



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 08:38 pm BST

PDB ID : 5LYB
Title : Crystal structure of the *S.cerevisiae* 80S ribosome in complex with the A-site bound aminoacyl-tRNA analog ACCPmn
Authors : Melnikov, S.; Mailliot, J.
Deposited on : 2016-09-26
Resolution : 3.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

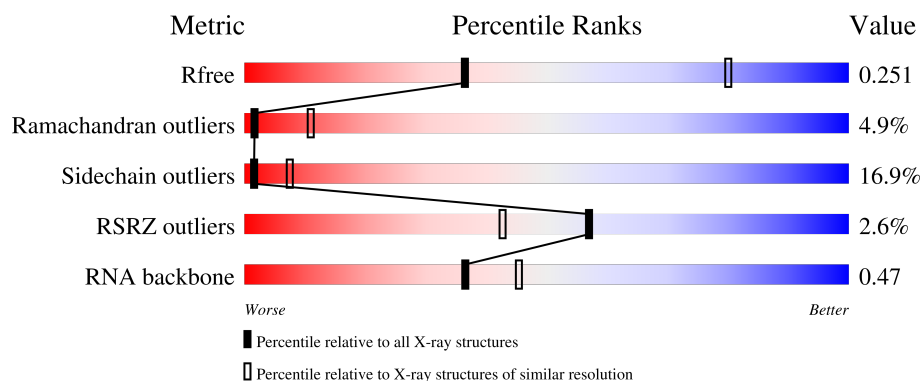
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	164625	1482 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (3.30-3.22)
RNA backbone	3690	1028 (3.60-2.92)

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

Mol	Chain	Length	Quality of chain
1	2	1800	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
1	6	1800	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>.</div> </div> </div>
2	S0	206	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
2	s0	206	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
3	S1	216	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	s1	216	
4	S2	217	
4	s2	217	
5	S3	223	
5	s3	223	
6	S4	260	
6	s4	260	
7	S5	206	
7	s5	206	
8	S6	226	
8	s6	226	
9	S7	186	
9	s7	186	
10	S8	199	
10	s8	199	
11	S9	185	
11	s9	185	
12	C0	96	
13	C1	155	
13	c1	155	
14	C2	124	
15	C3	150	
15	c3	150	
16	C4	128	
16	c4	128	

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Mol	Chain	Length	Quality of chain
17	C5	131	
18	C6	142	
18	c6	142	
19	C7	125	
19	c7	125	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	110	
22	d0	110	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	70	
27	d5	70	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	


















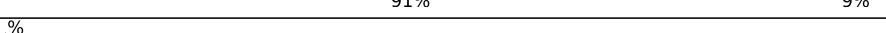







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Mol	Chain	Length	Quality of chain
30	D8	63	
30	d8	63	
31	D9	53	
31	d9	53	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
35	SM	159	
36	1	3394	
36	5	3394	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	252	
39	l2	252	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	

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Mol	Chain	Length	Quality of chain
43	l6	175	 78%10%10%
44	L7	223	 89%10%
44	l7	223	 86%13%
45	L8	233	 4%81%18%
46	L9	191	 5%81%19%
46	l9	191	 %79%20%
47	M0	220	 3%79%16%1%
47	m0	220	 5%79%16%1%
48	M1	169	 4%80%17%
48	m1	169	 %79%19%2%
49	M3	194	 5%79%19%
49	m3	194	 2%84%16%
50	M4	137	 %82%15%1%
50	m4	137	 3%86%13%
51	M5	203	 2%80%19%
51	m5	203	 %86%13%
52	M6	197	 2%91%9%
52	m6	197	 %89%10%1%
53	M7	183	 7%81%18%
53	m7	183	 %69%15%15%
54	M8	185	 %88%12%
54	m8	185	 %84%16%
55	M9	188	 5%85%15%
55	m9	188	 3%85%15%
56	N0	172	 %81%18%

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Mol	Chain	Length	Quality of chain
56	n0	172	<div> <div></div> <div>83%</div> <div>17%</div> </div>
57	N1	159	<div> <div></div> <div>80%</div> <div>19%</div> </div>
57	n1	159	<div> <div></div> <div>81%</div> <div>18%</div> </div>
58	N2	100	<div> <div></div> <div>86%</div> <div>14%</div> </div>
58	n2	100	<div> <div></div> <div>82%</div> <div>16%</div> </div>
59	N3	136	<div> <div></div> <div>85%</div> <div>15%</div> </div>
59	n3	136	<div> <div></div> <div>91%</div> <div>8%</div> </div>
60	N4	98	<div> <div></div> <div>87%</div> <div>13%</div> </div>
61	N5	121	<div> <div></div> <div>81%</div> <div>18%</div> </div>
61	n5	121	<div> <div></div> <div>79%</div> <div>18%</div> </div>
62	N6	126	<div> <div></div> <div>75%</div> <div>24%</div> </div>
62	n6	126	<div> <div></div> <div>75%</div> <div>24%</div> </div>
63	N7	135	<div> <div></div> <div>81%</div> <div>16%</div> </div>
63	n7	135	<div> <div></div> <div>76%</div> <div>21%</div> </div>
64	N8	148	<div> <div></div> <div>81%</div> <div>18%</div> </div>
64	n8	148	<div> <div></div> <div>84%</div> <div>16%</div> </div>
65	N9	58	<div> <div></div> <div>81%</div> <div>16%</div> </div>
65	n9	58	<div> <div></div> <div>72%</div> <div>22%</div> <div>5%</div> </div>
66	O0	100	<div> <div></div> <div>83%</div> <div>14%</div> </div>
66	o0	100	<div> <div></div> <div>84%</div> <div>16%</div> </div>
67	O1	109	<div> <div></div> <div>84%</div> <div>14%</div> </div>
67	o1	109	<div> <div></div> <div>80%</div> <div>20%</div> </div>
68	O2	127	<div> <div></div> <div>89%</div> <div>11%</div> </div>
68	o2	127	<div> <div></div> <div>84%</div> <div>15%</div> </div>
69	O3	106	<div> <div></div> <div>89%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
69	o3	106	<div> <div></div> <div>86%</div> <div>13%</div> <div></div> </div>
70	O4	112	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div></div> </div>
70	o4	112	<div> <div>4%</div> <div>87%</div> <div>13%</div> <div></div> </div>
71	O5	119	<div> <div>3%</div> <div>82%</div> <div>18%</div> <div></div> </div>
71	o5	119	<div> <div></div> <div>81%</div> <div>18%</div> <div></div> </div>
72	O6	99	<div> <div></div> <div>76%</div> <div>23%</div> <div></div> </div>
72	o6	99	<div> <div></div> <div>74%</div> <div>21%</div> <div>5%</div> </div>
73	O7	87	<div> <div>5%</div> <div>87%</div> <div>13%</div> <div></div> </div>
73	o7	87	<div> <div>2%</div> <div>77%</div> <div>22%</div> <div></div> </div>
74	O8	77	<div> <div></div> <div>75%</div> <div>25%</div> <div></div> </div>
74	o8	77	<div> <div></div> <div>83%</div> <div>17%</div> <div></div> </div>
75	O9	50	<div> <div>6%</div> <div>84%</div> <div>16%</div> <div></div> </div>
75	o9	50	<div> <div>8%</div> <div>86%</div> <div>14%</div> <div></div> </div>
76	Q0	52	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div></div> </div>
76	q0	52	<div> <div></div> <div>83%</div> <div>15%</div> <div></div> </div>
77	Q1	25	<div> <div></div> <div>76%</div> <div>24%</div> <div></div> </div>
77	q1	25	<div> <div></div> <div>72%</div> <div>28%</div> <div></div> </div>
78	Q2	105	<div> <div></div> <div>77%</div> <div>20%</div> <div></div> </div>
78	q2	105	<div> <div></div> <div>79%</div> <div>20%</div> <div></div> </div>
79	Q3	91	<div> <div>4%</div> <div>86%</div> <div>14%</div> <div></div> </div>
79	q3	91	<div> <div></div> <div>82%</div> <div>18%</div> <div></div> </div>
80	c0	96	<div> <div>5%</div> <div>79%</div> <div>21%</div> <div></div> </div>
81	c2	124	<div> <div>10%</div> <div>75%</div> <div>22%</div> <div></div> </div>
82	c5	142	<div> <div>5%</div> <div>72%</div> <div>21%</div> <div>5%</div> </div>
83	sR	318	<div> <div></div> <div>91%</div> <div>9%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
84	sM	104	
85	l8	231	
86	m2	150	
87	n4	135	
88	p0	219	
89	p1	47	
89	p2	47	
90	A	3	
90	a	3	

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
91	MG	1	3538	-	-	-	X
91	MG	1	3603	-	-	-	X
91	MG	1	3621	-	-	-	X
91	MG	1	3666	-	-	-	X
91	MG	1	3681	-	-	-	X
91	MG	1	3688	-	-	-	X
91	MG	1	3822	-	-	-	X
91	MG	1	3949	-	-	-	X
91	MG	1	4021	-	-	-	X
91	MG	1	4082	-	-	-	X
91	MG	2	1929	-	-	-	X
91	MG	2	1955	-	-	-	X
91	MG	2	1972	-	-	-	X
91	MG	3	208	-	-	-	X
91	MG	4	206	-	-	-	X
91	MG	5	3491	-	-	-	X
91	MG	5	3550	-	-	-	X
91	MG	5	3652	-	-	-	X
91	MG	5	3767	-	-	-	X
91	MG	5	3909	-	-	-	X
91	MG	5	4093	-	-	-	X
91	MG	6	1926	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	6	1945	-	-	-	X
91	MG	6	1960	-	-	-	X
91	MG	6	2000	-	-	-	X
91	MG	6	2111	-	-	-	X
91	MG	E1	502	-	-	-	X
91	MG	M7	203	-	-	-	X
91	MG	c8	202	-	-	-	X
91	MG	l3	404	-	-	-	X
91	MG	o4	202	-	-	-	X
92	OHX	1	4297	-	-	-	X
92	OHX	1	4307	-	-	-	X
92	OHX	1	4337	-	-	-	X
92	OHX	1	4361	-	-	-	X
92	OHX	1	4385	-	-	-	X
92	OHX	1	4394	-	-	-	X
92	OHX	1	4396	-	-	-	X
92	OHX	1	4413	-	-	-	X
92	OHX	1	4418	-	-	-	X
92	OHX	1	4423	-	-	-	X
92	OHX	1	4427	-	-	-	X
92	OHX	1	4429	-	-	-	X
92	OHX	1	4445	-	-	-	X
92	OHX	1	4449	-	-	-	X
92	OHX	1	4453	-	-	-	X
92	OHX	1	4455	-	-	-	X
92	OHX	1	4456	-	-	-	X
92	OHX	1	4460	-	-	-	X
92	OHX	1	4465	-	-	-	X
92	OHX	1	4483	-	-	-	X
92	OHX	1	4504	-	-	-	X
92	OHX	2	2227	-	-	-	X
92	OHX	2	2247	-	-	-	X
92	OHX	5	4324	-	-	-	X
92	OHX	5	4385	-	-	-	X
92	OHX	5	4391	-	-	-	X
92	OHX	5	4414	-	-	-	X
92	OHX	5	4425	-	-	-	X
92	OHX	5	4433	-	-	-	X
92	OHX	5	4437	-	-	-	X
92	OHX	5	4441	-	-	-	X
92	OHX	5	4461	-	-	-	X
92	OHX	5	4473	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
92	OHX	5	4479	-	-	-	X
92	OHX	5	4488	-	-	-	X
92	OHX	5	4490	-	-	-	X
92	OHX	5	4495	-	-	-	X
92	OHX	5	4498	-	-	-	X
92	OHX	5	4499	-	-	-	X
92	OHX	5	4505	-	-	-	X
92	OHX	5	4513	-	-	-	X
92	OHX	5	4520	-	-	-	X
92	OHX	5	4528	-	-	-	X
92	OHX	5	4533	-	-	-	X
92	OHX	5	4536	-	-	-	X
92	OHX	5	4537	-	-	-	X
92	OHX	5	4541	-	-	-	X
92	OHX	5	4543	-	-	-	X
92	OHX	5	4544	-	-	-	X
92	OHX	5	4548	-	-	-	X
92	OHX	5	4562	-	-	-	X
92	OHX	5	4565	-	-	-	X
92	OHX	6	2301	-	-	-	X
92	OHX	6	2303	-	-	-	X
92	OHX	6	2307	-	-	-	X
92	OHX	6	2323	-	-	-	X
92	OHX	7	239	-	-	-	X
92	OHX	8	237	-	-	-	X
92	OHX	A	102	-	-	-	X
92	OHX	M0	306	-	-	-	X
92	OHX	M0	307	-	-	-	X
92	OHX	l4	405	-	-	-	X
92	OHX	m0	303	-	-	-	X
92	OHX	o9	102	-	-	-	X

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 414290 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	1	0
			37970	16975	6720	12493	1782			
1	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

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

- Molecule 4 is a protein called 40S ribosomal protein S2.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 12 is a protein called 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S Ribosomal Protein S12.

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

- Molecule 15 is a protein called 40S ribosomal protein S13.

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

- Molecule 16 is a protein called 40S Ribosomal Protein S14.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	654	221	229			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	134	LEU	ASP	conflict	UNP P39015

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	0	0	0
			796	516	131	149			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	n2	98	Total	C	N	O	0	0	0
			778	505	127	146			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein S10-A, 40S ribosomal protein S10-A, 40S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

- Molecule 81 is a protein called 40S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	c2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			

- Molecule 82 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 83 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 84 is a protein called Suppressor protein STM1,Suppressor protein STM1,Ribosome-bound protein Stm1.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
sM	59	ALA	GLY	conflict	UNP P39015

- Molecule 85 is a protein called 60S ribosomal protein L8-A,60S ribosomal protein L8-A,60S Ribosomal Protein L8.

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

- Molecule 86 is a protein called 60S Ribosomal Protein L12.

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

- Molecule 87 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
87	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 88 is a protein called 60S acidic ribosomal protein P0,60S acidic ribosomal protein P0,60S Ribosomal Protein P0.

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

- Molecule 89 is a protein called 60S Ribosomal Protein P1/2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
89	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			
89	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 90 is a RNA chain called aminoacyl-tRNA fragment ACCPmn.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
90	A	3	Total	C	N	O	P	0	0	0
			77	40	13	21	3			
90	a	3	Total	C	N	O	P	0	0	0
			77	40	13	21	3			

- Molecule 91 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	2	169	Total	Mg	0	0
			169	169		
91	S1	1	Total	Mg	0	0
			1	1		
91	S2	2	Total	Mg	0	0
			2	2		
91	S4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	S6	1	Total 1	Mg 1	0	0
91	S8	2	Total 2	Mg 2	0	0
91	C1	2	Total 2	Mg 2	0	0
91	C5	1	Total 1	Mg 1	0	0
91	C8	1	Total 1	Mg 1	0	0
91	D0	1	Total 1	Mg 1	0	0
91	D3	1	Total 1	Mg 1	0	0
91	D6	1	Total 1	Mg 1	0	0
91	D9	2	Total 2	Mg 2	0	0
91	E1	1	Total 1	Mg 1	0	0
91	1	700	Total 700	Mg 700	1	0
91	3	18	Total 18	Mg 18	0	0
91	4	32	Total 32	Mg 32	0	0
91	L2	4	Total 4	Mg 4	0	0
91	L3	6	Total 6	Mg 6	0	0
91	L4	7	Total 7	Mg 7	0	0
91	L6	1	Total 1	Mg 1	0	0
91	L7	1	Total 1	Mg 1	0	0
91	L8	1	Total 1	Mg 1	0	0
91	M0	4	Total 4	Mg 4	0	0
91	M1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	M3	4	Total 4	Mg 4	0	0
91	M4	1	Total 1	Mg 1	0	0
91	M5	8	Total 8	Mg 8	0	0
91	M6	4	Total 4	Mg 4	0	0
91	M7	8	Total 8	Mg 8	0	0
91	M8	3	Total 3	Mg 3	0	0
91	M9	3	Total 3	Mg 3	0	0
91	N0	2	Total 2	Mg 2	0	0
91	N1	1	Total 1	Mg 1	0	0
91	N3	4	Total 4	Mg 4	0	0
91	N6	1	Total 1	Mg 1	0	0
91	N8	7	Total 7	Mg 7	0	0
91	N9	1	Total 1	Mg 1	0	0
91	O1	1	Total 1	Mg 1	0	0
91	O2	2	Total 2	Mg 2	0	0
91	O3	3	Total 3	Mg 3	0	0
91	O4	1	Total 1	Mg 1	0	0
91	O7	5	Total 5	Mg 5	0	0
91	O9	1	Total 1	Mg 1	0	0
91	Q0	2	Total 2	Mg 2	0	0
91	Q2	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	6	242	Total 242	Mg 242	0	0
91	s1	1	Total 1	Mg 1	0	0
91	s4	1	Total 1	Mg 1	0	0
91	s8	4	Total 4	Mg 4	0	0
91	c6	3	Total 3	Mg 3	0	0
91	c8	3	Total 3	Mg 3	0	0
91	c9	1	Total 1	Mg 1	0	0
91	d2	1	Total 1	Mg 1	0	0
91	d3	1	Total 1	Mg 1	0	0
91	d5	1	Total 1	Mg 1	0	0
91	d6	1	Total 1	Mg 1	0	0
91	d9	2	Total 2	Mg 2	0	0
91	sM	1	Total 1	Mg 1	0	0
91	5	758	Total 758	Mg 758	0	0
91	7	27	Total 27	Mg 27	0	0
91	8	21	Total 21	Mg 21	0	0
91	l2	5	Total 5	Mg 5	0	0
91	l3	11	Total 11	Mg 11	0	0
91	l4	3	Total 3	Mg 3	0	0
91	l5	7	Total 7	Mg 7	0	0
91	l7	4	Total 4	Mg 4	0	0

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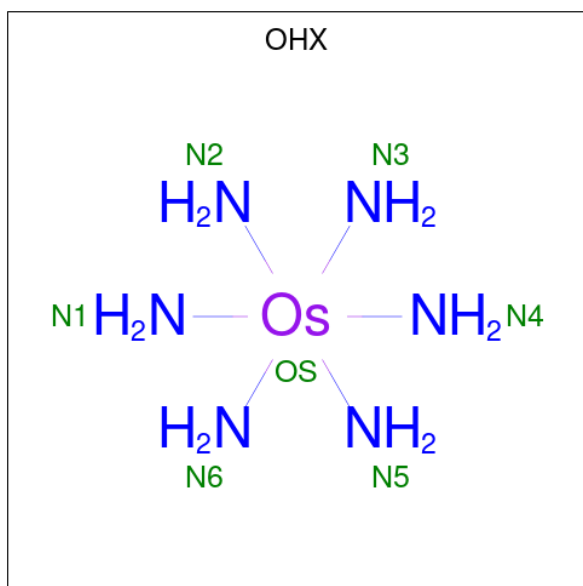
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	l8	1	Total 1	Mg 1	0	0
91	l9	3	Total 3	Mg 3	0	0
91	m0	1	Total 1	Mg 1	0	0
91	m1	2	Total 2	Mg 2	0	0
91	m3	2	Total 2	Mg 2	0	0
91	m4	1	Total 1	Mg 1	0	0
91	m5	2	Total 2	Mg 2	0	0
91	m6	6	Total 6	Mg 6	0	0
91	m7	7	Total 7	Mg 7	0	0
91	m8	2	Total 2	Mg 2	0	0
91	m9	1	Total 1	Mg 1	0	0
91	n0	5	Total 5	Mg 5	0	0
91	n1	3	Total 3	Mg 3	0	0
91	n3	3	Total 3	Mg 3	0	0
91	n6	1	Total 1	Mg 1	0	0
91	n8	4	Total 4	Mg 4	0	0
91	n9	2	Total 2	Mg 2	0	0
91	o2	3	Total 3	Mg 3	0	0
91	o3	5	Total 5	Mg 5	0	0
91	o4	3	Total 3	Mg 3	0	0
91	o6	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	o7	3	Total	Mg	0	0
			3	3		
91	o9	1	Total	Mg	0	0
			1	1		
91	q0	1	Total	Mg	0	0
			1	1		
91	q1	1	Total	Mg	0	0
			1	1		
91	q2	1	Total	Mg	0	0
			1	1		
91	q3	2	Total	Mg	0	0
			2	2		
91	p0	1	Total	Mg	0	0
			1	1		

- Molecule 92 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	2	1	Total	N	Os	0	0
			7	6	1		
92	S2	1	Total	N	Os	0	0
			7	6	1		
92	S6	1	Total	N	Os	0	0
			7	6	1		
92	S8	1	Total	N	Os	0	0
			7	6	1		
92	C3	1	Total	N	Os	0	0
			7	6	1		
92	C5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	C8	1	Total	N	Os	0	0
			7	6	1		
92	C8	1	Total	N	Os	0	0
			7	6	1		
92	D9	1	Total	N	Os	0	0
			7	6	1		
92	SR	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
			7	6	1		
92	1	1	Total	N	Os	0	0
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92	1	1	Total	N	Os	0	0
			7	6	1		
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92	1	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
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			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	3	1	Total	N	Os	0	0
			7	6	1		
92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
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92	3	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	4	1	Total	N	Os	0	0
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92	4	1	Total	N	Os	0	0
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92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
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			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		
92	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	L2	1	Total	N	Os	0	0
			7	6	1		
92	L3	1	Total	N	Os	0	0
			7	6	1		
92	L3	1	Total	N	Os	0	0
			7	6	1		
92	L3	1	Total	N	Os	0	0
			7	6	1		
92	L4	1	Total	N	Os	0	0
			7	6	1		
92	L5	1	Total	N	Os	0	0
			7	6	1		
92	M0	1	Total	N	Os	0	0
			7	6	1		
92	M0	1	Total	N	Os	0	0
			7	6	1		
92	M0	1	Total	N	Os	0	0
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92	M0	1	Total	N	Os	0	0
			7	6	1		
92	M5	1	Total	N	Os	0	0
			7	6	1		
92	M5	1	Total	N	Os	0	0
			7	6	1		
92	M7	1	Total	N	Os	0	0
			7	6	1		
92	M9	1	Total	N	Os	0	0
			7	6	1		
92	N1	1	Total	N	Os	0	0
			7	6	1		
92	N8	1	Total	N	Os	0	0
			7	6	1		
92	N9	1	Total	N	Os	0	0
			7	6	1		
92	O1	1	Total	N	Os	0	0
			7	6	1		
92	O3	1	Total	N	Os	0	0
			7	6	1		
92	O7	1	Total	N	Os	0	0
			7	6	1		
92	O7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	Q2	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
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92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		
92	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	6	1	Total 7	N 6	Os 1	0	0
92	s1	1	Total 7	N 6	Os 1	0	0
92	s4	1	Total 7	N 6	Os 1	0	0
92	s8	1	Total 7	N 6	Os 1	0	0
92	c1	1	Total 7	N 6	Os 1	0	0
92	c3	1	Total 7	N 6	Os 1	0	0
92	c5	1	Total 7	N 6	Os 1	0	0
92	c5	1	Total 7	N 6	Os 1	0	0
92	c8	1	Total 7	N 6	Os 1	0	0
92	d4	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	sR	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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92	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	5	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	7	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		
92	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	8	1	Total 7	N 6	Os 1	0	0
92	12	1	Total 7	N 6	Os 1	0	0
92	13	1	Total 7	N 6	Os 1	0	0
92	13	1	Total 7	N 6	Os 1	0	0
92	14	1	Total 7	N 6	Os 1	0	0
92	14	1	Total 7	N 6	Os 1	0	0
92	15	1	Total 7	N 6	Os 1	0	0
92	15	1	Total 7	N 6	Os 1	0	0
92	15	1	Total 7	N 6	Os 1	0	0
92	19	1	Total 7	N 6	Os 1	0	0
92	m0	1	Total 7	N 6	Os 1	0	0
92	m0	1	Total 7	N 6	Os 1	0	0
92	m0	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	m0	1	Total	N	Os	0	0
			7	6	1		
92	m1	1	Total	N	Os	0	0
			7	6	1		
92	m4	1	Total	N	Os	0	0
			7	6	1		
92	m5	1	Total	N	Os	0	0
			7	6	1		
92	m5	1	Total	N	Os	0	0
			7	6	1		
92	m7	1	Total	N	Os	0	0
			7	6	1		
92	m9	1	Total	N	Os	0	0
			7	6	1		
92	n1	1	Total	N	Os	0	0
			7	6	1		
92	n3	1	Total	N	Os	0	0
			7	6	1		
92	n9	1	Total	N	Os	0	0
			7	6	1		
92	o2	1	Total	N	Os	0	0
			7	6	1		
92	o3	1	Total	N	Os	0	0
			7	6	1		
92	o7	1	Total	N	Os	0	0
			7	6	1		
92	o9	1	Total	N	Os	0	0
			7	6	1		
92	q2	1	Total	N	Os	0	0
			7	6	1		
92	A	1	Total	N	Os	0	0
			7	6	1		
92	A	1	Total	N	Os	0	0
			7	6	1		
92	a	1	Total	N	Os	0	0
			7	6	1		

- Molecule 93 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	D6	1	Total	Zn	0	0
			1	1		

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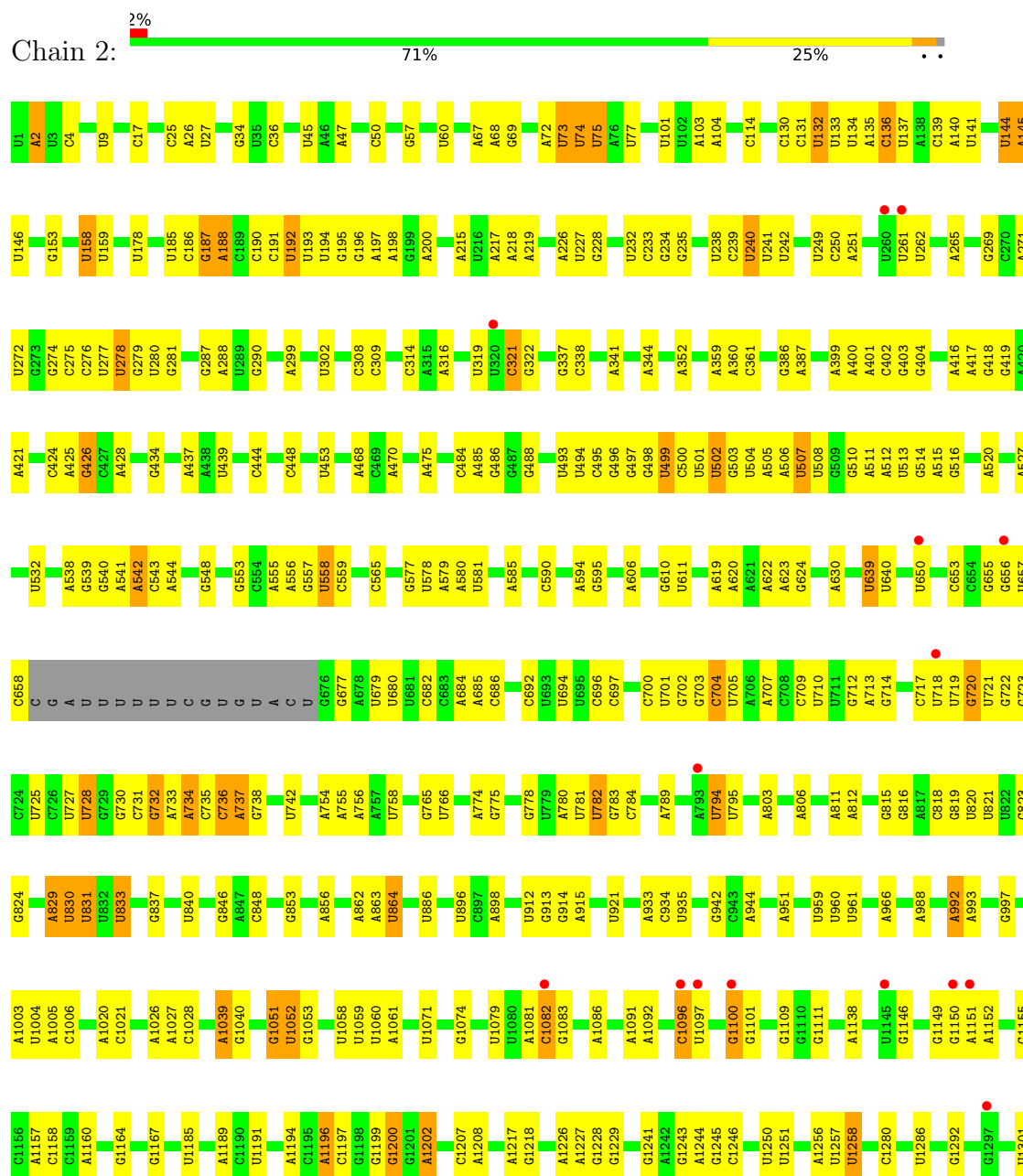
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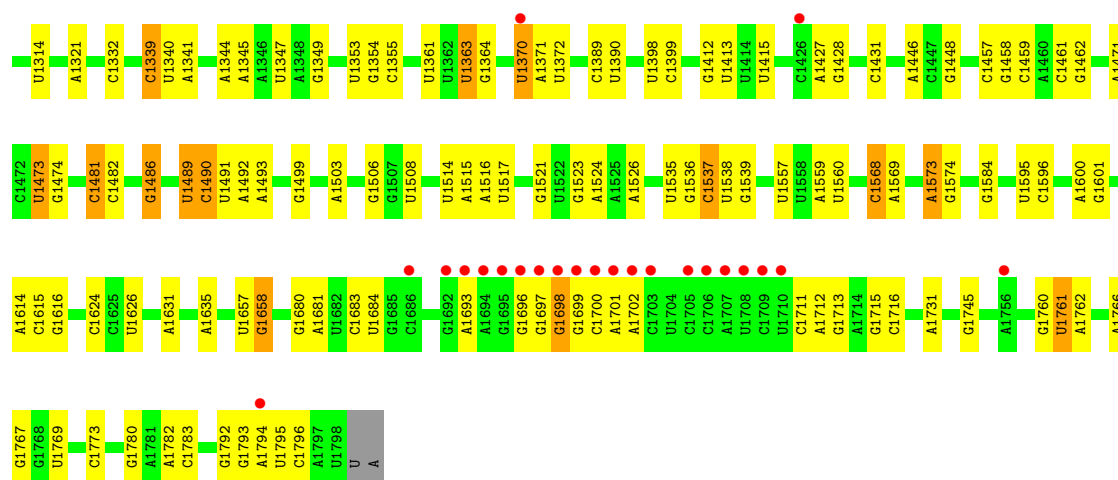
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			1	1		
93	D9	1	Total	Zn	0	0
			1	1		
93	E1	1	Total	Zn	0	0
			1	1		
93	O7	1	Total	Zn	0	0
			1	1		
93	Q0	1	Total	Zn	0	0
			1	1		
93	Q2	1	Total	Zn	0	0
			1	1		
93	Q3	1	Total	Zn	0	0
			1	1		
93	d6	1	Total	Zn	0	0
			1	1		
93	d7	1	Total	Zn	0	0
			1	1		
93	d9	1	Total	Zn	0	0
			1	1		
93	e1	1	Total	Zn	0	0
			1	1		
93	o7	1	Total	Zn	0	0
			1	1		
93	q0	1	Total	Zn	0	0
			1	1		
93	q2	1	Total	Zn	0	0
			1	1		
93	q3	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

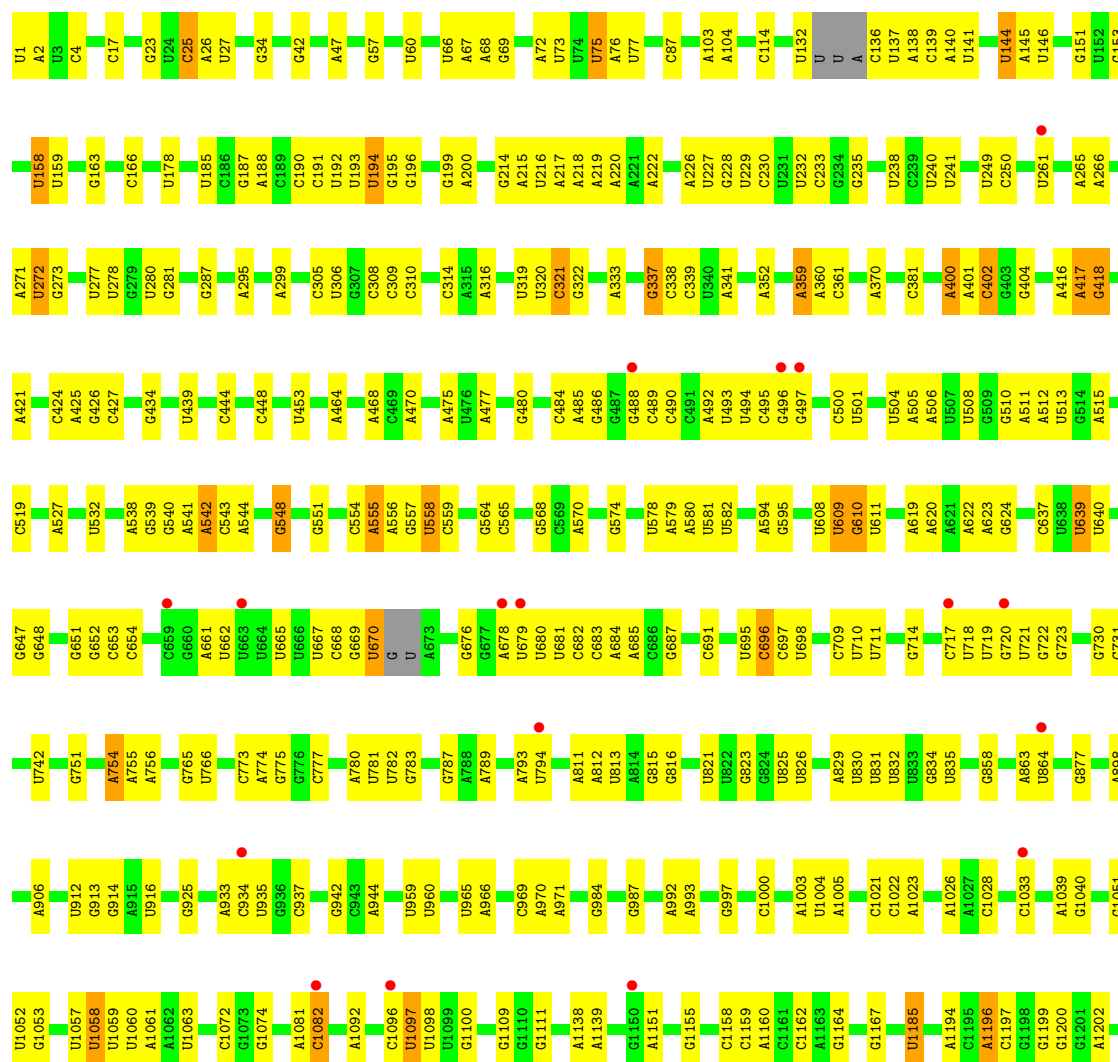
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

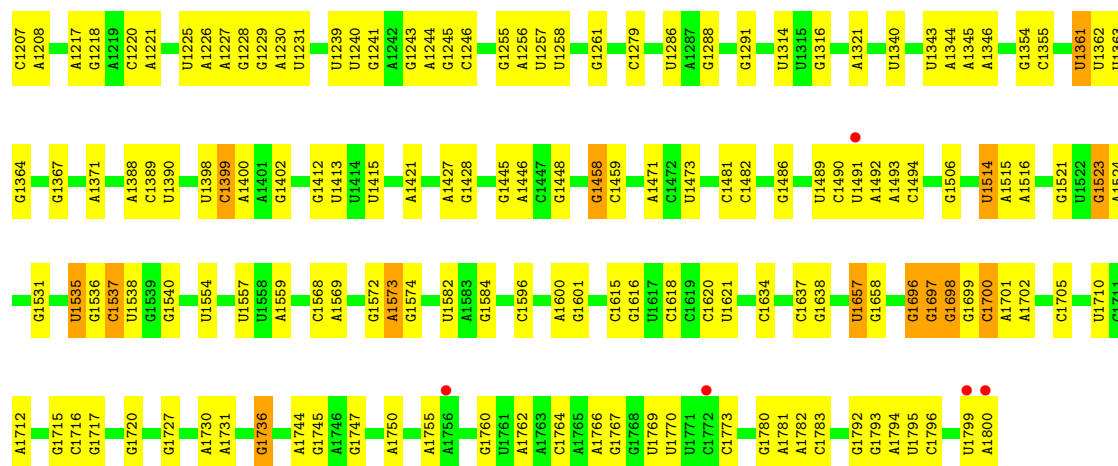
• Molecule 1: 18S rRNA



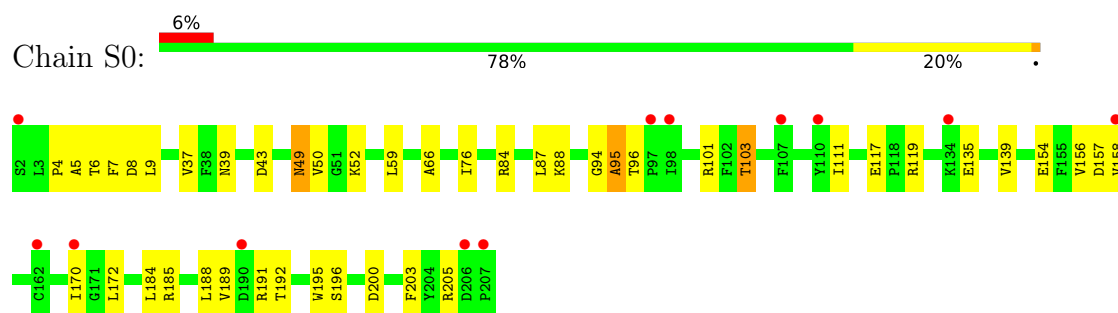


• Molecule 1: 18S rRNA

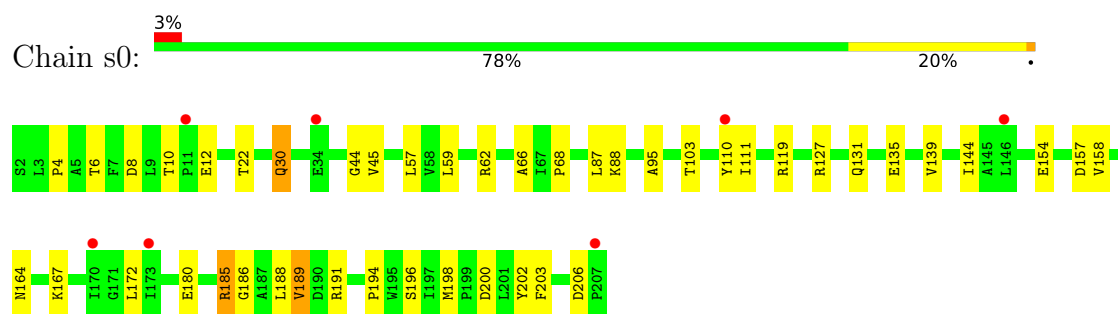




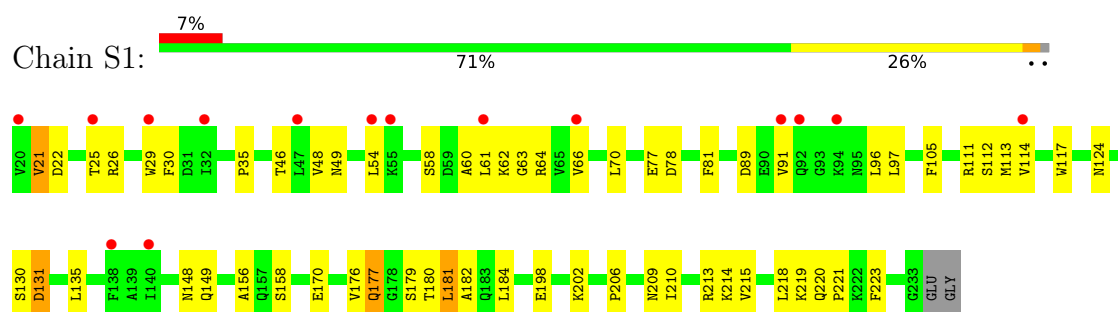
• Molecule 2: 40S ribosomal protein S0-A



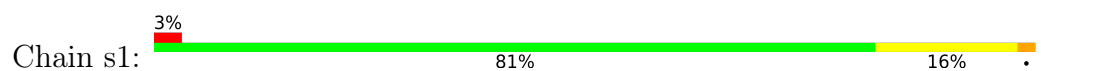
• Molecule 2: 40S ribosomal protein S0-A

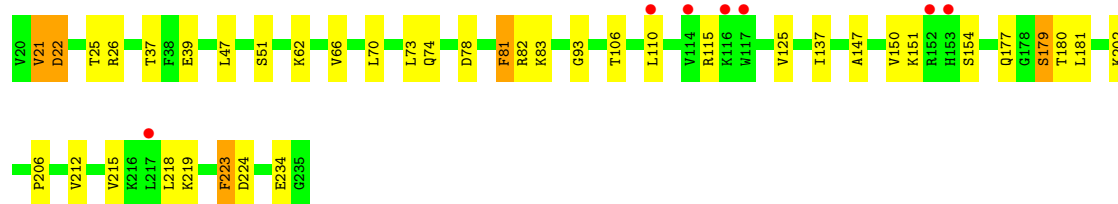


• Molecule 3: 40S ribosomal protein S1-A

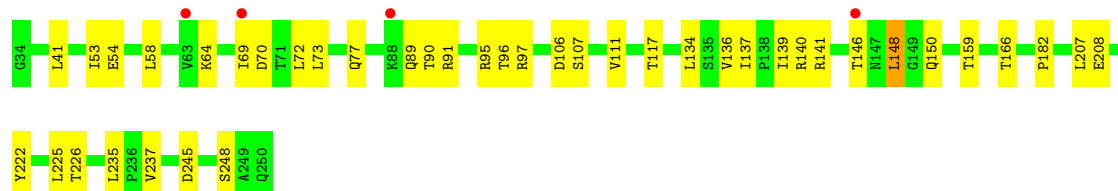
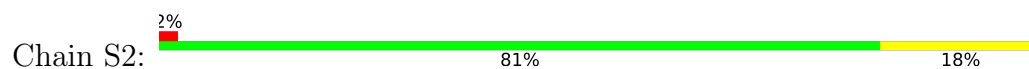


• Molecule 3: 40S ribosomal protein S1-A

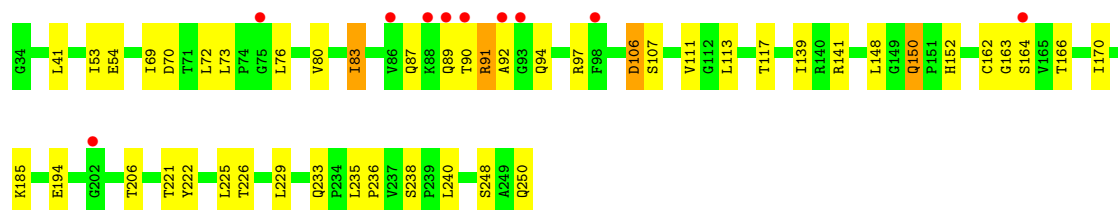
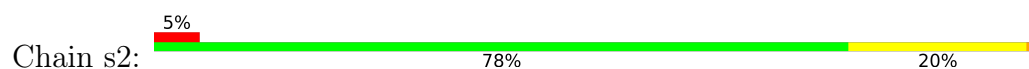




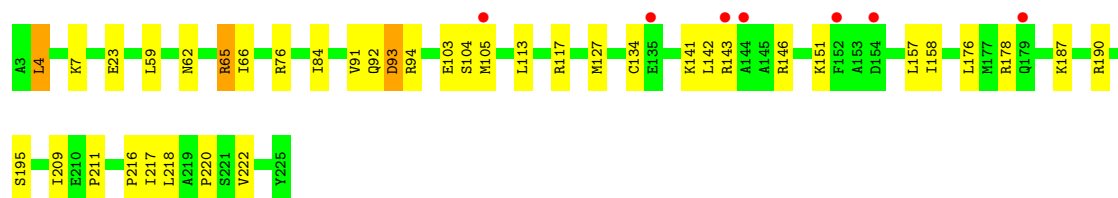
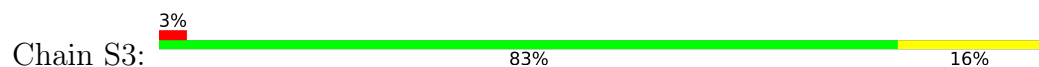
• Molecule 4: 40S ribosomal protein S2



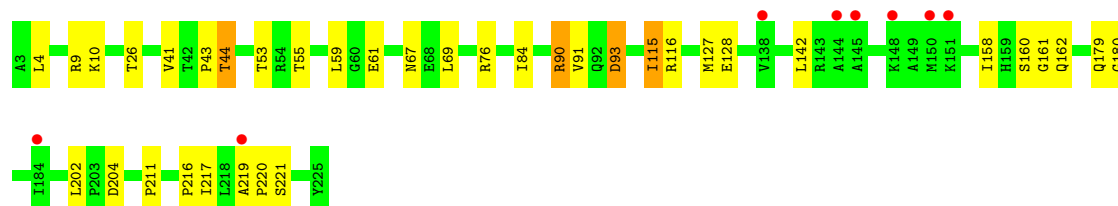
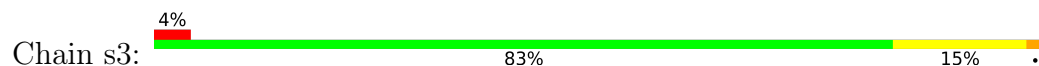
• Molecule 4: 40S ribosomal protein S2



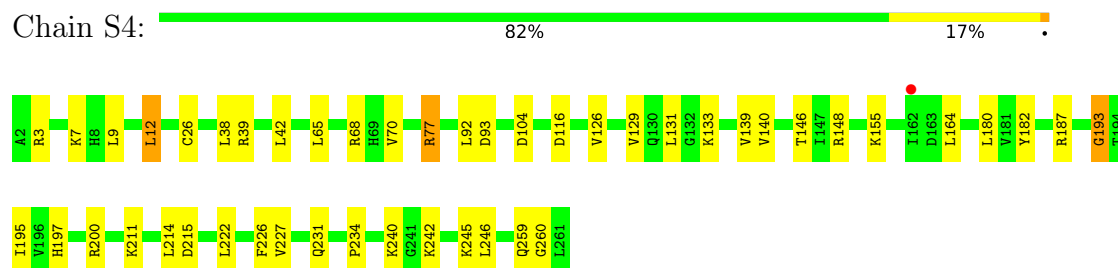
• Molecule 5: 40S ribosomal protein S3



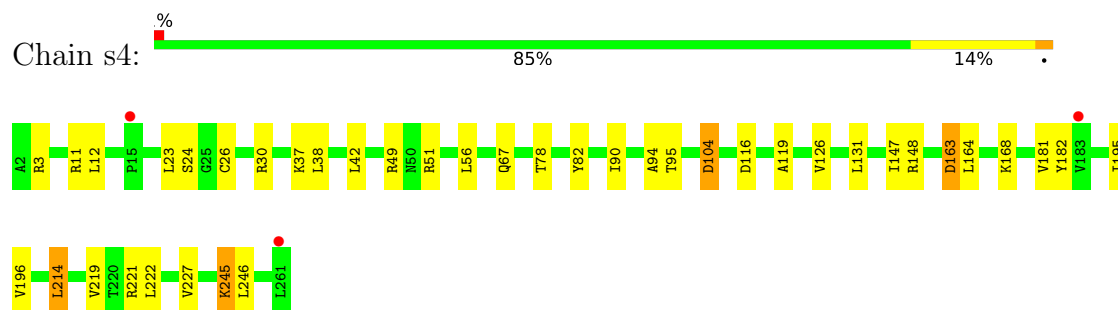
• Molecule 5: 40S ribosomal protein S3



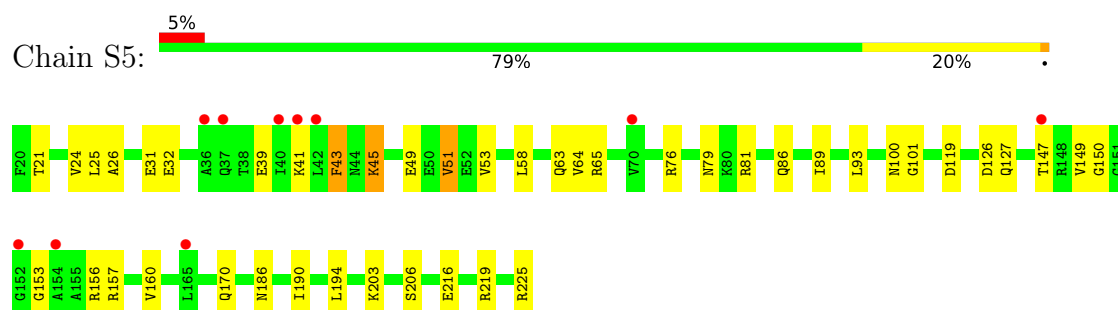
- Molecule 6: 40S ribosomal protein S4-A



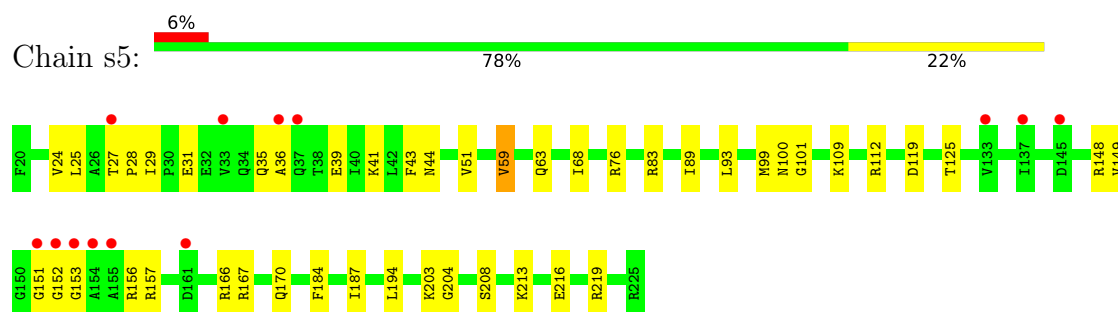
- Molecule 6: 40S ribosomal protein S4-A



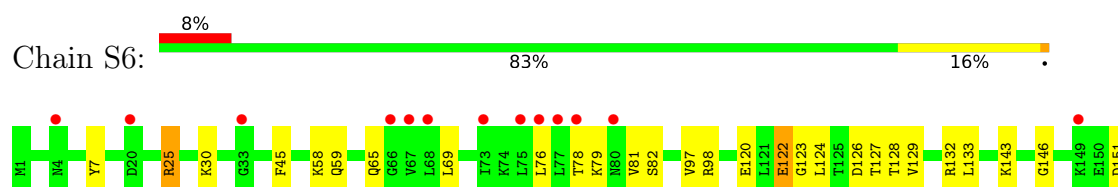
- Molecule 7: 40S ribosomal protein S5

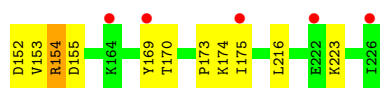


- Molecule 7: 40S ribosomal protein S5

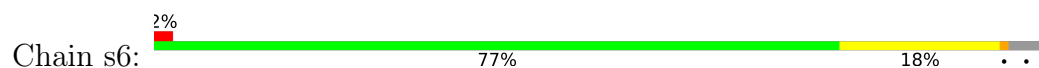


- Molecule 8: 40S ribosomal protein S6-A

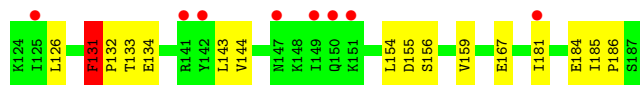
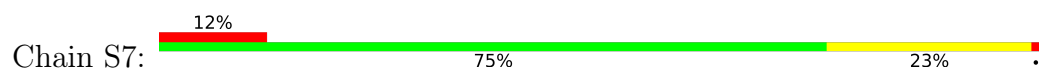




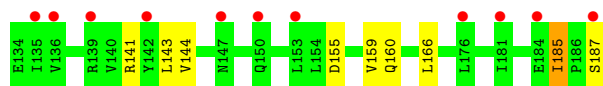
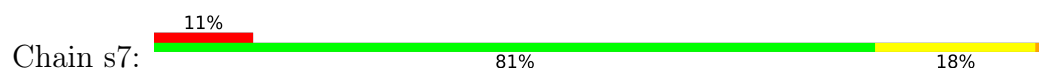
- Molecule 8: 40S ribosomal protein S6-A



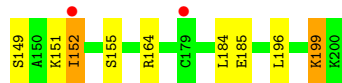
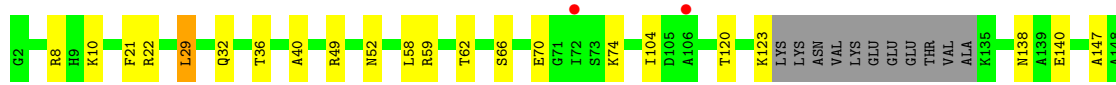
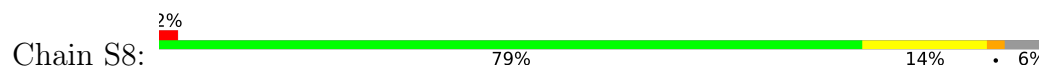
- Molecule 9: 40S ribosomal protein S7-A



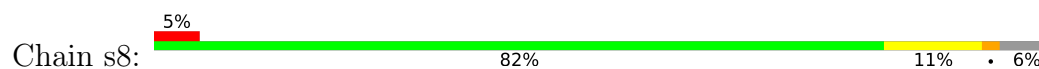
- Molecule 9: 40S ribosomal protein S7-A

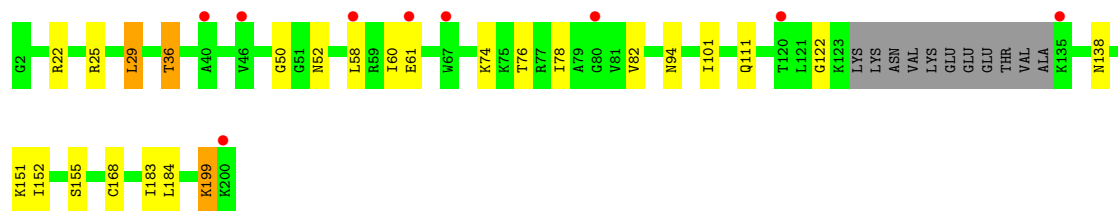


- Molecule 10: 40S ribosomal protein S8-A

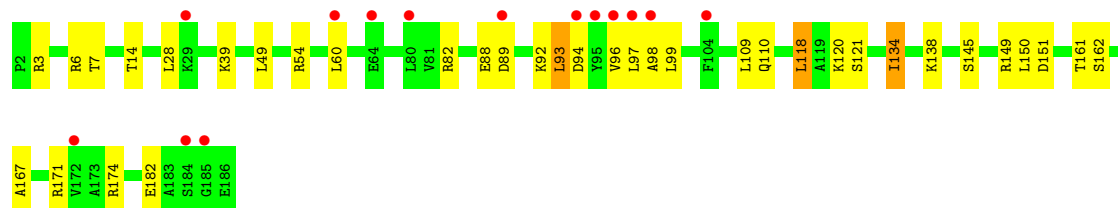
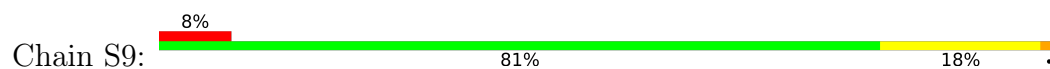


- Molecule 10: 40S ribosomal protein S8-A

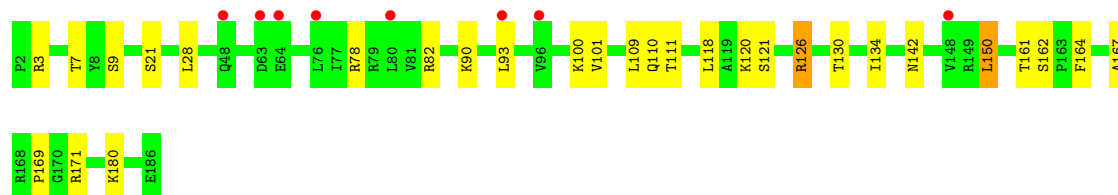
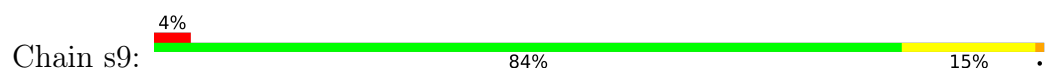




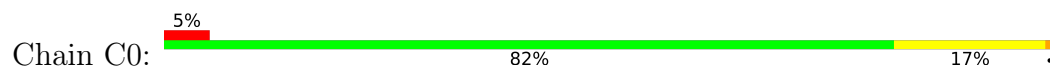
• Molecule 11: 40S ribosomal protein S9-A



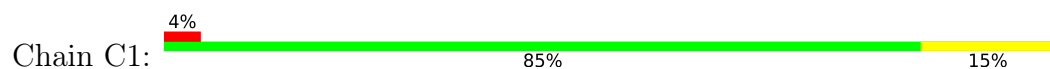
• Molecule 11: 40S ribosomal protein S9-A



• Molecule 12: 40S ribosomal protein S10-A, 40S ribosomal protein S10-A, 40S Ribosomal Protein S10-A

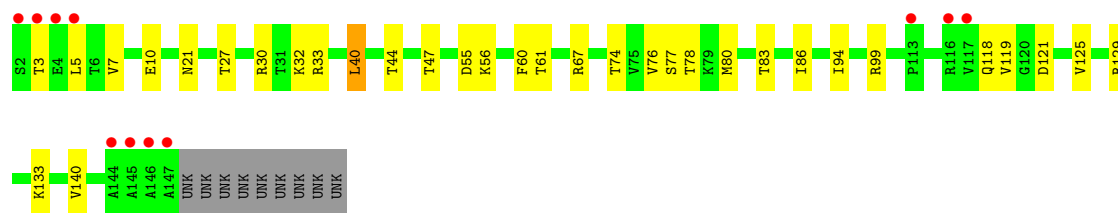


• Molecule 13: 40S ribosomal protein S11-A, 40S ribosomal protein S11-A, 40S Ribosomal Protein S11-A

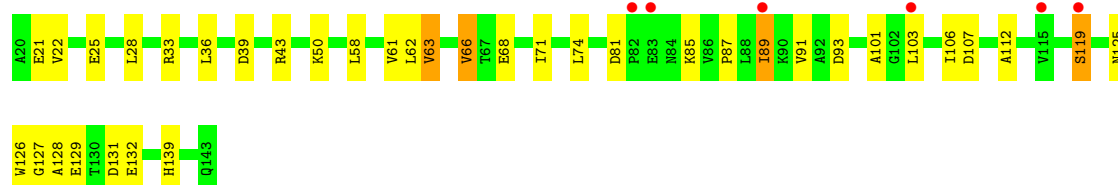


• Molecule 13: 40S ribosomal protein S11-A, 40S ribosomal protein S11-A, 40S Ribosomal Protein S11-A

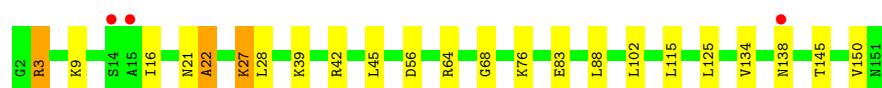
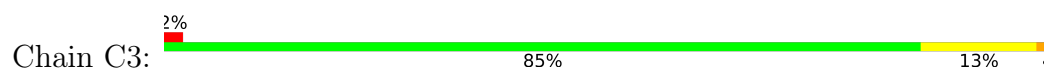




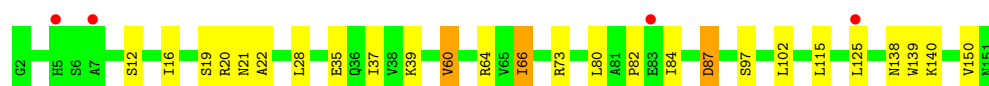
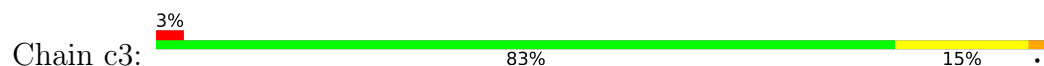
• Molecule 14: 40S Ribosomal Protein S12



