105	GLN	2.3
47	S1	220	GLN	2.3
49	s3	38	GLU	2.3
55	S9	33	GLU	2.3
1	1	1578	C	2.3
1	5	1812	G	2.3
37	o6	70	ARG	2.3
49	s3	190	ARG	2.3
64	C8	145	ARG	2.3
74	d8	42	ARG	2.3
47	s1	218	LEU	2.3
49	s3	176	LEU	2.3
49	s3	205	ALA	2.3
77	sR	232	TYR	2.3
11	L9	55	VAL	2.3
48	S2	101	VAL	2.3
49	s3	126	VAL	2.3
50	S4	31	PRO	2.3
58	C2	90	LYS	2.3
65	c9	20	SER	2.3
66	D0	118	VAL	2.3
69	d3	145	SER	2.3
77	sR	37	SER	2.3
7	L5	170	GLY	2.3
22	N1	146	ASN	2.3
49	s3	103	GLU	2.3
63	C7	76	GLU	2.3
50	S4	159	THR	2.3
28	n7	73	LYS	2.3
48	s2	187	LEU	2.3
56	c0	11	ILE	2.3
61	c5	123	TYR	2.3
63	C7	41	ILE	2.3
74	D8	40	ILE	2.3
32	O1	107	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
64	c8	128	PHE	2.3
77	SR	290	VAL	2.3
45	2	143	G	2.3
53	s7	106	SER	2.3
7	l5	186	GLU	2.3
51	S5	192	GLU	2.3
55	S9	126	ARG	2.3
59	c3	58	HIS	2.3
62	c6	82	ARG	2.3
37	o6	91	ASN	2.3
7	l5	49	TYR	2.3
7	l5	163	LEU	2.3
18	M7	180	LYS	2.3
10	l8	75	ILE	2.3
50	s4	45	ILE	2.3
51	s5	174	LEU	2.3
58	c2	124	LYS	2.3
79	s6	115	LYS	2.3
57	C1	131	ILE	2.3
77	sR	238	ASP	2.3
10	l8	151	VAL	2.3
11	L9	167	VAL	2.3
23	n2	96	VAL	2.3
32	O1	93	VAL	2.3
59	c3	60	VAL	2.3
60	c4	44	GLY	2.3
77	SR	97	GLY	2.3
29	N8	93	SER	2.3
32	O1	11	GLU	2.3
51	s5	143	ARG	2.3
66	D0	76	SER	2.3
66	d0	68	ARG	2.3
66	d0	76	SER	2.3
71	d5	68	ARG	2.3
7	l5	120	LYS	2.3
47	s1	216	LYS	2.3
19	m8	140	LEU	2.3
27	N6	45	ILE	2.3
7	L5	215	ASP	2.3
7	l5	76	ALA	2.3
33	O2	2	ALA	2.3
35	O4	89	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
43	Q2	70	LEU	2.3
46	s0	184	LEU	2.3
65	C9	138	GLN	2.3
58	c2	27	ALA	2.3
65	C9	131	ASP	2.3
68	D2	20	THR	2.3
68	D2	27	ILE	2.3
79	s6	111	LEU	2.3
34	o3	59	VAL	2.3
46	s0	14	ALA	2.3
78	SM	100	THR	2.3
68	D2	121	VAL	2.3
57	c1	87	ARG	2.3
77	sR	298	GLY	2.3
47	s1	85	LYS	2.3
55	s9	21	SER	2.3
7	l5	131	LEU	2.3
50	s4	44	LEU	2.3
8	l6	9	TRP	2.3
51	S5	63	GLN	2.3
64	c8	12	GLN	2.3
70	D4	74	LEU	2.3
77	SR	195	HIS	2.3
77	sR	64	HIS	2.3
11	L9	181	VAL	2.3
46	S0	187	ALA	2.3
56	C0	16	PHE	2.3
56	c0	54	TYR	2.3
49	S3	124	ARG	2.3
64	c8	123	ARG	2.3
70	D4	33	ALA	2.3
77	SR	36	ALA	2.3
51	S5	141	GLY	2.3
1	1	2535	A	2.3
48	s2	79	GLU	2.3
77	sR	179	LYS	2.3
13	m1	91	LEU	2.3
62	c6	53	LEU	2.3
64	C8	131	LEU	2.3
77	SR	33	LEU	2.3
77	SR	42	LEU	2.3
77	sR	246	SER	2.3

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Mol	Chain	Res	Type	RSRZ
7	l5	69	ILE	2.3
10	l8	52	TRP	2.3
13	M1	109	HIS	2.3
43	q2	81	ALA	2.3
49	s3	65	ARG	2.3
51	S5	65	ARG	2.3
51	s5	77	TYR	2.3
54	s8	21	PHE	2.3
73	D7	32	PHE	2.3
77	sR	113	VAL	2.3
22	n1	60	LYS	2.3
49	S3	187	LYS	2.3
57	C1	43	LYS	2.3
77	sR	194	GLY	2.3
53	s7	134	GLU	2.3
46	S0	182	LEU	2.3
60	C4	112	ILE	2.3
12	m0	95	HIS	2.3
46	S0	74	VAL	2.3
50	S4	13	ALA	2.3
51	S5	171	ALA	2.3
52	S6	131	LYS	2.3
77	sR	236	ALA	2.3
79	s6	7	TYR	2.3
16	m5	131	GLU	2.3
48	s2	194	GLU	2.3
1	5	1023	C	2.3
22	n1	77	ASN	2.3
22	n1	90	ASN	2.3
50	S4	151	ASP	2.3
51	s5	60	ASP	2.3
63	c7	25	THR	2.3
46	S0	120	LEU	2.3
63	c7	24	LEU	2.3
71	D5	68	ARG	2.3
6	l4	299	ILE	2.3
11	L9	187	ILE	2.3
61	C5	58	LYS	2.3
70	d4	128	LYS	2.3
78	SM	23	LYS	2.3
6	l4	142	VAL	2.3
12	m0	114	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
21	N0	88	HIS	2.3
33	o2	77	ALA	2.3
51	s5	163	SER	2.3
54	s8	82	VAL	2.3
48	s2	230	TRP	2.2
54	s8	167	ALA	2.3
58	c2	61	VAL	2.3
60	C4	121	VAL	2.3
62	c6	131	GLY	2.2
77	SR	289	ALA	2.3
25	n4	92	GLU	2.2
45	2	1364	G	2.2
45	6	235	G	2.2
77	sR	160	GLU	2.2
11	L9	91	ARG	2.2
27	n6	109	LEU	2.2
36	o5	17	LEU	2.2
38	o7	73	ARG	2.2
47	S1	37	THR	2.2
51	S5	60	ASP	2.2
52	S6	69	LEU	2.2
45	6	1686	C	2.2
46	S0	141	ILE	2.2
47	s1	193	ILE	2.2
48	s2	69	ILE	2.2
48	s2	83	ILE	2.2
52	S6	64	LYS	2.2
54	s8	101	ILE	2.2
56	C0	11	ILE	2.2
62	C6	109	PHE	2.2
71	D5	78	ILE	2.2
15	M4	44	VAL	2.2
20	m9	17	VAL	2.2
12	m0	195	ALA	2.2
27	n6	81	GLN	2.2
51	S5	132	VAL	2.2
74	D8	41	VAL	2.2
25	n4	114	GLU	2.2
76	e0	59	GLY	2.2
25	n4	74	LYS	2.2
28	N7	87	LEU	2.2
47	s1	96	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
71	D5	75	LEU	2.2
76	e0	39	LEU	2.2
27	N6	98	ASN	2.2
7	l5	64	ILE	2.2
14	M3	95	ILE	2.2
39	o8	22	THR	2.2
45	2	503	G	2.2
49	s3	57	ASP	2.2
61	c5	82	ASN	2.2
78	sM	43	ASP	2.2
79	s6	18	ILE	2.2
43	Q2	4	VAL	2.2
58	c2	22	VAL	2.2
10	L8	131	ALA	2.2
13	M1	98	ALA	2.2
46	s0	99	ALA	2.2
62	C6	133	GLY	2.2
79	s6	40	ALA	2.2
12	M0	143	SER	2.2
37	o6	64	SER	2.2
47	s1	87	ARG	2.2
55	s9	184	SER	2.2
64	C8	10	SER	2.2
72	d6	82	ARG	2.2
77	SR	147	HIS	2.2
10	l8	109	LEU	2.2
39	o8	73	LEU	2.2
64	C8	49	LYS	2.2
77	sR	40	LYS	2.2
28	n7	101	PHE	2.2
35	o4	54	ILE	2.2
48	S2	66	PHE	2.2
28	n7	70	PRO	2.2
46	S0	121	VAL	2.2
51	s5	33	VAL	2.2
51	s5	146	THR	2.2
61	C5	84	ILE	2.2
64	C8	21	ASN	2.2
72	d6	79	ILE	2.2
74	d8	7	VAL	2.2
77	SR	94	VAL	2.2
15	M4	41	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
16	m5	129	TYR	2.2
49	s3	23	GLU	2.2
51	S5	195	ALA	2.2
53	S7	95	GLU	2.2
54	S8	117	TYR	2.2
66	D0	74	GLU	2.2
69	d3	29	TYR	2.2
75	D9	26	SER	2.2
77	SR	66	HIS	2.2
26	n5	126	LEU	2.2
46	S0	17	LEU	2.2
48	s2	190	LEU	2.2
64	c8	61	LEU	2.2
48	s2	115	ILE	2.2
68	D2	50	PHE	2.2
14	m3	188	ARG	2.2
28	N7	45	GLY	2.2
51	S5	139	ASN	2.2
61	c5	41	VAL	2.2
66	d0	62	VAL	2.2
36	o5	20	GLN	2.2
36	o5	83	LYS	2.2
54	s8	55	TYR	2.2
60	c4	91	THR	2.2
71	d5	58	ARG	2.2
61	C5	54	ALA	2.2
73	D7	64	CYS	2.2
79	s6	2	LYS	2.2
1	1	2206	G	2.2
8	L6	9	TRP	2.2
45	6	647	G	2.2
48	S2	248	SER	2.2
1	1	2572	C	2.2
45	2	1359	C	2.2
16	M5	60	VAL	2.2
41	Q0	106	ARG	2.2
47	S1	64	ARG	2.2
47	s1	88	VAL	2.2
57	c1	86	ILE	2.2
60	C4	83	ILE	2.2
72	D6	22	ARG	2.2
77	SR	56	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
77	SR	193	ILE	2.2
77	sR	131	ILE	2.2
79	s6	191	ARG	2.2
26	n5	60	TYR	2.2
27	N6	86	THR	2.2
30	n9	24	PRO	2.2
55	S9	89	ASP	2.2
77	SR	105	GLY	2.2
49	S3	172	THR	2.2
51	S5	131	GLN	2.2
62	C6	8	GLN	2.2
4	l2	71	LEU	2.2
7	L5	222	LEU	2.2
10	l8	189	LEU	2.2
13	m1	30	LEU	2.2
26	n5	40	LEU	2.2
46	s0	17	LEU	2.2
13	M1	115	LYS	2.2
13	m1	161	SER	2.2
33	o2	117	ILE	2.2
39	O8	45	VAL	2.2
39	o8	5	ILE	2.2
59	C3	65	VAL	2.2
63	C7	120	SER	2.2
70	d4	21	LYS	2.2
71	D5	46	LYS	2.2
1	5	1803	C	2.2
22	n1	94	GLU	2.2
28	n7	18	TYR	2.2
7	L5	151	GLN	2.2
7	L5	233	ALA	2.2
13	M1	93	ASP	2.2
49	s3	93	ASP	2.2
69	d3	113	ALA	2.2
48	s2	156	THR	2.2
52	S6	56	ASN	2.2
55	S9	93	LEU	2.2
64	C8	86	LEU	2.2
77	sR	209	THR	2.2
54	S8	8	ARG	2.2
14	m3	95	ILE	2.2
22	n1	71	SER	2.2

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Mol	Chain	Res	Type	RSRZ
35	O4	105	VAL	2.2
48	s2	178	ILE	2.2
66	D0	69	LYS	2.2
51	s5	206	SER	2.2
10	l8	178	ALA	2.2
23	n2	78	TYR	2.2
22	n1	106	LEU	2.2
55	s9	139	GLN	2.2
75	D9	41	GLN	2.2
28	n7	133	LYS	2.2
48	s2	49	LYS	2.2
58	c2	49	THR	2.2
62	c6	128	LYS	2.2
66	d0	78	THR	2.2
70	D4	119	PHE	2.2
79	s6	30	LYS	2.2
13	m1	157	GLU	2.2
39	o8	45	VAL	2.2
64	c8	92	ILE	2.2
70	D4	25	VAL	2.2
70	D4	57	VAL	2.2
77	SR	219	GLU	2.2
77	sR	290	VAL	2.2
79	s6	49	VAL	2.2
47	s1	233	GLY	2.2
30	n9	57	ALA	2.2
58	c2	94	ALA	2.2
59	C3	45	LEU	2.2
63	C7	15	ALA	2.2
67	D1	58	TYR	2.2
50	S4	20	LEU	2.2
10	l8	42	PRO	2.2
59	c3	62	GLN	2.2
66	D0	77	LYS	2.2
67	D1	87	ARG	2.2
79	s6	182	GLN	2.2
48	s2	226	THR	2.2
77	SR	130	THR	2.2
77	SR	159	ASN	2.2
13	M1	148	VAL	2.2
35	o4	34	HIS	2.2
50	s4	36	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
55	S9	72	GLU	2.2
62	c6	55	VAL	2.2
65	c9	64	HIS	2.2
50	s4	124	GLY	2.2
14	M3	132	ALA	2.2
19	m8	76	ALA	2.2
26	N5	87	SER	2.2
48	S2	222	TYR	2.2
49	s3	108	LYS	2.2
51	S5	209	TYR	2.2
51	s5	175	LEU	2.2
53	S7	52	ALA	2.2
68	D2	68	ARG	2.2
70	d4	117	LYS	2.2
7	L5	232	ASP	2.2
27	N6	58	VAL	2.2
46	S0	58	VAL	2.2
47	s1	43	VAL	2.2
54	s8	169	ILE	2.2
65	c9	16	ASN	2.2
70	D4	24	VAL	2.2
74	D8	44	VAL	2.2
35	o4	78	GLY	2.2
50	s4	4	GLY	2.2
55	s9	73	GLY	2.2
29	n8	117	ARG	2.2
7	l5	195	LEU	2.2
10	l8	169	LEU	2.2
13	M1	75	LYS	2.2
14	m3	193	ALA	2.2
55	s9	109	LEU	2.2
56	C0	15	LEU	2.2
77	SR	281	TYR	2.2
21	N0	75	PHE	2.2
53	s7	42	GLN	2.2
37	o6	88	GLU	2.2
57	c1	121	ASP	2.2
60	c4	28	VAL	2.2
60	c4	112	ILE	2.2
63	C7	18	GLU	2.2
77	SR	262	VAL	2.2
39	o8	6	THR	2.2