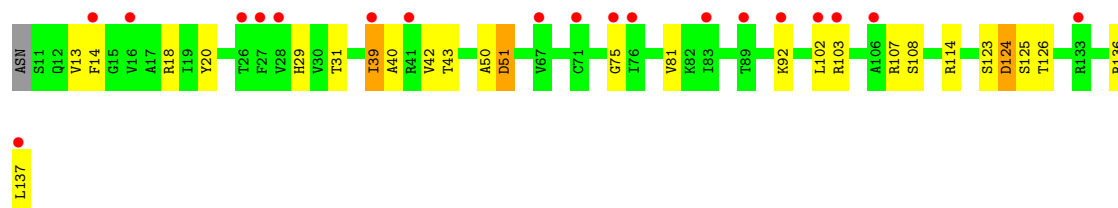
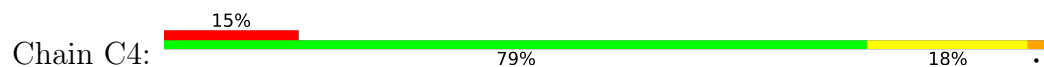
• Molecule 15: 40S ribosomal protein S13



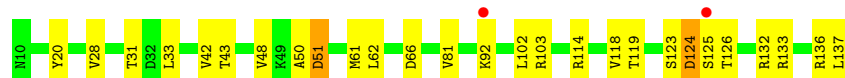
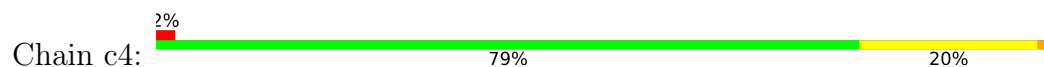
• Molecule 15: 40S ribosomal protein S13



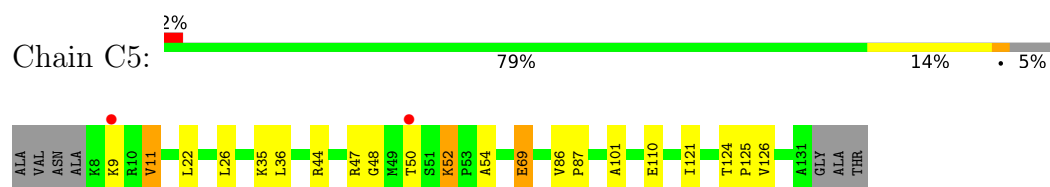
• Molecule 16: 40S Ribosomal Protein S14



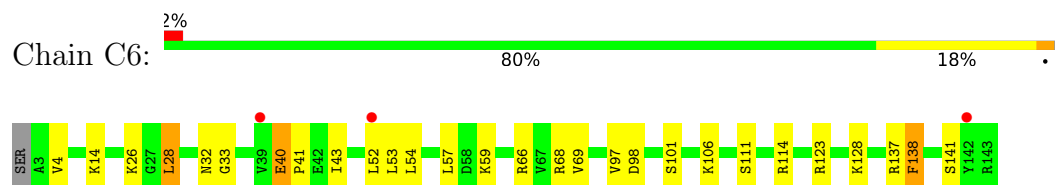
• Molecule 16: 40S Ribosomal Protein S14



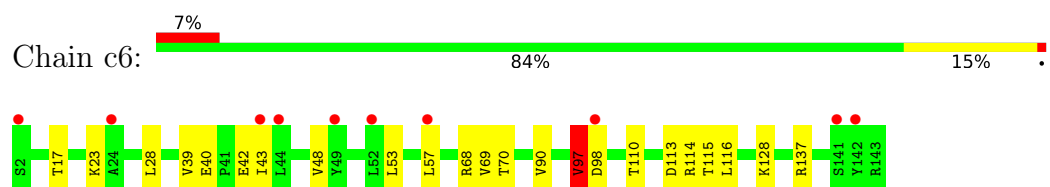
- Molecule 17: 40S ribosomal protein S15



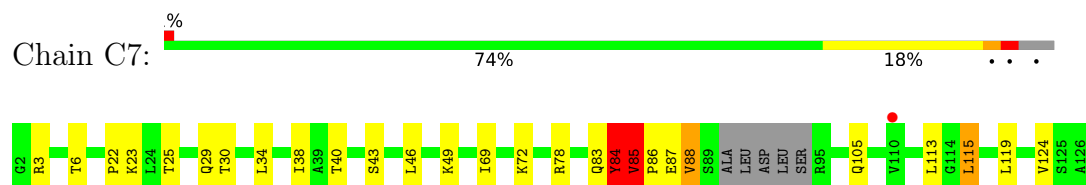
- Molecule 18: 40S ribosomal protein S16-A



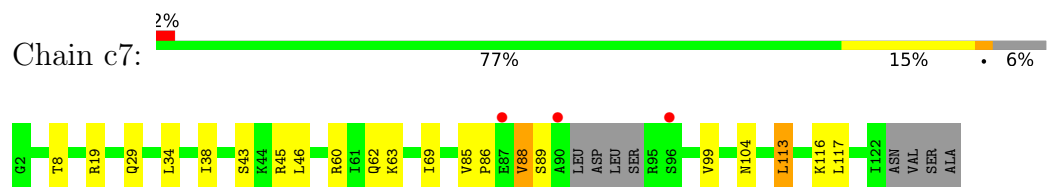
- Molecule 18: 40S ribosomal protein S16-A



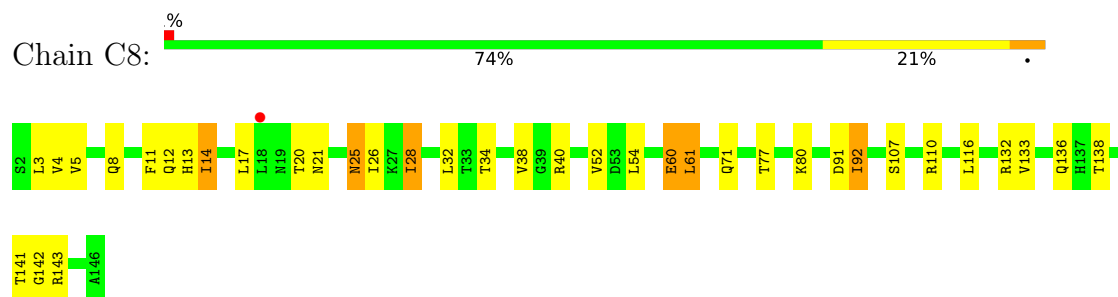
- Molecule 19: 40S ribosomal protein S17-A



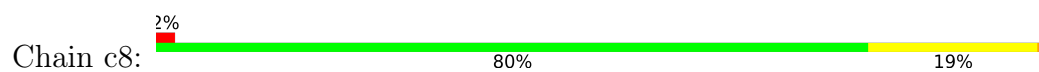
- Molecule 19: 40S ribosomal protein S17-A



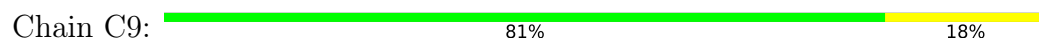
- Molecule 20: 40S ribosomal protein S18-A



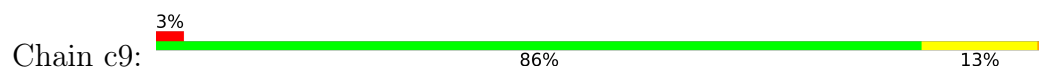
- Molecule 20: 40S ribosomal protein S18-A



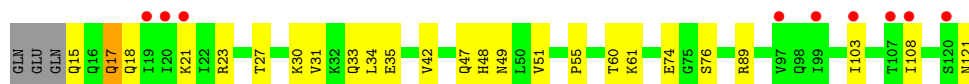
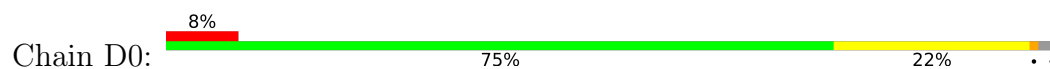
- Molecule 21: 40S ribosomal protein S19-A



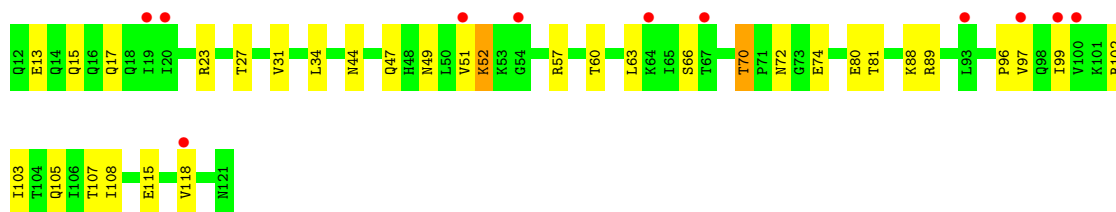
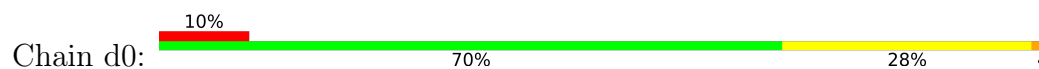
- Molecule 21: 40S ribosomal protein S19-A



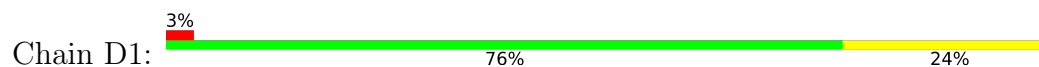
- Molecule 22: 40S ribosomal protein S20



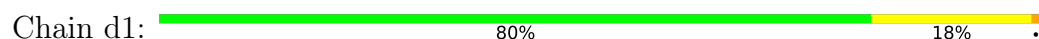
- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A

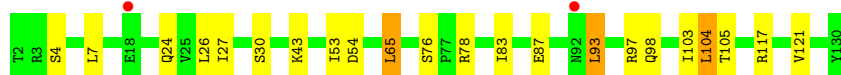
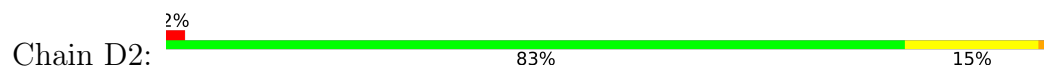


- Molecule 23: 40S ribosomal protein S21-A





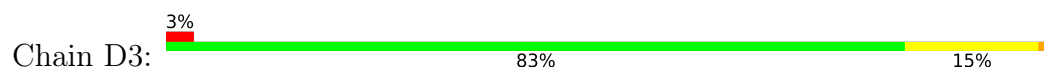
- Molecule 24: 40S ribosomal protein S22-A



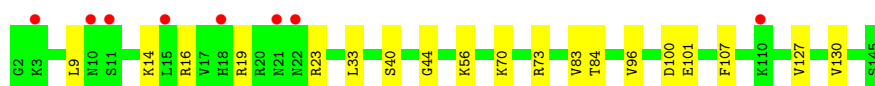
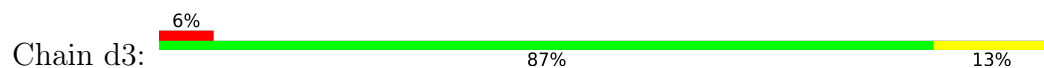
- Molecule 24: 40S ribosomal protein S22-A



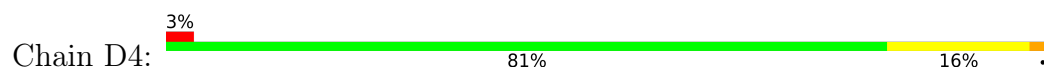
- Molecule 25: 40S ribosomal protein S23-A



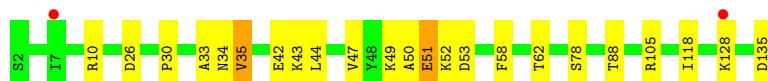
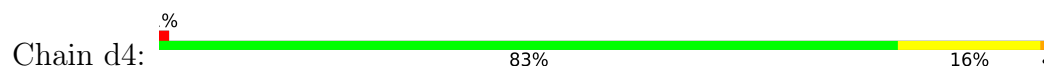
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A



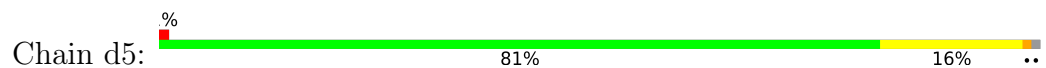
- Molecule 26: 40S ribosomal protein S24-A



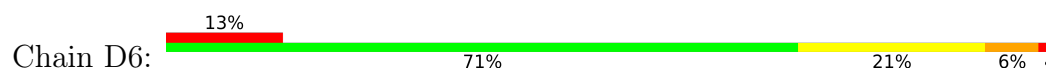
- Molecule 27: 40S ribosomal protein S25-A



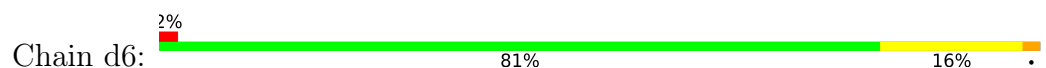
- Molecule 27: 40S ribosomal protein S25-A



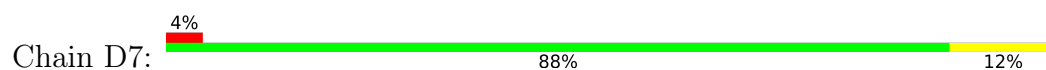
- Molecule 28: 40S ribosomal protein S26-B



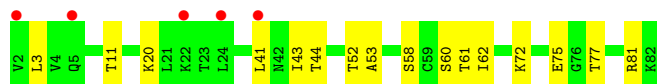
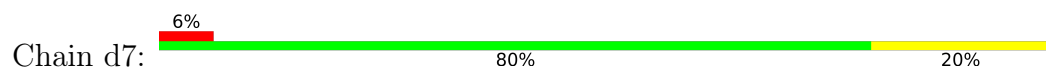
- Molecule 28: 40S ribosomal protein S26-B



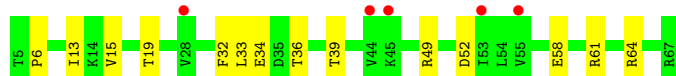
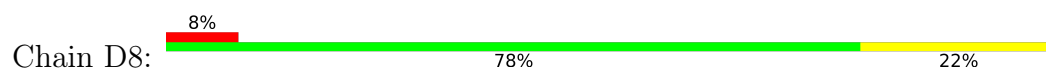
- Molecule 29: 40S ribosomal protein S27-A



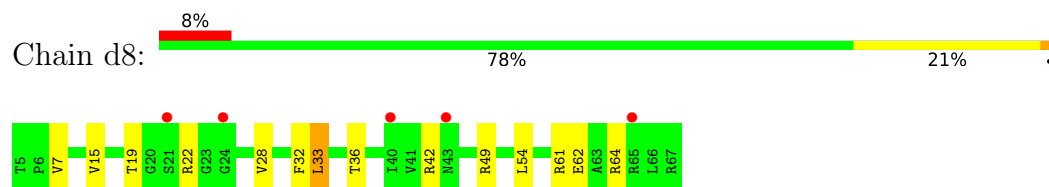
- Molecule 29: 40S ribosomal protein S27-A



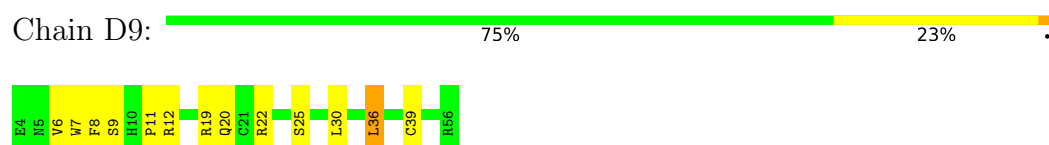
- Molecule 30: 40S ribosomal protein S28-A



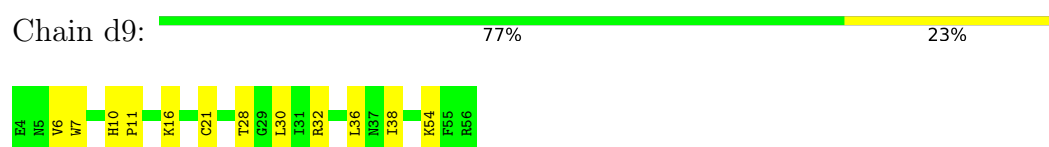
- Molecule 30: 40S ribosomal protein S28-A



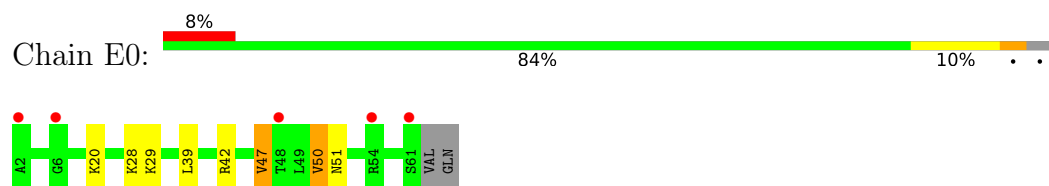
- Molecule 31: 40S ribosomal protein S29-A



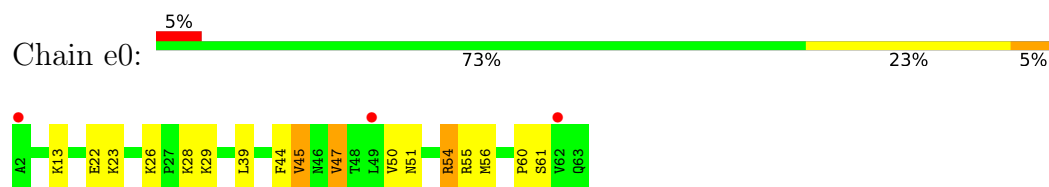
- Molecule 31: 40S ribosomal protein S29-A



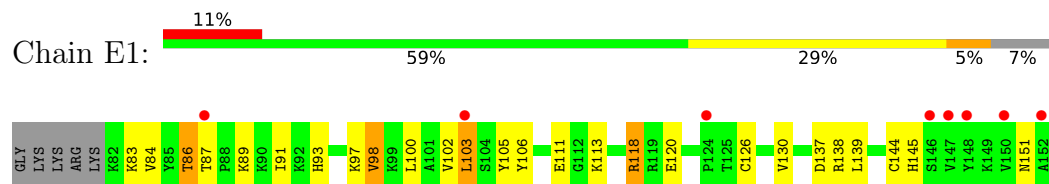
- Molecule 32: 40S ribosomal protein S30-A



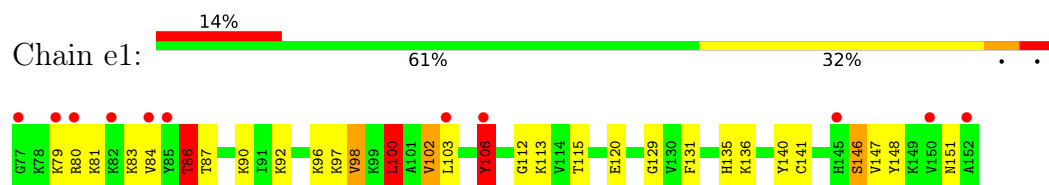
- Molecule 32: 40S ribosomal protein S30-A



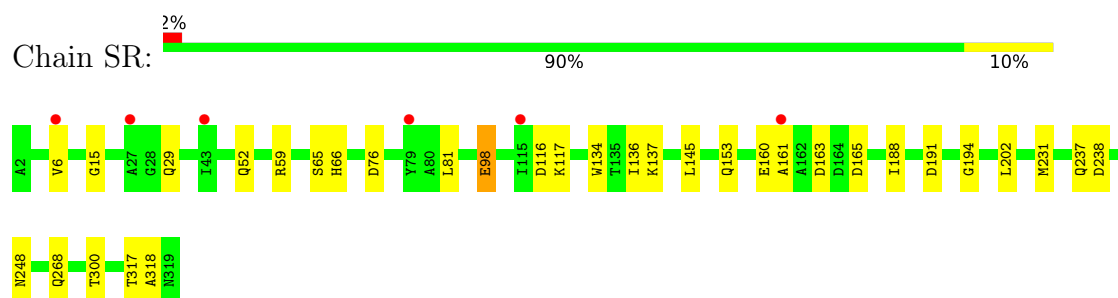
- Molecule 33: Ubiquitin-40S ribosomal protein S31



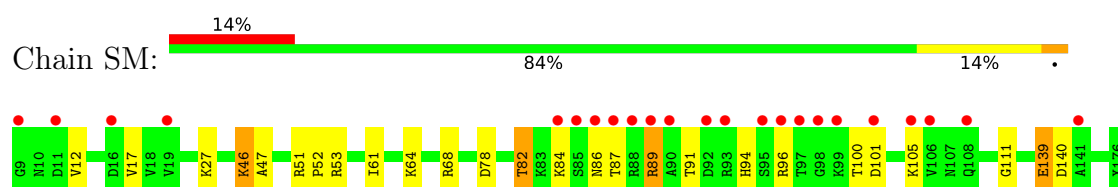
- Molecule 33: Ubiquitin-40S ribosomal protein S31



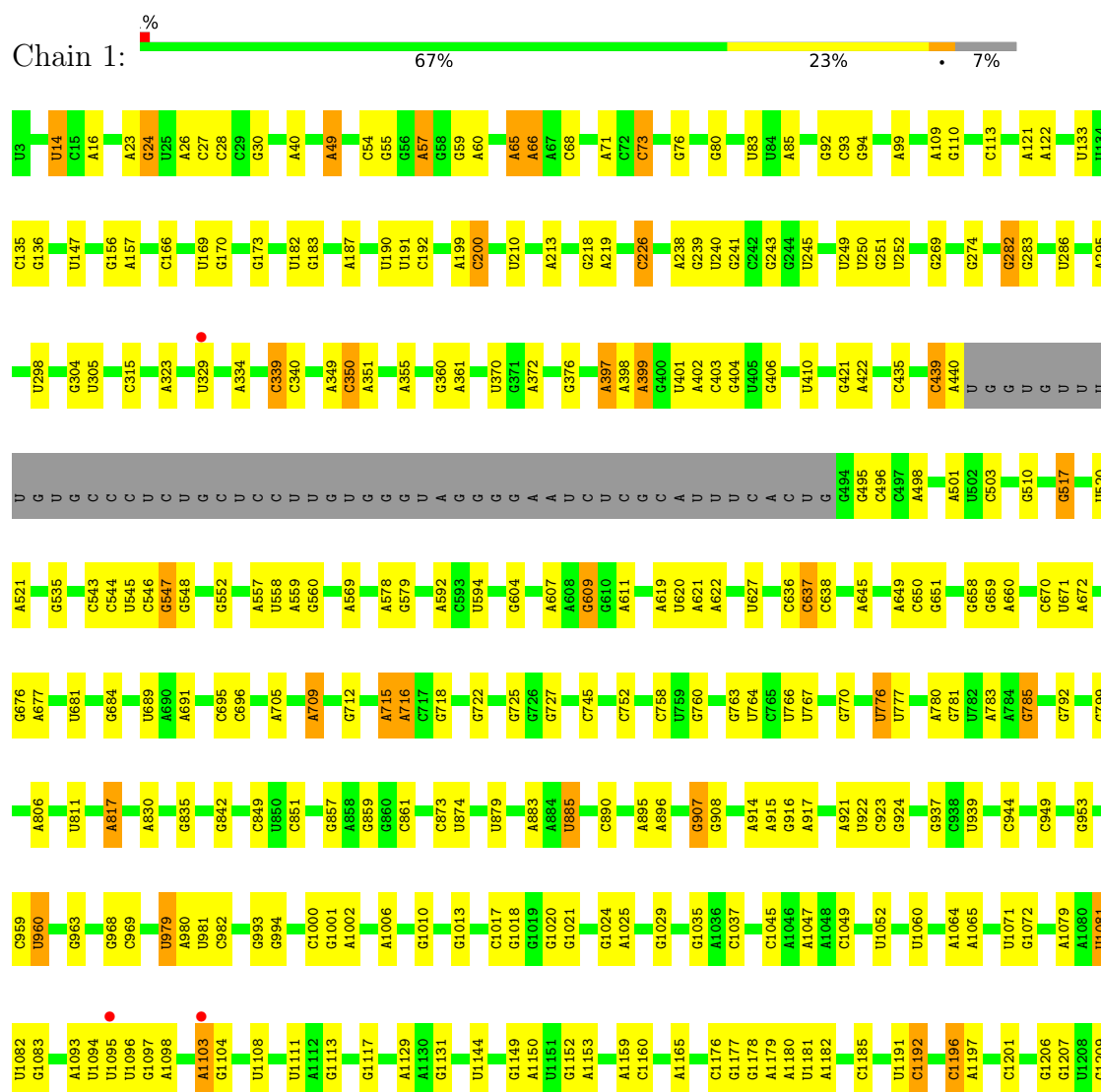
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



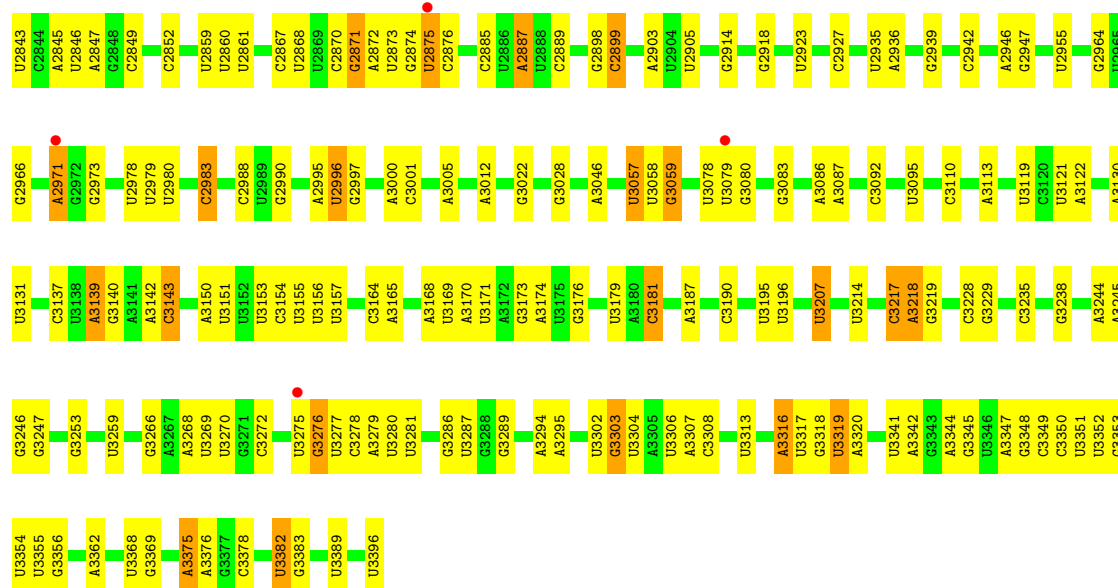
- Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1



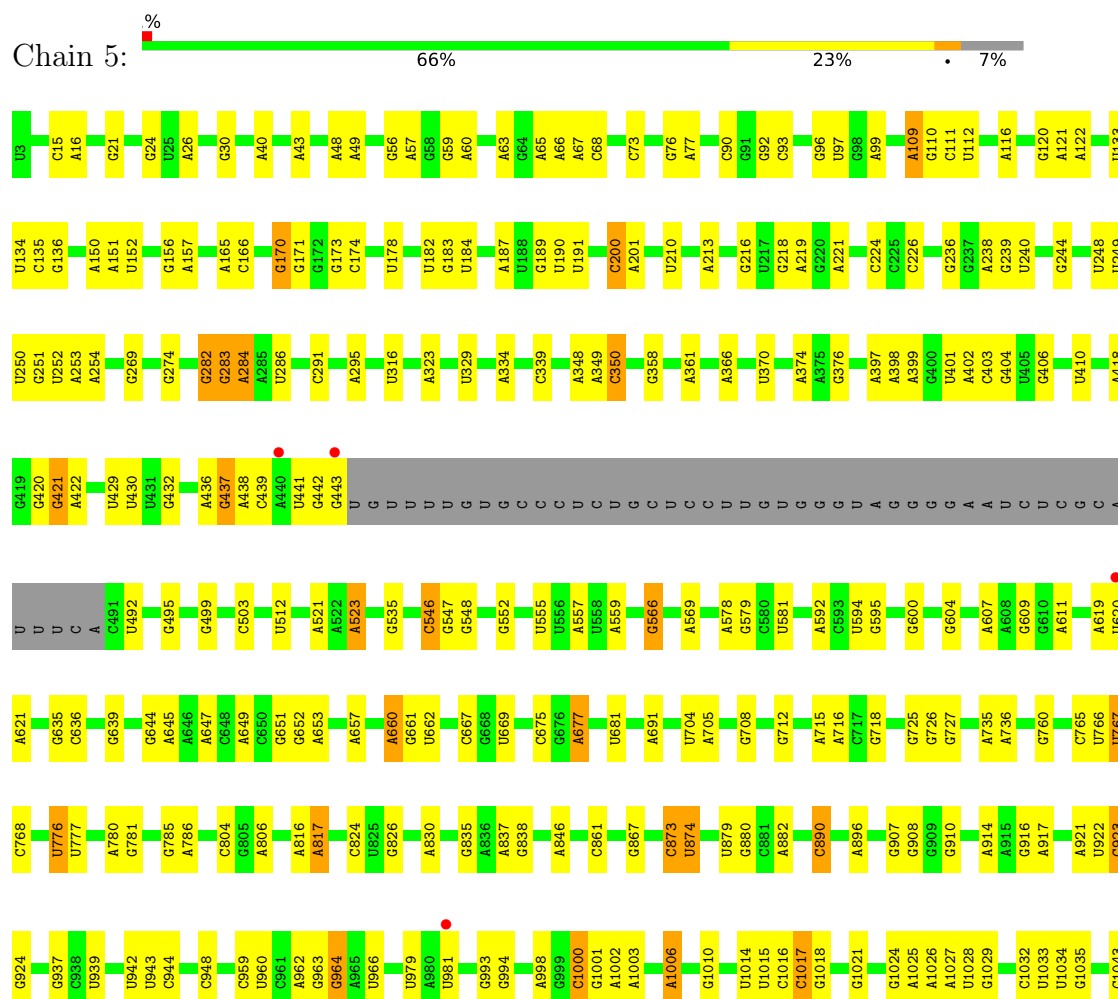
- Molecule 36: 25S rRNA



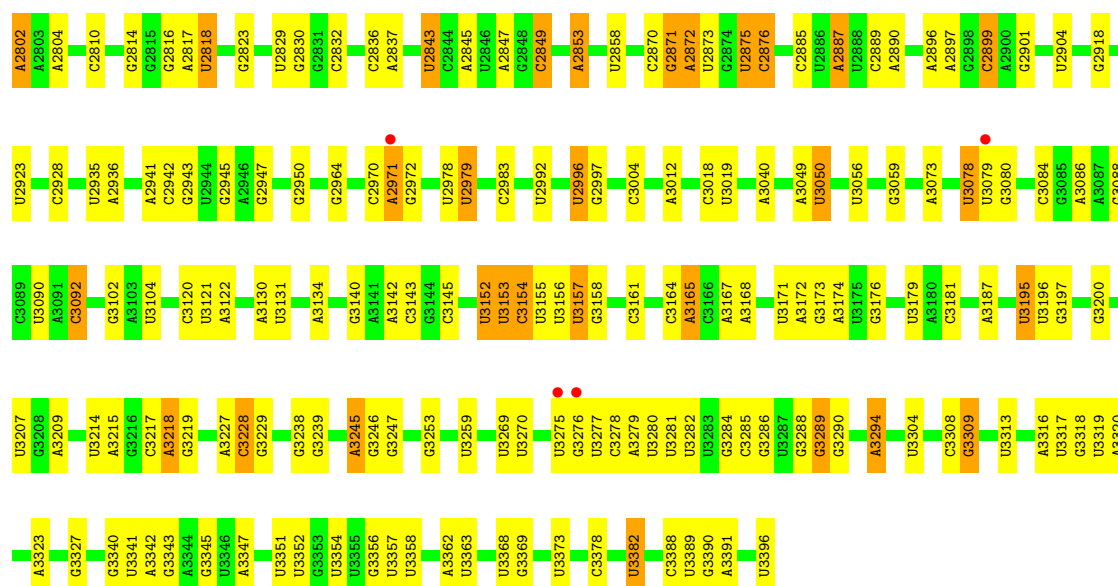
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G2728	A2593	A2594	G2418	U2298	A2144	G	C	G1780	A1587	G1434	G1307	G1213
C2737	C2594	C2594	A2419	U2298	A2144	U	U	C1781	A1588	A1435	A1308	
G2745	G2603	G2603	U2426	C2306	A2147	G	G	G1905	A1589	U1436	U1309	C1216
G2606	G2607	G2607	U2434	C2307	U2148	G	U	G1906	G1590	C1437		A1217
G2752	U2501	U2501	G2436	U2310	A2149	C	U		G1443		U1324	G1221
G2753	A2502	A2502	U2437	A2313	A2158	U	G	C1805	U1595	U1446	U1329	G1222
G2754	G2503	G2503	U2437	U2314	G2169	C	G	A1810	G1604	G1450	A1330	A1225
C2755	U2504	U2504	C2444	U2315	U2170	G	G	G1812	A1605	U1331	G1226	G1227
A2758	U2504	U2504	A2445	G2316	G2171	U	U	A1813	U1606	A1460	C1332	
U2759	C2507	C2507	U	U2334	U2172	U	U	U1950	U1607	C1333		C1232
G2760	U2513	U2513	A	U2335	A2173	A	G	C1951	U1620	A1468	G1345	G1233
G2761	U2514	U2514	G	U2336	U2174	G	U	G1952	A1814	A1481	U1347	G1236
A2762	A2515	A2515	G	C2337	U2175	C	C	G1953	G1817	A1482	U1348	G1237
U2766	G2522	G2522	G	G2355	G2187	C	U	U1955	U1818	G1483	U1349	
U2771	A2523	A2523	G	A2341	C2197	U	G	A	C1639	U1484	A1350	U1241
C2772	U2524	U2524	U	C2342	A2198	C	C	U1820	G1640	G1485	U1351	G1242
G2777	G2525	G2525	G	C2343	U2205	C	U	U1821	U1641	U1494	A1352	G1243
G2778	C2526	C2526	A	G2355	G2206	C	A	C1822	A1642	U1495	U1353	A1244
A2779	U2537	U2537	U	U2361	U2207	U	G	A1835	G1644	C1497	G1354	A1245
C2788	U2538	U2538	G	A2361	A2208	G	G	G1838	U1645	C1502	A1355	G1246
G2796	C2539	C2539	A	A2362	U2209	C	C	A1839	C1657	C1508	U1356	U1247
A2799	A2540	A2540	U	A2363	G2210	U	A	U1840	C1663	U1512	G1367	G1249
G2800	U2541	U2541	U	U2364	A2222	A	U	A1841	U1702	C1527	U1368	G1262
A2801	U2542	U2542	G	C2365	U2225	U	C	G1842	C1548	G1371	U1371	A1263
A2802	U2543	U2543	G	C2366	U2226	U	U	C1843	U1716	G1377	U1367	G1264
A2803	A2547	A2547	A	C2367	C2227	A	G	G1844	U1717	U1557	G1380	U1267
C2808	C2548	C2548	G	A2372	A2228	C	A	A1851	U1724	C1556	U1269	G1268
C2809	G2549	G2549	C	G2375	U2231	C	G	G1858	C1725	A1557	A1386	A1270
A2810	C2552	C2552	U	U2231	A2244	U	C	A1864	G1727	G1392	A1271	C1272
A2811	U2553	U2553	G	A2244	G2249	C	C	A1865	G1733	U1398	A1273	A1274
A2812	A2554	A2554	C	G2249	G2280	U	U	C1866	G1736	A1399	A1278	
A2813	G2555	G2555	C	G2280	A2255	G	G		A1741	G1400	C1279	C1280
G2814	A2561	A2561	G	A2255	A2256	U	C	A1874	A1750	G1404	G1285	
G2815	C2561	C2561	C	A2256	G2272	U	A	G1875	G1751	G1417	A1286	A1287
A2816	G2562	G2562	U	G2272	G2273	G	C	A1879	U1568	A1419	U1292	
A2817	C2563	C2563	C	G2273	G2123	C	U	U1880	U1569	U1427	U1293	U1294
U2818	A2564	A2564	A	A2262	A2131	G	G	A1886	U1570	U1428	U1295	A1294
A2819	U2569	U2569	U	A2262	A2131	U	U	A1891	U1571	G1576	A1429	
A2704	U2570	U2570	G	G2279	G2137	C	C	A1895	U1572	U1430	G1300	
A2705	U2571	U2571	G	A2281	U2137	G	G	A1896	G1577	C1581		
G2706	C2572	C2572	A	U2282		C	C	G1897	U1578	C1582		
U2829	G2573	G2573	A	C2284		U	U	G1898	G1770			
G2714	A2402	A2402	U									
A2715	G2403	G2403	A									
U2719	A2404	A2404	A									
U2725	C2405	C2405	C									



- Molecule 36: 25S rRNA

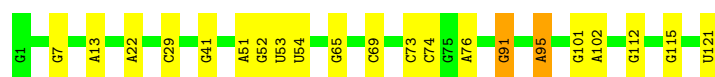


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G2663	G2549	A2398	C2293	U2176	G	U	G1775	A1580	A1452	C1314	C1192	A1048
A2667	C2552	A2401	U2298	A2188	C	U	G1778	C1581	A1453	U1329	A1193	C1049
A2674	G2555	G2402	A2303	U2189	U	G	G1779	A1583	U1457	A1330	C1196	A1064
G2677	C2566	G2403	U2297	C2197	U	G	G1780	A1588	A1460	U1331	A1200	A1065
A2678	C2567	A2404	G2307	A2198	U	G	G1781	A1589	A1461	C1201	C1201	U1071
C2681	U2681	C2405	U2310	C2199	C	C	G1794	A1593	A1462	A1202	A1203	G1072
C2682	U2682	U2411	U2311	A2201	A	U	G1795	A1597	A1465	U1351	G1209	U1081
U2683	C2572	G2418	A2313	C2204	G	C	G1796	C1597	G1480	U1352	U1082	U1082
A2689	C2573	A2419	U2314	U2205	C	U	G1797	G1604	A1481	U1353	C1216	A1085
G2690	G2574	C2420	G2315	U2209	U	U	A1812	A1605	A1482	G1354	G1222	U1085
A2691	U2570	U2421	U2316	C2210	C	U	A1813	U1606	G1483	A1355	A1223	U1088
A2694	C2584	G2435	U2317	U2211	U	C	A1814	U1607	U1484	G1357	G1232	A1093
A2695	G2585	U2436	A2320	C2212	C	A	A1815	C1608	G1487	U1367	U1241	U1094
A2696	U2589	A2437	U2327	A2213	U	G	A1816	U1609	A1490	A1373	G1236	U1095
A2704	C2593	A2438	C2330	U2222	G	G	A1817	U1620	U1495	G1374	G1237	U1096
G2705	C2594	A2439	U2334	A2223	C	C	U1818	C1628	U1496	U1379	C1238	G1097
A2706	U2594	U2441	G2335	U2224	C	C	U1819	U1629	C1496	G1380	A1240	A1098
C2707	A2601	G2442	U2336	U2225	U	U	A1820	C1639	A1503	U1241	U1241	A1103
G2714	G2606	A2443	U2337	A2228	C	C	U1821	A1643	A1506	G1242	G1242	G1104
U2719	U2505	A	C2337	U2229	A	U	A1842	U1644	A1507	G1116	G1116	G1116
C2726	G2607	U	C2338	C2231	U	C	A1846	U1645	G1507	G1117	G1117	G1117
A2727	U2506	U	U2339	G2234	U	U	A1847	G1655	G1508	C1118	C1118	C1118
G2728	C2507	A	U2340	U2235	A	U	A1848	G1656	G1509	C1119	C1119	C1119
U2729	U2508	G	A2341	U2236	U	U	A1849	C1657	A1539	A1129	A1129	A1129
G2730	G2610	G	U2342	U2237	U	U	A1850	C1658	U1540	A1130	A1130	A1130
C2742	U2614	G	G2343	U2238	U	U	C1856	C1665	G1541	G1131	G1131	G1131
A2743	G2615	U	U2344	U2239	C	C	A1867	A1683	U1553	G1134	G1134	G1134
U2752	G2618	U	A2345	U2240	C	C	U1868	A1704	U1554	A1143	A1143	A1143
G2753	G2621	G	U2346	U2241	U	U	C1872	U1716	U1555	G1148	G1148	G1148
A2762	C2625	A	G2347	U2242	U	U	A1879	U1717	G1560	G1152	G1152	G1152
U2771	A2634	A	A2348	U2243	U	U	U1880	U1724	G1561	A1153	A1153	A1153
C2772	G2635	G	U2349	U2244	A	A	U1885	C1725	C1562	A1154	A1154	A1154
C2773	A2636	U	G2350	U2245	C	C	A1886	G1736	A1566	C1155	C1155	C1155
G2777	C2637	C	U2351	U2246	C	C	A1891	U1750	U1567	G1295	G1295	G1295
G2778	U2638	G	U2352	U2247	U	U	G1892	G1751	U1568	C1296	C1296	C1296
A2779	G2639	A	U2353	U2248	C	C	A1893	U1752	U1569	C1297	C1297	C1297
G2796	C2644	C	G2354	U2249	U	U	G1894	A1760	A1571	G1300	G1300	G1300
C2797	U2652	U	U2355	U2250	C	C	U1897	C1761	U1572	U1305	U1305	U1305
C2798	A2656	U	U2356	U2251	U	U	A1901	G1762	G1573	G1306	G1306	G1306
A2799	G2659	C	U2357	U2252	C	C	C1904	U1763	G1574	G1307	G1307	G1307
G2800	U2541	G	U2358	U2253	U	U	G1905	U1764	A1575	U1308	U1308	U1308
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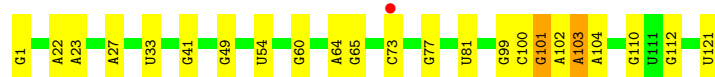
• Molecule 37: 5S rRNA

Chain 3: 83% 16% .



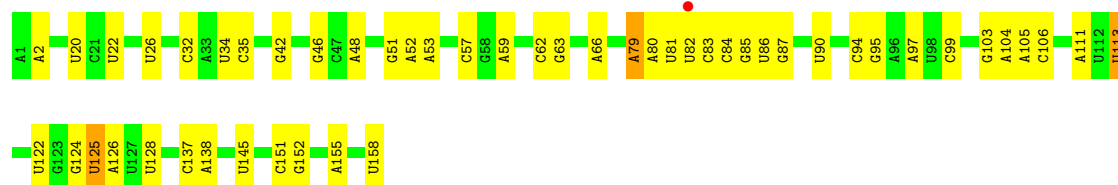
• Molecule 37: 5S rRNA

Chain 7: 81% 17% .



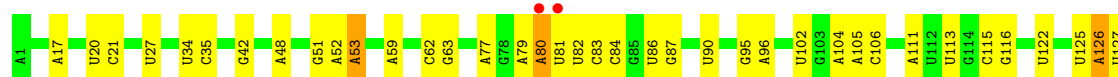
• Molecule 38: 5.8S rRNA

Chain 4: 68% 30% .



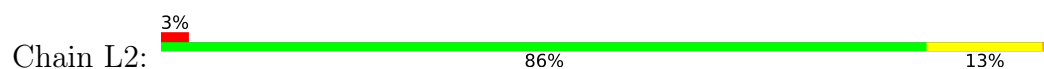
• Molecule 38: 5.8S rRNA

Chain 8: 73% 25% .

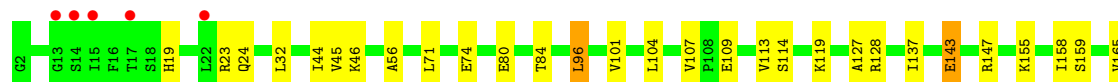
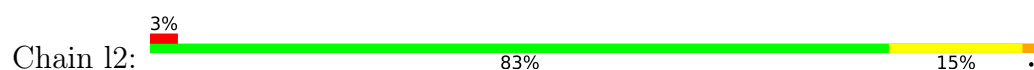




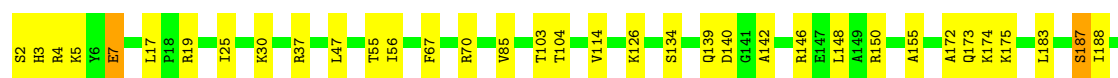
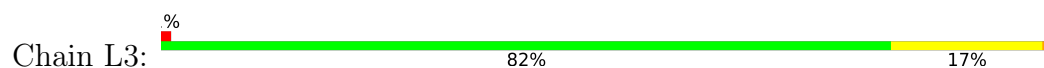
- Molecule 39: 60S ribosomal protein L2-A



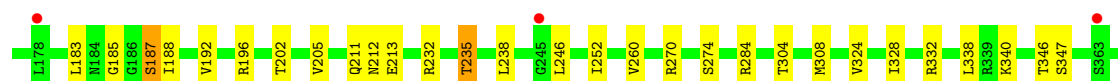
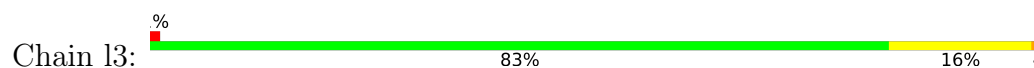
- Molecule 39: 60S ribosomal protein L2-A

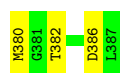


- Molecule 40: 60S ribosomal protein L3

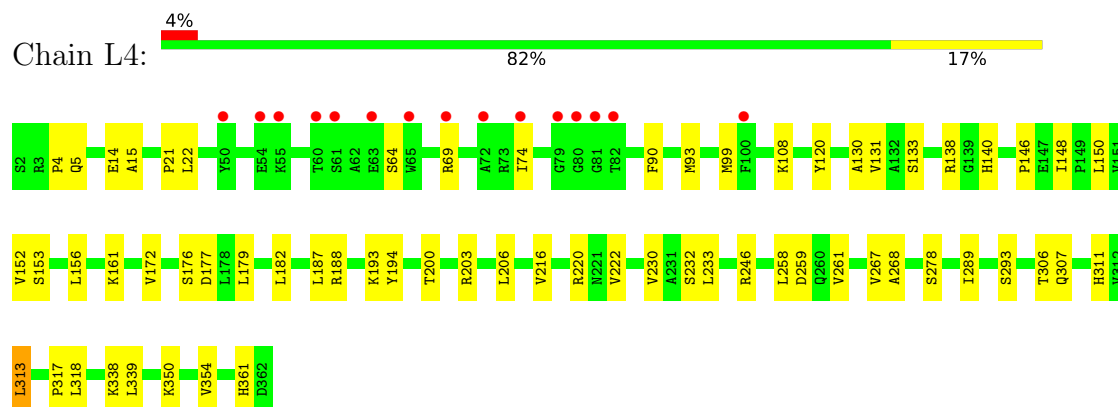


- Molecule 40: 60S ribosomal protein L3

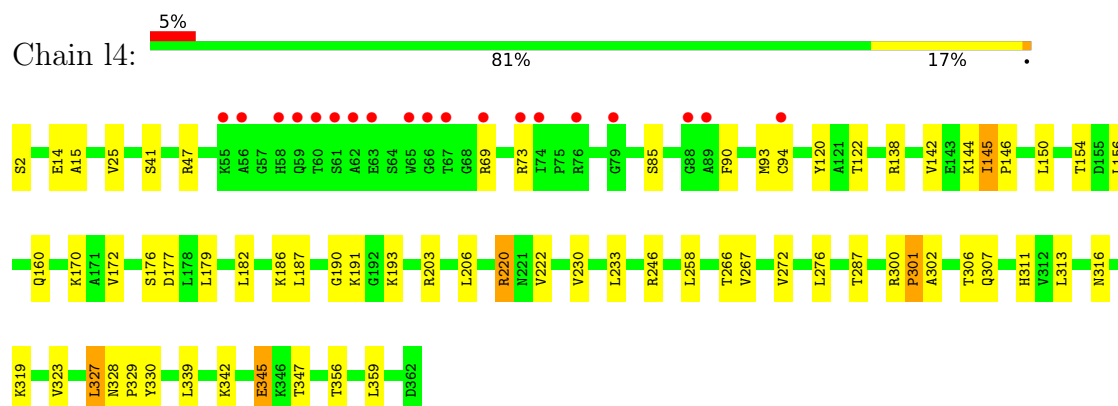




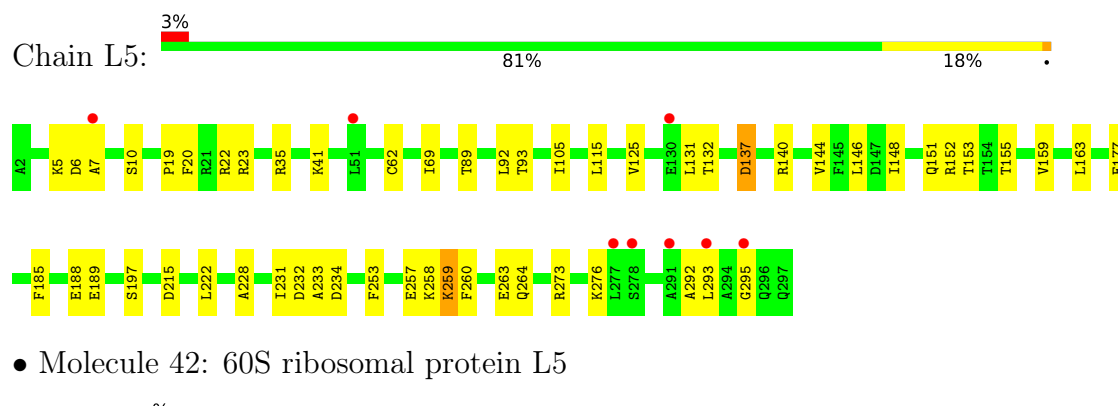
- Molecule 41: 60S ribosomal protein L4-A



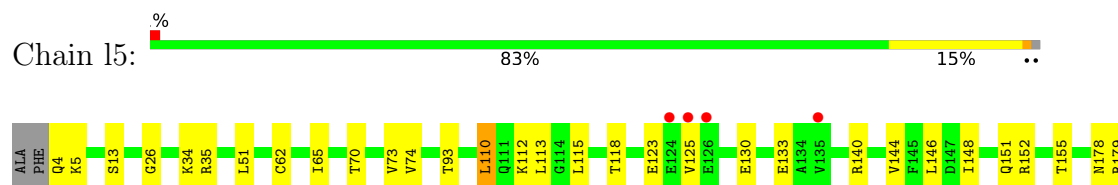
- Molecule 41: 60S ribosomal protein L4-A

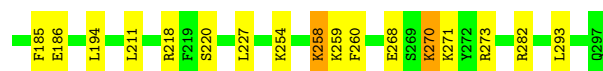


- Molecule 42: 60S ribosomal protein L5

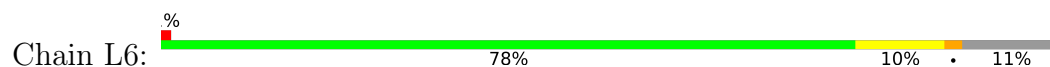


- Molecule 42: 60S ribosomal protein L5

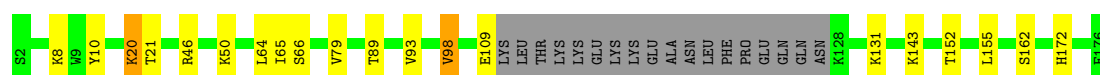
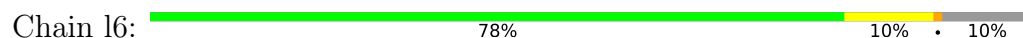




- Molecule 43: 60S ribosomal protein L6-A



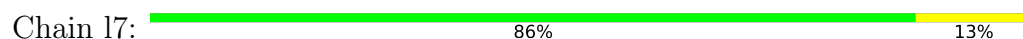
- Molecule 43: 60S ribosomal protein L6-A



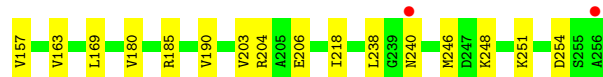
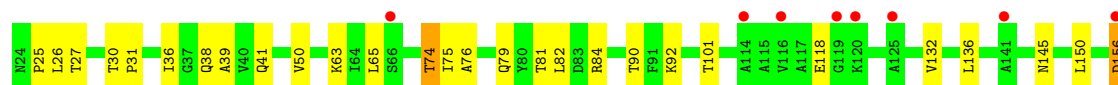
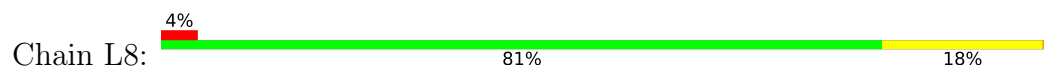
- Molecule 44: 60S ribosomal protein L7-A



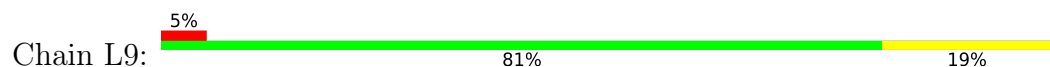
- Molecule 44: 60S ribosomal protein L7-A



- Molecule 45: 60S ribosomal protein L8-A

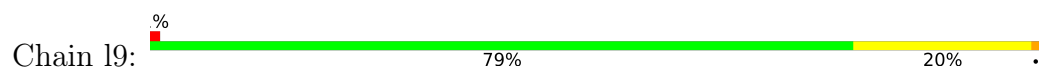


- Molecule 46: 60S ribosomal protein L9-A

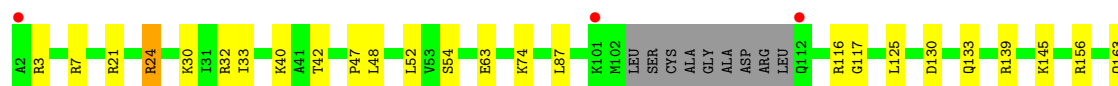
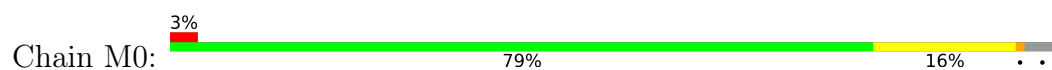




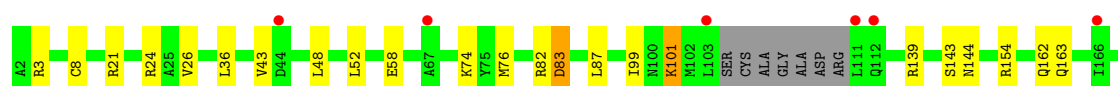
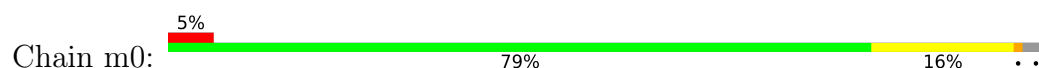
- Molecule 46: 60S ribosomal protein L9-A



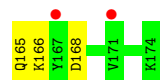
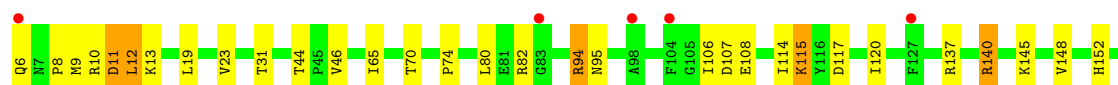
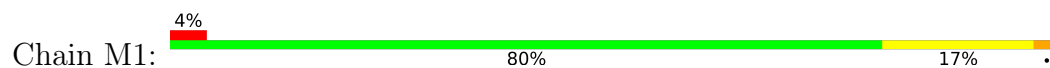
- Molecule 47: 60S ribosomal protein L10



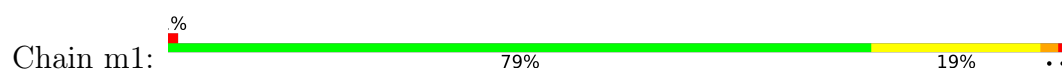
- Molecule 47: 60S ribosomal protein L10

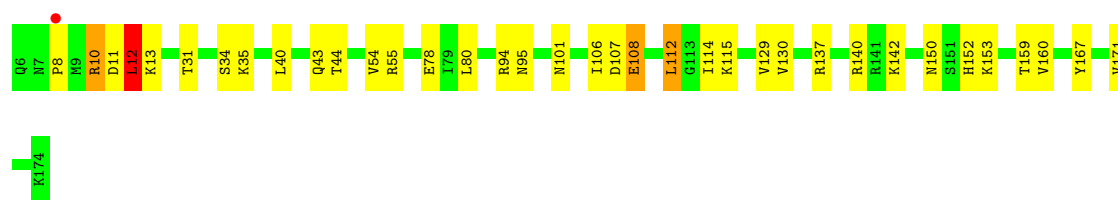


- Molecule 48: 60S ribosomal protein L11-B

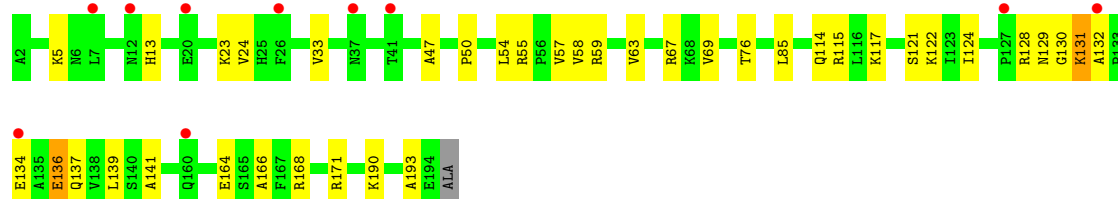
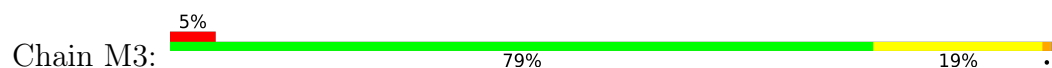


- Molecule 48: 60S ribosomal protein L11-B

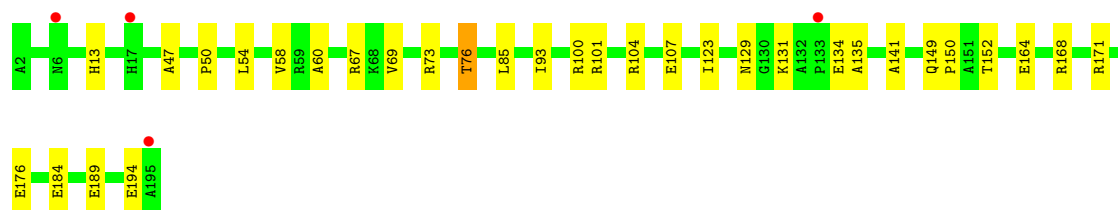
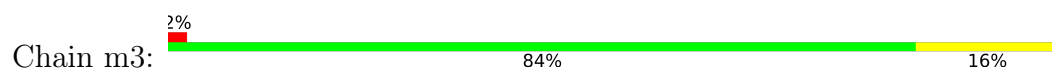




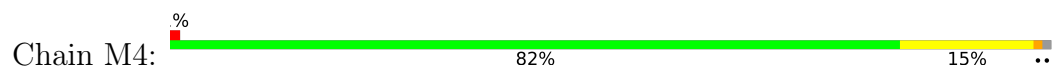
- Molecule 49: 60S ribosomal protein L13-A



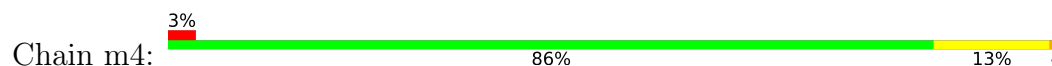
- Molecule 49: 60S ribosomal protein L13-A



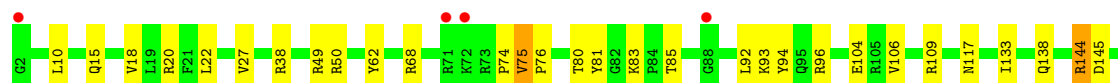
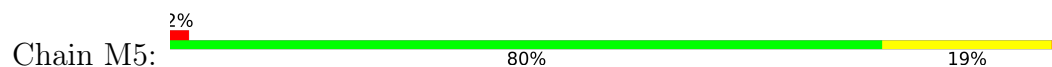
- Molecule 50: 60S ribosomal protein L14-A



- Molecule 50: 60S ribosomal protein L14-A

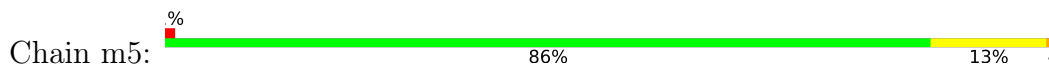


- Molecule 51: 60S ribosomal protein L15-A

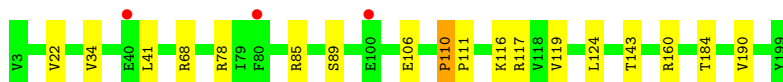




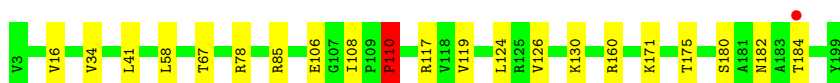
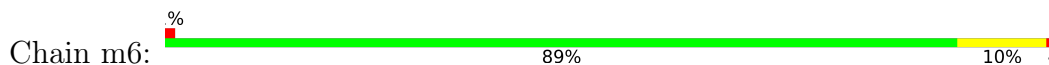
- Molecule 51: 60S ribosomal protein L15-A



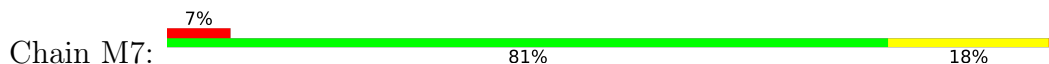
- Molecule 52: 60S ribosomal protein L16-A



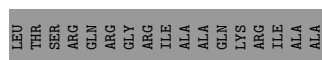
- Molecule 52: 60S ribosomal protein L16-A



- Molecule 53: 60S ribosomal protein L17-A



- Molecule 53: 60S ribosomal protein L17-A

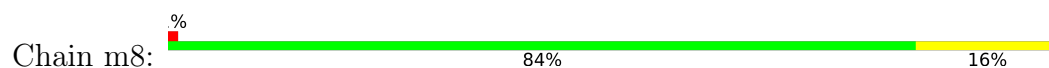


- Molecule 54: 60S ribosomal protein L18-A

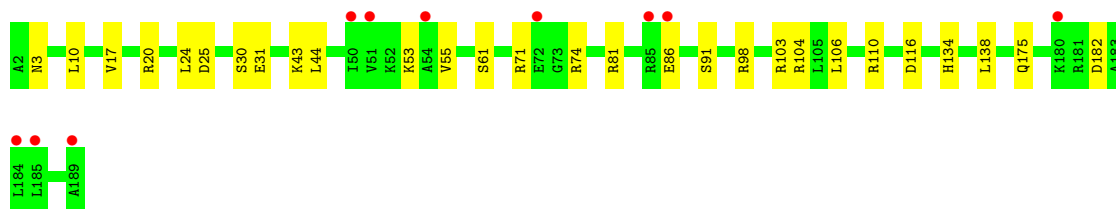
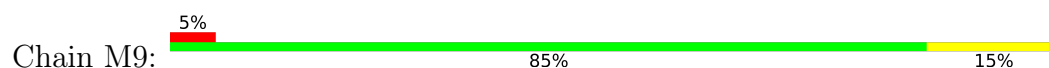




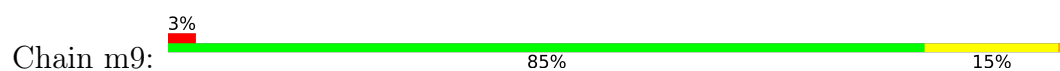
- Molecule 54: 60S ribosomal protein L18-A



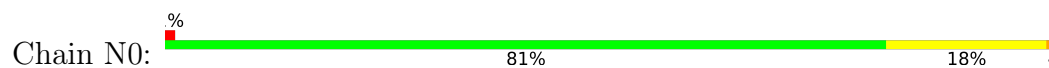
- Molecule 55: 60S ribosomal protein L19-A



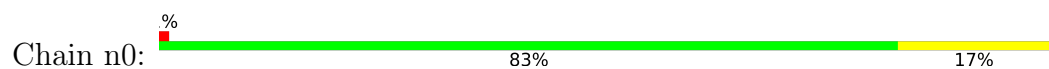
- Molecule 55: 60S ribosomal protein L19-A



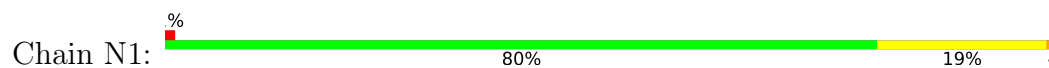
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 56: 60S ribosomal protein L20-A

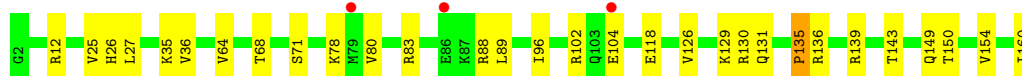
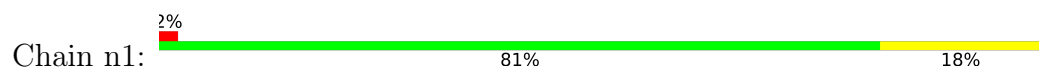


- Molecule 57: 60S ribosomal protein L21-A

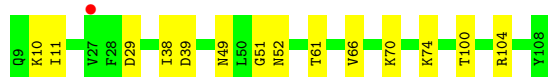
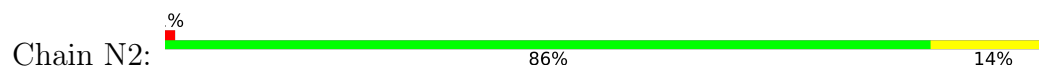




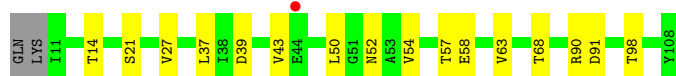
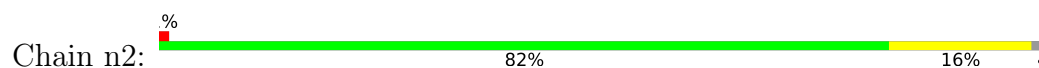
- Molecule 57: 60S ribosomal protein L21-A



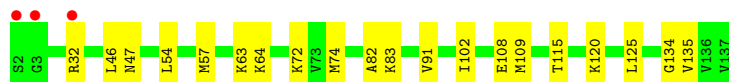
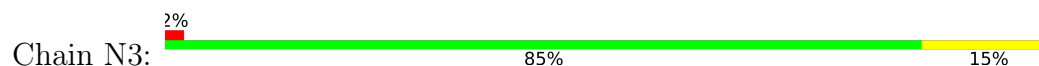
- Molecule 58: 60S ribosomal protein L22-A



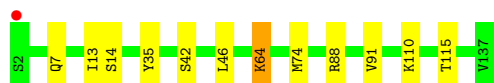
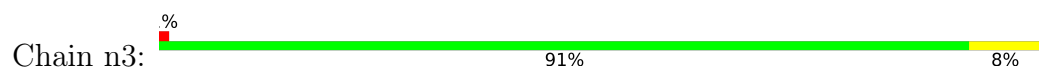
- Molecule 58: 60S ribosomal protein L22-A



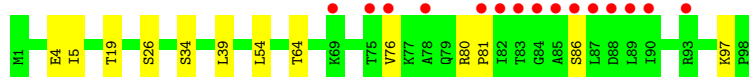
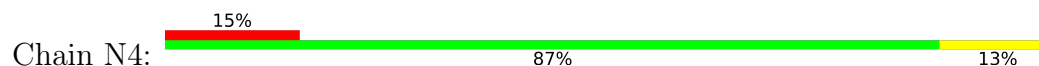
- Molecule 59: 60S ribosomal protein L23-A



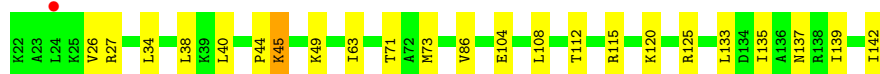
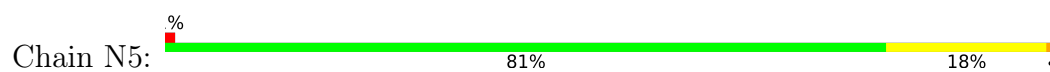
- Molecule 59: 60S ribosomal protein L23-A



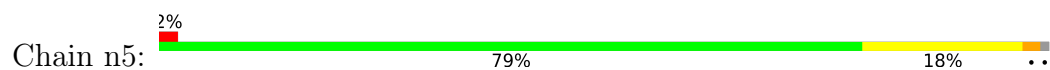
- Molecule 60: 60S ribosomal protein L24-A



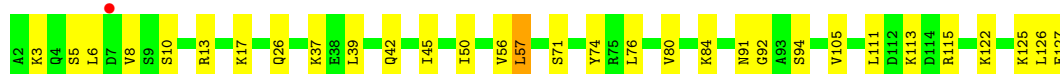
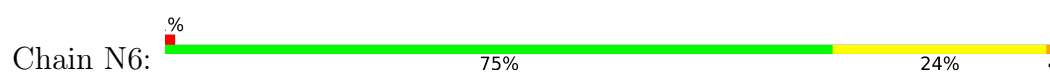
- Molecule 61: 60S ribosomal protein L25



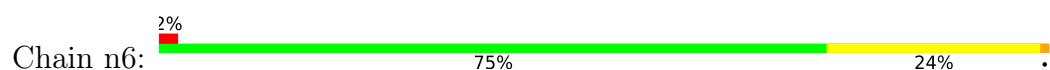
- Molecule 61: 60S ribosomal protein L25



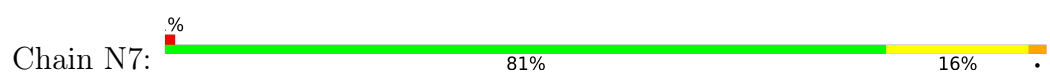
- Molecule 62: 60S ribosomal protein L26-A



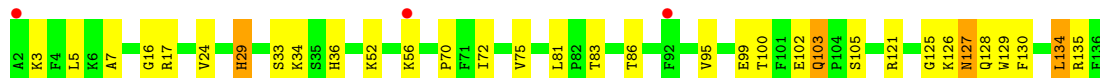
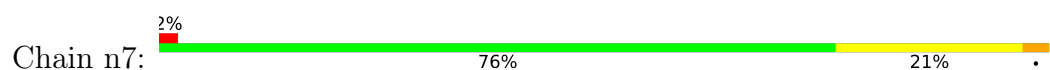
- Molecule 62: 60S ribosomal protein L26-A



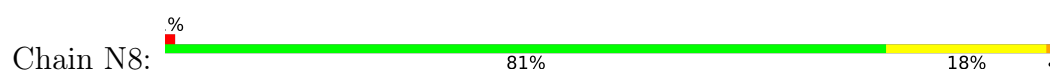
- Molecule 63: 60S ribosomal protein L27-A



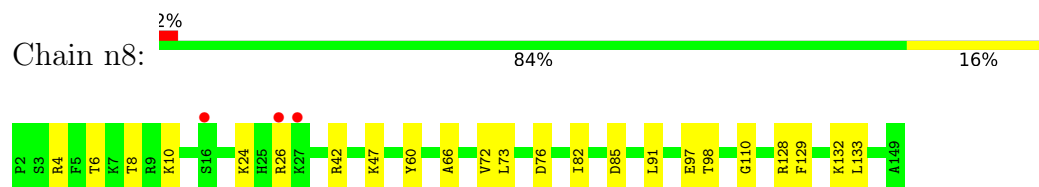
- Molecule 63: 60S ribosomal protein L27-A



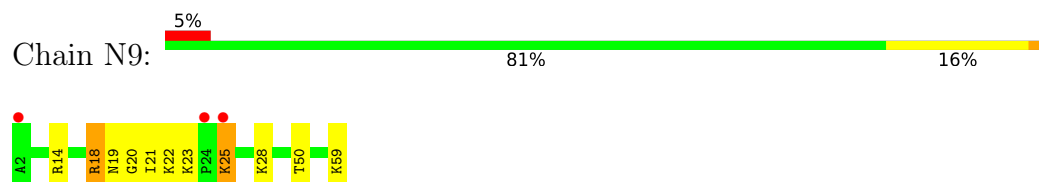
- Molecule 64: 60S ribosomal protein L28



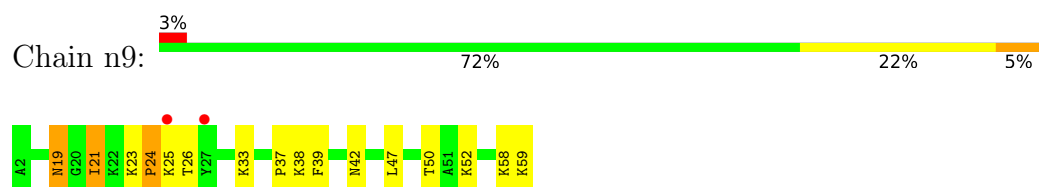
• Molecule 64: 60S ribosomal protein L28



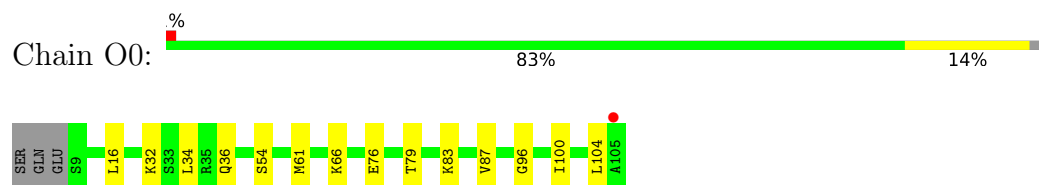
• Molecule 65: 60S ribosomal protein L29



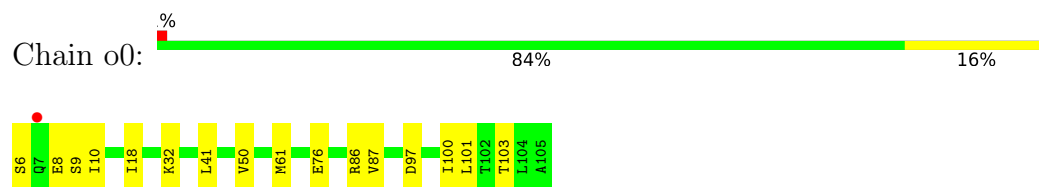
• Molecule 65: 60S ribosomal protein L29



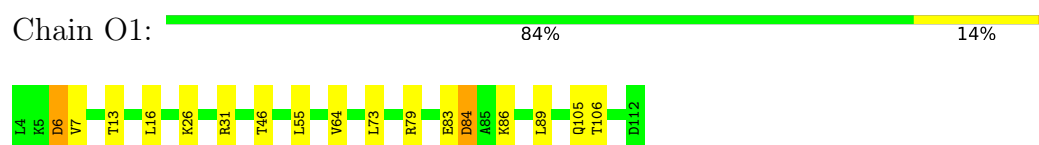
• Molecule 66: 60S ribosomal protein L30



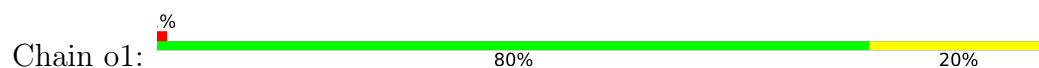
• Molecule 66: 60S ribosomal protein L30



• Molecule 67: 60S ribosomal protein L31-A

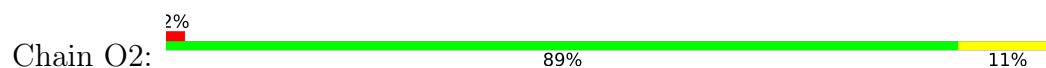


• Molecule 67: 60S ribosomal protein L31-A

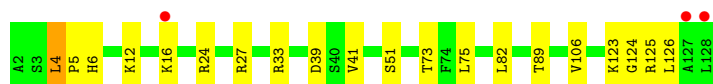
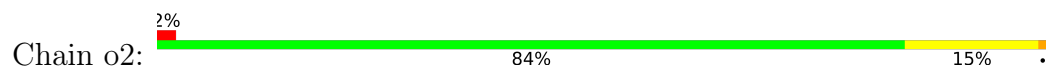




- Molecule 68: 60S ribosomal protein L32



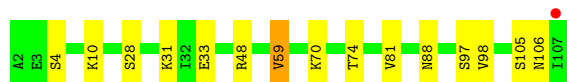
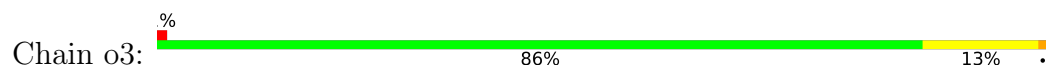
- Molecule 68: 60S ribosomal protein L32



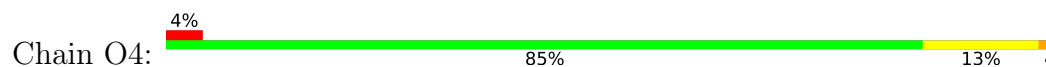
- Molecule 69: 60S ribosomal protein L33-A



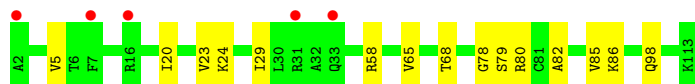
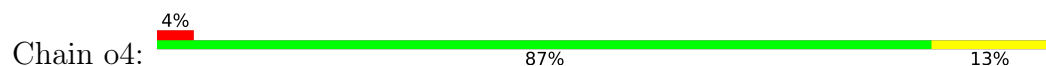
- Molecule 69: 60S ribosomal protein L33-A



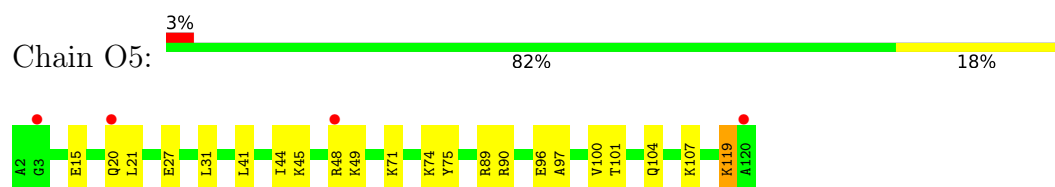
- Molecule 70: 60S ribosomal protein L34-A



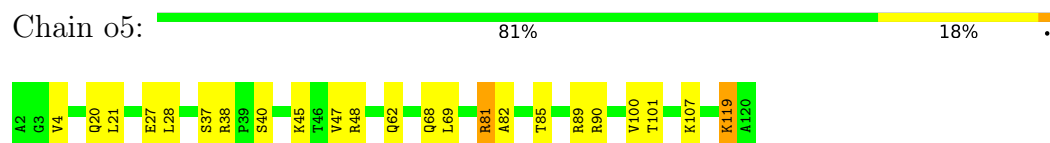
- Molecule 70: 60S ribosomal protein L34-A



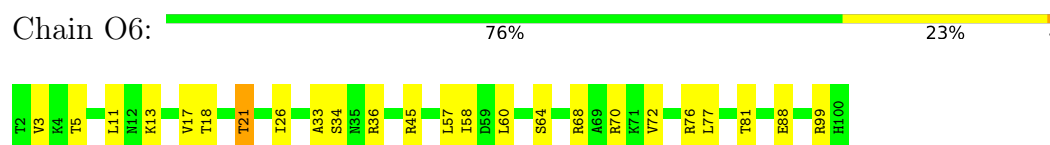
- Molecule 71: 60S ribosomal protein L35-A



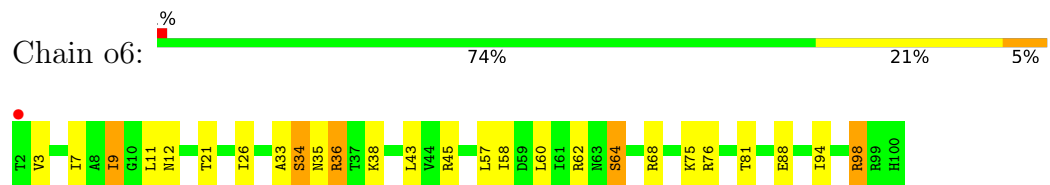
- Molecule 71: 60S ribosomal protein L35-A



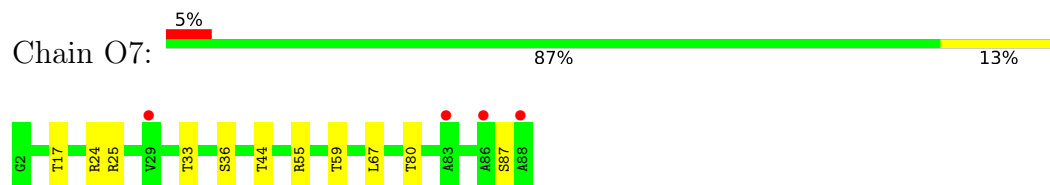
- Molecule 72: 60S ribosomal protein L36-A



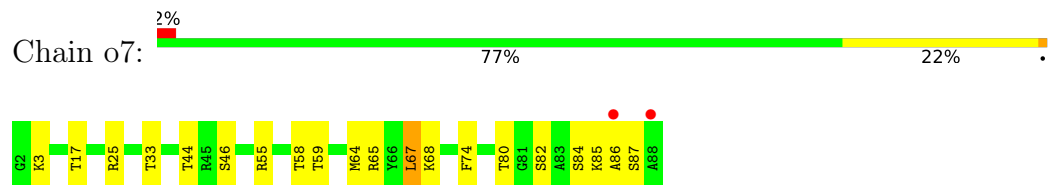
- Molecule 72: 60S ribosomal protein L36-A



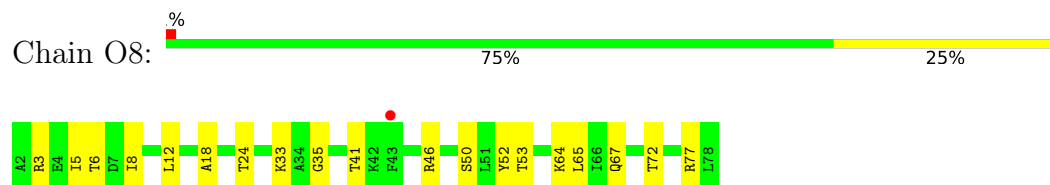
- Molecule 73: 60S ribosomal protein L37-A



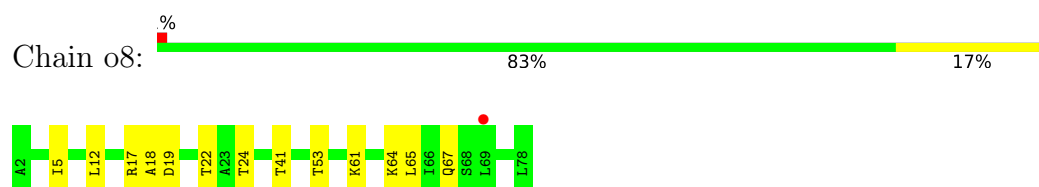
- Molecule 73: 60S ribosomal protein L37-A



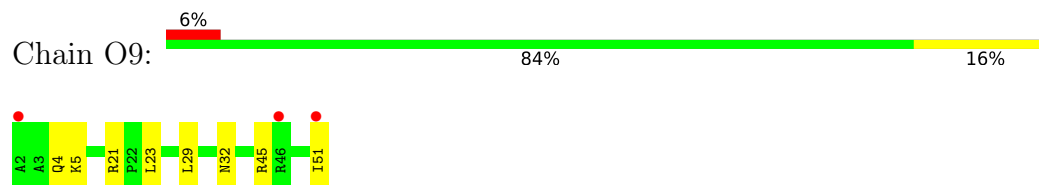
- Molecule 74: 60S ribosomal protein L38



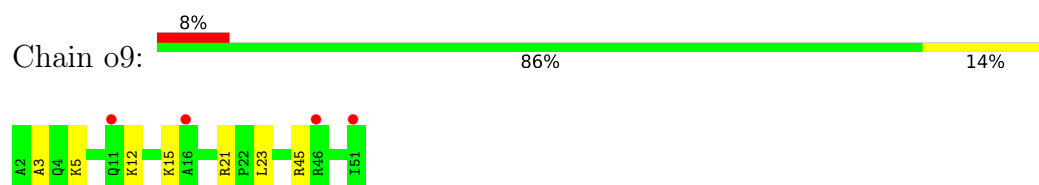
- Molecule 74: 60S ribosomal protein L38



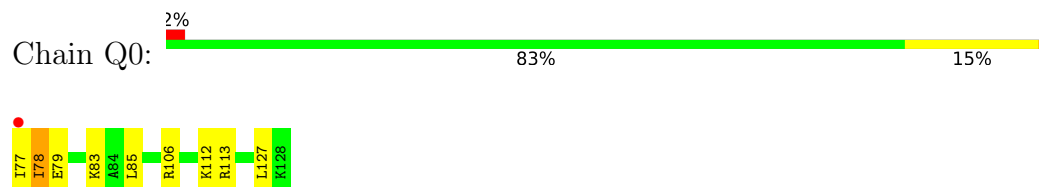
- Molecule 75: 60S ribosomal protein L39



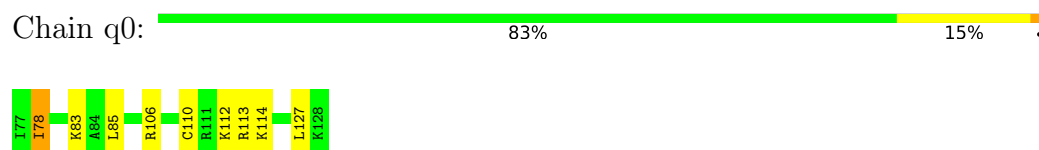
- Molecule 75: 60S ribosomal protein L39



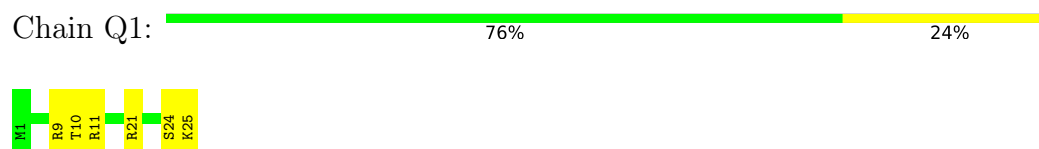
- Molecule 76: Ubiquitin-60S ribosomal protein L40



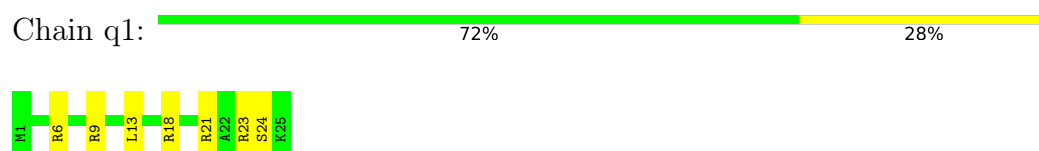
- Molecule 76: Ubiquitin-60S ribosomal protein L40



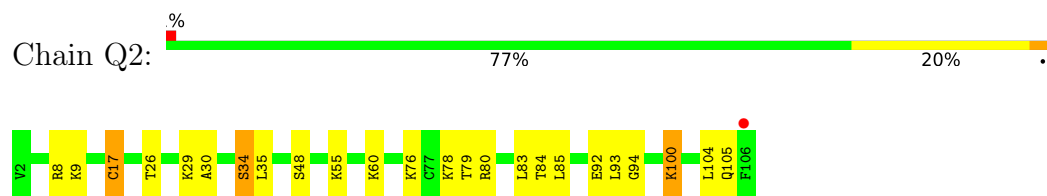
- Molecule 77: 60S ribosomal protein L41-A



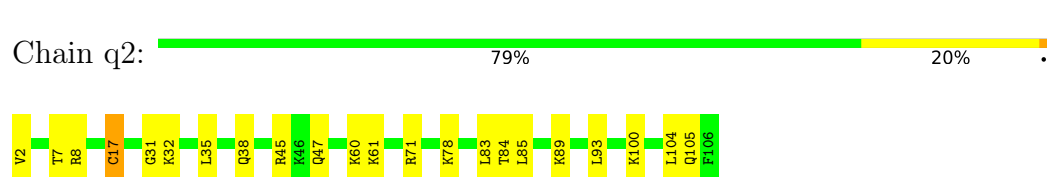
- Molecule 77: 60S ribosomal protein L41-A



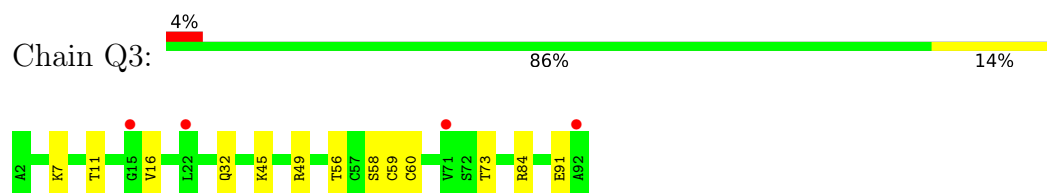
- Molecule 78: 60S ribosomal protein L42-A



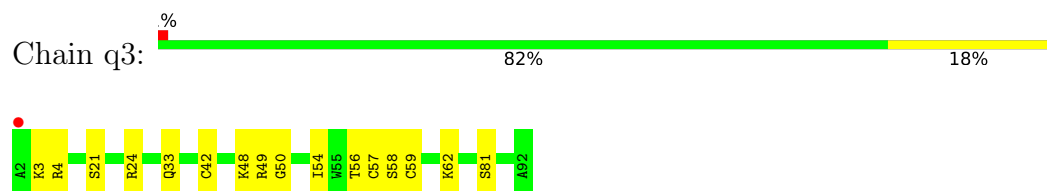
- Molecule 78: 60S ribosomal protein L42-A



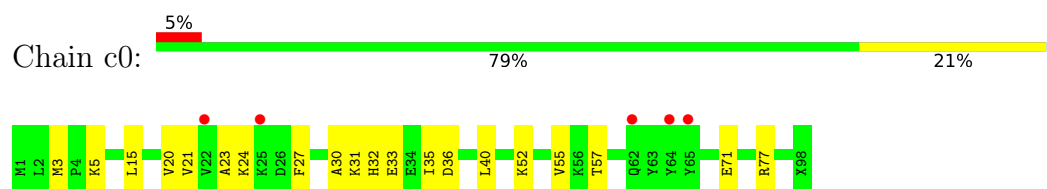
- Molecule 79: 60S ribosomal protein L43-A



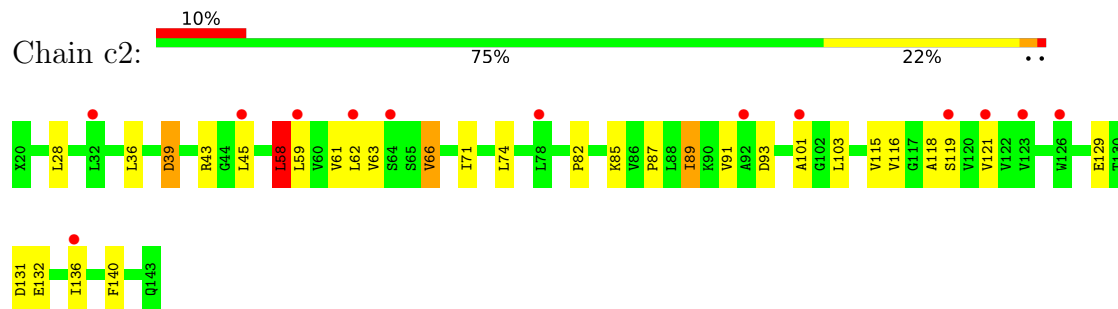
- Molecule 79: 60S ribosomal protein L43-A




- Molecule 80: 40S ribosomal protein S10-A, 40S ribosomal protein S10-A, 40S Ribosomal Protein S10

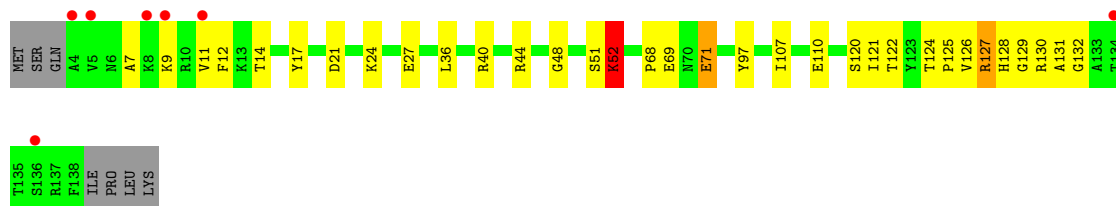


- Molecule 81: 40S Ribosomal Protein S12

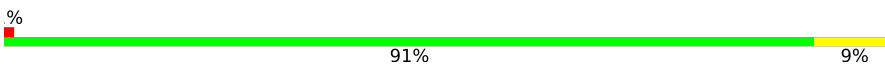


- Molecule 82: 40S ribosomal protein S15

Chain c5: 




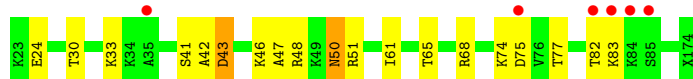
- Molecule 83: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR: 




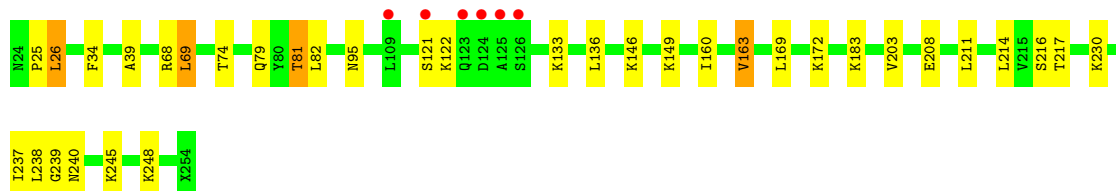
- Molecule 84: Suppressor protein STM1, Suppressor protein STM1, Ribosome-bound protein Stm1

Chain sM: 



- Molecule 85: 60S ribosomal protein L8-A, 60S ribosomal protein L8-A, 60S Ribosomal Protein L8

Chain l8: 




- Molecule 86: 60S Ribosomal Protein L12

Chain m2: 

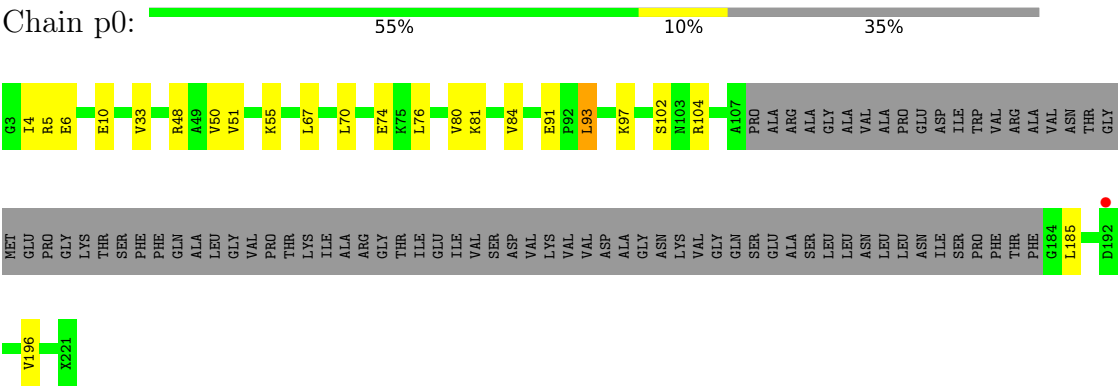
There are no outlier residues recorded for this chain.

- Molecule 87: 60S ribosomal protein L24-A

Chain n4: 



- Molecule 88: 60S acidic ribosomal protein P0, 60S acidic ribosomal protein P0, 60S Ribosomal Protein P0



- Molecule 89: 60S Ribosomal Protein P1/2



There are no outlier residues recorded for this chain.

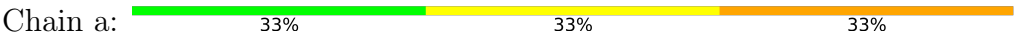
- Molecule 89: 60S Ribosomal Protein P1/2



- Molecule 90: aminoacyl-tRNA fragment ACCPmn



- Molecule 90: aminoacyl-tRNA fragment ACCPmn



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.18Å 288.24Å 303.58Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	172.59 – 3.25 172.59 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (172.59-3.25) 99.9 (172.59-3.25)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.208 , 0.249 0.210 , 0.251	Depositor DCC
R_{free} test set	23194 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	414290	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.56	1/42468 (0.0%)	1.09	161/66173 (0.2%)
1	6	0.64	3/42790 (0.0%)	1.13	143/66673 (0.2%)
2	S0	0.38	1/1617 (0.1%)	0.54	0/2215
2	s0	0.39	0/1623	0.57	0/2222
3	S1	0.31	0/1735	0.58	2/2335 (0.1%)
3	s1	0.39	0/1748	0.58	0/2352
4	S2	0.36	0/1665	0.56	0/2263
4	s2	0.44	0/1665	0.64	1/2263 (0.0%)
5	S3	0.38	0/1759	0.54	0/2368
5	s3	0.37	0/1759	0.55	0/2368
6	S4	0.38	0/2109	0.61	0/2839
6	s4	0.44	1/2109 (0.0%)	0.62	1/2839 (0.0%)
7	S5	0.34	0/1629	0.55	0/2202
7	s5	0.36	0/1629	0.54	0/2202
8	S6	0.38	0/1823	0.55	0/2439
8	s6	0.43	0/1779	0.62	0/2379
9	S7	0.36	0/1506	0.58	0/2028
9	s7	0.36	0/1516	0.58	0/2043
10	S8	0.41	0/1514	0.59	1/2021 (0.0%)
10	s8	0.46	0/1514	0.63	1/2021 (0.0%)
11	S9	0.36	0/1519	0.55	0/2035
11	s9	0.43	0/1519	0.60	0/2035
12	C0	0.31	0/725	0.54	1/978 (0.1%)
13	C1	0.39	0/1195	0.57	0/1612
13	c1	0.45	0/1194	0.62	0/1610
14	C2	0.33	0/898	0.60	0/1220
15	C3	0.38	0/1215	0.58	1/1638 (0.1%)
15	c3	0.39	0/1215	0.59	0/1638
16	C4	0.35	0/901	0.56	0/1217
16	c4	0.40	0/960	0.59	0/1290
17	C5	0.39	0/998	0.57	0/1341
18	C6	0.36	0/1125	0.64	2/1510 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	c6	0.34	0/1131	0.58	1/1518 (0.1%)
19	C7	0.38	0/935	0.58	1/1254 (0.1%)
19	c7	0.33	0/914	0.56	0/1224
20	C8	0.37	0/1211	0.59	0/1628
20	c8	0.36	0/1211	0.60	2/1628 (0.1%)
21	C9	0.39	1/1130 (0.1%)	0.54	1/1517 (0.1%)
21	c9	0.38	0/1130	0.54	0/1517
22	D0	0.37	0/865	0.56	0/1169
22	d0	0.37	0/892	0.59	0/1205
23	D1	0.36	0/693	0.55	0/935
23	d1	0.43	0/693	0.59	0/935
24	D2	0.37	0/1038	0.63	3/1395 (0.2%)
24	d2	0.42	0/1038	0.62	1/1395 (0.1%)
25	D3	0.43	0/1139	0.61	0/1518
25	d3	0.50	0/1139	0.67	0/1518
26	D4	0.38	0/1087	0.54	0/1449
26	d4	0.42	0/1087	0.61	0/1449
27	D5	0.32	0/571	0.60	0/768
27	d5	0.31	0/566	0.52	0/761
28	D6	0.35	0/782	0.63	0/1047
28	d6	0.42	0/782	0.57	0/1047
29	D7	0.35	0/620	0.55	0/838
29	d7	0.35	0/620	0.55	0/838
30	D8	0.34	0/499	0.54	0/670
30	d8	0.33	0/499	0.56	0/670
31	D9	0.43	0/452	0.65	1/600 (0.2%)
31	d9	0.43	0/452	0.58	0/600
32	E0	0.35	0/483	0.55	0/643
32	e0	0.40	0/499	0.60	0/665
33	E1	0.35	0/577	0.66	0/770
33	e1	0.34	0/619	0.68	2/822 (0.2%)
34	SR	0.32	0/2490	0.54	0/3389
35	SM	0.40	0/984	0.59	0/1323
36	1	0.81	15/75394 (0.0%)	1.28	488/117545 (0.4%)
36	5	0.84	23/75414 (0.0%)	1.31	508/117575 (0.4%)
37	3	0.70	0/2883	1.16	6/4491 (0.1%)
37	7	0.81	0/2883	1.32	19/4491 (0.4%)
38	4	0.77	0/3746	1.27	23/5832 (0.4%)
38	8	0.74	0/3746	1.19	11/5832 (0.2%)
39	L2	0.51	1/1948 (0.1%)	0.66	0/2617
39	l2	0.50	0/1946	0.70	2/2614 (0.1%)
40	L3	0.51	1/3146 (0.0%)	0.65	0/4228
40	l3	0.56	0/3146	0.69	1/4228 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	L4	0.54	0/2800	0.70	0/3790
41	l4	0.51	1/2800 (0.0%)	0.68	2/3790 (0.1%)
42	L5	0.45	1/2425 (0.0%)	0.59	0/3271
42	l5	0.56	1/2408 (0.0%)	0.64	2/3248 (0.1%)
43	L6	0.50	0/1260	0.65	0/1694
43	l6	0.55	0/1269	0.66	0/1705
44	L7	0.54	0/1821	0.67	1/2451 (0.0%)
44	l7	0.57	0/1828	0.65	2/2461 (0.1%)
45	L8	0.42	0/1836	0.58	1/2481 (0.0%)
46	L9	0.47	0/1539	0.63	0/2073
46	l9	0.54	0/1539	0.65	0/2073
47	M0	0.55	0/1741	0.65	1/2335 (0.0%)
47	m0	0.60	1/1758 (0.1%)	0.71	1/2358 (0.0%)
48	M1	0.40	0/1374	0.58	0/1842
48	m1	0.54	0/1374	0.69	3/1842 (0.2%)
49	M3	0.54	1/1568 (0.1%)	0.68	0/2106
49	m3	0.48	0/1573	0.67	0/2113
50	M4	0.49	0/1068	0.64	0/1438
50	m4	0.52	0/1074	0.62	0/1446
51	M5	0.52	0/1757	0.68	0/2354
51	m5	0.47	0/1757	0.63	0/2354
52	M6	0.60	0/1585	0.67	0/2128
52	m6	0.66	0/1585	0.69	0/2128
53	M7	0.54	0/1443	0.67	1/1944 (0.1%)
53	m7	0.62	0/1250	0.69	0/1683
54	M8	0.51	0/1465	0.66	0/1965
54	m8	0.50	0/1465	0.69	0/1965
55	M9	0.41	0/1538	0.57	0/2050
55	m9	0.42	0/1538	0.55	0/2050
56	N0	0.51	0/1481	0.66	1/1990 (0.1%)
56	n0	0.56	0/1481	0.66	0/1990
57	N1	0.51	0/1300	0.64	0/1743
57	n1	0.58	0/1300	0.66	0/1743
58	N2	0.36	0/812	0.53	0/1099
58	n2	0.38	0/794	0.55	0/1076
59	N3	0.51	0/1018	0.70	0/1369
59	n3	0.60	0/1018	0.71	0/1369
60	N4	0.45	0/712	0.57	0/958
61	N5	0.45	0/979	0.65	0/1321
61	n5	0.45	0/974	0.63	0/1314
62	N6	0.51	0/1004	0.72	2/1341 (0.1%)
62	n6	0.48	0/1004	0.70	0/1341
63	N7	0.44	0/1118	0.57	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	n7	0.48	1/1118 (0.1%)	0.55	0/1497
64	N8	0.50	0/1204	0.70	1/1612 (0.1%)
64	n8	0.52	1/1204 (0.1%)	0.67	1/1612 (0.1%)
65	N9	0.50	0/473	0.62	0/629
65	n9	0.52	0/473	0.77	0/629
66	O0	0.38	0/751	0.52	0/1008
66	o0	0.39	0/775	0.59	0/1040
67	O1	0.47	0/890	0.58	0/1196
67	o1	0.57	0/897	0.61	0/1205
68	O2	0.54	0/1041	0.67	0/1394
68	o2	0.57	0/1041	0.68	0/1394
69	O3	0.64	0/868	0.65	0/1168
69	o3	0.62	0/868	0.66	0/1168
70	O4	0.47	0/890	0.61	0/1189
70	o4	0.43	0/890	0.59	0/1189
71	O5	0.51	0/978	0.62	0/1301
71	o5	0.44	0/974	0.56	0/1297
72	O6	0.45	0/778	0.64	0/1034
72	o6	0.41	0/777	0.59	0/1033
73	O7	0.49	0/696	0.63	0/923
73	o7	0.49	0/696	0.67	0/923
74	O8	0.39	0/618	0.53	0/826
74	o8	0.38	0/614	0.52	0/822
75	O9	0.52	0/443	0.72	0/588
75	o9	0.52	0/443	0.68	0/588
76	Q0	0.57	0/423	0.65	0/562
76	q0	0.63	0/423	0.72	0/562
77	Q1	0.46	0/234	0.67	0/300
77	q1	0.60	0/234	0.65	0/300
78	Q2	0.72	1/860 (0.1%)	0.67	0/1136
78	q2	0.69	1/860 (0.1%)	0.71	1/1136 (0.1%)
79	Q3	0.50	0/701	0.65	0/934
79	q3	0.56	0/701	0.64	0/934
80	c0	0.33	0/693	0.52	0/933
81	c2	0.30	0/824	0.58	1/1116 (0.1%)
82	c5	0.41	0/1060	0.58	0/1426
83	sR	0.32	0/2495	0.53	0/3395
84	sM	0.44	0/481	0.57	0/644
85	l8	0.41	0/1765	0.59	1/2387 (0.0%)
87	n4	0.47	0/1052	0.58	0/1398
88	p0	0.36	0/977	0.57	0/1313
90	A	0.74	0/43	1.56	1/64 (1.6%)
90	a	0.79	0/43	2.00	2/64 (3.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.65	56/430203 (0.0%)	1.04	1409/631685 (0.2%)

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
3	S1	0	1
6	S4	0	1
7	s5	0	2
9	S7	0	1
10	s8	0	1
11	s9	0	1
13	c1	0	1
18	c6	0	1
19	C7	0	2
22	d0	0	1
24	D2	0	1
25	D3	0	1
25	d3	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	2
33	E1	0	1
33	e1	0	1
39	L2	0	1
39	l2	0	3
40	L3	0	1
40	l3	0	1
42	l5	0	2
43	L6	0	2
44	l7	0	2
45	L8	0	1
49	M3	0	1
50	m4	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
53	m7	0	1
56	N0	0	2
56	n0	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
57	N1	0	1
61	N5	0	1
63	n7	0	1
64	n8	0	1
65	N9	0	2
65	n9	0	2
68	o2	0	1
70	O4	0	1
82	c5	0	1
87	n4	0	1
All	All	0	56

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	14.16	2.06	1.82
78	q2	17	CYS	CB-SG	11.98	2.02	1.82
36	5	2971	A	N9-C4	11.70	1.44	1.37
63	n7	36	HIS	C-N	9.18	1.51	1.34
36	5	1152	G	N9-C4	-8.42	1.31	1.38
36	5	3019	U	C4-O4	8.39	1.30	1.23
36	5	2971	A	N3-C4	8.28	1.39	1.34
6	s4	82	TYR	C-N	-7.47	1.20	1.34
36	1	2971	A	N9-C4	7.32	1.42	1.37
36	5	430	U	P-OP2	7.17	1.61	1.49
36	5	2875	U	N1-C2	6.81	1.44	1.38
36	1	2401	A	N3-C4	6.80	1.39	1.34
42	l5	179	ARG	C-N	-6.79	1.18	1.34
36	5	2996	U	N1-C2	6.64	1.44	1.38
36	5	2404	A	N7-C5	6.59	1.43	1.39
36	1	2207	A	N9-C4	6.55	1.41	1.37
2	S0	95	ALA	C-N	6.52	1.49	1.34
36	5	2401	A	N3-C4	6.47	1.38	1.34
36	1	2404	A	N3-C4	6.35	1.38	1.34
36	5	2404	A	C5-C6	6.32	1.46	1.41
36	5	566	G	C8-N7	6.22	1.34	1.30
36	1	2714	G	N9-C4	-6.12	1.33	1.38
36	5	1152	G	N3-C4	-6.12	1.31	1.35
36	5	1152	G	N9-C8	6.01	1.42	1.37
49	M3	132	ALA	C-N	5.89	1.45	1.34
36	5	1159	A	N3-C4	-5.84	1.31	1.34
1	6	1720	G	C6-O6	5.83	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1143	A	N9-C4	-5.80	1.34	1.37
36	5	2401	A	N9-C4	5.75	1.41	1.37
41	l4	94	CYS	CB-SG	-5.57	1.72	1.81
36	1	1103	A	N9-C4	5.55	1.41	1.37
39	L2	118	GLU	C-N	-5.53	1.21	1.34
36	5	1192	C	N1-C2	5.45	1.45	1.40
36	1	2208	A	N9-C4	5.45	1.41	1.37
36	5	2372	A	N7-C5	-5.44	1.35	1.39
36	5	1922	A	N9-C4	-5.41	1.34	1.37
36	1	2401	A	N7-C5	5.35	1.42	1.39
40	L3	7	GLU	CG-CD	5.30	1.59	1.51
47	m0	8	CYS	CB-SG	-5.25	1.73	1.81
36	5	523	A	N9-C4	-5.25	1.34	1.37
21	C9	116	ILE	C-N	-5.18	1.22	1.34
36	1	2401	A	C6-N1	5.18	1.39	1.35
64	n8	98	THR	C-N	5.18	1.46	1.34
42	L5	62	CYS	CB-SG	-5.17	1.73	1.81
36	1	2404	A	N7-C5	5.15	1.42	1.39
36	1	361	A	C6-N1	-5.14	1.31	1.35
1	6	754	A	N3-C4	5.12	1.38	1.34
1	2	1508	U	C4-O4	5.11	1.27	1.23
36	5	2404	A	N9-C4	5.09	1.41	1.37
36	5	2941	A	N9-C4	-5.08	1.34	1.37
36	1	2875	U	N1-C2	5.07	1.43	1.38
1	6	359	A	N9-C4	-5.06	1.34	1.37
36	1	1399	A	N9-C4	-5.04	1.34	1.37
36	1	2726	C	N3-C4	-5.04	1.30	1.33
36	1	2147	A	N9-C4	-5.02	1.34	1.37
36	5	2872	A	C6-N1	5.01	1.39	1.35