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Mol	Chain	Res	Type	RSRZ
51	S5	109	LYS	2.2
52	S6	174	LYS	2.2
57	C1	6	THR	2.2
61	C5	64	LYS	2.2
61	c5	98	ASN	2.2
64	c8	20	THR	2.2
64	c8	144	ARG	2.2
54	S8	96	LEU	2.1
4	L2	90	ALA	2.1
16	m5	110	ALA	2.1
78	SM	80	ALA	2.1
10	l8	79	GLN	2.1
18	M7	172	GLN	2.1
35	o4	73	SER	2.1
47	S1	30	PHE	2.1
47	S1	138	PHE	2.1
53	s7	24	PHE	2.1
77	sR	235	SER	2.1
43	q2	73	GLU	2.1
47	S1	59	ASP	2.1
49	S3	58	VAL	2.1
43	q2	76	LYS	2.1
50	S4	122	LYS	2.1
50	s4	39	ARG	2.1
51	s5	148	ARG	2.1
56	c0	43	ILE	2.1
57	c1	122	ILE	2.1
66	d0	13	GLU	2.1
70	D4	35	VAL	2.1
76	E0	23	LYS	2.1
77	sR	297	ASP	2.1
23	N2	33	TYR	2.1
32	O1	16	LEU	2.1
45	6	1800	A	2.1
46	S0	202	TYR	2.1
51	s5	21	THR	2.1
52	S6	180	THR	2.1
59	C3	61	THR	2.1
61	c5	15	HIS	2.1
66	D0	27	THR	2.1
55	S9	159	ALA	2.1
61	C5	37	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
48	S2	57	PHE	2.1
23	n2	77	LYS	2.1
25	n4	73	ARG	2.1
25	n4	110	LYS	2.1
26	n5	25	LYS	2.1
47	S1	165	ARG	2.1
54	S8	78	ILE	2.1
58	C2	83	GLU	2.1
63	C7	23	LYS	2.1
63	C7	79	GLU	2.1
72	D6	2	PRO	2.1
25	n4	84	GLY	2.1
77	sR	97	GLY	2.1
39	O8	54	LEU	2.1
47	s1	70	LEU	2.1
50	s4	123	LEU	2.1
7	L5	55	PHE	2.1
39	o8	23	ALA	2.1
51	s5	72	HIS	2.1
50	S4	226	PHE	2.1
53	S7	78	THR	2.1
62	C6	115	THR	2.1
74	d8	19	THR	2.1
77	SR	319	ASN	2.1
79	s6	16	PHE	2.1
22	n1	92	ARG	2.1
15	M4	58	ILE	2.1
28	n7	12	VAL	2.1
35	O4	108	GLN	2.1
47	S1	55	LYS	2.1
51	s5	114	ILE	2.1
51	s5	170	GLN	2.1
64	C8	57	ARG	2.1
67	d1	33	GLN	2.1
77	SR	69	GLN	2.1
7	l5	182	GLY	2.1
52	S6	90	GLY	2.1
77	SR	291	SER	2.1
77	SR	316	MET	2.1
10	l8	238	LEU	2.1
36	o5	21	LEU	2.1
43	Q2	85	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
55	s9	76	LEU	2.1
4	l2	115	ASN	2.1
22	n1	35	LYS	2.1
27	N6	87	LYS	2.1
32	O1	50	ARG	2.1
43	Q2	71	ARG	2.1
54	S8	139	ALA	2.1
57	c1	138	ASN	2.1
58	c2	130	THR	2.1
64	C8	16	ARG	2.1
64	C8	96	LYS	2.1
74	d8	11	LYS	2.1
77	SR	285	ALA	2.1
77	sR	12	THR	2.1
27	N6	88	GLU	2.1
46	s0	121	VAL	2.1
55	s9	110	GLN	2.1
65	c9	111	ILE	2.1
29	n8	116	GLY	2.1
34	o3	61	GLY	2.1
46	S0	44	GLY	2.1
48	S2	154	LEU	2.1
50	S4	167	GLY	2.1
58	c2	82	PRO	2.1
70	D4	125	LEU	2.1
7	L5	78	ALA	2.1
35	o4	43	LYS	2.1
49	s3	102	ALA	2.1
49	s3	225	TYR	2.1
50	S4	108	ARG	2.1
61	C5	123	TYR	2.1
73	D7	82	LYS	2.1
74	D8	10	ALA	2.1
47	s1	215	VAL	2.1
48	s2	96	THR	2.1
68	d2	70	ASN	2.1
4	l2	102	LEU	2.1
7	l5	146	LEU	2.1
13	m1	103	GLY	2.1
61	c5	91	GLY	2.1
63	C7	57	LEU	2.1
66	D0	26	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
13	M1	119	SER	2.1
47	s1	51	SER	2.1
77	sR	166	SER	2.1
70	D4	85	PHE	2.1
17	M6	185	ALA	2.1
58	c2	35	ALA	2.1
58	c2	128	ALA	2.1
77	sR	284	ALA	2.1
16	m5	91	GLU	2.1
50	S4	17	HIS	2.1
56	c0	22	VAL	2.1
64	c8	137	HIS	2.1
58	C2	130	THR	2.1
62	C6	70	THR	2.1
65	c9	100	ILE	2.1
66	D0	62	VAL	2.1
68	d2	63	VAL	2.1
78	sM	58	GLU	2.1
11	l9	144	ILE	2.1
39	o8	40	GLN	2.1
22	n1	85	LEU	2.1
12	M0	49	CYS	2.1
43	Q2	89	LYS	2.1
47	S1	219	LYS	2.1
48	s2	133	LYS	2.1
49	S3	21	LEU	2.1
53	s7	40	PRO	2.1
54	S8	168	CYS	2.1
55	s9	39	LYS	2.1
77	SR	107	LYS	2.1
79	s6	137	ARG	2.1
58	c2	87	PRO	2.1
53	S7	115	SER	2.1
7	L5	76	ALA	2.1
53	S7	94	ALA	2.1
54	S8	106	ALA	2.1
59	C3	90	TYR	2.1
16	m5	66	VAL	2.1
28	n7	24	VAL	2.1
10	l8	65	LEU	2.1
50	S4	39	ARG	2.1
51	S5	106	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
54	s8	138	ASN	2.1
55	S9	79	ARG	2.1
63	C7	29	GLN	2.1
46	S0	142	PRO	2.1
46	s0	155	PHE	2.1
51	s5	129	PRO	2.1
19	M8	65	SER	2.1
62	C6	6	SER	2.1
65	C9	58	ALA	2.1
7	l5	37	VAL	2.1
13	M1	110	ILE	2.1
27	n6	108	LYS	2.1
28	n7	64	LYS	2.1
29	n8	138	ILE	2.1
4	l2	58	LEU	2.1
22	N1	151	LEU	2.1
37	o6	82	ARG	2.1
46	S0	122	ILE	2.1
47	S1	214	LYS	2.1
47	s1	62	LYS	2.1
49	S3	204	ASP	2.1
51	s5	168	VAL	2.1
53	s7	90	VAL	2.1
55	s9	138	LYS	2.1
62	C6	74	HIS	2.1
64	C8	127	HIS	2.1
77	SR	176	LYS	2.1
31	O0	14	LEU	2.1
31	o0	12	GLN	2.1
48	s2	114	GLY	2.1
49	s3	21	LEU	2.1
77	sR	223	TRP	2.1
35	o4	25	THR	2.1
46	s0	49	ASN	2.1
1	1	1562	C	2.1
16	m5	30	TYR	2.1
78	SM	38	PRO	2.1
58	c2	90	LYS	2.1
62	c6	119	ALA	2.1
77	sR	14	GLU	2.1
51	S5	111	VAL	2.1
53	s7	51	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
63	C7	80	ARG	2.1
64	c8	72	ILE	2.1
67	D1	39	VAL	2.1
70	d4	8	ARG	2.1
74	D8	29	ARG	2.1
76	e0	45	VAL	2.1
7	l5	170	GLY	2.1
13	m1	24	GLY	2.1
14	m3	153	ASP	2.1
46	S0	157	ASP	2.1
67	d1	66	ASP	2.1
77	sR	136	ILE	2.1
73	D7	21	LEU	2.1
77	sR	202	LEU	2.1
48	S2	87	GLN	2.1
77	SR	177	MET	2.1
47	S1	119	THR	2.1
51	S5	122	ASN	2.1
64	C8	11	PHE	2.1
77	SR	174	ASN	2.1
16	m5	119	TYR	2.1
45	6	225	A	2.1
53	S7	148	LYS	2.1
57	C1	17	PRO	2.1
65	c9	144	GLU	2.1
77	sR	30	PRO	2.1
7	l5	53	VAL	2.1
46	s0	73	VAL	2.1
28	n7	68	ILE	2.1
33	o2	128	LEU	2.1
50	s4	206	ASP	2.1
55	s9	97	LEU	2.1
59	c3	54	LEU	2.1
67	D1	18	SER	2.1
28	n7	122	HIS	2.1
68	D2	127	GLY	2.1
39	o8	10	GLN	2.1
65	c9	23	GLN	2.1
10	l8	125	ALA	2.1
12	M0	140	THR	2.1
19	M8	123	THR	2.1
25	N4	47	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
47	s1	82	ARG	2.1
49	S3	67	ASN	2.1
54	S8	54	LYS	2.1
79	s6	174	LYS	2.1
28	N7	59	ALA	2.1
32	O1	40	ALA	2.1
46	s0	22	THR	2.1
49	s3	18	TYR	2.1
50	s4	15	PRO	2.1
52	S6	157	VAL	2.1
54	s8	100	ALA	2.1
56	C0	57	THR	2.1
77	SR	204	ALA	2.1
11	L9	41	ILE	2.1
16	M5	133	ILE	2.1
39	o8	54	LEU	2.1
49	s3	110	LEU	2.1
55	s9	137	GLY	2.1
59	c3	139	TRP	2.0
62	c6	138	PHE	2.0
63	c7	58	MET	2.1
77	sR	70	ASP	2.1
23	n2	90	ARG	2.0
37	o6	75	LYS	2.0
45	6	234	G	2.0
49	S3	61	GLU	2.0
12	M0	68	ALA	2.0
13	M1	45	PRO	2.0
35	o4	68	THR	2.0
77	sR	151	VAL	2.0
79	s6	128	THR	2.0
14	M3	130	GLY	2.0
28	n7	80	LEU	2.0
29	n8	148	ILE	2.0
32	o1	75	ILE	2.0
63	c7	50	ILE	2.0
35	o4	3	GLN	2.0
46	S0	23	HIS	2.0
52	S6	31	ARG	2.0
52	S6	142	ARG	2.0
54	S8	56	ARG	2.0
64	c8	78	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
32	O1	68	GLU	2.0
45	2	239	C	2.0
55	s9	186	GLU	2.0
4	l2	35	ALA	2.0
48	S2	249	ALA	2.0
69	D3	12	ALA	2.0
75	D9	6	VAL	2.0
77	SR	232	TYR	2.0
77	sR	226	ALA	2.0
46	S0	103	THR	2.0
47	S1	49	ASN	2.0
51	s5	142	PRO	2.0
63	C7	100	LEU	2.0
77	SR	310	ILE	2.0
11	L9	174	LYS	2.0
28	n7	118	PHE	2.0
45	2	766	U	2.0
70	d4	122	GLY	2.0
79	s6	116	LYS	2.0
53	S7	70	PHE	2.0
68	D2	79	PHE	2.0
77	sR	241	PHE	2.0
10	l8	41	GLN	2.0
50	S4	142	HIS	2.0
63	C7	20	TYR	2.0
27	n6	39	LEU	2.0
32	O1	4	LEU	2.0
37	o6	86	LYS	2.0
46	S0	76	ILE	2.0
46	S0	146	LEU	2.0
49	s3	151	LYS	2.0
50	s4	173	ILE	2.0
54	S8	165	LEU	2.0
55	S9	118	LEU	2.0
63	C7	39	ALA	2.0
68	D2	82	LYS	2.0
19	m8	92	ARG	2.0
32	O1	39	PHE	2.0
36	o5	105	ARG	2.0
72	d6	69	ASN	2.0
75	D9	56	ARG	2.0
79	s6	83	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	5	2542	U	2.0
4	l2	109	GLU	2.0
62	c6	77	GLN	2.0
50	S4	209	HIS	2.0
57	C1	92	HIS	2.0
77	SR	112	SER	2.0
77	SR	205	SER	2.0
77	sR	92	TRP	2.0
20	m9	45	VAL	2.0
41	Q0	107	ALA	2.0
46	S0	98	ILE	2.0
47	S1	137	ILE	2.0
49	S3	50	ILE	2.0
50	S4	22	LYS	2.0
56	C0	75	TYR	2.0
62	c6	48	VAL	2.0
62	c6	91	ALA	2.0
66	d0	90	TYR	2.0
69	d3	72	VAL	2.0
49	S3	76	ARG	2.0
50	S4	162	ILE	2.0
51	s5	76	ARG	2.0
53	s7	16	LEU	2.0
54	s8	96	LEU	2.0
66	d0	86	ILE	2.0
51	s5	69	PHE	2.0
57	C1	137	PHE	2.0
48	S2	82	ASN	2.0
48	S2	90	THR	2.0
69	d3	27	ASN	2.0
64	C8	8	GLN	2.0
65	C9	141	GLU	2.0
73	d7	51	GLN	2.0
78	sM	120	GLU	2.0
11	L9	54	LYS	2.0
45	2	1473	U	2.0
45	6	499	U	2.0
13	M1	18	VAL	2.0
13	m1	153	LYS	2.0
29	n8	99	ALA	2.0
30	N9	57	ALA	2.0
40	o9	36	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
48	S2	240	LEU	2.0
50	s4	82	TYR	2.0
76	e0	21	VAL	2.0
77	SR	312	VAL	2.0
77	sR	229	LYS	2.0
54	S8	99	ALA	2.0
63	C7	17	ILE	2.0
78	SM	20	LEU	2.0
79	s6	154	ARG	2.0
5	l3	298	PHE	2.0
45	2	539	G	2.0
43	Q2	5	PRO	2.0
77	sR	276	PRO	2.0
21	N0	8	GLN	2.0
53	s7	108	GLN	2.0
14	m3	159	VAL	2.0
23	n2	79	LEU	2.0
46	s0	37	VAL	2.0
49	s3	182	LEU	2.0
61	C5	26	LEU	2.0
61	c5	115	TYR	2.0
71	d5	40	VAL	2.0
74	D8	55	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	5	3796	1/1	-0.24	0.33	165,165,165,165	0
81	MG	8	220	1/1	0.09	0.42	88,88,88,88	0
81	MG	2	2059	1/1	0.13	0.58	114,114,114,114	0
81	MG	5	3878	1/1	0.18	0.62	118,118,118,118	0
81	MG	2	1947	1/1	0.18	0.27	110,110,110,110	0
81	MG	5	4057	1/1	0.19	0.62	117,117,117,117	0
81	MG	1	4093	1/1	0.23	0.32	86,86,86,86	0
81	MG	1	4118	1/1	0.26	0.45	88,88,88,88	0
81	MG	2	2084	1/1	0.26	0.35	105,105,105,105	0
81	MG	1	3968	1/1	0.27	0.18	81,81,81,81	0
81	MG	1	3853	1/1	0.27	0.28	62,62,62,62	0
81	MG	5	3944	1/1	0.31	0.26	118,118,118,118	0
81	MG	5	3839	1/1	0.36	1.23	88,88,88,88	0
81	MG	2	2048	1/1	0.38	0.83	84,84,84,84	0
81	MG	6	2009	1/1	0.39	0.17	126,126,126,126	0
81	MG	5	3983	1/1	0.39	0.46	92,92,92,92	0
81	MG	m5	302	1/1	0.40	0.39	82,82,82,82	0
81	MG	5	3942	1/1	0.40	0.29	108,108,108,108	0
81	MG	1	4155	1/1	0.40	0.76	40,40,40,40	1
81	MG	1	4043	1/1	0.40	0.17	91,91,91,91	0
81	MG	5	4090	1/1	0.42	0.76	85,85,85,85	0
81	MG	1	4036	1/1	0.43	0.34	80,80,80,80	0
81	MG	8	213	1/1	0.43	0.38	67,67,67,67	0
81	MG	18	301	1/1	0.44	0.39	109,109,109,109	0
81	MG	5	3536	1/1	0.44	0.57	51,51,51,51	1
81	MG	5	3893	1/1	0.44	0.30	68,68,68,68	0
81	MG	6	1944	1/1	0.45	0.34	95,95,95,95	0
81	MG	1	3998	1/1	0.45	0.50	86,86,86,86	0
81	MG	5	3966	1/1	0.45	0.62	92,92,92,92	0
81	MG	5	4079	1/1	0.46	0.55	105,105,105,105	0
81	MG	2	2007	1/1	0.46	0.33	67,67,67,67	0
81	MG	1	3851	1/1	0.47	0.28	86,86,86,86	0
81	MG	3	206	1/1	0.47	0.27	87,87,87,87	0
81	MG	1	3903	1/1	0.47	0.50	68,68,68,68	0
81	MG	5	3967	1/1	0.47	0.31	100,100,100,100	0
81	MG	6	1943	1/1	0.48	0.29	89,89,89,89	0
81	MG	1	4100	1/1	0.48	0.63	94,94,94,94	0
81	MG	1	4117	1/1	0.50	0.16	114,114,114,114	0
81	MG	D3	202	1/1	0.51	0.45	79,79,79,79	0
81	MG	1	4035	1/1	0.52	0.18	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3507	1/1	0.52	0.23	65,65,65,65	0
81	MG	5	3789	1/1	0.52	0.37	70,70,70,70	0
81	MG	c9	201	1/1	0.53	0.09	115,115,115,115	0
81	MG	1	3857	1/1	0.53	0.30	57,57,57,57	0
81	MG	6	2028	1/1	0.53	0.24	126,126,126,126	0
81	MG	5	4059	1/1	0.53	0.43	98,98,98,98	0
81	MG	1	4099	1/1	0.53	0.58	85,85,85,85	0
81	MG	1	4114	1/1	0.53	0.38	76,76,76,76	0
81	MG	6	1952	1/1	0.54	0.17	103,103,103,103	0
81	MG	6	1946	1/1	0.54	0.23	84,84,84,84	0
81	MG	1	3502	1/1	0.54	0.22	66,66,66,66	0
81	MG	5	4091	1/1	0.55	0.55	75,75,75,75	0
81	MG	1	3521	1/1	0.55	0.41	49,49,49,49	1
81	MG	1	3849	1/1	0.55	0.20	56,56,56,56	0
81	MG	6	2063	1/1	0.55	0.37	88,88,88,88	0
81	MG	2	2069	1/1	0.55	0.28	96,96,96,96	0
81	MG	5	4033	1/1	0.56	0.18	88,88,88,88	0
81	MG	c1	201	1/1	0.56	0.35	78,78,78,78	0
81	MG	5	3685	1/1	0.56	0.64	59,59,59,59	0
81	MG	5	4025	1/1	0.56	0.50	71,71,71,71	0
81	MG	5	3914	1/1	0.57	0.34	97,97,97,97	0
81	MG	5	4019	1/1	0.57	0.80	86,86,86,86	0
81	MG	2	2061	1/1	0.57	0.50	105,105,105,105	0
81	MG	1	3924	1/1	0.57	0.56	58,58,58,58	0
81	MG	d3	202	1/1	0.57	0.27	87,87,87,87	0
81	MG	5	3999	1/1	0.57	0.47	71,71,71,71	0
81	MG	5	4085	1/1	0.57	0.42	88,88,88,88	0
81	MG	6	1937	1/1	0.57	0.76	72,72,72,72	0
81	MG	8	223	1/1	0.57	0.53	99,99,99,99	0
81	MG	6	2064	1/1	0.57	0.95	65,65,65,65	0
81	MG	5	4105	1/1	0.58	0.59	54,54,54,54	0
81	MG	5	3647	1/1	0.58	0.29	56,56,56,56	0
81	MG	6	2045	1/1	0.58	0.24	117,117,117,117	0
81	MG	5	3896	1/1	0.58	0.19	68,68,68,68	0
81	MG	5	3646	1/1	0.58	0.15	66,66,66,66	0
81	MG	5	3927	1/1	0.59	0.67	75,75,75,75	0
81	MG	5	4009	1/1	0.59	0.20	97,97,97,97	0
81	MG	5	3619	1/1	0.59	0.36	70,70,70,70	0
81	MG	5	3874	1/1	0.59	0.35	75,75,75,75	0
81	MG	1	3752	1/1	0.59	0.36	46,46,46,46	0
81	MG	1	4133	1/1	0.59	0.31	69,69,69,69	0
81	MG	3	209	1/1	0.59	0.26	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	q3	502	1/1	0.59	0.41	81,81,81,81	0
81	MG	n0	206	1/1	0.59	0.27	72,72,72,72	0
81	MG	o1	201	1/1	0.59	0.21	72,72,72,72	0
81	MG	L7	302	1/1	0.59	0.56	62,62,62,62	0
81	MG	6	2075	1/1	0.60	0.23	98,98,98,98	0
81	MG	1	3632	1/1	0.60	0.55	45,45,45,45	0
81	MG	2	1954	1/1	0.60	0.11	133,133,133,133	0
81	MG	2	2043	1/1	0.60	0.20	85,85,85,85	0
81	MG	17	305	1/1	0.60	0.30	62,62,62,62	0
81	MG	5	3855	1/1	0.60	0.40	74,74,74,74	0
81	MG	1	3963	1/1	0.60	0.45	52,52,52,52	0
81	MG	1	4033	1/1	0.60	0.41	55,55,55,55	0
81	MG	8	216	1/1	0.60	0.28	82,82,82,82	0
81	MG	2	2044	1/1	0.61	0.55	67,67,67,67	0
81	MG	1	4107	1/1	0.61	0.45	64,64,64,64	0
81	MG	5	3906	1/1	0.61	0.32	92,92,92,92	0
81	MG	N8	203	1/1	0.61	0.43	61,61,61,61	1
81	MG	5	3794	1/1	0.61	0.95	124,124,124,124	0
81	MG	5	4068	1/1	0.61	0.47	75,75,75,75	0
81	MG	1	3640	1/1	0.61	0.27	57,57,57,57	0
81	MG	2	1929	1/1	0.61	0.23	78,78,78,78	0
81	MG	6	2054	1/1	0.61	0.18	110,110,110,110	0
81	MG	1	3605	1/1	0.61	0.25	61,61,61,61	0
81	MG	L5	301	1/1	0.61	0.34	84,84,84,84	0
81	MG	5	3840	1/1	0.61	0.91	89,89,89,89	0
81	MG	5	4099	1/1	0.61	0.59	58,58,58,58	0
81	MG	5	3945	1/1	0.62	0.18	103,103,103,103	0
81	MG	5	4066	1/1	0.62	0.68	88,88,88,88	0
81	MG	1	3593	1/1	0.62	0.63	50,50,50,50	0
81	MG	2	2025	1/1	0.62	0.41	75,75,75,75	0
81	MG	8	225	1/1	0.62	0.22	77,77,77,77	0
81	MG	5	4044	1/1	0.62	0.33	64,64,64,64	0
81	MG	5	3994	1/1	0.62	0.51	59,59,59,59	0
81	MG	1	3654	1/1	0.62	0.35	47,47,47,47	0
81	MG	2	2020	1/1	0.62	0.37	83,83,83,83	0
81	MG	5	3890	1/1	0.62	0.36	78,78,78,78	0
81	MG	2	2054	1/1	0.62	0.28	86,86,86,86	0
81	MG	O1	202	1/1	0.62	0.33	63,63,63,63	0
81	MG	l3	408	1/1	0.62	0.25	71,71,71,71	0
81	MG	1	4020	1/1	0.62	0.49	49,49,49,49	1
81	MG	1	3526	1/1	0.63	0.36	48,48,48,48	0
81	MG	L9	201	1/1	0.63	0.14	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	m9	204	1/1	0.63	0.52	79,79,79,79	0
81	MG	1	4091	1/1	0.63	0.36	82,82,82,82	0
81	MG	m8	201	1/1	0.63	0.36	72,72,72,72	0
81	MG	1	4004	1/1	0.63	0.21	89,89,89,89	0
81	MG	5	4070	1/1	0.63	0.30	113,113,113,113	0
81	MG	2	2070	1/1	0.63	0.31	119,119,119,119	0
81	MG	1	3982	1/1	0.63	0.48	62,62,62,62	0
81	MG	1	4184	1/1	0.63	0.87	67,67,67,67	0
81	MG	1	3957	1/1	0.64	0.41	55,55,55,55	0
81	MG	1	4121	1/1	0.64	0.56	88,88,88,88	0
81	MG	5	3887	1/1	0.64	0.37	79,79,79,79	0
81	MG	n6	204	1/1	0.64	0.21	83,83,83,83	0
81	MG	5	3660	1/1	0.64	0.18	86,86,86,86	0
81	MG	1	3840	1/1	0.64	0.39	58,58,58,58	0
81	MG	1	4180	1/1	0.64	0.49	55,55,55,55	1
81	MG	5	3877	1/1	0.64	0.39	66,66,66,66	0
81	MG	2	2074	1/1	0.64	0.22	89,89,89,89	0
81	MG	6	2037	1/1	0.65	0.33	102,102,102,102	0
81	MG	8	222	1/1	0.65	0.42	78,78,78,78	0
81	MG	5	4067	1/1	0.65	0.80	94,94,94,94	0
81	MG	5	4125	1/1	0.65	0.21	78,78,78,78	0
81	MG	8	215	1/1	0.65	0.32	72,72,72,72	0
81	MG	1	4113	1/1	0.65	0.39	79,79,79,79	0
81	MG	8	212	1/1	0.65	0.54	74,74,74,74	0
81	MG	5	4037	1/1	0.65	0.23	65,65,65,65	0
81	MG	2	1932	1/1	0.65	0.47	83,83,83,83	0
81	MG	1	3711	1/1	0.65	0.41	44,44,44,44	0
81	MG	2	2083	1/1	0.65	0.38	101,101,101,101	0
81	MG	5	4073	1/1	0.65	0.25	77,77,77,77	0
81	MG	5	3841	1/1	0.65	1.24	82,82,82,82	0
81	MG	5	3581	1/1	0.65	0.40	55,55,55,55	0
81	MG	N1	202	1/1	0.66	0.33	61,61,61,61	0
81	MG	1	4065	1/1	0.66	0.37	69,69,69,69	0
81	MG	5	3903	1/1	0.66	0.35	87,87,87,87	0
81	MG	7	213	1/1	0.66	0.34	76,76,76,76	0
81	MG	1	3559	1/1	0.66	0.39	47,47,47,47	0
81	MG	1	4160	1/1	0.66	0.34	65,65,65,65	0
81	MG	6	1915	1/1	0.66	0.25	73,73,73,73	0
81	MG	1	4186	1/1	0.66	0.74	43,43,43,43	0
81	MG	5	3989	1/1	0.66	0.60	77,77,77,77	0
81	MG	7	204	1/1	0.66	0.44	65,65,65,65	0
81	MG	2	1931	1/1	0.66	0.25	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3827	1/1	0.66	0.90	70,70,70,70	0
81	MG	5	3901	1/1	0.66	0.29	94,94,94,94	0
81	MG	6	1981	1/1	0.66	0.33	77,77,77,77	0
81	MG	6	2067	1/1	0.66	0.78	75,75,75,75	0
81	MG	6	1998	1/1	0.66	0.39	74,74,74,74	0
81	MG	5	3842	1/1	0.67	1.44	78,78,78,78	0
81	MG	5	3677	1/1	0.67	0.70	55,55,55,55	0
81	MG	4	230	1/1	0.67	0.24	61,61,61,61	0
81	MG	6	1972	1/1	0.67	0.15	107,107,107,107	0
81	MG	L4	402	1/1	0.67	0.33	54,54,54,54	0
81	MG	6	2060	1/1	0.67	0.60	88,88,88,88	0
81	MG	2	2103	1/1	0.67	0.49	73,73,73,73	0
81	MG	2	2081	1/1	0.67	0.31	79,79,79,79	0
81	MG	5	4000	1/1	0.67	0.44	78,78,78,78	0
81	MG	5	4034	1/1	0.67	0.09	102,102,102,102	0
81	MG	5	3871	1/1	0.68	0.32	75,75,75,75	0
81	MG	6	1921	1/1	0.68	0.42	70,70,70,70	0
81	MG	1	3795	1/1	0.68	0.79	68,68,68,68	1
81	MG	4	223	1/1	0.68	0.33	65,65,65,65	0
81	MG	5	3911	1/1	0.68	0.33	63,63,63,63	0
81	MG	6	2065	1/1	0.68	0.59	66,66,66,66	0
81	MG	6	1966	1/1	0.68	0.41	88,88,88,88	0
81	MG	8	219	1/1	0.68	0.45	60,60,60,60	0
81	MG	1	4038	1/1	0.68	0.32	83,83,83,83	0
81	MG	2	2111	1/1	0.68	0.58	72,72,72,72	0
81	MG	2	2113	1/1	0.68	0.40	95,95,95,95	0
81	MG	5	4108	1/1	0.68	0.31	70,70,70,70	0
81	MG	1	4166	1/1	0.69	0.36	77,77,77,77	0
81	MG	O1	201	1/1	0.69	0.30	64,64,64,64	0
81	MG	2	2094	1/1	0.69	0.43	95,95,95,95	0
81	MG	1	3847	1/1	0.69	0.43	77,77,77,77	0
81	MG	d3	204	1/1	0.69	0.47	69,69,69,69	0
81	MG	5	3853	1/1	0.69	0.63	68,68,68,68	0
81	MG	o0	203	1/1	0.69	0.23	102,102,102,102	0
81	MG	5	3910	1/1	0.69	0.57	74,74,74,74	0
81	MG	6	2071	1/1	0.69	0.91	78,78,78,78	0
81	MG	1	3591	1/1	0.69	1.09	77,77,77,77	0
81	MG	1	3884	1/1	0.69	0.42	62,62,62,62	0
81	MG	6	2020	1/1	0.69	0.40	101,101,101,101	0
81	MG	5	4119	1/1	0.69	0.18	89,89,89,89	0
81	MG	2	1950	1/1	0.70	0.14	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	4098	1/1	0.70	0.46	48,48,48,48	0
81	MG	5	3529	1/1	0.70	0.58	55,55,55,55	0
81	MG	5	3701	1/1	0.70	0.72	70,70,70,70	0
81	MG	2	2115	1/1	0.70	0.38	118,118,118,118	0
81	MG	3	215	1/1	0.70	0.31	72,72,72,72	0
81	MG	5	4076	1/1	0.70	0.14	99,99,99,99	0
81	MG	1	4018	1/1	0.70	0.46	50,50,50,50	0
81	MG	1	4057	1/1	0.70	0.11	89,89,89,89	0
81	MG	5	3729	1/1	0.70	0.42	63,63,63,63	0
81	MG	1	4089	1/1	0.71	0.43	89,89,89,89	0
81	MG	1	3975	1/1	0.71	0.49	71,71,71,71	0
81	MG	2	2024	1/1	0.71	0.23	78,78,78,78	0
81	MG	1	3876	1/1	0.71	0.19	66,66,66,66	1
81	MG	5	3955	1/1	0.71	0.29	54,54,54,54	0
81	MG	2	1937	1/1	0.71	0.42	69,69,69,69	0
81	MG	5	3559	1/1	0.71	0.22	75,75,75,75	0
81	MG	2	1976	1/1	0.71	0.17	113,113,113,113	0
81	MG	5	3700	1/1	0.71	0.90	62,62,62,62	0
81	MG	3	210	1/1	0.71	0.13	91,91,91,91	0
81	MG	2	1940	1/1	0.71	0.96	78,78,78,78	0
81	MG	5	3625	1/1	0.71	0.34	68,68,68,68	0
81	MG	5	3828	1/1	0.71	0.62	64,64,64,64	0
81	MG	5	4013	1/1	0.71	0.42	87,87,87,87	0
81	MG	1	3860	1/1	0.71	0.43	54,54,54,54	0
81	MG	5	4061	1/1	0.71	0.32	64,64,64,64	0
81	MG	6	1953	1/1	0.71	0.23	96,96,96,96	0
81	MG	1	4123	1/1	0.72	0.25	70,70,70,70	1
81	MG	1	4095	1/1	0.72	0.41	86,86,86,86	0
81	MG	2	1986	1/1	0.72	0.32	82,82,82,82	0
81	MG	5	3561	1/1	0.72	0.68	81,81,81,81	0
81	MG	o1	203	1/1	0.72	0.14	74,74,74,74	0
81	MG	6	1947	1/1	0.72	0.20	113,113,113,113	0
81	MG	2	2019	1/1	0.72	0.50	81,81,81,81	0
81	MG	5	3875	1/1	0.72	0.34	75,75,75,75	0
81	MG	1	3965	1/1	0.72	0.27	53,53,53,53	1
81	MG	5	4045	1/1	0.72	0.24	67,67,67,67	0
81	MG	2	2091	1/1	0.72	0.20	81,81,81,81	0
81	MG	1	3548	1/1	0.72	0.46	67,67,67,67	0
81	MG	1	4131	1/1	0.72	0.20	71,71,71,71	0
81	MG	6	1965	1/1	0.72	0.24	104,104,104,104	0
81	MG	2	2016	1/1	0.72	0.32	84,84,84,84	0
81	MG	6	2070	1/1	0.72	0.79	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	6	2029	1/1	0.72	0.31	77,77,77,77	0
81	MG	1	4183	1/1	0.72	0.16	96,96,96,96	0
81	MG	17	304	1/1	0.72	0.24	66,66,66,66	0
81	MG	5	3615	1/1	0.72	0.31	82,82,82,82	0
81	MG	6	2041	1/1	0.72	0.18	101,101,101,101	0
81	MG	5	3846	1/1	0.72	1.03	89,89,89,89	0
81	MG	o2	204	1/1	0.72	0.41	62,62,62,62	0
81	MG	5	3960	1/1	0.72	0.39	44,44,44,44	0
81	MG	1	3967	1/1	0.72	0.18	77,77,77,77	0
81	MG	6	2011	1/1	0.72	0.52	69,69,69,69	0
81	MG	1	3634	1/1	0.73	0.72	48,48,48,48	0
81	MG	6	1941	1/1	0.73	0.30	80,80,80,80	0
81	MG	1	3955	1/1	0.73	0.25	59,59,59,59	0
81	MG	1	3785	1/1	0.73	0.32	69,69,69,69	0
81	MG	5	3980	1/1	0.73	0.28	97,97,97,97	0
81	MG	1	4187	1/1	0.73	0.29	50,50,50,50	0
81	MG	6	1992	1/1	0.73	0.32	86,86,86,86	0
81	MG	2	2078	1/1	0.73	0.11	100,100,100,100	0
81	MG	6	1924	1/1	0.73	0.33	83,83,83,83	0
81	MG	O2	202	1/1	0.73	0.64	44,44,44,44	0
81	MG	m9	203	1/1	0.73	0.14	78,78,78,78	0
81	MG	5	4038	1/1	0.73	0.51	68,68,68,68	0
81	MG	2	1991	1/1	0.73	0.33	91,91,91,91	0
81	MG	6	2053	1/1	0.73	0.26	123,123,123,123	0
81	MG	2	2071	1/1	0.73	0.25	67,67,67,67	0
81	MG	5	3572	1/1	0.73	0.29	72,72,72,72	0
81	MG	5	3959	1/1	0.73	0.43	59,59,59,59	0
81	MG	1	4070	1/1	0.73	0.17	84,84,84,84	0
81	MG	5	3998	1/1	0.73	0.56	63,63,63,63	0
81	MG	n8	201	1/1	0.73	0.18	55,55,55,55	0
81	MG	2	2026	1/1	0.73	0.46	69,69,69,69	0
81	MG	5	3769	1/1	0.73	0.58	53,53,53,53	0
81	MG	5	3622	1/1	0.73	0.31	69,69,69,69	0
81	MG	n6	201	1/1	0.73	0.31	71,71,71,71	0
81	MG	6	2024	1/1	0.73	0.11	119,119,119,119	0
81	MG	6	2014	1/1	0.73	0.37	89,89,89,89	0
81	MG	1	3806	1/1	0.73	0.35	50,50,50,50	0
81	MG	2	2010	1/1	0.74	0.48	64,64,64,64	0
81	MG	1	4173	1/1	0.74	0.41	58,58,58,58	0
81	MG	1	4098	1/1	0.74	0.83	89,89,89,89	0
81	MG	5	4087	1/1	0.74	0.26	85,85,85,85	0
81	MG	2	1923	1/1	0.74	0.41	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	4116	1/1	0.74	0.49	61,61,61,61	0
81	MG	5	3952	1/1	0.74	0.60	57,57,57,57	0
81	MG	5	3951	1/1	0.74	0.48	55,55,55,55	0
81	MG	5	3812	1/1	0.74	0.34	55,55,55,55	0
81	MG	6	2034	1/1	0.74	0.36	70,70,70,70	0
81	MG	5	3679	1/1	0.74	0.50	52,52,52,52	0
81	MG	1	4085	1/1	0.74	0.36	62,62,62,62	0
80	PAR	5	3423	42/42	0.74	0.41	86,86,86,86	42
81	MG	2	1912	1/1	0.74	0.23	92,92,92,92	0
81	MG	1	3715	1/1	0.74	0.37	46,46,46,46	0
81	MG	1	3974	1/1	0.74	0.39	58,58,58,58	0
81	MG	1	4198	1/1	0.74	0.49	68,68,68,68	0
81	MG	1	4174	1/1	0.74	0.34	54,54,54,54	0
81	MG	5	3586	1/1	0.74	0.30	64,64,64,64	0
81	MG	1	3904	1/1	0.74	0.40	63,63,63,63	0
81	MG	1	4079	1/1	0.74	0.28	59,59,59,59	0
81	MG	5	4126	1/1	0.75	0.30	78,78,78,78	0
81	MG	2	2011	1/1	0.75	0.48	101,101,101,101	0
81	MG	d3	205	1/1	0.75	0.34	78,78,78,78	0
81	MG	5	4115	1/1	0.75	0.70	74,74,74,74	0
81	MG	3	216	1/1	0.75	0.13	72,72,72,72	0
81	MG	5	4092	1/1	0.75	0.29	67,67,67,67	0
81	MG	2	2108	1/1	0.75	0.22	110,110,110,110	0
81	MG	5	3844	1/1	0.75	0.89	81,81,81,81	0
81	MG	1	4111	1/1	0.75	0.35	65,65,65,65	0
81	MG	l3	405	1/1	0.75	0.37	66,66,66,66	0
81	MG	Q2	505	1/1	0.75	0.28	42,42,42,42	0
81	MG	1	3993	1/1	0.75	0.41	46,46,46,46	0
81	MG	6	1949	1/1	0.75	0.21	83,83,83,83	0
81	MG	5	3631	1/1	0.75	0.32	62,62,62,62	0
81	MG	5	4050	1/1	0.75	0.26	57,57,57,57	1
81	MG	5	4082	1/1	0.75	0.51	79,79,79,79	0
81	MG	1	4139	1/1	0.75	0.46	50,50,50,50	0
81	MG	1	3979	1/1	0.75	0.40	63,63,63,63	0
81	MG	5	4111	1/1	0.75	1.12	75,75,75,75	0
81	MG	5	3987	1/1	0.75	0.69	77,77,77,77	0
81	MG	5	3924	1/1	0.75	0.31	75,75,75,75	0
81	MG	6	1919	1/1	0.75	0.35	85,85,85,85	1
81	MG	1	4115	1/1	0.75	0.22	98,98,98,98	0
81	MG	4	236	1/1	0.75	0.35	50,50,50,50	0
81	MG	6	1956	1/1	0.75	0.14	105,105,105,105	0
81	MG	1	4062	1/1	0.75	0.44	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3964	1/1	0.75	0.27	58,58,58,58	0
81	MG	5	3708	1/1	0.75	0.59	59,59,59,59	0
80	PAR	6	1902	42/42	0.76	0.38	87,87,87,87	42
81	MG	5	4031	1/1	0.76	0.16	91,91,91,91	0
81	MG	1	4031	1/1	0.76	0.32	44,44,44,44	1
81	MG	1	3660	1/1	0.76	0.25	55,55,55,55	0
81	MG	1	3728	1/1	0.76	0.39	49,49,49,49	0
81	MG	8	209	1/1	0.76	0.40	66,66,66,66	0
81	MG	5	3756	1/1	0.76	0.32	55,55,55,55	0
81	MG	1	4112	1/1	0.76	0.32	73,73,73,73	0
81	MG	1	3873	1/1	0.76	0.32	69,69,69,69	0
81	MG	3	214	1/1	0.76	0.14	73,73,73,73	0
82	ZN	d7	101	1/1	0.76	0.14	261,261,261,261	0
81	MG	S2	302	1/1	0.76	0.15	84,84,84,84	0
81	MG	l3	404	1/1	0.76	0.21	65,65,65,65	0
81	MG	5	3633	1/1	0.76	0.38	56,56,56,56	0
81	MG	2	1992	1/1	0.76	0.38	75,75,75,75	0
81	MG	6	1922	1/1	0.76	0.49	73,73,73,73	0
81	MG	5	3915	1/1	0.76	0.41	97,97,97,97	0
81	MG	5	4123	1/1	0.76	0.21	84,84,84,84	0
81	MG	m0	303	1/1	0.76	0.32	69,69,69,69	0
81	MG	1	3513	1/1	0.76	0.25	56,56,56,56	0
81	MG	2	2085	1/1	0.77	0.39	76,76,76,76	0
81	MG	1	3590	1/1	0.77	0.40	49,49,49,49	0
81	MG	5	3962	1/1	0.77	0.18	81,81,81,81	0
81	MG	2	1982	1/1	0.77	0.46	63,63,63,63	0
81	MG	5	3658	1/1	0.77	0.55	61,61,61,61	0
81	MG	1	4108	1/1	0.77	0.70	83,83,83,83	0
81	MG	2	2062	1/1	0.77	0.27	124,124,124,124	0
81	MG	5	3913	1/1	0.77	0.32	74,74,74,74	0
81	MG	5	3845	1/1	0.77	0.91	68,68,68,68	0
81	MG	5	3909	1/1	0.77	0.38	62,62,62,62	0
81	MG	1	4034	1/1	0.77	0.31	66,66,66,66	0
81	MG	5	3614	1/1	0.77	0.24	94,94,94,94	0
81	MG	6	2026	1/1	0.77	0.25	76,76,76,76	0
81	MG	1	3969	1/1	0.77	0.31	77,77,77,77	0
81	MG	1	3989	1/1	0.77	0.32	60,60,60,60	0
80	PAR	5	3403	42/42	0.77	0.34	84,84,84,84	42
81	MG	5	3953	1/1	0.77	0.51	49,49,49,49	0
81	MG	L3	402	1/1	0.77	0.52	55,55,55,55	0
81	MG	5	3793	1/1	0.77	0.67	89,89,89,89	0
81	MG	1	4109	1/1	0.77	0.50	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	5	3681	1/1	0.77	0.91	56,56,56,56	0
81	MG	6	1986	1/1	0.77	0.41	81,81,81,81	0
81	MG	5	3928	1/1	0.77	0.47	76,76,76,76	0
81	MG	n9	101	1/1	0.77	0.37	65,65,65,65	0
81	MG	5	3988	1/1	0.77	0.36	60,60,60,60	0
81	MG	1	4026	1/1	0.77	0.43	37,37,37,37	1
81	MG	5	4012	1/1	0.77	0.42	80,80,80,80	0
81	MG	1	3905	1/1	0.77	0.62	44,44,44,44	1
81	MG	6	2058	1/1	0.77	0.40	121,121,121,121	0
81	MG	2	2093	1/1	0.77	0.34	69,69,69,69	0
81	MG	5	4062	1/1	0.77	0.55	85,85,85,85	0
81	MG	1	3830	1/1	0.77	0.51	45,45,45,45	0
81	MG	5	3982	1/1	0.77	0.19	75,75,75,75	0
80	PAR	5	3428	42/42	0.78	0.23	120,120,120,120	0
81	MG	7	214	1/1	0.78	0.21	89,89,89,89	0
81	MG	6	2062	1/1	0.78	0.14	108,108,108,108	0
81	MG	1	3890	1/1	0.78	0.11	52,52,52,52	0
81	MG	5	4058	1/1	0.78	0.41	75,75,75,75	0
81	MG	5	3537	1/1	0.78	0.41	49,49,49,49	0
81	MG	1	3621	1/1	0.78	0.37	49,49,49,49	0
81	MG	1	4136	1/1	0.78	0.44	47,47,47,47	1
81	MG	1	3914	1/1	0.78	0.40	75,75,75,75	0
81	MG	1	4119	1/1	0.78	0.23	80,80,80,80	0
81	MG	3	213	1/1	0.78	0.14	89,89,89,89	0
81	MG	M6	202	1/1	0.78	0.31	52,52,52,52	0
81	MG	Q2	506	1/1	0.78	0.29	51,51,51,51	0
81	MG	6	2013	1/1	0.78	0.43	83,83,83,83	0
81	MG	1	3900	1/1	0.78	0.12	70,70,70,70	0
81	MG	2	1961	1/1	0.78	0.31	76,76,76,76	0
81	MG	N7	202	1/1	0.78	0.14	72,72,72,72	0
81	MG	1	3669	1/1	0.78	0.35	55,55,55,55	0
81	MG	4	226	1/1	0.78	0.38	60,60,60,60	0
81	MG	N6	204	1/1	0.78	0.23	56,56,56,56	0
81	MG	1	4056	1/1	0.78	0.21	69,69,69,69	0
81	MG	5	3937	1/1	0.78	0.24	76,76,76,76	0
81	MG	2	1963	1/1	0.78	0.26	112,112,112,112	0
80	PAR	3	201	42/42	0.78	0.20	95,95,95,95	42
81	MG	5	4030	1/1	0.78	0.14	88,88,88,88	0
81	MG	6	1939	1/1	0.78	0.14	104,104,104,104	0
81	MG	L8	301	1/1	0.79	0.25	73,73,73,73	0
80	PAR	6	1906	42/42	0.79	0.27	120,120,120,120	0
81	MG	5	3981	1/1	0.79	0.30	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
80	PAR	2	1905	42/42	0.79	0.32	80,80,80,80	42
81	MG	1	3491	1/1	0.79	0.45	58,58,58,58	0
81	MG	5	3792	1/1	0.79	0.40	50,50,50,50	0
81	MG	1	3946	1/1	0.79	0.50	56,56,56,56	0
81	MG	4	232	1/1	0.79	0.25	51,51,51,51	0
81	MG	1	3682	1/1	0.79	0.46	61,61,61,61	0
81	MG	5	3985	1/1	0.79	0.61	79,79,79,79	0
81	MG	5	4122	1/1	0.79	0.34	68,68,68,68	0
81	MG	5	3902	1/1	0.79	0.36	80,80,80,80	0
81	MG	1	3615	1/1	0.79	0.33	72,72,72,72	0
81	MG	5	3510	1/1	0.79	0.32	68,68,68,68	0
81	MG	1	3875	1/1	0.79	0.21	64,64,64,64	1
81	MG	4	203	1/1	0.79	0.30	44,44,44,44	0
81	MG	4	216	1/1	0.79	0.31	41,41,41,41	0
81	MG	1	3935	1/1	0.79	0.27	56,56,56,56	0
81	MG	M4	201	1/1	0.79	0.24	59,59,59,59	0
81	MG	1	3852	1/1	0.79	0.17	63,63,63,63	0
81	MG	5	3535	1/1	0.79	0.53	53,53,53,53	0
81	MG	5	3826	1/1	0.79	0.77	78,78,78,78	0
81	MG	6	2055	1/1	0.79	0.20	106,106,106,106	0
81	MG	4	205	1/1	0.79	0.39	46,46,46,46	0
81	MG	1	4164	1/1	0.79	0.27	69,69,69,69	0
81	MG	5	4100	1/1	0.79	0.42	60,60,60,60	0
81	MG	5	3872	1/1	0.79	0.34	72,72,72,72	0
81	MG	N6	203	1/1	0.79	0.27	55,55,55,55	0
81	MG	2	1968	1/1	0.79	0.15	129,129,129,129	0
81	MG	5	3964	1/1	0.79	0.20	67,67,67,67	1
81	MG	5	3883	1/1	0.79	0.37	73,73,73,73	0
81	MG	2	1910	1/1	0.79	0.32	80,80,80,80	0
81	MG	5	3879	1/1	0.79	0.18	137,137,137,137	0
81	MG	5	3774	1/1	0.79	0.38	59,59,59,59	1
81	MG	5	3741	1/1	0.79	0.29	58,58,58,58	0
81	MG	5	3946	1/1	0.79	0.29	72,72,72,72	0
81	MG	M6	203	1/1	0.79	0.34	56,56,56,56	0
81	MG	1	4175	1/1	0.79	0.62	69,69,69,69	0
81	MG	6	1920	1/1	0.79	0.26	70,70,70,70	1
81	MG	2	2003	1/1	0.79	0.51	66,66,66,66	0
81	MG	7	211	1/1	0.79	0.50	72,72,72,72	0
81	MG	2	1924	1/1	0.80	0.23	63,63,63,63	0
81	MG	5	4043	1/1	0.80	0.31	66,66,66,66	0
81	MG	1	3791	1/1	0.80	0.28	62,62,62,62	0
81	MG	2	2109	1/1	0.80	0.32	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3871	1/1	0.80	0.65	59,59,59,59	0
81	MG	5	3886	1/1	0.80	0.14	75,75,75,75	0
81	MG	1	4080	1/1	0.80	0.31	64,64,64,64	0
81	MG	5	3690	1/1	0.80	0.81	59,59,59,59	0
81	MG	1	4084	1/1	0.80	0.42	62,62,62,62	0
81	MG	5	3805	1/1	0.80	0.33	68,68,68,68	0
81	MG	5	3585	1/1	0.80	0.27	73,73,73,73	0
81	MG	1	3680	1/1	0.80	0.36	62,62,62,62	0
81	MG	1	3577	1/1	0.80	0.44	48,48,48,48	0
81	MG	1	4104	1/1	0.80	0.34	55,55,55,55	0
81	MG	1	3894	1/1	0.80	0.27	60,60,60,60	0
81	MG	1	3990	1/1	0.80	0.32	56,56,56,56	0
81	MG	1	4015	1/1	0.80	0.78	65,65,65,65	0
81	MG	1	4076	1/1	0.80	0.38	61,61,61,61	0
81	MG	2	1917	1/1	0.80	0.49	88,88,88,88	0
81	MG	5	3814	1/1	0.80	0.36	63,63,63,63	0
81	MG	5	4011	1/1	0.80	0.72	63,63,63,63	0
81	MG	M6	204	1/1	0.80	0.25	65,65,65,65	0
81	MG	1	3948	1/1	0.80	0.43	42,42,42,42	0
81	MG	1	3786	1/1	0.80	0.34	67,67,67,67	0
81	MG	2	2014	1/1	0.80	0.35	67,67,67,67	0
81	MG	1	3883	1/1	0.80	0.35	67,67,67,67	0
81	MG	S2	301	1/1	0.80	0.32	91,91,91,91	0
81	MG	1	4102	1/1	0.80	0.47	66,66,66,66	0
81	MG	c4	201	1/1	0.80	0.14	118,118,118,118	0
81	MG	1	4042	1/1	0.80	0.18	63,63,63,63	0
81	MG	1	3586	1/1	0.80	0.35	41,41,41,41	0
81	MG	6	2042	1/1	0.80	0.34	98,98,98,98	0
81	MG	5	4003	1/1	0.80	0.41	64,64,64,64	0
81	MG	n0	203	1/1	0.80	0.22	60,60,60,60	0
81	MG	5	3922	1/1	0.80	0.16	87,87,87,87	0
81	MG	1	3768	1/1	0.80	0.26	77,77,77,77	0
81	MG	2	1973	1/1	0.80	0.44	82,82,82,82	0
81	MG	1	3508	1/1	0.80	0.11	72,72,72,72	0
81	MG	1	4039	1/1	0.80	0.26	72,72,72,72	0
81	MG	2	1957	1/1	0.80	0.23	81,81,81,81	0
81	MG	1	3564	1/1	0.80	0.29	48,48,48,48	0
80	PAR	5	3427	42/42	0.80	0.35	94,94,94,94	42
81	MG	2	2058	1/1	0.80	0.54	58,58,58,58	0
81	MG	6	2049	1/1	0.81	0.25	74,74,74,74	0
81	MG	1	4007	1/1	0.81	0.46	46,46,46,46	0
81	MG	8	210	1/1	0.81	0.28	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3669	1/1	0.81	0.25	48,48,48,48	0
81	MG	2	2089	1/1	0.81	0.22	93,93,93,93	0
81	MG	2	1980	1/1	0.81	0.39	66,66,66,66	0
81	MG	1	3809	1/1	0.81	0.27	59,59,59,59	0
81	MG	5	3785	1/1	0.81	0.38	53,53,53,53	0
81	MG	6	1977	1/1	0.81	0.12	107,107,107,107	0
81	MG	1	3698	1/1	0.81	0.52	62,62,62,62	0
81	MG	1	4013	1/1	0.81	0.70	70,70,70,70	0
81	MG	D6	102	1/1	0.81	0.36	79,79,79,79	0
81	MG	6	2035	1/1	0.81	0.24	87,87,87,87	0
81	MG	N3	201	1/1	0.81	0.29	82,82,82,82	0
81	MG	5	3941	1/1	0.81	0.26	113,113,113,113	0
81	MG	5	4069	1/1	0.81	0.28	69,69,69,69	1
81	MG	1	3683	1/1	0.81	0.56	49,49,49,49	0
81	MG	5	3904	1/1	0.81	0.42	89,89,89,89	0
81	MG	1	4125	1/1	0.81	0.41	58,58,58,58	0
81	MG	5	3990	1/1	0.81	0.14	91,91,91,91	0
81	MG	C9	202	1/1	0.81	0.11	133,133,133,133	0
81	MG	1	3861	1/1	0.81	0.24	44,44,44,44	0
81	MG	2	2072	1/1	0.81	0.16	83,83,83,83	0
81	MG	2	1907	1/1	0.81	0.14	81,81,81,81	0
81	MG	2	2092	1/1	0.81	0.23	71,71,71,71	0
81	MG	5	3560	1/1	0.81	0.09	92,92,92,92	0
81	MG	5	3611	1/1	0.81	0.33	67,67,67,67	0
81	MG	6	2059	1/1	0.81	0.20	118,118,118,118	0
81	MG	2	2028	1/1	0.81	0.37	73,73,73,73	0
81	MG	1	4161	1/1	0.81	0.18	61,61,61,61	1
81	MG	2	2018	1/1	0.81	0.10	99,99,99,99	0
81	MG	1	4029	1/1	0.81	0.42	40,40,40,40	0
81	MG	L3	405	1/1	0.81	0.18	73,73,73,73	0
81	MG	c4	203	1/1	0.81	0.19	118,118,118,118	0
81	MG	5	3972	1/1	0.81	0.28	68,68,68,68	0
80	PAR	5	3405	42/42	0.81	0.23	131,131,131,131	0
81	MG	q0	202	1/1	0.81	0.40	67,67,67,67	0
81	MG	1	3525	1/1	0.81	0.45	54,54,54,54	0
81	MG	N7	201	1/1	0.81	0.22	64,64,64,64	0
81	MG	2	2001	1/1	0.81	0.17	80,80,80,80	0
81	MG	5	3580	1/1	0.81	0.29	60,60,60,60	0
81	MG	5	4024	1/1	0.81	0.37	52,52,52,52	0
81	MG	1	3985	1/1	0.81	0.46	61,61,61,61	0
81	MG	1	4105	1/1	0.81	0.23	63,63,63,63	0
81	MG	2	1919	1/1	0.81	0.24	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	5	3935	1/1	0.81	0.71	59,59,59,59	0
81	MG	1	3639	1/1	0.81	0.20	78,78,78,78	0
81	MG	5	4112	1/1	0.81	0.82	69,69,69,69	0
81	MG	2	1964	1/1	0.81	0.15	102,102,102,102	0
81	MG	M9	201	1/1	0.81	0.43	65,65,65,65	0
81	MG	n8	202	1/1	0.81	0.42	52,52,52,52	1
81	MG	1	4048	1/1	0.81	0.22	50,50,50,50	0
81	MG	1	3947	1/1	0.82	0.33	54,54,54,54	0
81	MG	6	1962	1/1	0.82	0.37	110,110,110,110	0
81	MG	5	3899	1/1	0.82	0.21	73,73,73,73	0
81	MG	L9	203	1/1	0.82	0.19	71,71,71,71	0
81	MG	2	2063	1/1	0.82	0.44	89,89,89,89	0
81	MG	1	4140	1/1	0.82	0.27	56,56,56,56	1
81	MG	5	4097	1/1	0.82	0.43	52,52,52,52	0
81	MG	1	3949	1/1	0.82	0.45	38,38,38,38	1
81	MG	6	1995	1/1	0.82	0.36	71,71,71,71	0
81	MG	5	3772	1/1	0.82	0.35	73,73,73,73	0
81	MG	6	1997	1/1	0.82	0.38	80,80,80,80	0
81	MG	5	3693	1/1	0.82	0.38	51,51,51,51	0
80	PAR	5	3422	42/42	0.82	0.20	105,105,105,105	0
81	MG	5	3620	1/1	0.82	0.54	79,79,79,79	0
81	MG	5	4010	1/1	0.82	0.32	74,74,74,74	0
81	MG	5	3880	1/1	0.82	0.58	77,77,77,77	0
81	MG	1	3962	1/1	0.82	0.41	44,44,44,44	0
81	MG	m6	201	1/1	0.82	0.35	52,52,52,52	0
81	MG	6	2016	1/1	0.82	0.34	95,95,95,95	0
81	MG	2	2000	1/1	0.82	0.13	78,78,78,78	0
81	MG	l3	406	1/1	0.82	0.25	62,62,62,62	0
81	MG	1	4002	1/1	0.82	0.56	75,75,75,75	0
81	MG	Q3	502	1/1	0.82	0.34	51,51,51,51	0
81	MG	1	3862	1/1	0.82	0.25	62,62,62,62	0
81	MG	6	2001	1/1	0.82	0.24	105,105,105,105	0
81	MG	2	2004	1/1	0.82	0.34	69,69,69,69	0
81	MG	M7	205	1/1	0.82	0.26	45,45,45,45	0
81	MG	1	3592	1/1	0.82	0.71	63,63,63,63	0
81	MG	5	3573	1/1	0.82	0.22	76,76,76,76	0
81	MG	1	3638	1/1	0.82	0.30	68,68,68,68	0
81	MG	2	2037	1/1	0.82	0.10	123,123,123,123	0
81	MG	1	3821	1/1	0.82	0.26	52,52,52,52	0
81	MG	2	2098	1/1	0.82	0.29	79,79,79,79	0
81	MG	1	3981	1/1	0.82	0.34	57,57,57,57	0
81	MG	1	3954	1/1	0.82	0.24	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	4120	1/1	0.82	0.21	58,58,58,58	0
81	MG	2	2100	1/1	0.82	0.60	58,58,58,58	0
80	PAR	1	3413	42/42	0.82	0.27	64,64,64,64	42
81	MG	5	3734	1/1	0.82	0.73	65,65,65,65	0
81	MG	2	2104	1/1	0.82	0.77	82,82,82,82	0
81	MG	5	3837	1/1	0.82	0.30	53,53,53,53	0
81	MG	5	3724	1/1	0.82	0.51	78,78,78,78	0
81	MG	5	3738	1/1	0.82	0.41	54,54,54,54	0
81	MG	O9	101	1/1	0.82	0.45	48,48,48,48	1
81	MG	6	1975	1/1	0.82	0.07	104,104,104,104	1
81	MG	1	3864	1/1	0.82	0.24	47,47,47,47	0
81	MG	1	4073	1/1	0.82	0.13	80,80,80,80	0
81	MG	5	3639	1/1	0.82	0.39	54,54,54,54	0
81	MG	2	1922	1/1	0.82	0.27	60,60,60,60	1
81	MG	1	4192	1/1	0.82	0.71	62,62,62,62	0
81	MG	6	2039	1/1	0.82	0.33	69,69,69,69	0
81	MG	6	2044	1/1	0.83	0.22	87,87,87,87	0
81	MG	1	4078	1/1	0.83	0.25	71,71,71,71	0
81	MG	2	2095	1/1	0.83	0.42	78,78,78,78	0
81	MG	5	4084	1/1	0.83	0.20	69,69,69,69	0
80	PAR	1	3433	42/42	0.83	0.27	64,64,64,64	42
81	MG	5	4035	1/1	0.83	0.17	85,85,85,85	0
81	MG	5	3598	1/1	0.83	0.38	82,82,82,82	0
81	MG	5	3892	1/1	0.83	0.25	66,66,66,66	0
81	MG	1	3818	1/1	0.83	0.27	54,54,54,54	0
81	MG	1	4014	1/1	0.83	0.90	70,70,70,70	0
81	MG	4	231	1/1	0.83	0.28	49,49,49,49	0
81	MG	6	2036	1/1	0.83	0.43	80,80,80,80	0
81	MG	5	3673	1/1	0.83	0.33	51,51,51,51	0
81	MG	M5	303	1/1	0.83	0.32	44,44,44,44	1
81	MG	2	2049	1/1	0.83	0.56	88,88,88,88	0
81	MG	2	2031	1/1	0.83	0.13	98,98,98,98	0
81	MG	1	4010	1/1	0.83	0.50	53,53,53,53	0
81	MG	M7	202	1/1	0.83	0.47	40,40,40,40	0
81	MG	5	3767	1/1	0.83	0.37	66,66,66,66	0
81	MG	1	4097	1/1	0.83	0.25	63,63,63,63	0
81	MG	5	4021	1/1	0.83	0.61	64,64,64,64	0
81	MG	5	4016	1/1	0.83	0.37	77,77,77,77	0
81	MG	M8	201	1/1	0.83	0.32	63,63,63,63	0
81	MG	7	212	1/1	0.83	0.22	60,60,60,60	0
81	MG	1	4096	1/1	0.83	0.30	62,62,62,62	0
81	MG	l3	407	1/1	0.83	0.40	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	5	3822	1/1	0.83	0.11	65,65,65,65	0
81	MG	1	3695	1/1	0.83	0.38	50,50,50,50	1
81	MG	5	3986	1/1	0.83	0.61	78,78,78,78	0
81	MG	1	3530	1/1	0.83	0.34	37,37,37,37	0
81	MG	2	1979	1/1	0.83	0.30	77,77,77,77	0
81	MG	5	3873	1/1	0.83	0.39	66,66,66,66	0
81	MG	6	2066	1/1	0.83	0.37	55,55,55,55	0
81	MG	M4	203	1/1	0.83	0.15	64,64,64,64	0
81	MG	6	2072	1/1	0.83	0.42	74,74,74,74	0
81	MG	1	4171	1/1	0.83	0.36	52,52,52,52	0
81	MG	5	3974	1/1	0.83	0.42	59,59,59,59	0
81	MG	1	4027	1/1	0.83	0.41	42,42,42,42	0
81	MG	5	3513	1/1	0.83	0.57	76,76,76,76	0
81	MG	5	3483	1/1	0.83	0.33	53,53,53,53	0
81	MG	2	1978	1/1	0.83	0.21	79,79,79,79	0
81	MG	1	3503	1/1	0.83	0.26	56,56,56,56	0
81	MG	1	4005	1/1	0.83	0.33	64,64,64,64	0
81	MG	1	4053	1/1	0.83	0.35	55,55,55,55	0
81	MG	n6	202	1/1	0.83	0.10	69,69,69,69	0
80	PAR	n3	201	42/42	0.83	0.30	63,63,63,63	42
81	MG	5	3861	1/1	0.83	0.38	64,64,64,64	0
81	MG	5	4118	1/1	0.83	0.27	66,66,66,66	0
81	MG	5	3697	1/1	0.83	0.69	60,60,60,60	0
81	MG	6	2051	1/1	0.83	0.26	110,110,110,110	0
81	MG	6	1938	1/1	0.83	0.09	99,99,99,99	0
81	MG	1	4000	1/1	0.83	0.24	54,54,54,54	0
81	MG	1	3789	1/1	0.83	0.44	54,54,54,54	0
81	MG	1	3882	1/1	0.83	0.17	74,74,74,74	0
81	MG	L5	303	1/1	0.83	0.20	86,86,86,86	0
80	PAR	o2	201	42/42	0.83	0.32	51,51,51,51	42
81	MG	1	3987	1/1	0.83	0.33	54,54,54,54	0
81	MG	L4	401	1/1	0.84	0.23	49,49,49,49	0
82	ZN	D7	101	1/1	0.84	0.16	173,173,173,173	0
81	MG	1	4030	1/1	0.84	0.37	48,48,48,48	0
81	MG	1	3500	1/1	0.84	0.76	71,71,71,71	0
81	MG	1	3896	1/1	0.84	0.28	76,76,76,76	0
81	MG	1	4041	1/1	0.84	0.15	69,69,69,69	0
81	MG	1	4001	1/1	0.84	0.22	62,62,62,62	0
81	MG	3	218	1/1	0.84	0.40	57,57,57,57	0
80	PAR	1	3403	42/42	0.84	0.31	58,58,58,58	42
81	MG	5	3713	1/1	0.84	0.48	56,56,56,56	0
81	MG	5	3995	1/1	0.84	0.26	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3549	1/1	0.84	0.34	49,49,49,49	0
81	MG	5	3835	1/1	0.84	0.37	57,57,57,57	0
81	MG	5	3991	1/1	0.84	0.17	66,66,66,66	0
81	MG	1	3984	1/1	0.84	0.36	52,52,52,52	0
81	MG	5	4014	1/1	0.84	0.39	71,71,71,71	0
81	MG	2	2066	1/1	0.84	0.35	82,82,82,82	0
81	MG	2	1936	1/1	0.84	0.54	59,59,59,59	0
81	MG	1	4054	1/1	0.84	0.29	75,75,75,75	0
81	MG	17	303	1/1	0.84	0.25	69,69,69,69	0
81	MG	5	3936	1/1	0.84	0.54	60,60,60,60	1
81	MG	1	3855	1/1	0.84	0.23	51,51,51,51	0
81	MG	1	4055	1/1	0.84	0.20	60,60,60,60	0
81	MG	1	3899	1/1	0.84	0.22	76,76,76,76	0
81	MG	5	3469	1/1	0.84	0.36	46,46,46,46	0
81	MG	5	3707	1/1	0.84	0.60	58,58,58,58	0
81	MG	1	3630	1/1	0.84	0.29	51,51,51,51	0
81	MG	5	4027	1/1	0.84	0.52	69,69,69,69	0
81	MG	1	3868	1/1	0.84	0.32	39,39,39,39	0
81	MG	M4	202	1/1	0.84	0.30	60,60,60,60	0
81	MG	o1	202	1/1	0.84	0.50	69,69,69,69	0
81	MG	5	3852	1/1	0.84	0.41	55,55,55,55	0
81	MG	1	4146	1/1	0.84	0.46	55,55,55,55	0
81	MG	1	3889	1/1	0.84	0.32	54,54,54,54	0
80	PAR	5	3404	42/42	0.84	0.23	90,90,90,90	0
81	MG	6	2004	1/1	0.84	0.74	77,77,77,77	0
80	PAR	1	3426	42/42	0.84	0.28	82,82,82,82	0
81	MG	1	3614	1/1	0.84	0.26	71,71,71,71	0
81	MG	1	3971	1/1	0.84	0.19	69,69,69,69	0
81	MG	5	3667	1/1	0.84	0.37	53,53,53,53	0
80	PAR	1	3401	42/42	0.84	0.22	87,87,87,87	42
81	MG	5	3847	1/1	0.84	0.33	96,96,96,96	0
81	MG	1	4092	1/1	0.84	0.20	62,62,62,62	0
81	MG	1	3788	1/1	0.84	0.27	68,68,68,68	0
81	MG	2	1987	1/1	0.84	0.59	81,81,81,81	0
81	MG	1	3501	1/1	0.84	0.57	78,78,78,78	0
81	MG	1	4145	1/1	0.84	0.28	52,52,52,52	0
81	MG	1	4116	1/1	0.84	0.31	107,107,107,107	0
81	MG	5	3603	1/1	0.84	0.24	65,65,65,65	0
81	MG	1	3972	1/1	0.84	0.39	84,84,84,84	0
81	MG	5	3764	1/1	0.84	0.34	56,56,56,56	0
81	MG	5	3867	1/1	0.84	0.26	66,66,66,66	0
81	MG	s8	301	1/1	0.84	0.32	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3956	1/1	0.84	0.23	67,67,67,67	0
81	MG	1	3874	1/1	0.84	0.20	67,67,67,67	1
81	MG	1	3930	1/1	0.84	0.40	45,45,45,45	0
81	MG	2	2080	1/1	0.84	0.17	81,81,81,81	0
81	MG	n0	202	1/1	0.85	0.23	59,59,59,59	0
81	MG	l7	302	1/1	0.85	0.41	57,57,57,57	0
80	PAR	2	1901	42/42	0.85	0.32	82,82,82,82	42
80	PAR	1	3405	42/42	0.85	0.35	44,44,44,44	42
81	MG	1	3797	1/1	0.85	0.19	53,53,53,53	0
81	MG	1	4103	1/1	0.85	0.49	57,57,57,57	0
81	MG	5	4004	1/1	0.85	0.27	72,72,72,72	0
81	MG	5	3747	1/1	0.85	0.60	60,60,60,60	0
80	PAR	4	201	42/42	0.85	0.31	43,43,43,43	42
81	MG	6	2074	1/1	0.85	0.32	81,81,81,81	0
81	MG	n1	202	1/1	0.85	0.50	63,63,63,63	0
81	MG	5	3947	1/1	0.85	0.28	57,57,57,57	0
81	MG	1	3973	1/1	0.85	0.36	71,71,71,71	0
81	MG	6	1954	1/1	0.85	0.16	98,98,98,98	0
80	PAR	1	3436	42/42	0.85	0.22	85,85,85,85	0
81	MG	6	1959	1/1	0.85	0.29	119,119,119,119	0
81	MG	5	3938	1/1	0.85	0.25	74,74,74,74	0
81	MG	5	3597	1/1	0.85	0.32	65,65,65,65	0
81	MG	2	1941	1/1	0.85	0.28	75,75,75,75	0
80	PAR	8	202	42/42	0.85	0.30	62,62,62,62	42
81	MG	1	3538	1/1	0.85	0.38	35,35,35,35	0
81	MG	8	217	1/1	0.85	0.24	69,69,69,69	0
81	MG	6	2017	1/1	0.85	0.20	93,93,93,93	0
81	MG	2	2116	1/1	0.85	0.38	93,93,93,93	0
81	MG	5	3771	1/1	0.85	0.37	88,88,88,88	0
81	MG	1	3511	1/1	0.85	0.11	73,73,73,73	0
81	MG	5	3950	1/1	0.85	0.34	61,61,61,61	0
81	MG	5	3521	1/1	0.85	0.28	55,55,55,55	0
81	MG	5	3530	1/1	0.85	0.29	43,43,43,43	0
81	MG	1	3932	1/1	0.85	0.28	44,44,44,44	0
81	MG	1	4181	1/1	0.85	0.26	49,49,49,49	0
81	MG	5	3616	1/1	0.85	0.14	81,81,81,81	0
81	MG	2	1915	1/1	0.85	0.33	82,82,82,82	0
81	MG	5	3546	1/1	0.85	0.30	59,59,59,59	0
81	MG	L2	306	1/1	0.85	0.37	51,51,51,51	0
81	MG	1	3923	1/1	0.85	0.42	45,45,45,45	0
81	MG	1	3546	1/1	0.85	0.18	43,43,43,43	0
81	MG	2	2106	1/1	0.85	0.17	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3541	1/1	0.85	0.47	41,41,41,41	0
81	MG	O7	104	1/1	0.85	0.31	43,43,43,43	0
81	MG	2	2041	1/1	0.85	0.11	126,126,126,126	0
81	MG	1	4199	1/1	0.85	0.19	47,47,47,47	0
81	MG	6	2068	1/1	0.85	0.63	71,71,71,71	0
81	MG	1	3941	1/1	0.85	0.36	72,72,72,72	0
81	MG	1	4176	1/1	0.85	0.71	78,78,78,78	0
81	MG	M9	202	1/1	0.85	0.34	61,61,61,61	0
80	PAR	1	3435	42/42	0.85	0.31	40,40,40,40	42
81	MG	1	4177	1/1	0.85	0.39	57,57,57,57	0
81	MG	1	3496	1/1	0.85	0.50	52,52,52,52	0
81	MG	6	1940	1/1	0.85	0.11	100,100,100,100	0
81	MG	5	3876	1/1	0.85	0.28	74,74,74,74	0
81	MG	5	3621	1/1	0.85	0.49	65,65,65,65	0
80	PAR	1	3431	42/42	0.85	0.25	67,67,67,67	42
80	PAR	5	3411	42/42	0.85	0.29	83,83,83,83	0
81	MG	M5	309	1/1	0.85	0.37	43,43,43,43	0
81	MG	Q1	1301	1/1	0.85	0.44	58,58,58,58	0
81	MG	1	4147	1/1	0.85	0.32	51,51,51,51	0
80	PAR	8	201	42/42	0.85	0.28	79,79,79,79	42
81	MG	2	1911	1/1	0.85	0.14	79,79,79,79	0
81	MG	1	3499	1/1	0.85	0.51	52,52,52,52	0
81	MG	5	3643	1/1	0.85	0.24	60,60,60,60	0
81	MG	5	3626	1/1	0.85	0.32	60,60,60,60	0
81	MG	L4	403	1/1	0.85	0.36	39,39,39,39	0
81	MG	5	3916	1/1	0.85	0.29	96,96,96,96	0
81	MG	1	4061	1/1	0.85	0.32	41,41,41,41	1
81	MG	5	3777	1/1	0.85	0.42	45,45,45,45	0
81	MG	1	4195	1/1	0.85	0.31	60,60,60,60	0
81	MG	5	3898	1/1	0.85	0.24	66,66,66,66	0
81	MG	2	1943	1/1	0.85	0.64	82,82,82,82	0
81	MG	2	1956	1/1	0.85	0.23	119,119,119,119	0
81	MG	5	3743	1/1	0.85	0.29	54,54,54,54	1
81	MG	L9	204	1/1	0.85	0.29	60,60,60,60	0
81	MG	5	4109	1/1	0.85	0.87	79,79,79,79	0
81	MG	5	4101	1/1	0.85	0.81	67,67,67,67	0
81	MG	1	3848	1/1	0.85	0.58	62,62,62,62	0
81	MG	1	3839	1/1	0.85	0.29	47,47,47,47	0
81	MG	5	3553	1/1	0.85	0.32	64,64,64,64	0
81	MG	5	3807	1/1	0.86	0.23	60,60,60,60	0
81	MG	5	4015	1/1	0.86	0.30	78,78,78,78	0
81	MG	1	3623	1/1	0.86	0.19	63,63,63,63	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3683	1/1	0.86	0.55	53,53,53,53	0
80	PAR	6	1905	42/42	0.86	0.20	112,112,112,112	0
81	MG	c9	202	1/1	0.86	0.15	124,124,124,124	0
81	MG	2	1999	1/1	0.86	0.17	74,74,74,74	0
81	MG	1	3996	1/1	0.86	0.49	78,78,78,78	0
81	MG	2	1969	1/1	0.86	0.16	114,114,114,114	0
81	MG	2	1972	1/1	0.86	0.55	92,92,92,92	0
81	MG	5	4104	1/1	0.86	0.42	52,52,52,52	0
81	MG	5	3961	1/1	0.86	0.22	60,60,60,60	0
81	MG	5	3851	1/1	0.86	0.68	61,61,61,61	0
81	MG	7	208	1/1	0.86	0.11	117,117,117,117	0
81	MG	2	1970	1/1	0.86	0.09	118,118,118,118	0
81	MG	1	3628	1/1	0.86	0.65	54,54,54,54	0
81	MG	5	3993	1/1	0.86	0.28	64,64,64,64	0
81	MG	6	1993	1/1	0.86	0.35	76,76,76,76	0
81	MG	5	4095	1/1	0.86	0.29	56,56,56,56	1
80	PAR	1	3406	42/42	0.86	0.38	68,68,68,68	42
81	MG	6	1951	1/1	0.86	0.20	78,78,78,78	0
81	MG	6	1979	1/1	0.86	0.13	90,90,90,90	0
81	MG	1	3781	1/1	0.86	0.33	51,51,51,51	1
81	MG	2	2060	1/1	0.86	0.41	103,103,103,103	0
81	MG	1	3953	1/1	0.86	0.18	54,54,54,54	0
81	MG	2	2112	1/1	0.86	0.51	72,72,72,72	0
81	MG	1	4154	1/1	0.86	0.35	38,38,38,38	0
81	MG	8	204	1/1	0.86	0.69	69,69,69,69	0
81	MG	5	4007	1/1	0.86	0.61	76,76,76,76	0
80	PAR	1	3437	42/42	0.86	0.31	64,64,64,64	42
81	MG	1	3560	1/1	0.86	0.17	42,42,42,42	0
81	MG	m9	201	1/1	0.86	0.22	63,63,63,63	0
81	MG	6	2030	1/1	0.86	0.39	71,71,71,71	0
81	MG	1	3784	1/1	0.86	0.39	56,56,56,56	0
81	MG	2	2052	1/1	0.86	0.25	95,95,95,95	0
81	MG	2	1958	1/1	0.86	0.18	114,114,114,114	0
81	MG	m7	205	1/1	0.86	0.26	60,60,60,60	0
81	MG	5	3720	1/1	0.86	0.33	65,65,65,65	0
81	MG	6	1980	1/1	0.86	0.14	105,105,105,105	0
81	MG	M8	202	1/1	0.86	0.67	52,52,52,52	0
81	MG	2	2065	1/1	0.86	0.36	76,76,76,76	0
81	MG	1	3603	1/1	0.86	0.33	52,52,52,52	0
81	MG	6	2052	1/1	0.86	0.22	72,72,72,72	0
80	PAR	1	3410	42/42	0.86	0.33	52,52,52,52	42
81	MG	5	3723	1/1	0.86	0.32	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	4072	1/1	0.86	0.19	65,65,65,65	0
81	MG	4	212	1/1	0.86	0.19	57,57,57,57	0
81	MG	5	3824	1/1	0.86	0.34	59,59,59,59	0
81	MG	5	3954	1/1	0.86	0.45	55,55,55,55	0
81	MG	1	3532	1/1	0.86	0.28	48,48,48,48	0
81	MG	O4	202	1/1	0.86	0.24	59,59,59,59	0
81	MG	5	4113	1/1	0.86	0.88	74,74,74,74	0
81	MG	1	3612	1/1	0.86	0.17	74,74,74,74	0
81	MG	2	1938	1/1	0.86	0.27	85,85,85,85	0
80	PAR	5	3409	42/42	0.87	0.32	56,56,56,56	42
81	MG	2	2086	1/1	0.87	0.33	95,95,95,95	0
80	PAR	5	3402	42/42	0.87	0.23	81,81,81,81	42
81	MG	1	3558	1/1	0.87	0.53	36,36,36,36	0
81	MG	5	3751	1/1	0.87	0.42	50,50,50,50	0
81	MG	m9	205	1/1	0.87	0.39	75,75,75,75	0
81	MG	1	4037	1/1	0.87	0.21	97,97,97,97	0
80	PAR	5	3413	42/42	0.87	0.29	72,72,72,72	42
81	MG	5	3979	1/1	0.87	0.31	73,73,73,73	0
81	MG	1	3782	1/1	0.87	0.21	82,82,82,82	0
81	MG	5	3857	1/1	0.87	0.23	60,60,60,60	0
81	MG	O1	203	1/1	0.87	0.27	74,74,74,74	0
81	MG	5	3624	1/1	0.87	0.39	76,76,76,76	0
81	MG	5	3825	1/1	0.87	0.93	67,67,67,67	0
81	MG	5	3821	1/1	0.87	0.26	62,62,62,62	0
81	MG	2	1988	1/1	0.87	0.14	86,86,86,86	0
81	MG	1	3665	1/1	0.87	0.32	54,54,54,54	0
81	MG	L3	403	1/1	0.87	0.29	57,57,57,57	0
81	MG	5	4071	1/1	0.87	0.14	56,56,56,56	0
81	MG	5	3799	1/1	0.87	0.23	47,47,47,47	0
81	MG	5	3645	1/1	0.87	0.30	62,62,62,62	0
81	MG	1	3678	1/1	0.87	0.25	58,58,58,58	1
81	MG	1	3523	1/1	0.87	0.31	50,50,50,50	0
81	MG	6	2040	1/1	0.87	0.42	66,66,66,66	0
81	MG	5	3550	1/1	0.87	0.28	55,55,55,55	0
81	MG	6	1983	1/1	0.87	0.32	88,88,88,88	0
81	MG	5	3644	1/1	0.87	0.48	59,59,59,59	0
81	MG	2	2097	1/1	0.87	0.49	62,62,62,62	0
81	MG	1	3895	1/1	0.87	0.24	65,65,65,65	0
81	MG	3	217	1/1	0.87	0.18	60,60,60,60	0
81	MG	1	3642	1/1	0.87	0.17	63,63,63,63	0
81	MG	5	3680	1/1	0.87	0.24	60,60,60,60	0
80	PAR	3	203	42/42	0.87	0.26	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	M3	201	1/1	0.87	0.27	36,36,36,36	0
81	MG	n0	201	1/1	0.87	0.14	59,59,59,59	0
81	MG	5	4055	1/1	0.87	0.21	56,56,56,56	0
81	MG	5	3856	1/1	0.87	0.24	51,51,51,51	0
81	MG	1	3631	1/1	0.87	0.34	47,47,47,47	0
81	MG	Q2	504	1/1	0.87	0.22	42,42,42,42	0
81	MG	2	2101	1/1	0.87	0.52	61,61,61,61	0
81	MG	1	3702	1/1	0.87	0.42	42,42,42,42	0
80	PAR	5	3421	42/42	0.87	0.19	102,102,102,102	0
81	MG	1	3714	1/1	0.87	0.22	44,44,44,44	0
81	MG	5	3925	1/1	0.87	0.34	73,73,73,73	0
81	MG	1	3961	1/1	0.87	0.20	40,40,40,40	0
81	MG	1	3600	1/1	0.87	0.42	52,52,52,52	0
81	MG	5	3838	1/1	0.87	0.25	57,57,57,57	0
81	MG	6	2050	1/1	0.87	0.42	80,80,80,80	0
81	MG	5	3726	1/1	0.87	0.62	69,69,69,69	0
81	MG	1	4148	1/1	0.87	0.35	47,47,47,47	0
81	MG	5	4046	1/1	0.87	0.34	68,68,68,68	0
81	MG	1	4008	1/1	0.87	0.47	50,50,50,50	0
81	MG	6	1958	1/1	0.87	0.33	81,81,81,81	0
81	MG	1	3451	1/1	0.87	0.33	36,36,36,36	0
81	MG	1	3701	1/1	0.87	0.30	46,46,46,46	0
80	PAR	1	3404	42/42	0.87	0.27	53,53,53,53	42
81	MG	1	3676	1/1	0.87	0.21	64,64,64,64	0
81	MG	14	401	1/1	0.87	0.18	62,62,62,62	0
81	MG	5	4065	1/1	0.87	0.17	100,100,100,100	0
81	MG	4	214	1/1	0.87	0.35	63,63,63,63	0
81	MG	5	3818	1/1	0.87	0.33	60,60,60,60	0
81	MG	5	3823	1/1	0.87	0.33	78,78,78,78	0
81	MG	6	1988	1/1	0.87	0.64	62,62,62,62	0
81	MG	5	3958	1/1	0.87	0.24	61,61,61,61	1
80	PAR	5	3425	42/42	0.87	0.29	75,75,75,75	42
81	MG	2	1959	1/1	0.87	0.31	92,92,92,92	0
81	MG	5	4006	1/1	0.88	0.61	68,68,68,68	0
81	MG	1	3713	1/1	0.88	0.28	53,53,53,53	0
81	MG	o2	203	1/1	0.88	0.26	49,49,49,49	0
80	PAR	7	202	42/42	0.88	0.27	59,59,59,59	42
81	MG	5	4121	1/1	0.88	0.17	65,65,65,65	0
81	MG	5	3921	1/1	0.88	0.26	91,91,91,91	0
81	MG	5	3773	1/1	0.88	0.32	80,80,80,80	0
81	MG	2	1948	1/1	0.88	0.21	85,85,85,85	0
81	MG	1	3909	1/1	0.88	0.86	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3709	1/1	0.88	0.36	54,54,54,54	0
81	MG	2	2056	1/1	0.88	0.42	80,80,80,80	0
81	MG	M5	304	1/1	0.88	0.28	61,61,61,61	0
81	MG	1	3756	1/1	0.88	0.21	47,47,47,47	0
81	MG	6	2002	1/1	0.88	0.60	64,64,64,64	0
81	MG	1	3913	1/1	0.88	0.39	66,66,66,66	0
81	MG	1	3915	1/1	0.88	0.40	69,69,69,69	0
81	MG	2	1935	1/1	0.88	0.35	78,78,78,78	0
81	MG	5	3984	1/1	0.88	0.56	85,85,85,85	0
81	MG	5	3547	1/1	0.88	0.25	59,59,59,59	0
81	MG	1	3539	1/1	0.88	0.21	30,30,30,30	0
81	MG	1	4046	1/1	0.88	0.23	49,49,49,49	0
81	MG	6	2046	1/1	0.88	0.33	118,118,118,118	0
80	PAR	1	3432	42/42	0.88	0.30	51,51,51,51	42
81	MG	1	3841	1/1	0.88	0.31	60,60,60,60	0
81	MG	2	2036	1/1	0.88	0.12	127,127,127,127	0
81	MG	4	233	1/1	0.88	0.36	57,57,57,57	0
81	MG	1	4142	1/1	0.88	0.20	83,83,83,83	0
81	MG	1	3783	1/1	0.88	0.22	57,57,57,57	0
81	MG	1	4022	1/1	0.88	0.26	47,47,47,47	1
81	MG	5	3770	1/1	0.88	0.48	59,59,59,59	0
81	MG	5	3813	1/1	0.88	1.07	70,70,70,70	0
81	MG	1	3881	1/1	0.88	0.22	72,72,72,72	0
81	MG	N6	205	1/1	0.88	0.36	67,67,67,67	0
81	MG	1	3635	1/1	0.88	0.31	49,49,49,49	0
81	MG	1	3958	1/1	0.88	0.26	59,59,59,59	0
81	MG	1	3897	1/1	0.88	0.19	56,56,56,56	0
81	MG	1	3945	1/1	0.88	0.18	49,49,49,49	0
81	MG	1	3769	1/1	0.88	0.25	54,54,54,54	0
81	MG	1	4162	1/1	0.88	0.24	63,63,63,63	0
81	MG	5	3881	1/1	0.88	0.23	58,58,58,58	0
81	MG	1	3596	1/1	0.88	0.18	44,44,44,44	0
81	MG	1	4126	1/1	0.88	0.34	35,35,35,35	0
81	MG	1	3527	1/1	0.88	0.25	32,32,32,32	0
81	MG	l3	402	1/1	0.88	0.13	59,59,59,59	0
81	MG	5	3531	1/1	0.88	0.48	49,49,49,49	0
81	MG	1	4069	1/1	0.88	0.21	74,74,74,74	0
81	MG	2	2034	1/1	0.88	0.09	113,113,113,113	0
81	MG	2	1967	1/1	0.88	0.32	100,100,100,100	0
81	MG	5	4017	1/1	0.88	0.88	67,67,67,67	0
81	MG	2	2075	1/1	0.88	0.14	95,95,95,95	0
80	PAR	5	3426	42/42	0.88	0.26	56,56,56,56	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	2	1981	1/1	0.88	0.29	61,61,61,61	0
81	MG	1	4094	1/1	0.88	0.24	84,84,84,84	0
81	MG	1	4024	1/1	0.88	0.66	61,61,61,61	0
81	MG	O6	201	1/1	0.88	0.37	56,56,56,56	0
81	MG	2	2117	1/1	0.88	0.30	90,90,90,90	0
80	PAR	1	3434	42/42	0.88	0.20	85,85,85,85	42
81	MG	8	214	1/1	0.88	0.17	61,61,61,61	0
81	MG	N3	204	1/1	0.88	0.34	53,53,53,53	0
81	MG	2	1984	1/1	0.88	0.74	59,59,59,59	0
81	MG	5	3565	1/1	0.88	0.22	80,80,80,80	0
80	PAR	1	3417	42/42	0.88	0.31	66,66,66,66	42
81	MG	1	3731	1/1	0.88	0.52	52,52,52,52	0
81	MG	1	3663	1/1	0.88	0.34	48,48,48,48	0
81	MG	5	3467	1/1	0.88	0.49	49,49,49,49	0
81	MG	1	4044	1/1	0.88	0.25	48,48,48,48	0
81	MG	5	3613	1/1	0.88	0.23	80,80,80,80	0
81	MG	1	3917	1/1	0.88	0.31	69,69,69,69	0
81	MG	O7	102	1/1	0.88	0.25	43,43,43,43	0
81	MG	1	4060	1/1	0.88	0.24	58,58,58,58	0
81	MG	1	4047	1/1	0.88	0.20	50,50,50,50	0
81	MG	1	3617	1/1	0.88	0.20	75,75,75,75	0
81	MG	2	1996	1/1	0.88	0.21	80,80,80,80	0
81	MG	2	1951	1/1	0.88	0.09	134,134,134,134	0
81	MG	1	3519	1/1	0.88	0.31	43,43,43,43	0
81	MG	2	2082	1/1	0.88	0.26	119,119,119,119	0
81	MG	6	1984	1/1	0.88	0.17	89,89,89,89	0
81	MG	1	3520	1/1	0.88	0.40	51,51,51,51	0
81	MG	1	3653	1/1	0.88	0.32	51,51,51,51	0
80	PAR	3	202	42/42	0.88	0.31	55,55,55,55	42
81	MG	3	211	1/1	0.88	0.24	86,86,86,86	0
81	MG	1	3610	1/1	0.88	0.20	58,58,58,58	0
81	MG	2	2046	1/1	0.88	0.29	60,60,60,60	0
81	MG	5	4114	1/1	0.88	0.29	52,52,52,52	0
81	MG	5	3517	1/1	0.88	0.30	57,57,57,57	0
81	MG	2	2042	1/1	0.88	0.12	126,126,126,126	0
81	MG	M6	205	1/1	0.88	0.37	53,53,53,53	0
81	MG	5	3788	1/1	0.88	0.24	68,68,68,68	0
81	MG	6	1974	1/1	0.88	0.12	110,110,110,110	0
81	MG	5	3640	1/1	0.88	0.26	49,49,49,49	0
81	MG	6	2006	1/1	0.89	0.48	76,76,76,76	0
81	MG	2	2105	1/1	0.89	0.27	62,62,62,62	0
81	MG	6	1971	1/1	0.89	0.16	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	4159	1/1	0.89	0.16	55,55,55,55	1
81	MG	5	3610	1/1	0.89	0.20	81,81,81,81	0
81	MG	o4	202	1/1	0.89	0.16	89,89,89,89	0
81	MG	5	3978	1/1	0.89	0.27	72,72,72,72	0
81	MG	5	3809	1/1	0.89	0.34	49,49,49,49	0
81	MG	1	3997	1/1	0.89	0.38	80,80,80,80	0
81	MG	1	3481	1/1	0.89	0.24	48,48,48,48	0
81	MG	1	3550	1/1	0.89	0.24	64,64,64,64	0
81	MG	5	3506	1/1	0.89	0.25	55,55,55,55	0
81	MG	5	3969	1/1	0.89	0.28	55,55,55,55	0
81	MG	O7	105	1/1	0.89	0.28	41,41,41,41	0
81	MG	1	3727	1/1	0.89	0.51	39,39,39,39	1
81	MG	5	3648	1/1	0.89	0.24	59,59,59,59	0
81	MG	1	4120	1/1	0.89	0.28	81,81,81,81	0
81	MG	L2	305	1/1	0.89	0.35	47,47,47,47	0
81	MG	S9	201	1/1	0.89	0.24	126,126,126,126	0
81	MG	6	2023	1/1	0.89	0.29	90,90,90,90	0
81	MG	5	3868	1/1	0.89	0.16	57,57,57,57	0
81	MG	5	4080	1/1	0.89	0.16	64,64,64,64	0
81	MG	2	1971	1/1	0.89	0.43	73,73,73,73	0
81	MG	6	1987	1/1	0.89	0.21	68,68,68,68	0
81	MG	1	3854	1/1	0.89	0.27	52,52,52,52	0
81	MG	1	3641	1/1	0.89	0.20	57,57,57,57	0
81	MG	6	1976	1/1	0.89	0.37	89,89,89,89	0
81	MG	5	3558	1/1	0.89	0.31	70,70,70,70	0
81	MG	2	2067	1/1	0.89	0.25	75,75,75,75	0
81	MG	1	3870	1/1	0.89	0.23	36,36,36,36	1
81	MG	1	3498	1/1	0.89	0.49	66,66,66,66	0
81	MG	5	3970	1/1	0.89	0.28	59,59,59,59	0
81	MG	1	4032	1/1	0.89	0.34	41,41,41,41	0
81	MG	1	4106	1/1	0.89	0.57	68,68,68,68	0
81	MG	2	2039	1/1	0.89	0.23	113,113,113,113	0
81	MG	2	2076	1/1	0.89	0.46	92,92,92,92	0
81	MG	5	3740	1/1	0.89	0.44	68,68,68,68	0
81	MG	m7	206	1/1	0.89	0.28	50,50,50,50	0
81	MG	5	4063	1/1	0.89	0.36	80,80,80,80	0
80	PAR	1	3414	42/42	0.89	0.24	63,63,63,63	42
81	MG	N1	203	1/1	0.89	0.21	62,62,62,62	0
81	MG	1	3893	1/1	0.89	0.24	71,71,71,71	0
81	MG	5	3656	1/1	0.89	0.35	40,40,40,40	0
81	MG	1	3994	1/1	0.89	0.49	61,61,61,61	0
81	MG	5	3815	1/1	0.89	0.34	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	4049	1/1	0.89	0.18	73,73,73,73	0
81	MG	1	3568	1/1	0.89	0.26	55,55,55,55	0
81	MG	5	3992	1/1	0.89	0.37	59,59,59,59	0
81	MG	5	3888	1/1	0.89	0.30	61,61,61,61	0
81	MG	1	3587	1/1	0.89	0.50	53,53,53,53	0
81	MG	5	4018	1/1	0.89	0.56	95,95,95,95	0
81	MG	1	4122	1/1	0.89	0.24	68,68,68,68	0
81	MG	5	4102	1/1	0.89	0.24	48,48,48,48	1
81	MG	n3	204	1/1	0.89	0.35	50,50,50,50	0
80	PAR	1	3427	42/42	0.89	0.26	65,65,65,65	42
81	MG	1	4157	1/1	0.89	0.35	44,44,44,44	0
81	MG	5	3975	1/1	0.89	0.33	57,57,57,57	0
81	MG	1	3952	1/1	0.89	0.19	63,63,63,63	0
81	MG	1	3504	1/1	0.89	0.36	58,58,58,58	0
81	MG	1	4158	1/1	0.89	0.20	55,55,55,55	0
80	PAR	5	3415	42/42	0.89	0.23	83,83,83,83	0
81	MG	4	206	1/1	0.89	0.31	48,48,48,48	0
81	MG	1	3730	1/1	0.89	0.70	47,47,47,47	0
80	PAR	2	1904	42/42	0.89	0.18	107,107,107,107	0
81	MG	1	3729	1/1	0.89	0.47	44,44,44,44	0
81	MG	2	2053	1/1	0.89	0.20	100,100,100,100	0
81	MG	8	224	1/1	0.89	0.60	59,59,59,59	0
81	MG	6	2025	1/1	0.89	0.23	85,85,85,85	0
81	MG	1	3858	1/1	0.89	0.17	106,106,106,106	0
81	MG	5	4008	1/1	0.89	0.70	59,59,59,59	0
81	MG	1	3991	1/1	0.89	0.30	41,41,41,41	1
81	MG	5	3689	1/1	0.89	0.31	59,59,59,59	0
80	PAR	6	1901	42/42	0.89	0.27	90,90,90,90	0
81	MG	M5	307	1/1	0.89	0.37	43,43,43,43	0
81	MG	6	1927	1/1	0.89	0.43	73,73,73,73	0
81	MG	5	3754	1/1	0.89	0.18	53,53,53,53	0
81	MG	1	3537	1/1	0.89	0.37	31,31,31,31	0
81	MG	1	4067	1/1	0.89	0.16	54,54,54,54	0
81	MG	1	3940	1/1	0.89	0.41	37,37,37,37	0
81	MG	5	4083	1/1	0.89	0.29	78,78,78,78	0
81	MG	1	3837	1/1	0.89	0.35	63,63,63,63	0
81	MG	1	3744	1/1	0.89	0.31	39,39,39,39	0
81	MG	o7	503	1/1	0.89	0.28	58,58,58,58	0
81	MG	5	3752	1/1	0.89	0.12	60,60,60,60	0
81	MG	1	3670	1/1	0.89	0.27	57,57,57,57	1
81	MG	1	3927	1/1	0.89	0.18	53,53,53,53	0
81	MG	m6	203	1/1	0.89	0.27	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3493	1/1	0.89	0.18	50,50,50,50	0
81	MG	5	3745	1/1	0.89	0.69	54,54,54,54	0
81	MG	5	3939	1/1	0.89	0.29	74,74,74,74	0
81	MG	5	3806	1/1	0.89	0.24	65,65,65,65	0
81	MG	1	3465	1/1	0.89	0.26	34,34,34,34	0
81	MG	6	2038	1/1	0.89	0.25	105,105,105,105	0
80	PAR	5	3401	42/42	0.89	0.20	78,78,78,78	42
81	MG	n0	205	1/1	0.89	0.12	62,62,62,62	0
81	MG	5	3748	1/1	0.89	0.24	50,50,50,50	0
81	MG	5	4074	1/1	0.90	0.13	71,71,71,71	0
81	MG	o2	202	1/1	0.90	0.47	53,53,53,53	0
81	MG	Q2	502	1/1	0.90	0.28	38,38,38,38	0
81	MG	1	4134	1/1	0.90	0.36	69,69,69,69	0
81	MG	2	2002	1/1	0.90	0.16	79,79,79,79	0
81	MG	5	4029	1/1	0.90	0.35	57,57,57,57	0
81	MG	2	2073	1/1	0.90	0.16	99,99,99,99	0
81	MG	1	4124	1/1	0.90	0.40	69,69,69,69	0
80	PAR	1	3407	42/42	0.90	0.33	69,69,69,69	42
81	MG	5	3653	1/1	0.90	0.57	45,45,45,45	0
81	MG	5	4048	1/1	0.90	0.27	66,66,66,66	0
81	MG	6	2032	1/1	0.90	0.23	78,78,78,78	0
81	MG	1	3569	1/1	0.90	0.17	61,61,61,61	0
81	MG	5	3750	1/1	0.90	0.37	46,46,46,46	0
81	MG	1	3820	1/1	0.90	0.21	54,54,54,54	0
81	MG	5	4103	1/1	0.90	0.47	52,52,52,52	0
81	MG	5	3976	1/1	0.90	0.34	58,58,58,58	0
80	PAR	5	3424	42/42	0.90	0.28	65,65,65,65	42
81	MG	1	3825	1/1	0.90	0.21	65,65,65,65	0
81	MG	1	3891	1/1	0.90	0.23	59,59,59,59	0
81	MG	6	1934	1/1	0.90	0.41	83,83,83,83	0
81	MG	4	224	1/1	0.90	0.34	55,55,55,55	0
80	PAR	5	3414	42/42	0.90	0.22	67,67,67,67	42
81	MG	4	220	1/1	0.90	0.30	45,45,45,45	0
81	MG	1	4128	1/1	0.90	0.33	47,47,47,47	0
81	MG	1	4017	1/1	0.90	0.35	57,57,57,57	0
81	MG	5	4052	1/1	0.90	0.21	53,53,53,53	0
81	MG	1	3773	1/1	0.90	0.38	47,47,47,47	0
81	MG	5	3490	1/1	0.90	0.35	50,50,50,50	0
81	MG	5	3602	1/1	0.90	0.14	87,87,87,87	0
81	MG	5	3504	1/1	0.90	0.23	53,53,53,53	0
81	MG	d2	201	1/1	0.90	0.43	84,84,84,84	0
81	MG	2	2079	1/1	0.90	0.29	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	8	206	1/1	0.90	0.20	56,56,56,56	0
81	MG	5	3684	1/1	0.90	0.57	55,55,55,55	0
81	MG	5	3736	1/1	0.90	0.37	46,46,46,46	0
81	MG	6	1969	1/1	0.90	0.31	101,101,101,101	0
81	MG	1	3983	1/1	0.90	0.30	51,51,51,51	1
81	MG	5	3859	1/1	0.90	0.41	51,51,51,51	0
81	MG	5	4096	1/1	0.90	0.25	52,52,52,52	0
81	MG	5	3742	1/1	0.90	0.25	53,53,53,53	0
81	MG	5	3674	1/1	0.90	0.31	49,49,49,49	0
81	MG	5	3834	1/1	0.90	0.12	77,77,77,77	0
81	MG	5	4002	1/1	0.90	0.32	66,66,66,66	0
81	MG	O2	203	1/1	0.90	0.16	38,38,38,38	0
81	MG	1	4068	1/1	0.90	0.33	51,51,51,51	0
81	MG	1	3944	1/1	0.90	0.44	48,48,48,48	0
81	MG	6	2021	1/1	0.90	0.46	85,85,85,85	0
81	MG	5	3781	1/1	0.90	0.40	49,49,49,49	0
80	PAR	1	3422	42/42	0.90	0.27	51,51,51,51	42
81	MG	1	4130	1/1	0.90	0.26	38,38,38,38	1
81	MG	2	2012	1/1	0.90	0.10	104,104,104,104	0
81	MG	5	3836	1/1	0.90	0.28	51,51,51,51	0
81	MG	1	3535	1/1	0.90	0.42	36,36,36,36	1
81	MG	5	3651	1/1	0.90	0.17	63,63,63,63	1
81	MG	2	1983	1/1	0.90	0.74	68,68,68,68	0
81	MG	5	3714	1/1	0.90	0.28	58,58,58,58	0
81	MG	5	3533	1/1	0.90	0.24	50,50,50,50	0
81	MG	1	3740	1/1	0.90	0.36	42,42,42,42	0
81	MG	1	3892	1/1	0.90	0.14	72,72,72,72	0
81	MG	5	4110	1/1	0.90	0.77	82,82,82,82	0
81	MG	1	3607	1/1	0.90	0.71	57,57,57,57	1
81	MG	5	4081	1/1	0.90	0.28	102,102,102,102	0
81	MG	5	3884	1/1	0.90	0.15	67,67,67,67	0
81	MG	1	3649	1/1	0.90	0.51	37,37,37,37	0
81	MG	6	1916	1/1	0.90	0.21	79,79,79,79	0
81	MG	M0	301	1/1	0.90	0.21	54,54,54,54	0
81	MG	5	3763	1/1	0.90	0.36	42,42,42,42	0
81	MG	5	3931	1/1	0.90	0.46	54,54,54,54	0
81	MG	5	3949	1/1	0.90	0.15	58,58,58,58	1
81	MG	1	3739	1/1	0.90	0.27	43,43,43,43	0
81	MG	4	204	1/1	0.90	0.53	51,51,51,51	0
81	MG	1	3542	1/1	0.90	0.24	38,38,38,38	0
81	MG	1	4088	1/1	0.90	0.69	79,79,79,79	0
81	MG	5	3933	1/1	0.90	0.60	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	5	3930	1/1	0.90	0.34	50,50,50,50	0
81	MG	5	3662	1/1	0.90	0.41	56,56,56,56	0
81	MG	1	4190	1/1	0.90	0.21	73,73,73,73	0
81	MG	1	3775	1/1	0.90	0.35	47,47,47,47	0
81	MG	1	4011	1/1	0.90	0.77	54,54,54,54	0
81	MG	5	3795	1/1	0.90	0.12	106,106,106,106	0
81	MG	2	2040	1/1	0.90	0.30	123,123,123,123	0
80	PAR	5	3419	42/42	0.90	0.27	57,57,57,57	0
81	MG	1	4059	1/1	0.90	0.33	53,53,53,53	0
81	MG	1	3919	1/1	0.90	0.32	48,48,48,48	0
81	MG	5	3804	1/1	0.90	0.26	48,48,48,48	0
81	MG	5	4005	1/1	0.90	0.25	85,85,85,85	0
81	MG	1	3563	1/1	0.90	0.10	55,55,55,55	0
81	MG	2	1945	1/1	0.90	0.17	88,88,88,88	0
80	PAR	6	1904	42/42	0.90	0.28	72,72,72,72	0
81	MG	Q3	503	1/1	0.90	0.28	54,54,54,54	0
80	PAR	5	3418	42/42	0.90	0.24	98,98,98,98	0
81	MG	1	3583	1/1	0.90	0.25	49,49,49,49	0
80	PAR	1	3418	42/42	0.90	0.21	69,69,69,69	42
81	MG	1	3681	1/1	0.90	0.37	53,53,53,53	0
80	PAR	1	3420	42/42	0.90	0.21	65,65,65,65	42
81	MG	1	3921	1/1	0.90	0.28	40,40,40,40	0
81	MG	5	3595	1/1	0.90	0.15	83,83,83,83	0
81	MG	2	1975	1/1	0.90	0.31	94,94,94,94	0
81	MG	6	1950	1/1	0.90	0.23	83,83,83,83	0
81	MG	1	3970	1/1	0.90	0.20	55,55,55,55	0
81	MG	1	3933	1/1	0.91	0.15	65,65,65,65	1
81	MG	1	3810	1/1	0.91	0.36	96,96,96,96	0
81	MG	5	3891	1/1	0.91	0.17	68,68,68,68	0
81	MG	1	4009	1/1	0.91	0.42	46,46,46,46	0
81	MG	1	3885	1/1	0.91	0.17	67,67,67,67	0
80	PAR	6	1903	42/42	0.91	0.26	74,74,74,74	0
80	PAR	1	3402	42/42	0.91	0.19	62,62,62,62	42
81	MG	5	3889	1/1	0.91	0.36	66,66,66,66	0
81	MG	5	3604	1/1	0.91	0.23	62,62,62,62	0
81	MG	1	4063	1/1	0.91	0.38	47,47,47,47	0
81	MG	1	3625	1/1	0.91	0.23	36,36,36,36	1
81	MG	2	2055	1/1	0.91	0.35	56,56,56,56	0
81	MG	5	3666	1/1	0.91	0.18	44,44,44,44	0
81	MG	8	207	1/1	0.91	0.12	79,79,79,79	0
81	MG	5	3555	1/1	0.91	0.46	54,54,54,54	0
81	MG	5	3905	1/1	0.91	0.21	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	4081	1/1	0.91	0.23	63,63,63,63	0
81	MG	1	3492	1/1	0.91	0.36	47,47,47,47	0
81	MG	1	3910	1/1	0.91	0.54	48,48,48,48	0
81	MG	6	1933	1/1	0.91	0.70	92,92,92,92	0
81	MG	5	3965	1/1	0.91	0.36	58,58,58,58	0
81	MG	5	3649	1/1	0.91	0.35	50,50,50,50	0
81	MG	5	3548	1/1	0.91	0.38	52,52,52,52	0
81	MG	N6	202	1/1	0.91	0.30	50,50,50,50	0
81	MG	5	3973	1/1	0.91	0.32	47,47,47,47	1
81	MG	1	3570	1/1	0.91	0.34	60,60,60,60	0
80	PAR	1	3415	42/42	0.91	0.27	46,46,46,46	42
81	MG	5	3858	1/1	0.91	0.28	62,62,62,62	0
81	MG	1	4087	1/1	0.91	0.49	67,67,67,67	0
80	PAR	7	201	42/42	0.91	0.21	85,85,85,85	0
81	MG	M5	305	1/1	0.91	0.28	52,52,52,52	0
81	MG	m0	302	1/1	0.91	0.20	66,66,66,66	0
81	MG	2	2033	1/1	0.91	0.23	75,75,75,75	0
81	MG	1	4194	1/1	0.91	0.25	50,50,50,50	0
81	MG	6	1908	1/1	0.91	0.23	76,76,76,76	0
81	MG	1	3867	1/1	0.91	0.53	47,47,47,47	0
81	MG	1	3760	1/1	0.91	0.13	43,43,43,43	0
81	MG	1	4051	1/1	0.91	0.33	51,51,51,51	0
81	MG	1	3803	1/1	0.91	0.27	55,55,55,55	0
81	MG	1	4170	1/1	0.91	0.43	56,56,56,56	0
81	MG	1	3790	1/1	0.91	0.15	62,62,62,62	0
81	MG	5	3481	1/1	0.91	0.24	47,47,47,47	0
81	MG	5	3854	1/1	0.91	0.21	65,65,65,65	0
81	MG	2	1909	1/1	0.91	0.20	88,88,88,88	0
81	MG	5	3820	1/1	0.91	0.19	59,59,59,59	0
81	MG	2	2006	1/1	0.91	0.14	66,66,66,66	0
81	MG	1	3622	1/1	0.91	0.43	54,54,54,54	0
81	MG	5	3768	1/1	0.91	0.26	55,55,55,55	0
81	MG	5	3500	1/1	0.91	0.52	56,56,56,56	0
81	MG	1	4074	1/1	0.91	0.49	57,57,57,57	0
81	MG	5	3607	1/1	0.91	0.24	49,49,49,49	0
81	MG	1	3719	1/1	0.91	0.16	42,42,42,42	0
81	MG	l2	303	1/1	0.91	0.43	66,66,66,66	0
81	MG	1	3888	1/1	0.91	0.21	42,42,42,42	0
80	PAR	2	1902	42/42	0.91	0.27	74,74,74,74	0
81	MG	1	3811	1/1	0.91	0.07	64,64,64,64	0
81	MG	d4	201	1/1	0.91	0.22	91,91,91,91	0
81	MG	6	2000	1/1	0.91	0.09	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	5	3627	1/1	0.91	0.27	59,59,59,59	0
81	MG	8	208	1/1	0.91	0.21	71,71,71,71	0
81	MG	5	3917	1/1	0.91	0.47	72,72,72,72	0
81	MG	5	3588	1/1	0.91	0.20	69,69,69,69	0
81	MG	5	3650	1/1	0.91	0.40	46,46,46,46	0
81	MG	2	2099	1/1	0.91	0.35	57,57,57,57	0
81	MG	1	3929	1/1	0.91	0.32	47,47,47,47	1
81	MG	1	3943	1/1	0.91	0.32	40,40,40,40	0
81	MG	1	3551	1/1	0.91	0.36	46,46,46,46	0
81	MG	6	1968	1/1	0.91	0.23	77,77,77,77	0
81	MG	1	3918	1/1	0.91	0.20	70,70,70,70	0
81	MG	2	1977	1/1	0.91	0.10	96,96,96,96	0
81	MG	5	3635	1/1	0.91	0.16	59,59,59,59	0
81	MG	4	228	1/1	0.91	0.17	47,47,47,47	0
81	MG	1	4143	1/1	0.91	0.47	62,62,62,62	0
81	MG	5	3638	1/1	0.91	0.25	58,58,58,58	0
81	MG	1	3976	1/1	0.91	0.22	56,56,56,56	0
81	MG	5	3920	1/1	0.91	0.40	65,65,65,65	0
81	MG	5	4020	1/1	0.91	0.41	100,100,100,100	0
81	MG	5	3779	1/1	0.91	0.38	52,52,52,52	0
81	MG	2	1993	1/1	0.91	0.26	83,83,83,83	0
81	MG	1	4196	1/1	0.91	0.24	46,46,46,46	1
81	MG	L7	301	1/1	0.91	0.24	52,52,52,52	0
81	MG	5	3753	1/1	0.91	0.31	57,57,57,57	0
81	MG	1	4188	1/1	0.91	0.20	57,57,57,57	0
81	MG	6	1910	1/1	0.91	0.19	78,78,78,78	0
81	MG	N8	202	1/1	0.91	0.15	59,59,59,59	0
81	MG	5	3671	1/1	0.91	0.45	56,56,56,56	0
80	PAR	1	3419	42/42	0.91	0.24	59,59,59,59	0
81	MG	m9	202	1/1	0.91	0.21	80,80,80,80	0
81	MG	1	3850	1/1	0.91	0.14	57,57,57,57	0
81	MG	5	4051	1/1	0.91	0.31	61,61,61,61	0
81	MG	5	3447	1/1	0.91	0.21	45,45,45,45	0
81	MG	5	3918	1/1	0.91	0.44	60,60,60,60	0
81	MG	2	1942	1/1	0.91	0.20	77,77,77,77	0
81	MG	5	3934	1/1	0.91	0.46	58,58,58,58	0
80	PAR	1	3430	42/42	0.91	0.20	65,65,65,65	42
81	MG	4	213	1/1	0.91	0.13	41,41,41,41	0
81	MG	6	2043	1/1	0.91	0.18	97,97,97,97	0
81	MG	4	217	1/1	0.91	0.32	72,72,72,72	0
81	MG	5	4086	1/1	0.91	0.16	79,79,79,79	0
81	MG	5	3907	1/1	0.91	0.28	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	5	3544	1/1	0.91	0.41	55,55,55,55	0
80	PAR	1	3412	42/42	0.91	0.25	67,67,67,67	0
81	MG	5	3542	1/1	0.91	0.62	50,50,50,50	0
81	MG	5	3885	1/1	0.91	0.19	65,65,65,65	0
81	MG	5	4094	1/1	0.91	0.28	48,48,48,48	0
81	MG	1	3911	1/1	0.91	0.35	43,43,43,43	0
81	MG	1	3926	1/1	0.91	0.31	53,53,53,53	0
81	MG	n2	201	1/1	0.91	0.15	97,97,97,97	0
81	MG	2	1997	1/1	0.91	0.16	81,81,81,81	0
81	MG	1	3522	1/1	0.91	0.31	52,52,52,52	0
81	MG	5	3895	1/1	0.91	0.19	56,56,56,56	0
81	MG	1	3978	1/1	0.91	0.20	68,68,68,68	0
81	MG	1	4049	1/1	0.91	0.26	51,51,51,51	0
81	MG	5	3688	1/1	0.91	0.31	59,59,59,59	0
81	MG	5	3468	1/1	0.91	0.32	44,44,44,44	0
81	MG	s2	301	1/1	0.91	0.12	95,95,95,95	0
81	MG	S6	301	1/1	0.91	0.33	118,118,118,118	0
81	MG	5	3737	1/1	0.91	0.36	43,43,43,43	0
81	MG	1	3540	1/1	0.91	0.34	33,33,33,33	0
81	MG	1	3908	1/1	0.92	0.65	49,49,49,49	0
81	MG	5	3652	1/1	0.92	0.41	49,49,49,49	0
80	PAR	1	3425	42/42	0.92	0.23	48,48,48,48	42
81	MG	1	3652	1/1	0.92	0.35	41,41,41,41	0
81	MG	5	3912	1/1	0.92	0.20	63,63,63,63	0
81	MG	5	3810	1/1	0.92	0.21	50,50,50,50	0
81	MG	5	3563	1/1	0.92	0.26	85,85,85,85	0
81	MG	5	3732	1/1	0.92	0.50	50,50,50,50	0
81	MG	5	3869	1/1	0.92	0.14	64,64,64,64	0
81	MG	1	3869	1/1	0.92	0.28	44,44,44,44	0
80	PAR	5	3420	42/42	0.92	0.29	77,77,77,77	0
81	MG	1	3643	1/1	0.92	0.32	55,55,55,55	0
81	MG	1	3581	1/1	0.92	0.34	42,42,42,42	0
80	PAR	4	202	42/42	0.92	0.24	49,49,49,49	42
81	MG	1	4101	1/1	0.92	0.23	113,113,113,113	0
81	MG	1	3959	1/1	0.92	0.29	52,52,52,52	0
81	MG	1	3494	1/1	0.92	0.41	44,44,44,44	0
81	MG	L9	202	1/1	0.92	0.29	58,58,58,58	0
81	MG	5	3678	1/1	0.92	0.23	50,50,50,50	0
81	MG	2	1952	1/1	0.92	0.20	132,132,132,132	0
81	MG	M6	201	1/1	0.92	0.30	53,53,53,53	0
81	MG	5	3940	1/1	0.92	0.16	73,73,73,73	0
81	MG	2	2029	1/1	0.92	0.34	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	4193	1/1	0.92	0.34	66,66,66,66	0
81	MG	5	3692	1/1	0.92	0.38	56,56,56,56	0
81	MG	2	2088	1/1	0.92	0.35	64,64,64,64	0
81	MG	2	2050	1/1	0.92	0.44	67,67,67,67	0
81	MG	5	3696	1/1	0.92	0.29	59,59,59,59	0
81	MG	2	2022	1/1	0.92	0.22	79,79,79,79	0
81	MG	1	3509	1/1	0.92	0.10	74,74,74,74	0
81	MG	1	4152	1/1	0.92	0.17	47,47,47,47	1
80	PAR	5	3412	42/42	0.92	0.21	47,47,47,47	42
81	MG	1	4153	1/1	0.92	0.81	50,50,50,50	0
81	MG	o3	201	1/1	0.92	0.36	59,59,59,59	0
81	MG	1	3578	1/1	0.92	0.24	41,41,41,41	0
81	MG	6	1999	1/1	0.92	0.30	82,82,82,82	0
81	MG	1	3776	1/1	0.92	0.46	52,52,52,52	0
81	MG	5	3570	1/1	0.92	0.21	110,110,110,110	0
81	MG	5	3819	1/1	0.92	0.21	60,60,60,60	0
81	MG	2	2057	1/1	0.92	0.29	75,75,75,75	0
81	MG	1	4028	1/1	0.92	0.28	45,45,45,45	0
81	MG	2	2077	1/1	0.92	0.06	121,121,121,121	0
81	MG	1	3672	1/1	0.92	0.29	57,57,57,57	0
81	MG	5	4124	1/1	0.92	0.40	81,81,81,81	0
81	MG	1	3928	1/1	0.92	0.21	46,46,46,46	0
81	MG	d6	102	1/1	0.92	0.26	85,85,85,85	0
81	MG	4	219	1/1	0.92	0.27	54,54,54,54	0
81	MG	5	3567	1/1	0.92	0.18	73,73,73,73	0
81	MG	1	3659	1/1	0.92	0.16	53,53,53,53	0
81	MG	1	3939	1/1	0.92	0.30	49,49,49,49	1
81	MG	1	3467	1/1	0.92	0.28	31,31,31,31	0
81	MG	5	3540	1/1	0.92	0.24	48,48,48,48	0
81	MG	1	3470	1/1	0.92	0.26	42,42,42,42	0
81	MG	5	3894	1/1	0.92	0.15	57,57,57,57	0
81	MG	1	3556	1/1	0.92	0.28	36,36,36,36	0
81	MG	5	4039	1/1	0.92	0.64	56,56,56,56	0
81	MG	1	3826	1/1	0.92	0.23	37,37,37,37	1
81	MG	1	3812	1/1	0.92	0.21	52,52,52,52	0
81	MG	1	3886	1/1	0.92	0.34	38,38,38,38	0
81	MG	5	3897	1/1	0.92	0.31	55,55,55,55	0
81	MG	5	4023	1/1	0.92	0.43	60,60,60,60	0
81	MG	1	3986	1/1	0.92	0.30	51,51,51,51	0
81	MG	2	2038	1/1	0.92	0.13	109,109,109,109	0
81	MG	5	3843	1/1	0.92	0.64	86,86,86,86	0
81	MG	17	301	1/1	0.92	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	4151	1/1	0.92	0.24	40,40,40,40	0
80	PAR	5	3416	42/42	0.92	0.23	75,75,75,75	0
81	MG	5	3605	1/1	0.92	0.12	71,71,71,71	0
81	MG	s6	302	1/1	0.92	0.33	68,68,68,68	0
81	MG	1	3693	1/1	0.92	0.31	46,46,46,46	0
81	MG	1	3722	1/1	0.92	0.29	50,50,50,50	0
81	MG	L5	302	1/1	0.92	0.23	68,68,68,68	0
81	MG	5	3612	1/1	0.92	0.14	70,70,70,70	0
81	MG	6	1907	1/1	0.92	0.28	93,93,93,93	0
81	MG	5	3782	1/1	0.92	0.26	46,46,46,46	0
81	MG	1	3545	1/1	0.92	0.28	37,37,37,37	0
81	MG	1	4169	1/1	0.92	0.28	48,48,48,48	0
81	MG	5	3698	1/1	0.92	0.28	49,49,49,49	0
81	MG	5	3730	1/1	0.92	0.47	55,55,55,55	0
81	MG	5	3948	1/1	0.92	0.27	53,53,53,53	0
81	MG	5	3744	1/1	0.92	0.79	58,58,58,58	0
81	MG	1	4052	1/1	0.92	0.22	50,50,50,50	0
81	MG	14	403	1/1	0.92	0.31	80,80,80,80	0
80	PAR	1	3429	42/42	0.92	0.24	58,58,58,58	42
81	MG	1	3863	1/1	0.92	0.17	46,46,46,46	0
81	MG	5	3687	1/1	0.92	0.24	58,58,58,58	0
81	MG	5	3706	1/1	0.92	0.39	64,64,64,64	0
81	MG	5	3431	1/1	0.92	0.25	42,42,42,42	0
81	MG	1	3916	1/1	0.92	0.28	68,68,68,68	0
81	MG	1	3838	1/1	0.92	0.27	53,53,53,53	0
81	MG	6	1923	1/1	0.92	0.41	65,65,65,65	0
81	MG	N6	201	1/1	0.92	0.11	57,57,57,57	1
81	MG	6	2008	1/1	0.92	0.59	98,98,98,98	0
81	MG	5	3659	1/1	0.92	0.34	43,43,43,43	0
81	MG	5	3746	1/1	0.92	0.30	50,50,50,50	0
81	MG	5	3617	1/1	0.92	0.20	69,69,69,69	0
81	MG	1	3633	1/1	0.92	0.41	49,49,49,49	0
81	MG	1	3486	1/1	0.92	0.20	38,38,38,38	0
81	MG	1	4090	1/1	0.92	0.38	66,66,66,66	0
81	MG	1	3646	1/1	0.92	0.19	42,42,42,42	0
81	MG	5	3932	1/1	0.92	0.35	54,54,54,54	1
81	MG	5	3437	1/1	0.92	0.22	43,43,43,43	0
81	MG	L2	304	1/1	0.92	0.29	44,44,44,44	0
81	MG	5	3848	1/1	0.92	0.27	95,95,95,95	0
81	MG	1	3616	1/1	0.92	0.24	53,53,53,53	0
81	MG	1	3544	1/1	0.92	0.28	32,32,32,32	0
81	MG	1	3505	1/1	0.92	0.22	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3588	1/1	0.92	0.35	47,47,47,47	0
81	MG	5	3757	1/1	0.92	0.22	57,57,57,57	0
81	MG	2	2051	1/1	0.92	0.21	96,96,96,96	0
81	MG	1	3898	1/1	0.92	0.09	70,70,70,70	0
81	MG	6	1917	1/1	0.92	0.35	71,71,71,71	0
81	MG	1	4072	1/1	0.92	0.23	80,80,80,80	0
81	MG	c4	202	1/1	0.92	0.22	119,119,119,119	0
81	MG	1	4138	1/1	0.92	0.27	55,55,55,55	0
81	MG	2	1928	1/1	0.92	0.22	75,75,75,75	0
81	MG	6	2056	1/1	0.92	0.08	126,126,126,126	0
81	MG	1	3762	1/1	0.92	0.17	54,54,54,54	0
81	MG	1	4075	1/1	0.92	0.34	55,55,55,55	0
81	MG	6	1936	1/1	0.93	0.23	84,84,84,84	0
81	MG	2	1925	1/1	0.93	0.33	58,58,58,58	0
81	MG	5	3791	1/1	0.93	0.16	70,70,70,70	0
81	MG	5	3775	1/1	0.93	0.59	60,60,60,60	0
81	MG	5	4107	1/1	0.93	0.28	52,52,52,52	0
81	MG	6	2031	1/1	0.93	0.75	64,64,64,64	0
81	MG	7	205	1/1	0.93	0.12	93,93,93,93	0
81	MG	6	2005	1/1	0.93	0.67	62,62,62,62	0
81	MG	1	3804	1/1	0.93	0.28	45,45,45,45	0
81	MG	5	4041	1/1	0.93	0.18	70,70,70,70	0
80	PAR	5	3407	42/42	0.93	0.23	51,51,51,51	42
81	MG	1	4006	1/1	0.93	0.25	64,64,64,64	0
81	MG	5	3568	1/1	0.93	0.11	74,74,74,74	0
81	MG	6	1960	1/1	0.93	0.24	110,110,110,110	0
81	MG	5	3929	1/1	0.93	0.52	55,55,55,55	0
81	MG	7	206	1/1	0.93	0.20	116,116,116,116	0
81	MG	2	2021	1/1	0.93	0.28	73,73,73,73	0
81	MG	6	1989	1/1	0.93	0.22	75,75,75,75	0
81	MG	2	1974	1/1	0.93	0.19	101,101,101,101	0
81	MG	5	3725	1/1	0.93	0.31	63,63,63,63	0
81	MG	2	2087	1/1	0.93	0.27	70,70,70,70	0
81	MG	n0	204	1/1	0.93	0.20	63,63,63,63	0
81	MG	5	3518	1/1	0.93	0.22	52,52,52,52	0
81	MG	5	3702	1/1	0.93	0.56	61,61,61,61	0
81	MG	1	3906	1/1	0.93	0.31	38,38,38,38	0
80	PAR	1	3416	42/42	0.93	0.23	52,52,52,52	0
81	MG	1	4064	1/1	0.93	0.17	44,44,44,44	0
81	MG	5	3728	1/1	0.93	0.29	61,61,61,61	1
81	MG	5	4093	1/1	0.93	0.31	60,60,60,60	0
81	MG	1	4012	1/1	0.93	0.40	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	4	209	1/1	0.93	0.18	36,36,36,36	0
80	PAR	1	3428	42/42	0.93	0.21	58,58,58,58	0
81	MG	1	4150	1/1	0.93	0.25	62,62,62,62	0
81	MG	1	3637	1/1	0.93	0.49	45,45,45,45	0
81	MG	8	211	1/1	0.93	0.24	66,66,66,66	0
81	MG	8	203	1/1	0.93	0.18	56,56,56,56	0
81	MG	1	3807	1/1	0.93	0.20	49,49,49,49	0
81	MG	1	3675	1/1	0.93	0.32	64,64,64,64	0
81	MG	5	3456	1/1	0.93	0.28	43,43,43,43	0
81	MG	2	2047	1/1	0.93	0.38	94,94,94,94	0
81	MG	5	3797	1/1	0.93	0.36	51,51,51,51	0
81	MG	1	3441	1/1	0.93	0.28	30,30,30,30	0
81	MG	5	3628	1/1	0.93	0.20	59,59,59,59	0
81	MG	2	1955	1/1	0.93	0.09	133,133,133,133	0
81	MG	1	3787	1/1	0.93	0.11	97,97,97,97	0
81	MG	5	3956	1/1	0.93	0.51	56,56,56,56	0
81	MG	1	3980	1/1	0.93	0.21	54,54,54,54	0
81	MG	1	3772	1/1	0.93	0.37	49,49,49,49	0
81	MG	2	2017	1/1	0.93	0.23	93,93,93,93	0
81	MG	5	3833	1/1	0.93	0.30	56,56,56,56	0
81	MG	1	3780	1/1	0.93	0.32	42,42,42,42	0
81	MG	2	1965	1/1	0.93	0.19	95,95,95,95	0
81	MG	1	3524	1/1	0.93	0.07	52,52,52,52	0
81	MG	n1	201	1/1	0.93	0.24	70,70,70,70	0
81	MG	6	2069	1/1	0.93	0.28	54,54,54,54	0
81	MG	5	3943	1/1	0.93	0.25	75,75,75,75	0
81	MG	5	3480	1/1	0.93	0.28	45,45,45,45	0
81	MG	1	3755	1/1	0.93	0.18	51,51,51,51	0
81	MG	1	4163	1/1	0.93	0.33	39,39,39,39	1
80	PAR	1	3408	42/42	0.93	0.24	44,44,44,44	42
81	MG	1	3573	1/1	0.93	0.30	45,45,45,45	0
81	MG	2	1953	1/1	0.93	0.15	131,131,131,131	0
81	MG	1	3704	1/1	0.93	0.19	42,42,42,42	0
81	MG	4	221	1/1	0.93	0.15	46,46,46,46	1
81	MG	5	3600	1/1	0.93	0.15	93,93,93,93	0
81	MG	5	3676	1/1	0.93	0.28	42,42,42,42	0
81	MG	5	3578	1/1	0.93	0.26	48,48,48,48	0
81	MG	5	3971	1/1	0.93	0.17	58,58,58,58	0
81	MG	5	3800	1/1	0.93	0.39	62,62,62,62	0
81	MG	1	4144	1/1	0.93	0.34	40,40,40,40	1
81	MG	5	3501	1/1	0.93	0.22	58,58,58,58	0
81	MG	1	4040	1/1	0.93	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3582	1/1	0.93	0.57	40,40,40,40	0
81	MG	5	3923	1/1	0.93	0.11	112,112,112,112	0
81	MG	d3	201	1/1	0.93	0.33	68,68,68,68	0
81	MG	2	1990	1/1	0.93	0.28	88,88,88,88	0
81	MG	1	4167	1/1	0.93	0.20	65,65,65,65	0
81	MG	N5	201	1/1	0.93	0.19	61,61,61,61	0
81	MG	6	2061	1/1	0.93	0.29	110,110,110,110	0
81	MG	1	3536	1/1	0.93	0.31	37,37,37,37	0
81	MG	2	2009	1/1	0.93	0.29	70,70,70,70	0
81	MG	2	1906	1/1	0.93	0.25	80,80,80,80	0
81	MG	5	4117	1/1	0.93	0.24	62,62,62,62	0
81	MG	C8	201	1/1	0.93	0.18	137,137,137,137	0
81	MG	1	3988	1/1	0.93	0.22	56,56,56,56	0
81	MG	1	4023	1/1	0.93	0.30	49,49,49,49	0
81	MG	N0	201	1/1	0.93	0.46	60,60,60,60	0
81	MG	1	4172	1/1	0.93	0.27	41,41,41,41	0
81	MG	5	3434	1/1	0.93	0.34	46,46,46,46	0
81	MG	5	3657	1/1	0.93	0.26	47,47,47,47	0
81	MG	1	3462	1/1	0.93	0.40	30,30,30,30	0
81	MG	5	3562	1/1	0.93	0.12	94,94,94,94	0
81	MG	5	3780	1/1	0.93	0.32	51,51,51,51	0
81	MG	1	3736	1/1	0.93	0.24	58,58,58,58	0
81	MG	1	4165	1/1	0.93	0.33	42,42,42,42	0
81	MG	1	3624	1/1	0.93	0.22	34,34,34,34	0
80	PAR	5	3406	42/42	0.93	0.22	51,51,51,51	42
81	MG	1	4003	1/1	0.93	0.27	40,40,40,40	0
81	MG	5	4088	1/1	0.93	0.17	70,70,70,70	0
81	MG	2	1916	1/1	0.93	0.26	86,86,86,86	0
81	MG	1	4025	1/1	0.93	0.20	41,41,41,41	0
81	MG	1	3602	1/1	0.93	0.22	55,55,55,55	0
80	PAR	5	3408	42/42	0.93	0.22	58,58,58,58	42
81	MG	5	3790	1/1	0.93	0.11	76,76,76,76	0
81	MG	m6	204	1/1	0.93	0.38	49,49,49,49	0
81	MG	5	3672	1/1	0.93	0.23	40,40,40,40	0
80	PAR	5	3410	42/42	0.93	0.23	75,75,75,75	0
81	MG	1	3856	1/1	0.93	0.18	49,49,49,49	0
81	MG	1	4019	1/1	0.93	0.38	52,52,52,52	0
81	MG	5	3908	1/1	0.93	0.12	86,86,86,86	0
80	PAR	1	3424	42/42	0.93	0.28	76,76,76,76	0
81	MG	5	3492	1/1	0.93	0.33	47,47,47,47	0
81	MG	5	3722	1/1	0.93	0.16	74,74,74,74	0
81	MG	1	3576	1/1	0.93	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	4189	1/1	0.93	0.30	77,77,77,77	0
81	MG	6	1955	1/1	0.93	0.30	91,91,91,91	0
81	MG	5	3566	1/1	0.93	0.42	81,81,81,81	0
81	MG	1	4191	1/1	0.93	0.32	48,48,48,48	0
81	MG	O7	103	1/1	0.93	0.31	37,37,37,37	0
81	MG	1	3724	1/1	0.93	0.37	31,31,31,31	0
81	MG	5	3811	1/1	0.93	0.49	54,54,54,54	0
81	MG	4	227	1/1	0.93	0.08	76,76,76,76	0
81	MG	2	1921	1/1	0.93	0.27	72,72,72,72	0
81	MG	5	4040	1/1	0.93	0.24	49,49,49,49	0
81	MG	1	3770	1/1	0.93	0.38	45,45,45,45	1
81	MG	1	3936	1/1	0.93	0.14	65,65,65,65	0
81	MG	5	3519	1/1	0.93	0.30	48,48,48,48	0
81	MG	1	3613	1/1	0.93	0.19	63,63,63,63	0
81	MG	5	3703	1/1	0.93	0.55	58,58,58,58	0
81	MG	6	1991	1/1	0.93	0.40	62,62,62,62	0
81	MG	1	3912	1/1	0.93	0.39	44,44,44,44	0
81	MG	8	205	1/1	0.93	0.27	55,55,55,55	0
81	MG	5	3466	1/1	0.93	0.31	45,45,45,45	0
81	MG	5	3787	1/1	0.93	0.30	59,59,59,59	0
81	MG	4	218	1/1	0.93	0.15	39,39,39,39	0
81	MG	1	3650	1/1	0.93	0.50	31,31,31,31	0
81	MG	1	3733	1/1	0.94	0.29	41,41,41,41	0
81	MG	6	2018	1/1	0.94	0.23	89,89,89,89	0
81	MG	1	3589	1/1	0.94	0.63	49,49,49,49	0
81	MG	1	3920	1/1	0.94	0.34	50,50,50,50	0
81	MG	6	1996	1/1	0.94	0.09	96,96,96,96	0
81	MG	1	3865	1/1	0.94	0.21	46,46,46,46	1
81	MG	2	2114	1/1	0.94	0.22	104,104,104,104	0
81	MG	O4	203	1/1	0.94	0.10	59,59,59,59	0
81	MG	1	3746	1/1	0.94	0.40	36,36,36,36	0
81	MG	6	1994	1/1	0.94	0.29	79,79,79,79	0
81	MG	1	3566	1/1	0.94	0.23	43,43,43,43	0
81	MG	1	3673	1/1	0.94	0.28	52,52,52,52	0
81	MG	5	3569	1/1	0.94	0.26	78,78,78,78	0
81	MG	1	3658	1/1	0.94	0.23	41,41,41,41	0
81	MG	2	2068	1/1	0.94	0.21	78,78,78,78	0
81	MG	5	4106	1/1	0.94	0.37	73,73,73,73	0
81	MG	2	1926	1/1	0.94	0.36	62,62,62,62	0
81	MG	m0	301	1/1	0.94	0.09	58,58,58,58	0
81	MG	n8	204	1/1	0.94	0.22	48,48,48,48	0
81	MG	1	3606	1/1	0.94	0.24	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3827	1/1	0.94	0.30	35,35,35,35	0
80	PAR	1	3409	42/42	0.94	0.22	38,38,38,38	42
81	MG	1	3721	1/1	0.94	0.26	47,47,47,47	1
81	MG	1	3934	1/1	0.94	0.19	57,57,57,57	0
81	MG	n3	202	1/1	0.94	0.31	59,59,59,59	0
81	MG	1	3547	1/1	0.94	0.17	65,65,65,65	0
80	PAR	2	1903	42/42	0.94	0.24	69,69,69,69	0
81	MG	6	2048	1/1	0.94	0.29	88,88,88,88	0
81	MG	7	207	1/1	0.94	0.18	118,118,118,118	0
81	MG	1	3887	1/1	0.94	0.13	40,40,40,40	0
81	MG	5	3776	1/1	0.94	0.49	48,48,48,48	0
81	MG	1	3552	1/1	0.94	0.36	61,61,61,61	0
81	MG	6	1961	1/1	0.94	0.20	98,98,98,98	0
81	MG	5	3803	1/1	0.94	0.18	47,47,47,47	0
81	MG	1	3691	1/1	0.94	0.28	42,42,42,42	0
81	MG	1	3668	1/1	0.94	0.25	53,53,53,53	0
81	MG	1	3488	1/1	0.94	0.23	43,43,43,43	0
81	MG	2	1913	1/1	0.94	0.23	87,87,87,87	0
81	MG	5	3534	1/1	0.94	0.30	46,46,46,46	0
81	MG	5	3515	1/1	0.94	0.17	61,61,61,61	0
81	MG	1	3835	1/1	0.94	0.36	45,45,45,45	0
81	MG	1	4178	1/1	0.94	0.32	54,54,54,54	0
81	MG	1	4197	1/1	0.94	0.33	44,44,44,44	0
81	MG	1	3878	1/1	0.94	0.38	54,54,54,54	1
81	MG	4	208	1/1	0.94	0.27	55,55,55,55	0
81	MG	1	3938	1/1	0.94	0.38	49,49,49,49	0
81	MG	1	3877	1/1	0.94	0.42	46,46,46,46	0
81	MG	5	3509	1/1	0.94	0.13	72,72,72,72	0
81	MG	5	3721	1/1	0.94	0.28	67,67,67,67	0
81	MG	5	3882	1/1	0.94	0.38	55,55,55,55	0
81	MG	6	1930	1/1	0.94	0.25	86,86,86,86	0
81	MG	6	1913	1/1	0.94	0.14	72,72,72,72	0
81	MG	1	3960	1/1	0.94	0.25	43,43,43,43	0
81	MG	1	3661	1/1	0.94	0.26	46,46,46,46	0
81	MG	1	3831	1/1	0.94	0.24	37,37,37,37	0
81	MG	6	2073	1/1	0.94	0.46	94,94,94,94	0
81	MG	N1	201	1/1	0.94	0.16	59,59,59,59	0
81	MG	1	3779	1/1	0.94	0.30	41,41,41,41	0
81	MG	M5	308	1/1	0.94	0.39	58,58,58,58	0
81	MG	4	207	1/1	0.94	0.16	58,58,58,58	0
81	MG	1	3801	1/1	0.94	0.30	47,47,47,47	0
80	PAR	5	3417	42/42	0.94	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	2	1966	1/1	0.94	0.18	99,99,99,99	0
81	MG	M7	204	1/1	0.94	0.22	42,42,42,42	0
81	MG	1	4071	1/1	0.94	0.18	78,78,78,78	0
81	MG	1	3793	1/1	0.94	0.27	43,43,43,43	0
81	MG	5	4042	1/1	0.94	0.27	69,69,69,69	0
81	MG	2	1962	1/1	0.94	0.12	106,106,106,106	0
81	MG	5	3592	1/1	0.94	0.26	61,61,61,61	1
81	MG	o7	502	1/1	0.94	0.34	48,48,48,48	0
81	MG	5	4089	1/1	0.94	0.30	69,69,69,69	0
81	MG	2	1908	1/1	0.94	0.24	104,104,104,104	0
81	MG	5	3668	1/1	0.94	0.31	47,47,47,47	1
81	MG	5	4077	1/1	0.94	0.28	74,74,74,74	0
81	MG	1	3629	1/1	0.94	0.58	53,53,53,53	0
81	MG	1	4045	1/1	0.94	0.30	44,44,44,44	0
81	MG	1	3757	1/1	0.94	0.31	45,45,45,45	0
81	MG	5	3866	1/1	0.94	0.19	68,68,68,68	0
81	MG	5	3489	1/1	0.94	0.26	46,46,46,46	0
81	MG	4	211	1/1	0.94	0.18	47,47,47,47	0
81	MG	1	3480	1/1	0.94	0.22	39,39,39,39	0
81	MG	6	1914	1/1	0.94	0.17	81,81,81,81	0
81	MG	5	3435	1/1	0.94	0.25	44,44,44,44	0
81	MG	O3	202	1/1	0.94	0.20	56,56,56,56	0
81	MG	5	4078	1/1	0.94	0.28	63,63,63,63	0
81	MG	1	3626	1/1	0.94	0.39	36,36,36,36	0
81	MG	o0	201	1/1	0.94	0.25	89,89,89,89	0
81	MG	m7	208	1/1	0.94	0.30	43,43,43,43	0
81	MG	5	3832	1/1	0.94	0.55	52,52,52,52	0
81	MG	n8	203	1/1	0.94	0.84	51,51,51,51	1
81	MG	5	3865	1/1	0.94	0.13	58,58,58,58	0
80	PAR	1	3411	42/42	0.94	0.24	44,44,44,44	0
81	MG	5	4026	1/1	0.94	0.50	69,69,69,69	0
81	MG	1	3712	1/1	0.94	0.33	43,43,43,43	0
81	MG	1	3792	1/1	0.94	0.22	45,45,45,45	0
81	MG	5	3996	1/1	0.94	0.33	54,54,54,54	0
81	MG	1	3452	1/1	0.94	0.35	30,30,30,30	0
81	MG	2	2027	1/1	0.94	0.20	69,69,69,69	0
81	MG	L3	404	1/1	0.94	0.29	43,43,43,43	0
81	MG	n5	201	1/1	0.94	0.35	60,60,60,60	0
81	MG	4	215	1/1	0.94	0.24	42,42,42,42	0
81	MG	1	3618	1/1	0.94	0.19	68,68,68,68	0
80	PAR	1	3421	42/42	0.94	0.24	43,43,43,43	42
81	MG	5	3571	1/1	0.94	0.15	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	6	1929	1/1	0.94	0.25	80,80,80,80	0
81	MG	1	4135	1/1	0.94	0.31	37,37,37,37	1
81	MG	1	4086	1/1	0.94	0.47	55,55,55,55	0
81	MG	1	3684	1/1	0.94	0.35	43,43,43,43	0
81	MG	1	3707	1/1	0.94	0.36	40,40,40,40	0
81	MG	1	3662	1/1	0.94	0.34	45,45,45,45	0
81	MG	5	4036	1/1	0.94	0.51	68,68,68,68	0
81	MG	5	3661	1/1	0.94	0.35	47,47,47,47	0
81	MG	n3	203	1/1	0.94	0.27	76,76,76,76	0
81	MG	1	3925	1/1	0.94	0.20	52,52,52,52	1
81	MG	1	4077	1/1	0.94	0.28	51,51,51,51	0
81	MG	5	4056	1/1	0.94	0.22	48,48,48,48	0
81	MG	5	3808	1/1	0.94	0.18	54,54,54,54	1
81	MG	n6	203	1/1	0.94	0.23	76,76,76,76	0
81	MG	1	3666	1/1	0.94	0.30	49,49,49,49	0
81	MG	5	3484	1/1	0.94	0.27	58,58,58,58	0
81	MG	1	3747	1/1	0.94	0.28	36,36,36,36	0
81	MG	5	3463	1/1	0.94	0.43	44,44,44,44	0
81	MG	6	2019	1/1	0.94	0.19	107,107,107,107	0
81	MG	1	4168	1/1	0.94	0.13	64,64,64,64	0
80	PAR	1	3423	42/42	0.94	0.23	54,54,54,54	0
81	MG	2	2110	1/1	0.94	0.46	78,78,78,78	0
81	MG	5	3470	1/1	0.94	0.26	45,45,45,45	0
81	MG	6	1931	1/1	0.94	0.20	94,94,94,94	0
81	MG	1	3655	1/1	0.94	0.29	52,52,52,52	0
81	MG	5	3609	1/1	0.94	0.29	59,59,59,59	0
81	MG	1	3450	1/1	0.94	0.28	29,29,29,29	0
81	MG	L2	303	1/1	0.94	0.24	38,38,38,38	0
81	MG	s4	301	1/1	0.94	0.10	96,96,96,96	0
81	MG	1	3688	1/1	0.94	0.29	39,39,39,39	0
81	MG	6	1945	1/1	0.94	0.31	71,71,71,71	0
81	MG	5	3453	1/1	0.94	0.24	45,45,45,45	0
81	MG	L2	301	1/1	0.94	0.31	31,31,31,31	0
81	MG	m7	209	1/1	0.94	0.29	47,47,47,47	0
81	MG	1	3697	1/1	0.94	0.69	58,58,58,58	0
81	MG	5	3494	1/1	0.94	0.17	64,64,64,64	0
81	MG	1	3562	1/1	0.94	0.40	44,44,44,44	0
81	MG	2	2015	1/1	0.94	0.09	140,140,140,140	0
81	MG	6	1942	1/1	0.94	0.19	105,105,105,105	0
81	MG	1	3796	1/1	0.94	0.29	52,52,52,52	0
81	MG	5	3816	1/1	0.94	0.18	58,58,58,58	0
81	MG	2	2005	1/1	0.94	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3794	1/1	0.94	0.23	55,55,55,55	0
81	MG	5	3587	1/1	0.94	0.20	66,66,66,66	0
81	MG	6	1918	1/1	0.94	0.31	71,71,71,71	0
81	MG	5	3830	1/1	0.94	0.27	56,56,56,56	0
81	MG	1	3735	1/1	0.94	0.55	62,62,62,62	0
81	MG	M5	301	1/1	0.94	0.22	39,39,39,39	0
81	MG	1	4137	1/1	0.94	0.21	61,61,61,61	0
81	MG	1	3741	1/1	0.94	0.28	37,37,37,37	0
81	MG	1	3765	1/1	0.94	0.18	68,68,68,68	0
81	MG	5	3549	1/1	0.94	0.49	50,50,50,50	0
81	MG	1	4156	1/1	0.94	0.21	44,44,44,44	1
81	MG	1	3510	1/1	0.94	0.11	68,68,68,68	0
81	MG	5	3758	1/1	0.95	0.33	48,48,48,48	0
81	MG	5	3432	1/1	0.95	0.37	43,43,43,43	0
81	MG	5	4053	1/1	0.95	0.18	59,59,59,59	0
81	MG	l3	403	1/1	0.95	0.28	43,43,43,43	1
81	MG	5	3760	1/1	0.95	0.23	50,50,50,50	0
81	MG	8	221	1/1	0.95	0.11	86,86,86,86	0
81	MG	1	3674	1/1	0.95	0.37	46,46,46,46	0
81	MG	5	3514	1/1	0.95	0.26	57,57,57,57	0
81	MG	5	3430	1/1	0.95	0.22	45,45,45,45	0
81	MG	6	1911	1/1	0.95	0.26	73,73,73,73	0
81	MG	6	2057	1/1	0.95	0.09	126,126,126,126	0
81	MG	8	218	1/1	0.95	0.22	73,73,73,73	0
81	MG	5	3849	1/1	0.95	0.57	88,88,88,88	0
81	MG	1	3594	1/1	0.95	0.38	45,45,45,45	0
81	MG	1	3555	1/1	0.95	0.26	38,38,38,38	0
81	MG	5	3584	1/1	0.95	0.31	67,67,67,67	0
81	MG	C9	201	1/1	0.95	0.16	121,121,121,121	0
81	MG	1	3438	1/1	0.95	0.33	36,36,36,36	0
81	MG	6	1963	1/1	0.95	0.39	97,97,97,97	0
81	MG	1	3866	1/1	0.95	0.31	38,38,38,38	0
81	MG	5	3482	1/1	0.95	0.45	44,44,44,44	0
81	MG	5	3525	1/1	0.95	0.32	52,52,52,52	0
81	MG	1	3644	1/1	0.95	0.35	46,46,46,46	0
81	MG	2	1946	1/1	0.95	0.24	74,74,74,74	0
81	MG	5	4032	1/1	0.95	0.16	75,75,75,75	0
81	MG	5	4022	1/1	0.95	0.87	64,64,64,64	0
81	MG	1	4179	1/1	0.95	0.24	42,42,42,42	0
81	MG	5	3665	1/1	0.95	0.24	46,46,46,46	0
81	MG	5	3487	1/1	0.95	0.32	43,43,43,43	0
81	MG	5	3473	1/1	0.95	0.32	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3699	1/1	0.95	0.24	48,48,48,48	0
81	MG	N3	202	1/1	0.95	0.43	68,68,68,68	0
81	MG	5	3477	1/1	0.95	0.23	49,49,49,49	0
81	MG	5	3444	1/1	0.95	0.18	52,52,52,52	0
81	MG	5	3712	1/1	0.95	0.39	57,57,57,57	0
81	MG	5	3488	1/1	0.95	0.21	44,44,44,44	0
81	MG	1	3814	1/1	0.95	0.27	47,47,47,47	0
81	MG	2	2035	1/1	0.95	0.11	116,116,116,116	0
81	MG	1	3572	1/1	0.95	0.31	41,41,41,41	0
81	MG	5	3863	1/1	0.95	0.31	55,55,55,55	0
81	MG	1	3834	1/1	0.95	0.29	31,31,31,31	0
81	MG	1	3942	1/1	0.95	0.16	52,52,52,52	0
81	MG	5	3629	1/1	0.95	0.10	66,66,66,66	0
81	MG	1	3686	1/1	0.95	0.20	45,45,45,45	0
81	MG	6	2033	1/1	0.95	0.34	70,70,70,70	0
81	MG	2	2064	1/1	0.95	0.12	111,111,111,111	0
81	MG	5	3454	1/1	0.95	0.24	40,40,40,40	0
81	MG	m7	202	1/1	0.95	0.23	48,48,48,48	0
81	MG	5	4028	1/1	0.95	0.20	78,78,78,78	0
81	MG	1	3778	1/1	0.95	0.29	50,50,50,50	1
81	MG	1	3696	1/1	0.95	0.47	51,51,51,51	0
81	MG	1	3808	1/1	0.95	0.23	51,51,51,51	0
81	MG	5	3593	1/1	0.95	0.32	64,64,64,64	0
81	MG	5	3691	1/1	0.95	0.55	58,58,58,58	0
81	MG	1	3611	1/1	0.95	0.13	60,60,60,60	0
81	MG	1	3802	1/1	0.95	0.14	42,42,42,42	0
81	MG	5	3591	1/1	0.95	0.28	58,58,58,58	0
81	MG	6	1926	1/1	0.95	0.31	70,70,70,70	0
81	MG	1	3620	1/1	0.95	0.22	68,68,68,68	0
81	MG	s6	301	1/1	0.95	0.09	121,121,121,121	0
81	MG	1	3754	1/1	0.95	0.14	52,52,52,52	0
81	MG	6	2007	1/1	0.95	0.48	90,90,90,90	0
81	MG	1	3598	1/1	0.95	0.29	41,41,41,41	0
81	MG	5	3575	1/1	0.95	0.24	58,58,58,58	0
81	MG	5	3765	1/1	0.95	0.17	52,52,52,52	1
81	MG	O4	204	1/1	0.95	0.24	63,63,63,63	0
81	MG	M7	203	1/1	0.95	0.28	45,45,45,45	0
81	MG	1	3479	1/1	0.95	0.35	37,37,37,37	0
81	MG	4	237	1/1	0.95	0.39	68,68,68,68	0
81	MG	1	3872	1/1	0.95	0.27	63,63,63,63	0
81	MG	1	3732	1/1	0.95	0.37	50,50,50,50	0
81	MG	1	4132	1/1	0.95	0.25	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3709	1/1	0.95	0.24	32,32,32,32	0
81	MG	S7	201	1/1	0.95	0.13	89,89,89,89	0
81	MG	6	2022	1/1	0.95	0.41	64,64,64,64	0
81	MG	5	3551	1/1	0.95	0.43	54,54,54,54	1
81	MG	1	3737	1/1	0.95	0.33	61,61,61,61	0
81	MG	5	3582	1/1	0.95	0.31	54,54,54,54	0
81	MG	4	222	1/1	0.95	0.18	49,49,49,49	0
81	MG	2	1985	1/1	0.95	0.36	46,46,46,46	0
81	MG	5	3443	1/1	0.95	0.24	42,42,42,42	0
81	MG	6	1990	1/1	0.95	0.27	69,69,69,69	0
81	MG	5	3545	1/1	0.95	0.24	55,55,55,55	0
81	MG	6	1967	1/1	0.95	0.31	80,80,80,80	0
81	MG	5	3735	1/1	0.95	0.27	49,49,49,49	0
81	MG	1	4021	1/1	0.95	0.38	45,45,45,45	0
81	MG	1	3734	1/1	0.95	0.35	43,43,43,43	0
81	MG	1	3608	1/1	0.95	0.25	50,50,50,50	0
81	MG	1	3879	1/1	0.95	0.33	61,61,61,61	0
81	MG	7	210	1/1	0.95	0.24	53,53,53,53	0
81	MG	5	3831	1/1	0.95	0.32	66,66,66,66	0
81	MG	1	3571	1/1	0.95	0.27	40,40,40,40	0
81	MG	1	3671	1/1	0.95	0.43	52,52,52,52	0
81	MG	5	3761	1/1	0.95	0.33	45,45,45,45	0
81	MG	1	3664	1/1	0.95	0.37	50,50,50,50	0
81	MG	2	1944	1/1	0.95	0.23	84,84,84,84	0
81	MG	5	3641	1/1	0.95	0.18	45,45,45,45	0
81	MG	6	2047	1/1	0.95	0.19	109,109,109,109	0
81	MG	1	3506	1/1	0.95	0.12	65,65,65,65	0
81	MG	5	3589	1/1	0.95	0.22	63,63,63,63	0
81	MG	1	3823	1/1	0.95	0.25	42,42,42,42	0
81	MG	3	204	1/1	0.95	0.16	84,84,84,84	0
81	MG	1	4185	1/1	0.95	0.09	56,56,56,56	0
81	MG	2	2008	1/1	0.95	0.30	76,76,76,76	0
81	MG	6	1964	1/1	0.95	0.18	108,108,108,108	0
81	MG	1	3531	1/1	0.95	0.31	41,41,41,41	0
81	MG	5	4001	1/1	0.95	0.24	63,63,63,63	0
81	MG	5	3663	1/1	0.95	0.24	57,57,57,57	0
81	MG	o0	202	1/1	0.95	0.46	88,88,88,88	0
81	MG	5	3817	1/1	0.95	0.32	57,57,57,57	0
81	MG	Q2	503	1/1	0.95	0.28	42,42,42,42	0
81	MG	5	3634	1/1	0.95	0.14	55,55,55,55	0
81	MG	m7	203	1/1	0.95	0.20	49,49,49,49	0
81	MG	5	3802	1/1	0.95	0.23	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	1	3645	1/1	0.95	0.20	44,44,44,44	0
81	MG	2	2096	1/1	0.95	0.18	76,76,76,76	0
81	MG	2	1920	1/1	0.95	0.35	68,68,68,68	0
81	MG	1	3992	1/1	0.95	0.24	47,47,47,47	1
81	MG	5	3718	1/1	0.95	0.29	63,63,63,63	0
81	MG	1	3478	1/1	0.95	0.31	37,37,37,37	0
81	MG	1	3824	1/1	0.95	0.32	58,58,58,58	0
81	MG	1	4082	1/1	0.95	0.24	54,54,54,54	0
81	MG	5	3564	1/1	0.95	0.16	85,85,85,85	0
81	MG	1	3705	1/1	0.95	0.38	44,44,44,44	0
81	MG	1	3843	1/1	0.95	0.14	48,48,48,48	0
81	MG	1	3609	1/1	0.95	0.15	56,56,56,56	0
81	MG	4	225	1/1	0.95	0.10	62,62,62,62	1
81	MG	m6	202	1/1	0.95	0.22	53,53,53,53	0
81	MG	1	3842	1/1	0.95	0.22	43,43,43,43	1
81	MG	1	3763	1/1	0.95	0.10	56,56,56,56	0
81	MG	1	3516	1/1	0.95	0.18	47,47,47,47	0
81	MG	1	4016	1/1	0.95	0.47	57,57,57,57	0
81	MG	q2	502	1/1	0.95	0.23	70,70,70,70	0
81	MG	6	1932	1/1	0.95	0.41	87,87,87,87	0
81	MG	2	1927	1/1	0.95	0.14	75,75,75,75	0
82	ZN	o4	201	1/1	0.96	0.10	102,102,102,102	0
81	MG	1	3561	1/1	0.96	0.18	43,43,43,43	0
81	MG	5	3870	1/1	0.96	0.19	63,63,63,63	0
81	MG	4	235	1/1	0.96	0.37	43,43,43,43	0
81	MG	5	3543	1/1	0.96	0.20	56,56,56,56	0
81	MG	1	3745	1/1	0.96	0.43	33,33,33,33	0
81	MG	5	3583	1/1	0.96	0.26	54,54,54,54	0
81	MG	5	4075	1/1	0.96	0.16	66,66,66,66	0
81	MG	1	3977	1/1	0.96	0.30	49,49,49,49	0
81	MG	5	3682	1/1	0.96	0.32	52,52,52,52	0
81	MG	5	3522	1/1	0.96	0.21	54,54,54,54	0
81	MG	1	3599	1/1	0.96	0.20	52,52,52,52	0
81	MG	5	3664	1/1	0.96	0.26	50,50,50,50	0
81	MG	3	212	1/1	0.96	0.19	85,85,85,85	0
81	MG	1	3685	1/1	0.96	0.31	41,41,41,41	0
81	MG	1	3902	1/1	0.96	0.21	61,61,61,61	0
81	MG	3	205	1/1	0.96	0.17	73,73,73,73	0
81	MG	1	3457	1/1	0.96	0.30	36,36,36,36	0
81	MG	1	3766	1/1	0.96	0.15	55,55,55,55	0
81	MG	5	3458	1/1	0.96	0.30	40,40,40,40	0
81	MG	5	3997	1/1	0.96	0.55	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	m5	301	1/1	0.96	0.26	72,72,72,72	0
81	MG	1	3999	1/1	0.96	0.31	58,58,58,58	0
81	MG	1	3758	1/1	0.96	0.23	45,45,45,45	0
81	MG	5	3433	1/1	0.96	0.36	46,46,46,46	0
81	MG	1	3859	1/1	0.96	0.16	53,53,53,53	0
81	MG	1	3584	1/1	0.96	0.37	43,43,43,43	0
81	MG	5	3479	1/1	0.96	0.15	48,48,48,48	0
81	MG	1	3699	1/1	0.96	0.61	51,51,51,51	0
81	MG	6	1970	1/1	0.96	0.23	86,86,86,86	0
81	MG	l3	401	1/1	0.96	0.22	44,44,44,44	0
81	MG	5	3485	1/1	0.96	0.26	47,47,47,47	0
81	MG	l4	402	1/1	0.96	0.45	57,57,57,57	0
81	MG	1	3517	1/1	0.96	0.23	43,43,43,43	0
81	MG	1	3995	1/1	0.96	0.22	47,47,47,47	0
81	MG	d3	203	1/1	0.96	0.15	80,80,80,80	0
81	MG	5	3511	1/1	0.96	0.17	45,45,45,45	0
81	MG	5	3438	1/1	0.96	0.25	47,47,47,47	0
81	MG	5	3449	1/1	0.96	0.18	56,56,56,56	0
81	MG	1	3750	1/1	0.96	0.23	38,38,38,38	0
81	MG	1	4083	1/1	0.96	0.34	44,44,44,44	0
81	MG	5	3499	1/1	0.96	0.14	56,56,56,56	0
81	MG	6	2015	1/1	0.96	0.30	91,91,91,91	0
81	MG	5	3686	1/1	0.96	0.21	55,55,55,55	0
81	MG	1	3690	1/1	0.96	0.21	44,44,44,44	0
81	MG	1	3515	1/1	0.96	0.26	44,44,44,44	0
81	MG	6	2012	1/1	0.96	0.42	65,65,65,65	0
82	ZN	D9	101	1/1	0.96	0.12	112,112,112,112	0
81	MG	1	3656	1/1	0.96	0.29	48,48,48,48	0
81	MG	1	3931	1/1	0.96	0.16	40,40,40,40	0
81	MG	5	3520	1/1	0.96	0.42	47,47,47,47	0
81	MG	1	4149	1/1	0.96	0.22	44,44,44,44	0
81	MG	D3	201	1/1	0.96	0.14	75,75,75,75	0
81	MG	1	3580	1/1	0.96	0.20	38,38,38,38	0
81	MG	1	3951	1/1	0.96	0.17	60,60,60,60	0
81	MG	6	1948	1/1	0.96	0.21	111,111,111,111	0
81	MG	1	3679	1/1	0.96	0.25	70,70,70,70	0
81	MG	6	1978	1/1	0.96	0.10	111,111,111,111	0
81	MG	1	3828	1/1	0.96	0.42	43,43,43,43	0
81	MG	1	3708	1/1	0.96	0.28	39,39,39,39	0
81	MG	5	3636	1/1	0.96	0.21	53,53,53,53	0
81	MG	1	3456	1/1	0.96	0.28	36,36,36,36	0
81	MG	m7	207	1/1	0.96	0.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3799	1/1	0.96	0.30	35,35,35,35	0
81	MG	1	3836	1/1	0.96	0.22	63,63,63,63	0
81	MG	5	3717	1/1	0.96	0.24	55,55,55,55	1
81	MG	5	3475	1/1	0.96	0.29	39,39,39,39	0
81	MG	O2	201	1/1	0.96	0.22	43,43,43,43	0
81	MG	1	3832	1/1	0.96	0.27	45,45,45,45	0
81	MG	2	1914	1/1	0.96	0.11	92,92,92,92	0
81	MG	5	3516	1/1	0.96	0.21	55,55,55,55	0
81	MG	5	3496	1/1	0.96	0.21	44,44,44,44	0
81	MG	5	3486	1/1	0.96	0.55	45,45,45,45	0
81	MG	1	3749	1/1	0.96	0.26	36,36,36,36	0
81	MG	M5	306	1/1	0.96	0.23	40,40,40,40	0
81	MG	5	4064	1/1	0.96	0.47	99,99,99,99	0
81	MG	6	2027	1/1	0.96	0.08	131,131,131,131	0
81	MG	5	3554	1/1	0.96	0.21	55,55,55,55	0
81	MG	5	3528	1/1	0.96	0.33	52,52,52,52	0
81	MG	5	3446	1/1	0.96	0.27	43,43,43,43	0
81	MG	M7	206	1/1	0.96	0.17	39,39,39,39	0
81	MG	1	3651	1/1	0.96	0.31	35,35,35,35	0
81	MG	1	3771	1/1	0.96	0.32	40,40,40,40	0
81	MG	5	3762	1/1	0.96	0.41	45,45,45,45	0
81	MG	1	3710	1/1	0.96	0.23	33,33,33,33	0
81	MG	1	3529	1/1	0.96	0.44	38,38,38,38	0
81	MG	5	3623	1/1	0.96	0.25	59,59,59,59	0
81	MG	1	3463	1/1	0.96	0.39	39,39,39,39	0
81	MG	5	3957	1/1	0.96	0.21	54,54,54,54	0
81	MG	5	3512	1/1	0.96	0.42	61,61,61,61	0
81	MG	1	3907	1/1	0.96	0.27	39,39,39,39	0
81	MG	1	3574	1/1	0.96	0.21	42,42,42,42	0
81	MG	1	3798	1/1	0.96	0.18	56,56,56,56	0
81	MG	L2	302	1/1	0.96	0.28	46,46,46,46	0
81	MG	6	1935	1/1	0.96	0.32	78,78,78,78	0
81	MG	1	3725	1/1	0.96	0.27	40,40,40,40	1
81	MG	1	3482	1/1	0.96	0.20	40,40,40,40	0
81	MG	5	4060	1/1	0.96	0.22	72,72,72,72	0
81	MG	1	3458	1/1	0.96	0.24	40,40,40,40	0
81	MG	5	3442	1/1	0.96	0.21	40,40,40,40	0
81	MG	1	3677	1/1	0.96	0.36	48,48,48,48	0
81	MG	2	2030	1/1	0.96	0.15	74,74,74,74	0
81	MG	1	3694	1/1	0.96	0.15	41,41,41,41	0
81	MG	5	3532	1/1	0.96	0.40	46,46,46,46	0
81	MG	6	1928	1/1	0.96	0.36	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3491	1/1	0.96	0.28	49,49,49,49	0
81	MG	1	3453	1/1	0.96	0.28	40,40,40,40	0
81	MG	6	1982	1/1	0.96	0.19	86,86,86,86	0
81	MG	5	3579	1/1	0.96	0.28	49,49,49,49	0
81	MG	1	4129	1/1	0.96	0.28	56,56,56,56	0
81	MG	6	1925	1/1	0.96	0.29	76,76,76,76	0
81	MG	5	3655	1/1	0.96	0.25	43,43,43,43	0
81	MG	1	3461	1/1	0.96	0.26	37,37,37,37	0
81	MG	1	3966	1/1	0.96	0.62	50,50,50,50	0
81	MG	1	3901	1/1	0.96	0.20	32,32,32,32	0
81	MG	5	3860	1/1	0.96	0.14	68,68,68,68	0
81	MG	O3	201	1/1	0.96	0.39	56,56,56,56	0
81	MG	5	3524	1/1	0.96	0.12	54,54,54,54	1
81	MG	1	3487	1/1	0.96	0.38	37,37,37,37	0
81	MG	7	209	1/1	0.96	0.11	96,96,96,96	0
81	MG	5	3526	1/1	0.96	0.41	52,52,52,52	0
81	MG	5	3801	1/1	0.96	0.21	52,52,52,52	0
81	MG	1	3597	1/1	0.96	0.50	43,43,43,43	0
81	MG	5	3695	1/1	0.96	0.31	56,56,56,56	0
81	MG	5	3963	1/1	0.96	0.14	58,58,58,58	0
81	MG	2	1995	1/1	0.96	0.14	81,81,81,81	0
81	MG	1	3937	1/1	0.96	0.10	59,59,59,59	0
81	MG	12	302	1/1	0.96	0.23	56,56,56,56	0
81	MG	5	3630	1/1	0.96	0.12	59,59,59,59	0
81	MG	1	3534	1/1	0.96	0.28	46,46,46,46	0
81	MG	5	3450	1/1	0.96	0.36	49,49,49,49	0
81	MG	5	3829	1/1	0.96	0.30	76,76,76,76	0
81	MG	1	3601	1/1	0.96	0.31	49,49,49,49	0
81	MG	1	4182	1/1	0.96	0.12	51,51,51,51	0
81	MG	5	3556	1/1	0.96	0.30	71,71,71,71	0
81	MG	5	3523	1/1	0.96	0.28	44,44,44,44	0
81	MG	5	3749	1/1	0.96	0.26	45,45,45,45	0
81	MG	12	301	1/1	0.96	0.13	53,53,53,53	0
81	MG	1	3541	1/1	0.96	0.47	29,29,29,29	0
81	MG	6	1957	1/1	0.96	0.22	102,102,102,102	0
81	MG	2	1933	1/1	0.97	0.21	78,78,78,78	0
81	MG	2	2023	1/1	0.97	0.21	81,81,81,81	0
81	MG	5	3601	1/1	0.97	0.25	93,93,93,93	0
81	MG	2	1998	1/1	0.97	0.24	79,79,79,79	0
81	MG	O0	201	1/1	0.97	0.12	63,63,63,63	0
81	MG	1	4110	1/1	0.97	0.33	63,63,63,63	0
81	MG	5	3755	1/1	0.97	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3575	1/1	0.97	0.33	38,38,38,38	0
81	MG	5	3440	1/1	0.97	0.27	47,47,47,47	0
81	MG	6	1912	1/1	0.97	0.21	76,76,76,76	0
81	MG	5	3538	1/1	0.97	0.38	46,46,46,46	0
82	ZN	q3	501	1/1	0.97	0.19	96,96,96,96	0
81	MG	5	3778	1/1	0.97	0.34	44,44,44,44	0
81	MG	7	203	1/1	0.97	0.27	47,47,47,47	0
81	MG	1	3485	1/1	0.97	0.26	32,32,32,32	0
81	MG	5	3455	1/1	0.97	0.23	47,47,47,47	0
81	MG	1	3777	1/1	0.97	0.20	44,44,44,44	0
81	MG	1	3579	1/1	0.97	0.16	51,51,51,51	0
81	MG	5	3476	1/1	0.97	0.23	44,44,44,44	0
81	MG	2	1949	1/1	0.97	0.15	102,102,102,102	0
81	MG	1	3753	1/1	0.97	0.23	47,47,47,47	0
81	MG	l3	409	1/1	0.97	0.21	55,55,55,55	1
81	MG	2	2102	1/1	0.97	0.19	78,78,78,78	0
81	MG	M5	302	1/1	0.97	0.25	35,35,35,35	0
81	MG	5	3508	1/1	0.97	0.25	59,59,59,59	0
81	MG	1	3922	1/1	0.97	0.25	43,43,43,43	0
81	MG	1	3700	1/1	0.97	0.29	38,38,38,38	0
81	MG	5	3727	1/1	0.97	0.43	55,55,55,55	0
81	MG	1	3819	1/1	0.97	0.11	53,53,53,53	0
81	MG	1	3767	1/1	0.97	0.07	62,62,62,62	0
81	MG	5	3460	1/1	0.97	0.23	42,42,42,42	0
81	MG	5	3783	1/1	0.97	0.14	55,55,55,55	0
81	MG	5	3715	1/1	0.97	0.38	57,57,57,57	0
81	MG	5	3900	1/1	0.97	0.41	75,75,75,75	0
81	MG	5	3694	1/1	0.97	0.40	52,52,52,52	0
81	MG	6	1973	1/1	0.97	0.10	113,113,113,113	0
81	MG	1	3748	1/1	0.97	0.33	31,31,31,31	0
81	MG	3	207	1/1	0.97	0.19	83,83,83,83	0
81	MG	5	3798	1/1	0.97	0.31	50,50,50,50	1
81	MG	1	3455	1/1	0.97	0.32	45,45,45,45	0
81	MG	5	3919	1/1	0.97	0.59	58,58,58,58	0
81	MG	5	3439	1/1	0.97	0.26	45,45,45,45	0
81	MG	1	3497	1/1	0.97	0.24	51,51,51,51	0
81	MG	1	3439	1/1	0.97	0.29	37,37,37,37	0
81	MG	1	3454	1/1	0.97	0.21	40,40,40,40	0
81	MG	M7	201	1/1	0.97	0.34	38,38,38,38	0
81	MG	5	4054	1/1	0.97	0.40	49,49,49,49	0
81	MG	1	3445	1/1	0.97	0.42	28,28,28,28	0
81	MG	2	2032	1/1	0.97	0.22	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3606	1/1	0.97	0.16	67,67,67,67	0
81	MG	5	3451	1/1	0.97	0.24	42,42,42,42	0
81	MG	1	3449	1/1	0.97	0.29	35,35,35,35	0
81	MG	1	3689	1/1	0.97	0.35	48,48,48,48	1
81	MG	5	3474	1/1	0.97	0.29	55,55,55,55	0
81	MG	5	3577	1/1	0.97	0.21	54,54,54,54	0
81	MG	5	3478	1/1	0.97	0.28	49,49,49,49	0
81	MG	1	3489	1/1	0.97	0.30	37,37,37,37	0
81	MG	1	3667	1/1	0.97	0.21	52,52,52,52	0
81	MG	5	3497	1/1	0.97	0.30	50,50,50,50	0
81	MG	5	3594	1/1	0.97	0.23	75,75,75,75	0
81	MG	5	3552	1/1	0.97	0.15	56,56,56,56	1
81	MG	6	2003	1/1	0.97	0.60	71,71,71,71	0
81	MG	2	1918	1/1	0.97	0.28	69,69,69,69	0
81	MG	1	3738	1/1	0.97	0.22	43,43,43,43	0
81	MG	1	3459	1/1	0.97	0.36	34,34,34,34	0
81	MG	5	3637	1/1	0.97	0.39	53,53,53,53	0
81	MG	5	3784	1/1	0.97	0.16	50,50,50,50	0
81	MG	1	3533	1/1	0.97	0.29	33,33,33,33	0
81	MG	1	3726	1/1	0.97	0.18	39,39,39,39	1
81	MG	5	3471	1/1	0.97	0.32	47,47,47,47	0
81	MG	5	3493	1/1	0.97	0.25	66,66,66,66	0
81	MG	2	2045	1/1	0.97	0.26	74,74,74,74	0
81	MG	5	3596	1/1	0.97	0.25	71,71,71,71	0
81	MG	5	3436	1/1	0.97	0.32	43,43,43,43	0
81	MG	1	3604	1/1	0.97	0.18	54,54,54,54	0
81	MG	5	3704	1/1	0.97	0.24	51,51,51,51	0
81	MG	1	3817	1/1	0.97	0.31	39,39,39,39	0
81	MG	1	3720	1/1	0.97	0.28	40,40,40,40	0
81	MG	5	3472	1/1	0.97	0.32	52,52,52,52	0
81	MG	6	1985	1/1	0.97	0.28	85,85,85,85	0
81	MG	5	3459	1/1	0.97	0.32	45,45,45,45	0
81	MG	1	4066	1/1	0.97	0.26	47,47,47,47	0
81	MG	1	3490	1/1	0.97	0.29	49,49,49,49	0
81	MG	1	3443	1/1	0.97	0.26	32,32,32,32	0
81	MG	1	3833	1/1	0.97	0.29	39,39,39,39	0
81	MG	1	3716	1/1	0.97	0.19	44,44,44,44	0
81	MG	19	201	1/1	0.97	0.26	56,56,56,56	0
81	MG	5	3632	1/1	0.97	0.27	59,59,59,59	0
81	MG	1	3880	1/1	0.97	0.32	43,43,43,43	0
81	MG	1	4050	1/1	0.97	0.18	48,48,48,48	0
81	MG	1	3543	1/1	0.97	0.40	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	17	306	1/1	0.97	0.33	65,65,65,65	0
81	MG	5	4047	1/1	0.97	0.40	68,68,68,68	0
81	MG	5	3608	1/1	0.97	0.34	52,52,52,52	0
81	MG	1	3554	1/1	0.97	0.29	34,34,34,34	0
81	MG	3	208	1/1	0.97	0.32	43,43,43,43	0
81	MG	1	3743	1/1	0.97	0.37	35,35,35,35	0
81	MG	6	2010	1/1	0.97	0.09	124,124,124,124	0
81	MG	1	3595	1/1	0.97	0.27	46,46,46,46	0
81	MG	1	3475	1/1	0.97	0.30	32,32,32,32	0
81	MG	4	229	1/1	0.97	0.11	57,57,57,57	0
81	MG	5	3926	1/1	0.97	0.12	78,78,78,78	0
81	MG	5	3557	1/1	0.97	0.22	67,67,67,67	0
81	MG	5	3539	1/1	0.97	0.42	44,44,44,44	0
81	MG	5	3731	1/1	0.97	0.44	54,54,54,54	0
81	MG	1	3829	1/1	0.97	0.29	40,40,40,40	0
81	MG	5	3642	1/1	0.98	0.15	56,56,56,56	0
81	MG	1	3585	1/1	0.98	0.15	46,46,46,46	0
81	MG	5	3464	1/1	0.98	0.51	44,44,44,44	0
81	MG	5	3864	1/1	0.98	0.34	42,42,42,42	0
81	MG	5	3574	1/1	0.98	0.28	65,65,65,65	0
81	MG	1	3440	1/1	0.98	0.11	39,39,39,39	0
81	MG	1	3448	1/1	0.98	0.23	35,35,35,35	0
82	ZN	Q3	501	1/1	0.98	0.17	64,64,64,64	0
81	MG	5	3786	1/1	0.98	0.32	53,53,53,53	0
81	MG	1	3813	1/1	0.98	0.23	50,50,50,50	0
81	MG	5	3527	1/1	0.98	0.44	54,54,54,54	0
81	MG	5	3675	1/1	0.98	0.19	50,50,50,50	0
81	MG	5	3462	1/1	0.98	0.36	39,39,39,39	0
81	MG	1	3514	1/1	0.98	0.16	63,63,63,63	1
81	MG	4	234	1/1	0.98	0.26	46,46,46,46	0
81	MG	2	1934	1/1	0.98	0.12	75,75,75,75	0
81	MG	5	3618	1/1	0.98	0.16	87,87,87,87	0
81	MG	5	3968	1/1	0.98	0.38	48,48,48,48	0
81	MG	1	3751	1/1	0.98	0.26	42,42,42,42	0
81	MG	1	3468	1/1	0.98	0.40	33,33,33,33	0
81	MG	2	2107	1/1	0.98	0.12	120,120,120,120	0
81	MG	5	3505	1/1	0.98	0.27	59,59,59,59	0
81	MG	1	3447	1/1	0.98	0.25	39,39,39,39	0
81	MG	5	3502	1/1	0.98	0.33	52,52,52,52	0
81	MG	2	1960	1/1	0.98	0.17	90,90,90,90	0
81	MG	5	3654	1/1	0.98	0.33	48,48,48,48	0
81	MG	1	3518	1/1	0.98	0.22	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3460	1/1	0.98	0.41	33,33,33,33	0
82	ZN	q2	501	1/1	0.98	0.08	113,113,113,113	0
82	ZN	o7	501	1/1	0.98	0.16	71,71,71,71	0
81	MG	1	3477	1/1	0.98	0.22	35,35,35,35	0
81	MG	1	3567	1/1	0.98	0.29	48,48,48,48	0
81	MG	1	3761	1/1	0.98	0.24	51,51,51,51	0
81	MG	5	3452	1/1	0.98	0.27	47,47,47,47	0
81	MG	1	3484	1/1	0.98	0.30	35,35,35,35	0
81	MG	5	3977	1/1	0.98	0.18	71,71,71,71	0
81	MG	1	3495	1/1	0.98	0.27	41,41,41,41	0
81	MG	2	1994	1/1	0.98	0.19	79,79,79,79	0
81	MG	5	3507	1/1	0.98	0.25	64,64,64,64	0
81	MG	1	3627	1/1	0.98	0.19	34,34,34,34	0
81	MG	1	3717	1/1	0.98	0.25	35,35,35,35	0
81	MG	1	3759	1/1	0.98	0.30	38,38,38,38	0
81	MG	1	3718	1/1	0.98	0.28	34,34,34,34	0
81	MG	1	3815	1/1	0.98	0.25	44,44,44,44	0
81	MG	5	3710	1/1	0.98	0.28	50,50,50,50	0
81	MG	5	3461	1/1	0.98	0.38	39,39,39,39	0
81	MG	1	3471	1/1	0.98	0.46	37,37,37,37	0
81	MG	5	3465	1/1	0.98	0.31	46,46,46,46	0
81	MG	1	3687	1/1	0.98	0.25	45,45,45,45	0
81	MG	1	3816	1/1	0.98	0.33	43,43,43,43	0
81	MG	1	3483	1/1	0.98	0.17	41,41,41,41	0
81	MG	5	3766	1/1	0.98	0.33	50,50,50,50	0
81	MG	5	3850	1/1	0.98	0.19	51,51,51,51	0
81	MG	1	3822	1/1	0.98	0.21	50,50,50,50	0
81	MG	2	2013	1/1	0.98	0.11	86,86,86,86	0
81	MG	5	3599	1/1	0.98	0.21	84,84,84,84	0
81	MG	1	3657	1/1	0.98	0.18	49,49,49,49	0
81	MG	m7	204	1/1	0.98	0.41	53,53,53,53	0
81	MG	1	3647	1/1	0.98	0.21	39,39,39,39	0
81	MG	5	3719	1/1	0.98	0.43	63,63,63,63	0
81	MG	1	3442	1/1	0.98	0.30	35,35,35,35	0
81	MG	1	4141	1/1	0.98	0.15	51,51,51,51	0
81	MG	4	210	1/1	0.98	0.17	47,47,47,47	0
81	MG	N3	203	1/1	0.98	0.33	45,45,45,45	0
81	MG	2	1989	1/1	0.98	0.18	88,88,88,88	0
81	MG	5	3759	1/1	0.98	0.28	46,46,46,46	0
81	MG	1	3648	1/1	0.98	0.42	40,40,40,40	0
81	MG	5	3503	1/1	0.98	0.53	51,51,51,51	0
81	MG	1	3703	1/1	0.98	0.26	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
81	MG	5	3670	1/1	0.98	0.19	46,46,46,46	0
81	MG	5	3711	1/1	0.98	0.34	54,54,54,54	0
81	MG	5	3716	1/1	0.98	0.23	58,58,58,58	0
81	MG	1	3950	1/1	0.98	0.17	53,53,53,53	1
81	MG	2	1939	1/1	0.98	0.40	84,84,84,84	0
81	MG	1	3845	1/1	0.98	0.28	38,38,38,38	0
81	MG	5	3862	1/1	0.98	0.10	65,65,65,65	0
81	MG	1	4127	1/1	0.98	0.16	39,39,39,39	0
81	MG	1	4058	1/1	0.98	0.42	73,73,73,73	0
81	MG	L3	401	1/1	0.98	0.26	46,46,46,46	0
81	MG	5	3739	1/1	0.98	0.18	50,50,50,50	0
82	ZN	D6	101	1/1	0.98	0.17	84,84,84,84	0
81	MG	1	3464	1/1	0.98	0.39	34,34,34,34	0
81	MG	1	3636	1/1	0.98	0.43	48,48,48,48	0
81	MG	5	3448	1/1	0.98	0.23	49,49,49,49	0
81	MG	5	3429	1/1	0.98	0.29	42,42,42,42	0
81	MG	1	3446	1/1	0.98	0.21	35,35,35,35	0
81	MG	2	1930	1/1	0.98	0.35	70,70,70,70	0
81	MG	1	3742	1/1	0.98	0.38	32,32,32,32	0
81	MG	1	3472	1/1	0.98	0.28	39,39,39,39	0
81	MG	1	3846	1/1	0.98	0.22	42,42,42,42	0
81	MG	5	3445	1/1	0.98	0.28	48,48,48,48	0
81	MG	1	3444	1/1	0.98	0.30	32,32,32,32	0
81	MG	1	3844	1/1	0.98	0.20	44,44,44,44	1
81	MG	5	3590	1/1	0.98	0.33	62,62,62,62	0
81	MG	5	3457	1/1	0.99	0.26	44,44,44,44	0
81	MG	5	3498	1/1	0.99	0.10	53,53,53,53	0
81	MG	1	3512	1/1	0.99	0.15	59,59,59,59	0
81	MG	1	3800	1/1	0.99	0.32	35,35,35,35	0
82	ZN	d9	101	1/1	0.99	0.11	123,123,123,123	0
81	MG	1	3474	1/1	0.99	0.27	43,43,43,43	0
81	MG	m7	201	1/1	0.99	0.32	44,44,44,44	0
81	MG	5	3495	1/1	0.99	0.29	46,46,46,46	0
81	MG	1	3764	1/1	0.99	0.18	55,55,55,55	0
81	MG	5	3576	1/1	0.99	0.14	56,56,56,56	0
82	ZN	O7	101	1/1	0.99	0.19	50,50,50,50	0
81	MG	5	3441	1/1	0.99	0.21	44,44,44,44	0
81	MG	1	3469	1/1	0.99	0.25	30,30,30,30	0
81	MG	1	3528	1/1	0.99	0.38	33,33,33,33	0
82	ZN	q0	201	1/1	0.99	0.16	58,58,58,58	0
81	MG	1	3565	1/1	0.99	0.21	46,46,46,46	0
81	MG	1	3619	1/1	0.99	0.30	58,58,58,58	0