All (1409) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-18.57	114.86	126.00
36	5	1152	G	N3-C4-C5	17.62	137.41	128.60
36	5	1152	G	C2-N3-C4	-14.18	104.81	111.90
36	1	1495	U	C5-C6-N1	-12.24	116.58	122.70
36	5	2704	A	O5'-P-OP1	-11.99	94.91	105.70
36	1	2714	G	N3-C4-N9	-11.85	118.89	126.00
36	5	1305	U	O5'-P-OP1	-11.66	95.21	105.70
36	1	2714	G	N3-C4-C5	11.50	134.35	128.60
36	1	2704	A	O5'-P-OP1	-11.08	95.73	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2726	C	C6-N1-C2	-10.14	116.25	120.30
36	1	1177	G	N1-C6-O6	10.07	125.94	119.90
38	8	80	A	C8-N9-C4	-9.97	101.81	105.80
38	8	80	A	N7-C8-N9	9.96	118.78	113.80
1	2	1096	C	N1-C2-O2	9.92	124.85	118.90
36	1	2617	U	C4-C5-C6	9.92	125.65	119.70
36	5	546	C	N1-C2-O2	9.88	124.83	118.90
36	1	2403	G	N1-C6-O6	9.75	125.75	119.90
36	5	2392	C	C6-N1-C2	9.73	124.19	120.30
36	5	2377	G	C8-N9-C4	9.65	110.26	106.40
36	5	2283	G	N1-C6-O6	9.63	125.68	119.90
36	1	609	G	O5'-P-OP2	-9.59	97.07	105.70
37	7	101	G	N1-C6-O6	9.55	125.63	119.90
36	5	2726	C	C5-C4-N4	9.53	126.87	120.20
36	1	3217	C	C2-N1-C1'	9.52	129.27	118.80
1	6	1720	G	C5-C6-N1	-9.52	106.74	111.50
36	5	3245	A	C5-N7-C8	-9.40	99.20	103.90
36	5	2872	A	O5'-P-OP1	-9.38	97.26	105.70
36	1	2572	C	N1-C2-O2	9.27	124.46	118.90
36	5	1152	G	C8-N9-C1'	9.25	139.03	127.00
36	5	2964	G	N1-C6-O6	-9.07	114.45	119.90
36	1	2726	C	C6-N1-C2	-9.04	116.68	120.30
36	1	2816	G	N1-C6-O6	9.01	125.30	119.90
36	5	2971	A	C2-N3-C4	9.01	115.10	110.60
36	5	3245	A	C2-N3-C4	-8.97	106.11	110.60
36	1	645	A	N1-C6-N6	-8.96	113.22	118.60
1	2	73	U	O4'-C1'-N1	8.96	115.37	108.20
36	1	1495	U	C2-N1-C1'	-8.91	107.01	117.70
36	5	546	C	N3-C2-O2	-8.90	115.67	121.90
36	5	2816	G	N1-C6-O6	8.88	125.23	119.90
36	5	1403	C	C6-N1-C2	8.87	123.85	120.30
36	5	2816	G	C5-C6-O6	-8.87	123.28	128.60
36	1	650	C	N1-C2-O2	-8.83	113.60	118.90
90	a	75	C	C6-N1-C2	-8.82	116.77	120.30
36	1	776	U	C4-C5-C6	8.76	124.96	119.70
36	1	372	A	O5'-P-OP2	-8.74	97.83	105.70
36	5	2871	G	O5'-P-OP2	-8.74	97.83	105.70
36	1	2726	C	C5-C4-N4	8.72	126.31	120.20
36	5	2572	C	N1-C2-O2	8.67	124.10	118.90
36	5	3245	A	N7-C8-N9	8.67	118.13	113.80
36	1	2617	U	N1-C2-N3	8.63	120.08	114.90
36	5	1481	A	C8-N9-C4	-8.56	102.37	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2524	A	O4'-C1'-N9	8.55	115.04	108.20
36	1	2827	U	C2-N1-C1'	-8.54	107.45	117.70
36	1	2726	C	N3-C4-N4	-8.54	112.03	118.00
36	1	716	A	O5'-P-OP1	-8.52	98.03	105.70
1	6	144	U	N3-C2-O2	-8.50	116.25	122.20
36	1	2406	C	C6-N1-C2	8.50	123.70	120.30
36	5	1192	C	N1-C2-O2	8.49	124.00	118.90
36	5	3154	C	N1-C2-O2	8.47	123.98	118.90
1	2	74	U	O4'-C1'-N1	8.40	114.92	108.20
36	1	3238	G	N1-C6-O6	8.38	124.93	119.90
36	1	2355	G	N1-C6-O6	8.37	124.92	119.90
36	5	3245	A	N1-C6-N6	8.34	123.61	118.60
36	1	65	A	P-O3'-C3'	8.33	129.70	119.70
36	5	922	U	C5-C6-N1	-8.33	118.54	122.70
36	1	1177	G	C5-C6-O6	-8.31	123.61	128.60
36	5	776	U	C5-C6-N1	-8.29	118.56	122.70
36	1	2816	G	C5-C6-O6	-8.29	123.63	128.60
38	4	94	C	C6-N1-C2	8.28	123.61	120.30
36	1	2871	G	O5'-P-OP2	-8.28	98.25	105.70
36	5	2376	G	C5-C6-O6	-8.27	123.64	128.60
36	5	645	A	N1-C6-N6	-8.26	113.64	118.60
36	5	3004	C	C6-N1-C2	8.26	123.60	120.30
36	5	2996	U	N1-C2-O2	8.25	128.57	122.80
1	2	1096	C	C2-N1-C1'	8.25	127.87	118.80
36	1	406	G	O4'-C1'-N9	8.24	114.79	108.20
36	5	566	G	C5-N7-C8	-8.23	100.18	104.30
36	5	2964	G	C5-C6-O6	8.20	133.52	128.60
36	1	2868	U	N1-C2-O2	8.18	128.53	122.80
36	1	2314	U	C2-N1-C1'	8.17	127.50	117.70
36	5	1152	G	C5-N7-C8	-8.16	100.22	104.30
36	1	406	G	N3-C4-N9	-8.15	121.11	126.00
36	1	637	C	P-O3'-C3'	8.14	129.47	119.70
36	1	1949	G	O5'-P-OP1	-8.14	98.38	105.70
1	2	453	U	C2-N1-C1'	8.14	127.46	117.70
36	1	3306	U	N3-C2-O2	-8.12	116.51	122.20
36	5	1152	G	C4-N9-C1'	-8.10	115.97	126.50
1	6	453	U	C2-N1-C1'	8.08	127.39	117.70
36	1	2973	G	N1-C6-O6	8.07	124.74	119.90
37	7	101	G	C5-C6-O6	-8.04	123.77	128.60
36	5	1897	G	C4-C5-N7	8.03	114.01	110.80
36	5	2372	A	N1-C6-N6	8.01	123.41	118.60
36	1	2572	C	N3-C2-O2	-8.00	116.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	17	229	PHE	CB-CG-CD1	7.98	126.39	120.80
36	1	2715	A	O5'-P-OP1	-7.96	98.54	105.70
36	5	1308	A	OP1-P-OP2	-7.94	107.69	119.60
36	1	3217	C	N1-C2-O2	7.94	123.66	118.90
1	6	194	U	C2-N1-C1'	7.94	127.22	117.70
1	2	453	U	N3-C2-O2	-7.92	116.66	122.20
36	1	885	U	C5-C6-N1	-7.89	118.75	122.70
36	1	517	G	N3-C4-C5	-7.87	124.67	128.60
36	5	2978	U	O4'-C1'-N1	7.87	114.49	108.20
36	5	2726	C	N3-C2-O2	-7.86	116.40	121.90
36	5	1307	G	P-O3'-C3'	7.83	129.09	119.70
36	5	2572	C	C2-N1-C1'	7.79	127.38	118.80
36	5	776	U	C4-C5-C6	7.79	124.38	119.70
36	5	1607	U	P-O3'-C3'	7.79	129.05	119.70
36	5	1879	A	O5'-P-OP1	7.79	120.05	110.70
36	1	3139	A	O5'-P-OP1	-7.78	98.70	105.70
36	1	1904	C	C6-N1-C2	-7.75	117.20	120.30
36	5	552	G	N1-C6-O6	7.74	124.55	119.90
1	6	1730	A	N1-C6-N6	7.74	123.25	118.60
36	1	1150	A	O5'-P-OP2	-7.73	98.74	105.70
36	1	2572	C	C2-N1-C1'	7.73	127.30	118.80
36	1	2827	U	C5-C6-N1	-7.70	118.85	122.70
36	5	1116	G	O5'-P-OP1	-7.69	98.78	105.70
36	5	2392	C	N3-C4-C5	7.69	124.98	121.90
36	1	1495	U	C4-C5-C6	7.67	124.30	119.70
1	2	558	U	N1-C2-O2	7.67	128.16	122.80
1	2	1389	C	N1-C2-O2	7.66	123.50	118.90
1	2	830	U	N3-C2-O2	-7.64	116.85	122.20
36	5	1604	G	C4-N9-C1'	7.64	136.44	126.50
36	1	439	C	N1-C2-O2	7.62	123.47	118.90
36	1	2868	U	N3-C2-O2	-7.61	116.87	122.20
36	5	1200	A	N1-C6-N6	7.58	123.15	118.60
1	2	1596	C	N3-C2-O2	-7.55	116.62	121.90
36	5	2683	U	N1-C2-O2	7.55	128.08	122.80
36	1	1365	G	C8-N9-C4	-7.54	103.39	106.40
1	2	145	A	C8-N9-C4	-7.52	102.79	105.80
1	2	321	C	C6-N1-C2	-7.51	117.30	120.30
1	2	639	U	N3-C2-O2	-7.50	116.95	122.20
36	5	2978	U	C5-C6-N1	-7.50	118.95	122.70
1	2	934	C	C2-N1-C1'	7.50	127.05	118.80
36	5	3154	C	C2-N1-C1'	7.49	127.04	118.80
36	5	3019	U	N3-C4-C5	-7.49	110.11	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2621	G	N1-C6-O6	7.49	124.39	119.90
1	2	1096	C	N3-C2-O2	-7.47	116.67	121.90
31	D9	36	LEU	CA-CB-CG	7.46	132.47	115.30
36	5	880	G	C4-N9-C1'	-7.45	116.82	126.50
36	1	650	C	N3-C2-O2	7.43	127.10	121.90
1	6	163	G	N3-C4-N9	-7.43	121.54	126.00
36	1	2978	U	O4'-C1'-N1	7.42	114.14	108.20
36	5	3152	U	N1-C2-N3	-7.42	110.45	114.90
36	1	835	G	O4'-C1'-N9	7.42	114.13	108.20
36	5	2385	G	N3-C4-C5	7.41	132.31	128.60
36	1	3319	U	P-O3'-C3'	7.39	128.57	119.70
36	5	635	G	C5-C6-O6	-7.39	124.17	128.60
1	2	831	U	C5-C6-N1	7.37	126.39	122.70
36	1	3344	A	O4'-C1'-N9	7.36	114.09	108.20
36	1	2819	A	O5'-P-OP2	-7.35	99.08	105.70
36	5	2327	U	C5-C6-N1	-7.35	119.03	122.70
36	5	3019	U	N3-C4-O4	7.30	124.51	119.40
36	1	3217	C	C6-N1-C1'	-7.29	112.05	120.80
36	1	645	A	N9-C4-C5	7.29	108.72	105.80
36	5	546	C	C6-N1-C2	-7.29	117.39	120.30
1	2	1537	C	C5-C4-N4	-7.27	115.11	120.20
1	2	558	U	N3-C2-O2	-7.27	117.11	122.20
37	7	101	G	C4-C5-N7	7.26	113.70	110.80
36	1	2714	G	C2-N3-C4	-7.25	108.27	111.90
36	5	437	G	C5-C6-O6	-7.25	124.25	128.60
36	1	1111	U	C6-N1-C2	7.22	125.33	121.00
36	5	2644	C	O5'-P-OP1	-7.21	99.21	105.70
36	1	2973	G	C5-C6-O6	-7.21	124.28	128.60
36	5	1879	A	C4-C5-N7	7.21	114.30	110.70
1	6	639	U	C2-N1-C1'	7.20	126.34	117.70
37	7	49	G	N1-C6-O6	7.20	124.22	119.90
36	1	3306	U	N3-C4-O4	-7.20	114.36	119.40
36	1	2996	U	N1-C2-O2	7.19	127.84	122.80
36	5	429	U	OP2-P-O3'	7.19	121.02	105.20
1	6	163	G	C2-N3-C4	-7.18	108.31	111.90
36	5	1006	A	O5'-P-OP2	-7.18	99.23	105.70
36	1	1308	A	N7-C8-N9	7.17	117.39	113.80
36	5	2531	C	N1-C2-O2	7.17	123.20	118.90
36	5	1308	A	N7-C8-N9	7.17	117.38	113.80
1	2	453	U	N1-C2-O2	7.16	127.81	122.80
1	2	1389	C	N3-C2-O2	-7.16	116.89	121.90
36	1	2719	U	C5-C6-N1	-7.15	119.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3275	U	C5-C6-N1	7.15	126.27	122.70
36	1	410	U	N3-C4-C5	-7.13	110.32	114.60
36	1	2617	U	C5-C4-O4	7.13	130.18	125.90
36	1	745	C	C6-N1-C2	7.12	123.15	120.30
1	2	507	U	N1-C2-O2	7.11	127.78	122.80
36	5	3197	G	N3-C4-N9	-7.10	121.74	126.00
1	2	577	G	C4-C5-N7	7.09	113.64	110.80
1	2	1200	G	N1-C6-O6	7.09	124.16	119.90
36	5	2728	G	O5'-P-OP2	-7.09	99.32	105.70
36	1	1897	G	OP2-P-O3'	7.09	120.80	105.20
36	1	3344	A	C8-N9-C4	-7.09	102.96	105.80
36	5	2377	G	N7-C8-N9	-7.09	109.55	113.10
36	5	607	A	N1-C6-N6	-7.09	114.35	118.60
36	1	3217	C	N3-C2-O2	-7.08	116.94	121.90
36	1	3306	U	C5-C4-O4	7.08	130.15	125.90
36	5	1879	A	N1-C6-N6	7.06	122.84	118.60
36	1	3022	G	O4'-C1'-N9	7.06	113.84	108.20
36	5	1879	A	C6-C5-N7	-7.06	127.36	132.30
36	5	3245	A	C6-C5-N7	-7.06	127.36	132.30
36	1	406	G	C5-C6-O6	7.05	132.83	128.60
36	1	2827	U	C5-C4-O4	7.05	130.13	125.90
36	1	718	G	N3-C4-C5	7.05	132.12	128.60
36	5	2283	G	C5-C6-O6	-7.05	124.37	128.60
36	5	3152	U	N1-C2-O2	7.05	127.73	122.80
78	q2	17	CYS	CA-CB-SG	7.03	126.65	114.00
1	6	1361	U	C2-N1-C1'	7.02	126.13	117.70
36	1	2706	G	C5-C6-O6	-7.02	124.39	128.60
36	5	2943	G	C6-C5-N7	-7.01	126.19	130.40
36	5	2531	C	C2-N1-C1'	7.00	126.50	118.80
1	2	736	C	C2-N1-C1'	7.00	126.50	118.80
38	4	32	C	N3-C4-C5	6.99	124.70	121.90
36	1	3382	U	N1-C2-O2	6.98	127.69	122.80
1	6	1747	G	C8-N9-C4	6.98	109.19	106.40
36	5	3140	G	C4-C5-N7	6.96	113.59	110.80
38	4	125	U	C2-N1-C1'	6.95	126.04	117.70
36	5	2272	G	O4'-C1'-N9	6.95	113.76	108.20
36	1	435	C	C6-N1-C2	6.95	123.08	120.30
1	2	507	U	N3-C2-O2	-6.94	117.34	122.20
36	1	1838	G	N1-C6-O6	6.94	124.06	119.90
36	5	406	G	N3-C4-N9	-6.94	121.84	126.00
36	1	2418	G	OP1-P-O3'	6.93	120.45	105.20
37	3	101	G	C8-N9-C4	6.92	109.17	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	880	G	C8-N9-C1'	6.92	135.99	127.00
36	5	948	C	C6-N1-C2	6.91	123.06	120.30
1	6	1700	C	C2-N1-C1'	6.90	126.39	118.80
36	5	358	G	N1-C6-O6	6.89	124.04	119.90
1	6	144	U	C2-N1-C1'	6.88	125.96	117.70
36	1	3344	A	N7-C8-N9	6.87	117.23	113.80
36	1	2355	G	C5-C6-O6	-6.87	124.48	128.60
36	5	3368	U	C2-N1-C1'	-6.86	109.47	117.70
36	5	1879	A	C5-N7-C8	-6.85	100.47	103.90
36	1	3362	A	O4'-C1'-N9	6.84	113.67	108.20
36	1	282	G	C8-N9-C4	-6.84	103.67	106.40
36	5	2404	A	N1-C6-N6	-6.83	114.50	118.60
1	2	1039	A	O4'-C1'-N9	6.82	113.66	108.20
36	5	2943	G	N1-C6-O6	6.82	123.99	119.90
1	2	1481	C	C6-N1-C2	-6.81	117.58	120.30
36	5	1192	C	C2-N1-C1'	6.81	126.29	118.80
1	2	590	C	C6-N1-C2	-6.81	117.58	120.30
1	2	1560	U	N3-C2-O2	-6.81	117.44	122.20
36	1	2818	U	C5-C6-N1	6.81	126.10	122.70
36	5	3078	U	N3-C2-O2	-6.80	117.44	122.20
36	5	3245	A	C4-C5-N7	6.80	114.10	110.70
1	6	1745	G	N3-C4-N9	6.80	130.08	126.00
36	1	410	U	N3-C4-O4	6.80	124.16	119.40
36	5	2872	A	C4-C5-C6	-6.80	113.60	117.00
36	5	420	G	C8-N9-C4	6.79	109.12	106.40
37	7	1	G	N3-C4-N9	6.79	130.08	126.00
1	2	639	U	N1-C2-O2	6.79	127.55	122.80
36	5	404	G	O5'-P-OP2	-6.78	99.60	105.70
36	1	355	A	C8-N9-C4	6.78	108.51	105.80
36	1	1437	C	C6-N1-C2	-6.77	117.59	120.30
36	5	1582	C	C6-N1-C2	-6.75	117.60	120.30
1	6	158	U	P-O3'-C3'	6.74	127.79	119.70
36	1	2983	C	N3-C4-N4	-6.74	113.28	118.00
38	8	115	C	C6-N1-C2	6.73	122.99	120.30
36	1	2760	C	N1-C2-O2	-6.73	114.86	118.90
36	1	1308	A	C8-N9-C4	-6.71	103.12	105.80
36	1	1495	U	N1-C2-O2	-6.71	118.10	122.80
36	1	1741	A	C2-N3-C4	-6.71	107.25	110.60
1	6	1473	U	N3-C2-O2	-6.71	117.50	122.20
36	1	3207	U	C5-C4-O4	6.71	129.92	125.90
36	5	2376	G	N1-C6-O6	6.70	123.92	119.90
37	7	100	C	C6-N1-C2	6.69	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	103	G	N3-C4-C5	-6.68	125.26	128.60
1	2	732	G	C5-C6-O6	-6.68	124.59	128.60
36	5	2372	A	C6-C5-N7	-6.67	127.63	132.30
36	5	3214	U	N3-C2-O2	-6.67	117.53	122.20
36	5	645	A	N9-C4-C5	6.67	108.47	105.80
36	5	1148	G	C5-C6-O6	-6.66	124.60	128.60
36	5	3245	A	C8-N9-C4	-6.66	103.13	105.80
36	1	23	A	N1-C6-N6	-6.66	114.61	118.60
36	1	1306	G	N9-C4-C5	-6.66	102.74	105.40
36	5	3153	U	N3-C2-O2	-6.65	117.54	122.20
36	1	2209	U	C5-C6-N1	6.65	126.02	122.70
1	6	1389	C	N1-C2-O2	6.65	122.89	118.90
36	1	2946	A	N1-C6-N6	6.62	122.57	118.60
36	1	2617	U	N3-C4-C5	-6.62	110.63	114.60
24	d2	93	LEU	CA-CB-CG	6.62	130.53	115.30
36	1	1306	G	N1-C6-O6	6.62	123.87	119.90
36	1	2827	U	N3-C4-O4	-6.62	114.77	119.40
36	1	3278	C	N1-C2-O2	6.62	122.87	118.90
36	5	1604	G	C8-N9-C1'	-6.62	118.40	127.00
36	1	2979	U	N1-C2-O2	6.61	127.43	122.80
36	1	2617	U	C5-C6-N1	-6.61	119.39	122.70
1	6	1	U	N1-C2-O2	6.61	127.43	122.80
37	7	101	G	C6-C5-N7	-6.61	126.43	130.40
36	5	3084	C	O5'-P-OP1	-6.61	99.75	105.70
36	5	2572	C	N3-C2-O2	-6.61	117.27	121.90
1	2	558	U	C2-N1-C1'	6.60	125.62	117.70
36	5	2875	U	N3-C2-O2	-6.60	117.58	122.20
36	5	350	C	N1-C2-O2	6.59	122.86	118.90
36	5	1897	G	C5-N7-C8	-6.59	101.00	104.30
36	1	2726	C	N3-C2-O2	-6.59	117.29	121.90
36	1	24	G	C8-N9-C4	6.59	109.03	106.40
1	2	507	U	C2-N1-C1'	6.58	125.60	117.70
1	6	1033	C	C6-N1-C2	6.58	122.93	120.30
1	6	1	U	C2-N1-C1'	6.58	125.60	117.70
38	8	17	A	N1-C6-N6	6.58	122.55	118.60
1	6	1473	U	N1-C2-O2	6.57	127.40	122.80
36	5	2858	U	N3-C2-O2	-6.57	117.60	122.20
90	A	75	C	C6-N1-C2	-6.57	117.67	120.30
1	2	704	C	C2-N1-C1'	6.56	126.02	118.80
1	2	132	U	P-O3'-C3'	6.55	127.56	119.70
36	1	3278	C	N3-C2-O2	-6.55	117.31	121.90
36	1	406	G	C4-N9-C1'	-6.55	117.99	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1311	G	O5'-P-OP2	-6.54	99.81	105.70
36	5	2573	G	N1-C6-O6	6.54	123.83	119.90
18	C6	40	GLU	C-N-CD	-6.54	106.20	120.60
36	5	284	A	O5'-P-OP1	-6.54	99.81	105.70
85	18	69	LEU	CA-CB-CG	6.54	130.35	115.30
38	4	125	U	N1-C2-O2	6.54	127.38	122.80
1	6	194	U	N1-C2-O2	6.54	127.38	122.80
36	5	1481	A	N7-C8-N9	6.53	117.07	113.80
36	1	2123	G	C8-N9-C4	6.53	109.01	106.40
1	2	1537	C	N3-C4-N4	6.53	122.57	118.00
36	5	1189	C	N1-C2-O2	-6.53	114.98	118.90
36	5	1604	G	N3-C4-C5	-6.53	125.33	128.60
36	1	969	C	N1-C2-O2	-6.53	114.98	118.90
1	6	1097	U	P-O3'-C3'	6.53	127.53	119.70
36	1	2314	U	C5-C6-N1	6.52	125.96	122.70
1	6	1473	U	C2-N1-C1'	6.52	125.53	117.70
36	1	817	A	N9-C4-C5	-6.52	103.19	105.80
1	6	1596	C	C6-N1-C2	-6.52	117.69	120.30
36	1	85	A	C2-N3-C4	-6.51	107.34	110.60
36	5	1152	G	N3-C2-N2	-6.51	115.34	119.90
36	1	2874	G	C5-C6-O6	6.51	132.50	128.60
36	5	3197	G	N3-C2-N2	-6.51	115.34	119.90
1	2	9	U	O5'-P-OP1	-6.50	99.85	105.70
36	1	2571	U	N3-C2-O2	-6.49	117.66	122.20
36	5	3154	C	N3-C2-O2	-6.49	117.35	121.90
1	2	1347	U	N1-C2-O2	-6.48	118.26	122.80
1	2	1773	C	C6-N1-C2	-6.48	117.71	120.30
36	5	3209	A	O4'-C1'-N9	6.48	113.38	108.20
36	1	1368	U	C5-C4-O4	-6.48	122.01	125.90
36	5	3197	G	N3-C4-C5	6.47	131.84	128.60
36	1	2719	U	C2-N3-C4	-6.47	123.12	127.00
36	1	2400	G	C8-N9-C4	6.46	108.98	106.40
36	1	979	U	N3-C2-O2	-6.46	117.68	122.20
53	M7	3	ARG	NE-CZ-NH2	-6.46	117.07	120.30
39	12	246	LEU	CA-CB-CG	6.45	130.15	115.30
36	1	350	C	N3-C2-O2	-6.44	117.39	121.90
1	6	453	U	N3-C2-O2	-6.44	117.69	122.20
36	5	406	G	O4'-C1'-N9	6.44	113.35	108.20
36	5	2281	A	N1-C6-N6	6.44	122.46	118.60
36	5	1367	G	N1-C6-O6	6.43	123.76	119.90
36	1	3214	U	N1-C2-O2	6.43	127.30	122.80
1	2	830	U	N1-C2-O2	6.43	127.30	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D2	93	LEU	CA-CB-CG	6.43	130.08	115.30
36	5	2363	A	C8-N9-C4	-6.43	103.23	105.80
36	1	1351	U	N1-C2-O2	6.42	127.30	122.80
36	1	2988	C	C6-N1-C2	6.42	122.87	120.30
36	5	361	A	N1-C6-N6	-6.42	114.75	118.60
36	1	1149	G	C4-N9-C1'	-6.42	118.16	126.50
36	5	566	G	C4-C5-N7	6.42	113.37	110.80
36	5	1847	A	O5'-P-OP2	-6.41	99.93	105.70
36	5	3228	C	N1-C2-O2	6.41	122.75	118.90
36	5	2996	U	N3-C2-O2	-6.41	117.71	122.20
1	6	1657	U	O5'-P-OP2	-6.41	99.93	105.70
36	5	552	G	C5-C6-N1	-6.40	108.30	111.50
36	1	2758	A	N1-C6-N6	-6.40	114.76	118.60
10	s8	29	LEU	CA-CB-CG	6.40	130.02	115.30
36	5	2524	A	N7-C8-N9	6.40	117.00	113.80
1	6	1	U	N3-C2-O2	-6.40	117.72	122.20
36	1	3277	U	N3-C2-O2	-6.40	117.72	122.20
1	2	1339	C	OP2-P-O3'	6.39	119.27	105.20
36	1	406	G	C6-C5-N7	6.38	134.23	130.40
62	N6	57	LEU	CA-CB-CG	6.38	129.98	115.30
36	1	2363	A	N1-C6-N6	-6.38	114.77	118.60
36	1	1495	U	C2-N3-C4	-6.37	123.18	127.00
37	7	110	G	C8-N9-C4	6.37	108.95	106.40
36	1	2812	C	O5'-P-OP1	-6.37	99.97	105.70
36	1	1891	A	C8-N9-C4	6.36	108.35	105.80
36	5	776	U	N1-C2-N3	6.36	118.72	114.90
36	1	2306	C	N1-C2-O2	6.36	122.72	118.90
36	1	2870	C	C6-N1-C1'	6.35	128.42	120.80
36	5	1904	C	N1-C2-O2	6.35	122.71	118.90
36	5	1152	G	C5-C6-N1	-6.35	108.33	111.50
1	2	1508	U	N3-C4-C5	-6.34	110.79	114.60
1	6	321	C	N3-C2-O2	-6.34	117.46	121.90
1	2	1370	U	P-O3'-C3'	6.34	127.31	119.70
1	2	1246	C	C6-N1-C2	-6.34	117.76	120.30
1	2	1745	G	N3-C4-N9	6.33	129.80	126.00
1	6	542	A	O4'-C1'-N9	6.33	113.26	108.20
36	1	439	C	C2-N1-C1'	6.33	125.76	118.80
36	5	1481	A	P-O3'-C3'	6.32	127.28	119.70
36	5	2726	C	N3-C4-N4	-6.32	113.58	118.00
36	5	3308	C	N1-C2-O2	-6.32	115.11	118.90
1	6	1700	C	N1-C2-O2	6.32	122.69	118.90
1	2	1389	C	C2-N1-C1'	6.32	125.75	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2887	A	C2-N3-C4	6.32	113.76	110.60
36	5	1483	G	O4'-C1'-N9	6.32	113.25	108.20
36	5	2411	U	C5-C6-N1	-6.32	119.54	122.70
37	7	49	G	C5-C6-O6	-6.31	124.81	128.60
1	2	75	U	C2-N1-C1'	6.31	125.27	117.70
36	5	2349	U	OP1-P-O3'	6.31	119.08	105.20
36	1	1060	U	C5-C6-N1	-6.31	119.55	122.70
1	6	272	U	C2-N1-C1'	6.30	125.27	117.70
1	6	609	U	C5-C4-O4	6.30	129.68	125.90
4	s2	113	LEU	CA-CB-CG	6.30	129.79	115.30
1	6	75	U	P-O3'-C3'	6.30	127.26	119.70
1	6	1000	C	C2-N1-C1'	6.30	125.73	118.80
1	2	1761	U	C5-C4-O4	6.29	129.67	125.90
36	5	1196	C	C6-N1-C2	6.28	122.81	120.30
36	1	3375	A	C8-N9-C4	-6.28	103.29	105.80
36	5	2376	G	N3-C4-N9	6.28	129.76	126.00
36	1	496	C	C6-N1-C2	-6.27	117.79	120.30
1	2	1258	U	N3-C2-O2	-6.27	117.81	122.20
36	5	2327	U	C6-N1-C2	6.27	124.76	121.00
36	5	2830	G	N1-C2-N3	6.26	127.66	123.90
36	5	2971	A	N1-C2-N3	-6.26	126.17	129.30
36	1	2875	U	N3-C2-O2	-6.25	117.83	122.20
1	2	1389	C	C6-N1-C2	-6.24	117.80	120.30
36	1	960	U	C6-N1-C2	6.24	124.75	121.00
36	1	2827	U	C6-N1-C1'	6.24	129.93	121.20
36	1	1196	C	C6-N1-C2	6.24	122.79	120.30
36	5	3215	A	N1-C6-N6	6.24	122.34	118.60
36	1	2816	G	C6-C5-N7	-6.23	126.66	130.40
36	5	966	U	N3-C2-O2	-6.23	117.84	122.20
1	6	687	G	N3-C4-N9	-6.23	122.26	126.00
36	5	1452	A	C5-C6-N6	-6.22	118.72	123.70
36	1	1192	C	N1-C2-O2	6.22	122.63	118.90
36	1	895	A	C5-N7-C8	-6.22	100.79	103.90
36	5	1129	A	O5'-P-OP2	-6.21	100.11	105.70
36	1	3000	A	C8-N9-C4	6.21	108.28	105.80
36	1	2282	U	O5'-P-OP2	-6.20	100.12	105.70
1	6	610	G	C8-N9-C1'	-6.20	118.94	127.00
36	1	857	G	N1-C6-O6	6.20	123.62	119.90
36	1	3382	U	N3-C2-O2	-6.20	117.86	122.20
36	5	2211	U	C4-C5-C6	6.20	123.42	119.70
36	1	3110	C	C6-N1-C2	-6.19	117.82	120.30
36	1	979	U	C6-N1-C2	-6.19	117.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	882	A	N1-C2-N3	6.19	132.40	129.30
36	1	2899	C	C2-N1-C1'	6.19	125.61	118.80
36	5	224	C	C6-N1-C2	-6.18	117.83	120.30
1	2	287	G	O4'-C1'-N9	6.18	113.15	108.20
36	5	1495	U	C2-N1-C1'	6.18	125.12	117.70
36	5	1437	C	C2-N1-C1'	6.18	125.60	118.80
1	6	1745	G	N9-C4-C5	-6.17	102.93	105.40
36	1	2621	G	O5'-P-OP2	-6.17	100.14	105.70
36	1	3095	U	O5'-P-OP1	-6.17	100.15	105.70
36	5	1389	G	N9-C4-C5	-6.17	102.93	105.40
36	1	2719	U	N1-C2-O2	-6.16	118.49	122.80
36	5	1849	C	C6-N1-C2	6.16	122.77	120.30
36	5	923	C	C6-N1-C2	6.16	122.77	120.30
1	6	934	C	N1-C2-O2	6.16	122.60	118.90
36	5	2372	A	C5-C6-N6	-6.16	118.77	123.70
36	5	3152	U	C6-N1-C1'	-6.16	112.58	121.20
36	5	2601	A	C8-N9-C4	6.15	108.26	105.80
36	5	3120	C	O5'-P-OP1	-6.15	100.16	105.70
36	1	1820	U	P-O3'-C3'	6.15	127.08	119.70
36	1	3266	G	N9-C4-C5	6.15	107.86	105.40
37	7	101	G	N9-C4-C5	-6.13	102.95	105.40
38	8	80	A	C5-N7-C8	-6.13	100.84	103.90
36	5	2197	C	C6-N1-C2	6.13	122.75	120.30
36	5	3245	A	N1-C2-N3	6.13	132.36	129.30
36	1	3057	U	N3-C2-O2	-6.12	117.91	122.20
37	7	103	A	C5-C6-N6	-6.12	118.80	123.70
36	1	3375	A	N7-C8-N9	6.12	116.86	113.80
36	5	2330	C	O5'-P-OP2	-6.11	100.20	105.70
1	2	934	C	C6-N1-C1'	-6.11	113.47	120.80
36	1	1351	U	C2-N1-C1'	6.11	125.03	117.70
36	5	3323	A	N1-C6-N6	-6.11	114.94	118.60
36	1	1306	G	C8-N9-C4	6.10	108.84	106.40
36	5	1940	G	C8-N9-C4	6.10	108.84	106.40
1	2	1698	G	P-O3'-C3'	6.10	127.02	119.70
1	6	308	C	C5-C6-N1	-6.10	117.95	121.00
37	3	115	G	C8-N9-C4	6.10	108.84	106.40
36	1	1727	G	C8-N9-C4	-6.09	103.96	106.40
36	5	3382	U	C2-N1-C1'	6.09	125.01	117.70
36	5	2726	C	N1-C2-N3	6.09	123.46	119.20
36	5	3040	A	C8-N9-C4	6.08	108.23	105.80
36	5	2403	G	O5'-P-OP2	-6.08	100.22	105.70
1	6	558	U	P-O3'-C3'	6.08	127.00	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	610	G	C4-N9-C1'	6.07	134.40	126.50
36	5	1014	U	C2-N1-C1'	6.07	124.99	117.70
36	5	1484	U	C5-C6-N1	-6.07	119.67	122.70
36	5	1604	G	N3-C4-N9	6.07	129.64	126.00
1	2	1006	C	C6-N1-C2	-6.07	117.87	120.30
36	5	2719	U	C2-N1-C1'	-6.06	110.43	117.70
1	2	732	G	N3-C4-N9	6.06	129.63	126.00
36	1	1333	C	C6-N1-C2	-6.06	117.88	120.30
36	1	2679	A	O4'-C1'-N9	6.06	113.05	108.20
36	5	63	A	N1-C6-N6	6.06	122.24	118.60
36	5	1597	C	C6-N1-C2	-6.06	117.88	120.30
36	1	1206	G	O5'-P-OP2	-6.06	100.25	105.70
36	5	3018	C	O5'-P-OP2	-6.05	100.26	105.70
36	1	2714	G	C8-N9-C1'	6.04	134.86	127.00
1	6	858	G	O4'-C1'-N9	6.04	113.03	108.20
36	5	1239	C	C5-C6-N1	6.04	124.02	121.00
1	2	704	C	N1-C2-O2	6.04	122.52	118.90
1	6	359	A	C4-N9-C1'	-6.04	115.43	126.30
41	14	339	LEU	CA-CB-CG	6.04	129.19	115.30
1	6	1745	G	C8-N9-C1'	-6.04	119.16	127.00
36	5	2541	U	C2-N1-C1'	6.04	124.94	117.70
36	1	406	G	N9-C4-C5	6.03	107.81	105.40
36	1	2836	C	C5-C4-N4	6.03	124.42	120.20
36	1	2403	G	O5'-P-OP2	-6.03	100.27	105.70
1	2	577	G	C5-C6-O6	-6.03	124.98	128.60
1	2	1096	C	C6-N1-C1'	-6.03	113.57	120.80
10	S8	29	LEU	CA-CB-CG	6.02	129.15	115.30
36	5	1006	A	O5'-P-OP1	6.02	117.92	110.70
36	5	2320	A	C2-N3-C4	-6.02	107.59	110.60
48	m1	12	LEU	CA-CB-CG	6.02	129.14	115.30
36	1	2174	G	C8-N9-C4	-6.01	104.00	106.40
36	1	282	G	C2'-C3'-O3'	6.01	123.31	113.70
36	1	340	C	N3-C4-C5	6.01	124.30	121.90
36	1	2618	G	N1-C6-O6	-6.01	116.30	119.90
36	1	2316	G	N1-C6-O6	6.01	123.50	119.90
36	1	715	A	C8-N9-C4	-6.00	103.40	105.80
1	6	42	G	O4'-C1'-N9	6.00	113.00	108.20
36	5	2231	C	C2-N1-C1'	6.00	125.40	118.80
36	5	2847	A	C8-N9-C4	6.00	108.20	105.80
36	1	907	G	O4'-C1'-N9	6.00	113.00	108.20
36	1	2620	G	N1-C6-O6	6.00	123.50	119.90
1	6	1389	C	C2-N1-C1'	6.00	125.39	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2707	C	C5-C4-N4	-6.00	116.00	120.20
36	5	2340	U	C5-C6-N1	5.99	125.70	122.70
40	13	102	LEU	CA-CB-CG	5.99	129.08	115.30
1	6	427	C	C6-N1-C2	5.99	122.70	120.30
1	6	542	A	P-O3'-C3'	5.99	126.89	119.70
36	5	669	U	N3-C2-O2	-5.99	118.01	122.20
36	5	2211	U	N3-C2-O2	-5.99	118.01	122.20
36	5	2853	A	C8-N9-C4	5.99	108.19	105.80
36	1	1556	C	N1-C2-O2	5.98	122.49	118.90
36	5	1148	G	N1-C6-O6	5.98	123.49	119.90
36	1	1427	U	C6-N1-C2	5.98	124.59	121.00
36	5	2798	C	C2-N1-C1'	-5.98	112.22	118.80
36	5	3153	U	N1-C2-O2	5.98	126.98	122.80
1	2	75	U	N1-C2-O2	5.97	126.98	122.80
36	5	350	C	N3-C2-O2	-5.97	117.72	121.90
36	1	55	G	C8-N9-C4	5.97	108.79	106.40
36	1	1346	G	O5'-P-OP2	-5.97	100.33	105.70
1	2	728	U	C2-N1-C1'	5.97	124.86	117.70
1	6	1537	C	C5-C4-N4	-5.96	116.03	120.20
36	1	2979	U	C2-N3-C4	5.96	130.58	127.00
36	1	3382	U	C2-N1-C1'	5.96	124.85	117.70
36	1	922	U	N1-C2-O2	5.96	126.97	122.80
36	1	2364	G	N1-C6-O6	-5.96	116.33	119.90
36	5	1885	U	C6-N1-C2	5.96	124.57	121.00
1	6	610	G	N3-C4-N9	5.95	129.57	126.00
36	5	3200	G	N1-C6-O6	5.95	123.47	119.90
36	1	2706	G	N1-C6-O6	5.95	123.47	119.90
36	5	2659	G	C5-C6-O6	-5.95	125.03	128.60
47	M0	24	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	2	499	U	C2-N1-C1'	5.94	124.83	117.70
36	5	1938	U	C6-N1-C2	5.94	124.56	121.00
1	2	1241	G	O4'-C1'-N9	5.94	112.95	108.20
36	5	652	G	OP2-P-O3'	5.94	118.27	105.20
36	5	2730	G	N1-C6-O6	5.94	123.46	119.90
36	1	979	U	P-O3'-C3'	5.94	126.83	119.70
36	5	667	C	OP1-P-O3'	5.94	118.26	105.20
36	5	2872	A	C4-N9-C1'	-5.93	115.62	126.30
36	1	2364	G	C6-C5-N7	5.93	133.96	130.40
36	1	2227	C	P-O3'-C3'	5.93	126.81	119.70
36	5	406	G	C4-N9-C1'	-5.92	118.80	126.50
1	2	864	U	C6-N1-C2	-5.92	117.45	121.00
1	6	609	U	C5-C6-N1	-5.92	119.74	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1332	C	C6-N1-C2	-5.92	117.93	120.30
36	1	1404	G	C8-N9-C4	5.91	108.76	106.40
36	1	2808	A	N9-C4-C5	-5.91	103.44	105.80
36	5	826	G	C5-C6-O6	-5.91	125.06	128.60
36	5	2593	A	P-O3'-C3'	5.91	126.79	119.70
36	5	1496	C	O5'-P-OP1	5.91	117.79	110.70
36	5	48	A	N1-C6-N6	-5.91	115.06	118.60
36	5	2189	U	O5'-P-OP1	-5.91	100.39	105.70
36	5	2197	C	N3-C2-O2	5.91	126.03	121.90
42	l5	110	LEU	CA-CB-CG	5.91	128.88	115.30
36	1	696	C	C6-N1-C2	5.90	122.66	120.30
1	2	1761	U	P-O3'-C3'	5.89	126.77	119.70
36	1	1604	G	C4-N9-C1'	5.89	134.16	126.50
36	5	1433	A	C8-N9-C4	-5.89	103.44	105.80
36	1	28	C	C6-N1-C2	5.89	122.66	120.30
36	1	510	G	N1-C6-O6	5.89	123.43	119.90
36	1	2314	U	N3-C4-O4	5.89	123.52	119.40
1	2	934	C	N1-C2-O2	5.88	122.43	118.90
36	1	2112	U	P-O3'-C3'	5.88	126.76	119.70
36	1	3059	G	OP1-P-O3'	5.88	118.14	105.20
36	5	3368	U	C5-C6-N1	-5.88	119.76	122.70
1	2	1490	C	C6-N1-C2	-5.88	117.95	120.30
36	1	895	A	C4-C5-N7	5.88	113.64	110.70
36	5	1452	A	N1-C6-N6	5.88	122.12	118.60
1	6	1458	G	C4-N9-C1'	5.87	134.13	126.50
36	5	2524	A	N9-C1'-C2'	5.87	121.64	114.00
36	1	439	C	C6-N1-C1'	-5.87	113.75	120.80
36	1	1152	G	O4'-C1'-N9	5.87	112.90	108.20
36	5	1816	A	OP1-P-O3'	5.87	118.12	105.20
36	1	1308	A	C2-N3-C4	-5.87	107.67	110.60
36	5	2726	C	N3-C4-C5	-5.87	119.55	121.90
1	2	833	U	O5'-P-OP2	5.87	117.74	110.70
36	1	1149	G	C8-N9-C4	5.87	108.75	106.40
36	1	2873	U	O4'-C1'-N1	5.87	112.89	108.20
1	6	25	C	C2-N1-C1'	5.87	125.25	118.80
36	5	1437	C	C6-N1-C2	-5.86	117.95	120.30
1	2	736	C	C5-C6-N1	5.86	123.93	121.00
36	1	1324	U	O5'-P-OP2	-5.86	100.43	105.70
1	2	734	A	P-O3'-C3'	5.86	126.73	119.70
20	c8	116	LEU	CA-CB-CG	5.86	128.78	115.30
36	1	671	U	O5'-P-OP2	-5.86	100.43	105.70
1	2	720	G	P-O3'-C3'	5.86	126.73	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	406	G	N1-C6-O6	-5.85	116.39	119.90
36	5	1901	A	C8-N9-C4	-5.85	103.46	105.80
15	C3	22	ALA	C-N-CD	-5.85	107.73	120.60
36	5	282	G	P-O3'-C3'	5.85	126.72	119.70
41	14	327	LEU	CA-CB-CG	5.85	128.75	115.30
36	5	1308	A	C8-N9-C4	-5.85	103.46	105.80
36	5	2625	C	C6-N1-C2	5.84	122.64	120.30
1	6	144	U	C6-N1-C2	-5.84	117.49	121.00
36	5	2406	C	N3-C2-O2	5.84	125.99	121.90
36	1	1313	G	C5-C6-O6	-5.84	125.10	128.60
36	1	2885	C	C6-N1-C2	5.84	122.64	120.30
36	5	1017	C	C2-N1-C1'	5.84	125.22	118.80
1	6	548	G	N1-C6-O6	5.83	123.40	119.90
36	5	943	U	O5'-P-OP1	-5.83	100.45	105.70
36	1	1377	G	C5-C6-O6	-5.83	125.10	128.60
36	1	517	G	N3-C4-N9	5.83	129.50	126.00
36	1	410	U	C6-N1-C2	-5.82	117.51	121.00
36	5	804	C	N3-C4-C5	-5.82	119.57	121.90
36	1	1494	U	C2-N1-C1'	-5.82	110.71	117.70
36	5	1203	A	N1-C6-N6	5.82	122.09	118.60
36	5	2341	A	C8-N9-C4	5.82	108.13	105.80
36	5	2843	U	N3-C2-O2	-5.81	118.13	122.20
36	1	695	C	C6-N1-C2	5.81	122.62	120.30
36	1	1846	C	N1-C2-O2	-5.81	115.41	118.90
36	1	1371	G	C8-N9-C4	5.81	108.72	106.40
20	c8	15	LEU	CA-CB-CG	5.81	128.66	115.30
36	5	1716	U	P-O3'-C3'	5.81	126.67	119.70
36	1	406	G	C8-N9-C1'	5.81	134.55	127.00
36	5	56	G	O5'-P-OP2	-5.81	100.47	105.70
36	1	1548	C	N1-C2-O2	-5.80	115.42	118.90
36	1	2918	G	C8-N9-C4	-5.80	104.08	106.40
1	6	151	G	N3-C4-N9	-5.80	122.52	126.00
36	5	1152	G	N9-C4-C5	5.80	107.72	105.40
36	5	2872	A	C6-C5-N7	5.80	136.36	132.30
36	5	1350	A	N1-C6-N6	-5.80	115.12	118.60
36	5	437	G	C4-C5-N7	5.80	113.12	110.80
1	6	163	G	N3-C4-C5	5.80	131.50	128.60
36	5	1379	G	N9-C4-C5	-5.80	103.08	105.40
1	6	1764	C	C6-N1-C2	5.79	122.62	120.30
36	5	2899	C	N3-C2-O2	-5.79	117.84	121.90
1	2	1339	C	P-O3'-C3'	5.79	126.65	119.70
36	1	949	C	N1-C2-O2	-5.79	115.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	785	G	N3-C4-C5	-5.79	125.71	128.60
36	1	2571	U	N1-C2-O2	5.79	126.85	122.80
36	1	1838	G	C6-C5-N7	-5.79	126.93	130.40
36	1	3143	C	N3-C2-O2	5.79	125.95	121.90
1	6	647	G	N3-C4-N9	-5.79	122.53	126.00
36	5	3294	A	N1-C6-N6	-5.79	115.13	118.60
1	2	1189	A	C8-N9-C4	5.78	108.11	105.80
36	5	1495	U	C5-C6-N1	5.78	125.59	122.70
36	5	3161	C	C6-N1-C2	-5.78	117.99	120.30
1	2	1332	C	C5-C6-N1	5.78	123.89	121.00
36	1	627	U	C2-N1-C1'	-5.78	110.77	117.70
1	6	453	U	N1-C2-O2	5.77	126.84	122.80
1	2	1052	U	C2-N1-C1'	5.77	124.62	117.70
36	1	2355	G	C6-C5-N7	-5.77	126.94	130.40
36	1	979	U	N1-C2-N3	5.77	118.36	114.90
36	1	3218	A	P-O3'-C3'	5.77	126.62	119.70
36	5	406	G	C6-C5-N7	5.77	133.86	130.40
37	3	95	A	C8-N9-C4	-5.76	103.50	105.80
36	5	1433	A	C2-N3-C4	5.76	113.48	110.60
36	5	2897	A	C5-C6-N6	-5.76	119.09	123.70
36	1	2873	U	N3-C2-O2	-5.76	118.17	122.20
36	1	1417	G	C8-N9-C4	5.76	108.70	106.40
36	1	517	G	C4-N9-C1'	5.76	133.98	126.50
36	1	1177	G	N3-C2-N2	-5.76	115.87	119.90
37	7	77	G	C8-N9-C4	5.76	108.70	106.40
36	1	2873	U	C5-C4-O4	5.75	129.35	125.90
36	5	1503	A	C8-N9-C4	5.75	108.10	105.80
36	5	2364	G	N1-C6-O6	-5.75	116.45	119.90
36	5	2870	C	C2-N3-C4	-5.75	117.02	119.90
36	5	2876	C	O5'-P-OP1	-5.75	100.52	105.70
36	1	2996	U	C2-N1-C1'	5.74	124.59	117.70
36	1	645	A	C8-N9-C4	-5.74	103.50	105.80
36	5	2113	A	C8-N9-C4	5.74	108.09	105.80
36	5	1379	G	N3-C4-N9	5.73	129.44	126.00
36	5	1119	C	C6-N1-C2	5.73	122.59	120.30
36	5	1437	C	C5-C6-N1	5.73	123.87	121.00
1	2	1761	U	C6-N1-C2	-5.73	117.56	121.00
36	5	661	G	O5'-P-OP1	-5.73	100.54	105.70
1	2	145	A	N9-C4-C5	5.73	108.09	105.80
36	1	2364	G	N3-C4-N9	-5.73	122.56	126.00
36	5	1373	A	N1-C6-N6	5.73	122.04	118.60
36	5	2797	C	N3-C4-C5	-5.73	119.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2832	C	C6-N1-C2	5.73	122.59	120.30
36	5	2943	G	C5-C6-O6	-5.73	125.16	128.60
36	1	2818	U	C6-N1-C2	-5.72	117.57	121.00
36	5	3050	U	C5-C4-O4	5.71	129.33	125.90
36	1	2197	C	C6-N1-C2	5.71	122.58	120.30
36	1	1604	G	N3-C4-N9	5.71	129.42	126.00
38	4	125	U	C6-N1-C1'	-5.71	113.21	121.20
36	1	73	C	N1-C2-O2	-5.70	115.48	118.90
36	1	3214	U	N3-C2-O2	-5.70	118.21	122.20
36	5	942	U	N3-C4-O4	5.70	123.39	119.40
36	1	1081	U	C2-N1-C1'	5.70	124.54	117.70
36	1	1663	C	C6-N1-C2	5.70	122.58	120.30
36	5	3218	A	P-O3'-C3'	5.70	126.53	119.70
36	1	2725	U	C5-C6-N1	-5.69	119.85	122.70
36	1	360	G	N3-C4-C5	-5.69	125.75	128.60
36	1	1365	G	N3-C4-C5	-5.69	125.75	128.60
1	6	144	U	N1-C2-O2	5.69	126.78	122.80
1	6	310	C	N3-C4-C5	-5.69	119.62	121.90
36	5	1429	G	N9-C4-C5	-5.69	103.12	105.40
36	5	3140	G	C6-C5-N7	-5.69	126.99	130.40
36	5	437	G	C5-N7-C8	-5.68	101.46	104.30
36	5	3228	C	C2-N1-C1'	5.68	125.05	118.80
33	e1	100	LEU	CA-CB-CG	5.68	128.36	115.30
36	5	1462	A	N1-C6-N6	5.68	122.01	118.60
36	5	890	C	O5'-P-OP2	-5.67	100.59	105.70
1	6	1000	C	N3-C2-O2	-5.67	117.93	121.90
1	6	1399	C	C6-N1-C2	-5.67	118.03	120.30
36	5	48	A	N9-C4-C5	5.67	108.07	105.80
36	5	835	G	O4'-C1'-N9	5.67	112.74	108.20
36	1	2572	C	C6-N1-C2	-5.67	118.03	120.30
36	5	2875	U	C6-N1-C2	-5.67	117.60	121.00
1	2	782	U	P-O3'-C3'	5.67	126.50	119.70
37	3	91	G	C8-N9-C4	-5.66	104.14	106.40
36	5	2943	G	O5'-P-OP2	-5.66	100.61	105.70
36	5	112	U	O5'-P-OP1	-5.65	100.61	105.70
36	5	718	G	C4-N9-C1'	5.65	133.85	126.50
36	5	2901	G	C5-C6-O6	-5.65	125.21	128.60
36	1	2434	U	C5-C4-O4	5.65	129.29	125.90
36	5	2440	G	C8-N9-C4	-5.65	104.14	106.40
36	5	2897	A	N1-C6-N6	5.65	121.99	118.60
36	1	1874	A	O5'-P-OP1	-5.65	100.62	105.70
1	2	959	U	N3-C2-O2	-5.65	118.25	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3238	G	C5-C6-O6	-5.65	125.21	128.60
36	5	2366	C	C6-N1-C2	-5.65	118.04	120.30
36	1	709	A	C8-N9-C4	5.64	108.06	105.80
36	1	2418	G	C2-N3-C4	5.64	114.72	111.90
36	1	2385	G	C8-N9-C4	5.64	108.66	106.40
36	5	1885	U	C5-C6-N1	-5.64	119.88	122.70
36	1	2231	C	C6-N1-C2	5.63	122.55	120.30
36	5	374	A	N9-C4-C5	5.63	108.05	105.80
36	1	2836	C	N3-C2-O2	-5.63	117.96	121.90
36	5	274	G	C8-N9-C4	5.63	108.65	106.40
36	5	2531	C	N3-C2-O2	-5.63	117.96	121.90
36	1	2355	G	N9-C4-C5	-5.62	103.15	105.40
36	1	1351	U	N3-C2-O2	-5.62	118.27	122.20
36	5	432	G	C8-N9-C4	5.62	108.65	106.40
36	5	998	A	OP2-P-O3'	5.62	117.57	105.20
36	5	1374	G	C8-N9-C4	5.62	108.65	106.40
36	5	2573	G	C5-C6-O6	-5.62	125.23	128.60
1	2	829	A	P-O3'-C3'	5.62	126.44	119.70
36	5	366	A	OP1-P-O3'	5.62	117.56	105.20
36	5	499	G	O5'-P-OP1	-5.62	100.64	105.70
36	5	170	G	C4-N9-C1'	5.61	133.80	126.50
36	5	3347	A	C8-N9-C4	5.61	108.05	105.80
36	5	2146	C	C6-N1-C2	-5.61	118.06	120.30
36	5	1429	G	C8-N9-C4	5.61	108.64	106.40
1	2	734	A	OP1-P-O3'	5.61	117.54	105.20
36	5	358	G	C5-C6-O6	-5.61	125.24	128.60
36	5	2353	G	C5-C6-O6	-5.61	125.24	128.60
36	5	2378	C	C6-N1-C2	-5.61	118.06	120.30
37	7	77	G	O5'-P-OP1	5.61	117.43	110.70
1	2	831	U	C6-N1-C2	-5.61	117.64	121.00
1	2	426	G	C4-N9-C1'	5.60	133.78	126.50
36	1	1294	A	O4'-C1'-N9	5.60	112.68	108.20
36	5	2406	C	C5-C4-N4	-5.60	116.28	120.20
1	2	17	C	C6-N1-C2	-5.60	118.06	120.30
36	5	817	A	C5-C6-N1	5.60	120.50	117.70
36	5	1014	U	C6-N1-C1'	-5.60	113.36	121.20
1	2	1100	G	N9-C4-C5	-5.59	103.16	105.40
36	5	410	U	N3-C4-C5	-5.59	111.24	114.60
36	5	677	A	N1-C6-N6	5.59	121.95	118.60
36	5	2376	G	O5'-P-OP2	-5.59	100.67	105.70
1	2	1363	U	N1-C2-O2	5.59	126.71	122.80
36	5	2283	G	N3-C4-C5	5.59	131.39	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1494	U	C5-C4-O4	5.58	129.25	125.90
36	5	1704	A	C8-N9-C4	5.58	108.03	105.80
36	1	1595	U	C2-N1-C1'	-5.58	111.00	117.70
36	1	1849	C	N1-C2-O2	-5.58	115.55	118.90
1	2	581	U	C2-N1-C1'	5.58	124.40	117.70
1	2	1596	C	N1-C2-O2	5.58	122.25	118.90
36	5	882	A	C6-N1-C2	-5.58	115.25	118.60
44	17	229	PHE	CB-CG-CD2	-5.58	116.89	120.80
36	1	817	A	C8-N9-C4	5.58	108.03	105.80
36	1	2387	A	C8-N9-C4	5.58	108.03	105.80
36	1	2905	U	N3-C2-O2	5.58	126.10	122.20
1	2	1600	A	C2-N3-C4	-5.57	107.81	110.60
36	1	1300	G	C4-C5-N7	5.57	113.03	110.80
36	5	1391	C	C6-N1-C2	5.57	122.53	120.30
36	1	1495	U	C6-N1-C1'	5.57	129.00	121.20
36	1	3190	C	C6-N1-C2	5.57	122.53	120.30
36	5	874	U	O5'-P-OP1	-5.57	100.69	105.70
36	5	2823	G	N1-C6-O6	5.57	123.24	119.90
36	1	3143	C	N1-C2-O2	-5.56	115.56	118.90
1	6	687	G	N3-C2-N2	-5.56	116.00	119.90
1	2	720	G	OP1-P-O3'	5.56	117.44	105.20
36	1	2966	G	N9-C4-C5	-5.56	103.17	105.40
1	6	453	U	C6-N1-C2	-5.56	117.66	121.00
1	6	1058	U	P-O3'-C3'	5.56	126.38	119.70
36	1	14	U	O5'-P-OP2	-5.56	100.69	105.70
36	1	1380	G	O5'-P-OP1	5.56	117.37	110.70
36	5	1192	C	N3-C2-O2	-5.56	118.01	121.90
36	1	1929	G	C8-N9-C4	5.56	108.62	106.40
38	4	53	A	C2-N3-C4	5.56	113.38	110.60
36	5	867	G	O5'-P-OP2	5.56	117.37	110.70
36	1	1875	G	N7-C8-N9	-5.56	110.32	113.10
36	1	3268	A	N1-C6-N6	5.56	121.93	118.60
36	5	2156	C	C6-N1-C2	5.56	122.52	120.30
36	1	2403	G	C6-C5-N7	-5.55	127.07	130.40
36	1	2726	C	N1-C2-N3	5.55	123.09	119.20
1	6	308	C	N3-C4-N4	-5.55	114.11	118.00
36	5	3140	G	N9-C4-C5	-5.55	103.18	105.40
36	1	2376	G	N7-C8-N9	5.55	115.88	113.10
36	5	406	G	C8-N9-C1'	5.55	134.22	127.00
36	1	2208	A	C6-N1-C2	-5.55	115.27	118.60
1	6	1022	C	O5'-P-OP1	-5.55	100.70	105.70
36	1	2861	U	O5'-P-OP1	-5.54	100.71	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3362	A	C2-N3-C4	-5.54	107.83	110.60
1	6	581	U	C2-N1-C1'	-5.54	111.05	117.70
36	5	2132	C	C6-N1-C2	-5.54	118.08	120.30
36	5	2621	G	C5-C6-O6	-5.54	125.28	128.60
36	5	2901	G	O5'-P-OP2	-5.54	100.71	105.70
1	2	158	U	P-O3'-C3'	5.54	126.35	119.70
36	5	2404	A	C6-C5-N7	5.54	136.18	132.30
36	5	2979	U	C2-N3-C4	5.54	130.32	127.00
36	1	2983	C	O4'-C1'-N1	5.54	112.63	108.20
12	C0	76	LEU	CA-CB-CG	5.54	128.03	115.30
36	1	3001	C	C6-N1-C2	5.54	122.51	120.30
1	6	1279	C	C6-N1-C2	-5.53	118.09	120.30
36	5	566	G	N7-C8-N9	5.53	115.87	113.10
36	1	1815	U	P-O3'-C3'	5.53	126.33	119.70
36	5	2772	C	P-O3'-C3'	5.53	126.34	119.70
36	5	2804	A	O5'-P-OP1	-5.53	100.72	105.70
36	1	2279	A	N1-C6-N6	5.53	121.92	118.60
36	1	1345	G	OP2-P-O3'	5.52	117.35	105.20
36	5	964	G	OP2-P-O3'	5.52	117.35	105.20
1	2	1573	A	P-O3'-C3'	5.52	126.33	119.70
38	8	77	A	C8-N9-C4	5.52	108.01	105.80
36	1	1207	G	C5-C6-O6	-5.52	125.29	128.60
36	1	953	G	N3-C4-C5	5.52	131.36	128.60
36	1	1368	U	O5'-P-OP1	-5.52	100.73	105.70
36	1	1484	U	P-O3'-C3'	5.52	126.32	119.70
36	1	2393	G	N3-C4-N9	5.52	129.31	126.00
36	5	2572	C	C6-N1-C1'	-5.52	114.18	120.80
36	1	2870	C	C2-N1-C1'	-5.51	112.73	118.80
36	5	1424	C	O5'-P-OP2	-5.51	100.74	105.70
36	5	645	A	C8-N9-C4	-5.51	103.59	105.80
36	5	2971	A	N3-C4-N9	5.51	131.81	127.40
37	7	1	G	C6-C5-N7	-5.51	127.09	130.40
36	1	2996	U	N3-C2-O2	-5.51	118.34	122.20
36	5	826	G	N1-C6-O6	5.51	123.21	119.90
36	5	3152	U	C2-N1-C1'	5.51	124.31	117.70
1	2	737	A	O4'-C1'-N9	5.51	112.61	108.20
36	1	57	A	C8-N9-C4	5.51	108.00	105.80
36	1	752	C	C6-N1-C2	5.51	122.50	120.30
1	2	74	U	P-O3'-C3'	5.50	126.30	119.70
1	2	502	U	C5-C6-N1	5.50	125.45	122.70
1	2	853	G	C4-C5-N7	5.50	113.00	110.80
36	5	922	U	C2-N3-C4	-5.50	123.70	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2385	G	N3-C4-N9	-5.50	122.70	126.00
36	5	2524	A	C5-N7-C8	-5.50	101.15	103.90
36	1	2875	U	N1-C1'-C2'	-5.50	105.95	112.00
36	5	2639	G	C8-N9-C4	-5.50	104.20	106.40
36	5	3214	U	O4'-C1'-N1	5.50	112.60	108.20
36	1	2283	G	N1-C6-O6	5.49	123.20	119.90
1	6	1736	G	N1-C6-O6	5.49	123.20	119.90
36	5	189	G	N1-C6-O6	-5.49	116.61	119.90
1	6	1596	C	N3-C2-O2	-5.49	118.06	121.90
36	5	1300	G	C5-C6-O6	-5.49	125.31	128.60
36	5	1487	G	N1-C6-O6	-5.49	116.61	119.90
36	1	2149	A	C8-N9-C4	5.49	108.00	105.80
1	6	214	G	N1-C6-O6	5.49	123.19	119.90
36	5	3195	U	N1-C2-O2	5.49	126.64	122.80
36	1	1929	G	N9-C4-C5	-5.48	103.21	105.40
36	1	2419	A	O5'-P-OP2	-5.48	100.77	105.70
36	1	226	C	C6-N1-C2	-5.48	118.11	120.30
36	1	1300	G	N9-C4-C5	-5.48	103.21	105.40
36	1	2314	U	C6-N1-C1'	-5.48	113.52	121.20
36	5	873	C	P-O3'-C3'	5.48	126.28	119.70
36	5	1445	U	C6-N1-C2	5.48	124.29	121.00
36	1	545	U	C2-N1-C1'	5.48	124.28	117.70
36	5	2298	U	C2-N1-C1'	-5.48	111.12	117.70
36	1	895	A	N7-C8-N9	5.48	116.54	113.80
36	5	2345	A	N1-C6-N6	5.48	121.89	118.60
36	1	2369	G	N3-C4-C5	-5.48	125.86	128.60
38	4	137	C	C6-N1-C2	5.48	122.49	120.30
1	2	1489	U	N3-C2-O2	-5.47	118.37	122.20
36	5	657	A	C8-N9-C4	5.47	107.99	105.80
36	5	1536	G	N1-C6-O6	5.47	123.18	119.90
36	1	1307	G	P-O3'-C3'	5.47	126.27	119.70
48	m1	43	GLN	C-N-CA	-5.47	108.02	121.70
1	2	1458	G	C4-N9-C1'	5.47	133.61	126.50
36	1	1300	G	C5-C6-O6	-5.47	125.32	128.60
1	6	359	A	C4-C5-C6	-5.47	114.27	117.00
1	2	1761	U	N3-C2-O2	-5.46	118.38	122.20
36	1	1741	A	N1-C2-N3	5.46	132.03	129.30
1	6	321	C	C6-N1-C2	-5.46	118.11	120.30
36	1	776	U	C5-C6-N1	-5.46	119.97	122.70
36	1	1269	U	C2-N1-C1'	5.46	124.25	117.70
62	N6	6	LEU	CA-CB-CG	-5.46	102.74	115.30
1	6	1421	A	C8-N9-C4	5.46	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1314	C	C5-C4-N4	-5.46	116.38	120.20
38	4	97	A	N1-C6-N6	-5.46	115.33	118.60
1	6	400	A	N1-C6-N6	5.46	121.88	118.60
36	1	2403	G	C5-C6-N1	-5.46	108.77	111.50
1	6	1458	G	C8-N9-C1'	-5.46	119.91	127.00
36	5	1367	G	C5-C6-N1	-5.46	108.77	111.50
36	1	1849	C	O5'-P-OP1	-5.45	100.79	105.70
1	6	1657	U	N1-C2-O2	5.45	126.62	122.80
36	1	1331	U	O4'-C1'-N1	-5.45	103.84	108.20
36	1	2766	U	N3-C2-O2	-5.45	118.39	122.20
36	1	2966	G	C4-C5-N7	5.45	112.98	110.80
1	6	1361	U	C6-N1-C1'	-5.45	113.57	121.20
36	5	2145	A	C8-N9-C4	-5.45	103.62	105.80
1	2	453	U	C6-N1-C2	-5.45	117.73	121.00
36	5	1867	A	N1-C6-N6	5.45	121.87	118.60
36	1	672	A	N1-C6-N6	5.45	121.87	118.60
36	5	282	G	C2'-C3'-O3'	5.45	122.42	113.70
36	1	2343	C	N3-C4-C5	5.44	124.08	121.90
36	1	3278	C	C6-N1-C2	-5.44	118.12	120.30
36	5	1453	A	C8-N9-C4	5.44	107.98	105.80
36	1	2593	A	P-O3'-C3'	5.44	126.23	119.70
36	1	397	A	N1-C6-N6	-5.44	115.34	118.60
36	1	2679	A	C2-N3-C4	-5.44	107.88	110.60
1	2	1596	C	C6-N1-C2	-5.44	118.13	120.30
36	1	651	G	N3-C4-C5	-5.44	125.88	128.60
1	2	75	U	N3-C2-O2	-5.43	118.40	122.20
36	1	760	G	O4'-C1'-N9	5.43	112.55	108.20
1	6	427	C	C5-C6-N1	-5.43	118.28	121.00
36	5	2618	G	C5-C6-N1	5.43	114.22	111.50
1	6	555	A	C8-N9-C4	-5.43	103.63	105.80
36	1	1306	G	C5-C6-O6	-5.43	125.34	128.60
36	1	1108	U	C5-C6-N1	-5.43	119.99	122.70
36	5	767	U	O4'-C1'-N1	5.43	112.54	108.20
36	5	1017	C	N1-C2-O2	5.43	122.16	118.90
36	1	2818	U	P-O3'-C3'	5.43	126.21	119.70
1	6	194	U	N3-C2-O2	-5.43	118.40	122.20
36	5	1506	A	C8-N9-C4	-5.43	103.63	105.80
36	5	2837	A	C8-N9-C4	5.43	107.97	105.80
36	1	1495	U	N1-C2-N3	5.42	118.16	114.90
1	6	339	C	C6-N1-C2	-5.42	118.13	120.30
36	1	1497	C	C6-N1-C2	-5.42	118.13	120.30
36	1	651	G	N3-C4-N9	5.42	129.25	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S1	181	LEU	CA-CB-CG	5.42	127.77	115.30
36	1	2650	U	C6-N1-C2	-5.42	117.75	121.00
36	5	2823	G	C5-C6-O6	-5.42	125.35	128.60
36	1	2714	G	C4-N9-C1'	-5.42	119.46	126.50
38	4	113	U	C2-N1-C1'	-5.42	111.20	117.70
1	6	1033	C	C5-C6-N1	-5.42	118.29	121.00
36	1	3214	U	C2-N1-C1'	5.41	124.20	117.70
38	4	57	C	C6-N1-C2	5.41	122.47	120.30
1	6	1514	U	N3-C2-O2	-5.41	118.41	122.20
36	5	2353	G	N1-C6-O6	5.41	123.15	119.90
36	1	501	A	C8-N9-C4	5.41	107.96	105.80
36	1	645	A	C5-C6-N1	5.41	120.41	117.70
1	2	1568	C	P-O3'-C3'	5.41	126.19	119.70
36	5	1794	G	N1-C2-N2	-5.41	111.33	116.20
36	1	30	G	N1-C6-O6	-5.41	116.66	119.90
36	1	1366	A	N1-C6-N6	5.41	121.84	118.60
36	1	1589	A	O4'-C1'-N9	-5.40	103.88	108.20
36	1	200	C	N3-C2-O2	-5.40	118.12	121.90
36	1	2808	A	N1-C6-N6	5.40	121.84	118.60
36	1	2873	U	N1-C2-N3	5.40	118.14	114.90
1	6	1657	U	N3-C2-O2	-5.40	118.42	122.20
36	5	2707	C	N3-C4-C5	5.40	124.06	121.90
1	2	1473	U	N3-C2-O2	-5.39	118.42	122.20
36	1	1377	G	C4-C5-N7	5.39	112.96	110.80
38	4	79	A	C8-N9-C4	-5.39	103.64	105.80
36	5	2950	G	O4'-C1'-N9	5.39	112.51	108.20
1	2	499	U	P-O3'-C3'	5.39	126.17	119.70
1	6	1340	U	N1-C2-O2	5.39	126.57	122.80
36	5	2519	A	O5'-P-OP1	-5.39	100.85	105.70
36	5	2802	A	OP2-P-O3'	5.38	117.04	105.20
36	1	2887	A	C5-C6-N6	-5.38	119.40	123.70
36	5	1000	C	C6-N1-C2	5.38	122.45	120.30
1	6	1745	G	C6-C5-N7	-5.38	127.17	130.40
36	1	3140	G	N1-C6-O6	5.38	123.12	119.90
36	5	283	G	C4-C5-N7	5.38	112.95	110.80
36	5	3323	A	N9-C4-C5	5.38	107.95	105.80
1	2	864	U	N3-C2-O2	-5.37	118.44	122.20
1	2	1361	U	N1-C2-O2	5.37	126.56	122.80
36	5	97	U	N3-C2-O2	5.37	125.96	122.20
36	5	2890	A	OP2-P-O3'	5.37	117.02	105.20
19	C7	84	TYR	C-N-CA	5.37	135.13	121.70
36	1	2745	G	C4-N9-C1'	-5.37	119.52	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	53	A	N1-C6-N6	-5.37	115.38	118.60
36	1	2366	C	O5'-P-OP2	-5.37	100.87	105.70
36	5	3073	A	C8-N9-C4	5.37	107.95	105.80
38	4	32	C	C6-N1-C2	5.37	122.45	120.30
1	2	830	U	C2-N1-C1'	5.36	124.14	117.70
36	1	645	A	C6-N1-C2	-5.36	115.38	118.60
36	1	1308	A	N1-C2-N3	5.36	131.98	129.30
36	5	2885	C	O5'-P-OP2	-5.36	100.87	105.70
36	1	274	G	C8-N9-C4	5.36	108.54	106.40
36	5	2402	A	C8-N9-C4	5.36	107.94	105.80
36	5	2280	A	N1-C6-N6	5.36	121.81	118.60
36	1	49	A	C5-C6-N1	-5.36	115.02	117.70
1	6	925	G	N1-C6-O6	5.36	123.11	119.90
36	5	1373	A	C5-C6-N6	-5.35	119.42	123.70
1	2	704	C	O4'-C1'-N1	5.35	112.48	108.20
1	6	934	C	C2-N1-C1'	5.35	124.69	118.80
36	5	639	G	C8-N9-C4	5.35	108.54	106.40
36	5	2211	U	C5-C4-O4	5.35	129.11	125.90
1	2	732	G	N9-C4-C5	-5.35	103.26	105.40
36	1	3308	C	N1-C2-O2	-5.35	115.69	118.90
38	4	124	G	P-O3'-C3'	-5.35	113.28	119.70
36	5	3195	U	P-O3'-C3'	5.35	126.12	119.70
36	1	1844	C	C6-N1-C2	5.35	122.44	120.30
38	4	20	U	C5-C6-N1	-5.34	120.03	122.70
36	1	2283	G	C5-C6-O6	-5.34	125.39	128.60
36	5	200	C	C6-N1-C2	-5.34	118.16	120.30
36	1	1733	G	N3-C4-C5	-5.34	125.93	128.60
36	1	1898	G	O5'-P-OP1	-5.34	100.89	105.70
36	1	1838	G	C5-C6-O6	-5.34	125.40	128.60
36	5	948	C	C5-C6-N1	-5.34	118.33	121.00
36	5	3104	U	N1-C2-O2	-5.34	119.06	122.80
36	5	3154	C	C6-N1-C1'	-5.34	114.40	120.80
1	6	1698	G	P-O3'-C3'	5.33	126.10	119.70
36	5	2385	G	O5'-P-OP1	-5.33	100.90	105.70
36	1	71	A	C8-N9-C4	-5.33	103.67	105.80
36	1	213	A	C8-N9-C4	5.33	107.93	105.80
1	6	214	G	C5-C6-O6	-5.33	125.40	128.60
36	1	3316	A	C2-N3-C4	-5.33	107.94	110.60
1	6	696	C	C2-N1-C1'	-5.33	112.94	118.80
36	5	2388	U	N3-C4-C5	-5.33	111.40	114.60
1	2	864	U	C5-C4-O4	5.33	129.10	125.90
36	1	2836	C	N3-C4-C5	-5.33	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2584	G	OP2-P-O3'	5.32	116.91	105.20
36	5	3088	G	O5'-P-OP2	5.32	117.09	110.70
36	1	859	G	N1-C2-N2	-5.32	111.41	116.20
36	1	2172	A	N1-C6-N6	5.32	121.79	118.60
1	6	194	U	C6-N1-C1'	-5.32	113.75	121.20
36	5	1462	A	C8-N9-C4	5.32	107.93	105.80
36	5	2514	U	O5'-P-OP1	-5.32	100.91	105.70
36	1	3362	A	N7-C8-N9	5.32	116.46	113.80
36	1	2946	A	C6-C5-N7	-5.32	128.58	132.30
36	5	1156	C	C6-N1-C2	-5.32	118.17	120.30
36	5	2385	G	C8-N9-C4	5.32	108.53	106.40
1	2	1051	G	P-O3'-C3'	5.32	126.08	119.70
36	1	1639	C	C6-N1-C2	-5.32	118.17	120.30
36	1	2700	G	C5-C6-O6	-5.32	125.41	128.60
1	6	25	C	N1-C2-O2	5.32	122.09	118.90
36	5	348	A	O5'-P-OP1	-5.32	100.92	105.70
36	5	2421	U	N1-C2-N3	5.32	118.09	114.90
1	2	1027	A	C4-C5-N7	5.31	113.36	110.70
36	1	27	C	O5'-P-OP1	-5.31	100.92	105.70
36	1	49	A	C2-N3-C4	-5.31	107.94	110.60
36	1	2846	U	N3-C2-O2	-5.31	118.48	122.20
1	2	386	G	N3-C4-C5	-5.31	125.95	128.60
36	1	2101	C	P-O3'-C3'	5.31	126.07	119.70
36	1	915	A	C8-N9-C4	-5.30	103.68	105.80
37	3	69	C	C6-N1-C2	-5.30	118.18	120.30
1	6	272	U	P-O3'-C3'	5.30	126.06	119.70
36	5	90	C	C6-N1-C2	-5.30	118.18	120.30
1	2	1503	A	O4'-C1'-N9	5.30	112.44	108.20
36	1	199	A	O4'-C1'-N9	5.30	112.44	108.20
36	5	2383	C	N1-C2-O2	-5.30	115.72	118.90
1	6	305	C	N1-C2-O2	-5.30	115.72	118.90
36	5	718	G	O4'-C1'-N9	5.30	112.44	108.20
1	2	1280	C	N3-C4-C5	-5.30	119.78	121.90
36	1	670	C	C6-N1-C2	5.30	122.42	120.30
36	1	2572	C	C6-N1-C1'	-5.30	114.44	120.80
36	5	1665	C	N1-C2-O2	5.30	122.08	118.90
36	5	2836	C	O4'-C1'-N1	5.30	112.44	108.20
1	2	577	G	N1-C6-O6	5.29	123.08	119.90
36	1	1604	G	C8-N9-C1'	-5.29	120.12	127.00
1	6	321	C	N1-C2-O2	5.29	122.08	118.90
36	1	334	A	N1-C6-N6	5.29	121.78	118.60
1	6	308	C	C2-N1-C1'	-5.29	112.98	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	188	A	O5'-P-OP1	-5.29	100.94	105.70
36	1	811	U	C4-C5-C6	5.29	122.87	119.70
36	1	3083	G	N3-C4-C5	-5.29	125.96	128.60
36	5	374	A	P-O3'-C3'	5.29	126.05	119.70
36	5	1628	C	C6-N1-C2	-5.29	118.19	120.30
36	1	3276	G	N3-C4-C5	5.29	131.24	128.60
1	6	558	U	C2-N1-C1'	5.29	124.04	117.70
1	6	877	G	N1-C6-O6	-5.29	116.73	119.90
36	5	922	U	N3-C2-O2	-5.29	118.50	122.20
1	2	1596	C	C2-N1-C1'	5.28	124.61	118.80
36	1	406	G	C4-C5-N7	-5.28	108.69	110.80
36	5	1430	U	C6-N1-C2	5.28	124.17	121.00
36	5	2231	C	O4'-C1'-N1	5.28	112.43	108.20
48	m1	112	LEU	CA-CB-CG	5.28	127.45	115.30
36	5	1448	U	C5-C6-N1	-5.28	120.06	122.70
36	5	2890	A	C8-N9-C4	-5.28	103.69	105.80
64	n8	73	LEU	CA-CB-CG	5.28	127.44	115.30
1	6	1750	A	O5'-P-OP2	-5.27	100.95	105.70
36	1	1822	C	C6-N1-C2	-5.27	118.19	120.30
64	N8	115	LYS	C-N-CA	-5.27	111.23	122.30
1	2	36	C	C6-N1-C2	5.27	122.41	120.30
36	1	2207	A	O4'-C1'-N9	5.27	112.42	108.20
38	4	22	U	C5-C6-N1	-5.27	120.06	122.70
36	1	547	G	P-O3'-C3'	5.27	126.02	119.70
1	6	609	U	N3-C4-O4	-5.27	115.71	119.40
1	6	965	U	N3-C2-O2	-5.27	118.51	122.20
36	1	304	G	N9-C4-C5	5.26	107.51	105.40
1	6	1523	G	N3-C4-N9	5.26	129.16	126.00
36	5	224	C	N1-C2-O2	5.26	122.06	118.90
36	5	1196	C	N1-C2-N3	-5.26	115.52	119.20
1	2	553	G	N1-C6-O6	5.26	123.06	119.90
18	c6	97	VAL	CA-CB-CG2	5.26	118.79	110.90
1	6	1361	U	N1-C2-O2	5.25	126.48	122.80
1	6	813	U	N1-C2-O2	5.25	126.48	122.80
36	5	3090	U	N3-C4-O4	-5.25	115.72	119.40
1	6	984	G	C8-N9-C4	5.25	108.50	106.40
36	5	2964	G	N9-C4-C5	5.25	107.50	105.40
1	2	610	G	C4-N9-C1'	5.25	133.32	126.50
1	2	704	C	C6-N1-C1'	-5.25	114.50	120.80
36	5	216	G	O5'-P-OP1	-5.25	100.98	105.70
36	1	2298	U	N3-C4-O4	-5.24	115.73	119.40
36	1	1113	G	N3-C2-N2	-5.24	116.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2872	A	N3-C4-C5	5.24	130.47	126.80
36	1	2809	C	C6-N1-C2	-5.24	118.20	120.30
36	5	418	A	N1-C6-N6	5.24	121.74	118.60
36	5	2744	U	O5'-P-OP2	-5.24	100.98	105.70
36	1	799	G	O5'-P-OP1	-5.24	100.98	105.70
36	1	2662	G	C6-C5-N7	-5.24	127.26	130.40
36	5	109	A	N1-C6-N6	-5.24	115.46	118.60
36	5	1379	G	C8-N9-C1'	-5.24	120.19	127.00
1	2	1027	A	C5-N7-C8	-5.23	101.28	103.90
36	1	2995	A	C8-N9-C4	5.23	107.89	105.80
24	D2	104	LEU	CA-CB-CG	5.23	127.33	115.30
36	1	715	A	P-O3'-C3'	5.23	125.98	119.70
36	5	2278	C	N1-C2-O2	5.23	122.04	118.90
36	5	3092	C	O4'-C1'-N1	5.23	112.39	108.20
36	5	2204	C	OP1-P-O3'	5.23	116.70	105.20
1	2	499	U	C6-N1-C1'	-5.23	113.88	121.20
36	1	2875	U	C4-C5-C6	5.23	122.84	119.70
36	5	1582	C	C5-C6-N1	5.23	123.61	121.00
36	5	1216	C	C6-N1-C2	-5.22	118.21	120.30
36	5	2663	G	C5-C6-O6	-5.22	125.47	128.60
36	1	658	G	C4-N9-C1'	5.22	133.29	126.50
36	1	676	G	N3-C4-C5	-5.22	125.99	128.60
36	1	1716	U	P-O3'-C3'	5.22	125.97	119.70
38	4	103	G	C8-N9-C4	-5.22	104.31	106.40
1	2	192	U	C2-N1-C1'	5.22	123.96	117.70
36	1	1433	A	N1-C6-N6	-5.22	115.47	118.60
36	1	2996	U	C6-N1-C1'	-5.22	113.89	121.20
1	6	1781	A	C8-N9-C4	-5.22	103.71	105.80
36	5	1117	G	C4-C5-N7	5.22	112.89	110.80
36	1	2852	C	C6-N1-C2	5.22	122.39	120.30
56	N0	24	LEU	CA-CB-CG	5.22	127.30	115.30
1	2	1658	G	C4-C5-N7	5.21	112.89	110.80
36	5	2372	A	C4-C5-C6	5.21	119.61	117.00
36	5	406	G	C5-C6-O6	5.21	131.73	128.60
36	5	2283	G	C8-N9-C4	5.21	108.48	106.40
36	1	2403	G	C5-C6-O6	-5.21	125.47	128.60
36	5	2388	U	N3-C4-O4	5.21	123.05	119.40
36	1	2620	G	C8-N9-C4	5.21	108.48	106.40
1	6	1696	G	C3'-C2'-C1'	5.21	105.66	101.50
36	5	3157	U	N1-C2-O2	5.20	126.44	122.80
3	S1	184	LEU	CA-CB-CG	5.20	127.26	115.30
1	2	1202	A	N1-C6-N6	-5.20	115.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	430	U	O5'-P-OP1	-5.20	101.02	105.70
36	5	660	A	OP1-P-OP2	5.20	127.40	119.60
36	5	2172	A	C8-N9-C4	5.20	107.88	105.80
36	1	76	G	N3-C4-C5	-5.20	126.00	128.60
36	1	883	A	N1-C2-N3	5.20	131.90	129.30
36	5	1879	A	N9-C4-C5	-5.20	103.72	105.80
36	5	2405	C	N3-C2-O2	-5.20	118.26	121.90
36	1	339	C	N3-C4-N4	-5.20	114.36	118.00
1	6	1185	U	N1-C2-O2	5.20	126.44	122.80
36	5	200	C	N3-C4-C5	-5.20	119.82	121.90
1	6	1535	U	N3-C2-O2	-5.19	118.56	122.20
36	1	968	G	C5-C6-O6	-5.19	125.48	128.60
36	1	2137	U	O4'-C1'-N1	5.19	112.35	108.20
36	1	2745	G	C8-N9-C4	5.19	108.48	106.40
33	e1	86	THR	C-N-CA	5.19	134.68	121.70
36	1	54	C	C6-N1-C2	5.19	122.38	120.30
36	5	2635	A	O5'-P-OP2	-5.19	101.03	105.70
36	5	2800	G	N1-C6-O6	5.19	123.01	119.90
36	1	783	A	N9-C4-C5	-5.19	103.73	105.80
36	5	2512	C	C5-C6-N1	5.19	123.59	121.00
1	2	1100	G	N1-C6-O6	5.18	123.01	119.90
36	1	1851	G	C5-C6-O6	-5.18	125.49	128.60
36	5	2662	G	N3-C4-C5	-5.18	126.01	128.60
36	5	3278	C	C6-N1-C2	5.18	122.37	120.30
36	5	1848	G	C4-C5-N7	5.18	112.87	110.80
36	5	1856	C	O5'-P-OP1	-5.18	101.04	105.70
1	6	1773	C	N1-C2-O2	-5.18	115.79	118.90
36	5	1885	U	N3-C2-O2	5.18	125.83	122.20
24	D2	65	LEU	CA-CB-CG	5.18	127.21	115.30
1	6	214	G	C4-C5-N7	5.18	112.87	110.80
1	6	295	A	C8-N9-C4	5.17	107.87	105.80
36	5	437	G	N7-C8-N9	5.17	115.69	113.10
1	2	321	C	O4'-C1'-N1	5.17	112.34	108.20
36	1	1604	G	N3-C4-C5	-5.17	126.01	128.60
36	1	2541	U	P-O3'-C3'	5.17	125.91	119.70
1	6	965	U	N1-C2-O2	5.17	126.42	122.80
37	7	81	U	C6-N1-C2	5.17	124.10	121.00
36	1	939	U	N3-C2-O2	5.17	125.82	122.20
36	1	1129	A	N1-C6-N6	5.17	121.70	118.60
36	1	2537	U	P-O3'-C3'	5.17	125.90	119.70
36	5	226	C	N1-C2-O2	5.17	122.00	118.90
36	5	2211	U	N3-C4-C5	-5.17	111.50	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	L7	207	LEU	CB-CG-CD1	-5.17	102.22	111.00
36	5	421	G	C4-N9-C1'	5.16	133.21	126.50
1	2	278	U	P-O3'-C3'	5.16	125.89	119.70
1	6	937	C	C6-N1-C2	-5.16	118.23	120.30
36	1	1838	G	N9-C4-C5	-5.16	103.34	105.40
37	3	115	G	N9-C4-C5	-5.16	103.34	105.40
1	2	187	G	P-O3'-C3'	5.16	125.89	119.70
36	1	2147	A	C8-N9-C4	5.16	107.86	105.80
36	5	2887	A	O4'-C1'-N9	-5.16	104.07	108.20
36	1	1111	U	C5-C6-N1	-5.16	120.12	122.70
37	7	1	G	C4-N9-C1'	5.16	133.20	126.50
36	1	1419	A	O5'-P-OP1	5.15	116.89	110.70
36	1	1902	G	N9-C4-C5	-5.15	103.34	105.40
36	5	1134	G	C8-N9-C4	5.15	108.46	106.40
36	1	2316	G	N9-C4-C5	-5.15	103.34	105.40
36	1	3046	A	C8-N9-C4	-5.15	103.74	105.80
1	6	987	G	N3-C4-N9	5.15	129.09	126.00
36	5	2234	G	N9-C4-C5	-5.15	103.34	105.40
36	5	3373	U	C5-C6-N1	-5.15	120.13	122.70
1	2	1363	U	N3-C2-O2	-5.14	118.60	122.20
36	1	1497	C	N3-C4-C5	-5.14	119.84	121.90
36	1	2983	C	C5-C4-N4	5.14	123.80	120.20
36	1	3276	G	O4'-C1'-N9	-5.14	104.08	108.20
36	5	2996	U	O5'-P-OP2	-5.14	101.07	105.70
1	2	240	U	OP2-P-O3'	5.14	116.51	105.20
36	1	817	A	N1-C6-N6	5.14	121.69	118.60
1	6	453	U	C5-C6-N1	5.14	125.27	122.70
1	6	1058	U	OP1-P-O3'	5.14	116.51	105.20
36	5	635	G	C4-C5-N7	5.14	112.86	110.80
36	5	1238	C	P-O3'-C3'	5.14	125.87	119.70
36	5	3228	C	C6-N1-C1'	-5.14	114.63	120.80
36	5	1389	G	C4-C5-N7	5.14	112.86	110.80
1	2	251	A	O5'-P-OP1	-5.14	101.08	105.70
1	6	813	U	N3-C2-O2	-5.14	118.61	122.20
1	2	136	C	C6-N1-C2	-5.13	118.25	120.30
1	2	1100	G	C5-C6-O6	-5.13	125.52	128.60
36	5	3362	A	C2-N3-C4	-5.13	108.03	110.60
1	6	1744	A	C8-N9-C4	5.13	107.85	105.80
36	5	939	U	O5'-P-OP1	5.13	116.86	110.70
1	2	321	C	C5-C6-N1	5.13	123.56	121.00
1	2	794	U	P-O3'-C3'	5.13	125.85	119.70
36	1	2816	G	N9-C4-C5	-5.13	103.35	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2828	G	N3-C2-N2	5.13	123.49	119.90
38	4	46	G	C4-N9-C1'	5.13	133.17	126.50
37	7	121	U	C2-N1-C1'	5.13	123.85	117.70
38	8	126	A	OP1-P-O3'	5.13	116.48	105.20
36	1	2809	C	N3-C2-O2	-5.13	118.31	121.90
37	7	100	C	C5-C6-N1	-5.13	118.44	121.00
36	5	2818	U	P-O3'-C3'	5.12	125.85	119.70
38	4	2	A	C8-N9-C4	-5.12	103.75	105.80
36	5	1429	G	C4-C5-N7	5.12	112.85	110.80
36	5	3309	G	C4-N9-C1'	5.12	133.16	126.50
36	5	3327	G	N3-C2-N2	-5.12	116.31	119.90
36	5	1457	U	O5'-P-OP2	5.12	116.84	110.70
36	5	2411	U	N3-C4-O4	-5.12	115.81	119.40
36	5	2621	G	N3-C2-N2	-5.12	116.32	119.90
1	2	1767	G	O4'-C1'-N9	5.12	112.29	108.20
36	1	57	A	N1-C6-N6	5.12	121.67	118.60
1	2	144	U	N3-C2-O2	-5.12	118.62	122.20
1	2	251	A	O5'-P-OP2	5.12	116.84	110.70
36	5	962	A	N1-C6-N6	5.12	121.67	118.60
1	2	782	U	OP2-P-O3'	5.12	116.45	105.20
1	6	1697	G	N3-C4-C5	-5.12	126.04	128.60
36	5	30	G	C4-C5-N7	5.12	112.85	110.80
36	5	2634	U	C2-N3-C4	-5.12	123.93	127.00
1	2	1773	C	N3-C4-C5	-5.11	119.86	121.90
36	1	355	A	N7-C8-N9	-5.11	111.25	113.80
36	1	2364	G	C4-N9-C1'	-5.11	119.86	126.50
36	5	2118	C	N1-C2-O2	5.11	121.97	118.90
38	8	27	U	C5-C6-N1	5.11	125.25	122.70
1	6	337	G	C6-C5-N7	-5.11	127.33	130.40
36	5	1065	A	C8-N9-C4	5.11	107.84	105.80
36	1	2966	G	C6-C5-N7	-5.11	127.34	130.40
36	5	77	A	OP2-P-O3'	5.11	116.43	105.20
36	5	2816	G	C6-C5-N7	-5.11	127.34	130.40
1	6	151	G	N3-C2-N2	-5.10	116.33	119.90
38	8	96	A	C8-N9-C4	5.10	107.84	105.80
1	2	1595	U	O4'-C1'-N1	5.10	112.28	108.20
1	2	1745	G	N9-C4-C5	-5.10	103.36	105.40
36	1	2337	C	C6-N1-C2	-5.10	118.26	120.30
36	5	1314	C	C6-N1-C1'	-5.10	114.68	120.80
36	1	399	A	OP1-P-OP2	-5.10	111.95	119.60
36	1	2399	A	OP1-P-O3'	5.10	116.42	105.20
36	1	3275	U	C2-N1-C1'	5.10	123.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	644	G	C5-C6-O6	5.10	131.66	128.60
1	6	359	A	C8-N9-C1'	5.10	136.88	127.70
38	4	145	U	N3-C2-O2	-5.10	118.63	122.20
36	1	689	U	O5'-P-OP2	-5.09	101.11	105.70
36	5	1043	C	O5'-P-OP1	5.09	116.81	110.70
1	6	421	A	N1-C6-N6	5.09	121.66	118.60
36	5	291	C	C6-N1-C2	5.09	122.34	120.30
37	7	1	G	C8-N9-C1'	-5.09	120.38	127.00
36	5	824	C	O5'-P-OP2	-5.09	101.12	105.70
36	5	2885	C	C6-N1-C2	5.09	122.34	120.30
36	1	2964	G	C2-N3-C4	-5.09	109.36	111.90
18	C6	28	LEU	CA-CB-CG	5.09	127.00	115.30
36	1	3306	U	N1-C2-O2	5.09	126.36	122.80
36	5	2257	C	C6-N1-C2	-5.09	118.27	120.30
36	5	2293	C	N1-C2-O2	5.09	121.95	118.90
36	1	503	C	C6-N1-C2	5.08	122.33	120.30
36	1	2918	G	C4-N9-C1'	5.08	133.11	126.50
1	6	402	C	O5'-P-OP1	5.08	116.80	110.70
1	2	736	C	C6-N1-C1'	-5.08	114.70	120.80
36	1	2874	G	N1-C6-O6	-5.08	116.85	119.90
36	1	922	U	N3-C2-O2	-5.08	118.64	122.20
42	l5	179	ARG	C-N-CA	5.08	134.40	121.70
1	2	639	U	C2-N1-C1'	5.08	123.80	117.70
36	5	1143	A	C2-N3-C4	-5.08	108.06	110.60
36	5	2818	U	C5'-C4'-O4'	-5.08	103.00	109.10
36	5	3309	G	N3-C4-C5	-5.08	126.06	128.60
36	1	350	C	C6-N1-C2	-5.08	118.27	120.30
1	6	548	G	C5-C6-O6	-5.08	125.56	128.60
36	5	1764	U	C5-C6-N1	5.08	125.24	122.70
36	5	1872	C	N1-C2-O2	5.08	121.94	118.90
1	2	1082	C	N1-C2-O2	5.07	121.94	118.90
1	6	418	G	O5'-P-OP1	-5.07	101.13	105.70
1	6	1523	G	N3-C4-C5	-5.07	126.06	128.60
1	2	1027	A	N1-C6-N6	5.07	121.64	118.60
36	1	3005	A	C8-N9-C4	-5.07	103.77	105.80
1	6	1730	A	C5-C6-N6	-5.07	119.64	123.70
36	1	1858	A	N3-C4-N9	5.07	131.46	127.40
1	6	417	A	P-O3'-C3'	5.07	125.78	119.70
36	5	838	G	C5-C6-O6	5.07	131.64	128.60
36	1	282	G	P-O3'-C3'	5.07	125.78	119.70
36	5	704	U	C6-N1-C2	-5.07	117.96	121.00
36	1	2283	G	C4-C5-N7	5.07	112.83	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	66	A	O5'-P-OP1	-5.07	101.14	105.70
36	5	1297	C	C6-N1-C2	-5.07	118.27	120.30
21	C9	28	LEU	CA-CB-CG	5.06	126.94	115.30
1	6	1196	A	P-O3'-C3'	5.06	125.78	119.70
36	1	859	G	N3-C2-N2	5.06	123.44	119.90
1	6	670	U	C2-N1-C1'	5.06	123.77	117.70
36	5	3343	G	N3-C4-N9	5.06	129.04	126.00
1	2	1489	U	C6-N1-C2	-5.06	117.96	121.00
36	1	2401	A	C4-C5-C6	-5.06	114.47	117.00
36	1	3181	C	C6-N1-C2	-5.06	118.28	120.30
36	5	1239	C	C6-N1-C2	-5.06	118.28	120.30
36	5	3004	C	N3-C2-O2	5.06	125.44	121.90
1	2	2	A	O4'-C1'-N9	-5.06	104.15	108.20
47	m0	48	LEU	CA-CB-CG	5.06	126.93	115.30
1	2	577	G	C5-N7-C8	-5.06	101.77	104.30
36	1	770	G	O4'-C1'-N9	5.05	112.24	108.20
1	6	306	U	C6-N1-C2	5.05	124.03	121.00
1	6	1700	C	C6-N1-C1'	-5.05	114.73	120.80
36	5	880	G	C6-C5-N7	5.05	133.43	130.40
38	4	46	G	C8-N9-C1'	-5.05	120.43	127.00
36	1	1849	C	N3-C2-O2	5.05	125.44	121.90
36	1	2966	G	N1-C6-O6	5.05	122.93	119.90
36	1	3057	U	C5-C4-O4	5.05	128.93	125.90
36	5	2512	C	C6-N1-C2	-5.05	118.28	120.30
1	2	992	A	O4'-C1'-N9	5.05	112.24	108.20
36	1	274	G	N1-C6-O6	5.05	122.93	119.90
6	s4	3	ARG	NE-CZ-NH1	-5.05	117.78	120.30
36	1	2903	A	C8-N9-C4	5.04	107.82	105.80
81	c2	58	LEU	CA-CB-CG	5.04	126.90	115.30
1	6	1573	A	P-O3'-C3'	5.04	125.75	119.70
36	5	2376	G	C8-N9-C1'	-5.04	120.44	127.00
36	1	1149	G	N7-C8-N9	-5.04	110.58	113.10
36	5	1300	G	N1-C6-O6	5.04	122.92	119.90
1	2	1486	G	C5-N7-C8	-5.04	101.78	104.30
38	4	99	C	C6-N1-C2	5.04	122.32	120.30
36	5	2611	U	C5-C6-N1	-5.04	120.18	122.70
36	5	3134	A	C5-C6-N6	-5.04	119.67	123.70
1	2	610	G	C8-N9-C1'	-5.04	120.45	127.00
36	1	3362	A	C5-N7-C8	-5.04	101.38	103.90
36	5	1604	G	C4-C5-C6	5.04	121.82	118.80
36	1	1595	U	C6-N1-C2	5.04	124.02	121.00
36	1	1875	G	C5-N7-C8	5.03	106.82	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	136	C	C2-N1-C1'	5.03	124.33	118.80
36	1	659	G	C2-N3-C4	5.03	114.42	111.90
36	1	1512	U	C6-N1-C2	-5.03	117.98	121.00
36	1	1590	G	N1-C6-O6	-5.03	116.88	119.90
39	12	238	ILE	CG1-CB-CG2	-5.03	100.34	111.40
36	1	2554	A	P-O3'-C3'	5.03	125.73	119.70
45	L8	65	LEU	CA-CB-CG	5.03	126.86	115.30
36	1	676	G	C8-N9-C4	-5.03	104.39	106.40
36	1	2939	G	OP2-P-O3'	5.03	116.26	105.20
36	5	1604	G	N1-C2-N3	5.03	126.92	123.90
36	5	2872	A	C8-N9-C1'	5.03	136.75	127.70
36	5	3289	G	N7-C8-N9	5.03	115.61	113.10
36	1	334	A	N9-C4-C5	-5.02	103.79	105.80
36	1	1433	A	N9-C4-C5	5.02	107.81	105.80
1	2	1196	A	P-O3'-C3'	5.02	125.73	119.70
36	1	851	C	C2-N1-C1'	5.02	124.33	118.80
36	5	1292	C	C6-N1-C2	5.02	122.31	120.30
38	8	53	A	C2-N3-C4	5.02	113.11	110.60
1	2	1745	G	N3-C2-N2	5.02	123.42	119.90
36	5	2659	G	N1-C6-O6	5.02	122.91	119.90
36	5	3382	U	N3-C2-O2	-5.02	118.69	122.20
36	1	2376	G	C8-N9-C4	-5.02	104.39	106.40
36	1	3276	G	C5-C6-O6	-5.02	125.59	128.60
36	1	3302	U	C6-N1-C2	5.02	124.01	121.00
1	6	1389	C	N3-C2-O2	-5.02	118.39	121.90
36	5	1155	C	N3-C4-C5	5.02	123.91	121.90
38	8	96	A	O5'-P-OP2	-5.02	101.18	105.70
36	1	80	G	C8-N9-C4	5.02	108.41	106.40
36	1	2808	A	O4'-C1'-N9	-5.02	104.19	108.20
1	6	1082	C	C6-N1-C2	-5.02	118.29	120.30
36	1	80	G	OP2-P-O3'	5.02	116.24	105.20
1	6	608	U	N3-C2-O2	-5.01	118.69	122.20
36	5	2118	C	C2-N1-C1'	5.01	124.31	118.80
90	a	75	C	N3-C2-O2	-5.01	118.39	121.90
36	5	3388	C	C5-C6-N1	-5.01	118.49	121.00
36	1	2426	U	C5-C4-O4	5.01	128.91	125.90
36	5	2978	U	N3-C4-O4	-5.01	115.89	119.40
36	1	545	U	N1-C2-O2	5.01	126.31	122.80
36	1	3143	C	C6-N1-C2	5.01	122.30	120.30
36	1	3303	G	O4'-C1'-N9	5.01	112.21	108.20
36	5	2440	G	N7-C8-N9	5.01	115.60	113.10
36	5	2849	C	N3-C2-O2	5.01	125.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	3137	C	C6-N1-C2	5.01	122.30	120.30
36	5	1561	G	O4'-C1'-N9	5.01	112.21	108.20
36	1	1176	C	O5'-P-OP2	5.01	116.71	110.70
36	5	2918	G	N1-C6-O6	5.01	122.90	119.90
1	2	1101	G	N1-C6-O6	-5.00	116.90	119.90
36	1	2811	A	C8-N9-C4	-5.00	103.80	105.80
36	5	1445	U	C5-C6-N1	-5.00	120.20	122.70
36	5	3368	U	N1-C2-O2	-5.00	119.30	122.80
36	1	1165	A	C8-N9-C4	5.00	107.80	105.80
36	5	546	C	C2-N1-C1'	5.00	124.30	118.80
1	2	542	A	O4'-C1'-N9	5.00	112.20	108.20
36	1	2603	G	N1-C6-O6	5.00	122.90	119.90
36	5	2832	C	C5-C6-N1	-5.00	118.50	121.00
36	5	2870	C	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
24	D2	54	ASP	Peptide
25	D3	44	GLY	Peptide
27	D5	54	VAL	Peptide
27	D5	94	LYS	Peptide
28	D6	84	VAL	Peptide
28	D6	85	ARG	Peptide
33	E1	105	TYR	Peptide
39	L2	19	HIS	Peptide
40	L3	172	ALA	Peptide
43	L6	129	GLU	Peptide
43	L6	89	THR	Peptide
45	L8	74	THR	Peptide
49	M3	137	GLN	Peptide
52	M6	110	PRO	Peptide
53	M7	120	ASN	Peptide
56	N0	133	ALA	Peptide
56	N0	22	PRO	Peptide
57	N1	16	GLN	Peptide
61	N5	137	ASN	Peptide
65	N9	19	ASN	Peptide
65	N9	20	GLY	Peptide

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Mol	Chain	Res	Type	Group
70	O4	71	THR	Peptide
3	S1	131	ASP	Peptide
6	S4	193	GLY	Peptide
9	S7	131	PHE	Peptide
13	c1	119	VAL	Peptide
82	c5	52	LYS	Peptide
18	c6	40	GLU	Peptide
22	d0	70	THR	Peptide
25	d3	44	GLY	Peptide
27	d5	85	LYS	Peptide
33	e1	106	TYR	Peptide
39	l2	143	GLU	Peptide
39	l2	171	GLY	Peptide
39	l2	211	HIS	Peptide
40	l3	185	GLY	Peptide
42	l5	270	LYS	Peptide
42	l5	271	LYS	Peptide
44	l7	192	GLY	Peptide
44	l7	226	GLY	Peptide
50	m4	20	VAL	Peptide
52	m6	110	PRO	Peptide
53	m7	119	VAL	Peptide
56	n0	133	ALA	Peptide
87	n4	75	THR	Peptide
63	n7	5	LEU	Peptide
64	n8	66	ALA	Peptide
65	n9	19	ASN	Peptide
65	n9	24	PRO	Peptide
68	o2	39	ASP	Peptide
7	s5	44	ASN	Peptide
7	s5	99	MET	Peptide
10	s8	60	ILE	Peptide
11	s9	100	LYS	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/206 (99%)	155 (76%)	34 (17%)	15 (7%)	1	5
2	s0	204/206 (99%)	163 (80%)	22 (11%)	19 (9%)	0	3
3	S1	212/216 (98%)	151 (71%)	35 (16%)	26 (12%)	0	1
3	s1	214/216 (99%)	173 (81%)	26 (12%)	15 (7%)	1	6
4	S2	215/217 (99%)	189 (88%)	19 (9%)	7 (3%)	3	18
4	s2	215/217 (99%)	179 (83%)	25 (12%)	11 (5%)	1	10
5	S3	221/223 (99%)	186 (84%)	25 (11%)	10 (4%)	2	12
5	s3	221/223 (99%)	177 (80%)	28 (13%)	16 (7%)	1	6
6	S4	258/260 (99%)	218 (84%)	30 (12%)	10 (4%)	2	15
6	s4	258/260 (99%)	218 (84%)	26 (10%)	14 (5%)	1	9
7	S5	204/206 (99%)	166 (81%)	22 (11%)	16 (8%)	1	5
7	s5	204/206 (99%)	160 (78%)	30 (15%)	14 (7%)	1	6
8	S6	224/226 (99%)	198 (88%)	16 (7%)	10 (4%)	2	12
8	s6	216/226 (96%)	190 (88%)	12 (6%)	14 (6%)	1	7
9	S7	182/186 (98%)	144 (79%)	19 (10%)	19 (10%)	0	2
9	s7	184/186 (99%)	150 (82%)	22 (12%)	12 (6%)	1	7
10	S8	184/199 (92%)	163 (89%)	10 (5%)	11 (6%)	1	8
10	s8	184/199 (92%)	159 (86%)	17 (9%)	8 (4%)	2	13
11	S9	183/185 (99%)	158 (86%)	17 (9%)	8 (4%)	2	12
11	s9	183/185 (99%)	157 (86%)	18 (10%)	8 (4%)	2	12
12	C0	82/96 (85%)	69 (84%)	9 (11%)	4 (5%)	2	11
13	C1	145/155 (94%)	119 (82%)	19 (13%)	7 (5%)	2	11
13	c1	144/155 (93%)	120 (83%)	18 (12%)	6 (4%)	2	13
14	C2	122/124 (98%)	74 (61%)	26 (21%)	22 (18%)	0	1
15	C3	148/150 (99%)	127 (86%)	15 (10%)	6 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	c3	148/150 (99%)	121 (82%)	19 (13%)	8 (5%)	1	9
16	C4	125/128 (98%)	97 (78%)	17 (14%)	11 (9%)	0	4
16	c4	126/128 (98%)	103 (82%)	17 (14%)	6 (5%)	2	11
17	C5	122/131 (93%)	96 (79%)	16 (13%)	10 (8%)	1	4
18	C6	139/142 (98%)	116 (84%)	15 (11%)	8 (6%)	1	8
18	c6	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	2	13
19	C7	116/125 (93%)	94 (81%)	14 (12%)	8 (7%)	1	6
19	c7	113/125 (90%)	92 (81%)	12 (11%)	9 (8%)	1	4
20	C8	143/145 (99%)	113 (79%)	22 (15%)	8 (6%)	1	9
20	c8	143/145 (99%)	121 (85%)	16 (11%)	6 (4%)	2	13
21	C9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	4	21
21	c9	141/143 (99%)	124 (88%)	14 (10%)	3 (2%)	5	26
22	D0	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	2	15
22	d0	108/110 (98%)	86 (80%)	12 (11%)	10 (9%)	0	3
23	D1	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	1
23	d1	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	1	8
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	5	23
24	d2	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	16	45
25	D3	142/144 (99%)	118 (83%)	14 (10%)	10 (7%)	1	6
25	d3	142/144 (99%)	128 (90%)	11 (8%)	3 (2%)	5	26
26	D4	132/134 (98%)	111 (84%)	13 (10%)	8 (6%)	1	8
26	d4	132/134 (98%)	106 (80%)	17 (13%)	9 (7%)	1	6
27	D5	68/70 (97%)	47 (69%)	12 (18%)	9 (13%)	0	1
27	d5	67/70 (96%)	53 (79%)	10 (15%)	4 (6%)	1	8
28	D6	95/97 (98%)	60 (63%)	22 (23%)	13 (14%)	0	1
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	0	4
29	D7	79/81 (98%)	65 (82%)	11 (14%)	3 (4%)	2	15
29	d7	79/81 (98%)	61 (77%)	11 (14%)	7 (9%)	0	3
30	D8	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	11
30	d8	61/63 (97%)	46 (75%)	12 (20%)	3 (5%)	2	11
31	D9	51/53 (96%)	40 (78%)	8 (16%)	3 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	d9	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	1	8
32	E0	58/62 (94%)	46 (79%)	9 (16%)	3 (5%)	1	10
32	e0	60/62 (97%)	47 (78%)	7 (12%)	6 (10%)	0	3
33	E1	69/76 (91%)	38 (55%)	18 (26%)	13 (19%)	0	0
33	e1	74/76 (97%)	33 (45%)	23 (31%)	18 (24%)	0	0
34	SR	316/318 (99%)	275 (87%)	32 (10%)	9 (3%)	4	21
35	SM	131/159 (82%)	100 (76%)	17 (13%)	14 (11%)	0	2
39	L2	250/252 (99%)	229 (92%)	13 (5%)	8 (3%)	3	19
39	l2	250/252 (99%)	215 (86%)	26 (10%)	9 (4%)	3	16
40	L3	384/386 (100%)	334 (87%)	35 (9%)	15 (4%)	2	15
40	l3	384/386 (100%)	349 (91%)	25 (6%)	10 (3%)	4	22
41	L4	359/361 (99%)	301 (84%)	37 (10%)	21 (6%)	1	8
41	l4	359/361 (99%)	300 (84%)	41 (11%)	18 (5%)	1	10
42	L5	294/296 (99%)	239 (81%)	37 (13%)	18 (6%)	1	8
42	l5	292/296 (99%)	257 (88%)	28 (10%)	7 (2%)	5	23
43	L6	152/175 (87%)	132 (87%)	17 (11%)	3 (2%)	6	27
43	l6	153/175 (87%)	135 (88%)	14 (9%)	4 (3%)	4	22
44	L7	220/223 (99%)	199 (90%)	15 (7%)	6 (3%)	4	21
44	l7	221/223 (99%)	201 (91%)	14 (6%)	6 (3%)	4	21
45	L8	231/233 (99%)	194 (84%)	26 (11%)	11 (5%)	2	11
46	L9	189/191 (99%)	167 (88%)	17 (9%)	5 (3%)	4	22
46	l9	189/191 (99%)	175 (93%)	8 (4%)	6 (3%)	3	19
47	M0	207/220 (94%)	180 (87%)	18 (9%)	9 (4%)	2	13
47	m0	209/220 (95%)	168 (80%)	31 (15%)	10 (5%)	2	11
48	M1	167/169 (99%)	127 (76%)	26 (16%)	14 (8%)	0	4
48	m1	167/169 (99%)	140 (84%)	17 (10%)	10 (6%)	1	8
49	M3	191/194 (98%)	159 (83%)	21 (11%)	11 (6%)	1	8
49	m3	192/194 (99%)	156 (81%)	24 (12%)	12 (6%)	1	7
50	M4	134/137 (98%)	118 (88%)	10 (8%)	6 (4%)	2	12
50	m4	135/137 (98%)	123 (91%)	9 (7%)	3 (2%)	5	25
51	M5	201/203 (99%)	182 (90%)	12 (6%)	7 (4%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	3	20
52	M6	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	13	41
52	m6	195/197 (99%)	181 (93%)	12 (6%)	2 (1%)	13	41
53	M7	181/183 (99%)	152 (84%)	20 (11%)	9 (5%)	1	10
53	m7	153/183 (84%)	136 (89%)	12 (8%)	5 (3%)	3	18
54	M8	183/185 (99%)	161 (88%)	18 (10%)	4 (2%)	5	25
54	m8	183/185 (99%)	156 (85%)	21 (12%)	6 (3%)	3	18
55	M9	186/188 (99%)	173 (93%)	11 (6%)	2 (1%)	12	39
55	m9	186/188 (99%)	180 (97%)	4 (2%)	2 (1%)	12	39
56	N0	170/172 (99%)	153 (90%)	13 (8%)	4 (2%)	5	23
56	n0	170/172 (99%)	159 (94%)	8 (5%)	3 (2%)	7	30
57	N1	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	6	29
57	n1	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	10	35
58	N2	98/100 (98%)	80 (82%)	16 (16%)	2 (2%)	6	27
58	n2	96/100 (96%)	85 (88%)	10 (10%)	1 (1%)	13	41
59	N3	134/136 (98%)	122 (91%)	8 (6%)	4 (3%)	3	20
59	n3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	8	33
60	N4	96/98 (98%)	76 (79%)	14 (15%)	6 (6%)	1	7
61	N5	119/121 (98%)	105 (88%)	12 (10%)	2 (2%)	7	30
61	n5	118/121 (98%)	99 (84%)	10 (8%)	9 (8%)	1	5
62	N6	124/126 (98%)	111 (90%)	10 (8%)	3 (2%)	5	23
62	n6	124/126 (98%)	112 (90%)	7 (6%)	5 (4%)	2	14
63	N7	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	1	9
63	n7	133/135 (98%)	106 (80%)	15 (11%)	12 (9%)	0	3
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	1	9
64	n8	146/148 (99%)	121 (83%)	20 (14%)	5 (3%)	3	18
65	N9	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	1	9
65	n9	56/58 (97%)	40 (71%)	10 (18%)	6 (11%)	0	2
66	O0	95/100 (95%)	89 (94%)	5 (5%)	1 (1%)	12	39
66	o0	98/100 (98%)	88 (90%)	6 (6%)	4 (4%)	2	13
67	O1	107/109 (98%)	98 (92%)	5 (5%)	4 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	o1	107/109 (98%)	94 (88%)	9 (8%)	4 (4%)	2	16
68	O2	125/127 (98%)	111 (89%)	11 (9%)	3 (2%)	5	23
68	o2	125/127 (98%)	108 (86%)	12 (10%)	5 (4%)	2	14
69	O3	104/106 (98%)	94 (90%)	8 (8%)	2 (2%)	6	29
69	o3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	3	20
70	O4	110/112 (98%)	97 (88%)	11 (10%)	2 (2%)	7	30
70	o4	110/112 (98%)	96 (87%)	11 (10%)	3 (3%)	4	21
71	O5	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	4	22
71	o5	117/119 (98%)	102 (87%)	11 (9%)	4 (3%)	3	18
72	O6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	1	6
72	o6	97/99 (98%)	83 (86%)	7 (7%)	7 (7%)	1	6
73	O7	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
73	o7	85/87 (98%)	76 (89%)	5 (6%)	4 (5%)	2	11
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	2	14
74	o8	75/77 (97%)	62 (83%)	12 (16%)	1 (1%)	10	35
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	5	26
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	5	26
76	Q0	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	2	14
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	6	27
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	85 (82%)	12 (12%)	6 (6%)	1	8
78	q2	103/105 (98%)	94 (91%)	5 (5%)	4 (4%)	2	15
79	Q3	89/91 (98%)	79 (89%)	7 (8%)	3 (3%)	3	18
79	q3	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	12	39
80	c0	78/96 (81%)	61 (78%)	10 (13%)	7 (9%)	0	3
81	c2	108/124 (87%)	67 (62%)	26 (24%)	15 (14%)	0	1
82	c5	133/142 (94%)	96 (72%)	19 (14%)	18 (14%)	0	1
83	sR	316/318 (99%)	268 (85%)	39 (12%)	9 (3%)	4	21
84	sM	61/104 (59%)	43 (70%)	10 (16%)	8 (13%)	0	1
85	l8	224/231 (97%)	184 (82%)	25 (11%)	15 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	n4	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	1	5
88	p0	117/219 (53%)	101 (86%)	12 (10%)	4 (3%)	3	18
All	All	22197/22912 (97%)	18787 (85%)	2314 (10%)	1096 (5%)	2	11

All (1096) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	5	ALA
2	S0	95	ALA
2	S0	158	VAL
2	S0	191	ARG
2	S0	203	PHE
3	S1	49	ASN
3	S1	113	MET
3	S1	148	ASN
3	S1	177	GLN
3	S1	179	SER
3	S1	206	PRO
4	S2	107	SER
4	S2	148	LEU
5	S3	62	ASN
5	S3	65	ARG
5	S3	93	ASP
5	S3	195	SER
5	S3	211	PRO
5	S3	220	PRO
6	S4	104	ASP
7	S5	26	ALA
7	S5	51	VAL
7	S5	101	GLY
7	S5	153	GLY
8	S6	25	ARG
8	S6	122	GLU
8	S6	154	ARG
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	111	LYS
9	S7	112	ARG

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Mol	Chain	Res	Type
9	S7	131	PHE
9	S7	133	THR
9	S7	134	GLU
10	S8	147	ALA
10	S8	149	SER
11	S9	93	LEU
11	S9	134	ILE
12	C0	60	SER
12	C0	81	ASN
14	C2	89	ILE
14	C2	93	ASP
14	C2	127	GLY
15	C3	28	LEU
15	C3	138	ASN
16	C4	39	ILE
16	C4	124	ASP
16	C4	125	SER
16	C4	126	THR
17	C5	54	ALA
17	C5	125	PRO
17	C5	126	VAL
18	C6	40	GLU
18	C6	41	PRO
18	C6	114	ARG
18	C6	138	PHE
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	25	ASN
20	C8	28	ILE
20	C8	60	GLU
20	C8	91	ASP
20	C8	92	ILE
21	C9	31	PRO
21	C9	53	TRP
23	D1	7	GLN
25	D3	114	LYS
25	D3	138	GLU
26	D4	36	SER
27	D5	39	ALA

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Mol	Chain	Res	Type
27	D5	44	GLN
27	D5	54	VAL
27	D5	71	ILE
27	D5	97	LYS
28	D6	36	ILE
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
29	D7	62	ILE
32	E0	47	VAL
33	E1	84	VAL
33	E1	102	VAL
33	E1	106	TYR
34	SR	318	ALA
35	SM	47	ALA
35	SM	52	PRO
35	SM	140	ASP
39	L2	47	GLN
40	L3	4	ARG
40	L3	5	LYS
40	L3	140	ASP
40	L3	142	ALA
40	L3	187	SER
40	L3	347	SER
40	L3	385	LYS
41	L4	130	ALA
41	L4	293	SER
41	L4	311	HIS
41	L4	317	PRO
42	L5	20	PHE
42	L5	234	ASP
42	L5	295	GLY
43	L6	6	ALA
43	L6	98	VAL
44	L7	26	VAL
44	L7	160	ARG
44	L7	164	SER
45	L8	25	PRO
45	L8	31	PRO
46	L9	50	ASN
47	M0	218	ALA

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Mol	Chain	Res	Type
48	M1	8	PRO
48	M1	11	ASP
48	M1	94	ARG
48	M1	115	LYS
48	M1	140	ARG
48	M1	165	GLN
49	M3	47	ALA
49	M3	129	ASN
49	M3	131	LYS
49	M3	136	GLU
50	M4	8	LYS
50	M4	9	ALA
50	M4	29	ALA
50	M4	36	VAL
51	M5	74	PRO
51	M5	144	ARG
52	M6	111	PRO
53	M7	67	ILE
53	M7	75	GLU
53	M7	157	VAL
60	N4	81	PRO
60	N4	86	SER
61	N5	44	PRO
63	N7	17	ARG
63	N7	30	ASP
63	N7	125	GLY
64	N8	57	GLY
64	N8	66	ALA
67	O1	6	ASP
67	O1	83	GLU
67	O1	84	ASP
71	O5	119	LYS
72	O6	13	LYS
72	O6	33	ALA
78	Q2	17	CYS
78	Q2	30	ALA
79	Q3	58	SER
2	s0	4	PRO
2	s0	95	ALA
2	s0	158	VAL
2	s0	164	ASN
2	s0	189	VAL

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Mol	Chain	Res	Type
2	s0	206	ASP
3	s1	106	THR
3	s1	154	SER
3	s1	206	PRO
3	s1	223	PHE
4	s2	92	ALA
4	s2	162	CYS
5	s3	61	GLU
5	s3	115	ILE
5	s3	211	PRO
5	s3	216	PRO
5	s3	217	ILE
5	s3	219	ALA
5	s3	220	PRO
6	s4	95	THR
6	s4	163	ASP
6	s4	164	LEU
6	s4	196	VAL
7	s5	28	PRO
7	s5	39	GLU
7	s5	184	PHE
7	s5	204	GLY
8	s6	70	PRO
8	s6	154	ARG
8	s6	173	PRO
8	s6	174	LYS
9	s7	10	SER
9	s7	64	VAL
9	s7	67	LEU
9	s7	74	GLN
9	s7	131	PHE
11	s9	150	LEU
80	c0	32	HIS
13	c1	133	LYS
81	c2	89	ILE
16	c4	126	THR
82	c5	11	VAL
82	c5	17	TYR
82	c5	52	LYS
82	c5	68	PRO
82	c5	125	PRO
82	c5	126	VAL

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Mol	Chain	Res	Type
82	c5	127	ARG
18	c6	42	GLU
18	c6	116	LEU
19	c7	63	LYS
19	c7	88	VAL
19	c7	99	VAL
19	c7	104	ASN
20	c8	91	ASP
20	c8	92	ILE
21	c9	29	GLU
21	c9	33	TYR
21	c9	34	VAL
22	d0	17	GLN
22	d0	49	ASN
22	d0	97	VAL
26	d4	30	PRO
26	d4	33	ALA
26	d4	52	LYS
27	d5	85	LYS
27	d5	104	ALA
28	d6	47	ALA
29	d7	60	SER
30	d8	61	ARG
31	d9	6	VAL
32	e0	60	PRO
33	e1	79	LYS
33	e1	83	LYS
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	106	TYR
83	sR	160	GLU
83	sR	163	ASP
83	sR	165	ASP
83	sR	318	ALA
84	sM	42	ALA
84	sM	50	ASN
39	l2	238	ILE
40	l3	22	ALA
40	l3	129	ALA
41	l4	301	PRO
41	l4	329	PRO

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Mol	Chain	Res	Type
42	l5	178	ASN
44	l7	159	GLN
85	l8	25	PRO
85	l8	34	PHE
85	l8	121	SER
85	l8	122	LYS
47	m0	82	ARG
47	m0	220	GLN
48	m1	8	PRO
48	m1	10	ARG
48	m1	94	ARG
48	m1	108	GLU
49	m3	47	ALA
49	m3	150	PRO
51	m5	76	PRO
52	m6	110	PRO
54	m8	99	THR
57	n1	136	ARG
87	n4	26	SER
87	n4	63	ILE
87	n4	71	ARG
87	n4	76	VAL
61	n5	24	LEU
61	n5	44	PRO
61	n5	45	LYS
61	n5	55	ASN
62	n6	83	ASP
62	n6	84	LYS
62	n6	125	LYS
62	n6	126	LEU
63	n7	7	ALA
63	n7	125	GLY
63	n7	129	TRP
64	n8	76	ASP
65	n9	21	ILE
65	n9	23	LYS
65	n9	39	PHE
67	o1	45	GLY
68	o2	6	HIS
69	o3	88	ASN
72	o6	33	ALA
72	o6	64	SER

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Mol	Chain	Res	Type
72	o6	98	ARG
78	q2	17	CYS
88	p0	93	LEU
2	S0	4	PRO
2	S0	39	ASN
2	S0	49	ASN
2	S0	94	GLY
3	S1	21	VAL
3	S1	26	ARG
3	S1	35	PRO
3	S1	58	SER
3	S1	60	ALA
3	S1	62	LYS
3	S1	63	GLY
3	S1	158	SER
3	S1	182	ALA
3	S1	221	PRO
4	S2	106	ASP
5	S3	59	LEU
5	S3	216	PRO
6	S4	12	LEU
6	S4	195	ILE
7	S5	43	PHE
7	S5	63	GLN
7	S5	127	GLN
7	S5	150	GLY
8	S6	152	ASP
9	S7	29	ASN
9	S7	155	ASP
9	S7	186	PRO
10	S8	40	ALA
10	S8	104	ILE
10	S8	199	LYS
11	S9	98	ALA
11	S9	121	SER
11	S9	167	ALA
13	C1	30	ARG
13	C1	55	ASP
14	C2	25	GLU
14	C2	91	VAL
15	C3	22	ALA
15	C3	68	GLY

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Mol	Chain	Res	Type
16	C4	50	ALA
16	C4	51	ASP
16	C4	114	ARG
17	C5	11	VAL
17	C5	48	GLY
17	C5	101	ALA
18	C6	59	LYS
19	C7	23	LYS
19	C7	87	GLU
19	C7	115	LEU
20	C8	61	LEU
20	C8	142	GLY
21	C9	28	LEU
22	D0	17	GLN
23	D1	2	GLU
23	D1	4	ASP
23	D1	15	ARG
25	D3	70	LYS
25	D3	112	LYS
26	D4	5	VAL
27	D5	43	ASP
28	D6	11	ASN
28	D6	65	PRO
28	D6	86	VAL
29	D7	63	LEU
30	D8	36	THR
31	D9	20	GLN
32	E0	51	ASN
33	E1	83	LYS
33	E1	86	THR
33	E1	98	VAL
33	E1	144	CYS
33	E1	145	HIS
34	SR	161	ALA
35	SM	86	ASN
35	SM	87	THR
35	SM	111	GLY
39	L2	13	GLY
40	L3	3	HIS
40	L3	289	ASP
40	L3	351	LEU
41	L4	318	LEU

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Mol	Chain	Res	Type
41	L4	338	LYS
42	L5	6	ASP
42	L5	125	VAL
42	L5	137	ASP
42	L5	153	THR
42	L5	233	ALA
42	L5	253	PHE
42	L5	258	LYS
42	L5	276	LYS
44	L7	25	GLN
45	L8	36	ILE
45	L8	39	ALA
45	L8	75	ILE
47	M0	117	GLY
47	M0	145	LYS
47	M0	194	GLY
47	M0	220	GLN
48	M1	12	LEU
48	M1	74	PRO
48	M1	114	ILE
48	M1	152	HIS
49	M3	13	HIS
49	M3	141	ALA
49	M3	193	ALA
50	M4	10	SER
54	M8	98	LYS
55	M9	3	ASN
55	M9	53	LYS
56	N0	166	LYS
57	N1	123	GLY
57	N1	124	VAL
58	N2	51	GLY
59	N3	82	ALA
59	N3	134	GLY
60	N4	64	THR
61	N5	45	LYS
62	N6	84	LYS
62	N6	92	GLY
63	N7	35	SER
63	N7	102	GLU
64	N8	76	ASP
64	N8	96	LYS

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Mol	Chain	Res	Type
68	O2	27	ARG
71	O5	97	ALA
74	O8	18	ALA
74	O8	33	LYS
76	Q0	78	ILE
78	Q2	60	LYS
78	Q2	94	GLY
78	Q2	100	LYS
2	s0	8	ASP
2	s0	44	GLY
2	s0	66	ALA
2	s0	68	PRO
2	s0	186	GLY
3	s1	81	PHE
3	s1	82	ARG
3	s1	93	GLY
3	s1	218	LEU
5	s3	179	GLN
6	s4	12	LEU
6	s4	104	ASP
6	s4	195	ILE
6	s4	214	LEU
7	s5	36	ALA
7	s5	101	GLY
8	s6	138	ALA
8	s6	175	ILE
9	s7	66	SER
9	s7	133	THR
9	s7	155	ASP
10	s8	36	THR
10	s8	122	GLY
10	s8	199	LYS
11	s9	118	LEU
80	c0	23	ALA
80	c0	35	ILE
13	c1	7	VAL
81	c2	58	LEU
81	c2	66	VAL
81	c2	87	PRO
81	c2	101	ALA
81	c2	119	SER
81	c2	131	ASP

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Mol	Chain	Res	Type
15	c3	19	SER
15	c3	66	ILE
15	c3	139	TRP
16	c4	51	ASP
82	c5	51	SER
82	c5	131	ALA
82	c5	132	GLY
18	c6	39	VAL
18	c6	115	THR
19	c7	116	LYS
20	c8	60	GLU
22	d0	15	GLN
22	d0	52	LYS
22	d0	96	PRO
22	d0	118	VAL
26	d4	35	VAL
27	d5	44	GLN
28	d6	28	LYS
29	d7	53	ALA
32	e0	47	VAL
32	e0	51	ASN
32	e0	61	SER
33	e1	100	LEU
33	e1	102	VAL
33	e1	112	GLY
33	e1	136	LYS
84	sM	65	THR
84	sM	83	LYS
39	l2	24	GLN
39	l2	96	LEU
39	l2	127	ALA
39	l2	212	GLY
40	l3	140	ASP
41	l4	14	GLU
41	l4	15	ALA
41	l4	90	PHE
41	l4	146	PRO
41	l4	311	HIS
41	l4	345	GLU
42	l5	26	GLY
42	l5	123	GLU
42	l5	258	LYS

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Mol	Chain	Res	Type
42	l5	260	PHE
43	l6	98	VAL
44	l7	158	LYS
85	l8	26	LEU
85	l8	203	VAL
46	l9	144	ILE
46	l9	189	GLU
47	m0	83	ASP
47	m0	193	ASP
48	m1	95	ASN
48	m1	115	LYS
48	m1	167	TYR
49	m3	50	PRO
49	m3	93	ILE
49	m3	101	ARG
49	m3	134	GLU
49	m3	135	ALA
49	m3	141	ALA
50	m4	136	ALA
51	m5	183	THR
51	m5	184	LYS
51	m5	187	ARG
52	m6	16	VAL
53	m7	66	SER
53	m7	77	GLY
54	m8	84	VAL
54	m8	167	SER
56	n0	142	GLN
59	n3	42	SER
87	n4	25	ASP
87	n4	83	THR
87	n4	133	THR
61	n5	25	LYS
61	n5	40	LEU
63	n7	29	HIS
63	n7	70	PRO
63	n7	130	PHE
64	n8	47	LYS
65	n9	24	PRO
65	n9	25	LYS
66	o0	10	ILE
67	o1	83	GLU

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Mol	Chain	Res	Type
68	o2	124	GLY
70	o4	79	SER
71	o5	119	LYS
73	o7	67	LEU
73	o7	87	SER
74	o8	18	ALA
75	o9	3	ALA
78	q2	31	GLY
78	q2	32	LYS
88	p0	33	VAL
2	S0	192	THR
2	S0	195	TRP
3	S1	54	LEU
3	S1	156	ALA
6	S4	3	ARG
6	S4	245	LYS
7	S5	31	GLU
7	S5	39	GLU
7	S5	45	LYS
8	S6	69	LEU
9	S7	30	SER
9	S7	36	ALA
9	S7	74	GLN
9	S7	98	ILE
10	S8	22	ARG
11	S9	150	LEU
12	C0	64	TYR
13	C1	7	VAL
13	C1	146	ALA
14	C2	21	GLU
14	C2	87	PRO
14	C2	106	ILE
14	C2	107	ASP
14	C2	119	SER
15	C3	27	LYS
16	C4	40	ALA
16	C4	42	VAL
17	C5	52	LYS
17	C5	69	GLU
18	C6	111	SER
21	C9	69	LYS
22	D0	55	PRO