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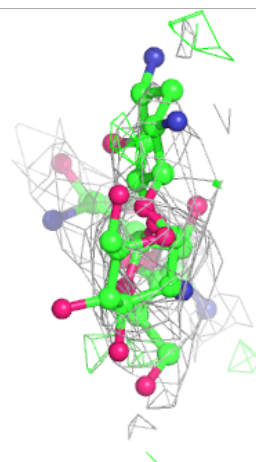
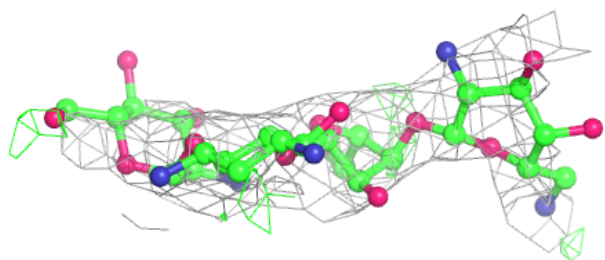
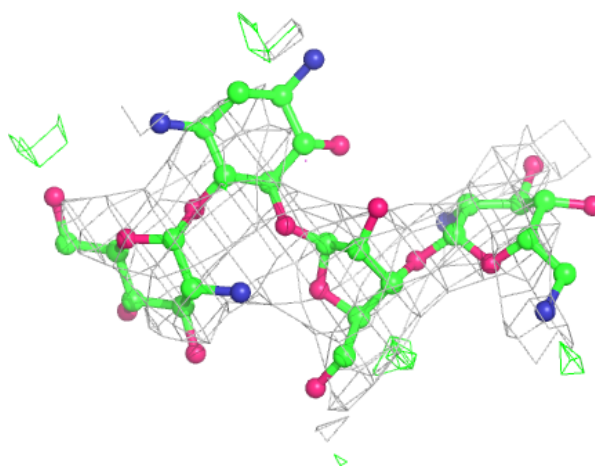
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	1	3473	1/1	0.99	0.42	38,38,38,38	0
82	ZN	O4	201	1/1	0.99	0.10	63,63,63,63	0
81	MG	2	2090	1/1	0.99	0.07	102,102,102,102	0
82	ZN	d6	101	1/1	0.99	0.14	91,91,91,91	0
81	MG	1	3723	1/1	0.99	0.38	34,34,34,34	0
81	MG	1	3706	1/1	0.99	0.27	44,44,44,44	0
81	MG	1	3476	1/1	0.99	0.27	34,34,34,34	0
82	ZN	Q2	501	1/1	0.99	0.10	90,90,90,90	0
81	MG	1	3466	1/1	0.99	0.21	39,39,39,39	0
81	MG	5	3733	1/1	0.99	0.33	55,55,55,55	0
81	MG	1	3805	1/1	0.99	0.12	51,51,51,51	0
81	MG	1	3774	1/1	0.99	0.29	41,41,41,41	0
81	MG	6	1909	1/1	0.99	0.22	71,71,71,71	0
81	MG	1	3553	1/1	0.99	0.21	37,37,37,37	0
81	MG	5	3705	1/1	0.99	0.29	54,54,54,54	0
81	MG	1	3557	1/1	0.99	0.26	34,34,34,34	0
81	MG	N8	201	1/1	0.99	0.17	41,41,41,41	0
81	MG	1	3692	1/1	0.99	0.35	33,33,33,33	0
82	ZN	Q0	500	1/1	1.00	0.15	67,67,67,67	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