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Mol	Chain	Res	Type
24	D2	78	ARG
25	D3	131	SER
27	D5	41	ILE
28	D6	18	VAL
28	D6	35	ALA
29	D7	51	GLN
30	D8	61	ARG
31	D9	8	PHE
32	E0	50	VAL
33	E1	103	LEU
33	E1	111	GLU
33	E1	118	ARG
34	SR	98	GLU
34	SR	163	ASP
35	SM	82	THR
39	L2	144	ASN
39	L2	251	LYS
40	L3	174	LYS
40	L3	221	THR
41	L4	15	ALA
41	L4	90	PHE
41	L4	146	PRO
41	L4	182	LEU
41	L4	232	SER
41	L4	268	ALA
42	L5	7	ALA
42	L5	215	ASP
42	L5	260	PHE
43	L6	5	LYS
45	L8	76	ALA
46	L9	190	ASP
47	M0	187	ALA
47	M0	207	GLU
48	M1	95	ASN
48	M1	108	GLU
48	M1	145	LYS
49	M3	50	PRO
49	M3	76	THR
49	M3	130	GLY
49	M3	166	ALA
51	M5	81	TYR
53	M7	162	GLU

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Mol	Chain	Res	Type
53	M7	164	LYS
57	N1	159	PHE
58	N2	11	ILE
59	N3	46	LEU
59	N3	47	ASN
60	N4	97	LYS
62	N6	91	ASN
63	N7	36	HIS
64	N8	97	GLU
64	N8	117	ARG
68	O2	12	LYS
68	O2	68	PRO
72	O6	64	SER
79	Q3	7	LYS
79	Q3	84	ARG
2	s0	10	THR
2	s0	30	GLN
2	s0	185	ARG
2	s0	194	PRO
2	s0	203	PHE
3	s1	21	VAL
3	s1	39	GLU
3	s1	147	ALA
4	s2	106	ASP
4	s2	107	SER
4	s2	238	SER
5	s3	44	THR
5	s3	161	GLY
6	s4	245	LYS
7	s5	43	PHE
7	s5	151	GLY
8	s6	65	GLN
8	s6	68	LEU
8	s6	126	ASP
8	s6	152	ASP
8	s6	165	GLY
11	s9	169	PRO
13	c1	40	LEU
13	c1	121	ASP
81	c2	93	ASP
15	c3	87	ASP
15	c3	140	LYS

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Mol	Chain	Res	Type
16	c4	50	ALA
82	c5	7	ALA
82	c5	9	LYS
18	c6	113	ASP
20	c8	61	LEU
24	d2	56	HIS
26	d4	50	ALA
26	d4	78	SER
28	d6	13	LYS
29	d7	62	ILE
30	d8	62	GLU
31	d9	7	TRP
33	e1	81	LYS
33	e1	86	THR
33	e1	129	GLY
33	e1	131	PHE
33	e1	148	TYR
83	sR	4	ASN
84	sM	47	ALA
39	l2	56	ALA
39	l2	216	HIS
40	l3	155	ALA
40	l3	235	THR
41	l4	142	VAL
41	l4	190	GLY
41	l4	220	ARG
41	l4	233	LEU
41	l4	302	ALA
42	l5	270	LYS
44	l7	191	VAL
44	l7	228	SER
85	l8	39	ALA
85	l8	133	LYS
85	l8	239	GLY
85	l8	240	ASN
46	l9	2	LYS
47	m0	170	LYS
47	m0	174	THR
47	m0	176	LEU
47	m0	204	GLY
51	m5	181	ASN
54	m8	112	ALA

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Mol	Chain	Res	Type
56	n0	154	HIS
58	n2	91	ASP
87	n4	58	HIS
63	n7	56	LYS
63	n7	128	GLN
66	o0	100	ILE
66	o0	103	THR
67	o1	5	LYS
67	o1	84	ASP
71	o5	81	ARG
72	o6	34	SER
76	q0	78	ILE
78	q2	60	LYS
79	q3	50	GLY
88	p0	102	SER
2	S0	103	THR
2	S0	205	ARG
3	S1	130	SER
3	S1	209	ASN
3	S1	213	ARG
4	S2	235	LEU
4	S2	248	SER
5	S3	217	ILE
6	S4	193	GLY
6	S4	200	ARG
6	S4	234	PRO
6	S4	260	GLY
7	S5	58	LEU
7	S5	64	VAL
9	S7	5	GLN
9	S7	156	SER
10	S8	10	LYS
10	S8	52	ASN
10	S8	120	THR
10	S8	152	ILE
11	S9	118	LEU
12	C0	34	GLU
13	C1	147	ALA
14	C2	22	VAL
14	C2	112	ALA
14	C2	125	ASN
15	C3	3	ARG

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Mol	Chain	Res	Type
18	C6	32	ASN
19	C7	84	TYR
23	D1	81	ASN
24	D2	30	SER
24	D2	83	ILE
25	D3	41	SER
26	D4	6	THR
26	D4	34	ASN
26	D4	51	GLU
28	D6	46	GLU
28	D6	64	LEU
30	D8	6	PRO
33	E1	87	THR
34	SR	15	GLY
34	SR	231	MET
35	SM	12	VAL
39	L2	143	GLU
39	L2	246	LEU
42	L5	228	ALA
42	L5	259	LYS
45	L8	156	ASP
45	L8	157	VAL
45	L8	254	ASP
46	L9	2	LYS
46	L9	110	LYS
47	M0	217	PHE
51	M5	75	VAL
51	M5	184	LYS
53	M7	160	ALA
53	M7	161	ALA
53	M7	163	LYS
54	M8	99	THR
56	N0	24	LEU
60	N4	76	VAL
63	N7	103	GLN
65	N9	18	ARG
66	O0	96	GLY
71	O5	75	TYR
72	O6	34	SER
74	O8	35	GLY
78	Q2	34	SER
2	s0	103	THR

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Mol	Chain	Res	Type
3	s1	26	ARG
3	s1	179	SER
3	s1	224	ASP
4	s2	150	GLN
4	s2	235	LEU
5	s3	90	ARG
5	s3	93	ASP
5	s3	221	SER
6	s4	30	ARG
6	s4	90	ILE
6	s4	168	LYS
7	s5	29	ILE
7	s5	100	ASN
7	s5	153	GLY
8	s6	25	ARG
10	s8	94	ASN
11	s9	121	SER
11	s9	164	PHE
11	s9	167	ALA
80	c0	24	LYS
80	c0	30	ALA
13	c1	55	ASP
81	c2	39	ASP
81	c2	45	LEU
15	c3	60	VAL
15	c3	82	PRO
16	c4	48	VAL
16	c4	132	ARG
82	c5	14	THR
18	c6	97	VAL
19	c7	62	GLN
19	c7	113	LEU
22	d0	13	GLU
22	d0	51	VAL
23	d1	42	GLU
23	d1	44	ARG
26	d4	58	PHE
28	d6	15	ARG
28	d6	59	TYR
29	d7	20	LYS
29	d7	75	GLU
30	d8	33	LEU

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Mol	Chain	Res	Type
31	d9	11	PRO
33	e1	84	VAL
33	e1	103	LEU
83	sR	161	LYS
39	l2	80	GLU
40	l3	23	ALA
40	l3	187	SER
40	l3	386	ASP
41	l4	145	ILE
41	l4	193	LYS
41	l4	330	TYR
43	l6	10	TYR
43	l6	20	LYS
43	l6	172	HIS
85	l8	82	LEU
85	l8	163	VAL
85	l8	237	ILE
46	l9	110	LYS
48	m1	114	ILE
49	m3	60	ALA
49	m3	76	THR
49	m3	129	ASN
53	m7	67	ILE
53	m7	75	GLU
53	m7	78	VAL
54	m8	108	ALA
54	m8	155	MET
55	m9	3	ASN
56	n0	2	ALA
57	n1	135	PRO
59	n3	64	LYS
61	n5	38	LEU
61	n5	47	ALA
62	n6	77	LYS
63	n7	103	GLN
63	n7	127	ASN
63	n7	134	LEU
64	n8	110	GLY
68	o2	4	LEU
68	o2	5	PRO
68	o2	12	LYS
71	o5	82	ALA

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Mol	Chain	Res	Type
73	o7	85	LYS
73	o7	86	ALA
2	S0	66	ALA
3	S1	64	ARG
4	S2	150	GLN
5	S3	4	LEU
6	S4	77	ARG
7	S5	81	ARG
8	S6	146	GLY
9	S7	73	VAL
10	S8	59	ARG
13	C1	95	PRO
14	C2	39	ASP
14	C2	66	VAL
14	C2	68	GLU
14	C2	101	ALA
16	C4	18	ARG
16	C4	75	GLY
17	C5	9	LYS
22	D0	21	LYS
22	D0	49	ASN
23	D1	10	GLU
23	D1	42	GLU
23	D1	44	ARG
25	D3	3	LYS
25	D3	89	ASN
31	D9	11	PRO
33	E1	100	LEU
34	SR	160	GLU
34	SR	237	GLN
35	SM	46	LYS
35	SM	101	ASP
39	L2	127	ALA
40	L3	155	ALA
41	L4	5	GLN
41	L4	14	GLU
41	L4	233	LEU
41	L4	313	LEU
41	L4	339	LEU
41	L4	361	HIS
42	L5	19	PRO
42	L5	292	ALA

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Mol	Chain	Res	Type
46	L9	96	HIS
48	M1	117	ASP
51	M5	94	TYR
51	M5	145	ASP
54	M8	162	ALA
56	N0	2	ALA
60	N4	80	ARG
64	N8	47	LYS
65	N9	25	LYS
67	O1	7	VAL
69	O3	91	ALA
70	O4	46	ASP
72	O6	3	VAL
72	O6	21	THR
72	O6	77	LEU
75	O9	4	GLN
76	Q0	79	GLU
2	s0	127	ARG
4	s2	91	ARG
6	s4	94	ALA
6	s4	119	ALA
7	s5	35	GLN
7	s5	152	GLY
9	s7	8	ILE
9	s7	11	GLN
10	s8	78	ILE
11	s9	126	ARG
80	c0	3	MET
80	c0	31	LYS
81	c2	59	LEU
81	c2	82	PRO
81	c2	118	ALA
15	c3	22	ALA
19	c7	86	PRO
20	c8	14	ILE
20	c8	135	GLY
22	d0	72	ASN
23	d1	4	ASP
23	d1	77	GLY
25	d3	101	GLU
26	d4	51	GLU
26	d4	53	ASP

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Mol	Chain	Res	Type
28	d6	35	ALA
29	d7	3	LEU
29	d7	58	SER
33	e1	146	SER
83	sR	146	GLY
84	sM	43	ASP
84	sM	46	LYS
39	l2	143	GLU
41	l4	328	ASN
46	l9	96	HIS
46	l9	167	VAL
47	m0	43	VAL
48	m1	153	LYS
50	m4	135	LEU
63	n7	16	GLY
64	n8	24	LYS
66	o0	101	LEU
69	o3	33	GLU
69	o3	59	VAL
3	S1	210	ILE
7	S5	100	ASN
8	S6	123	GLY
8	S6	153	VAL
11	S9	162	SER
13	C1	96	LYS
14	C2	63	VAL
14	C2	85	LYS
14	C2	128	ALA
14	C2	131	ASP
18	C6	33	GLY
25	D3	96	VAL
28	D6	63	ALA
35	SM	17	VAL
35	SM	53	ARG
35	SM	89	ARG
35	SM	139	GLU
39	L2	180	LEU
40	L3	175	LYS
40	L3	317	ILE
41	L4	4	PRO
41	L4	140	HIS
44	L7	178	ILE

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Mol	Chain	Res	Type
45	L8	190	VAL
50	M4	6	ILE
52	M6	110	PRO
64	N8	27	LYS
2	s0	191	ARG
4	s2	163	GLY
4	s2	236	PRO
5	s3	43	PRO
5	s3	160	SER
5	s3	180	GLY
9	s7	115	SER
9	s7	185	ILE
10	s8	52	ASN
11	s9	162	SER
13	c1	76	VAL
16	c4	124	ASP
82	c5	71	GLU
82	c5	128	HIS
82	c5	130	ARG
23	d1	10	GLU
25	d3	70	LYS
27	d5	103	ARG
28	d6	58	VAL
32	e0	45	VAL
32	e0	54	ARG
40	l3	3	HIS
44	l7	229	PHE
85	l8	69	LEU
85	l8	81	THR
47	m0	101	LYS
48	m1	12	LEU
49	m3	152	THR
50	m4	49	PRO
51	m5	68	ARG
55	m9	36	ASN
87	n4	72	SER
64	n8	129	PHE
70	o4	78	GLY
70	o4	82	ALA
72	o6	36	ARG
23	D1	82	VAL
25	D3	8	GLY

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Mol	Chain	Res	Type
26	D4	100	VAL
56	N0	167	ARG
65	N9	21	ILE
69	O3	59	VAL
70	O4	77	GLY
4	s2	83	ILE
10	s8	50	GLY
10	s8	101	ILE
81	c2	63	VAL
82	c5	129	GLY
28	d6	60	PRO
41	l4	272	VAL
42	l5	125	VAL
72	o6	3	VAL
3	S1	48	VAL
3	S1	176	VAL
4	S2	182	PRO
14	C2	81	ASP
23	D1	6	GLY
26	D4	47	VAL
41	L4	131	VAL
54	M8	183	GLY
8	s6	69	LEU
82	c5	48	GLY
83	sR	97	GLY
83	sR	105	GLY
44	l7	178	ILE
71	o5	4	VAL
2	S0	189	VAL
17	C5	87	PRO
26	D4	95	GLY
27	D5	55	PRO
44	L7	191	VAL
45	L8	30	THR
47	M0	47	PRO
3	s1	22	ASP
81	c2	115	VAL
19	c7	117	LEU
25	d3	130	VAL
87	n4	132	GLY
3	S1	114	VAL
7	S5	21	THR

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Mol	Chain	Res	Type
9	S7	132	PRO
27	D5	88	ILE
34	SR	194	GLY
53	M7	36	ILE
8	s6	153	VAL
40	l3	141	GLY
61	n5	62	VAL
65	n9	37	PRO
72	o6	9	ILE
88	p0	196	VAL
7	s5	59	VAL
84	sM	51	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/173 (95%)	132 (80%)	32 (20%)	1	4
2	s0	165/173 (95%)	136 (82%)	29 (18%)	1	6
3	S1	191/192 (100%)	155 (81%)	36 (19%)	1	5
3	s1	192/192 (100%)	162 (84%)	30 (16%)	2	9
4	S2	176/176 (100%)	141 (80%)	35 (20%)	1	4
4	s2	176/176 (100%)	137 (78%)	39 (22%)	1	3
5	S3	182/182 (100%)	150 (82%)	32 (18%)	1	6
5	s3	182/182 (100%)	157 (86%)	25 (14%)	3	13
6	S4	221/221 (100%)	182 (82%)	39 (18%)	1	6
6	s4	221/221 (100%)	193 (87%)	28 (13%)	3	15
7	S5	173/173 (100%)	142 (82%)	31 (18%)	1	6
7	s5	173/173 (100%)	142 (82%)	31 (18%)	1	6
8	S6	188/193 (97%)	156 (83%)	32 (17%)	1	7
8	s6	187/193 (97%)	154 (82%)	33 (18%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S7	165/166 (99%)	139 (84%)	26 (16%)	2	9
9	s7	165/166 (99%)	138 (84%)	27 (16%)	2	8
10	S8	150/160 (94%)	128 (85%)	22 (15%)	2	11
10	s8	150/160 (94%)	132 (88%)	18 (12%)	4	17
11	S9	158/158 (100%)	127 (80%)	31 (20%)	1	4
11	s9	158/158 (100%)	136 (86%)	22 (14%)	3	13
12	C0	77/77 (100%)	64 (83%)	13 (17%)	1	7
13	C1	129/129 (100%)	113 (88%)	16 (12%)	4	16
13	c1	129/129 (100%)	102 (79%)	27 (21%)	1	4
14	C2	88/100 (88%)	69 (78%)	19 (22%)	1	3
15	C3	127/127 (100%)	108 (85%)	19 (15%)	2	10
15	c3	127/127 (100%)	106 (84%)	21 (16%)	2	8
16	C4	81/97 (84%)	63 (78%)	18 (22%)	1	3
16	c4	97/97 (100%)	74 (76%)	23 (24%)	0	2
17	C5	101/107 (94%)	87 (86%)	14 (14%)	3	13
18	C6	117/118 (99%)	96 (82%)	21 (18%)	1	6
18	c6	118/118 (100%)	101 (86%)	17 (14%)	2	11
19	C7	94/113 (83%)	72 (77%)	22 (23%)	0	2
19	c7	92/113 (81%)	78 (85%)	14 (15%)	2	10
20	C8	128/128 (100%)	93 (73%)	35 (27%)	0	1
20	c8	128/128 (100%)	105 (82%)	23 (18%)	1	6
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	4
21	c9	115/115 (100%)	97 (84%)	18 (16%)	2	9
22	D0	100/103 (97%)	78 (78%)	22 (22%)	1	3
22	d0	103/103 (100%)	79 (77%)	24 (23%)	0	2
23	D1	74/74 (100%)	63 (85%)	11 (15%)	2	10
23	d1	74/74 (100%)	61 (82%)	13 (18%)	1	6
24	D2	110/110 (100%)	92 (84%)	18 (16%)	2	8
24	d2	110/110 (100%)	97 (88%)	13 (12%)	4	17
25	D3	119/119 (100%)	103 (87%)	16 (13%)	3	13
25	d3	119/119 (100%)	104 (87%)	15 (13%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1	5
26	d4	112/112 (100%)	96 (86%)	16 (14%)	2	12
27	D5	61/61 (100%)	44 (72%)	17 (28%)	0	1
27	d5	61/61 (100%)	53 (87%)	8 (13%)	3	14
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0	1
28	d6	83/83 (100%)	71 (86%)	12 (14%)	2	11
29	D7	70/70 (100%)	63 (90%)	7 (10%)	6	23
29	d7	70/70 (100%)	61 (87%)	9 (13%)	3	15
30	D8	56/56 (100%)	45 (80%)	11 (20%)	1	4
30	d8	56/56 (100%)	44 (79%)	12 (21%)	1	3
31	D9	47/47 (100%)	37 (79%)	10 (21%)	1	3
31	d9	47/47 (100%)	38 (81%)	9 (19%)	1	5
32	E0	51/53 (96%)	44 (86%)	7 (14%)	3	13
32	e0	53/53 (100%)	39 (74%)	14 (26%)	0	1
33	E1	62/66 (94%)	46 (74%)	16 (26%)	0	1
33	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
34	SR	259/260 (100%)	234 (90%)	25 (10%)	6	24
35	SM	97/107 (91%)	81 (84%)	16 (16%)	2	8
39	L2	193/194 (100%)	166 (86%)	27 (14%)	3	13
39	l2	192/194 (99%)	160 (83%)	32 (17%)	2	8
40	L3	321/322 (100%)	265 (83%)	56 (17%)	1	6
40	l3	321/322 (100%)	264 (82%)	57 (18%)	1	6
41	L4	288/288 (100%)	244 (85%)	44 (15%)	2	10
41	l4	288/288 (100%)	237 (82%)	51 (18%)	1	6
42	L5	244/244 (100%)	206 (84%)	38 (16%)	2	9
42	l5	243/244 (100%)	203 (84%)	40 (16%)	2	8
43	L6	134/152 (88%)	116 (87%)	18 (13%)	3	13
43	l6	135/152 (89%)	117 (87%)	18 (13%)	3	14
44	L7	186/187 (100%)	168 (90%)	18 (10%)	6	24
44	l7	187/187 (100%)	162 (87%)	25 (13%)	3	13
45	L8	187/191 (98%)	154 (82%)	33 (18%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	L9	171/171 (100%)	138 (81%)	33 (19%)	1	4
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	3
47	M0	177/186 (95%)	147 (83%)	30 (17%)	1	7
47	m0	179/186 (96%)	149 (83%)	30 (17%)	1	7
48	M1	147/147 (100%)	122 (83%)	25 (17%)	1	7
48	m1	147/147 (100%)	120 (82%)	27 (18%)	1	5
49	M3	154/154 (100%)	126 (82%)	28 (18%)	1	6
49	m3	154/154 (100%)	133 (86%)	21 (14%)	3	13
50	M4	107/108 (99%)	88 (82%)	19 (18%)	1	6
50	m4	108/108 (100%)	92 (85%)	16 (15%)	2	10
51	M5	175/175 (100%)	139 (79%)	36 (21%)	1	4
51	m5	175/175 (100%)	150 (86%)	25 (14%)	2	12
52	M6	160/160 (100%)	144 (90%)	16 (10%)	6	23
52	m6	160/160 (100%)	140 (88%)	20 (12%)	3	16
53	M7	140/145 (97%)	114 (81%)	26 (19%)	1	5
53	m7	125/145 (86%)	103 (82%)	22 (18%)	1	6
54	M8	150/150 (100%)	130 (87%)	20 (13%)	3	14
54	m8	150/150 (100%)	126 (84%)	24 (16%)	2	8
55	M9	153/153 (100%)	127 (83%)	26 (17%)	1	7
55	m9	153/153 (100%)	125 (82%)	28 (18%)	1	5
56	N0	156/156 (100%)	128 (82%)	28 (18%)	1	6
56	n0	156/156 (100%)	130 (83%)	26 (17%)	2	8
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	3
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	3
58	N2	87/87 (100%)	75 (86%)	12 (14%)	3	13
58	n2	85/87 (98%)	70 (82%)	15 (18%)	1	6
59	N3	104/104 (100%)	88 (85%)	16 (15%)	2	9
59	n3	104/104 (100%)	93 (89%)	11 (11%)	5	21
60	N4	57/86 (66%)	50 (88%)	7 (12%)	4	16
61	N5	104/105 (99%)	83 (80%)	21 (20%)	1	4
61	n5	104/105 (99%)	85 (82%)	19 (18%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	N6	109/109 (100%)	82 (75%)	27 (25%)	0	2
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	2
63	N7	115/115 (100%)	94 (82%)	21 (18%)	1	5
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	4
64	N8	118/118 (100%)	97 (82%)	21 (18%)	1	6
64	n8	118/118 (100%)	103 (87%)	15 (13%)	3	15
65	N9	46/46 (100%)	38 (83%)	8 (17%)	1	6
65	n9	46/46 (100%)	35 (76%)	11 (24%)	0	2
66	O0	81/84 (96%)	68 (84%)	13 (16%)	2	8
66	o0	84/84 (100%)	72 (86%)	12 (14%)	2	12
67	O1	92/96 (96%)	77 (84%)	15 (16%)	2	8
67	o1	94/96 (98%)	76 (81%)	18 (19%)	1	5
68	O2	109/109 (100%)	98 (90%)	11 (10%)	6	22
68	o2	109/109 (100%)	94 (86%)	15 (14%)	3	13
69	O3	90/90 (100%)	79 (88%)	11 (12%)	4	16
69	o3	90/90 (100%)	77 (86%)	13 (14%)	2	11
70	O4	95/95 (100%)	79 (83%)	16 (17%)	1	7
70	o4	95/95 (100%)	83 (87%)	12 (13%)	3	15
71	O5	104/104 (100%)	84 (81%)	20 (19%)	1	4
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	4
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	3
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	59 (84%)	11 (16%)	2	9
73	o7	70/70 (100%)	53 (76%)	17 (24%)	0	2
74	O8	68/68 (100%)	52 (76%)	16 (24%)	0	2
74	o8	67/68 (98%)	55 (82%)	12 (18%)	1	6
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	9
75	o9	45/45 (100%)	39 (87%)	6 (13%)	3	14
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	1	7
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1	5
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	70 (78%)	20 (22%)	1	3
78	q2	90/90 (100%)	72 (80%)	18 (20%)	1	4
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	12
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	3
80	c0	73/73 (100%)	60 (82%)	13 (18%)	1	6
81	c2	88/88 (100%)	68 (77%)	20 (23%)	0	2
82	c5	103/118 (87%)	85 (82%)	18 (18%)	1	6
83	sR	260/261 (100%)	241 (93%)	19 (7%)	11	34
84	sM	54/54 (100%)	41 (76%)	13 (24%)	0	2
85	l8	177/185 (96%)	154 (87%)	23 (13%)	3	14
87	n4	100/114 (88%)	91 (91%)	9 (9%)	8	27
88	p0	105/165 (64%)	85 (81%)	20 (19%)	1	5
All	All	18729/19106 (98%)	15556 (83%)	3173 (17%)	1	7

All (3173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	6	THR
2	S0	7	PHE
2	S0	8	ASP
2	S0	9	LEU
2	S0	37	VAL
2	S0	43	ASP
2	S0	49	ASN
2	S0	50	VAL
2	S0	52	LYS
2	S0	59	LEU
2	S0	76	ILE
2	S0	84	ARG
2	S0	87	LEU
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	103	THR
2	S0	111	ILE
2	S0	117	GLU

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Mol	Chain	Res	Type
2	S0	119	ARG
2	S0	135	GLU
2	S0	139	VAL
2	S0	154	GLU
2	S0	156	VAL
2	S0	157	ASP
2	S0	170	ILE
2	S0	172	LEU
2	S0	184	LEU
2	S0	185	ARG
2	S0	188	LEU
2	S0	196	SER
2	S0	200	ASP
3	S1	21	VAL
3	S1	22	ASP
3	S1	25	THR
3	S1	29	TRP
3	S1	30	PHE
3	S1	46	THR
3	S1	61	LEU
3	S1	66	VAL
3	S1	70	LEU
3	S1	77	GLU
3	S1	78	ASP
3	S1	81	PHE
3	S1	89	ASP
3	S1	91	VAL
3	S1	96	LEU
3	S1	97	LEU
3	S1	105	PHE
3	S1	111	ARG
3	S1	112	SER
3	S1	117	TRP
3	S1	124	ASN
3	S1	131	ASP
3	S1	135	LEU
3	S1	149	GLN
3	S1	170	GLU
3	S1	177	GLN
3	S1	180	THR
3	S1	181	LEU
3	S1	198	GLU

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Mol	Chain	Res	Type
3	S1	202	LYS
3	S1	214	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	219	LYS
3	S1	220	GLN
3	S1	223	PHE
4	S2	41	LEU
4	S2	53	ILE
4	S2	54	GLU
4	S2	58	LEU
4	S2	64	LYS
4	S2	69	ILE
4	S2	70	ASP
4	S2	72	LEU
4	S2	73	LEU
4	S2	77	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	91	ARG
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	111	VAL
4	S2	117	THR
4	S2	134	LEU
4	S2	136	VAL
4	S2	137	ILE
4	S2	139	ILE
4	S2	140	ARG
4	S2	141	ARG
4	S2	146	THR
4	S2	148	LEU
4	S2	159	THR
4	S2	166	THR
4	S2	207	LEU
4	S2	208	GLU
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	237	VAL
4	S2	245	ASP

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Mol	Chain	Res	Type
5	S3	4	LEU
5	S3	7	LYS
5	S3	23	GLU
5	S3	65	ARG
5	S3	66	ILE
5	S3	76	ARG
5	S3	84	ILE
5	S3	91	VAL
5	S3	92	GLN
5	S3	93	ASP
5	S3	94	ARG
5	S3	103	GLU
5	S3	104	SER
5	S3	105	MET
5	S3	113	LEU
5	S3	117	ARG
5	S3	127	MET
5	S3	134	CYS
5	S3	141	LYS
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	151	LYS
5	S3	157	LEU
5	S3	158	ILE
5	S3	176	LEU
5	S3	178	ARG
5	S3	187	LYS
5	S3	190	ARG
5	S3	209	ILE
5	S3	218	LEU
5	S3	222	VAL
6	S4	7	LYS
6	S4	9	LEU
6	S4	12	LEU
6	S4	26	CYS
6	S4	38	LEU
6	S4	39	ARG
6	S4	42	LEU
6	S4	65	LEU
6	S4	68	ARG
6	S4	70	VAL

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Mol	Chain	Res	Type
6	S4	77	ARG
6	S4	92	LEU
6	S4	93	ASP
6	S4	116	ASP
6	S4	126	VAL
6	S4	129	VAL
6	S4	131	LEU
6	S4	133	LYS
6	S4	139	VAL
6	S4	140	VAL
6	S4	146	THR
6	S4	148	ARG
6	S4	155	LYS
6	S4	164	LEU
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	197	HIS
6	S4	211	LYS
6	S4	214	LEU
6	S4	215	ASP
6	S4	222	LEU
6	S4	226	PHE
6	S4	227	VAL
6	S4	231	GLN
6	S4	240	LYS
6	S4	242	LYS
6	S4	246	LEU
6	S4	259	GLN
7	S5	24	VAL
7	S5	25	LEU
7	S5	32	GLU
7	S5	41	LYS
7	S5	43	PHE
7	S5	45	LYS
7	S5	49	GLU
7	S5	51	VAL
7	S5	53	VAL
7	S5	65	ARG
7	S5	76	ARG
7	S5	79	ASN
7	S5	86	GLN

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Mol	Chain	Res	Type
7	S5	89	ILE
7	S5	93	LEU
7	S5	119	ASP
7	S5	126	ASP
7	S5	147	THR
7	S5	149	VAL
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	170	GLN
7	S5	186	ASN
7	S5	190	ILE
7	S5	194	LEU
7	S5	203	LYS
7	S5	206	SER
7	S5	216	GLU
7	S5	219	ARG
7	S5	225	ARG
8	S6	7	TYR
8	S6	25	ARG
8	S6	30	LYS
8	S6	45	PHE
8	S6	58	LYS
8	S6	59	GLN
8	S6	65	GLN
8	S6	76	LEU
8	S6	78	THR
8	S6	79	LYS
8	S6	81	VAL
8	S6	82	SER
8	S6	97	VAL
8	S6	98	ARG
8	S6	120	GLU
8	S6	122	GLU
8	S6	124	LEU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	129	VAL
8	S6	132	ARG
8	S6	133	LEU
8	S6	143	LYS

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Mol	Chain	Res	Type
8	S6	151	ASP
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	175	ILE
8	S6	216	LEU
8	S6	223	LYS
9	S7	9	LEU
9	S7	24	PHE
9	S7	37	GLU
9	S7	38	LEU
9	S7	50	ASP
9	S7	70	PHE
9	S7	77	LEU
9	S7	79	ARG
9	S7	80	GLU
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	105	THR
9	S7	109	VAL
9	S7	114	ARG
9	S7	116	ARG
9	S7	126	LEU
9	S7	131	PHE
9	S7	143	LEU
9	S7	144	VAL
9	S7	154	LEU
9	S7	159	VAL
9	S7	167	GLU
9	S7	181	ILE
9	S7	184	GLU
9	S7	185	ILE
10	S8	8	ARG
10	S8	21	PHE
10	S8	29	LEU
10	S8	32	GLN
10	S8	36	THR
10	S8	49	ARG
10	S8	58	LEU
10	S8	62	THR

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Mol	Chain	Res	Type
10	S8	66	SER
10	S8	70	GLU
10	S8	74	LYS
10	S8	123	LYS
10	S8	138	ASN
10	S8	140	GLU
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	164	ARG
10	S8	184	LEU
10	S8	185	GLU
10	S8	196	LEU
10	S8	199	LYS
11	S9	3	ARG
11	S9	6	ARG
11	S9	7	THR
11	S9	14	THR
11	S9	28	LEU
11	S9	39	LYS
11	S9	49	LEU
11	S9	54	ARG
11	S9	60	LEU
11	S9	82	ARG
11	S9	88	GLU
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	96	VAL
11	S9	97	LEU
11	S9	99	LEU
11	S9	109	LEU
11	S9	110	GLN
11	S9	118	LEU
11	S9	120	LYS
11	S9	134	ILE
11	S9	138	LYS
11	S9	145	SER
11	S9	149	ARG
11	S9	151	ASP
11	S9	161	THR

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Mol	Chain	Res	Type
11	S9	171	ARG
11	S9	174	ARG
11	S9	182	GLU
12	C0	8	ARG
12	C0	20	VAL
12	C0	22	VAL
12	C0	27	PHE
12	C0	28	ASN
12	C0	32	HIS
12	C0	46	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	71	GLU
12	C0	76	LEU
12	C0	78	GLU
12	C0	82	LEU
13	C1	21	ASN
13	C1	29	LYS
13	C1	40	LEU
13	C1	43	LYS
13	C1	44	THR
13	C1	54	ILE
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	83	THR
13	C1	99	ARG
13	C1	109	VAL
13	C1	123	VAL
13	C1	125	VAL
13	C1	136	ARG
13	C1	141	LYS
14	C2	28	LEU
14	C2	33	ARG
14	C2	36	LEU
14	C2	43	ARG
14	C2	50	LYS
14	C2	58	LEU
14	C2	61	VAL
14	C2	62	LEU
14	C2	63	VAL
14	C2	66	VAL

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Mol	Chain	Res	Type
14	C2	71	ILE
14	C2	74	LEU
14	C2	89	ILE
14	C2	103	LEU
14	C2	119	SER
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
14	C2	139	HIS
15	C3	3	ARG
15	C3	9	LYS
15	C3	16	ILE
15	C3	21	ASN
15	C3	27	LYS
15	C3	39	LYS
15	C3	42	ARG
15	C3	45	LEU
15	C3	56	ASP
15	C3	64	ARG
15	C3	76	LYS
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	115	LEU
15	C3	125	LEU
15	C3	134	VAL
15	C3	145	THR
15	C3	150	VAL
16	C4	13	VAL
16	C4	14	PHE
16	C4	20	TYR
16	C4	29	HIS
16	C4	31	THR
16	C4	39	ILE
16	C4	43	THR
16	C4	51	ASP
16	C4	81	VAL
16	C4	92	LYS
16	C4	102	LEU
16	C4	103	ARG
16	C4	107	ARG
16	C4	108	SER

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Mol	Chain	Res	Type
16	C4	123	SER
16	C4	124	ASP
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	22	LEU
17	C5	26	LEU
17	C5	35	LYS
17	C5	36	LEU
17	C5	44	ARG
17	C5	47	ARG
17	C5	50	THR
17	C5	52	LYS
17	C5	69	GLU
17	C5	86	VAL
17	C5	110	GLU
17	C5	121	ILE
17	C5	124	THR
18	C6	4	VAL
18	C6	14	LYS
18	C6	26	LYS
18	C6	28	LEU
18	C6	43	ILE
18	C6	52	LEU
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	68	ARG
18	C6	69	VAL
18	C6	97	VAL
18	C6	98	ASP
18	C6	101	SER
18	C6	106	LYS
18	C6	123	ARG
18	C6	128	LYS
18	C6	137	ARG
18	C6	138	PHE
18	C6	141	SER
19	C7	3	ARG
19	C7	6	THR
19	C7	25	THR

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Mol	Chain	Res	Type
19	C7	29	GLN
19	C7	30	THR
19	C7	34	LEU
19	C7	38	ILE
19	C7	40	THR
19	C7	43	SER
19	C7	46	LEU
19	C7	49	LYS
19	C7	69	ILE
19	C7	72	LYS
19	C7	78	ARG
19	C7	83	GLN
19	C7	84	TYR
19	C7	85	VAL
19	C7	88	VAL
19	C7	105	GLN
19	C7	113	LEU
19	C7	115	LEU
19	C7	119	LEU
20	C8	3	LEU
20	C8	4	VAL
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	12	GLN
20	C8	13	HIS
20	C8	14	ILE
20	C8	17	LEU
20	C8	20	THR
20	C8	21	ASN
20	C8	25	ASN
20	C8	26	ILE
20	C8	28	ILE
20	C8	32	LEU
20	C8	34	THR
20	C8	38	VAL
20	C8	40	ARG
20	C8	52	VAL
20	C8	54	LEU
20	C8	60	GLU
20	C8	61	LEU
20	C8	71	GLN

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Mol	Chain	Res	Type
20	C8	77	THR
20	C8	80	LYS
20	C8	92	ILE
20	C8	107	SER
20	C8	110	ARG
20	C8	116	LEU
20	C8	132	ARG
20	C8	133	VAL
20	C8	136	GLN
20	C8	138	THR
20	C8	141	THR
20	C8	143	ARG
21	C9	4	VAL
21	C9	13	ASP
21	C9	18	TYR
21	C9	22	LEU
21	C9	25	GLN
21	C9	28	LEU
21	C9	30	VAL
21	C9	33	TYR
21	C9	35	ASP
21	C9	36	ILE
21	C9	37	VAL
21	C9	57	ARG
21	C9	67	MET
21	C9	70	GLN
21	C9	94	ILE
21	C9	125	SER
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	132	LEU
21	C9	133	ASP
21	C9	134	ARG
21	C9	144	GLU
22	D0	15	GLN
22	D0	17	GLN
22	D0	18	GLN
22	D0	23	ARG
22	D0	27	THR
22	D0	30	LYS
22	D0	31	VAL

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Mol	Chain	Res	Type
22	D0	33	GLN
22	D0	34	LEU
22	D0	35	GLU
22	D0	42	VAL
22	D0	47	GLN
22	D0	48	HIS
22	D0	51	VAL
22	D0	60	THR
22	D0	61	LYS
22	D0	74	GLU
22	D0	76	SER
22	D0	89	ARG
22	D0	103	ILE
22	D0	108	ILE
22	D0	121	ASN
23	D1	3	ASN
23	D1	5	LYS
23	D1	32	VAL
23	D1	41	GLU
23	D1	49	GLU
23	D1	52	THR
23	D1	62	ARG
23	D1	65	SER
23	D1	68	SER
23	D1	78	LEU
23	D1	80	LYS
24	D2	4	SER
24	D2	7	LEU
24	D2	24	GLN
24	D2	26	LEU
24	D2	27	ILE
24	D2	43	LYS
24	D2	53	ILE
24	D2	65	LEU
24	D2	76	SER
24	D2	87	GLU
24	D2	93	LEU
24	D2	97	ARG
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR

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Mol	Chain	Res	Type
24	D2	117	ARG
24	D2	121	VAL
25	D3	7	ARG
25	D3	9	LEU
25	D3	18	HIS
25	D3	40	SER
25	D3	60	GLU
25	D3	73	ARG
25	D3	78	LYS
25	D3	82	LYS
25	D3	84	THR
25	D3	96	VAL
25	D3	107	PHE
25	D3	110	LYS
25	D3	114	LYS
25	D3	131	SER
25	D3	133	LEU
25	D3	144	ARG
26	D4	17	LEU
26	D4	29	HIS
26	D4	32	ARG
26	D4	34	ASN
26	D4	35	VAL
26	D4	36	SER
26	D4	47	VAL
26	D4	49	LYS
26	D4	51	GLU
26	D4	52	LYS
26	D4	57	VAL
26	D4	61	ARG
26	D4	84	LYS
26	D4	88	THR
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	121	THR
26	D4	124	ARG
26	D4	127	LYS
26	D4	128	LYS
27	D5	37	GLN
27	D5	38	HIS
27	D5	42	LEU

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Mol	Chain	Res	Type
27	D5	58	ARG
27	D5	59	TYR
27	D5	67	ASP
27	D5	68	ARG
27	D5	69	LEU
27	D5	71	ILE
27	D5	75	LEU
27	D5	85	LYS
27	D5	90	LYS
27	D5	92	ILE
27	D5	93	SER
27	D5	95	HIS
27	D5	96	SER
27	D5	100	ILE
28	D6	10	ARG
28	D6	12	LYS
28	D6	18	VAL
28	D6	36	ILE
28	D6	38	ARG
28	D6	41	ILE
28	D6	44	ILE
28	D6	45	VAL
28	D6	50	VAL
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	68	TYR
28	D6	69	ASN
28	D6	70	LYS
28	D6	79	ILE
28	D6	82	ARG
28	D6	83	ILE
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
28	D6	90	GLU
28	D6	91	ASP
29	D7	3	LEU
29	D7	4	VAL
29	D7	20	LYS
29	D7	33	LEU
29	D7	34	ASP

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Mol	Chain	Res	Type
29	D7	61	THR
29	D7	67	THR
30	D8	13	ILE
30	D8	15	VAL
30	D8	19	THR
30	D8	32	PHE
30	D8	33	LEU
30	D8	34	GLU
30	D8	39	THR
30	D8	49	ARG
30	D8	52	ASP
30	D8	58	GLU
30	D8	64	ARG
31	D9	6	VAL
31	D9	7	TRP
31	D9	9	SER
31	D9	12	ARG
31	D9	19	ARG
31	D9	22	ARG
31	D9	25	SER
31	D9	30	LEU
31	D9	36	LEU
31	D9	39	CYS
32	E0	20	LYS
32	E0	28	LYS
32	E0	29	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	47	VAL
32	E0	50	VAL
33	E1	86	THR
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	97	LYS
33	E1	98	VAL
33	E1	103	LEU
33	E1	113	LYS
33	E1	118	ARG
33	E1	120	GLU
33	E1	126	CYS
33	E1	130	VAL

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Mol	Chain	Res	Type
33	E1	137	ASP
33	E1	138	ARG
33	E1	139	LEU
33	E1	151	ASN
34	SR	6	VAL
34	SR	29	GLN
34	SR	52	GLN
34	SR	59	ARG
34	SR	65	SER
34	SR	66	HIS
34	SR	76	ASP
34	SR	81	LEU
34	SR	98	GLU
34	SR	116	ASP
34	SR	117	LYS
34	SR	134	TRP
34	SR	136	ILE
34	SR	137	LYS
34	SR	145	LEU
34	SR	153	GLN
34	SR	165	ASP
34	SR	188	ILE
34	SR	191	ASP
34	SR	202	LEU
34	SR	238	ASP
34	SR	248	ASN
34	SR	268	GLN
34	SR	300	THR
34	SR	317	THR
35	SM	27	LYS
35	SM	46	LYS
35	SM	51	ARG
35	SM	61	ILE
35	SM	64	LYS
35	SM	68	ARG
35	SM	78	ASP
35	SM	82	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	94	HIS
35	SM	96	ARG

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Mol	Chain	Res	Type
35	SM	100	THR
35	SM	105	LYS
35	SM	139	GLU
39	L2	14	SER
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	72	ARG
39	L2	74	GLU
39	L2	84	THR
39	L2	97	ASN
39	L2	101	VAL
39	L2	104	LEU
39	L2	107	VAL
39	L2	109	GLU
39	L2	113	VAL
39	L2	116	VAL
39	L2	143	GLU
39	L2	157	VAL
39	L2	165	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	191	LEU
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	224	THR
39	L2	227	ARG
39	L2	230	VAL
39	L2	241	ARG
40	L3	2	SER
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	30	LYS
40	L3	37	ARG
40	L3	47	LEU
40	L3	55	THR
40	L3	56	ILE
40	L3	67	PHE
40	L3	70	ARG

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Mol	Chain	Res	Type
40	L3	85	VAL
40	L3	103	THR
40	L3	104	THR
40	L3	114	VAL
40	L3	126	LYS
40	L3	134	SER
40	L3	139	GLN
40	L3	146	ARG
40	L3	148	LEU
40	L3	150	ARG
40	L3	173	GLN
40	L3	183	LEU
40	L3	187	SER
40	L3	188	ILE
40	L3	192	VAL
40	L3	200	GLU
40	L3	202	THR
40	L3	212	ASN
40	L3	229	VAL
40	L3	232	ARG
40	L3	235	THR
40	L3	236	LYS
40	L3	241	LYS
40	L3	244	ARG
40	L3	252	ILE
40	L3	260	VAL
40	L3	284	ARG
40	L3	296	THR
40	L3	300	ARG
40	L3	305	ILE
40	L3	317	ILE
40	L3	319	ASN
40	L3	320	ASP
40	L3	324	VAL
40	L3	325	LYS
40	L3	328	ILE
40	L3	332	ARG
40	L3	338	LEU
40	L3	347	SER
40	L3	354	VAL
40	L3	355	SER
40	L3	375	GLU

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Mol	Chain	Res	Type
40	L3	380	MET
40	L3	387	LEU
41	L4	21	PRO
41	L4	22	LEU
41	L4	64	SER
41	L4	69	ARG
41	L4	74	ILE
41	L4	93	MET
41	L4	99	MET
41	L4	108	LYS
41	L4	120	TYR
41	L4	133	SER
41	L4	138	ARG
41	L4	148	ILE
41	L4	150	LEU
41	L4	152	VAL
41	L4	153	SER
41	L4	156	LEU
41	L4	161	LYS
41	L4	172	VAL
41	L4	176	SER
41	L4	177	ASP
41	L4	179	LEU
41	L4	187	LEU
41	L4	188	ARG
41	L4	193	LYS
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	206	LEU
41	L4	216	VAL
41	L4	220	ARG
41	L4	222	VAL
41	L4	230	VAL
41	L4	246	ARG
41	L4	258	LEU
41	L4	259	ASP
41	L4	261	VAL
41	L4	267	VAL
41	L4	278	SER
41	L4	289	ILE
41	L4	306	THR

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Mol	Chain	Res	Type
41	L4	307	GLN
41	L4	313	LEU
41	L4	350	LYS
41	L4	354	VAL
42	L5	5	LYS
42	L5	10	SER
42	L5	22	ARG
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	69	ILE
42	L5	89	THR
42	L5	92	LEU
42	L5	93	THR
42	L5	105	ILE
42	L5	115	LEU
42	L5	131	LEU
42	L5	132	THR
42	L5	137	ASP
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	148	ILE
42	L5	151	GLN
42	L5	152	ARG
42	L5	155	THR
42	L5	159	VAL
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	188	GLU
42	L5	189	GLU
42	L5	197	SER
42	L5	222	LEU
42	L5	231	ILE
42	L5	232	ASP
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	264	GLN
42	L5	273	ARG
42	L5	293	LEU

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Mol	Chain	Res	Type
43	L6	2	SER
43	L6	5	LYS
43	L6	15	VAL
43	L6	21	THR
43	L6	28	GLN
43	L6	35	VAL
43	L6	52	VAL
43	L6	64	LEU
43	L6	65	ILE
43	L6	78	ARG
43	L6	79	VAL
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	93	VAL
43	L6	99	GLU
43	L6	129	GLU
43	L6	134	ARG
44	L7	24	GLU
44	L7	25	GLN
44	L7	82	LYS
44	L7	83	LEU
44	L7	84	VAL
44	L7	87	VAL
44	L7	93	ASN
44	L7	100	ARG
44	L7	108	LEU
44	L7	121	LYS
44	L7	158	LYS
44	L7	175	LYS
44	L7	179	LEU
44	L7	184	LEU
44	L7	189	ILE
44	L7	234	GLU
44	L7	239	LEU
44	L7	244	ASN
45	L8	26	LEU
45	L8	27	THR
45	L8	38	GLN
45	L8	41	GLN
45	L8	50	VAL
45	L8	63	LYS

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Mol	Chain	Res	Type
45	L8	74	THR
45	L8	79	GLN
45	L8	81	THR
45	L8	82	LEU
45	L8	84	ARG
45	L8	90	THR
45	L8	92	LYS
45	L8	101	THR
45	L8	118	GLU
45	L8	132	VAL
45	L8	136	LEU
45	L8	145	ASN
45	L8	150	LEU
45	L8	156	ASP
45	L8	163	VAL
45	L8	169	LEU
45	L8	180	VAL
45	L8	185	ARG
45	L8	203	VAL
45	L8	204	ARG
45	L8	206	GLU
45	L8	218	ILE
45	L8	238	LEU
45	L8	240	ASN
45	L8	246	MET
45	L8	248	LYS
45	L8	251	LYS
46	L9	1	MET
46	L9	5	GLN
46	L9	9	GLN
46	L9	16	VAL
46	L9	18	VAL
46	L9	20	ILE
46	L9	24	ILE
46	L9	33	THR
46	L9	41	ILE
46	L9	48	VAL
46	L9	49	ASN
46	L9	52	LEU
46	L9	65	VAL
46	L9	68	LEU
46	L9	69	ARG

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Mol	Chain	Res	Type
46	L9	70	THR
46	L9	90	MET
46	L9	92	TYR
46	L9	132	VAL
46	L9	135	GLU
46	L9	138	THR
46	L9	139	ASN
46	L9	140	VAL
46	L9	147	SER
46	L9	149	ASN
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN
46	L9	164	ILE
46	L9	172	ILE
46	L9	177	ASP
46	L9	189	GLU
46	L9	190	ASP
47	M0	3	ARG
47	M0	7	ARG
47	M0	21	ARG
47	M0	24	ARG
47	M0	30	LYS
47	M0	32	ARG
47	M0	33	ILE
47	M0	40	LYS
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	54	SER
47	M0	63	GLU
47	M0	74	LYS
47	M0	87	LEU
47	M0	116	ARG
47	M0	125	LEU
47	M0	130	ASP
47	M0	133	GLN
47	M0	139	ARG
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	169	LYS

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Mol	Chain	Res	Type
47	M0	177	ASP
47	M0	184	LYS
47	M0	192	ASP
47	M0	197	VAL
47	M0	203	LYS
47	M0	207	GLU
48	M1	6	GLN
48	M1	9	MET
48	M1	10	ARG
48	M1	11	ASP
48	M1	12	LEU
48	M1	13	LYS
48	M1	19	LEU
48	M1	23	VAL
48	M1	31	THR
48	M1	44	THR
48	M1	46	VAL
48	M1	65	ILE
48	M1	70	THR
48	M1	80	LEU
48	M1	82	ARG
48	M1	94	ARG
48	M1	106	ILE
48	M1	107	ASP
48	M1	115	LYS
48	M1	120	ILE
48	M1	137	ARG
48	M1	140	ARG
48	M1	148	VAL
48	M1	166	LYS
48	M1	168	ASP
49	M3	5	LYS
49	M3	23	LYS
49	M3	24	VAL
49	M3	33	VAL
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	58	VAL
49	M3	59	ARG
49	M3	63	VAL
49	M3	67	ARG

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Mol	Chain	Res	Type
49	M3	69	VAL
49	M3	85	LEU
49	M3	114	GLN
49	M3	115	ARG
49	M3	117	LYS
49	M3	121	SER
49	M3	122	LYS
49	M3	124	ILE
49	M3	128	ARG
49	M3	131	LYS
49	M3	134	GLU
49	M3	136	GLU
49	M3	139	LEU
49	M3	164	GLU
49	M3	168	ARG
49	M3	171	ARG
49	M3	190	LYS
50	M4	8	LYS
50	M4	10	SER
50	M4	11	ASN
50	M4	20	VAL
50	M4	21	VAL
50	M4	27	GLN
50	M4	50	LYS
50	M4	53	VAL
50	M4	58	ILE
50	M4	63	VAL
50	M4	74	ARG
50	M4	82	SER
50	M4	91	CYS
50	M4	93	LYS
50	M4	102	LYS
50	M4	105	GLN
50	M4	108	ARG
50	M4	113	THR
50	M4	135	LEU
51	M5	10	LEU
51	M5	15	GLN
51	M5	18	VAL
51	M5	20	ARG
51	M5	22	LEU
51	M5	27	VAL

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Mol	Chain	Res	Type
51	M5	38	ARG
51	M5	49	ARG
51	M5	50	ARG
51	M5	62	TYR
51	M5	68	ARG
51	M5	75	VAL
51	M5	76	PRO
51	M5	80	THR
51	M5	83	LYS
51	M5	85	THR
51	M5	92	LEU
51	M5	93	LYS
51	M5	96	ARG
51	M5	104	GLU
51	M5	106	VAL
51	M5	109	ARG
51	M5	117	ASN
51	M5	133	ILE
51	M5	138	GLN
51	M5	144	ARG
51	M5	151	ILE
51	M5	155	VAL
51	M5	159	ARG
51	M5	182	ASN
51	M5	183	THR
51	M5	187	ARG
51	M5	190	THR
51	M5	198	SER
51	M5	201	ARG
51	M5	204	LYS
52	M6	22	VAL
52	M6	34	VAL
52	M6	41	LEU
52	M6	68	ARG
52	M6	78	ARG
52	M6	85	ARG
52	M6	89	SER
52	M6	106	GLU
52	M6	116	LYS
52	M6	117	ARG
52	M6	119	VAL
52	M6	124	LEU

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Mol	Chain	Res	Type
52	M6	143	THR
52	M6	160	ARG
52	M6	184	THR
52	M6	190	VAL
53	M7	7	THR
53	M7	8	SER
53	M7	9	THR
53	M7	24	VAL
53	M7	32	THR
53	M7	36	ILE
53	M7	52	LEU
53	M7	56	ARG
53	M7	69	ARG
53	M7	70	THR
53	M7	111	LYS
53	M7	112	LEU
53	M7	115	SER
53	M7	118	GLN
53	M7	121	GLN
53	M7	126	ARG
53	M7	127	ARG
53	M7	144	SER
53	M7	149	VAL
53	M7	155	GLU
53	M7	157	VAL
53	M7	165	VAL
53	M7	168	LEU
53	M7	173	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	7	SER
54	M8	17	THR
54	M8	22	ASP
54	M8	26	LEU
54	M8	32	LEU
54	M8	41	ASP
54	M8	49	LEU
54	M8	69	ARG
54	M8	74	GLU
54	M8	81	VAL
54	M8	98	LYS
54	M8	100	THR

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Mol	Chain	Res	Type
54	M8	127	LEU
54	M8	135	GLN
54	M8	138	LEU
54	M8	141	ARG
54	M8	168	THR
54	M8	171	LYS
54	M8	174	ARG
54	M8	180	ARG
55	M9	10	LEU
55	M9	17	VAL
55	M9	20	ARG
55	M9	24	LEU
55	M9	25	ASP
55	M9	30	SER
55	M9	31	GLU
55	M9	43	LYS
55	M9	44	LEU
55	M9	55	VAL
55	M9	61	SER
55	M9	71	ARG
55	M9	74	ARG
55	M9	81	ARG
55	M9	86	GLU
55	M9	91	SER
55	M9	98	ARG
55	M9	103	ARG
55	M9	104	ARG
55	M9	106	LEU
55	M9	110	ARG
55	M9	116	ASP
55	M9	134	HIS
55	M9	138	LEU
55	M9	175	GLN
55	M9	182	ASP
56	N0	8	GLN
56	N0	12	ARG
56	N0	13	ARG
56	N0	40	ARG
56	N0	45	LEU
56	N0	51	VAL
56	N0	57	GLU
56	N0	61	ILE

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Mol	Chain	Res	Type
56	N0	63	GLN
56	N0	71	LYS
56	N0	79	VAL
56	N0	87	THR
56	N0	103	VAL
56	N0	105	THR
56	N0	106	LEU
56	N0	115	ARG
56	N0	117	ARG
56	N0	122	HIS
56	N0	123	ILE
56	N0	130	GLU
56	N0	137	ARG
56	N0	138	GLN
56	N0	144	LEU
56	N0	160	THR
56	N0	162	THR
56	N0	167	ARG
56	N0	171	PHE
56	N0	172	TYR
57	N1	4	SER
57	N1	9	SER
57	N1	12	ARG
57	N1	14	MET
57	N1	18	ASP
57	N1	27	LEU
57	N1	64	VAL
57	N1	68	THR
57	N1	71	SER
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	83	ARG
57	N1	88	ARG
57	N1	89	LEU
57	N1	97	LYS
57	N1	104	GLU
57	N1	106	LEU
57	N1	118	GLU
57	N1	122	GLN
57	N1	124	VAL

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Mol	Chain	Res	Type
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	139	ARG
57	N1	143	THR
57	N1	149	GLN
57	N1	154	VAL
57	N1	159	PHE
58	N2	10	LYS
58	N2	29	ASP
58	N2	38	ILE
58	N2	39	ASP
58	N2	49	ASN
58	N2	52	ASN
58	N2	61	THR
58	N2	66	VAL
58	N2	70	LYS
58	N2	74	LYS
58	N2	100	THR
58	N2	104	ARG
59	N3	32	ARG
59	N3	54	LEU
59	N3	57	MET
59	N3	63	LYS
59	N3	64	LYS
59	N3	72	LYS
59	N3	74	MET
59	N3	83	LYS
59	N3	91	VAL
59	N3	102	ILE
59	N3	108	GLU
59	N3	109	MET
59	N3	115	THR
59	N3	120	LYS
59	N3	125	LEU
59	N3	135	VAL
60	N4	4	GLU
60	N4	5	ILE
60	N4	19	THR
60	N4	26	SER
60	N4	34	SER
60	N4	39	LEU

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Mol	Chain	Res	Type
60	N4	54	LEU
61	N5	26	VAL
61	N5	27	ARG
61	N5	34	LEU
61	N5	38	LEU
61	N5	40	LEU
61	N5	45	LYS
61	N5	49	LYS
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET
61	N5	86	VAL
61	N5	104	GLU
61	N5	108	LEU
61	N5	112	THR
61	N5	115	ARG
61	N5	120	LYS
61	N5	125	ARG
61	N5	133	LEU
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	5	SER
62	N6	8	VAL
62	N6	10	SER
62	N6	13	ARG
62	N6	17	LYS
62	N6	26	GLN
62	N6	37	LYS
62	N6	39	LEU
62	N6	42	GLN
62	N6	45	ILE
62	N6	50	ILE
62	N6	56	VAL
62	N6	57	LEU
62	N6	71	SER
62	N6	74	TYR
62	N6	76	LEU
62	N6	80	VAL
62	N6	94	SER
62	N6	105	VAL

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Mol	Chain	Res	Type
62	N6	111	LEU
62	N6	113	LYS
62	N6	115	ARG
62	N6	122	LYS
62	N6	125	LYS
62	N6	126	LEU
62	N6	127	GLU
63	N7	3	LYS
63	N7	14	VAL
63	N7	17	ARG
63	N7	24	VAL
63	N7	34	LYS
63	N7	46	ILE
63	N7	53	VAL
63	N7	54	THR
63	N7	64	LYS
63	N7	75	VAL
63	N7	81	LEU
63	N7	83	THR
63	N7	86	THR
63	N7	90	GLU
63	N7	99	GLU
63	N7	102	GLU
63	N7	103	GLN
63	N7	107	ARG
63	N7	109	GLU
63	N7	121	ARG
63	N7	134	LEU
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	12	ARG
64	N8	14	HIS
64	N8	16	SER
64	N8	26	ARG
64	N8	42	ARG
64	N8	46	ASP
64	N8	56	VAL
64	N8	60	TYR
64	N8	72	VAL
64	N8	76	ASP
64	N8	84	GLU

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Mol	Chain	Res	Type
64	N8	91	LEU
64	N8	98	THR
64	N8	115	LYS
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
64	N8	139	ARG
65	N9	14	ARG
65	N9	18	ARG
65	N9	22	LYS
65	N9	23	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	16	LEU
66	O0	32	LYS
66	O0	34	LEU
66	O0	36	GLN
66	O0	54	SER
66	O0	61	MET
66	O0	66	LYS
66	O0	76	GLU
66	O0	79	THR
66	O0	83	LYS
66	O0	87	VAL
66	O0	100	ILE
66	O0	104	LEU
67	O1	6	ASP
67	O1	13	THR
67	O1	16	LEU
67	O1	26	LYS
67	O1	31	ARG
67	O1	46	THR
67	O1	55	LEU
67	O1	64	VAL
67	O1	73	LEU
67	O1	79	ARG
67	O1	84	ASP
67	O1	86	LYS
67	O1	89	LEU
67	O1	105	GLN

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Mol	Chain	Res	Type
67	O1	106	THR
68	O2	24	ARG
68	O2	31	ASN
68	O2	33	ARG
68	O2	61	LYS
68	O2	62	LYS
68	O2	73	THR
68	O2	75	LEU
68	O2	84	THR
68	O2	103	LYS
68	O2	106	VAL
68	O2	128	LEU
69	O3	4	SER
69	O3	15	SER
69	O3	20	LYS
69	O3	59	VAL
69	O3	70	LYS
69	O3	74	THR
69	O3	78	SER
69	O3	81	VAL
69	O3	86	ARG
69	O3	98	VAL
69	O3	106	ASN
70	O4	3	GLN
70	O4	5	VAL
70	O4	20	ILE
70	O4	21	LYS
70	O4	24	LYS
70	O4	29	ILE
70	O4	46	ASP
70	O4	49	SER
70	O4	55	SER
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	79	SER
70	O4	86	LYS
70	O4	87	GLU
70	O4	104	VAL
71	O5	15	GLU
71	O5	20	GLN
71	O5	21	LEU

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Mol	Chain	Res	Type
71	O5	27	GLU
71	O5	31	LEU
71	O5	41	LEU
71	O5	44	ILE
71	O5	45	LYS
71	O5	48	ARG
71	O5	49	LYS
71	O5	71	LYS
71	O5	74	LYS
71	O5	89	ARG
71	O5	90	ARG
71	O5	96	GLU
71	O5	100	VAL
71	O5	101	THR
71	O5	104	GLN
71	O5	107	LYS
71	O5	119	LYS
72	O6	5	THR
72	O6	11	LEU
72	O6	17	VAL
72	O6	18	THR
72	O6	21	THR
72	O6	26	ILE
72	O6	36	ARG
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	68	ARG
72	O6	70	ARG
72	O6	72	VAL
72	O6	76	ARG
72	O6	81	THR
72	O6	88	GLU
72	O6	99	ARG
73	O7	17	THR
73	O7	24	ARG
73	O7	25	ARG
73	O7	33	THR
73	O7	36	SER
73	O7	44	THR
73	O7	55	ARG