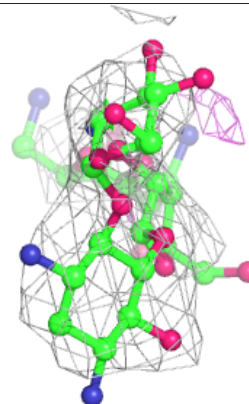
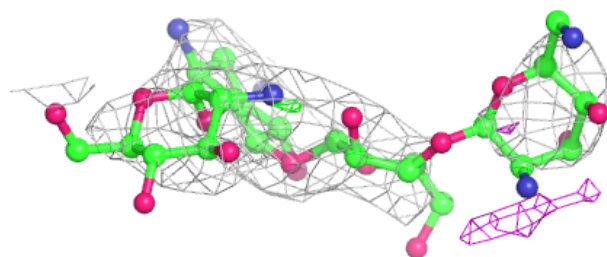
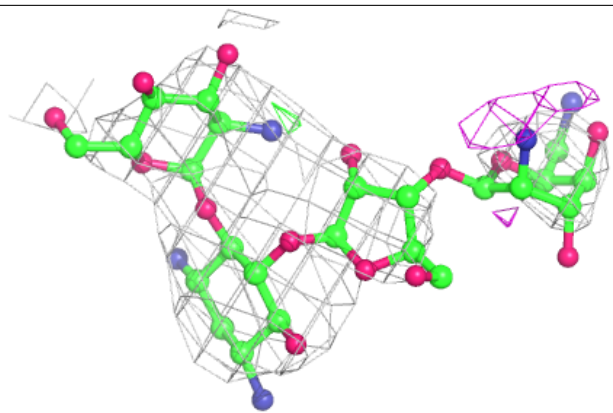
Electron density around PAR 5 3423:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



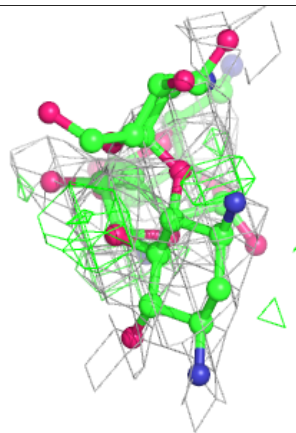
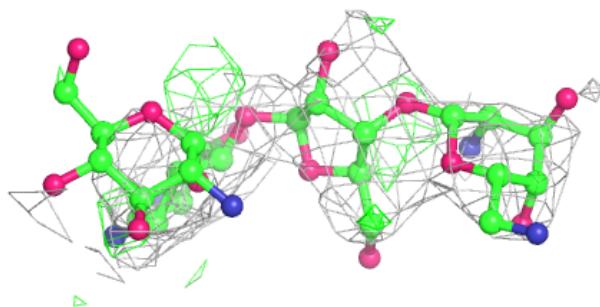
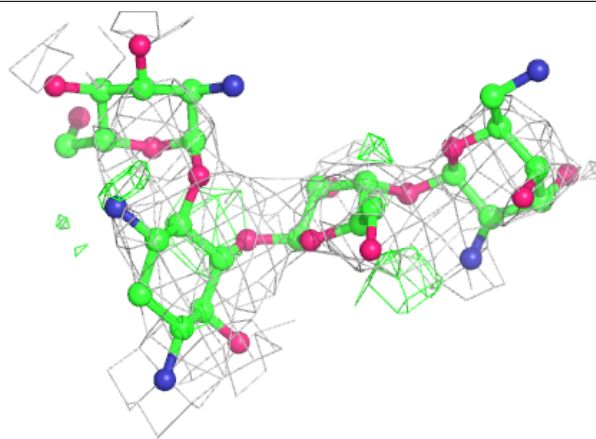
Electron density around PAR 6 1902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



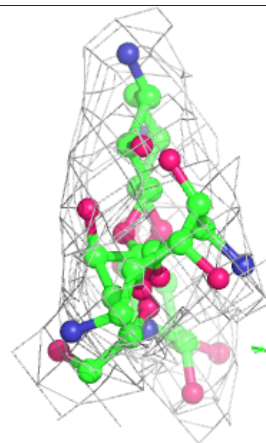
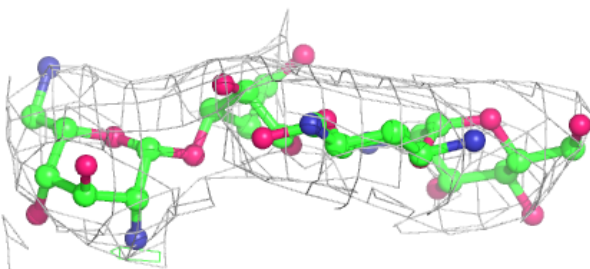
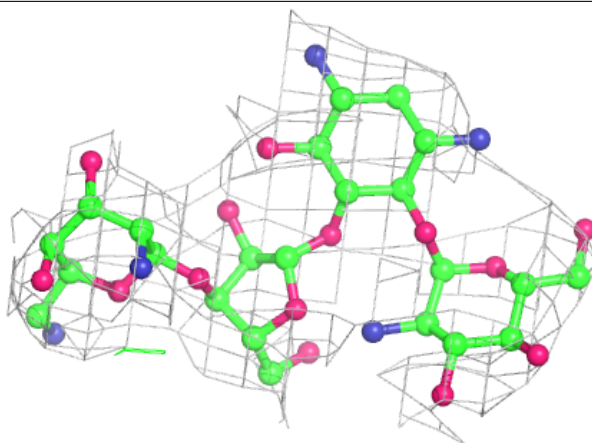
Electron density around PAR 5 3403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



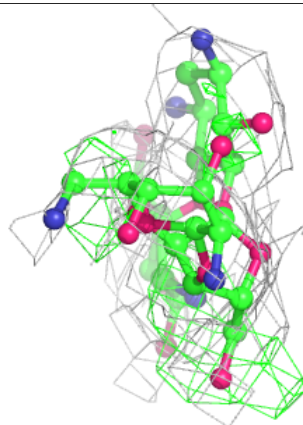
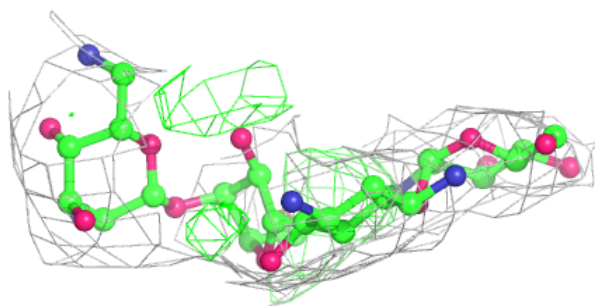
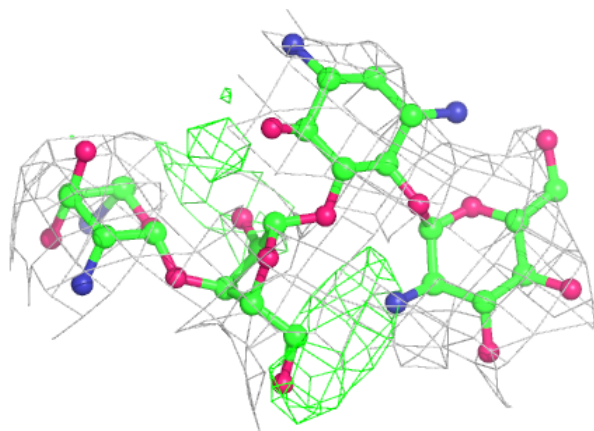
Electron density around PAR 5 3428:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



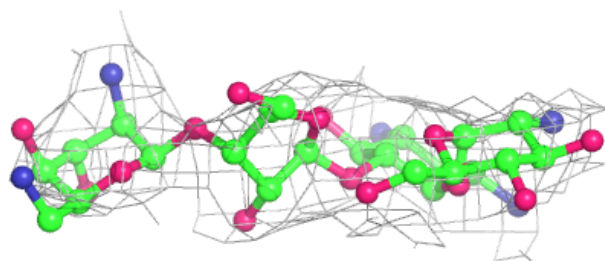
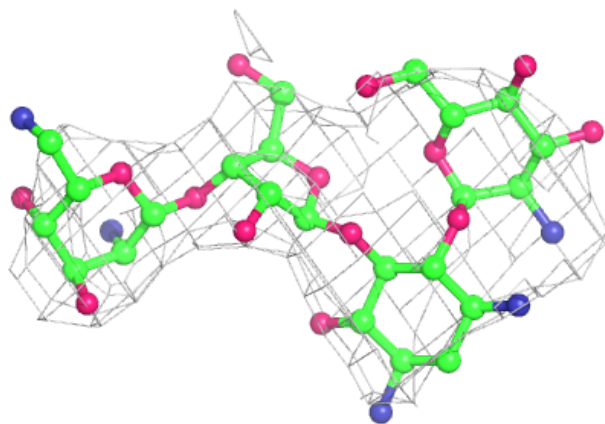
Electron density around PAR 3 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



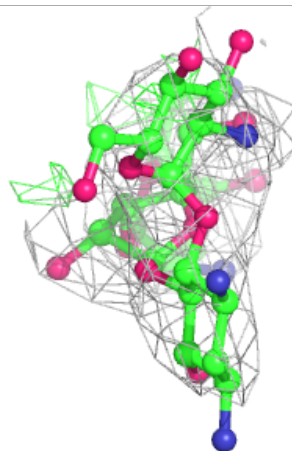
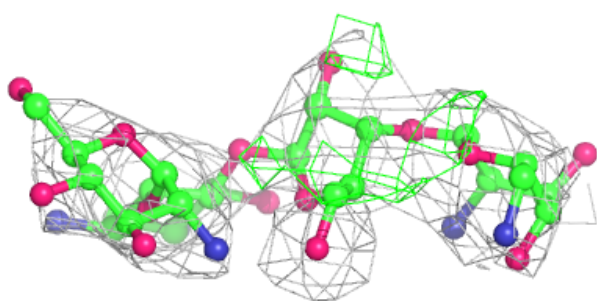
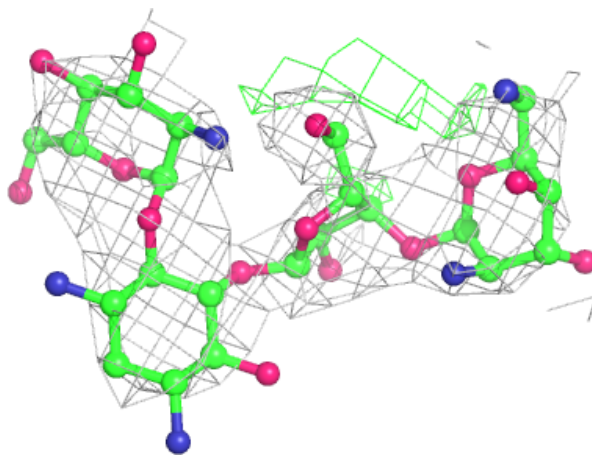
Electron density around PAR 6 1906:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



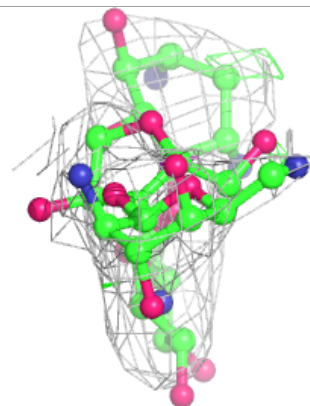
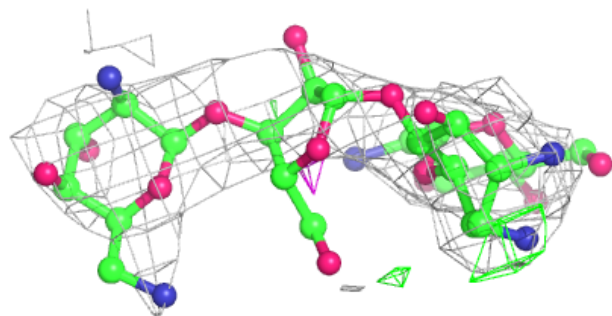
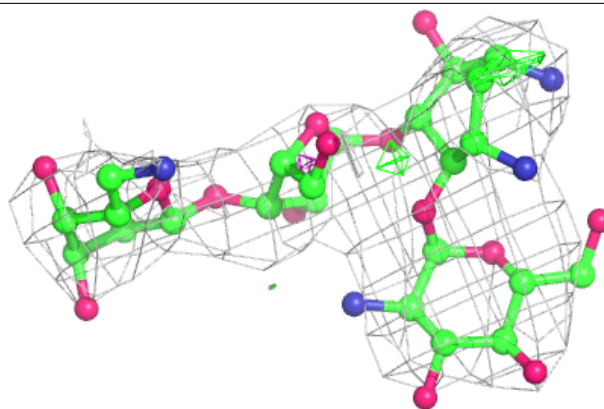
Electron density around PAR 2 1905:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

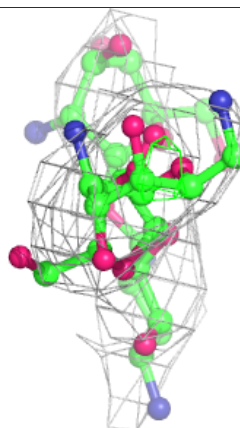
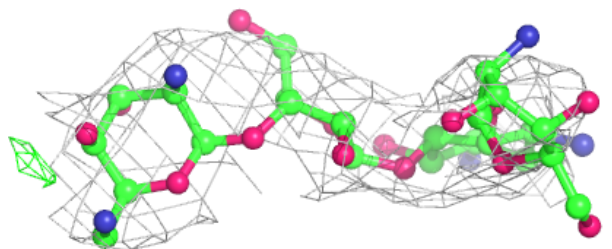
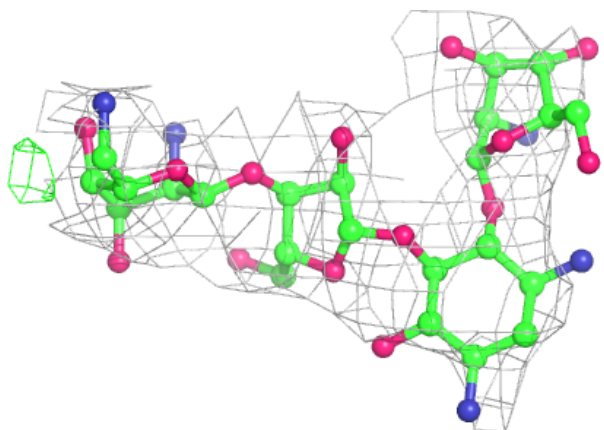


Electron density around PAR 5 3427:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

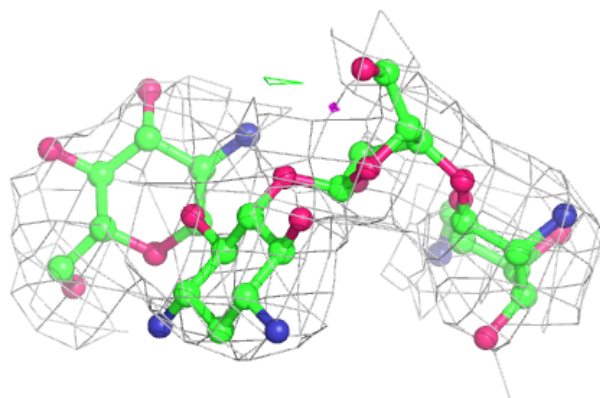
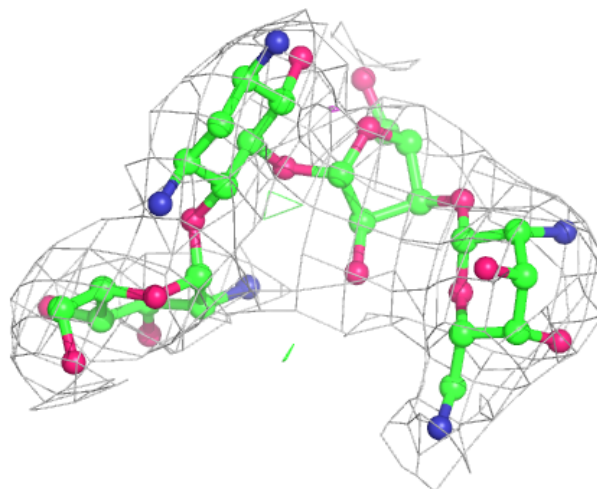
**Electron density around PAR 5 3405:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



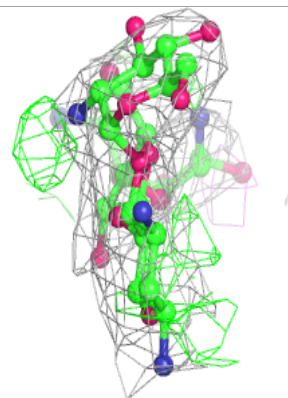
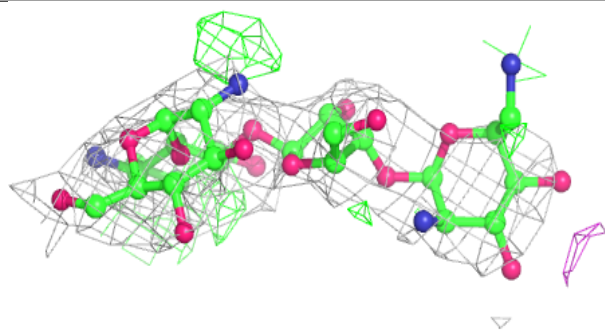
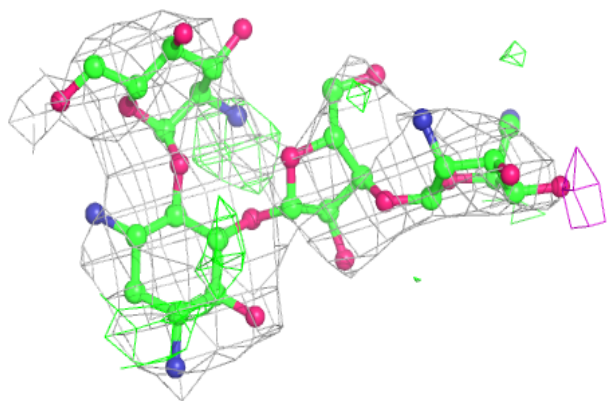
Electron density around PAR 5 3422:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

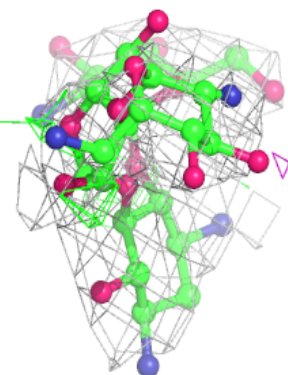
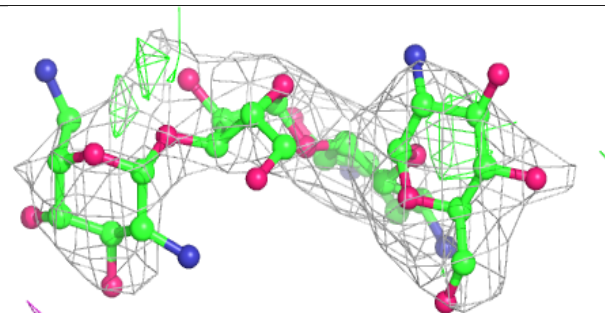
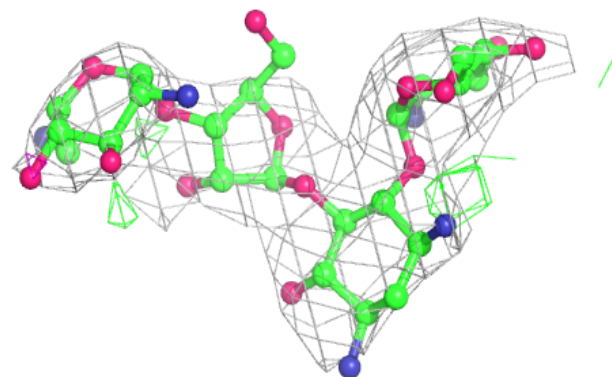


Electron density around PAR 1 3413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

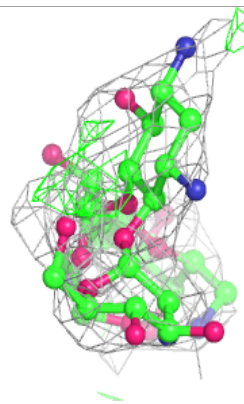
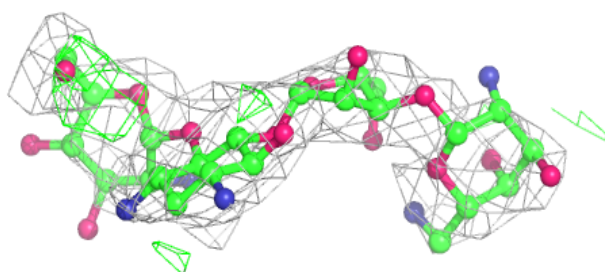
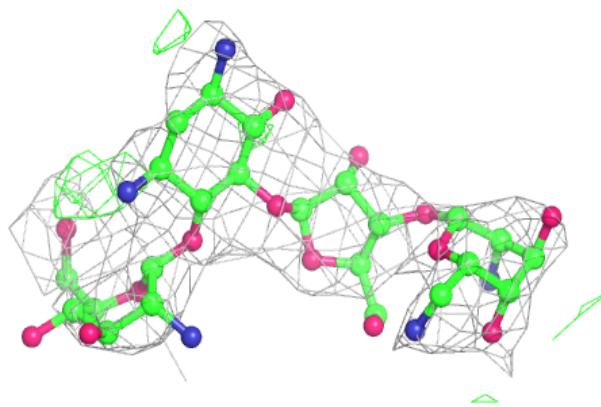
**Electron density around PAR 1 3433:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

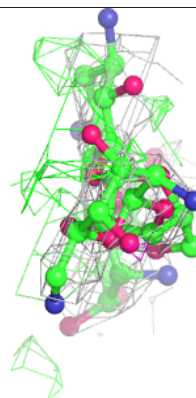
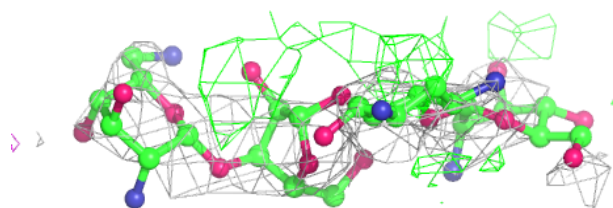
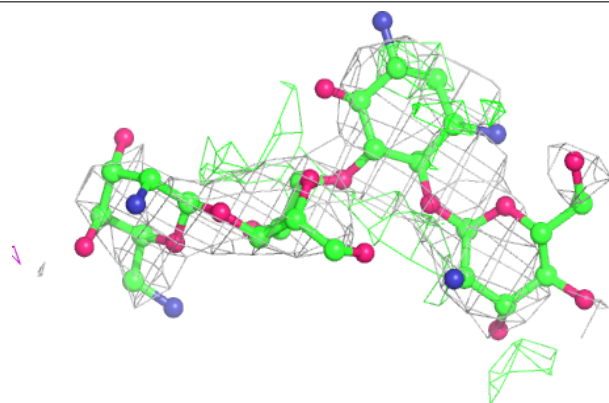


Electron density around PAR n3 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

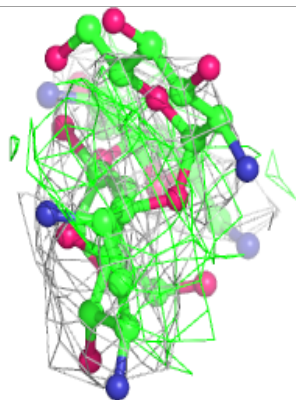
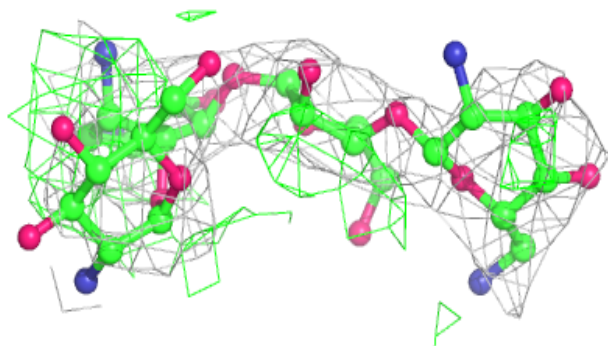
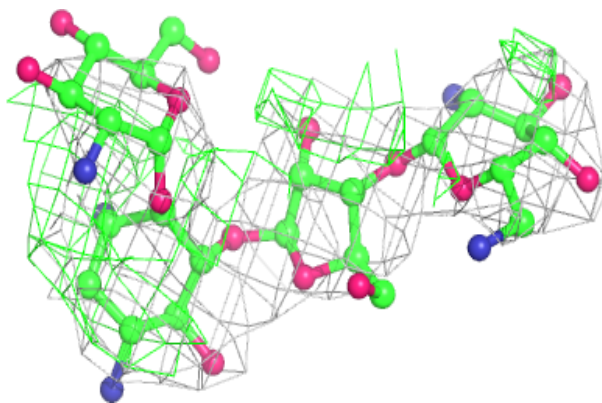
**Electron density around PAR o2 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



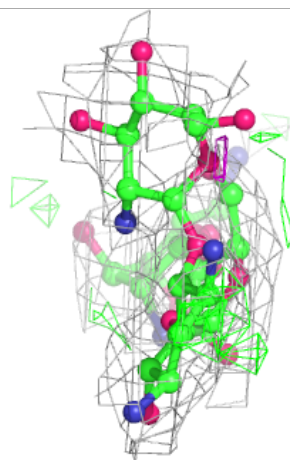
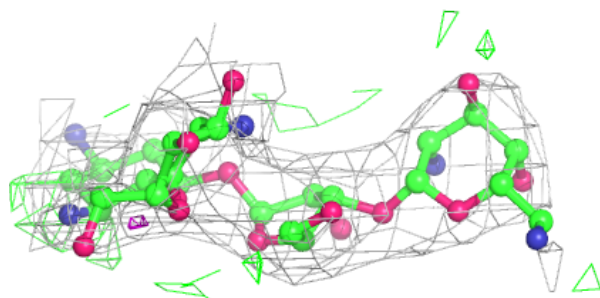
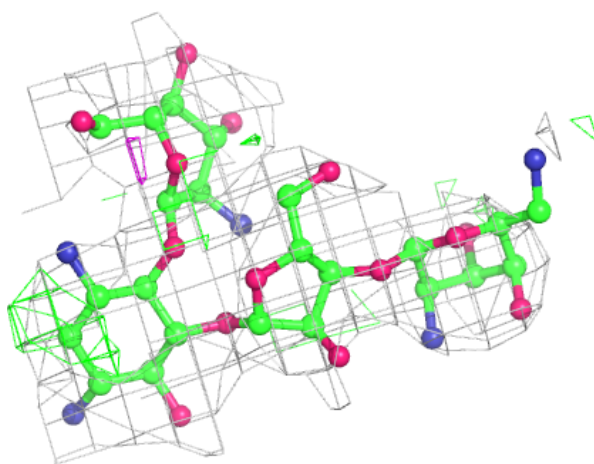
Electron density around PAR 1 3403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



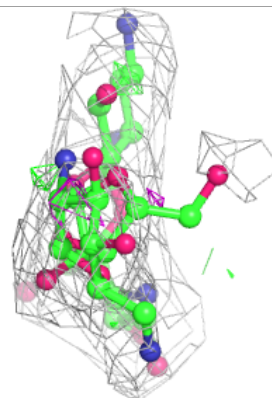
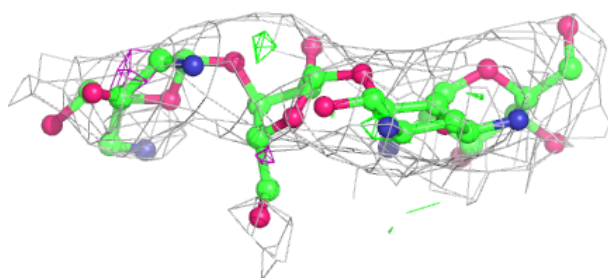
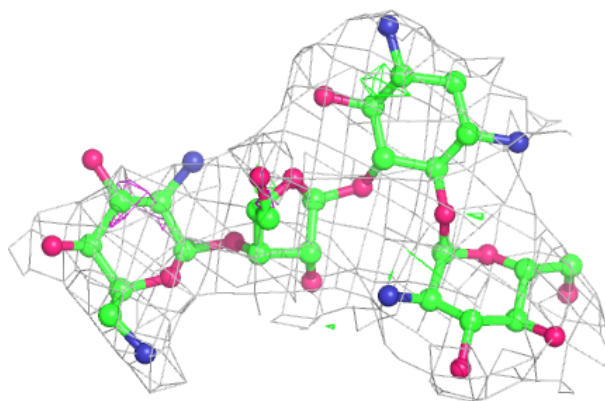
Electron density around PAR 5 3404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