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Mol	Chain	Res	Type
73	O7	59	THR
73	O7	67	LEU
73	O7	80	THR
73	O7	87	SER
74	O8	3	ARG
74	O8	5	ILE
74	O8	6	THR
74	O8	8	ILE
74	O8	12	LEU
74	O8	24	THR
74	O8	41	THR
74	O8	46	ARG
74	O8	50	SER
74	O8	52	TYR
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	72	THR
74	O8	77	ARG
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	29	LEU
75	O9	32	ASN
75	O9	45	ARG
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	106	ARG
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	127	LEU
77	Q1	9	ARG
77	Q1	10	THR
77	Q1	11	ARG
77	Q1	21	ARG
77	Q1	24	SER
77	Q1	25	LYS
78	Q2	8	ARG

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Mol	Chain	Res	Type
78	Q2	9	LYS
78	Q2	26	THR
78	Q2	29	LYS
78	Q2	34	SER
78	Q2	35	LEU
78	Q2	48	SER
78	Q2	55	LYS
78	Q2	76	LYS
78	Q2	78	LYS
78	Q2	79	THR
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	92	GLU
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
78	Q2	105	GLN
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	32	GLN
79	Q3	45	LYS
79	Q3	49	ARG
79	Q3	56	THR
79	Q3	59	CYS
79	Q3	60	CYS
79	Q3	73	THR
79	Q3	91	GLU
2	s0	6	THR
2	s0	12	GLU
2	s0	22	THR
2	s0	30	GLN
2	s0	45	VAL
2	s0	57	LEU
2	s0	59	LEU
2	s0	62	ARG
2	s0	87	LEU
2	s0	88	LYS
2	s0	110	TYR
2	s0	111	ILE
2	s0	119	ARG

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Mol	Chain	Res	Type
2	s0	131	GLN
2	s0	135	GLU
2	s0	139	VAL
2	s0	144	ILE
2	s0	154	GLU
2	s0	157	ASP
2	s0	167	LYS
2	s0	172	LEU
2	s0	180	GLU
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	196	SER
2	s0	198	MET
2	s0	200	ASP
2	s0	202	TYR
3	s1	21	VAL
3	s1	22	ASP
3	s1	25	THR
3	s1	37	THR
3	s1	47	LEU
3	s1	51	SER
3	s1	62	LYS
3	s1	66	VAL
3	s1	70	LEU
3	s1	73	LEU
3	s1	74	GLN
3	s1	78	ASP
3	s1	81	PHE
3	s1	83	LYS
3	s1	110	LEU
3	s1	115	ARG
3	s1	125	VAL
3	s1	137	ILE
3	s1	150	VAL
3	s1	151	LYS
3	s1	177	GLN
3	s1	179	SER
3	s1	180	THR
3	s1	181	LEU
3	s1	202	LYS
3	s1	212	VAL

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Mol	Chain	Res	Type
3	s1	215	VAL
3	s1	219	LYS
3	s1	223	PHE
3	s1	234	GLU
4	s2	41	LEU
4	s2	53	ILE
4	s2	54	GLU
4	s2	69	ILE
4	s2	70	ASP
4	s2	72	LEU
4	s2	73	LEU
4	s2	76	LEU
4	s2	80	VAL
4	s2	83	ILE
4	s2	87	GLN
4	s2	89	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	94	GLN
4	s2	97	ARG
4	s2	106	ASP
4	s2	111	VAL
4	s2	117	THR
4	s2	139	ILE
4	s2	141	ARG
4	s2	148	LEU
4	s2	150	GLN
4	s2	152	HIS
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	185	LYS
4	s2	194	GLU
4	s2	206	THR
4	s2	221	THR
4	s2	222	TYR
4	s2	225	LEU
4	s2	226	THR
4	s2	229	LEU
4	s2	233	GLN
4	s2	240	LEU
4	s2	248	SER

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Mol	Chain	Res	Type
4	s2	250	GLN
5	s3	4	LEU
5	s3	9	ARG
5	s3	10	LYS
5	s3	26	THR
5	s3	41	VAL
5	s3	44	THR
5	s3	53	THR
5	s3	55	THR
5	s3	59	LEU
5	s3	67	ASN
5	s3	69	LEU
5	s3	76	ARG
5	s3	84	ILE
5	s3	90	ARG
5	s3	91	VAL
5	s3	93	ASP
5	s3	115	ILE
5	s3	116	ARG
5	s3	127	MET
5	s3	128	GLU
5	s3	142	LEU
5	s3	158	ILE
5	s3	162	GLN
5	s3	202	LEU
5	s3	204	ASP
6	s4	11	ARG
6	s4	23	LEU
6	s4	24	SER
6	s4	26	CYS
6	s4	37	LYS
6	s4	38	LEU
6	s4	42	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	56	LEU
6	s4	67	GLN
6	s4	78	THR
6	s4	104	ASP
6	s4	116	ASP
6	s4	126	VAL
6	s4	131	LEU

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Mol	Chain	Res	Type
6	s4	147	ILE
6	s4	148	ARG
6	s4	163	ASP
6	s4	181	VAL
6	s4	182	TYR
6	s4	214	LEU
6	s4	219	VAL
6	s4	221	ARG
6	s4	222	LEU
6	s4	227	VAL
6	s4	245	LYS
6	s4	246	LEU
7	s5	24	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	41	LYS
7	s5	51	VAL
7	s5	59	VAL
7	s5	63	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	83	ARG
7	s5	89	ILE
7	s5	93	LEU
7	s5	109	LYS
7	s5	112	ARG
7	s5	119	ASP
7	s5	125	THR
7	s5	148	ARG
7	s5	149	VAL
7	s5	156	ARG
7	s5	157	ARG
7	s5	166	ARG
7	s5	167	ARG
7	s5	170	GLN
7	s5	187	ILE
7	s5	194	LEU
7	s5	203	LYS
7	s5	208	SER
7	s5	213	LYS
7	s5	216	GLU

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Mol	Chain	Res	Type
7	s5	219	ARG
8	s6	12	SER
8	s6	15	THR
8	s6	25	ARG
8	s6	30	LYS
8	s6	31	ARG
8	s6	69	LEU
8	s6	71	THR
8	s6	76	LEU
8	s6	78	THR
8	s6	93	LYS
8	s6	97	VAL
8	s6	108	VAL
8	s6	109	LEU
8	s6	111	LEU
8	s6	112	VAL
8	s6	115	LYS
8	s6	120	GLU
8	s6	121	LEU
8	s6	127	THR
8	s6	128	THR
8	s6	129	VAL
8	s6	137	ARG
8	s6	143	LYS
8	s6	151	ASP
8	s6	153	VAL
8	s6	155	ASP
8	s6	169	TYR
8	s6	170	THR
8	s6	171	LYS
8	s6	177	ARG
8	s6	182	GLN
8	s6	212	LEU
8	s6	215	ARG
9	s7	11	GLN
9	s7	28	GLU
9	s7	33	GLU
9	s7	41	LEU
9	s7	49	ILE
9	s7	67	LEU
9	s7	77	LEU
9	s7	81	LEU

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Mol	Chain	Res	Type
9	s7	86	GLN
9	s7	87	ASP
9	s7	97	ARG
9	s7	103	SER
9	s7	105	THR
9	s7	108	GLN
9	s7	109	VAL
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	126	LEU
9	s7	141	ARG
9	s7	143	LEU
9	s7	144	VAL
9	s7	159	VAL
9	s7	160	GLN
9	s7	166	LEU
9	s7	185	ILE
9	s7	187	SER
10	s8	22	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	58	LEU
10	s8	61	GLU
10	s8	74	LYS
10	s8	76	THR
10	s8	82	VAL
10	s8	111	GLN
10	s8	138	ASN
10	s8	151	LYS
10	s8	152	ILE
10	s8	155	SER
10	s8	168	CYS
10	s8	183	ILE
10	s8	184	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	21	SER
11	s9	28	LEU

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Mol	Chain	Res	Type
11	s9	78	ARG
11	s9	82	ARG
11	s9	90	LYS
11	s9	93	LEU
11	s9	101	VAL
11	s9	109	LEU
11	s9	110	GLN
11	s9	111	THR
11	s9	120	LYS
11	s9	126	ARG
11	s9	130	THR
11	s9	134	ILE
11	s9	142	ASN
11	s9	150	LEU
11	s9	161	THR
11	s9	171	ARG
11	s9	180	LYS
80	c0	5	LYS
80	c0	15	LEU
80	c0	20	VAL
80	c0	21	VAL
80	c0	27	PHE
80	c0	33	GLU
80	c0	36	ASP
80	c0	40	LEU
80	c0	52	LYS
80	c0	55	VAL
80	c0	57	THR
80	c0	71	GLU
80	c0	77	ARG
13	c1	3	THR
13	c1	5	LEU
13	c1	10	GLU
13	c1	21	ASN
13	c1	27	THR
13	c1	30	ARG
13	c1	32	LYS
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	56	LYS

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Mol	Chain	Res	Type
13	c1	60	PHE
13	c1	61	THR
13	c1	67	ARG
13	c1	74	THR
13	c1	77	SER
13	c1	78	THR
13	c1	80	MET
13	c1	83	THR
13	c1	86	ILE
13	c1	94	ILE
13	c1	99	ARG
13	c1	118	GLN
13	c1	125	VAL
13	c1	129	ARG
13	c1	140	VAL
81	c2	28	LEU
81	c2	36	LEU
81	c2	39	ASP
81	c2	43	ARG
81	c2	58	LEU
81	c2	61	VAL
81	c2	62	LEU
81	c2	66	VAL
81	c2	71	ILE
81	c2	74	LEU
81	c2	85	LYS
81	c2	89	ILE
81	c2	91	VAL
81	c2	103	LEU
81	c2	116	VAL
81	c2	121	VAL
81	c2	129	GLU
81	c2	132	GLU
81	c2	136	ILE
81	c2	140	PHE
15	c3	12	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	21	ASN
15	c3	28	LEU
15	c3	35	GLU
15	c3	37	ILE

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Mol	Chain	Res	Type
15	c3	39	LYS
15	c3	60	VAL
15	c3	64	ARG
15	c3	66	ILE
15	c3	73	ARG
15	c3	80	LEU
15	c3	84	ILE
15	c3	87	ASP
15	c3	97	SER
15	c3	102	LEU
15	c3	115	LEU
15	c3	125	LEU
15	c3	138	ASN
15	c3	150	VAL
16	c4	20	TYR
16	c4	28	VAL
16	c4	31	THR
16	c4	33	LEU
16	c4	42	VAL
16	c4	43	THR
16	c4	51	ASP
16	c4	61	MET
16	c4	62	LEU
16	c4	66	ASP
16	c4	81	VAL
16	c4	92	LYS
16	c4	102	LEU
16	c4	103	ARG
16	c4	114	ARG
16	c4	118	VAL
16	c4	119	THR
16	c4	123	SER
16	c4	124	ASP
16	c4	125	SER
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
82	c5	12	PHE
82	c5	21	ASP
82	c5	24	LYS
82	c5	27	GLU
82	c5	36	LEU

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Mol	Chain	Res	Type
82	c5	40	ARG
82	c5	44	ARG
82	c5	52	LYS
82	c5	69	GLU
82	c5	71	GLU
82	c5	97	TYR
82	c5	107	ILE
82	c5	110	GLU
82	c5	120	SER
82	c5	121	ILE
82	c5	122	THR
82	c5	124	THR
82	c5	127	ARG
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	43	ILE
18	c6	48	VAL
18	c6	53	LEU
18	c6	57	LEU
18	c6	68	ARG
18	c6	69	VAL
18	c6	70	THR
18	c6	90	VAL
18	c6	97	VAL
18	c6	98	ASP
18	c6	110	THR
18	c6	114	ARG
18	c6	128	LYS
18	c6	137	ARG
19	c7	8	THR
19	c7	19	ARG
19	c7	29	GLN
19	c7	34	LEU
19	c7	38	ILE
19	c7	43	SER
19	c7	45	ARG
19	c7	46	LEU
19	c7	60	ARG
19	c7	69	ILE
19	c7	85	VAL
19	c7	88	VAL

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Mol	Chain	Res	Type
19	c7	89	SER
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	13	HIS
20	c8	15	LEU
20	c8	25	ASN
20	c8	27	LYS
20	c8	28	ILE
20	c8	36	LYS
20	c8	40	ARG
20	c8	55	HIS
20	c8	63	GLN
20	c8	80	LYS
20	c8	85	PHE
20	c8	94	ASP
20	c8	104	ASN
20	c8	116	LEU
20	c8	134	ARG
20	c8	136	GLN
20	c8	138	THR
20	c8	144	ARG
21	c9	6	VAL
21	c9	13	ASP
21	c9	27	LYS
21	c9	28	LEU
21	c9	34	VAL
21	c9	37	VAL
21	c9	68	ARG
21	c9	70	GLN
21	c9	71	VAL
21	c9	75	LYS
21	c9	111	ILE
21	c9	116	ILE
21	c9	122	ARG
21	c9	123	ARG
21	c9	126	GLU
21	c9	140	LEU
21	c9	141	GLU

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Mol	Chain	Res	Type
21	c9	144	GLU
22	d0	23	ARG
22	d0	27	THR
22	d0	31	VAL
22	d0	34	LEU
22	d0	44	ASN
22	d0	47	GLN
22	d0	52	LYS
22	d0	57	ARG
22	d0	60	THR
22	d0	63	LEU
22	d0	66	SER
22	d0	70	THR
22	d0	74	GLU
22	d0	80	GLU
22	d0	81	THR
22	d0	88	LYS
22	d0	89	ARG
22	d0	99	ILE
22	d0	102	ARG
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	108	ILE
22	d0	115	GLU
23	d1	2	GLU
23	d1	5	LYS
23	d1	10	GLU
23	d1	11	LEU
23	d1	12	TYR
23	d1	32	VAL
23	d1	38	LYS
23	d1	50	TYR
23	d1	52	THR
23	d1	68	SER
23	d1	69	LEU
23	d1	78	LEU
23	d1	81	ASN
24	d2	4	SER
24	d2	7	LEU
24	d2	9	ASP
24	d2	23	ARG

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Mol	Chain	Res	Type
24	d2	37	PHE
24	d2	65	LEU
24	d2	74	VAL
24	d2	88	LYS
24	d2	93	LEU
24	d2	98	GLN
24	d2	103	ILE
24	d2	124	LYS
24	d2	126	LEU
25	d3	9	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	19	ARG
25	d3	23	ARG
25	d3	33	LEU
25	d3	40	SER
25	d3	56	LYS
25	d3	73	ARG
25	d3	83	VAL
25	d3	84	THR
25	d3	96	VAL
25	d3	100	ASP
25	d3	107	PHE
25	d3	127	VAL
26	d4	10	ARG
26	d4	26	ASP
26	d4	34	ASN
26	d4	35	VAL
26	d4	42	GLU
26	d4	43	LYS
26	d4	44	LEU
26	d4	47	VAL
26	d4	49	LYS
26	d4	51	GLU
26	d4	62	THR
26	d4	88	THR
26	d4	105	ARG
26	d4	118	ILE
26	d4	128	LYS
26	d4	135	ASP
27	d5	43	ASP
27	d5	46	LYS

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Mol	Chain	Res	Type
27	d5	53	GLU
27	d5	57	TYR
27	d5	60	VAL
27	d5	81	ARG
27	d5	86	GLU
27	d5	105	THR
28	d6	10	ARG
28	d6	24	VAL
28	d6	28	LYS
28	d6	33	ASP
28	d6	44	ILE
28	d6	53	LEU
28	d6	58	VAL
28	d6	67	THR
28	d6	82	ARG
28	d6	84	VAL
28	d6	85	ARG
28	d6	90	GLU
29	d7	11	THR
29	d7	41	LEU
29	d7	43	ILE
29	d7	44	THR
29	d7	52	THR
29	d7	61	THR
29	d7	72	LYS
29	d7	77	THR
29	d7	81	ARG
30	d8	7	VAL
30	d8	15	VAL
30	d8	19	THR
30	d8	22	ARG
30	d8	28	VAL
30	d8	32	PHE
30	d8	33	LEU
30	d8	36	THR
30	d8	42	ARG
30	d8	49	ARG
30	d8	54	LEU
30	d8	64	ARG
31	d9	10	HIS
31	d9	16	LYS
31	d9	21	CYS

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Mol	Chain	Res	Type
31	d9	28	THR
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	38	ILE
31	d9	54	LYS
32	e0	13	LYS
32	e0	22	GLU
32	e0	23	LYS
32	e0	26	LYS
32	e0	28	LYS
32	e0	29	LYS
32	e0	39	LEU
32	e0	44	PHE
32	e0	45	VAL
32	e0	47	VAL
32	e0	50	VAL
32	e0	54	ARG
32	e0	55	ARG
32	e0	56	MET
33	e1	80	ARG
33	e1	86	THR
33	e1	90	LYS
33	e1	96	LYS
33	e1	97	LYS
33	e1	98	VAL
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	113	LYS
33	e1	115	THR
33	e1	120	GLU
33	e1	135	HIS
33	e1	140	TYR
33	e1	141	CYS
33	e1	146	SER
33	e1	147	VAL
33	e1	151	ASN
83	sR	22	SER
83	sR	29	GLN
83	sR	52	GLN
83	sR	58	VAL

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Mol	Chain	Res	Type
83	sR	59	ARG
83	sR	64	HIS
83	sR	65	SER
83	sR	76	ASP
83	sR	96	THR
83	sR	145	LEU
83	sR	168	THR
83	sR	176	LYS
83	sR	188	ILE
83	sR	228	LYS
83	sR	232	TYR
83	sR	274	LEU
83	sR	278	PHE
83	sR	297	ASP
83	sR	309	VAL
84	sM	24	GLU
84	sM	30	THR
84	sM	33	LYS
84	sM	41	SER
84	sM	43	ASP
84	sM	48	ARG
84	sM	50	ASN
84	sM	61	ILE
84	sM	68	ARG
84	sM	74	LYS
84	sM	75	ASP
84	sM	77	THR
84	sM	82	THR
39	l2	19	HIS
39	l2	23	ARG
39	l2	32	LEU
39	l2	44	ILE
39	l2	45	VAL
39	l2	46	LYS
39	l2	71	LEU
39	l2	74	GLU
39	l2	84	THR
39	l2	96	LEU
39	l2	101	VAL
39	l2	104	LEU
39	l2	107	VAL
39	l2	109	GLU

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Mol	Chain	Res	Type
39	l2	113	VAL
39	l2	114	SER
39	l2	119	LYS
39	l2	128	ARG
39	l2	137	ILE
39	l2	147	ARG
39	l2	155	LYS
39	l2	158	ILE
39	l2	159	SER
39	l2	165	VAL
39	l2	180	LEU
39	l2	193	ARG
39	l2	202	VAL
39	l2	204	MET
39	l2	223	SER
39	l2	226	SER
39	l2	246	LEU
39	l2	249	SER
40	l3	3	HIS
40	l3	7	GLU
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	21	ARG
40	l3	24	SER
40	l3	25	ILE
40	l3	30	LYS
40	l3	37	ARG
40	l3	41	VAL
40	l3	47	LEU
40	l3	50	LYS
40	l3	56	ILE
40	l3	73	VAL
40	l3	84	VAL
40	l3	85	VAL
40	l3	95	THR
40	l3	103	THR
40	l3	114	VAL
40	l3	116	ARG
40	l3	125	SER
40	l3	139	GLN
40	l3	146	ARG

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Mol	Chain	Res	Type
40	l3	148	LEU
40	l3	150	ARG
40	l3	169	THR
40	l3	183	LEU
40	l3	187	SER
40	l3	188	ILE
40	l3	192	VAL
40	l3	196	ARG
40	l3	202	THR
40	l3	205	VAL
40	l3	211	GLN
40	l3	212	ASN
40	l3	213	GLU
40	l3	232	ARG
40	l3	235	THR
40	l3	238	LEU
40	l3	246	LEU
40	l3	252	ILE
40	l3	260	VAL
40	l3	270	ARG
40	l3	274	SER
40	l3	284	ARG
40	l3	304	THR
40	l3	308	MET
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	338	LEU
40	l3	340	LYS
40	l3	346	THR
40	l3	347	SER
40	l3	380	MET
40	l3	382	THR
41	l4	2	SER
41	l4	25	VAL
41	l4	41	SER
41	l4	47	ARG
41	l4	69	ARG
41	l4	73	ARG
41	l4	85	SER
41	l4	93	MET
41	l4	120	TYR

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Mol	Chain	Res	Type
41	l4	122	THR
41	l4	138	ARG
41	l4	144	LYS
41	l4	145	ILE
41	l4	150	LEU
41	l4	154	THR
41	l4	156	LEU
41	l4	160	GLN
41	l4	170	LYS
41	l4	172	VAL
41	l4	176	SER
41	l4	177	ASP
41	l4	179	LEU
41	l4	182	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	191	LYS
41	l4	203	ARG
41	l4	206	LEU
41	l4	220	ARG
41	l4	222	VAL
41	l4	230	VAL
41	l4	246	ARG
41	l4	258	LEU
41	l4	266	THR
41	l4	267	VAL
41	l4	276	LEU
41	l4	287	THR
41	l4	300	ARG
41	l4	301	PRO
41	l4	306	THR
41	l4	307	GLN
41	l4	313	LEU
41	l4	316	ASN
41	l4	319	LYS
41	l4	323	VAL
41	l4	327	LEU
41	l4	342	LYS
41	l4	345	GLU
41	l4	347	THR
41	l4	356	THR
41	l4	359	LEU

Continued on next page...

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Mol	Chain	Res	Type
42	15	4	GLN
42	15	5	LYS
42	15	13	SER
42	15	34	LYS
42	15	35	ARG
42	15	51	LEU
42	15	62	CYS
42	15	65	ILE
42	15	70	THR
42	15	73	VAL
42	15	74	VAL
42	15	93	THR
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	115	LEU
42	15	118	THR
42	15	130	GLU
42	15	133	GLU
42	15	140	ARG
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE
42	15	151	GLN
42	15	152	ARG
42	15	155	THR
42	15	185	PHE
42	15	186	GLU
42	15	194	LEU
42	15	211	LEU
42	15	218	ARG
42	15	220	SER
42	15	227	LEU
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS
42	15	268	GLU
42	15	273	ARG
42	15	282	ARG
42	15	293	LEU
43	16	8	LYS
43	16	20	LYS

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Mol	Chain	Res	Type
43	16	21	THR
43	16	46	ARG
43	16	50	LYS
43	16	64	LEU
43	16	65	ILE
43	16	66	SER
43	16	79	VAL
43	16	89	THR
43	16	93	VAL
43	16	98	VAL
43	16	109	GLU
43	16	131	LYS
43	16	143	LYS
43	16	152	THR
43	16	155	LEU
43	16	162	SER
44	17	22	THR
44	17	26	VAL
44	17	41	ARG
44	17	53	LYS
44	17	56	GLU
44	17	60	ARG
44	17	77	VAL
44	17	80	GLN
44	17	83	LEU
44	17	84	VAL
44	17	87	VAL
44	17	88	ARG
44	17	98	LYS
44	17	110	ARG
44	17	115	THR
44	17	121	LYS
44	17	156	ILE
44	17	158	LYS
44	17	173	LEU
44	17	175	LYS
44	17	179	LEU
44	17	184	LEU
44	17	196	LYS
44	17	229	PHE
44	17	239	LEU
85	18	26	LEU

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Mol	Chain	Res	Type
85	18	68	ARG
85	18	74	THR
85	18	79	GLN
85	18	81	THR
85	18	95	ASN
85	18	136	LEU
85	18	146	LYS
85	18	149	LYS
85	18	160	ILE
85	18	163	VAL
85	18	169	LEU
85	18	172	LYS
85	18	183	LYS
85	18	208	GLU
85	18	211	LEU
85	18	214	LEU
85	18	216	SER
85	18	217	THR
85	18	230	LYS
85	18	238	LEU
85	18	245	LYS
85	18	248	LYS
46	19	4	ILE
46	19	6	THR
46	19	18	VAL
46	19	22	SER
46	19	33	THR
46	19	44	THR
46	19	48	VAL
46	19	55	VAL
46	19	68	LEU
46	19	69	ARG
46	19	70	THR
46	19	80	THR
46	19	82	VAL
46	19	90	MET
46	19	92	TYR
46	19	105	GLU
46	19	120	ASP
46	19	129	ARG
46	19	130	ASP
46	19	132	VAL

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Mol	Chain	Res	Type
46	l9	133	THR
46	l9	137	SER
46	l9	138	THR
46	l9	140	VAL
46	l9	144	ILE
46	l9	151	VAL
46	l9	152	GLU
46	l9	157	ASN
46	l9	161	LEU
46	l9	162	GLN
46	l9	166	ARG
46	l9	167	VAL
46	l9	170	LYS
46	l9	173	ARG
46	l9	179	ILE
46	l9	184	LYS
46	l9	191	LEU
47	m0	3	ARG
47	m0	21	ARG
47	m0	24	ARG
47	m0	26	VAL
47	m0	36	LEU
47	m0	52	LEU
47	m0	58	GLU
47	m0	74	LYS
47	m0	76	MET
47	m0	83	ASP
47	m0	87	LEU
47	m0	99	ILE
47	m0	101	LYS
47	m0	139	ARG
47	m0	143	SER
47	m0	144	ASN
47	m0	154	ARG
47	m0	162	GLN
47	m0	163	GLN
47	m0	169	LYS
47	m0	176	LEU
47	m0	177	ASP
47	m0	178	ARG
47	m0	197	VAL
47	m0	200	LEU

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Mol	Chain	Res	Type
47	m0	208	ASN
47	m0	211	ARG
47	m0	212	GLU
47	m0	215	GLU
47	m0	217	PHE
48	m1	10	ARG
48	m1	11	ASP
48	m1	12	LEU
48	m1	13	LYS
48	m1	31	THR
48	m1	34	SER
48	m1	35	LYS
48	m1	40	LEU
48	m1	44	THR
48	m1	54	VAL
48	m1	55	ARG
48	m1	80	LEU
48	m1	101	ASN
48	m1	106	ILE
48	m1	107	ASP
48	m1	108	GLU
48	m1	112	LEU
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	150	ASN
48	m1	152	HIS
48	m1	159	THR
48	m1	160	VAL
48	m1	171	VAL
49	m3	13	HIS
49	m3	54	LEU
49	m3	58	VAL
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	85	LEU
49	m3	100	ARG
49	m3	104	ARG

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Mol	Chain	Res	Type
49	m3	107	GLU
49	m3	123	ILE
49	m3	131	LYS
49	m3	149	GLN
49	m3	164	GLU
49	m3	168	ARG
49	m3	171	ARG
49	m3	176	GLU
49	m3	184	GLU
49	m3	189	GLU
49	m3	194	GLU
50	m4	3	THR
50	m4	6	ILE
50	m4	16	GLU
50	m4	27	GLN
50	m4	28	SER
50	m4	43	LYS
50	m4	64	VAL
50	m4	66	THR
50	m4	69	THR
50	m4	72	LEU
50	m4	80	THR
50	m4	98	SER
50	m4	106	ARG
50	m4	124	ARG
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	8	GLU
51	m5	10	LEU
51	m5	15	GLN
51	m5	18	VAL
51	m5	22	LEU
51	m5	24	ARG
51	m5	41	ARG
51	m5	49	ARG
51	m5	75	VAL
51	m5	76	PRO
51	m5	80	THR
51	m5	85	THR
51	m5	97	SER
51	m5	105	ARG

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Mol	Chain	Res	Type
51	m5	106	VAL
51	m5	117	ASN
51	m5	138	GLN
51	m5	153	ASP
51	m5	155	VAL
51	m5	170	LYS
51	m5	174	ILE
51	m5	178	HIS
51	m5	183	THR
51	m5	190	THR
52	m6	34	VAL
52	m6	41	LEU
52	m6	58	LEU
52	m6	67	THR
52	m6	78	ARG
52	m6	85	ARG
52	m6	106	GLU
52	m6	108	ILE
52	m6	110	PRO
52	m6	117	ARG
52	m6	119	VAL
52	m6	124	LEU
52	m6	126	VAL
52	m6	130	LYS
52	m6	160	ARG
52	m6	171	LYS
52	m6	175	THR
52	m6	180	SER
52	m6	182	ASN
52	m6	184	THR
53	m7	7	THR
53	m7	8	SER
53	m7	9	THR
53	m7	13	LYS
53	m7	24	VAL
53	m7	32	THR
53	m7	41	LEU
53	m7	52	LEU
53	m7	65	SER
53	m7	76	PHE
53	m7	79	THR
53	m7	80	LYS

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Mol	Chain	Res	Type
53	m7	94	LEU
53	m7	103	GLU
53	m7	107	LEU
53	m7	112	LEU
53	m7	124	LYS
53	m7	126	ARG
53	m7	144	SER
53	m7	148	LEU
53	m7	150	VAL
53	m7	155	GLU
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	17	THR
54	m8	21	SER
54	m8	24	VAL
54	m8	26	LEU
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	41	ASP
54	m8	49	LEU
54	m8	57	ILE
54	m8	80	THR
54	m8	81	VAL
54	m8	100	THR
54	m8	113	LYS
54	m8	129	VAL
54	m8	135	GLN
54	m8	138	LEU
54	m8	147	ARG
54	m8	161	LYS
54	m8	165	ILE
54	m8	170	ARG
55	m9	7	GLN
55	m9	10	LEU
55	m9	17	VAL
55	m9	20	ARG
55	m9	29	THR
55	m9	36	ASN
55	m9	37	SER
55	m9	43	LYS

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Mol	Chain	Res	Type
55	m9	49	THR
55	m9	55	VAL
55	m9	56	THR
55	m9	63	THR
55	m9	70	LYS
55	m9	74	ARG
55	m9	88	ARG
55	m9	99	LEU
55	m9	105	LEU
55	m9	106	LEU
55	m9	126	GLU
55	m9	127	SER
55	m9	133	LYS
55	m9	138	LEU
55	m9	152	GLU
55	m9	153	LYS
55	m9	164	LEU
55	m9	171	ASP
55	m9	173	ARG
55	m9	186	LYS
56	n0	13	ARG
56	n0	17	GLU
56	n0	21	GLU
56	n0	23	LYS
56	n0	40	ARG
56	n0	45	LEU
56	n0	50	LYS
56	n0	51	VAL
56	n0	73	LYS
56	n0	80	ARG
56	n0	97	VAL
56	n0	100	VAL
56	n0	104	GLU
56	n0	107	TYR
56	n0	115	ARG
56	n0	117	ARG
56	n0	130	GLU
56	n0	132	THR
56	n0	136	LYS
56	n0	137	ARG
56	n0	148	LEU
56	n0	149	LYS

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Mol	Chain	Res	Type
56	n0	155	ARG
56	n0	162	THR
56	n0	166	LYS
56	n0	172	TYR
57	n1	12	ARG
57	n1	25	VAL
57	n1	26	HIS
57	n1	27	LEU
57	n1	35	LYS
57	n1	36	VAL
57	n1	64	VAL
57	n1	68	THR
57	n1	71	SER
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	102	ARG
57	n1	104	GLU
57	n1	118	GLU
57	n1	126	VAL
57	n1	129	LYS
57	n1	130	ARG
57	n1	131	GLN
57	n1	135	PRO
57	n1	139	ARG
57	n1	143	THR
57	n1	149	GLN
57	n1	150	THR
57	n1	154	VAL
57	n1	160	ILE
58	n2	14	THR
58	n2	21	SER
58	n2	27	VAL
58	n2	37	LEU
58	n2	39	ASP
58	n2	43	VAL
58	n2	50	LEU
58	n2	52	ASN
58	n2	54	VAL

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Mol	Chain	Res	Type
58	n2	57	THR
58	n2	58	GLU
58	n2	63	VAL
58	n2	68	THR
58	n2	90	ARG
58	n2	98	THR
59	n3	7	GLN
59	n3	13	ILE
59	n3	14	SER
59	n3	35	TYR
59	n3	46	LEU
59	n3	64	LYS
59	n3	74	MET
59	n3	88	ARG
59	n3	91	VAL
59	n3	110	LYS
59	n3	115	THR
87	n4	1	MET
87	n4	7	SER
87	n4	19	THR
87	n4	39	LEU
87	n4	63	ILE
87	n4	89	LEU
87	n4	95	SER
87	n4	126	GLU
87	n4	127	LYS
61	n5	24	LEU
61	n5	27	ARG
61	n5	34	LEU
61	n5	37	THR
61	n5	39	LYS
61	n5	40	LEU
61	n5	45	LYS
61	n5	56	ARG
61	n5	63	ILE
61	n5	71	THR
61	n5	73	MET
61	n5	86	VAL
61	n5	108	LEU
61	n5	109	LYS
61	n5	115	ARG
61	n5	125	ARG

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Mol	Chain	Res	Type
61	n5	133	LEU
61	n5	135	ILE
61	n5	142	ILE
62	n6	4	GLN
62	n6	8	VAL
62	n6	12	ARG
62	n6	13	ARG
62	n6	14	LYS
62	n6	17	LYS
62	n6	37	LYS
62	n6	39	LEU
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	52	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	66	GLN
62	n6	71	SER
62	n6	74	TYR
62	n6	76	LEU
62	n6	80	VAL
62	n6	83	ASP
62	n6	87	LYS
62	n6	90	VAL
62	n6	94	SER
62	n6	97	ILE
62	n6	102	SER
62	n6	115	ARG
62	n6	120	GLN
63	n7	3	LYS
63	n7	17	ARG
63	n7	24	VAL
63	n7	29	HIS
63	n7	33	SER
63	n7	34	LYS
63	n7	52	LYS
63	n7	72	ILE
63	n7	75	VAL
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR

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Mol	Chain	Res	Type
63	n7	95	VAL
63	n7	99	GLU
63	n7	100	THR
63	n7	102	GLU
63	n7	103	GLN
63	n7	105	SER
63	n7	121	ARG
63	n7	126	LYS
63	n7	127	ASN
63	n7	134	LEU
63	n7	135	ARG
64	n8	4	ARG
64	n8	6	THR
64	n8	8	THR
64	n8	10	LYS
64	n8	26	ARG
64	n8	42	ARG
64	n8	60	TYR
64	n8	72	VAL
64	n8	82	ILE
64	n8	85	ASP
64	n8	91	LEU
64	n8	97	GLU
64	n8	128	ARG
64	n8	132	LYS
64	n8	133	LEU
65	n9	19	ASN
65	n9	21	ILE
65	n9	26	THR
65	n9	33	LYS
65	n9	38	LYS
65	n9	42	ASN
65	n9	47	LEU
65	n9	50	THR
65	n9	52	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	6	SER
66	o0	8	GLU
66	o0	9	SER
66	o0	18	ILE
66	o0	32	LYS

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Mol	Chain	Res	Type
66	o0	41	LEU
66	o0	50	VAL
66	o0	61	MET
66	o0	76	GLU
66	o0	86	ARG
66	o0	87	VAL
66	o0	97	ASP
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	24	SER
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS
67	o1	44	MET
67	o1	50	ARG
67	o1	55	LEU
67	o1	68	GLU
67	o1	76	SER
67	o1	96	VAL
67	o1	100	SER
67	o1	102	LYS
67	o1	106	THR
67	o1	110	GLU
68	o2	4	LEU
68	o2	16	LYS
68	o2	24	ARG
68	o2	27	ARG
68	o2	33	ARG
68	o2	41	VAL
68	o2	51	SER
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	89	THR
68	o2	106	VAL
68	o2	123	LYS
68	o2	125	ARG
68	o2	126	LEU
69	o3	4	SER
69	o3	10	LYS

Continued on next page...

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Mol	Chain	Res	Type
69	o3	28	SER
69	o3	31	LYS
69	o3	48	ARG
69	o3	59	VAL
69	o3	70	LYS
69	o3	74	THR
69	o3	81	VAL
69	o3	97	SER
69	o3	98	VAL
69	o3	105	SER
69	o3	106	ASN
70	o4	5	VAL
70	o4	20	ILE
70	o4	23	VAL
70	o4	24	LYS
70	o4	29	ILE
70	o4	58	ARG
70	o4	65	VAL
70	o4	68	THR
70	o4	80	ARG
70	o4	85	VAL
70	o4	86	LYS
70	o4	98	GLN
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	28	LEU
71	o5	37	SER
71	o5	38	ARG
71	o5	40	SER
71	o5	45	LYS
71	o5	47	VAL
71	o5	48	ARG
71	o5	62	GLN
71	o5	68	GLN
71	o5	69	LEU
71	o5	81	ARG
71	o5	85	THR
71	o5	89	ARG
71	o5	90	ARG
71	o5	100	VAL
71	o5	101	THR

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Mol	Chain	Res	Type
71	o5	107	LYS
71	o5	119	LYS
72	o6	7	ILE
72	o6	9	ILE
72	o6	11	LEU
72	o6	12	ASN
72	o6	21	THR
72	o6	26	ILE
72	o6	34	SER
72	o6	35	ASN
72	o6	36	ARG
72	o6	38	LYS
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	60	LEU
72	o6	62	ARG
72	o6	64	SER
72	o6	68	ARG
72	o6	75	LYS
72	o6	76	ARG
72	o6	81	THR
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	3	LYS
73	o7	17	THR
73	o7	25	ARG
73	o7	33	THR
73	o7	44	THR
73	o7	46	SER
73	o7	55	ARG
73	o7	58	THR
73	o7	59	THR
73	o7	64	MET
73	o7	65	ARG
73	o7	67	LEU
73	o7	68	LYS
73	o7	74	PHE
73	o7	80	THR
73	o7	82	SER

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Mol	Chain	Res	Type
73	o7	84	SER
74	o8	5	ILE
74	o8	12	LEU
74	o8	17	ARG
74	o8	19	ASP
74	o8	22	THR
74	o8	24	THR
74	o8	41	THR
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
74	o8	67	GLN
75	o9	5	LYS
75	o9	12	LYS
75	o9	15	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	45	ARG
76	q0	78	ILE
76	q0	83	LYS
76	q0	85	LEU
76	q0	106	ARG
76	q0	110	CYS
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
76	q0	127	LEU
77	q1	6	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	18	ARG
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
78	q2	2	VAL
78	q2	7	THR
78	q2	8	ARG
78	q2	35	LEU
78	q2	38	GLN
78	q2	45	ARG
78	q2	47	GLN

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Mol	Chain	Res	Type
78	q2	61	LYS
78	q2	71	ARG
78	q2	78	LYS
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	89	LYS
78	q2	93	LEU
78	q2	100	LYS
78	q2	104	LEU
78	q2	105	GLN
79	q3	3	LYS
79	q3	4	ARG
79	q3	21	SER
79	q3	24	ARG
79	q3	33	GLN
79	q3	42	CYS
79	q3	48	LYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	57	CYS
79	q3	58	SER
79	q3	59	CYS
79	q3	62	LYS
79	q3	81	SER
88	p0	4	ILE
88	p0	5	ARG
88	p0	6	GLU
88	p0	10	GLU
88	p0	48	ARG
88	p0	50	VAL
88	p0	51	VAL
88	p0	55	LYS
88	p0	67	LEU
88	p0	70	LEU
88	p0	74	GLU
88	p0	76	LEU
88	p0	80	VAL
88	p0	81	LYS
88	p0	84	VAL
88	p0	91	GLU

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Mol	Chain	Res	Type
88	p0	93	LEU
88	p0	97	LYS
88	p0	104	ARG
88	p0	185	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	95	ASN
3	S1	149	GLN
6	S4	188	ASN
8	S6	59	GLN
9	S7	74	GLN
11	S9	110	GLN
19	C7	105	GLN
20	C8	136	GLN
27	D5	95	HIS
34	SR	159	ASN
43	L6	28	GLN
44	L7	244	ASN
47	M0	59	GLN
63	N7	127	ASN
74	O8	67	GLN
78	Q2	3	ASN
2	s0	140	ASN
3	s1	149	GLN
3	s1	209	ASN
11	s9	110	GLN
11	s9	142	ASN
80	c0	32	HIS
20	c8	12	GLN
22	d0	72	ASN
24	d2	56	HIS
26	d4	22	GLN
32	e0	17	GLN
41	l4	296	GLN
42	l5	81	HIS
42	l5	264	GLN
44	l7	112	ASN
51	m5	138	GLN
51	m5	178	HIS
55	m9	7	GLN

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Mol	Chain	Res	Type
61	n5	137	ASN
64	n8	25	HIS
64	n8	44	ASN
70	o4	3	GLN
72	o6	63	ASN
73	o7	13	ASN
74	o8	40	GLN
75	o9	4	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	458 (25%)	67 (3%)
1	6	1792/1800 (99%)	445 (24%)	51 (2%)
36	1	3146/3394 (92%)	647 (20%)	70 (2%)
36	5	3145/3394 (92%)	646 (20%)	82 (2%)
37	3	120/121 (99%)	17 (14%)	1 (0%)
37	7	120/121 (99%)	16 (13%)	0
38	4	157/158 (99%)	36 (22%)	2 (1%)
38	8	157/158 (99%)	38 (24%)	2 (1%)
90	A	1/3 (33%)	1 (100%)	0
90	a	1/3 (33%)	1 (100%)	0
All	All	10416/10952 (95%)	2305 (22%)	275 (2%)

All (2305) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	45	U
1	2	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	67	A
1	2	68	A
1	2	69	G

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Mol	Chain	Res	Type
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	101	U
1	2	104	A
1	2	114	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	178	U
1	2	185	U
1	2	186	C
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A

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Mol	Chain	Res	Type
1	2	227	U
1	2	228	G
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	249	U
1	2	250	C
1	2	261	U
1	2	262	U
1	2	265	A
1	2	269	G
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	299	A
1	2	302	U
1	2	308	C
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	341	A
1	2	344	A
1	2	352	A

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Mol	Chain	Res	Type
1	2	359	A
1	2	360	A
1	2	361	C
1	2	387	A
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	421	A
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	437	A
1	2	439	U
1	2	444	C
1	2	448	C
1	2	468	A
1	2	470	A
1	2	475	A
1	2	484	C
1	2	485	A
1	2	486	G
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A

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Mol	Chain	Res	Type
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	513	U
1	2	514	G
1	2	515	A
1	2	516	G
1	2	520	A
1	2	527	A
1	2	532	U
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	548	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	585	A
1	2	594	A
1	2	595	G
1	2	606	A
1	2	611	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	630	A
1	2	639	U
1	2	640	U

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Mol	Chain	Res	Type
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	682	C
1	2	684	A
1	2	685	A
1	2	686	C
1	2	692	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G

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Mol	Chain	Res	Type
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	758	U
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	794	U
1	2	795	U
1	2	803	A
1	2	806	A
1	2	811	A
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	837	G
1	2	840	U

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Mol	Chain	Res	Type
1	2	846	G
1	2	848	C
1	2	856	A
1	2	862	A
1	2	863	A
1	2	864	U
1	2	886	U
1	2	896	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	921	U
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	961	U
1	2	966	A
1	2	988	A
1	2	992	A
1	2	993	A
1	2	997	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1026	A
1	2	1028	C
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1071	U

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Mol	Chain	Res	Type
1	2	1074	G
1	2	1079	U
1	2	1082	C
1	2	1083	G
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1109	G
1	2	1111	G
1	2	1138	A
1	2	1146	G
1	2	1149	G
1	2	1150	G
1	2	1151	A
1	2	1152	A
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1243	G
1	2	1244	A
1	2	1245	G

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Mol	Chain	Res	Type
1	2	1250	U
1	2	1251	U
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1286	U
1	2	1292	G
1	2	1301	U
1	2	1314	U
1	2	1321	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1349	G
1	2	1354	G
1	2	1355	C
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1446	A
1	2	1448	G
1	2	1457	C
1	2	1459	C
1	2	1461	C
1	2	1462	G
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1482	C

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Mol	Chain	Res	Type
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1539	G
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1624	C
1	2	1626	U
1	2	1631	A
1	2	1635	A
1	2	1657	U
1	2	1658	G
1	2	1680	G
1	2	1681	A
1	2	1683	C
1	2	1684	U
1	2	1693	A
1	2	1696	G

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Mol	Chain	Res	Type
1	2	1697	G
1	2	1698	G
1	2	1699	G
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1712	A
1	2	1713	G
1	2	1715	G
1	2	1716	C
1	2	1731	A
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	14	U
36	1	16	A
36	1	24	G
36	1	26	A
36	1	40	A
36	1	49	A
36	1	57	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	73	C
36	1	83	U
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A

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Mol	Chain	Res	Type
36	1	109	A
36	1	110	G
36	1	113	C
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	147	U
36	1	156	G
36	1	157	A
36	1	166	C
36	1	169	U
36	1	170	G
36	1	173	G
36	1	182	U
36	1	183	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	200	C
36	1	210	U
36	1	218	G
36	1	219	A
36	1	226	C
36	1	238	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	245	U
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U
36	1	269	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	305	U
36	1	315	C

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Mol	Chain	Res	Type
36	1	323	A
36	1	329	U
36	1	339	C
36	1	349	A
36	1	350	C
36	1	351	A
36	1	370	U
36	1	376	G
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	404	G
36	1	421	G
36	1	422	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	498	A
36	1	517	G
36	1	520	U
36	1	521	A
36	1	535	G
36	1	543	C
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	552	G
36	1	557	A
36	1	558	U
36	1	559	A
36	1	560	G
36	1	569	A
36	1	578	A
36	1	579	G
36	1	592	A
36	1	594	U
36	1	604	G
36	1	607	A
36	1	609	G

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Mol	Chain	Res	Type
36	1	611	A
36	1	619	A
36	1	620	U
36	1	621	A
36	1	622	A
36	1	636	C
36	1	637	C
36	1	638	C
36	1	649	A
36	1	660	A
36	1	677	A
36	1	681	U
36	1	684	G
36	1	691	A
36	1	705	A
36	1	709	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	722	G
36	1	725	G
36	1	727	G
36	1	758	C
36	1	764	U
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	780	A
36	1	781	G
36	1	785	G
36	1	792	G
36	1	806	A
36	1	817	A
36	1	830	A
36	1	842	G
36	1	849	C
36	1	861	C
36	1	874	U
36	1	879	U
36	1	885	U
36	1	890	C

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Mol	Chain	Res	Type
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	944	C
36	1	959	C
36	1	960	U
36	1	963	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	993	G
36	1	994	G
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1035	G
36	1	1037	C
36	1	1045	C
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1064	A
36	1	1065	A
36	1	1071	U

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Mol	Chain	Res	Type
36	1	1072	G
36	1	1079	A
36	1	1081	U
36	1	1082	U
36	1	1083	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1131	G
36	1	1144	U
36	1	1153	A
36	1	1159	A
36	1	1160	C
36	1	1178	G
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1185	C
36	1	1191	U
36	1	1192	C
36	1	1196	C
36	1	1197	A
36	1	1201	C
36	1	1209	G
36	1	1212	A
36	1	1213	G
36	1	1216	C
36	1	1217	A
36	1	1221	A
36	1	1222	G
36	1	1225	A
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1236	G

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Mol	Chain	Res	Type
36	1	1237	G
36	1	1241	U
36	1	1242	G
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1267	U
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1272	C
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1307	G
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1330	A
36	1	1331	U
36	1	1345	G
36	1	1348	U
36	1	1349	G
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1386	A

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Mol	Chain	Res	Type
36	1	1392	G
36	1	1398	U
36	1	1399	A
36	1	1400	G
36	1	1417	G
36	1	1419	A
36	1	1429	G
36	1	1431	G
36	1	1433	A
36	1	1434	G
36	1	1436	U
36	1	1437	C
36	1	1443	G
36	1	1446	A
36	1	1450	G
36	1	1460	A
36	1	1468	A
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1502	C
36	1	1508	C
36	1	1527	C
36	1	1556	C
36	1	1557	A
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1572	U
36	1	1576	G
36	1	1580	A
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A

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Mol	Chain	Res	Type
36	1	1596	C
36	1	1605	A
36	1	1607	U
36	1	1620	U
36	1	1629	U
36	1	1639	C
36	1	1641	U
36	1	1643	A
36	1	1645	U
36	1	1657	C
36	1	1683	A
36	1	1702	U
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C
36	1	1736	G
36	1	1750	A
36	1	1751	G
36	1	1762	C
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G
36	1	1775	G
36	1	1780	G
36	1	1781	C
36	1	1797	A
36	1	1805	C
36	1	1810	A
36	1	1812	G
36	1	1813	A
36	1	1814	A
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A

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Mol	Chain	Res	Type
36	1	1846	C
36	1	1849	C
36	1	1850	A
36	1	1864	A
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1895	A
36	1	1901	A
36	1	1906	G
36	1	1935	G
36	1	1951	C
36	1	1952	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2106	A
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2116	G
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2134	G
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2169	G
36	1	2170	U
36	1	2175	U
36	1	2187	G
36	1	2198	A
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2222	A
36	1	2223	A
36	1	2225	U

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Mol	Chain	Res	Type
36	1	2228	A
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	A
36	1	2262	A
36	1	2272	G
36	1	2273	G
36	1	2281	A
36	1	2282	U
36	1	2283	G
36	1	2284	C
36	1	2288	G
36	1	2298	U
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2334	U
36	1	2335	G
36	1	2336	U
36	1	2341	A
36	1	2361	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2393	G
36	1	2395	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2435	G
36	1	2437	G

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Mol	Chain	Res	Type
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2507	C
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2525	G
36	1	2526	C
36	1	2532	U
36	1	2533	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2561	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2576	G
36	1	2581	U
36	1	2585	G
36	1	2586	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G

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Mol	Chain	Res	Type
36	1	2614	G
36	1	2626	A
36	1	2629	U
36	1	2637	A
36	1	2652	U
36	1	2656	A
36	1	2674	A
36	1	2677	G
36	1	2685	C
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2705	A
36	1	2714	G
36	1	2728	G
36	1	2737	C
36	1	2752	U
36	1	2753	G
36	1	2754	G
36	1	2755	C
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2779	A
36	1	2788	C
36	1	2796	G
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2803	A
36	1	2810	C
36	1	2814	G
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2829	U
36	1	2834	G
36	1	2836	C
36	1	2842	U

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Mol	Chain	Res	Type
36	1	2843	U
36	1	2845	A
36	1	2847	A
36	1	2849	C
36	1	2859	U
36	1	2860	U
36	1	2867	C
36	1	2871	G
36	1	2872	A
36	1	2875	U
36	1	2876	C
36	1	2887	A
36	1	2889	C
36	1	2898	G
36	1	2899	C
36	1	2914	G
36	1	2923	U
36	1	2927	C
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2947	G
36	1	2955	U
36	1	2971	A
36	1	2980	U
36	1	2983	C
36	1	2990	G
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3028	G
36	1	3057	U
36	1	3058	U
36	1	3059	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3086	A
36	1	3087	A
36	1	3092	C
36	1	3113	A
36	1	3119	U

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Mol	Chain	Res	Type
36	1	3122	A
36	1	3130	A
36	1	3131	U
36	1	3139	A
36	1	3142	A
36	1	3143	C
36	1	3150	A
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3168	A
36	1	3169	U
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3195	U
36	1	3196	U
36	1	3207	U
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3228	C
36	1	3229	G
36	1	3235	C
36	1	3244	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3269	U
36	1	3270	U

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Mol	Chain	Res	Type
36	1	3272	C
36	1	3276	G
36	1	3279	A
36	1	3280	U
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3289	G
36	1	3294	A
36	1	3295	A
36	1	3303	G
36	1	3304	U
36	1	3307	A
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3348	G
36	1	3349	C
36	1	3350	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3368	U
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3389	U
36	1	3396	U
37	3	7	G

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Mol	Chain	Res	Type
37	3	13	A
37	3	22	A
37	3	29	C
37	3	41	G
37	3	51	A
37	3	53	U
37	3	54	U
37	3	65	G
37	3	73	C
37	3	74	C
37	3	76	A
37	3	91	G
37	3	95	A
37	3	102	A
37	3	112	G
37	3	121	U
38	4	26	U
38	4	34	U
38	4	35	C
38	4	42	G
38	4	48	A
38	4	51	G
38	4	52	A
38	4	59	A
38	4	62	C
38	4	63	G
38	4	66	A
38	4	79	A
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A

Continued on next page...

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Mol	Chain	Res	Type
38	4	113	U
38	4	122	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	151	C
38	4	152	G
38	4	155	A
38	4	158	U
1	6	2	A
1	6	4	C
1	6	17	C
1	6	23	G
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	57	G
1	6	60	U
1	6	66	U
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	87	C
1	6	104	A
1	6	114	C
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	144	U
1	6	145	A
1	6	146	U
1	6	153	G

Continued on next page...

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Mol	Chain	Res	Type
1	6	158	U
1	6	159	U
1	6	166	C
1	6	178	U
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	196	G
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	229	U
1	6	230	C
1	6	232	U
1	6	233	C
1	6	235	G
1	6	238	U
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	261	U
1	6	265	A
1	6	266	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	277	U

Continued on next page...

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Mol	Chain	Res	Type
1	6	278	U
1	6	280	U
1	6	281	G
1	6	287	G
1	6	299	A
1	6	309	C
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	333	A
1	6	337	G
1	6	338	C
1	6	341	A
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	370	A
1	6	381	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	439	U
1	6	444	C
1	6	448	C
1	6	464	A
1	6	468	A
1	6	470	A
1	6	475	A
1	6	477	A
1	6	480	G
1	6	484	C

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Mol	Chain	Res	Type
1	6	485	A
1	6	486	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	495	C
1	6	496	G
1	6	497	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	515	A
1	6	519	C
1	6	527	A
1	6	532	U
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	551	G
1	6	554	C
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	564	G
1	6	565	C

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Mol	Chain	Res	Type
1	6	568	G
1	6	570	A
1	6	574	G
1	6	578	U
1	6	579	A
1	6	580	A
1	6	582	U
1	6	594	A
1	6	595	G
1	6	609	U
1	6	610	G
1	6	611	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	624	G
1	6	637	C
1	6	639	U
1	6	640	U
1	6	648	G
1	6	652	G
1	6	653	C
1	6	654	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	669	G
1	6	670	U
1	6	676	G
1	6	678	A
1	6	679	U
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	691	C
1	6	695	U

Continued on next page...