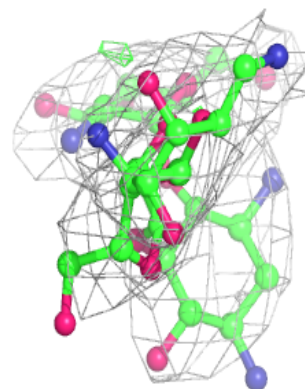
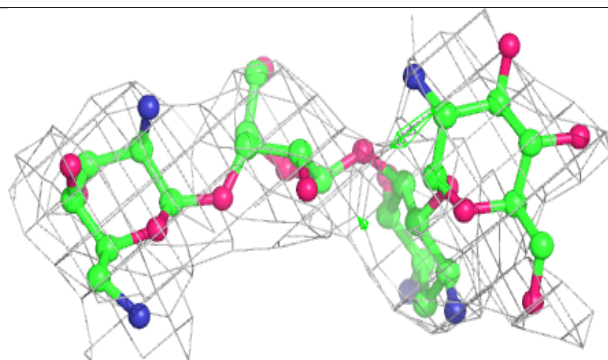
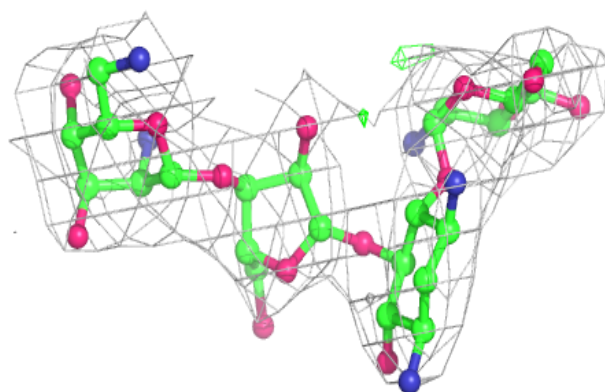


Electron density around PAR 1 3426:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

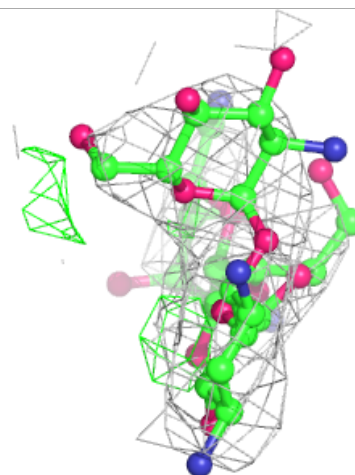
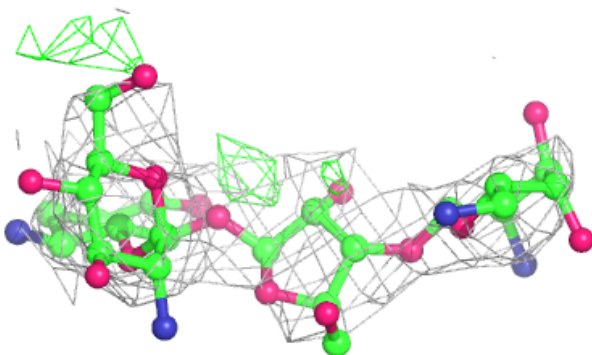
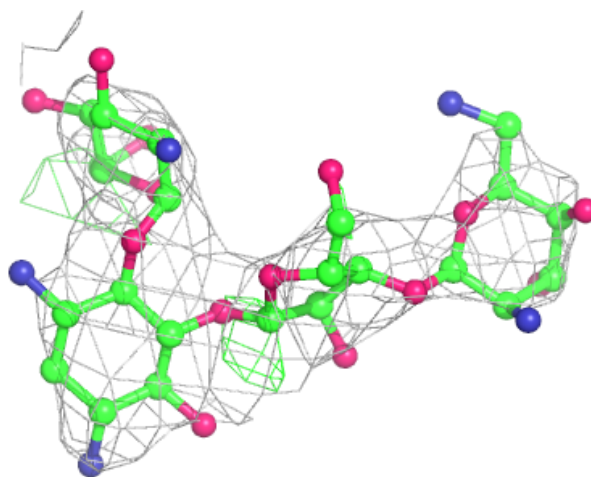
**Electron density around PAR 1 3401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



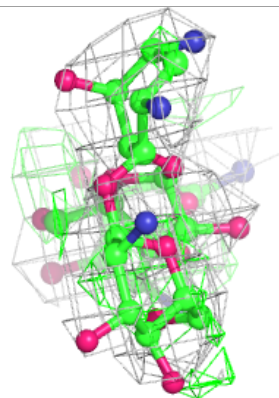
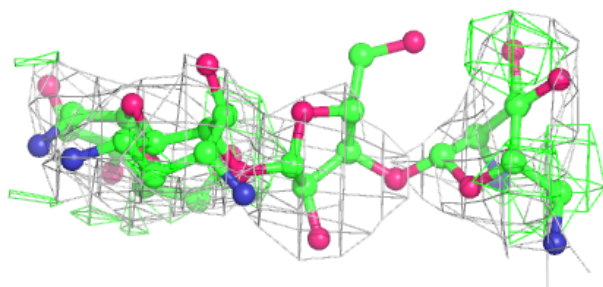
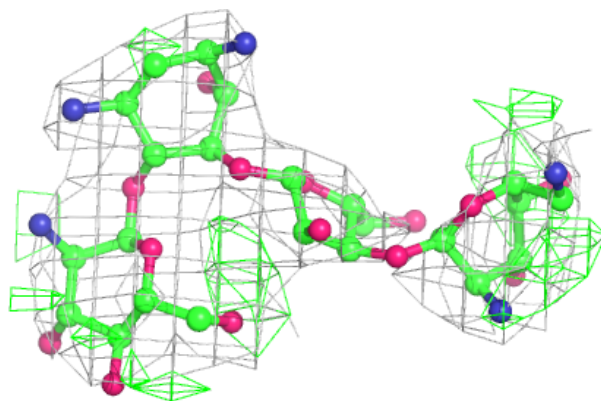
Electron density around PAR 2 1901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

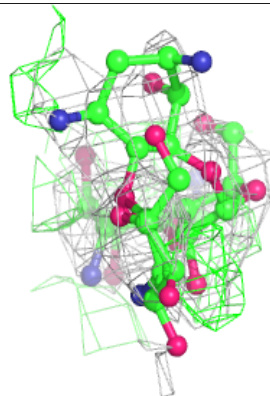
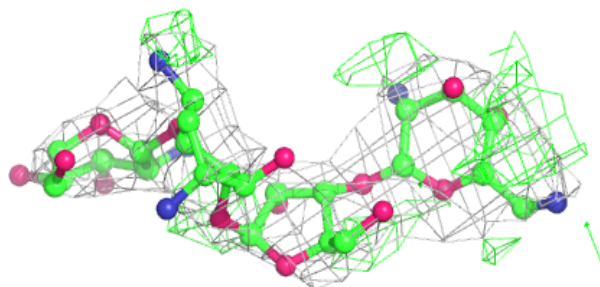
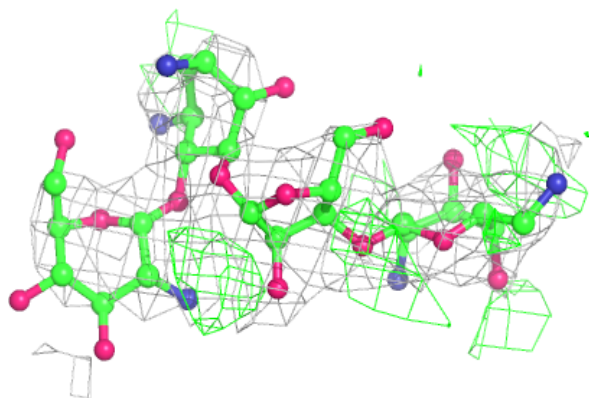


Electron density around PAR 1 3405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

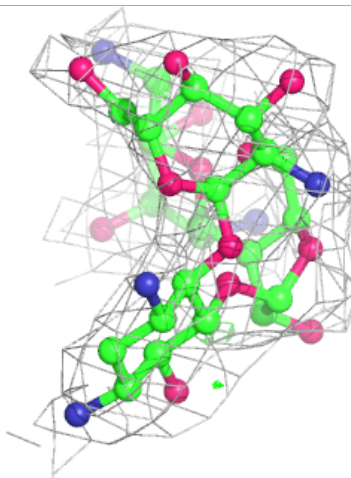
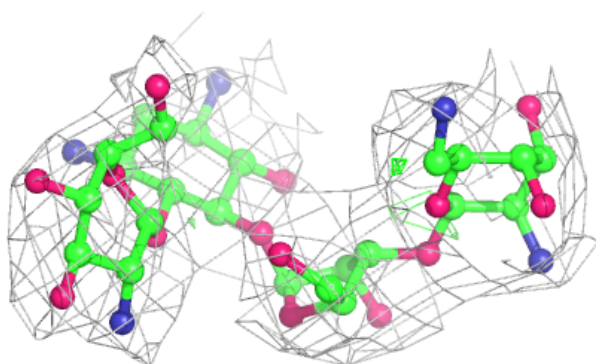
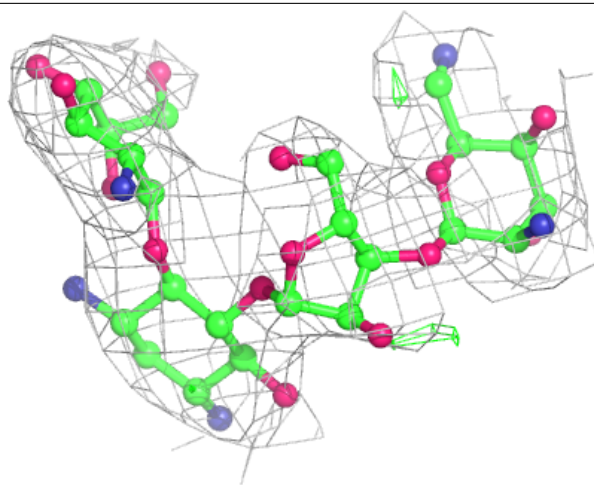
**Electron density around PAR 4 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



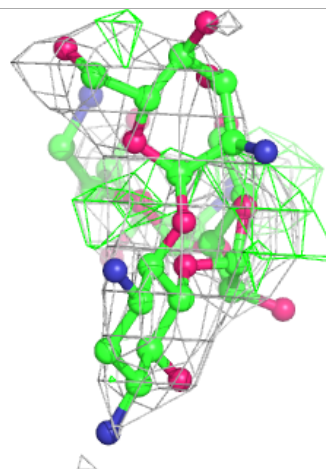
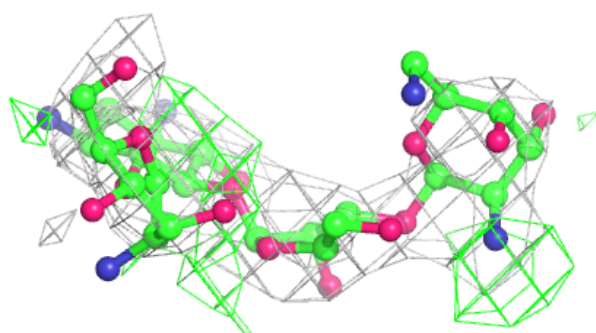
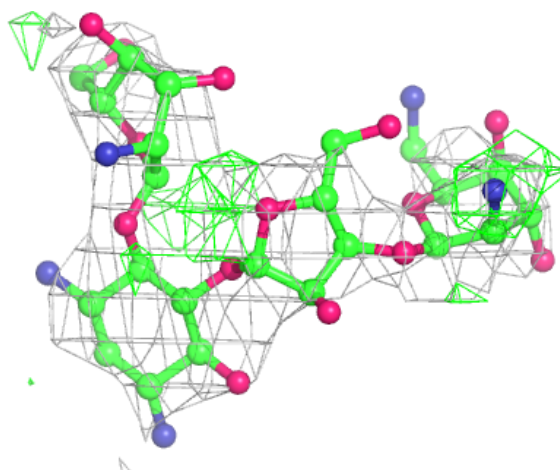
Electron density around PAR 1 3436:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



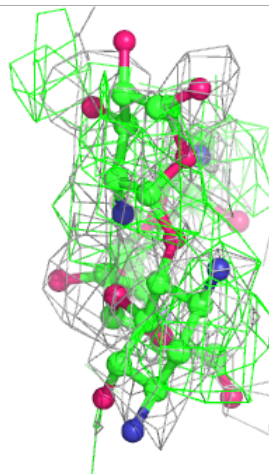
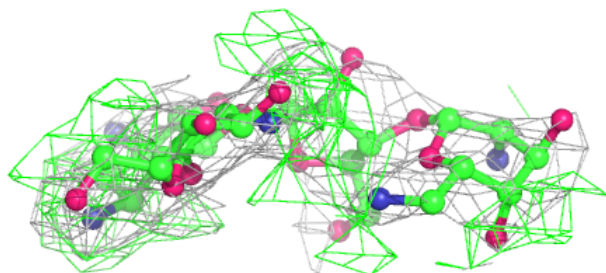
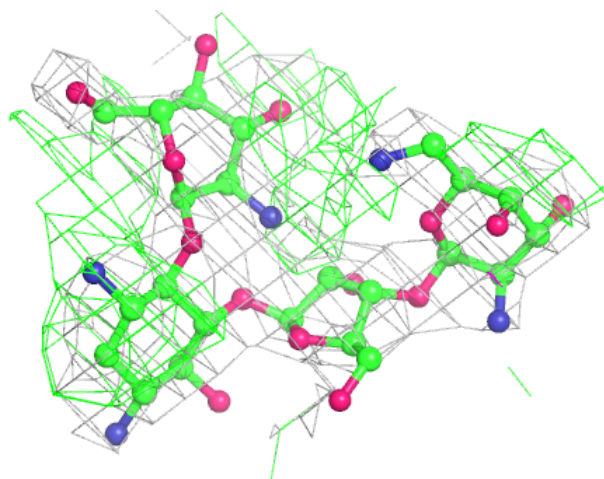
Electron density around PAR 8 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



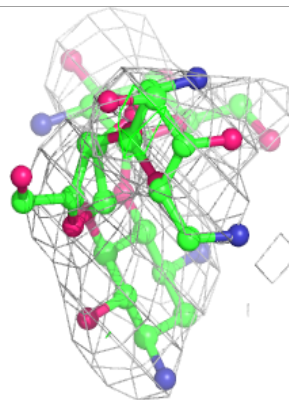
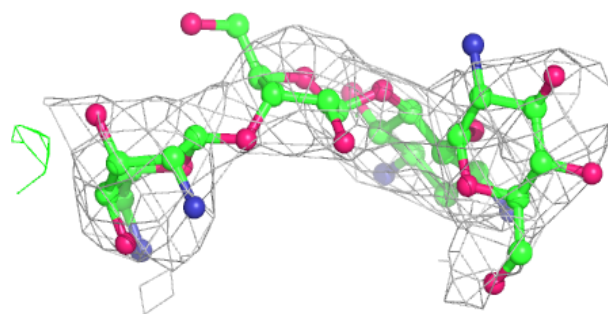
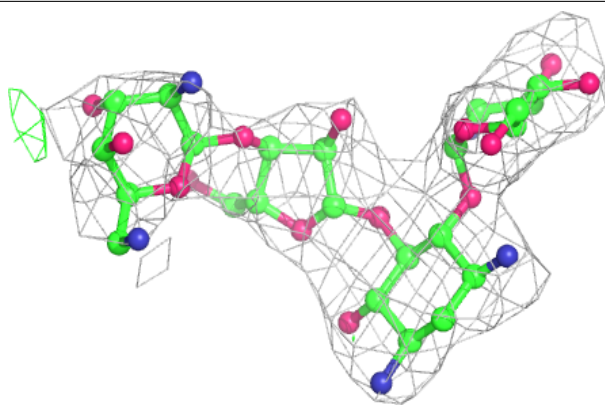
Electron density around PAR 1 3435:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



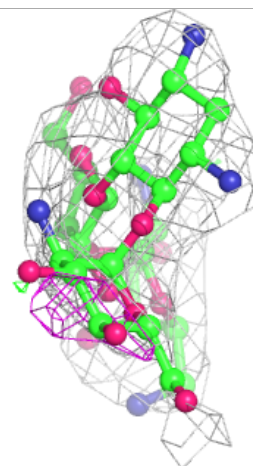
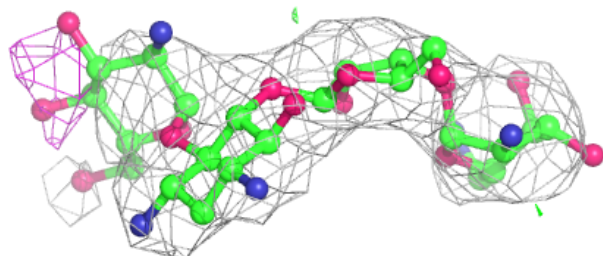
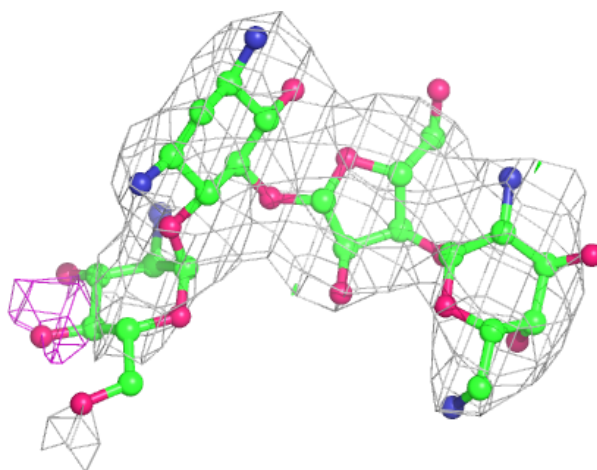
Electron density around PAR 1 3431:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



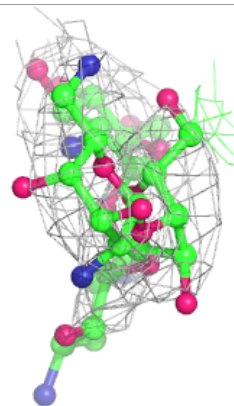
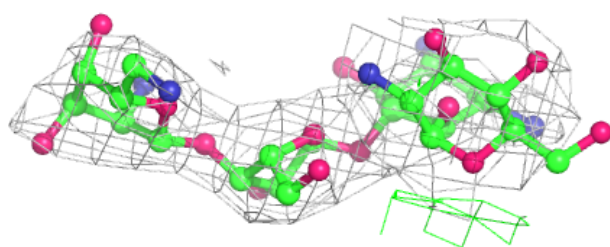
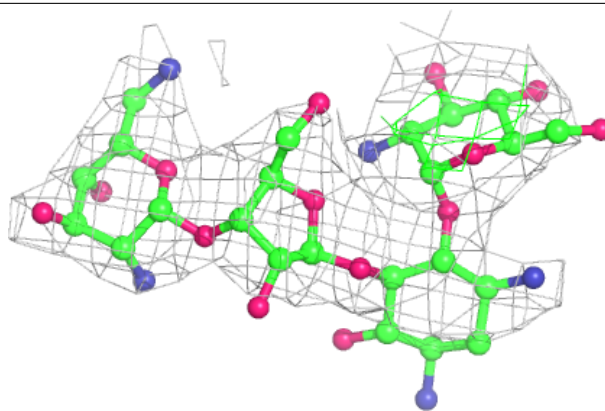
Electron density around PAR 5 3411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

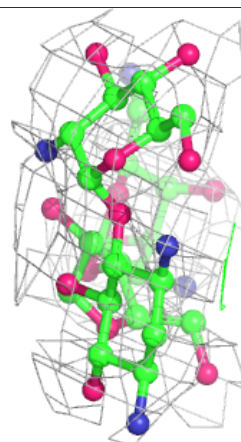
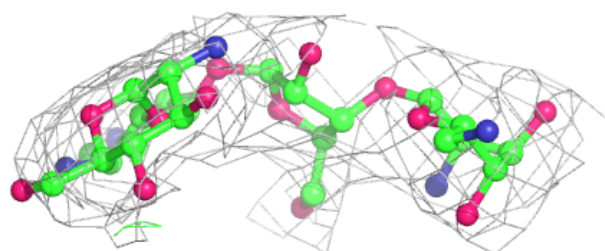
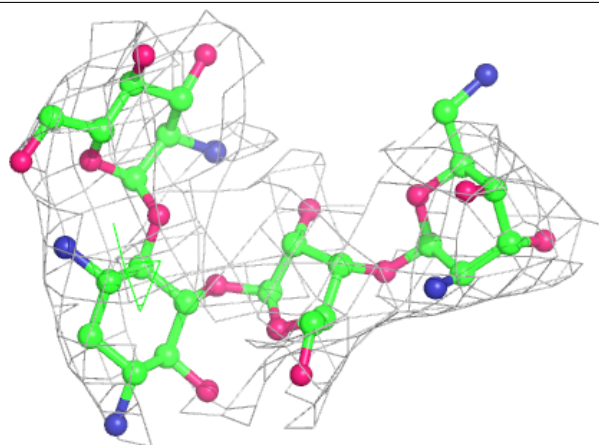


Electron density around PAR 8 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

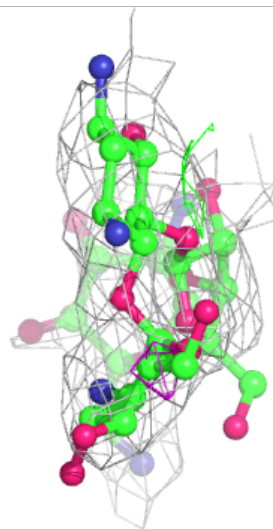
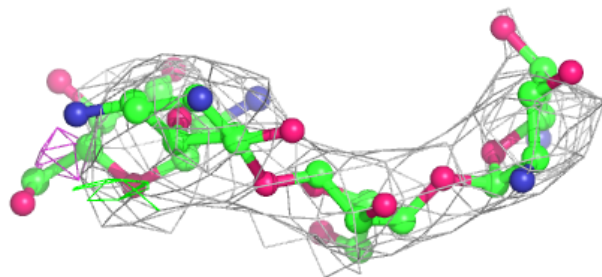
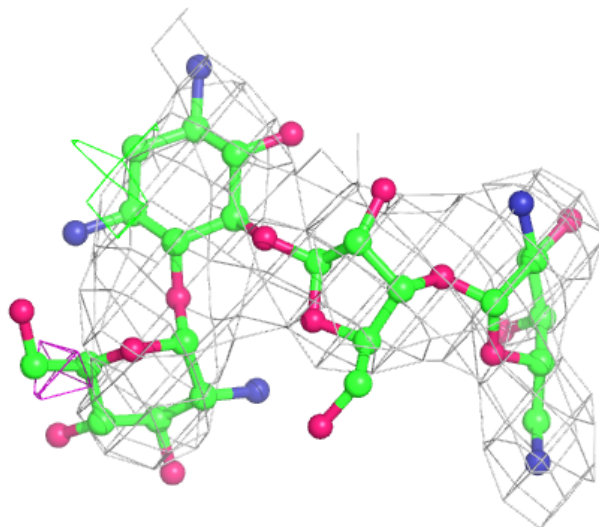
**Electron density around PAR 6 1905:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



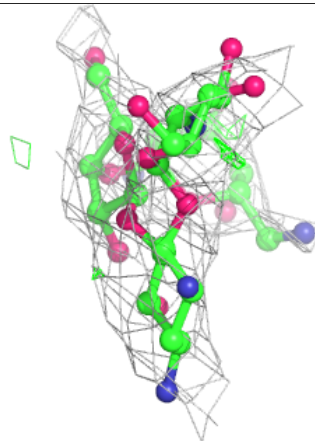
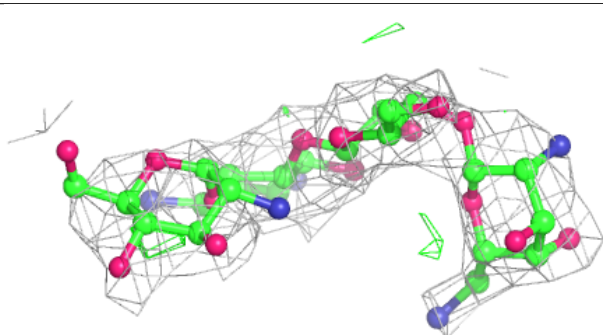
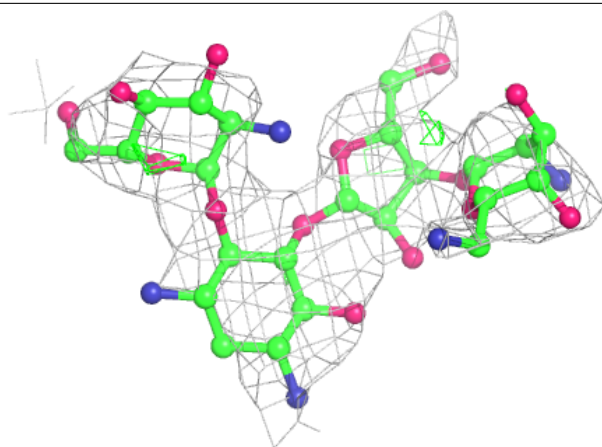
Electron density around PAR 1 3406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

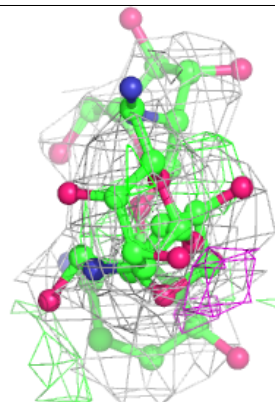
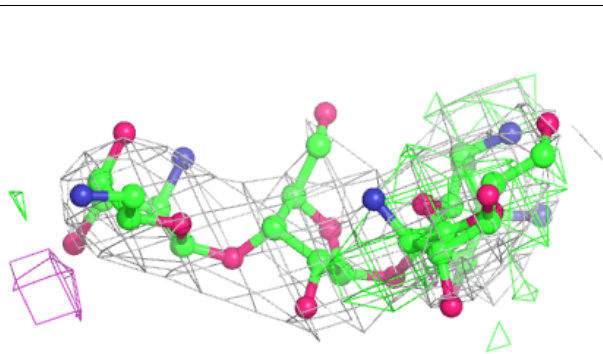
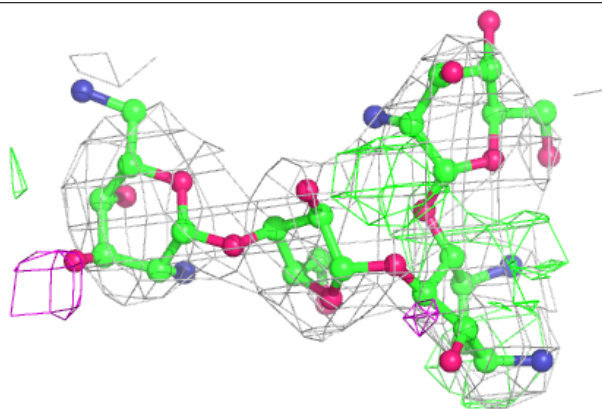


Electron density around PAR 1 3437:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

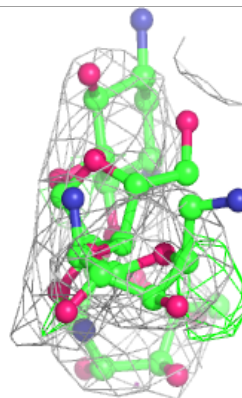
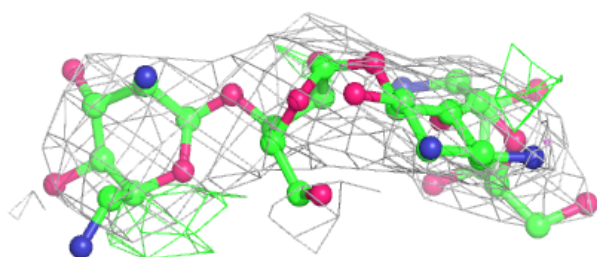
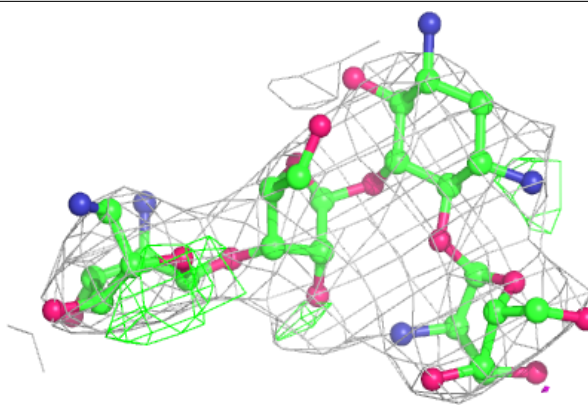
**Electron density around PAR 1 3410:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

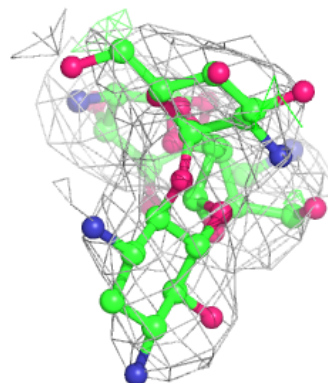
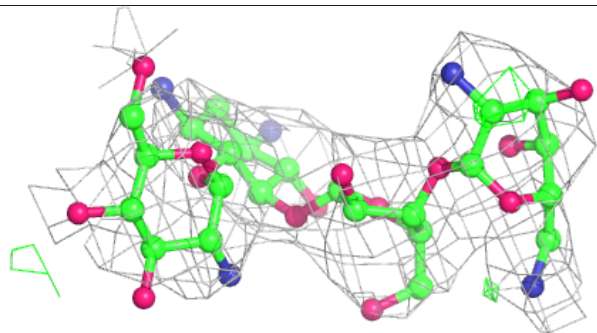
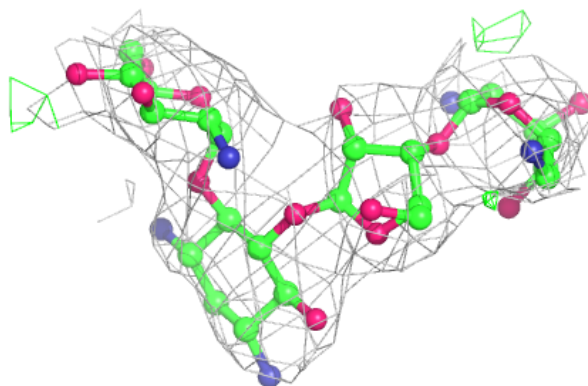


Electron density around PAR 5 3409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

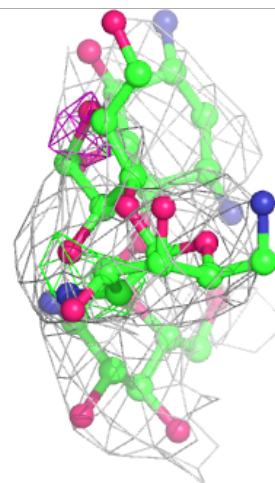
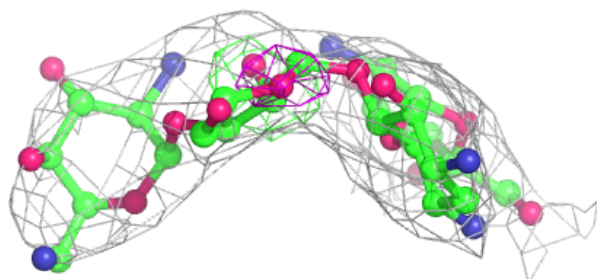
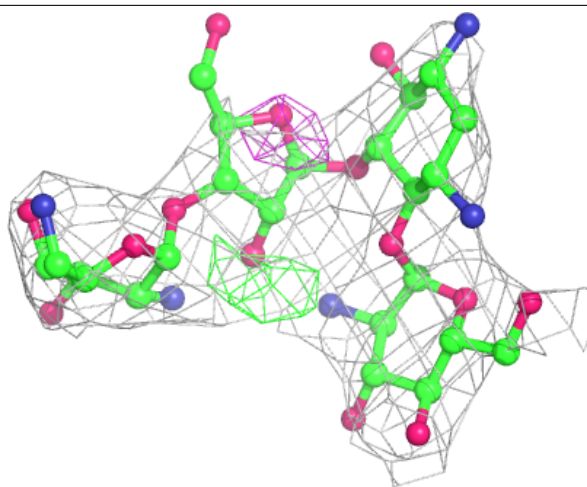
**Electron density around PAR 5 3402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



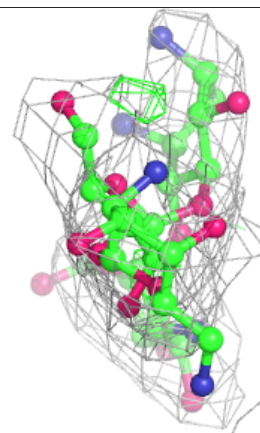
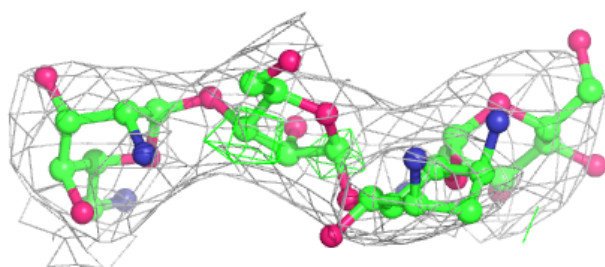
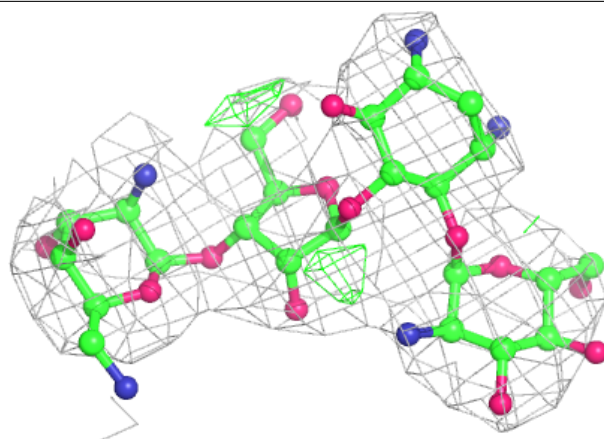
Electron density around PAR 5 3413:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



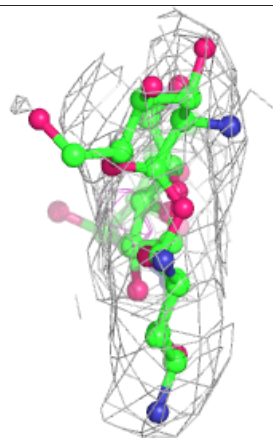
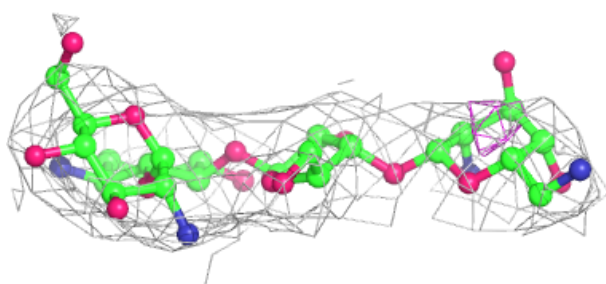
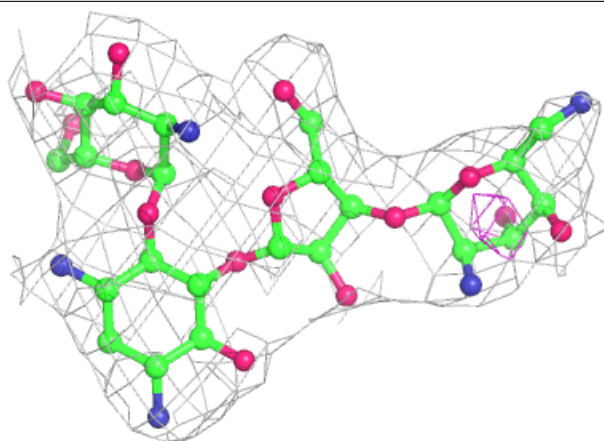
Electron density around PAR 3 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

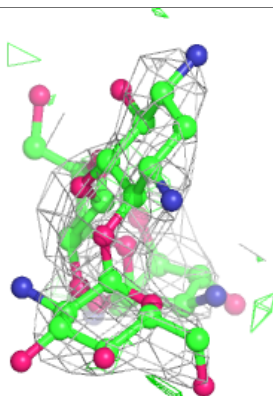
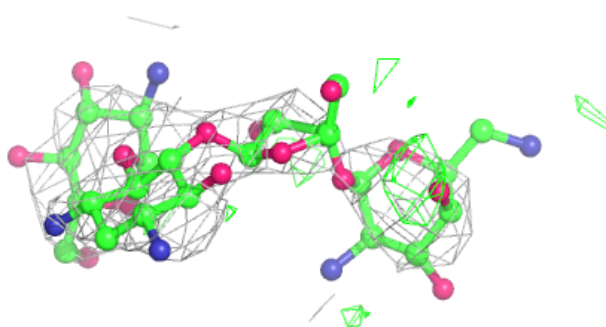
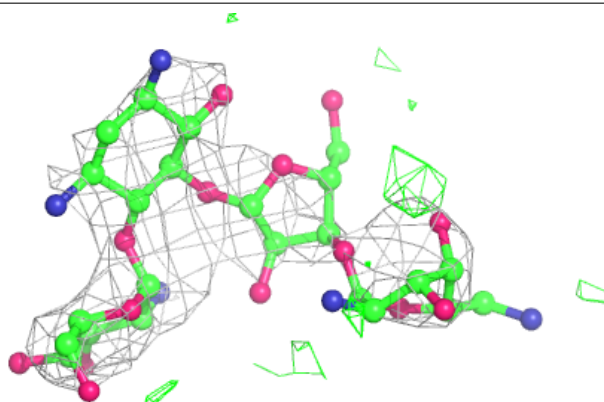


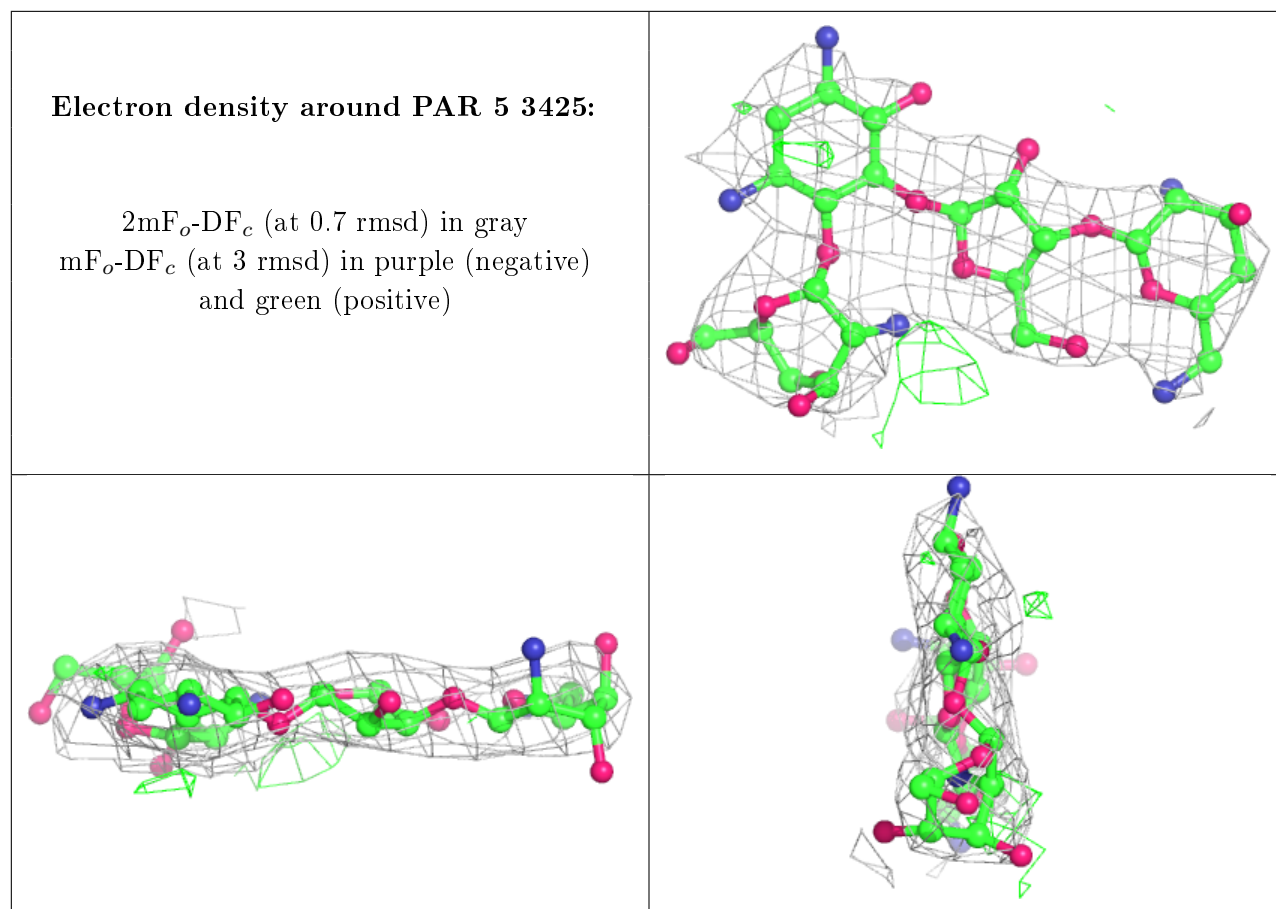
Electron density around PAR 5 3421:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PAR 1 3404:**

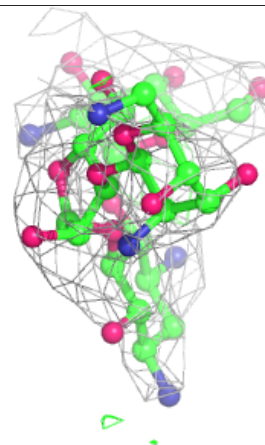
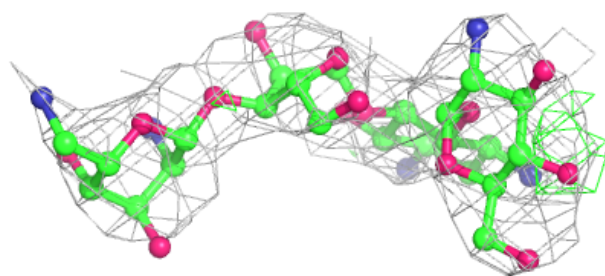
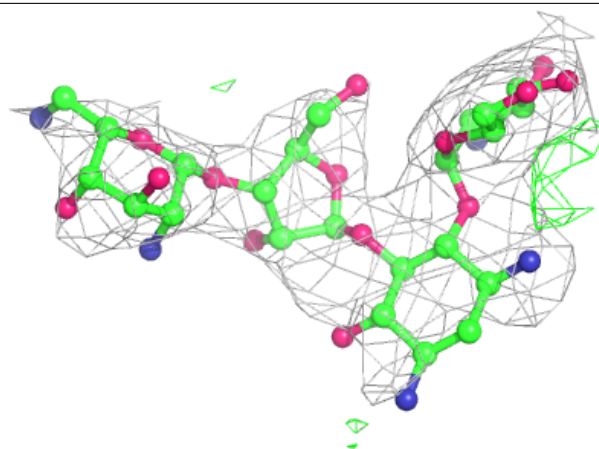
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





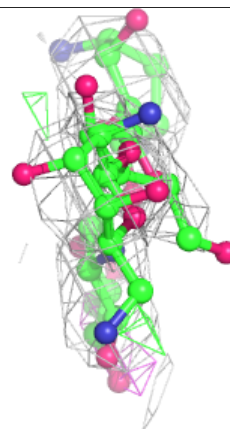
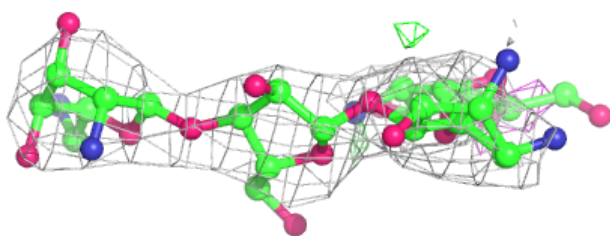
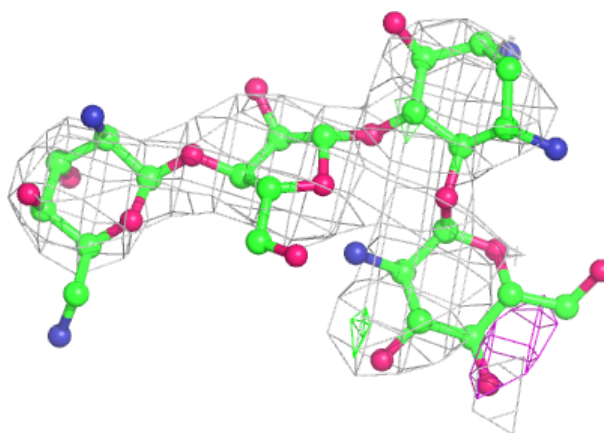
Electron density around PAR 7 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

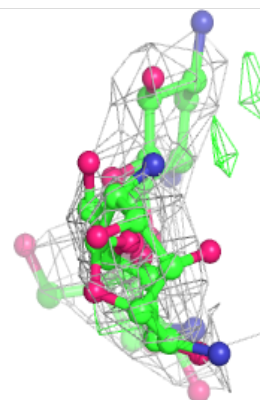
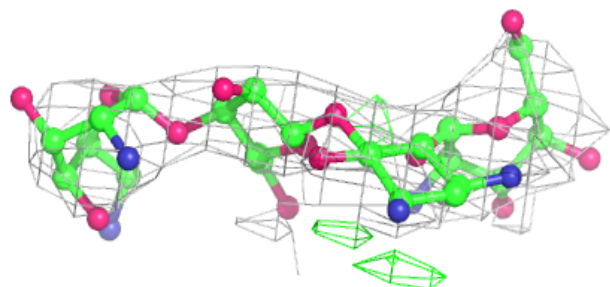
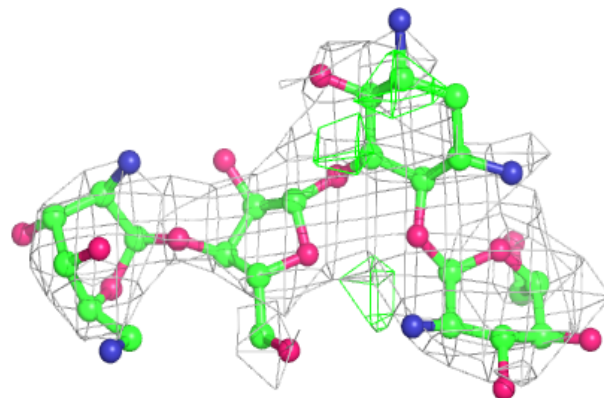


Electron density around PAR 1 3432:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

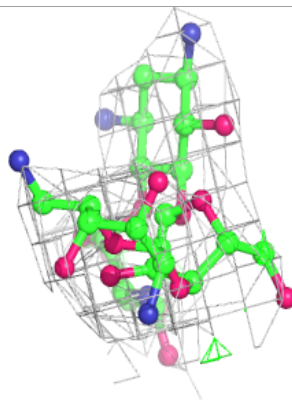
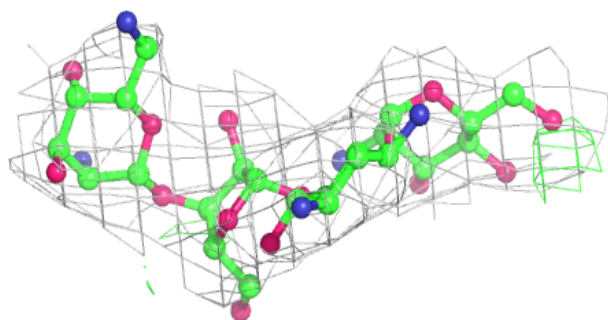
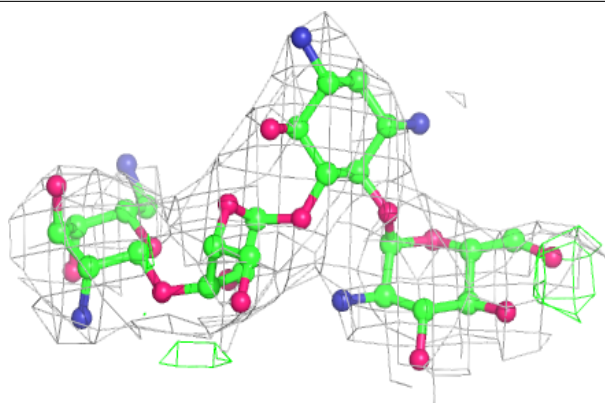
**Electron density around PAR 5 3426:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

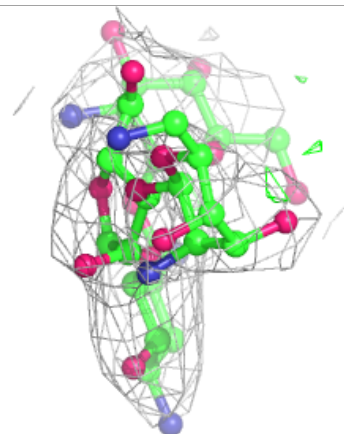
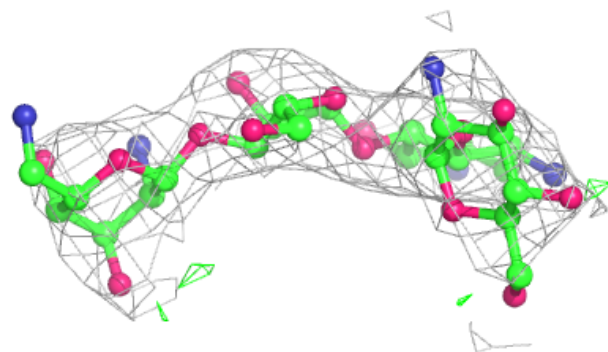
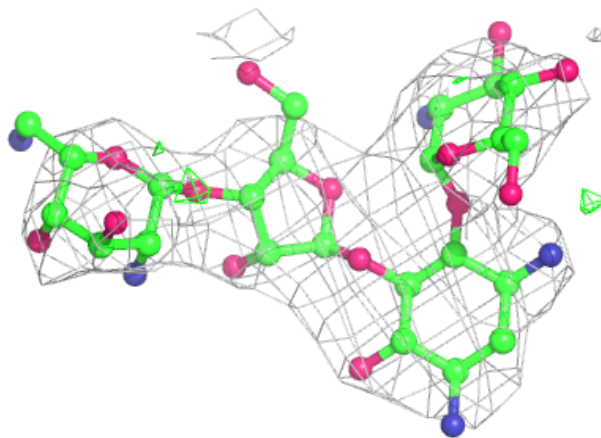


Electron density around PAR 1 3434:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

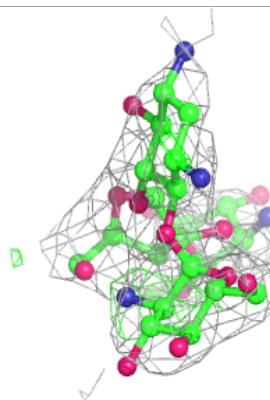
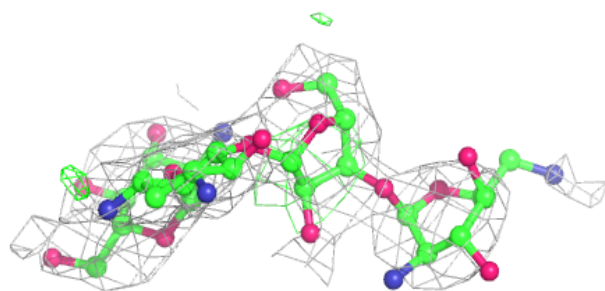
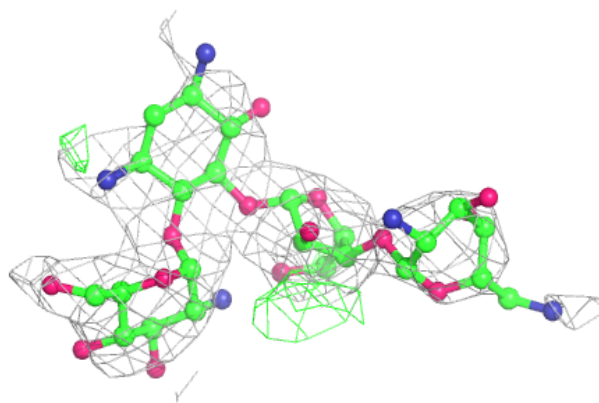
**Electron density around PAR 1 3417:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

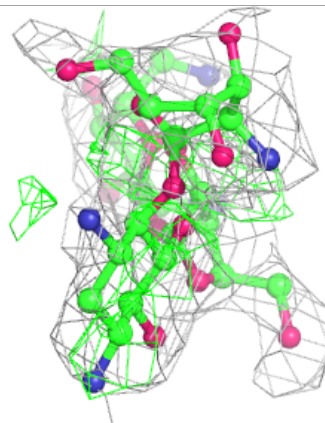
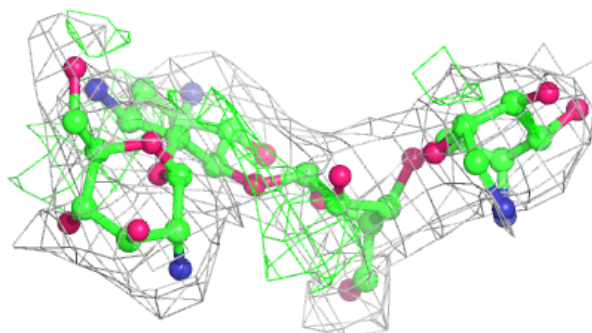
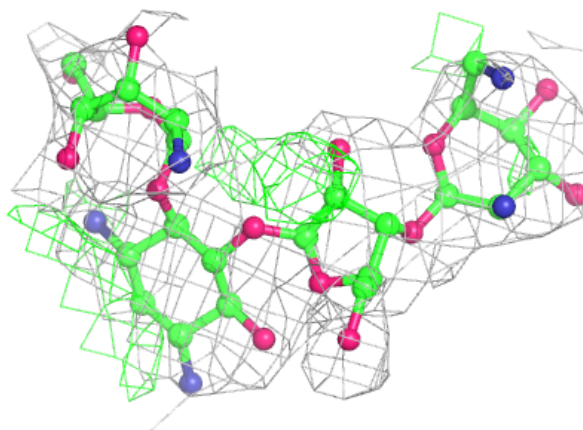


Electron density around PAR 3 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

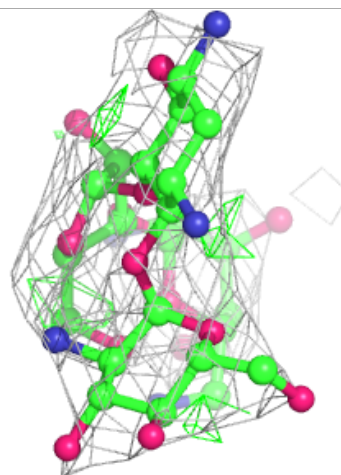
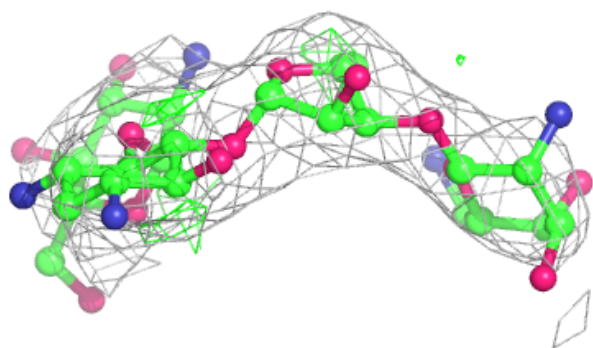
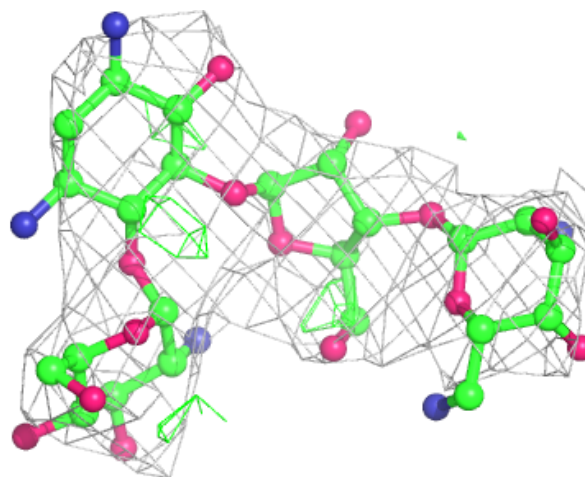
**Electron density around PAR 1 3414:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



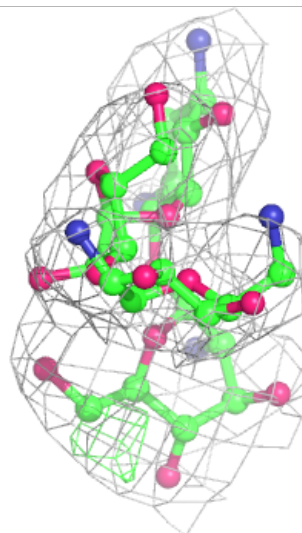
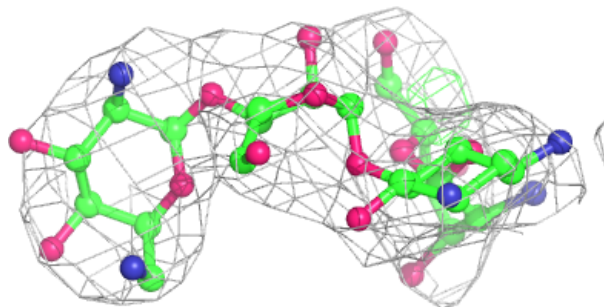
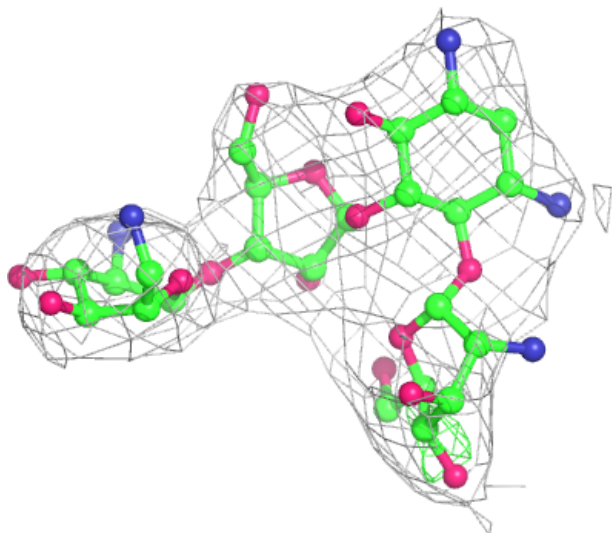
Electron density around PAR 1 3427:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



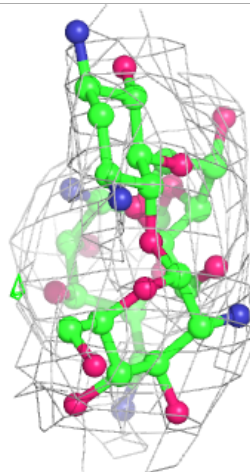
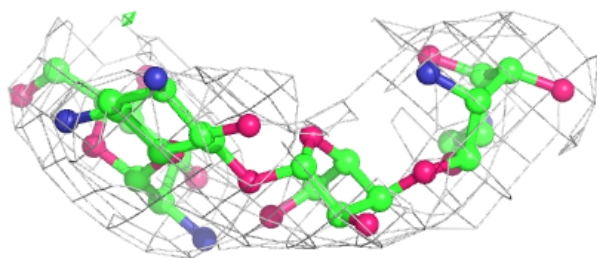
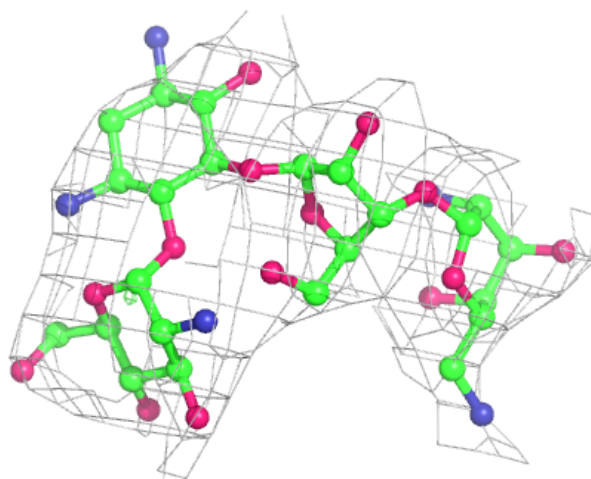
Electron density around PAR 5 3415:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



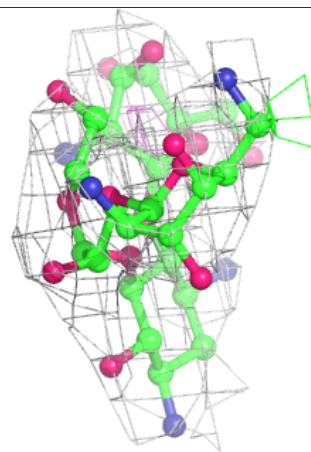
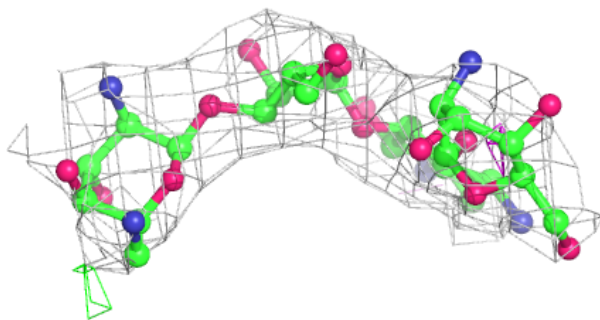
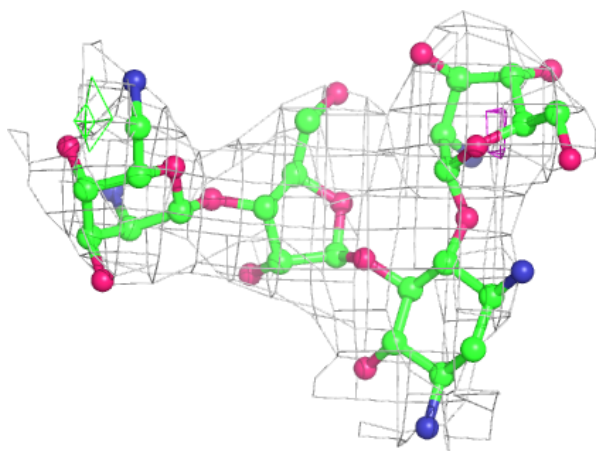
Electron density around PAR 2 1904:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



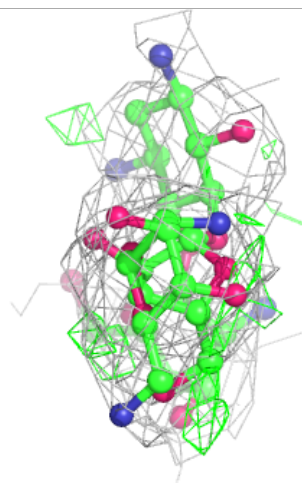
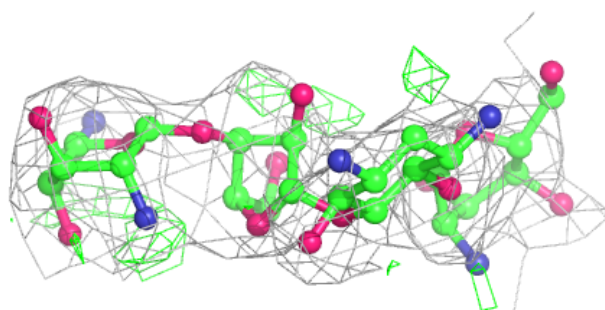
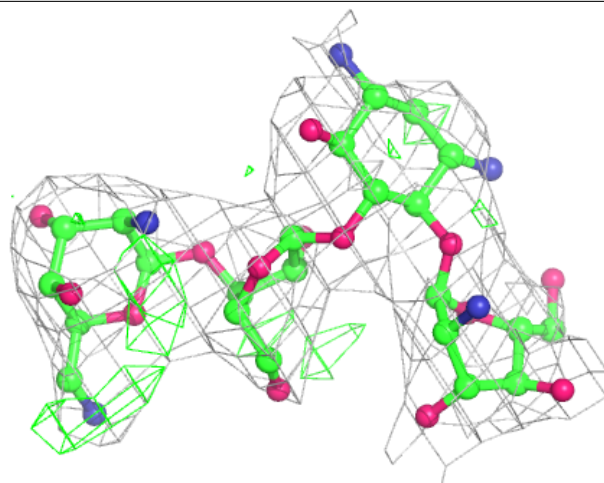
Electron density around PAR 6 1901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



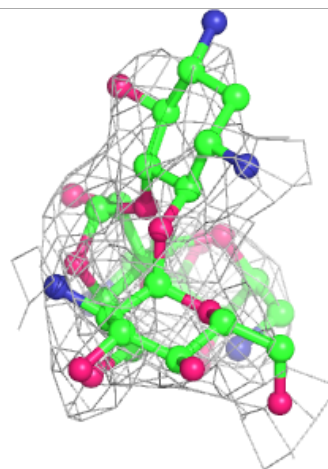
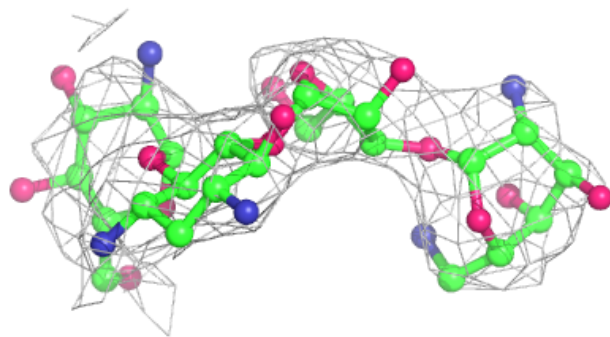
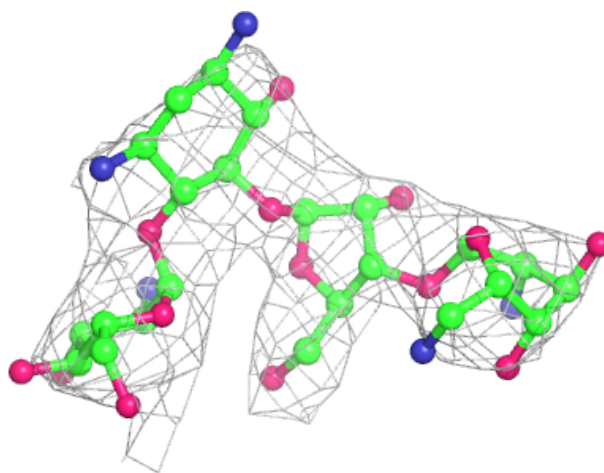
Electron density around PAR 5 3401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



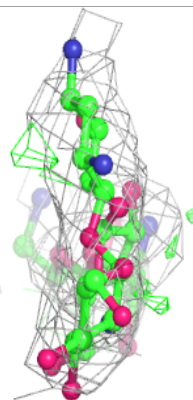
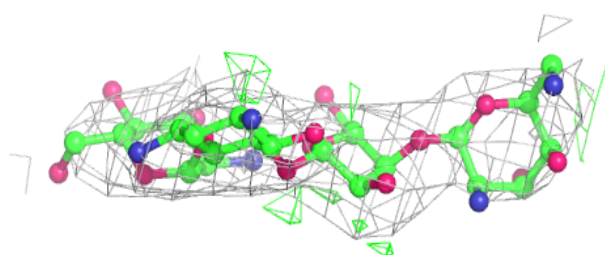
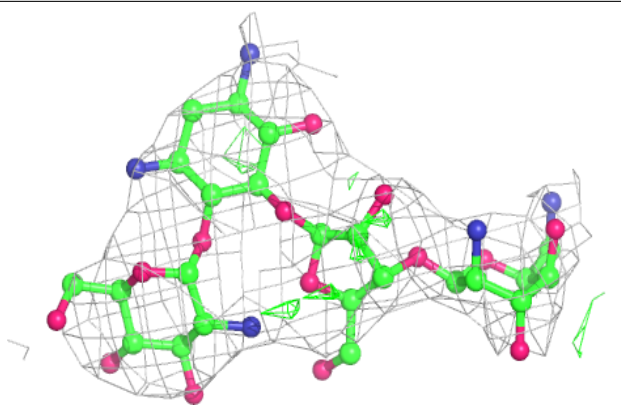
Electron density around PAR 1 3407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

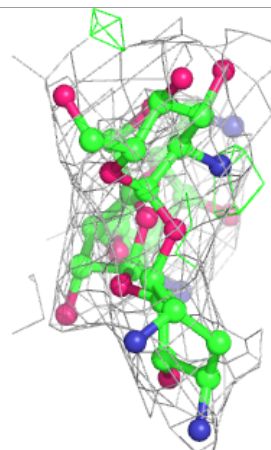
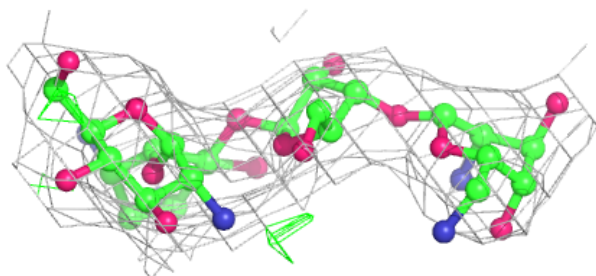
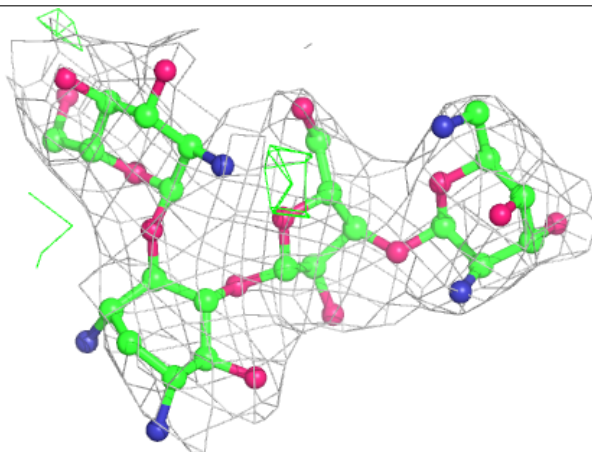


Electron density around PAR 5 3424:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

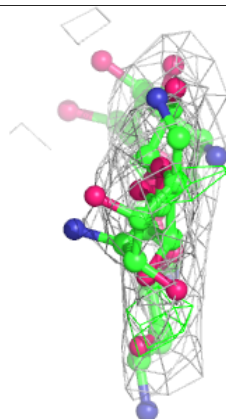
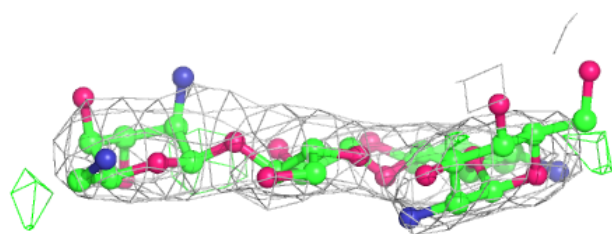
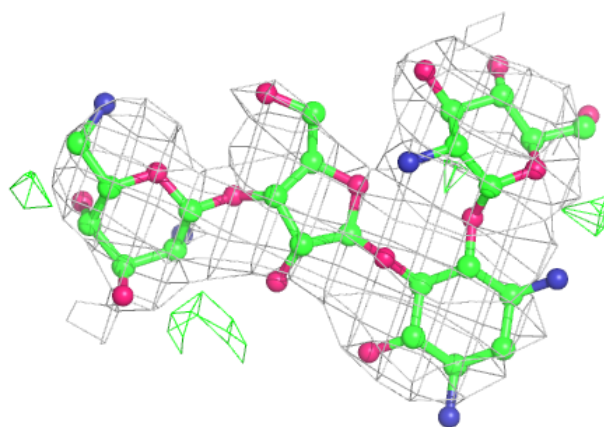
**Electron density around PAR 5 3414:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

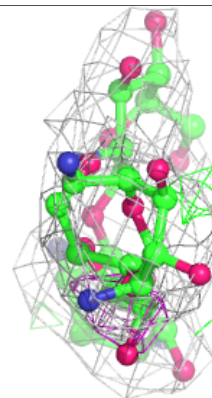
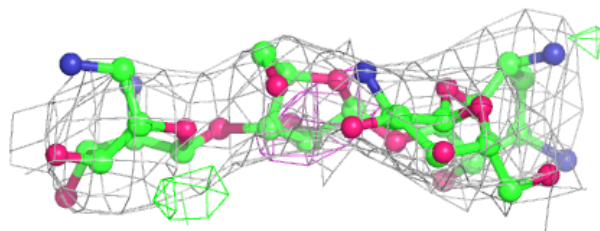
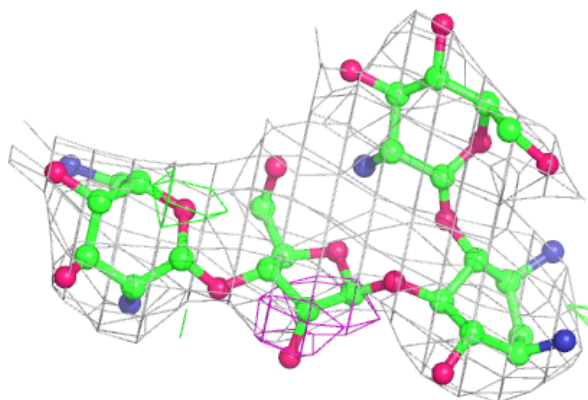


Electron density around PAR 1 3422:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

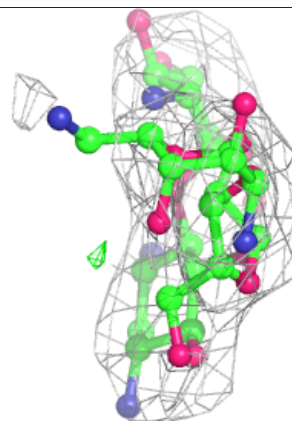
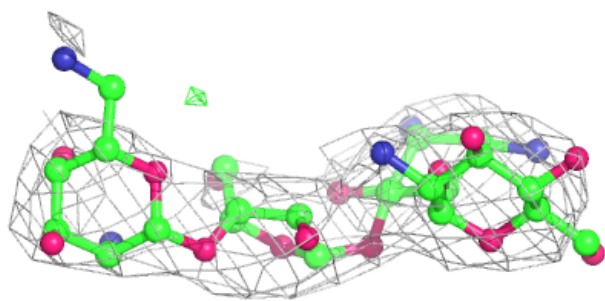
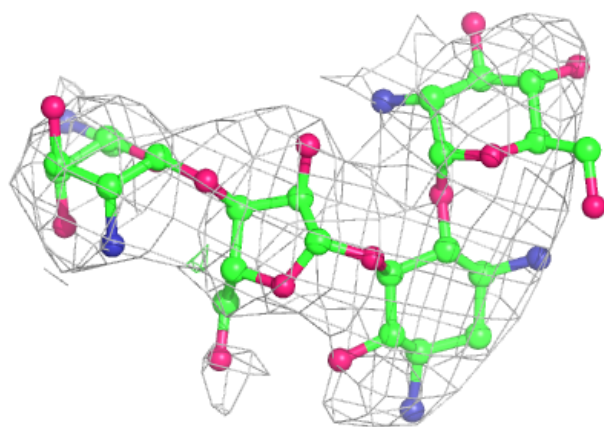
**Electron density around PAR 5 3419:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



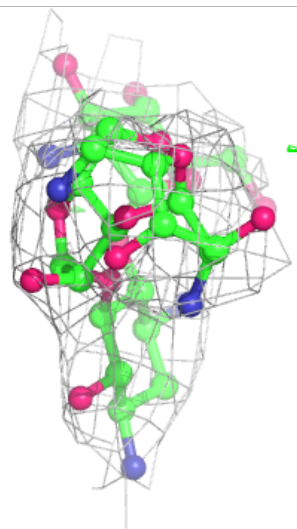
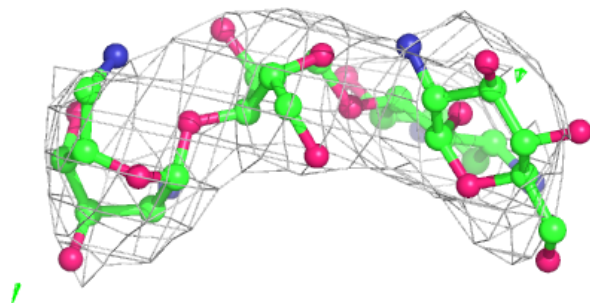
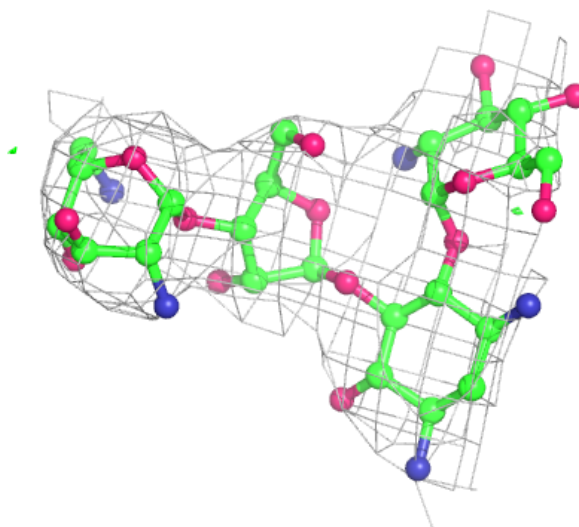
Electron density around PAR 6 1904:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



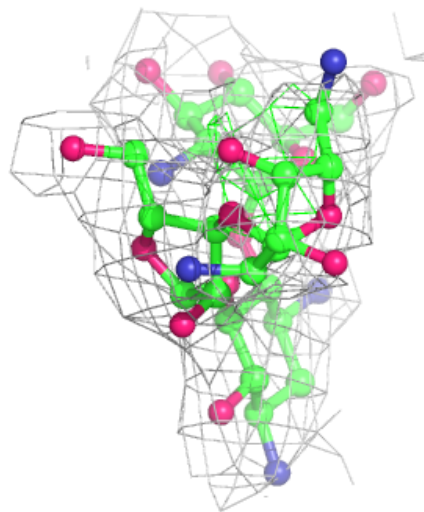
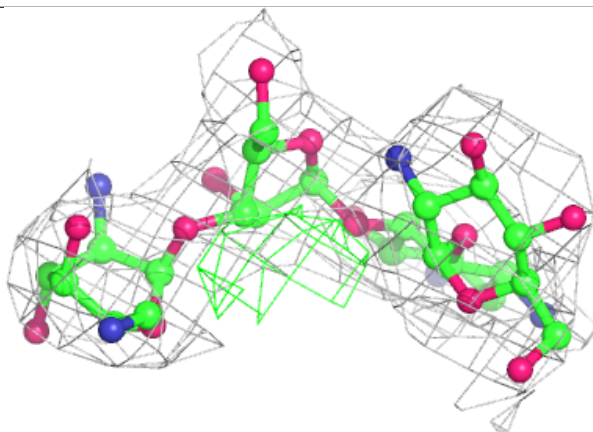
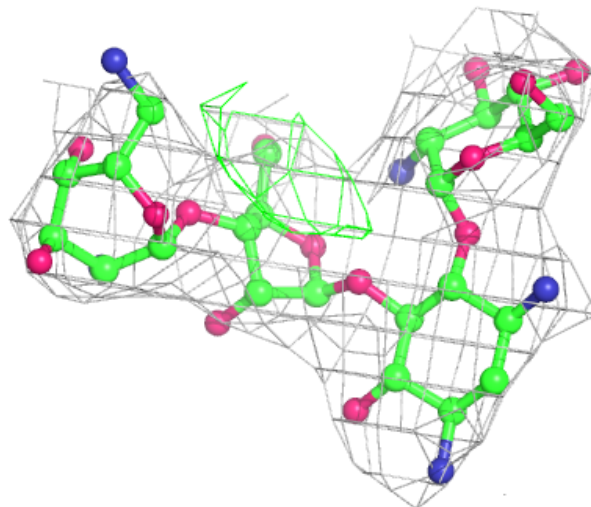
Electron density around PAR 5 3418:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



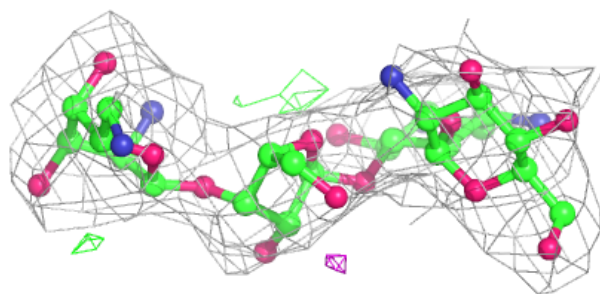
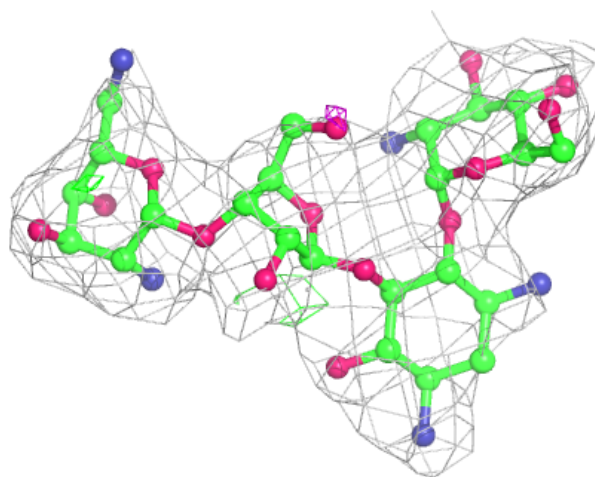
Electron density around PAR 1 3418:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



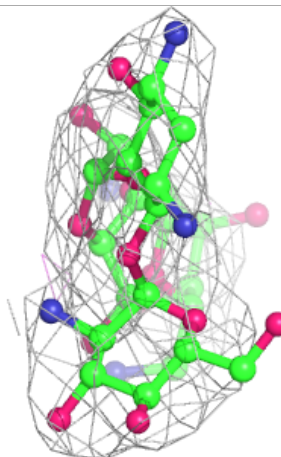
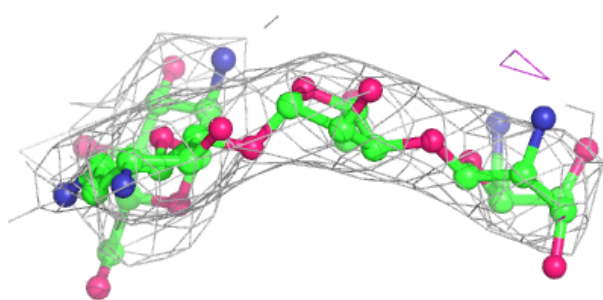
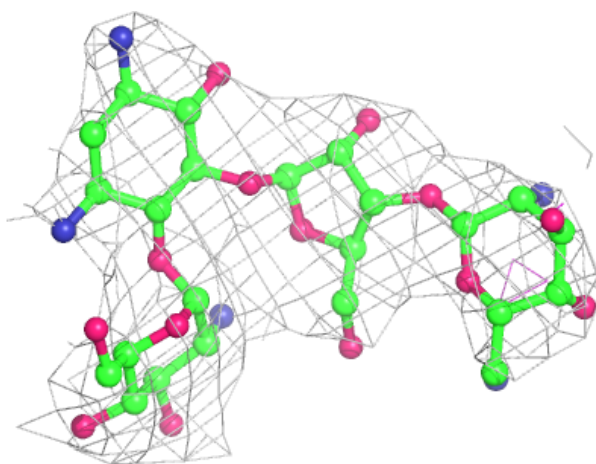
Electron density around PAR 1 3420:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



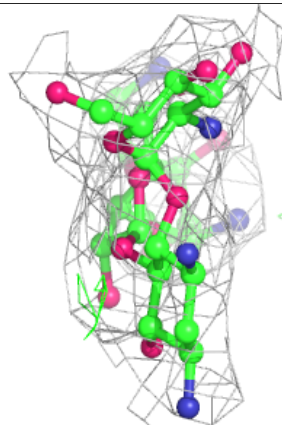
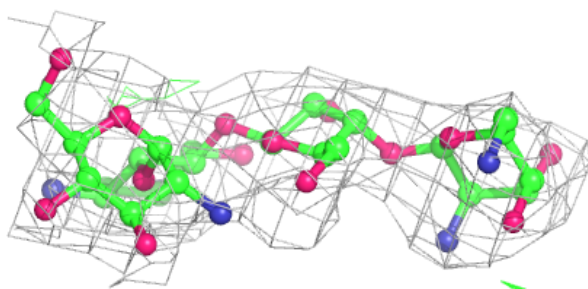
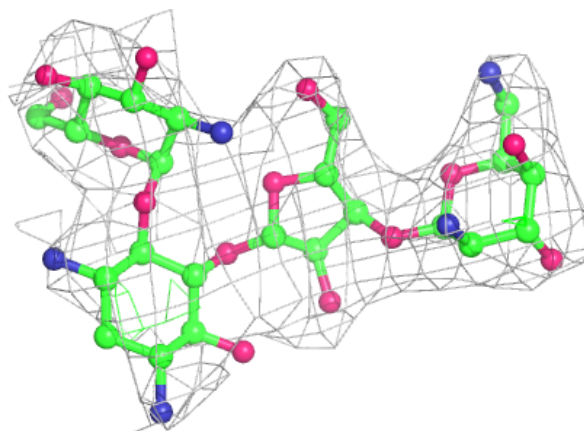
Electron density around PAR 6 1903:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

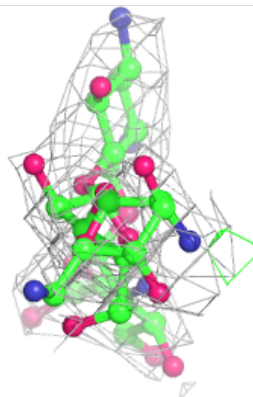
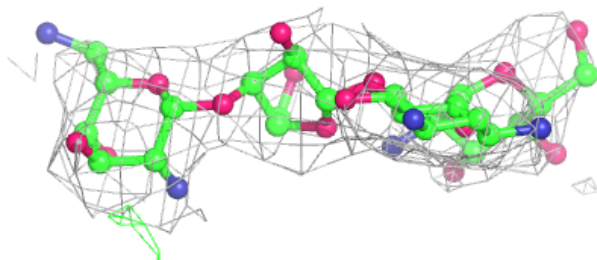
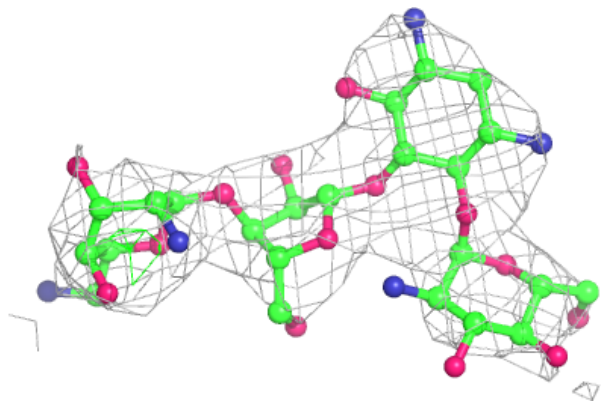


Electron density around PAR 1 3402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

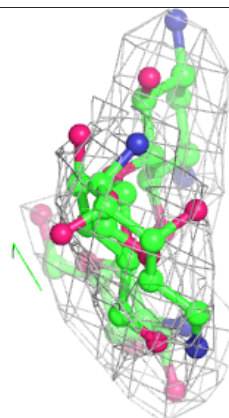
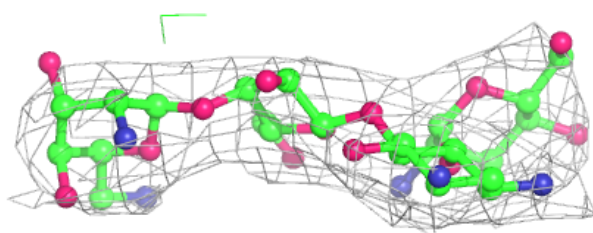
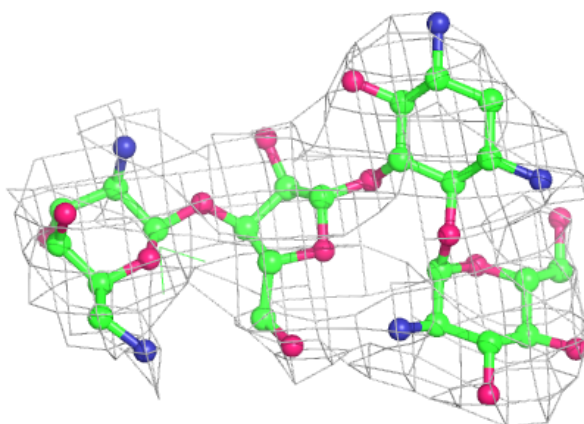
**Electron density around PAR 1 3415:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



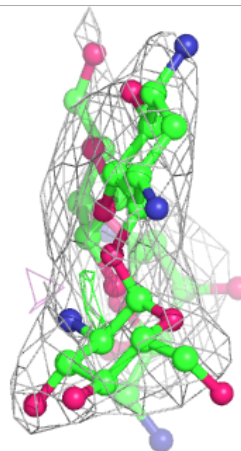
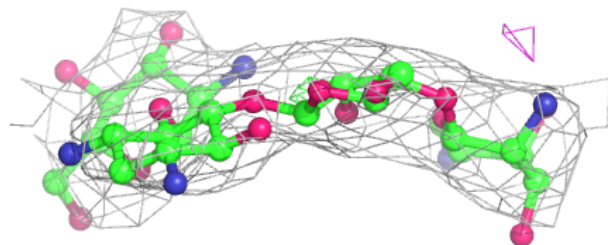
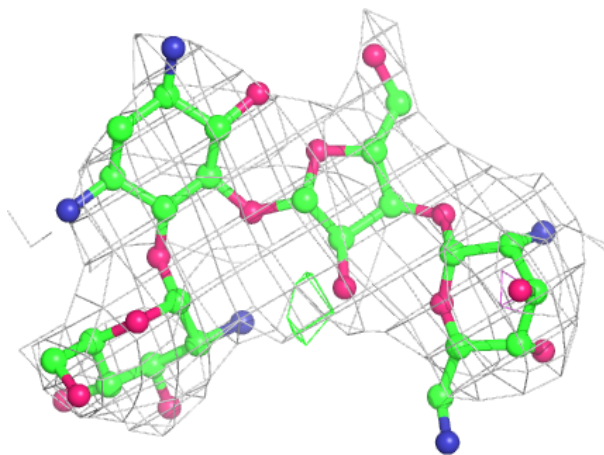
Electron density around PAR 7 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



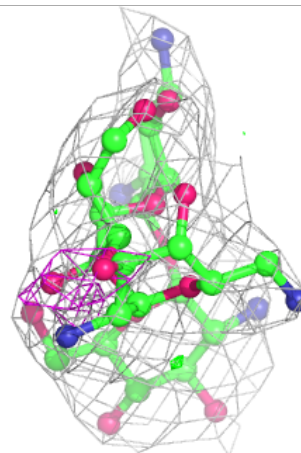
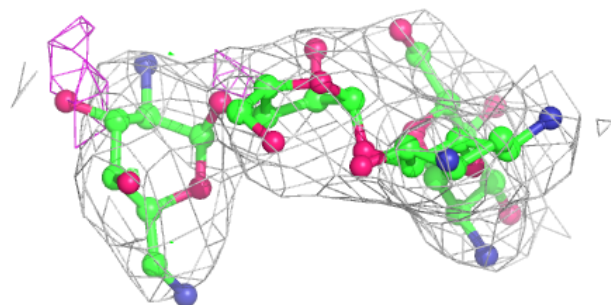
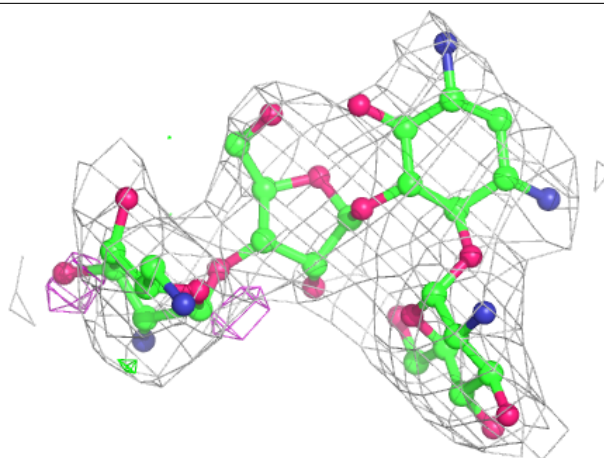
Electron density around PAR 2 1902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



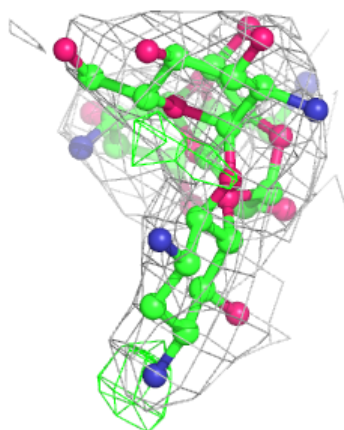
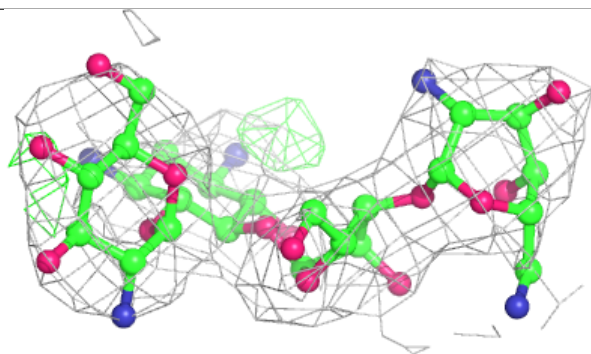
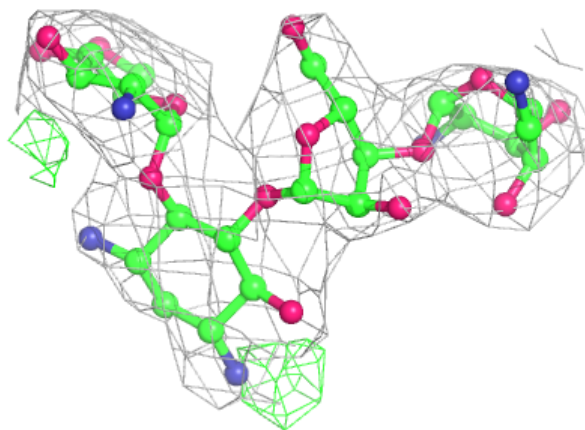
Electron density around PAR 1 3419:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



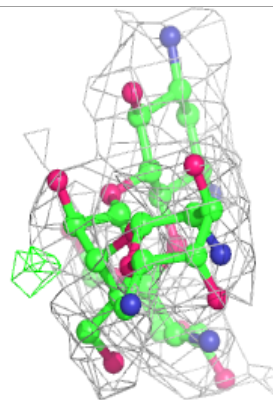
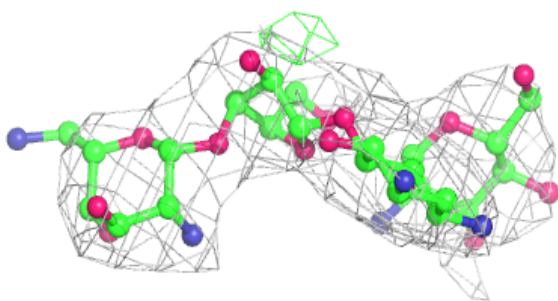
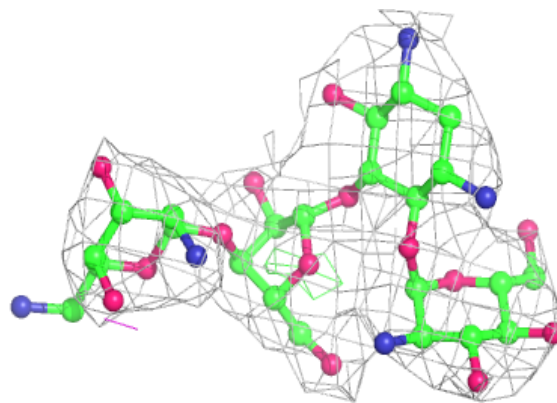
Electron density around PAR 1 3430:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



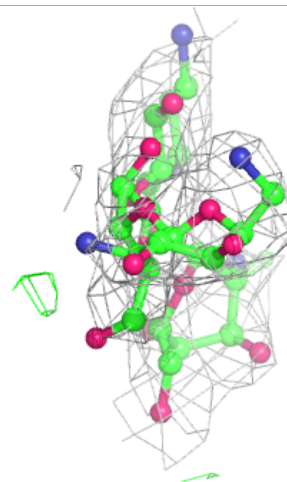
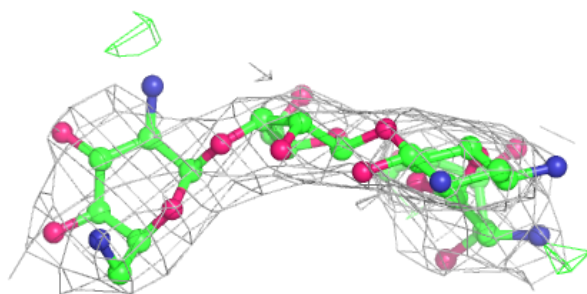
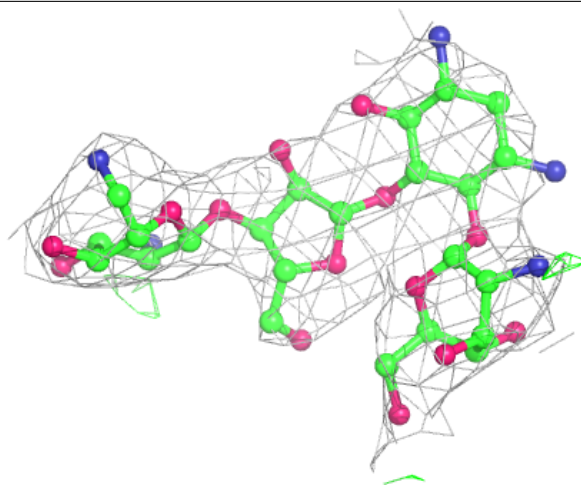
Electron density around PAR 1 3412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



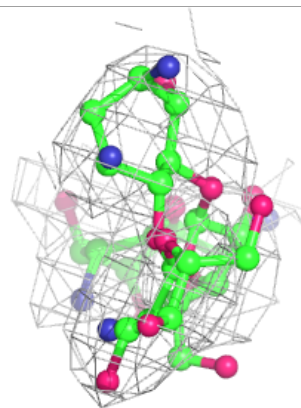
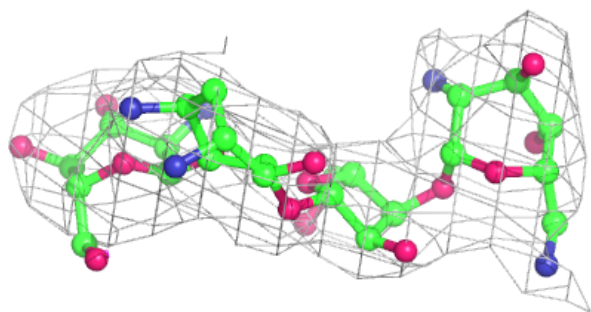
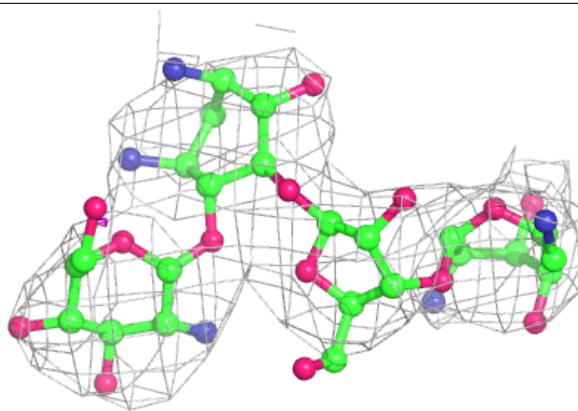
Electron density around PAR 1 3425:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

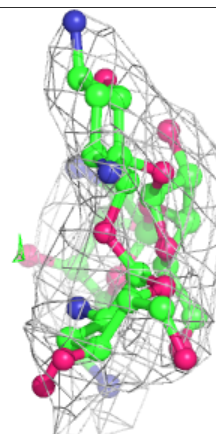
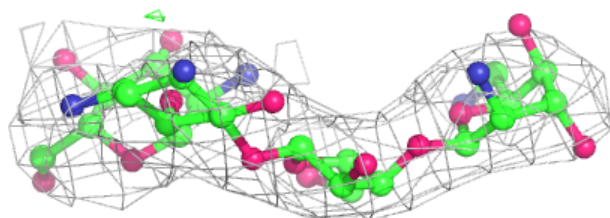
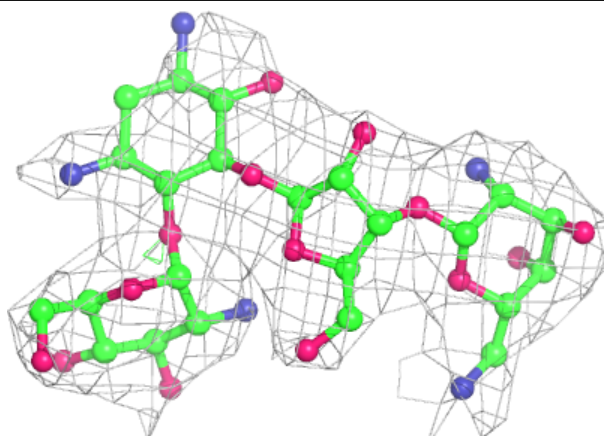


Electron density around PAR 5 3420:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

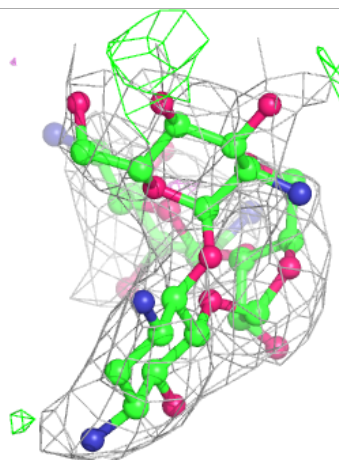
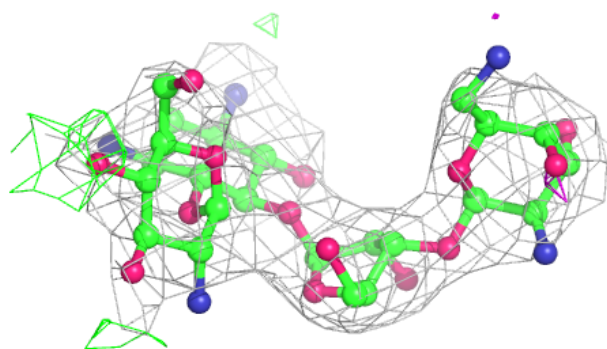
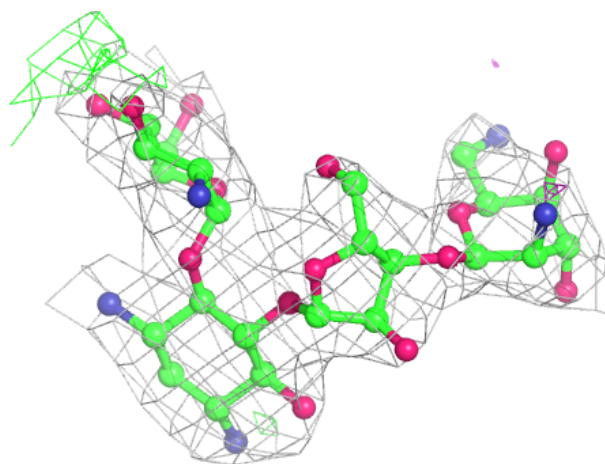
**Electron density around PAR 4 202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



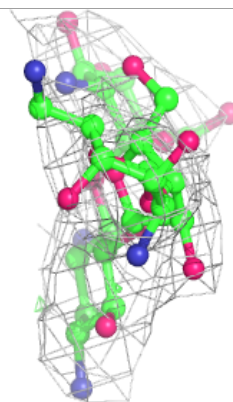
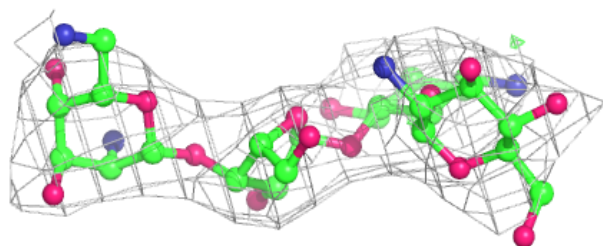
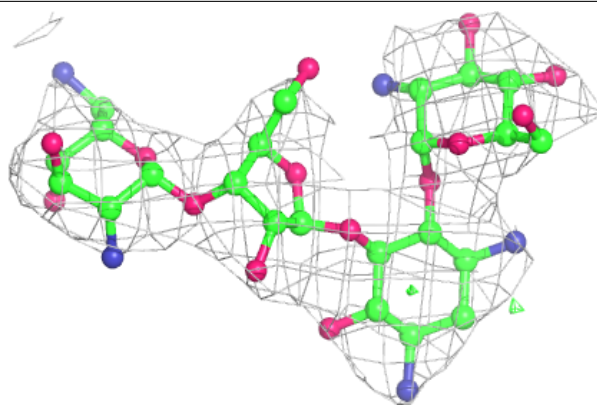
Electron density around PAR 5 3412:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



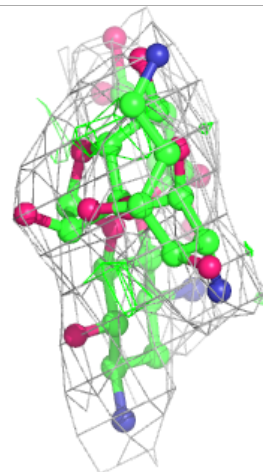
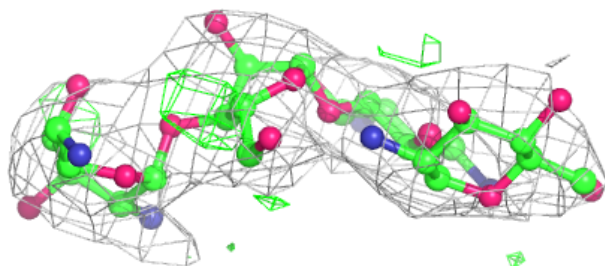
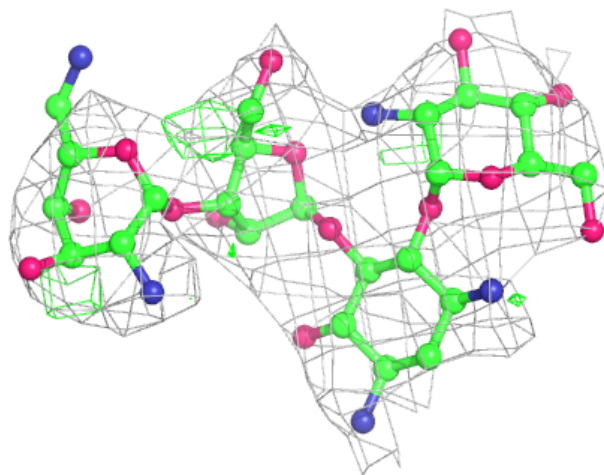
Electron density around PAR 5 3416:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



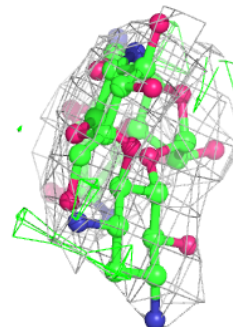
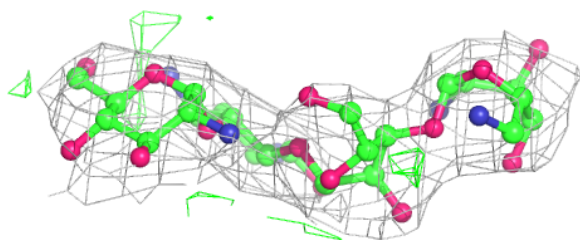
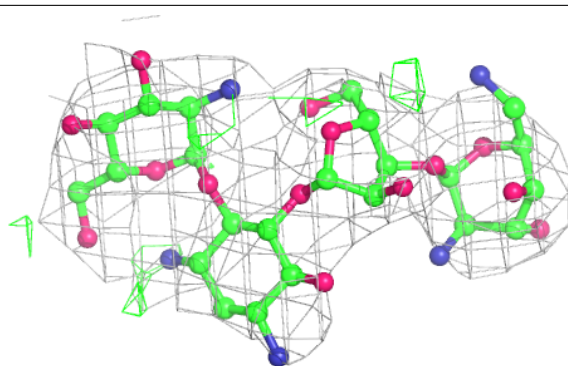
Electron density around PAR 1 3429:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

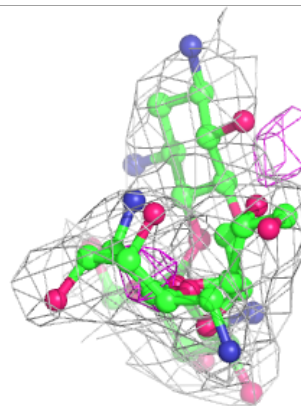
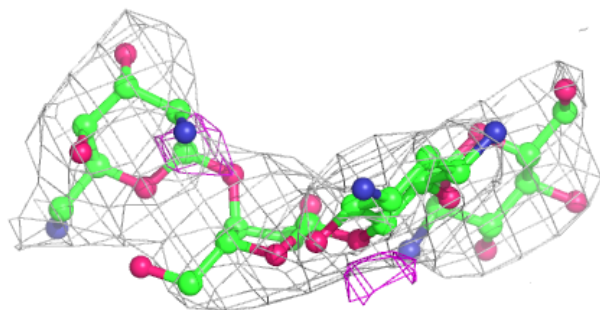
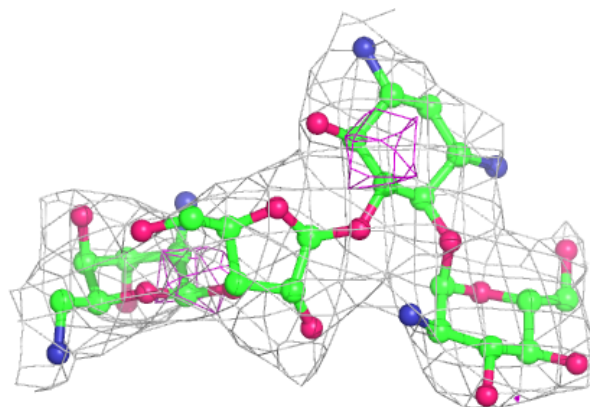


Electron density around PAR 5 3407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

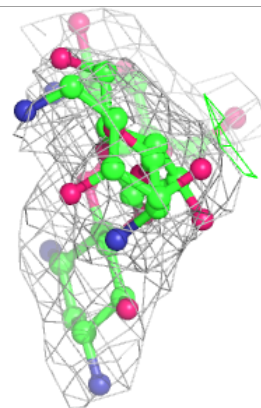
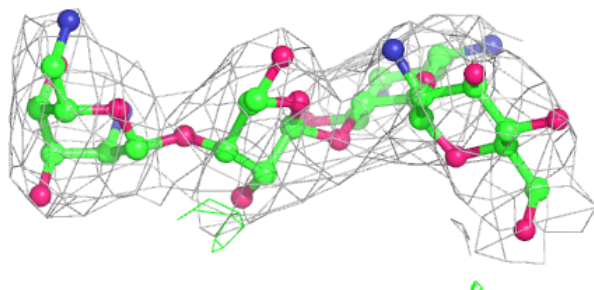
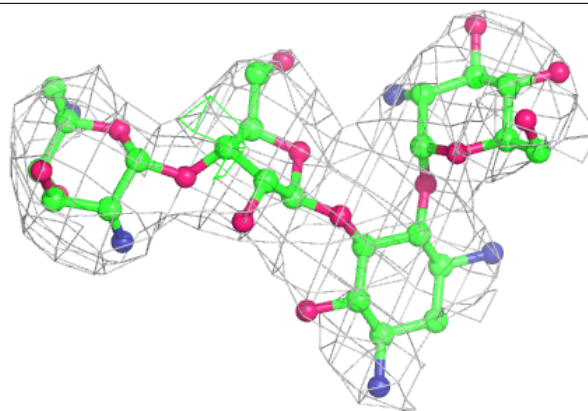
**Electron density around PAR 1 3416:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



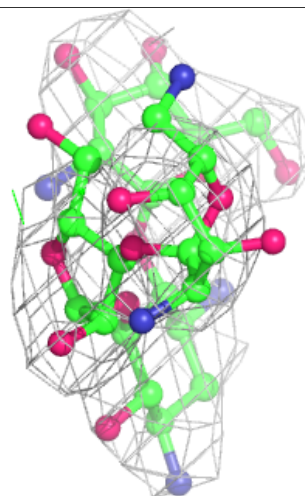
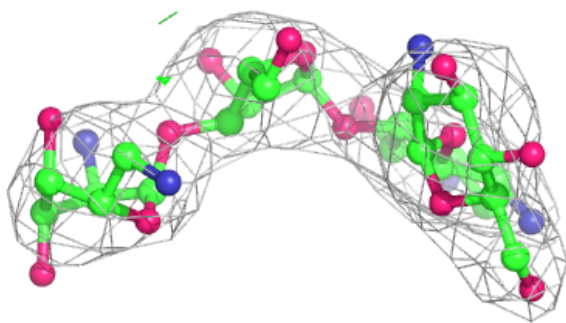
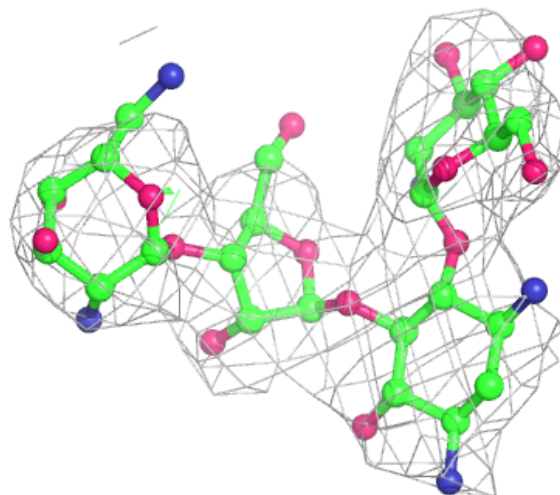
Electron density around PAR 1 3428:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



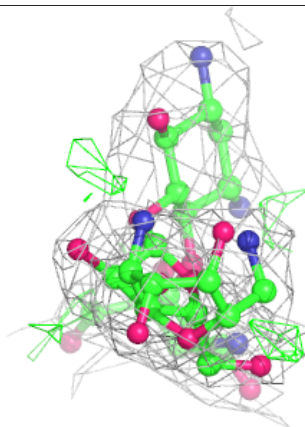
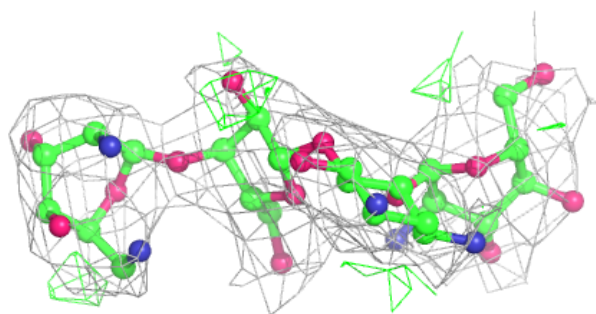
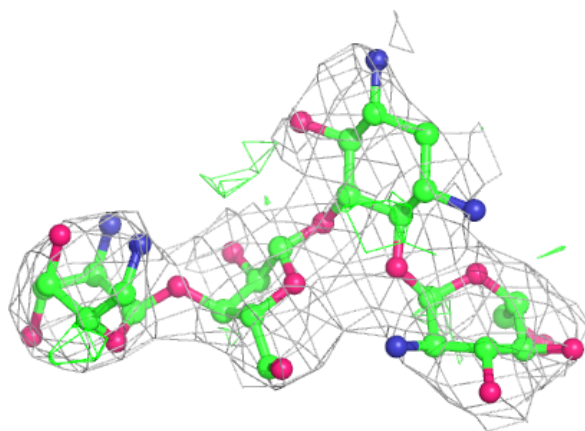
Electron density around PAR 1 3408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



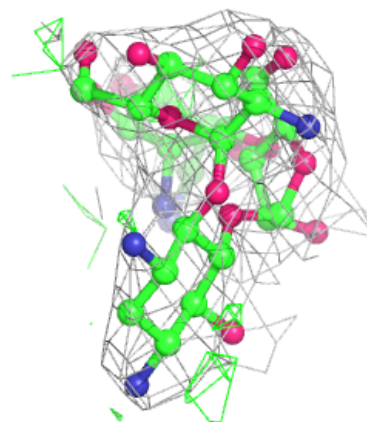
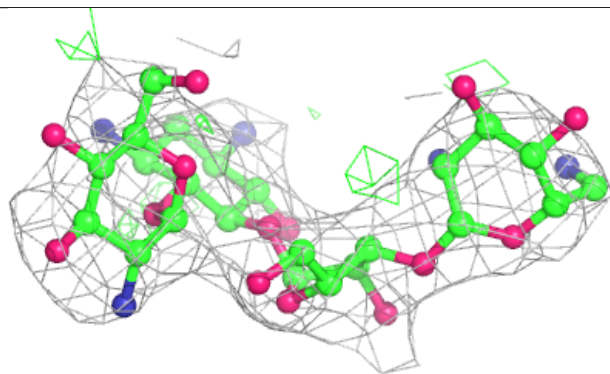
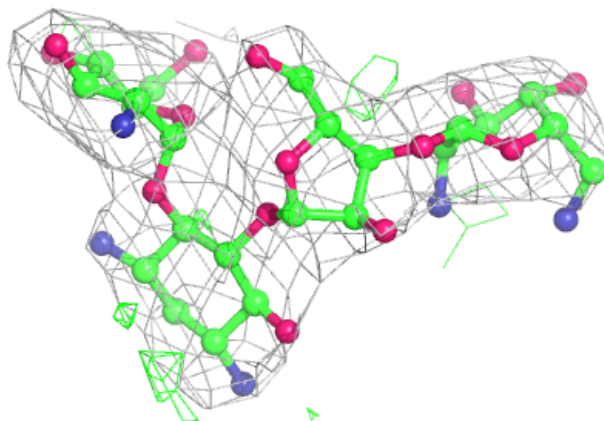
Electron density around PAR 5 3406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



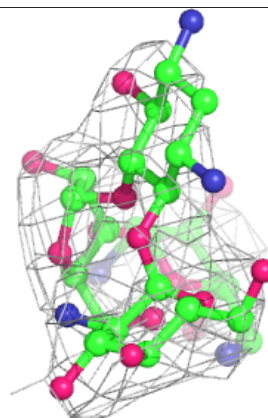
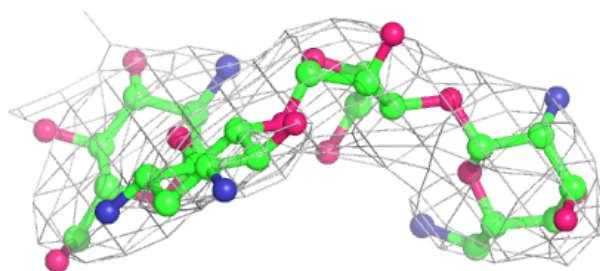
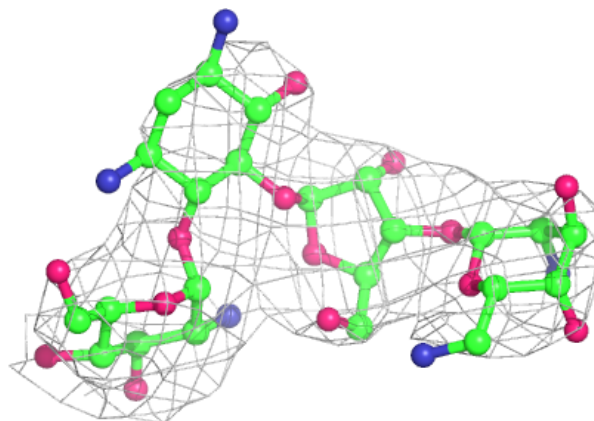
Electron density around PAR 5 3408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



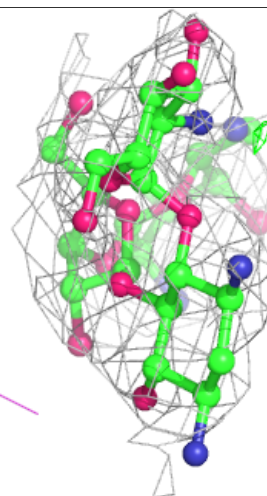
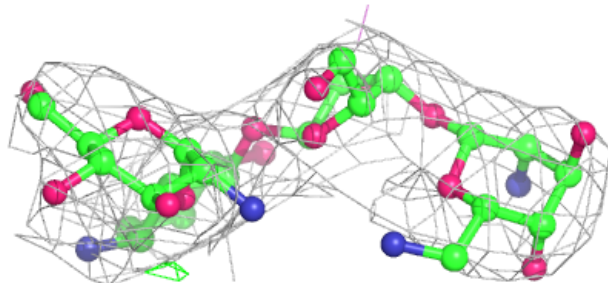
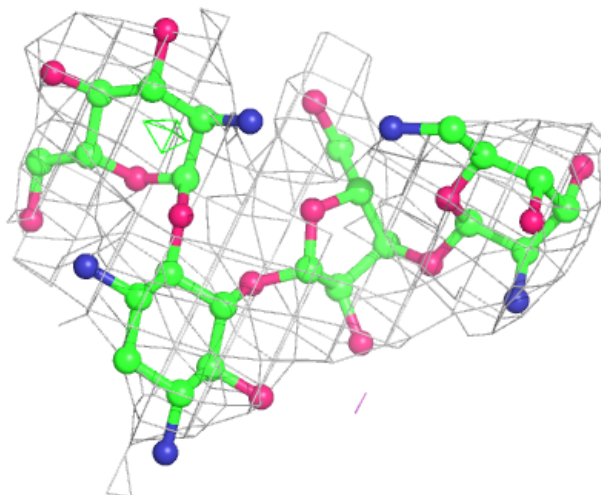
Electron density around PAR 5 3410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



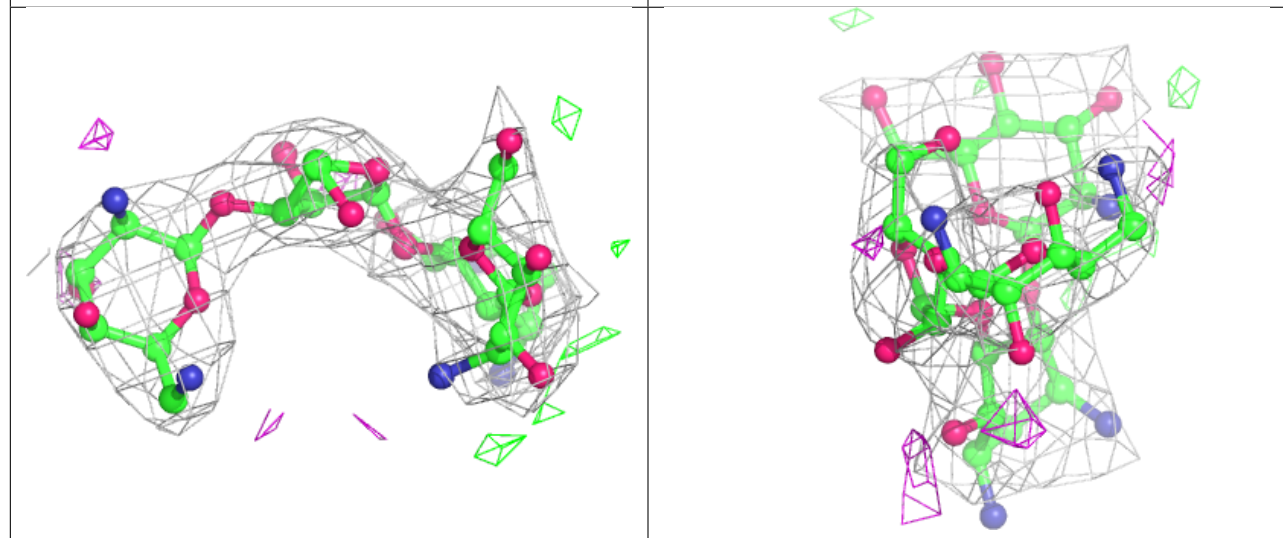
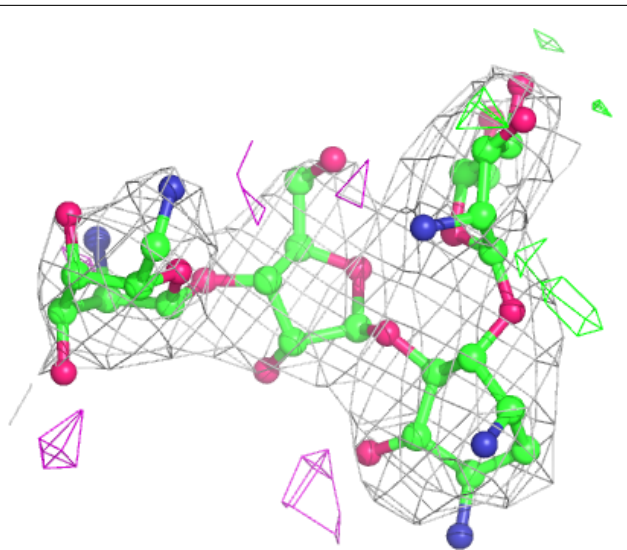
Electron density around PAR 1 3424:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



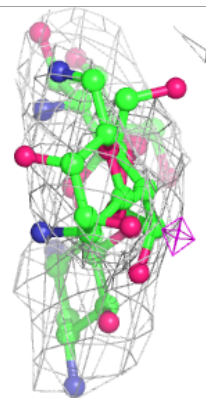
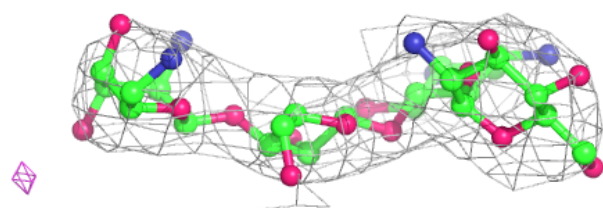
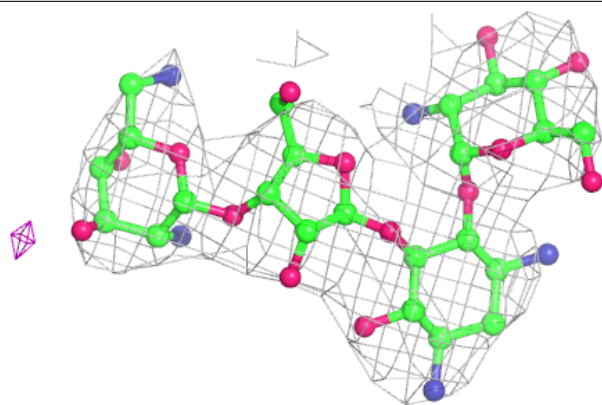
Electron density around PAR 1 3409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

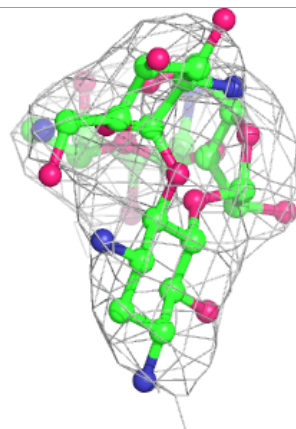
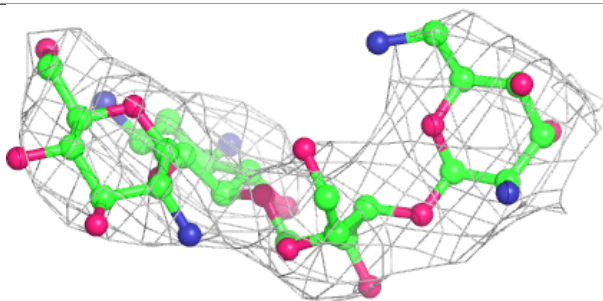
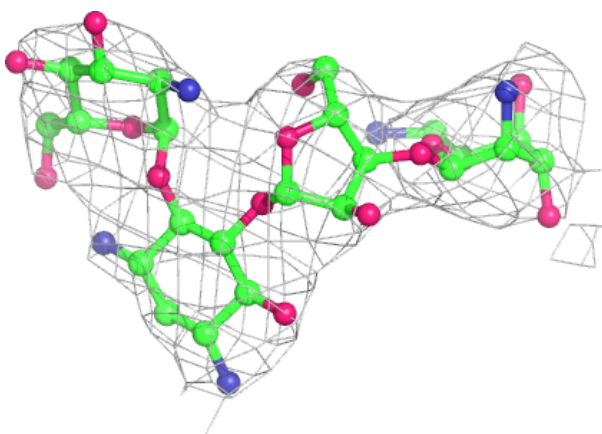


Electron density around PAR 2 1903:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

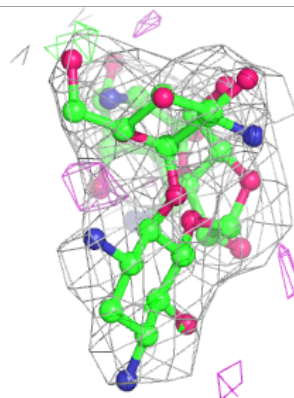
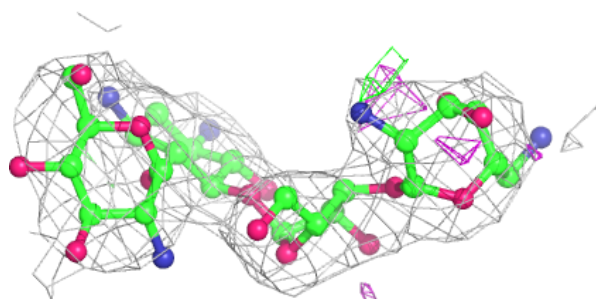
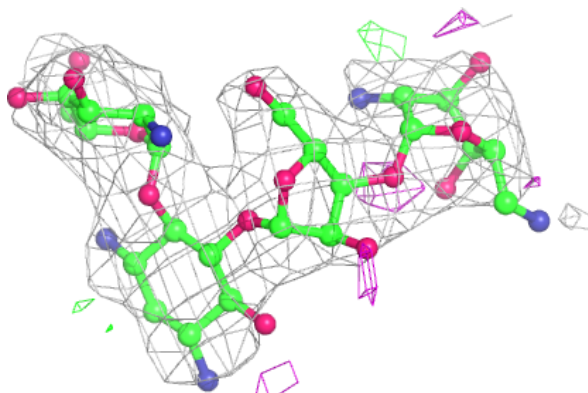
**Electron density around PAR 5 3417:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

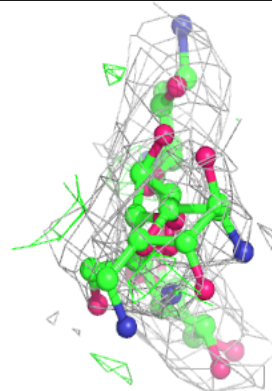
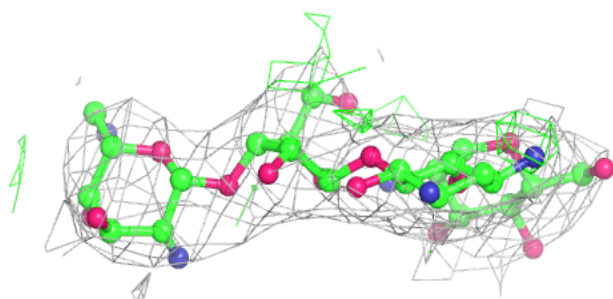
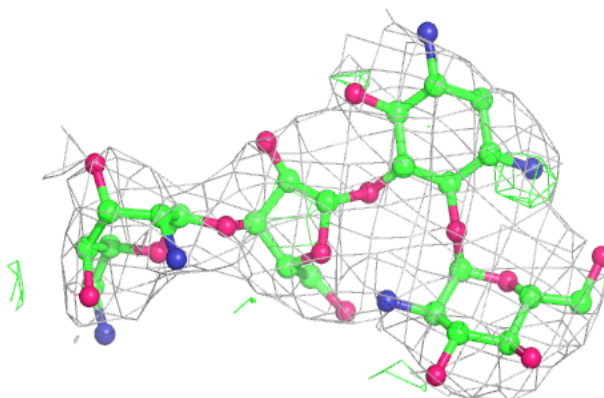


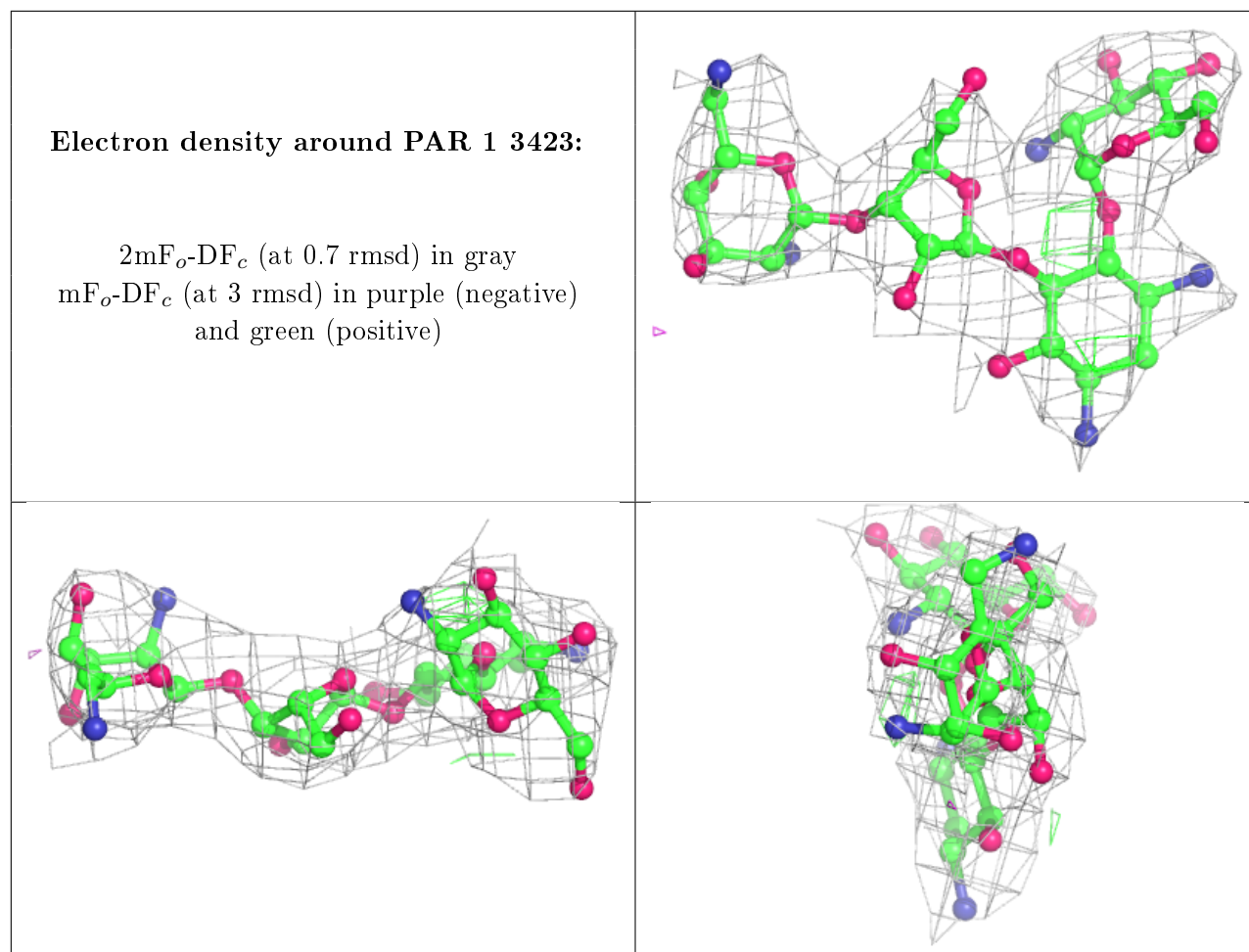
Electron density around PAR 1 3411:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PAR 1 3421:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.