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Mol	Chain	Res	Type
1	6	696	C
1	6	697	C
1	6	698	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	714	G
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	723	G
1	6	730	G
1	6	731	C
1	6	742	U
1	6	751	G
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	766	U
1	6	773	C
1	6	774	A
1	6	775	G
1	6	777	C
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	793	A
1	6	794	U
1	6	811	A
1	6	812	A
1	6	815	G
1	6	816	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	U

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Mol	Chain	Res	Type
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	863	A
1	6	864	U
1	6	898	A
1	6	906	A
1	6	912	U
1	6	913	G
1	6	914	G
1	6	916	U
1	6	933	A
1	6	935	U
1	6	942	G
1	6	944	A
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	992	A
1	6	993	A
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1021	C
1	6	1023	A
1	6	1026	A
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U

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Mol	Chain	Res	Type
1	6	1061	A
1	6	1063	U
1	6	1072	C
1	6	1074	G
1	6	1082	C
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1109	G
1	6	1111	G
1	6	1138	A
1	6	1139	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1162	C
1	6	1164	G
1	6	1167	G
1	6	1185	U
1	6	1194	A
1	6	1196	A
1	6	1197	C
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1208	A
1	6	1217	A
1	6	1218	G
1	6	1220	C
1	6	1221	A
1	6	1225	U
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1231	U
1	6	1239	U
1	6	1240	U

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Mol	Chain	Res	Type
1	6	1241	G
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1261	G
1	6	1286	U
1	6	1288	G
1	6	1291	G
1	6	1314	U
1	6	1316	G
1	6	1321	A
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1354	G
1	6	1355	C
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1367	G
1	6	1371	A
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G
1	6	1412	G
1	6	1413	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1445	G
1	6	1446	A
1	6	1448	G

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Mol	Chain	Res	Type
1	6	1458	G
1	6	1459	C
1	6	1471	A
1	6	1481	C
1	6	1482	C
1	6	1486	G
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1494	C
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1531	G
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1572	G
1	6	1573	A
1	6	1574	G
1	6	1582	U
1	6	1584	G
1	6	1600	A
1	6	1601	G
1	6	1616	G
1	6	1618	C
1	6	1621	U
1	6	1634	C
1	6	1637	C
1	6	1638	G

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Mol	Chain	Res	Type
1	6	1657	U
1	6	1658	G
1	6	1696	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1705	C
1	6	1710	U
1	6	1712	A
1	6	1715	G
1	6	1716	C
1	6	1717	G
1	6	1727	G
1	6	1731	A
1	6	1736	G
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1770	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	16	A
36	5	21	G
36	5	24	G
36	5	26	A
36	5	40	A
36	5	43	A

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Mol	Chain	Res	Type
36	5	49	A
36	5	57	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	68	C
36	5	73	C
36	5	76	G
36	5	92	G
36	5	93	C
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	111	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	150	A
36	5	152	U
36	5	156	G
36	5	157	A
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	173	G
36	5	174	C
36	5	178	U
36	5	182	U
36	5	183	G
36	5	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C

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Mol	Chain	Res	Type
36	5	201	A
36	5	210	U
36	5	213	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	236	G
36	5	239	G
36	5	240	U
36	5	244	G
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	269	G
36	5	283	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	316	U
36	5	323	A
36	5	329	U
36	5	334	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	370	U
36	5	376	G
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C

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Mol	Chain	Res	Type
36	5	441	U
36	5	442	G
36	5	443	G
36	5	492	U
36	5	495	G
36	5	503	C
36	5	512	U
36	5	521	A
36	5	523	A
36	5	535	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	555	U
36	5	557	A
36	5	559	A
36	5	566	G
36	5	569	A
36	5	578	A
36	5	579	G
36	5	581	U
36	5	592	A
36	5	594	U
36	5	595	G
36	5	600	G
36	5	604	G
36	5	609	G
36	5	611	A
36	5	619	A
36	5	620	U
36	5	621	A
36	5	636	C
36	5	649	A
36	5	651	G
36	5	653	A
36	5	660	A
36	5	662	U
36	5	675	C
36	5	677	A
36	5	681	U
36	5	691	A
36	5	705	A

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Mol	Chain	Res	Type
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	725	G
36	5	726	G
36	5	727	G
36	5	736	A
36	5	760	G
36	5	766	U
36	5	767	U
36	5	768	C
36	5	776	U
36	5	777	U
36	5	780	A
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	830	A
36	5	837	A
36	5	846	A
36	5	861	C
36	5	874	U
36	5	879	U
36	5	890	C
36	5	896	A
36	5	907	G
36	5	908	G
36	5	910	G
36	5	914	A
36	5	916	G
36	5	917	A
36	5	921	A
36	5	923	C
36	5	924	G
36	5	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	963	G

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Mol	Chain	Res	Type
36	5	964	G
36	5	979	U
36	5	981	U
36	5	994	G
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1003	A
36	5	1006	A
36	5	1010	G
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1027	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1034	U
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1071	U
36	5	1072	G
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1088	U
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1096	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G

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Mol	Chain	Res	Type
36	5	1117	G
36	5	1131	G
36	5	1153	A
36	5	1159	A
36	5	1160	C
36	5	1178	G
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1201	C
36	5	1202	A
36	5	1209	G
36	5	1222	G
36	5	1223	A
36	5	1232	C
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1254	C
36	5	1259	A
36	5	1262	G
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1285	G
36	5	1295	G
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1330	A
36	5	1349	G
36	5	1351	U
36	5	1352	A

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Mol	Chain	Res	Type
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1380	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1418	A
36	5	1419	A
36	5	1431	G
36	5	1432	C
36	5	1434	G
36	5	1437	C
36	5	1438	U
36	5	1446	A
36	5	1450	G
36	5	1460	A
36	5	1465	A
36	5	1480	G
36	5	1481	A
36	5	1482	A
36	5	1484	U
36	5	1490	A
36	5	1503	A
36	5	1508	C
36	5	1536	G
36	5	1539	A
36	5	1541	G
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1557	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1566	A
36	5	1567	U

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Mol	Chain	Res	Type
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1580	A
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1605	A
36	5	1607	U
36	5	1608	C
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1655	G
36	5	1657	C
36	5	1683	A
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1736	G
36	5	1750	A
36	5	1751	G
36	5	1760	A
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1770	G

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Mol	Chain	Res	Type
36	5	1775	G
36	5	1778	G
36	5	1780	G
36	5	1781	C
36	5	1795	U
36	5	1797	A
36	5	1812	G
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1820	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1886	A
36	5	1891	A
36	5	1893	A
36	5	1906	G
36	5	1918	C
36	5	1935	G
36	5	1952	G
36	5	1953	G
36	5	2101	C
36	5	2102	U
36	5	2112	U
36	5	2113	A
36	5	2114	C
36	5	2121	G
36	5	2122	G
36	5	2128	C
36	5	2131	A
36	5	2144	A
36	5	2158	A

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Mol	Chain	Res	Type
36	5	2169	G
36	5	2176	U
36	5	2188	A
36	5	2198	A
36	5	2201	G
36	5	2205	U
36	5	2210	G
36	5	2213	A
36	5	2222	A
36	5	2223	A
36	5	2225	U
36	5	2228	A
36	5	2244	A
36	5	2250	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2257	C
36	5	2258	U
36	5	2264	U
36	5	2273	G
36	5	2276	G
36	5	2279	A
36	5	2281	A
36	5	2288	G
36	5	2303	A
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2318	U
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2337	C
36	5	2338	C
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2393	G

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Mol	Chain	Res	Type
36	5	2397	A
36	5	2398	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2435	G
36	5	2436	U
36	5	2437	G
36	5	2438	A
36	5	2439	A
36	5	2440	G
36	5	2441	A
36	5	2443	A
36	5	2504	U
36	5	2505	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2513	U
36	5	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2524	A
36	5	2526	C
36	5	2530	G
36	5	2531	C
36	5	2532	U
36	5	2534	G
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G

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Mol	Chain	Res	Type
36	5	2552	C
36	5	2555	G
36	5	2566	C
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2609	A
36	5	2610	G
36	5	2614	G
36	5	2615	G
36	5	2626	A
36	5	2637	A
36	5	2639	G
36	5	2652	U
36	5	2656	A
36	5	2667	A
36	5	2674	A
36	5	2677	G
36	5	2678	A
36	5	2681	U
36	5	2683	U
36	5	2689	A
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2714	G
36	5	2726	C
36	5	2728	G
36	5	2729	U

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Mol	Chain	Res	Type
36	5	2742	C
36	5	2752	U
36	5	2753	G
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2779	A
36	5	2796	G
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2810	C
36	5	2814	G
36	5	2817	A
36	5	2818	U
36	5	2829	U
36	5	2843	U
36	5	2845	A
36	5	2849	C
36	5	2853	A
36	5	2871	G
36	5	2872	A
36	5	2873	U
36	5	2875	U
36	5	2876	C
36	5	2887	A
36	5	2889	C
36	5	2896	A
36	5	2899	C
36	5	2904	U
36	5	2923	U
36	5	2928	C
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2945	G
36	5	2947	G
36	5	2971	A
36	5	2972	G

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Mol	Chain	Res	Type
36	5	2979	U
36	5	2983	C
36	5	2992	U
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3049	A
36	5	3050	U
36	5	3056	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3080	G
36	5	3086	A
36	5	3092	C
36	5	3102	G
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3145	C
36	5	3152	U
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3179	U
36	5	3181	C
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3207	U

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Mol	Chain	Res	Type
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3227	A
36	5	3229	G
36	5	3238	G
36	5	3239	G
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3253	G
36	5	3259	U
36	5	3270	U
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3280	U
36	5	3281	U
36	5	3282	U
36	5	3284	G
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A
36	5	3304	U
36	5	3309	G
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3356	G

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Mol	Chain	Res	Type
36	5	3358	U
36	5	3363	U
36	5	3369	G
36	5	3378	C
36	5	3382	U
36	5	3389	U
36	5	3390	G
36	5	3391	A
36	5	3396	U
37	7	22	A
37	7	23	A
37	7	27	A
37	7	33	U
37	7	41	G
37	7	54	U
37	7	60	G
37	7	64	A
37	7	65	G
37	7	73	C
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	104	A
37	7	112	G
38	8	20	U
38	8	21	C
38	8	34	U
38	8	35	C
38	8	42	G
38	8	48	A
38	8	51	G
38	8	52	A
38	8	53	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C

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Mol	Chain	Res	Type
38	8	84	C
38	8	86	U
38	8	87	G
38	8	90	U
38	8	95	G
38	8	102	U
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	116	G
38	8	122	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	152	G
38	8	156	U
38	8	157	U
38	8	158	U
90	A	75	C
90	a	75	C

All (275) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	74	U
1	2	103	A
1	2	114	C
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	136	C
1	2	139	C
1	2	158	U
1	2	187	G

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Mol	Chain	Res	Type
1	2	217	A
1	2	218	A
1	2	232	U
1	2	240	U
1	2	278	U
1	2	280	U
1	2	321	C
1	2	417	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	622	A
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	734	A
1	2	755	A
1	2	781	U
1	2	782	U
1	2	794	U
1	2	811	A
1	2	829	A
1	2	913	G
1	2	1051	G
1	2	1058	U
1	2	1081	A
1	2	1157	A
1	2	1196	A
1	2	1207	C
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1339	C
1	2	1344	A
1	2	1370	U
1	2	1481	C

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Mol	Chain	Res	Type
1	2	1489	U
1	2	1490	C
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1696	G
1	2	1698	G
1	2	1711	C
1	2	1761	U
36	1	65	A
36	1	169	U
36	1	239	G
36	1	282	G
36	1	397	A
36	1	547	G
36	1	594	U
36	1	637	C
36	1	715	A
36	1	763	G
36	1	873	C
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1181	U
36	1	1196	C
36	1	1273	A
36	1	1307	G
36	1	1329	U
36	1	1352	A
36	1	1355	A
36	1	1484	U
36	1	1562	C
36	1	1582	C
36	1	1716	U
36	1	1751	G
36	1	1815	U

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Mol	Chain	Res	Type
36	1	1816	A
36	1	1820	U
36	1	1841	A
36	1	1842	A
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2227	C
36	1	2249	G
36	1	2281	A
36	1	2372	A
36	1	2374	C
36	1	2418	G
36	1	2501	U
36	1	2513	U
36	1	2525	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2801	A
36	1	2818	U
36	1	2859	U
36	1	3078	U
36	1	3121	U
36	1	3195	U
36	1	3207	U
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3276	G
36	1	3316	A
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	52	G
38	4	85	G
38	4	111	A
1	6	25	C

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Mol	Chain	Res	Type
1	6	66	U
1	6	75	U
1	6	76	A
1	6	103	A
1	6	114	C
1	6	136	C
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	240	U
1	6	272	U
1	6	277	U
1	6	417	A
1	6	512	A
1	6	542	A
1	6	555	A
1	6	558	U
1	6	651	G
1	6	667	U
1	6	678	A
1	6	697	C
1	6	717	C
1	6	755	A
1	6	829	A
1	6	834	G
1	6	1051	G
1	6	1058	U
1	6	1081	A
1	6	1097	U
1	6	1196	A
1	6	1207	C
1	6	1227	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C
1	6	1490	C
1	6	1491	U
1	6	1535	U
1	6	1568	C

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Mol	Chain	Res	Type
1	6	1573	A
1	6	1615	C
1	6	1620	C
1	6	1637	C
1	6	1657	U
1	6	1696	G
1	6	1698	G
1	6	1700	C
36	5	67	A
36	5	151	A
36	5	183	G
36	5	238	A
36	5	282	G
36	5	397	A
36	5	438	A
36	5	546	C
36	5	647	A
36	5	715	A
36	5	735	A
36	5	765	C
36	5	786	A
36	5	816	A
36	5	873	C
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1033	U
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1181	U
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1481	A
36	5	1554	U

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Mol	Chain	Res	Type
36	5	1560	G
36	5	1580	A
36	5	1607	U
36	5	1716	U
36	5	1724	U
36	5	1816	A
36	5	1819	U
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	2101	C
36	5	2112	U
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2372	A
36	5	2373	A
36	5	2401	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2531	C
36	5	2593	A
36	5	2682	C
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2872	A
36	5	2970	C
36	5	2971	A
36	5	2979	U
36	5	3078	U
36	5	3121	U
36	5	3154	C
36	5	3167	A
36	5	3195	U
36	5	3218	A
36	5	3228	C
36	5	3269	U

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Mol	Chain	Res	Type
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3340	G
36	5	3341	U
36	5	3357	U
38	8	111	A
38	8	126	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
90	PPU	a	76	36,90	32,40,41	1.04	2 (6%)	33,57,60	1.74	6 (18%)
90	PPU	A	76	36,90	32,40,41	1.07	2 (6%)	33,57,60	1.74	8 (24%)

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
90	PPU	a	76	36,90	-	4/21/43/44	0/4/4/4
90	PPU	A	76	36,90	-	3/21/43/44	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	a	76	PPU	C2'-C3'	-2.87	1.48	1.53
90	a	76	PPU	C5-C4	2.32	1.47	1.40
90	A	76	PPU	C2'-C3'	-2.23	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	A	76	PPU	C5-C4	2.19	1.46	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	a	76	PPU	C3'-N3'-C	-5.38	115.10	123.21
90	A	76	PPU	C3'-N3'-C	-4.92	115.79	123.21
90	a	76	PPU	CG-CB-CA	-4.45	104.87	114.13
90	A	76	PPU	CA-C-N3'	3.52	121.03	116.15
90	A	76	PPU	N3-C2-N1	-3.52	123.18	128.68
90	a	76	PPU	N3-C2-N1	-3.40	123.36	128.68
90	a	76	PPU	CA-C-N3'	2.83	120.08	116.15
90	A	76	PPU	O4'-C4'-C3'	2.77	108.04	104.06
90	a	76	PPU	O2'-C2'-C3'	-2.76	104.42	111.16
90	A	76	PPU	CG-CB-CA	-2.59	108.75	114.13
90	a	76	PPU	C4-C5-N7	-2.40	106.89	109.40
90	A	76	PPU	CD2-CG-CD1	2.40	121.94	118.17
90	A	76	PPU	N1-C6-N6	2.24	119.42	117.06
90	A	76	PPU	C4-C5-N7	-2.10	107.21	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	A	76	PPU	C3'-C4'-C5'-O5'
90	a	76	PPU	CE2-CZ-OC-CM
90	a	76	PPU	CE1-CZ-OC-CM
90	A	76	PPU	O4'-C4'-C5'-O5'
90	a	76	PPU	CA-CB-CG-CD1
90	a	76	PPU	CA-CB-CG-CD2
90	A	76	PPU	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3553 ligands modelled in this entry, 2208 are monoatomic - leaving 1345 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	$\# Z > 2$
92	OHX	6	2324	92	0,6,6	-	-	-		
92	OHX	1	4353	92	0,6,6	-	-	-		
92	OHX	5	4381	92	0,6,6	-	-	-		
92	OHX	6	2274	92	0,6,6	-	-	-		
92	OHX	6	2278	-	0,6,6	-	-	-		
92	OHX	5	4403	92	0,6,6	-	-	-		
92	OHX	5	4293	92	0,6,6	-	-	-		
92	OHX	1	4185	92	0,6,6	-	-	-		
92	OHX	1	4108	-	0,6,6	-	-	-		
92	OHX	6	2154	-	0,6,6	-	-	-		
92	OHX	5	4270	-	0,6,6	-	-	-		
92	OHX	6	2302	92	0,6,6	-	-	-		
92	OHX	1	4120	-	0,6,6	-	-	-		
92	OHX	6	2306	-	0,6,6	-	-	-		
92	OHX	1	4494	-	0,6,6	-	-	-		
92	OHX	2	2211	-	0,6,6	-	-	-		
92	OHX	M5	310	-	0,6,6	-	-	-		
92	OHX	5	4425	-	0,6,6	-	-	-		
92	OHX	1	4384	-	0,6,6	-	-	-		
92	OHX	1	4262	92	0,6,6	-	-	-		
92	OHX	1	4222	-	0,6,6	-	-	-		
92	OHX	5	4389	-	0,6,6	-	-	-		
92	OHX	1	4476	92	0,6,6	-	-	-		
92	OHX	2	2155	-	0,6,6	-	-	-		
92	OHX	5	4290	-	0,6,6	-	-	-		
92	OHX	1	4233	-	0,6,6	-	-	-		
92	OHX	1	4308	-	0,6,6	-	-	-		
92	OHX	1	4212	-	0,6,6	-	-	-		
92	OHX	1	4167	-	0,6,6	-	-	-		
92	OHX	5	4306	-	0,6,6	-	-	-		
92	OHX	6	2163	-	0,6,6	-	-	-		
92	OHX	5	4478	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4382	-	0,6,6	-	-	-		
92	OHX	5	4348	92	0,6,6	-	-	-		
92	OHX	1	4135	-	0,6,6	-	-	-		
92	OHX	2	2111	92	0,6,6	-	-	-		
92	OHX	1	4380	36	0,6,6	-	-	-		
92	OHX	2	2088	-	0,6,6	-	-	-		
92	OHX	5	4417	-	0,6,6	-	-	-		
92	OHX	5	4432	92,36	0,6,6	-	-	-		
92	OHX	5	4533	-	0,6,6	-	-	-		
92	OHX	6	2235	-	0,6,6	-	-	-		
92	OHX	5	4365	-	0,6,6	-	-	-		
92	OHX	5	4300	-	0,6,6	-	-	-		
92	OHX	5	4386	-	0,6,6	-	-	-		
92	OHX	6	2305	-	0,6,6	-	-	-		
92	OHX	2	2109	-	0,6,6	-	-	-		
92	OHX	2	2236	92	0,6,6	-	-	-		
92	OHX	7	235	-	0,6,6	-	-	-		
92	OHX	5	4276	92	0,6,6	-	-	-		
92	OHX	1	4128	-	0,6,6	-	-	-		
92	OHX	1	4455	-	0,6,6	-	-	-		
92	OHX	5	4332	-	0,6,6	-	-	-		
92	OHX	2	2083	92	0,6,6	-	-	-		
92	OHX	1	4508	92	0,6,6	-	-	-		
92	OHX	13	413	-	0,6,6	-	-	-		
92	OHX	1	4345	-	0,6,6	-	-	-		
92	OHX	2	2210	1	0,6,6	-	-	-		
92	OHX	5	4368	-	0,6,6	-	-	-		
92	OHX	2	2256	92	0,6,6	-	-	-		
92	OHX	2	2168	-	0,6,6	-	-	-		
92	OHX	5	4289	-	0,6,6	-	-	-		
92	OHX	1	4165	-	0,6,6	-	-	-		
92	OHX	1	4304	-	0,6,6	-	-	-		
92	OHX	6	2192	-	0,6,6	-	-	-		
92	OHX	6	2269	-	0,6,6	-	-	-		
92	OHX	5	4371	-	0,6,6	-	-	-		
92	OHX	5	4262	-	0,6,6	-	-	-		
92	OHX	4	237	38	0,6,6	-	-	-		
92	OHX	1	4360	-	0,6,6	-	-	-		
92	OHX	3	220	-	0,6,6	-	-	-		
92	OHX	1	4099	-	0,6,6	-	-	-		
92	OHX	5	4308	-	0,6,6	-	-	-		
92	OHX	5	4280	-	0,6,6	-	-	-		
92	OHX	1	4475	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2112	-	0,6,6	-	-	-		
92	OHX	5	4561	92	0,6,6	-	-	-		
92	OHX	5	4532	-	0,6,6	-	-	-		
92	OHX	2	2098	-	0,6,6	-	-	-		
92	OHX	6	2240	-	0,6,6	-	-	-		
92	OHX	1	4133	-	0,6,6	-	-	-		
92	OHX	2	2249	92	0,6,6	-	-	-		
92	OHX	1	4187	92	0,6,6	-	-	-		
92	OHX	5	4416	-	0,6,6	-	-	-		
92	OHX	5	4540	36	0,6,6	-	-	-		
92	OHX	1	4239	92	0,6,6	-	-	-		
92	OHX	5	4231	92	0,6,6	-	-	-		
92	OHX	5	4427	-	0,6,6	-	-	-		
92	OHX	1	4442	92	0,6,6	-	-	-		
92	OHX	2	2124	-	0,6,6	-	-	-		
92	OHX	5	4573	92	0,6,6	-	-	-		
92	OHX	1	4218	-	0,6,6	-	-	-		
92	OHX	1	4352	-	0,6,6	-	-	-		
92	OHX	1	4364	-	0,6,6	-	-	-		
92	OHX	5	4228	-	0,6,6	-	-	-		
92	OHX	2	2190	92	0,6,6	-	-	-		
92	OHX	6	2179	-	0,6,6	-	-	-		
92	OHX	1	4311	-	0,6,6	-	-	-		
92	OHX	6	2330	-	0,6,6	-	-	-		
92	OHX	5	4460	-	0,6,6	-	-	-		
92	OHX	1	4275	-	0,6,6	-	-	-		
92	OHX	5	4565	92	0,6,6	-	-	-		
92	OHX	C8	202	92	0,6,6	-	-	-		
92	OHX	5	4345	-	0,6,6	-	-	-		
92	OHX	C5	202	17	0,6,6	-	-	-		
92	OHX	2	2069	-	0,6,6	-	-	-		
92	OHX	7	201	92	0,6,6	-	-	-		
92	OHX	6	2195	-	0,6,6	-	-	-		
92	OHX	1	4261	-	0,6,6	-	-	-		
92	OHX	5	4354	-	0,6,6	-	-	-		
92	OHX	3	230	92	0,6,6	-	-	-		
92	OHX	1	4204	-	0,6,6	-	-	-		
92	OHX	6	2157	-	0,6,6	-	-	-		
92	OHX	5	4323	92,36	0,6,6	-	-	-		
92	OHX	5	4243	-	0,6,6	-	-	-		
92	OHX	6	2297	92	0,6,6	-	-	-		
92	OHX	6	2155	92	0,6,6	-	-	-		
92	OHX	1	4301	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4229	-	0,6,6	-	-	-		
92	OHX	1	4465	-	0,6,6	-	-	-		
92	OHX	1	4189	-	0,6,6	-	-	-		
92	OHX	5	4239	-	0,6,6	-	-	-		
92	OHX	5	4359	92	0,6,6	-	-	-		
92	OHX	5	4419	-	0,6,6	-	-	-		
92	OHX	1	4423	-	0,6,6	-	-	-		
92	OHX	3	224	-	0,6,6	-	-	-		
92	OHX	1	4179	-	0,6,6	-	-	-		
92	OHX	2	2216	92	0,6,6	-	-	-		
92	OHX	1	4321	-	0,6,6	-	-	-		
92	OHX	1	4291	92	0,6,6	-	-	-		
92	OHX	s8	305	-	0,6,6	-	-	-		
92	OHX	1	4424	92	0,6,6	-	-	-		
92	OHX	1	4282	-	0,6,6	-	-	-		
92	OHX	5	4318	-	0,6,6	-	-	-		
92	OHX	5	4288	92	0,6,6	-	-	-		
92	OHX	M7	209	-	0,6,6	-	-	-		
92	OHX	6	2205	-	0,6,6	-	-	-		
92	OHX	5	4311	-	0,6,6	-	-	-		
92	OHX	2	2145	92	0,6,6	-	-	-		
92	OHX	5	4421	-	0,6,6	-	-	-		
92	OHX	1	4410	-	0,6,6	-	-	-		
92	OHX	5	4495	-	0,6,6	-	-	-		
92	OHX	1	4205	-	0,6,6	-	-	-		
92	OHX	6	2310	92	0,6,6	-	-	-		
92	OHX	5	4508	-	0,6,6	-	-	-		
92	OHX	5	4435	-	0,6,6	-	-	-		
92	OHX	1	4184	-	0,6,6	-	-	-		
92	OHX	4	244	-	0,6,6	-	-	-		
92	OHX	5	4454	-	0,6,6	-	-	-		
92	OHX	2	2170	-	0,6,6	-	-	-		
92	OHX	1	4370	-	0,6,6	-	-	-		
92	OHX	1	4376	92	0,6,6	-	-	-		
92	OHX	1	4219	-	0,6,6	-	-	-		
92	OHX	6	2210	-	0,6,6	-	-	-		
92	OHX	5	4391	92	0,6,6	-	-	-		
92	OHX	1	4117	-	0,6,6	-	-	-		
92	OHX	5	4373	92	0,6,6	-	-	-		
92	OHX	1	4325	-	0,6,6	-	-	-		
92	OHX	6	2270	-	0,6,6	-	-	-		
92	OHX	1	4166	-	0,6,6	-	-	-		
92	OHX	5	4443	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2192	-	0,6,6	-	-	-		
92	OHX	6	2329	92	0,6,6	-	-	-		
92	OHX	2	2159	92,1	0,6,6	-	-	-		
92	OHX	2	2146	-	0,6,6	-	-	-		
92	OHX	6	2198	-	0,6,6	-	-	-		
92	OHX	1	4397	-	0,6,6	-	-	-		
92	OHX	5	4286	-	0,6,6	-	-	-		
92	OHX	2	2208	-	0,6,6	-	-	-		
92	OHX	5	4471	92	0,6,6	-	-	-		
92	OHX	5	4537	-	0,6,6	-	-	-		
92	OHX	5	4207	92	0,6,6	-	-	-		
92	OHX	1	4103	36	0,6,6	-	-	-		
92	OHX	1	4337	-	0,6,6	-	-	-		
92	OHX	6	2145	-	0,6,6	-	-	-		
92	OHX	5	4305	-	0,6,6	-	-	-		
92	OHX	14	404	-	0,6,6	-	-	-		
92	OHX	1	4307	92	0,6,6	-	-	-		
92	OHX	5	4314	-	0,6,6	-	-	-		
92	OHX	1	4372	92	0,6,6	-	-	-		
92	OHX	1	4486	-	0,6,6	-	-	-		
92	OHX	5	4197	-	0,6,6	-	-	-		
92	OHX	6	2144	-	0,6,6	-	-	-		
92	OHX	1	4283	-	0,6,6	-	-	-		
92	OHX	5	4513	-	0,6,6	-	-	-		
92	OHX	5	4357	-	0,6,6	-	-	-		
92	OHX	6	2296	-	0,6,6	-	-	-		
92	OHX	1	4203	92	0,6,6	-	-	-		
92	OHX	2	2103	-	0,6,6	-	-	-		
92	OHX	5	4303	-	0,6,6	-	-	-		
92	OHX	6	2161	92	0,6,6	-	-	-		
92	OHX	1	4104	-	0,6,6	-	-	-		
92	OHX	1	4267	-	0,6,6	-	-	-		
92	OHX	1	4289	92	0,6,6	-	-	-		
92	OHX	5	4447	-	0,6,6	-	-	-		
92	OHX	5	4245	-	0,6,6	-	-	-		
92	OHX	1	4246	-	0,6,6	-	-	-		
92	OHX	1	4258	-	0,6,6	-	-	-		
92	OHX	6	2325	92	0,6,6	-	-	-		
92	OHX	6	2267	-	0,6,6	-	-	-		
92	OHX	5	4229	92	0,6,6	-	-	-		
92	OHX	2	2215	-	0,6,6	-	-	-		
92	OHX	6	2166	-	0,6,6	-	-	-		
92	OHX	1	4499	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	3401	1	0,6,6	-	-	-		
92	OHX	1	4342	36	0,6,6	-	-	-		
92	OHX	6	2229	-	0,6,6	-	-	-		
92	OHX	2	2255	92	0,6,6	-	-	-		
92	OHX	1	4284	-	0,6,6	-	-	-		
92	OHX	1	4467	92	0,6,6	-	-	-		
92	OHX	5	4568	92	0,6,6	-	-	-		
92	OHX	2	2151	-	0,6,6	-	-	-		
92	OHX	2	2140	1	0,6,6	-	-	-		
92	OHX	1	4374	-	0,6,6	-	-	-		
92	OHX	1	4351	-	0,6,6	-	-	-		
92	OHX	5	4395	-	0,6,6	-	-	-		
92	OHX	1	4170	92	0,6,6	-	-	-		
92	OHX	5	4307	-	0,6,6	-	-	-		
92	OHX	2	2183	92,1	0,6,6	-	-	-		
92	OHX	5	4415	-	0,6,6	-	-	-		
92	OHX	6	2332	92	0,6,6	-	-	-		
92	OHX	2	2253	-	0,6,6	-	-	-		
92	OHX	5	4283	-	0,6,6	-	-	-		
92	OHX	1	4414	92	0,6,6	-	-	-		
92	OHX	1	4139	-	0,6,6	-	-	-		
92	OHX	5	4566	92	0,6,6	-	-	-		
92	OHX	1	4149	-	0,6,6	-	-	-		
92	OHX	A	101	90	0,6,6	-	-	-		
92	OHX	8	227	-	0,6,6	-	-	-		
92	OHX	1	4354	-	0,6,6	-	-	-		
92	OHX	1	4105	92	0,6,6	-	-	-		
92	OHX	5	4342	-	0,6,6	-	-	-		
92	OHX	2	2116	92	0,6,6	-	-	-		
92	OHX	5	4221	-	0,6,6	-	-	-		
92	OHX	6	2159	92	0,6,6	-	-	-		
92	OHX	5	4502	-	0,6,6	-	-	-		
92	OHX	1	4388	-	0,6,6	-	-	-		
92	OHX	1	4306	92	0,6,6	-	-	-		
92	OHX	6	2176	-	0,6,6	-	-	-		
92	OHX	c8	204	-	0,6,6	-	-	-		
92	OHX	5	4351	-	0,6,6	-	-	-		
92	OHX	5	4340	-	0,6,6	-	-	-		
92	OHX	1	4359	92	0,6,6	-	-	-		
92	OHX	1	4279	92	0,6,6	-	-	-		
92	OHX	1	4315	92	0,6,6	-	-	-		
92	OHX	6	2265	-	0,6,6	-	-	-		
92	OHX	5	4408	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2240	92	0,6,6	-	-	-		
92	OHX	1	4334	-	0,6,6	-	-	-		
92	OHX	1	4417	36	0,6,6	-	-	-		
92	OHX	5	4548	-	0,6,6	-	-	-		
92	OHX	m0	305	92	0,6,6	-	-	-		
92	OHX	6	2258	92	0,6,6	-	-	-		
92	OHX	O7	108	-	0,6,6	-	-	-		
92	OHX	5	4562	-	0,6,6	-	-	-		
92	OHX	5	4480	92	0,6,6	-	-	-		
92	OHX	6	2239	-	0,6,6	-	-	-		
92	OHX	6	2262	92	0,6,6	-	-	-		
92	OHX	d9	104	92	0,6,6	-	-	-		
92	OHX	1	4452	92	0,6,6	-	-	-		
92	OHX	5	4370	-	0,6,6	-	-	-		
92	OHX	2	2104	-	0,6,6	-	-	-		
92	OHX	2	2230	-	0,6,6	-	-	-		
92	OHX	2	2133	92	0,6,6	-	-	-		
92	OHX	5	4310	-	0,6,6	-	-	-		
92	OHX	6	2286	92	0,6,6	-	-	-		
92	OHX	6	2231	-	0,6,6	-	-	-		
92	OHX	6	2288	-	0,6,6	-	-	-		
92	OHX	5	4325	-	0,6,6	-	-	-		
92	OHX	6	2215	-	0,6,6	-	-	-		
92	OHX	6	2182	-	0,6,6	-	-	-		
92	OHX	5	4374	-	0,6,6	-	-	-		
92	OHX	5	4476	92	0,6,6	-	-	-		
92	OHX	5	4431	-	0,6,6	-	-	-		
92	OHX	2	2153	-	0,6,6	-	-	-		
92	OHX	5	4216	92	0,6,6	-	-	-		
92	OHX	5	4518	-	0,6,6	-	-	-		
92	OHX	5	4212	-	0,6,6	-	-	-		
92	OHX	1	4298	-	0,6,6	-	-	-		
92	OHX	1	4404	-	0,6,6	-	-	-		
92	OHX	1	4230	-	0,6,6	-	-	-		
92	OHX	5	4183	-	0,6,6	-	-	-		
92	OHX	5	4210	-	0,6,6	-	-	-		
92	OHX	3	227	-	0,6,6	-	-	-		
92	OHX	6	2313	-	0,6,6	-	-	-		
92	OHX	7	236	-	0,6,6	-	-	-		
92	OHX	4	241	-	0,6,6	-	-	-		
92	OHX	5	4563	-	0,6,6	-	-	-		
92	OHX	5	4406	92	0,6,6	-	-	-		
92	OHX	1	4451	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2233	-	0,6,6	-	-	-		
92	OHX	1	4242	-	0,6,6	-	-	-		
92	OHX	1	4440	92,36	0,6,6	-	-	-		
92	OHX	L3	407	-	0,6,6	-	-	-		
92	OHX	6	2170	1	0,6,6	-	-	-		
92	OHX	2	2142	-	0,6,6	-	-	-		
92	OHX	6	2295	-	0,6,6	-	-	-		
92	OHX	1	4333	-	0,6,6	-	-	-		
92	OHX	1	4112	-	0,6,6	-	-	-		
92	OHX	5	4317	-	0,6,6	-	-	-		
92	OHX	2	2143	92	0,6,6	-	-	-		
92	OHX	1	4326	-	0,6,6	-	-	-		
92	OHX	1	4392	-	0,6,6	-	-	-		
92	OHX	5	4312	92	0,6,6	-	-	-		
92	OHX	2	2169	-	0,6,6	-	-	-		
92	OHX	5	4224	-	0,6,6	-	-	-		
92	OHX	1	4441	-	0,6,6	-	-	-		
92	OHX	1	4110	-	0,6,6	-	-	-		
92	OHX	1	4211	92	0,6,6	-	-	-		
92	OHX	5	4349	92	0,6,6	-	-	-		
92	OHX	1	4263	-	0,6,6	-	-	-		
92	OHX	5	4450	36	0,6,6	-	-	-		
92	OHX	1	4491	92	0,6,6	-	-	-		
92	OHX	1	4168	92	0,6,6	-	-	-		
92	OHX	5	4459	92	0,6,6	-	-	-		
92	OHX	6	2227	-	0,6,6	-	-	-		
92	OHX	5	4378	-	0,6,6	-	-	-		
92	OHX	1	4412	92	0,6,6	-	-	-		
92	OHX	5	4187	92	0,6,6	-	-	-		
92	OHX	1	4400	-	0,6,6	-	-	-		
92	OHX	3	223	92	0,6,6	-	-	-		
92	OHX	6	2168	-	0,6,6	-	-	-		
92	OHX	5	4369	92	0,6,6	-	-	-		
92	OHX	2	2162	-	0,6,6	-	-	-		
92	OHX	1	4143	92	0,6,6	-	-	-		
92	OHX	5	4372	-	0,6,6	-	-	-		
92	OHX	5	4440	92	0,6,6	-	-	-		
92	OHX	5	4352	92	0,6,6	-	-	-		
92	OHX	5	4457	92	0,6,6	-	-	-		
92	OHX	5	4271	36	0,6,6	-	-	-		
92	OHX	5	4542	-	0,6,6	-	-	-		
92	OHX	1	4405	92	0,6,6	-	-	-		
92	OHX	1	4252	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4175	-	0,6,6	-	-	-		
92	OHX	6	2314	-	0,6,6	-	-	-		
92	OHX	1	4472	-	0,6,6	-	-	-		
92	OHX	5	4531	-	0,6,6	-	-	-		
92	OHX	8	224	-	0,6,6	-	-	-		
92	OHX	4	248	-	0,6,6	-	-	-		
92	OHX	5	4211	92	0,6,6	-	-	-		
92	OHX	6	2171	-	0,6,6	-	-	-		
92	OHX	1	4411	92	0,6,6	-	-	-		
92	OHX	1	4235	-	0,6,6	-	-	-		
92	OHX	1	4489	92	0,6,6	-	-	-		
92	OHX	5	4436	-	0,6,6	-	-	-		
92	OHX	1	4102	-	0,6,6	-	-	-		
92	OHX	8	232	-	0,6,6	-	-	-		
92	OHX	6	2196	92	0,6,6	-	-	-		
92	OHX	7	229	-	0,6,6	-	-	-		
92	OHX	5	4545	92	0,6,6	-	-	-		
92	OHX	5	4398	-	0,6,6	-	-	-		
92	OHX	6	2146	-	0,6,6	-	-	-		
92	OHX	6	2281	-	0,6,6	-	-	-		
92	OHX	1	4341	-	0,6,6	-	-	-		
92	OHX	3	228	92	0,6,6	-	-	-		
92	OHX	1	4155	-	0,6,6	-	-	-		
92	OHX	5	4400	92	0,6,6	-	-	-		
92	OHX	5	4437	92	0,6,6	-	-	-		
92	OHX	5	4410	92	0,6,6	-	-	-		
92	OHX	2	2102	-	0,6,6	-	-	-		
92	OHX	6	2236	-	0,6,6	-	-	-		
92	OHX	1	4429	-	0,6,6	-	-	-		
92	OHX	2	2202	-	0,6,6	-	-	-		
92	OHX	5	4555	92	0,6,6	-	-	-		
92	OHX	5	4554	92	0,6,6	-	-	-		
92	OHX	c3	201	-	0,6,6	-	-	-		
92	OHX	5	4257	92,36	0,6,6	-	-	-		
92	OHX	5	4376	-	0,6,6	-	-	-		
92	OHX	S2	303	92	0,6,6	-	-	-		
92	OHX	1	4196	92	0,6,6	-	-	-		
92	OHX	2	2101	92	0,6,6	-	-	-		
92	OHX	5	4164	-	0,6,6	-	-	-		
92	OHX	2	2173	-	0,6,6	-	-	-		
92	OHX	6	2199	1	0,6,6	-	-	-		
92	OHX	5	4218	-	0,6,6	-	-	-		
92	OHX	5	4559	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4274	-	0,6,6	-	-	-		
92	OHX	6	2304	-	0,6,6	-	-	-		
92	OHX	6	2328	-	0,6,6	-	-	-		
92	OHX	1	4367	-	0,6,6	-	-	-		
92	OHX	5	4219	92	0,6,6	-	-	-		
92	OHX	5	4549	-	0,6,6	-	-	-		
92	OHX	6	2246	-	0,6,6	-	-	-		
92	OHX	1	4339	-	0,6,6	-	-	-		
92	OHX	8	237	38	0,6,6	-	-	-		
92	OHX	1	4180	92	0,6,6	-	-	-		
92	OHX	5	4514	-	0,6,6	-	-	-		
92	OHX	5	4167	-	0,6,6	-	-	-		
92	OHX	5	4487	-	0,6,6	-	-	-		
92	OHX	5	4261	92	0,6,6	-	-	-		
92	OHX	l9	204	-	0,6,6	-	-	-		
92	OHX	D9	104	92	0,6,6	-	-	-		
92	OHX	1	4331	-	0,6,6	-	-	-		
92	OHX	1	4431	92	0,6,6	-	-	-		
92	OHX	4	247	92	0,6,6	-	-	-		
92	OHX	5	4527	-	0,6,6	-	-	-		
92	OHX	7	232	-	0,6,6	-	-	-		
92	OHX	m9	202	-	0,6,6	-	-	-		
92	OHX	7	237	-	0,6,6	-	-	-		
92	OHX	1	4241	-	0,6,6	-	-	-		
92	OHX	1	4444	-	0,6,6	-	-	-		
92	OHX	l5	308	-	0,6,6	-	-	-		
92	OHX	1	4328	-	0,6,6	-	-	-		
92	OHX	5	4230	-	0,6,6	-	-	-		
92	OHX	5	4529	-	0,6,6	-	-	-		
92	OHX	6	2284	-	0,6,6	-	-	-		
92	OHX	5	4474	92	0,6,6	-	-	-		
92	OHX	1	4109	-	0,6,6	-	-	-		
92	OHX	5	4182	-	0,6,6	-	-	-		
92	OHX	2	2244	92,1	0,6,6	-	-	-		
92	OHX	5	4363	-	0,6,6	-	-	-		
92	OHX	5	4453	92	0,6,6	-	-	-		
92	OHX	L3	409	-	0,6,6	-	-	-		
92	OHX	n3	204	-	0,6,6	-	-	-		
92	OHX	1	4226	-	0,6,6	-	-	-		
92	OHX	1	4483	-	0,6,6	-	-	-		
92	OHX	4	242	-	0,6,6	-	-	-		
92	OHX	1	4348	-	0,6,6	-	-	-		
92	OHX	5	4291	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4250	-	0,6,6	-	-	-		
92	OHX	7	231	92	0,6,6	-	-	-		
92	OHX	2	2099	-	0,6,6	-	-	-		
92	OHX	1	4327	-	0,6,6	-	-	-		
92	OHX	2	2221	92	0,6,6	-	-	-		
92	OHX	1	4278	36	0,6,6	-	-	-		
92	OHX	5	4260	-	0,6,6	-	-	-		
92	OHX	5	4360	-	0,6,6	-	-	-		
92	OHX	5	4339	-	0,6,6	-	-	-		
92	OHX	5	4328	-	0,6,6	-	-	-		
92	OHX	6	2234	-	0,6,6	-	-	-		
92	OHX	5	4277	-	0,6,6	-	-	-		
92	OHX	5	4547	92	0,6,6	-	-	-		
92	OHX	5	4233	92	0,6,6	-	-	-		
92	OHX	1	4101	-	0,6,6	-	-	-		
92	OHX	5	4284	-	0,6,6	-	-	-		
92	OHX	1	4214	-	0,6,6	-	-	-		
92	OHX	5	4552	92	0,6,6	-	-	-		
92	OHX	c5	202	-	0,6,6	-	-	-		
92	OHX	2	2090	92	0,6,6	-	-	-		
92	OHX	1	4361	92	0,6,6	-	-	-		
92	OHX	6	2226	-	0,6,6	-	-	-		
92	OHX	6	2323	92	0,6,6	-	-	-		
92	OHX	5	4466	-	0,6,6	-	-	-		
92	OHX	1	4368	-	0,6,6	-	-	-		
92	OHX	1	4296	92	0,6,6	-	-	-		
92	OHX	5	4560	92	0,6,6	-	-	-		
92	OHX	5	4387	36	0,6,6	-	-	-		
92	OHX	2	2207	92	0,6,6	-	-	-		
92	OHX	1	4137	-	0,6,6	-	-	-		
92	OHX	5	4467	36	0,6,6	-	-	-		
92	OHX	5	4254	36	0,6,6	-	-	-		
92	OHX	2	2228	-	0,6,6	-	-	-		
92	OHX	5	4511	92	0,6,6	-	-	-		
92	OHX	1	4280	-	0,6,6	-	-	-		
92	OHX	4	235	-	0,6,6	-	-	-		
92	OHX	6	2172	-	0,6,6	-	-	-		
92	OHX	L4	408	-	0,6,6	-	-	-		
92	OHX	1	4272	92	0,6,6	-	-	-		
92	OHX	1	4231	92	0,6,6	-	-	-		
92	OHX	1	4393	36	0,6,6	-	-	-		
92	OHX	5	4222	92	0,6,6	-	-	-		
92	OHX	5	4448	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4515	92	0,6,6	-	-	-		
92	OHX	5	4240	36	0,6,6	-	-	-		
92	OHX	M0	308	92	0,6,6	-	-	-		
92	OHX	1	4377	-	0,6,6	-	-	-		
92	OHX	2	2114	-	0,6,6	-	-	-		
92	OHX	2	2094	-	0,6,6	-	-	-		
92	OHX	5	4181	-	0,6,6	-	-	-		
92	OHX	l2	306	92	0,6,6	-	-	-		
92	OHX	1	4302	92	0,6,6	-	-	-		
92	OHX	5	4251	-	0,6,6	-	-	-		
92	OHX	5	4268	-	0,6,6	-	-	-		
92	OHX	1	4150	-	0,6,6	-	-	-		
92	OHX	2	2199	92	0,6,6	-	-	-		
92	OHX	M0	305	92	0,6,6	-	-	-		
92	OHX	5	4418	-	0,6,6	-	-	-		
92	OHX	5	4534	36	0,6,6	-	-	-		
92	OHX	1	4227	-	0,6,6	-	-	-		
92	OHX	5	4465	92	0,6,6	-	-	-		
92	OHX	1	4237	-	0,6,6	-	-	-		
92	OHX	5	4267	-	0,6,6	-	-	-		
92	OHX	2	2184	-	0,6,6	-	-	-		
92	OHX	2	2222	92	0,6,6	-	-	-		
92	OHX	6	2208	-	0,6,6	-	-	-		
92	OHX	l3	412	-	0,6,6	-	-	-		
92	OHX	6	2294	92,1	0,6,6	-	-	-		
92	OHX	q2	203	-	0,6,6	-	-	-		
92	OHX	5	4193	-	0,6,6	-	-	-		
92	OHX	5	4396	-	0,6,6	-	-	-		
92	OHX	1	4195	-	0,6,6	-	-	-		
92	OHX	2	2071	-	0,6,6	-	-	-		
92	OHX	1	4188	-	0,6,6	-	-	-		
92	OHX	2	2119	-	0,6,6	-	-	-		
92	OHX	2	2137	1	0,6,6	-	-	-		
92	OHX	1	4190	-	0,6,6	-	-	-		
92	OHX	1	4210	92	0,6,6	-	-	-		
92	OHX	2	2197	1	0,6,6	-	-	-		
92	OHX	1	4313	-	0,6,6	-	-	-		
92	OHX	1	4140	-	0,6,6	-	-	-		
92	OHX	1	4223	-	0,6,6	-	-	-		
92	OHX	5	4541	-	0,6,6	-	-	-		
92	OHX	6	2276	-	0,6,6	-	-	-		
92	OHX	1	4147	92	0,6,6	-	-	-		
92	OHX	5	4225	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2224	-	0,6,6	-	-	-		
92	OHX	5	4356	-	0,6,6	-	-	-		
92	OHX	5	4186	-	0,6,6	-	-	-		
92	OHX	1	4123	-	0,6,6	-	-	-		
92	OHX	5	4294	-	0,6,6	-	-	-		
92	OHX	5	4206	92	0,6,6	-	-	-		
92	OHX	1	4288	-	0,6,6	-	-	-		
92	OHX	d4	201	-	0,6,6	-	-	-		
92	OHX	5	4281	-	0,6,6	-	-	-		
92	OHX	6	2255	92,1	0,6,6	-	-	-		
92	OHX	6	2142	-	0,6,6	-	-	-		
92	OHX	5	4510	-	0,6,6	-	-	-		
92	OHX	1	4425	-	0,6,6	-	-	-		
92	OHX	1	4495	92	0,6,6	-	-	-		
92	OHX	5	4402	-	0,6,6	-	-	-		
92	OHX	5	4452	-	0,6,6	-	-	-		
92	OHX	8	229	-	0,6,6	-	-	-		
92	OHX	1	4161	92	0,6,6	-	-	-		
92	OHX	2	2187	-	0,6,6	-	-	-		
92	OHX	1	4469	92	0,6,6	-	-	-		
92	OHX	6	2169	-	0,6,6	-	-	-		
92	OHX	2	2234	-	0,6,6	-	-	-		
92	OHX	8	226	92	0,6,6	-	-	-		
92	OHX	5	4255	-	0,6,6	-	-	-		
92	OHX	1	4178	-	0,6,6	-	-	-		
92	OHX	2	2220	1	0,6,6	-	-	-		
92	OHX	1	4126	-	0,6,6	-	-	-		
92	OHX	6	2322	-	0,6,6	-	-	-		
92	OHX	5	4439	-	0,6,6	-	-	-		
92	OHX	5	4301	-	0,6,6	-	-	-		
92	OHX	2	2129	92,1	0,6,6	-	-	-		
92	OHX	5	4343	-	0,6,6	-	-	-		
92	OHX	6	2147	-	0,6,6	-	-	-		
92	OHX	5	4335	-	0,6,6	-	-	-		
92	OHX	2	2077	92,1	0,6,6	-	-	-		
92	OHX	3	229	-	0,6,6	-	-	-		
92	OHX	1	4157	92	0,6,6	-	-	-		
92	OHX	1	4119	-	0,6,6	-	-	-		
92	OHX	1	4457	92	0,6,6	-	-	-		
92	OHX	6	2339	92	0,6,6	-	-	-		
92	OHX	1	4158	-	0,6,6	-	-	-		
92	OHX	1	4428	92	0,6,6	-	-	-		
92	OHX	2	2148	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4183	-	0,6,6	-	-	-		
92	OHX	1	4391	-	0,6,6	-	-	-		
92	OHX	1	4265	-	0,6,6	-	-	-		
92	OHX	5	4451	-	0,6,6	-	-	-		
92	OHX	6	2211	-	0,6,6	-	-	-		
92	OHX	5	4493	-	0,6,6	-	-	-		
92	OHX	5	4557	92	0,6,6	-	-	-		
92	OHX	5	4242	36	0,6,6	-	-	-		
92	OHX	5	4500	-	0,6,6	-	-	-		
92	OHX	1	4371	-	0,6,6	-	-	-		
92	OHX	5	4489	36	0,6,6	-	-	-		
92	OHX	1	4146	-	0,6,6	-	-	-		
92	OHX	1	4357	-	0,6,6	-	-	-		
92	OHX	5	4237	92	0,6,6	-	-	-		
92	OHX	5	4169	-	0,6,6	-	-	-		
92	OHX	1	4390	92	0,6,6	-	-	-		
92	OHX	5	4161	-	0,6,6	-	-	-		
92	OHX	6	2206	-	0,6,6	-	-	-		
92	OHX	6	2282	92	0,6,6	-	-	-		
92	OHX	2	2087	-	0,6,6	-	-	-		
92	OHX	5	4539	92	0,6,6	-	-	-		
92	OHX	6	2312	92	0,6,6	-	-	-		
92	OHX	6	2184	-	0,6,6	-	-	-		
92	OHX	1	4449	-	0,6,6	-	-	-		
92	OHX	5	4214	-	0,6,6	-	-	-		
92	OHX	1	4264	-	0,6,6	-	-	-		
92	OHX	L2	305	92	0,6,6	-	-	-		
92	OHX	2	2191	-	0,6,6	-	-	-		
92	OHX	1	4163	-	0,6,6	-	-	-		
92	OHX	1	4316	-	0,6,6	-	-	-		
92	OHX	5	4524	36	0,6,6	-	-	-		
92	OHX	1	4383	-	0,6,6	-	-	-		
92	OHX	2	2131	-	0,6,6	-	-	-		
92	OHX	o7	105	-	0,6,6	-	-	-		
92	OHX	1	4245	92	0,6,6	-	-	-		
92	OHX	1	4409	-	0,6,6	-	-	-		
92	OHX	5	4490	-	0,6,6	-	-	-		
92	OHX	5	4412	-	0,6,6	-	-	-		
92	OHX	5	4397	-	0,6,6	-	-	-		
92	OHX	1	4273	36	0,6,6	-	-	-		
92	OHX	2	2205	-	0,6,6	-	-	-		
92	OHX	6	2309	92	0,6,6	-	-	-		
92	OHX	6	2197	1	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2249	92	0,6,6	-	-	-		
92	OHX	8	225	-	0,6,6	-	-	-		
92	OHX	5	4203	92	0,6,6	-	-	-		
92	OHX	2	2235	92	0,6,6	-	-	-		
92	OHX	6	2189	-	0,6,6	-	-	-		
92	OHX	5	4428	-	0,6,6	-	-	-		
92	OHX	6	2334	92	0,6,6	-	-	-		
92	OHX	2	2152	92	0,6,6	-	-	-		
92	OHX	5	4265	-	0,6,6	-	-	-		
92	OHX	6	2224	-	0,6,6	-	-	-		
92	OHX	1	4297	-	0,6,6	-	-	-		
92	OHX	5	4319	-	0,6,6	-	-	-		
92	OHX	5	4377	-	0,6,6	-	-	-		
92	OHX	5	4411	-	0,6,6	-	-	-		
92	OHX	1	4173	-	0,6,6	-	-	-		
92	OHX	4	243	-	0,6,6	-	-	-		
92	OHX	6	2218	-	0,6,6	-	-	-		
92	OHX	1	4199	-	0,6,6	-	-	-		
92	OHX	1	4220	-	0,6,6	-	-	-		
92	OHX	5	4388	36	0,6,6	-	-	-		
92	OHX	2	2177	-	0,6,6	-	-	-		
92	OHX	1	4505	92,36	0,6,6	-	-	-		
92	OHX	5	4252	92	0,6,6	-	-	-		
92	OHX	7	234	-	0,6,6	-	-	-		
92	OHX	6	2285	-	0,6,6	-	-	-		
92	OHX	5	4175	-	0,6,6	-	-	-		
92	OHX	1	4174	-	0,6,6	-	-	-		
92	OHX	1	4127	-	0,6,6	-	-	-		
92	OHX	5	4444	-	0,6,6	-	-	-		
92	OHX	5	4227	-	0,6,6	-	-	-		
92	OHX	6	2243	-	0,6,6	-	-	-		
92	OHX	1	4106	-	0,6,6	-	-	-		
92	OHX	1	4385	92	0,6,6	-	-	-		
92	OHX	1	4259	-	0,6,6	-	-	-		
92	OHX	5	4485	92	0,6,6	-	-	-		
92	OHX	5	4528	-	0,6,6	-	-	-		
92	OHX	5	4264	92	0,6,6	-	-	-		
92	OHX	m0	304	92	0,6,6	-	-	-		
92	OHX	5	4475	-	0,6,6	-	-	-		
92	OHX	5	4163	-	0,6,6	-	-	-		
92	OHX	2	2158	92	0,6,6	-	-	-		
92	OHX	5	4316	-	0,6,6	-	-	-		
92	OHX	m1	203	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4419	-	0,6,6	-	-	-		
92	OHX	1	4249	-	0,6,6	-	-	-		
92	OHX	2	2209	-	0,6,6	-	-	-		
92	OHX	5	4520	92	0,6,6	-	-	-		
92	OHX	1	4496	92	0,6,6	-	-	-		
92	OHX	1	4394	-	0,6,6	-	-	-		
92	OHX	6	2141	-	0,6,6	-	-	-		
92	OHX	1	4200	92	0,6,6	-	-	-		
92	OHX	5	4341	92	0,6,6	-	-	-		
92	OHX	1	4481	92	0,6,6	-	-	-		
92	OHX	1	4474	-	0,6,6	-	-	-		
92	OHX	8	236	-	0,6,6	-	-	-		
92	OHX	5	4501	-	0,6,6	-	-	-		
92	OHX	1	4209	-	0,6,6	-	-	-		
92	OHX	6	2261	-	0,6,6	-	-	-		
92	OHX	5	4226	-	0,6,6	-	-	-		
92	OHX	N1	202	-	0,6,6	-	-	-		
92	OHX	1	4197	92	0,6,6	-	-	-		
92	OHX	M9	204	-	0,6,6	-	-	-		
92	OHX	5	4429	-	0,6,6	-	-	-		
92	OHX	5	4530	92	0,6,6	-	-	-		
92	OHX	5	4546	-	0,6,6	-	-	-		
92	OHX	2	2161	1	0,6,6	-	-	-		
92	OHX	6	2216	92	0,6,6	-	-	-		
92	OHX	2	2223	-	0,6,6	-	-	-		
92	OHX	1	4125	-	0,6,6	-	-	-		
92	OHX	5	4285	92	0,6,6	-	-	-		
92	OHX	1	4159	-	0,6,6	-	-	-		
92	OHX	1	4293	-	0,6,6	-	-	-		
92	OHX	1	4198	92	0,6,6	-	-	-		
92	OHX	5	4220	-	0,6,6	-	-	-		
92	OHX	1	4462	-	0,6,6	-	-	-		
92	OHX	1	4497	-	0,6,6	-	-	-		
92	OHX	1	4270	-	0,6,6	-	-	-		
92	OHX	2	2092	-	0,6,6	-	-	-		
92	OHX	5	4180	-	0,6,6	-	-	-		
92	OHX	1	4121	-	0,6,6	-	-	-		
92	OHX	2	2097	-	0,6,6	-	-	-		
92	OHX	1	4445	92	0,6,6	-	-	-		
92	OHX	5	4479	-	0,6,6	-	-	-		
92	OHX	1	4344	-	0,6,6	-	-	-		
92	OHX	5	4367	-	0,6,6	-	-	-		
92	OHX	1	4458	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4420	-	0,6,6	-	-	-		
92	OHX	5	4362	-	0,6,6	-	-	-		
92	OHX	1	4255	-	0,6,6	-	-	-		
92	OHX	6	2191	92	0,6,6	-	-	-		
92	OHX	1	4450	-	0,6,6	-	-	-		
92	OHX	5	4200	92	0,6,6	-	-	-		
92	OHX	5	4331	-	0,6,6	-	-	-		
92	OHX	1	4153	92	0,6,6	-	-	-		
92	OHX	5	4330	-	0,6,6	-	-	-		
92	OHX	2	2237	92	0,6,6	-	-	-		
92	OHX	5	4517	92	0,6,6	-	-	-		
92	OHX	5	4215	92	0,6,6	-	-	-		
92	OHX	1	4208	-	0,6,6	-	-	-		
92	OHX	5	4536	-	0,6,6	-	-	-		
92	OHX	5	4544	-	0,6,6	-	-	-		
92	OHX	1	4240	-	0,6,6	-	-	-		
92	OHX	1	4478	92	0,6,6	-	-	-		
92	OHX	2	2150	-	0,6,6	-	-	-		
92	OHX	5	4462	92	0,6,6	-	-	-		
92	OHX	3	231	-	0,6,6	-	-	-		
92	OHX	2	2093	1	0,6,6	-	-	-		
92	OHX	5	4344	92	0,6,6	-	-	-		
92	OHX	1	4407	92	0,6,6	-	-	-		
92	OHX	5	4174	-	0,6,6	-	-	-		
92	OHX	5	4278	-	0,6,6	-	-	-		
92	OHX	5	4494	-	0,6,6	-	-	-		
92	OHX	2	2178	-	0,6,6	-	-	-		
92	OHX	5	4538	-	0,6,6	-	-	-		
92	OHX	5	4336	-	0,6,6	-	-	-		
92	OHX	2	2073	-	0,6,6	-	-	-		
92	OHX	6	2194	92	0,6,6	-	-	-		
92	OHX	N9	102	-	0,6,6	-	-	-		
92	OHX	1	4115	-	0,6,6	-	-	-		
92	OHX	2	2091	1	0,6,6	-	-	-		
92	OHX	2	2108	92	0,6,6	-	-	-		
92	OHX	5	4384	-	0,6,6	-	-	-		
92	OHX	6	2264	-	0,6,6	-	-	-		
92	OHX	1	4309	36	0,6,6	-	-	-		
92	OHX	5	4258	92	0,6,6	-	-	-		
92	OHX	5	4188	-	0,6,6	-	-	-		
92	OHX	1	4317	-	0,6,6	-	-	-		
92	OHX	1	4162	-	0,6,6	-	-	-		
92	OHX	6	2336	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2316	92	0,6,6	-	-	-		
92	OHX	5	4296	-	0,6,6	-	-	-		
92	OHX	2	2238	92	0,6,6	-	-	-		
92	OHX	1	4349	-	0,6,6	-	-	-		
92	OHX	1	4433	92	0,6,6	-	-	-		
92	OHX	1	4324	-	0,6,6	-	-	-		
92	OHX	2	2254	92	0,6,6	-	-	-		
92	OHX	5	4526	-	0,6,6	-	-	-		
92	OHX	6	2148	-	0,6,6	-	-	-		
92	OHX	6	2202	-	0,6,6	-	-	-		
92	OHX	1	4459	92,36	0,6,6	-	-	-		
92	OHX	5	4208	-	0,6,6	-	-	-		
92	OHX	2	2075	92	0,6,6	-	-	-		
92	OHX	1	4213	-	0,6,6	-	-	-		
92	OHX	1	4378	36	0,6,6	-	-	-		
92	OHX	1	4350	-	0,6,6	-	-	-		
92	OHX	2	2125	-	0,6,6	-	-	-		
92	OHX	6	2298	92,1	0,6,6	-	-	-		
92	OHX	1	4225	-	0,6,6	-	-	-		
92	OHX	1	4347	92	0,6,6	-	-	-		
92	OHX	1	4256	-	0,6,6	-	-	-		
92	OHX	4	233	-	0,6,6	-	-	-		
92	OHX	2	2144	92	0,6,6	-	-	-		
92	OHX	L3	408	-	0,6,6	-	-	-		
92	OHX	6	2213	92	0,6,6	-	-	-		
92	OHX	2	2138	92	0,6,6	-	-	-		
92	OHX	2	2248	92	0,6,6	-	-	-		
92	OHX	1	4134	92	0,6,6	-	-	-		
92	OHX	2	2076	-	0,6,6	-	-	-		
92	OHX	c1	201	92	0,6,6	-	-	-		
92	OHX	6	2271	-	0,6,6	-	-	-		
92	OHX	6	2320	-	0,6,6	-	-	-		
92	OHX	1	4299	-	0,6,6	-	-	-		
92	OHX	6	2241	-	0,6,6	-	-	-		
92	OHX	4	234	-	0,6,6	-	-	-		
92	OHX	5	4543	92	0,6,6	-	-	-		
92	OHX	6	2230	-	0,6,6	-	-	-		
92	OHX	2	2126	-	0,6,6	-	-	-		
92	OHX	6	2201	92	0,6,6	-	-	-		
92	OHX	2	2218	1	0,6,6	-	-	-		
92	OHX	2	2166	92	0,6,6	-	-	-		
92	OHX	5	4492	-	0,6,6	-	-	-		
92	OHX	2	2149	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2293	-	0,6,6	-	-	-		
92	OHX	M0	307	92	0,6,6	-	-	-		
92	OHX	2	2200	-	0,6,6	-	-	-		
92	OHX	1	4176	-	0,6,6	-	-	-		
92	OHX	3	222	-	0,6,6	-	-	-		
92	OHX	2	2127	-	0,6,6	-	-	-		
92	OHX	1	4217	-	0,6,6	-	-	-		
92	OHX	2	2110	-	0,6,6	-	-	-		
92	OHX	1	4340	-	0,6,6	-	-	-		
92	OHX	5	4213	-	0,6,6	-	-	-		
92	OHX	m5	303	-	0,6,6	-	-	-		
92	OHX	5	4503	92	0,6,6	-	-	-		
92	OHX	O1	202	92	0,6,6	-	-	-		
92	OHX	6	2292	-	0,6,6	-	-	-		
92	OHX	5	4499	92	0,6,6	-	-	-		
92	OHX	6	2177	-	0,6,6	-	-	-		
92	OHX	8	235	-	0,6,6	-	-	-		
92	OHX	2	2195	92	0,6,6	-	-	-		
92	OHX	SR	401	-	0,6,6	-	-	-		
92	OHX	S6	302	-	0,6,6	-	-	-		
92	OHX	2	2186	92	0,6,6	-	-	-		
92	OHX	5	4223	-	0,6,6	-	-	-		
92	OHX	6	2307	-	0,6,6	-	-	-		
92	OHX	6	2318	92	0,6,6	-	-	-		
92	OHX	5	4358	-	0,6,6	-	-	-		
92	OHX	2	2180	-	0,6,6	-	-	-		
92	OHX	6	2268	-	0,6,6	-	-	-		
92	OHX	1	4172	92	0,6,6	-	-	-		
92	OHX	6	2315	-	0,6,6	-	-	-		
92	OHX	1	4454	-	0,6,6	-	-	-		
92	OHX	5	4253	92	0,6,6	-	-	-		
92	OHX	1	4148	92	0,6,6	-	-	-		
92	OHX	6	2178	-	0,6,6	-	-	-		
92	OHX	1	4224	-	0,6,6	-	-	-		
92	OHX	1	4430	-	0,6,6	-	-	-		
92	OHX	1	4373	-	0,6,6	-	-	-		
92	OHX	2	2157	92	0,6,6	-	-	-		
92	OHX	6	2173	92	0,6,6	-	-	-		
92	OHX	1	4247	-	0,6,6	-	-	-		
92	OHX	2	2204	-	0,6,6	-	-	-		
92	OHX	3	225	92	0,6,6	-	-	-		
92	OHX	1	4186	92	0,6,6	-	-	-		
92	OHX	2	2188	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2139	-	0,6,6	-	-	-		
92	OHX	1	4330	92	0,6,6	-	-	-		
92	OHX	6	2287	-	0,6,6	-	-	-		
92	OHX	6	2253	-	0,6,6	-	-	-		
92	OHX	6	2290	1	0,6,6	-	-	-		
92	OHX	2	2105	-	0,6,6	-	-	-		
92	OHX	5	4302	-	0,6,6	-	-	-		
92	OHX	6	2228	-	0,6,6	-	-	-		
92	OHX	N8	208	-	0,6,6	-	-	-		
92	OHX	6	2321	-	0,6,6	-	-	-		
92	OHX	5	4458	36	0,6,6	-	-	-		
92	OHX	2	2132	-	0,6,6	-	-	-		
92	OHX	5	4464	92	0,6,6	-	-	-		
92	OHX	6	2277	-	0,6,6	-	-	-		
92	OHX	5	4178	-	0,6,6	-	-	-		
92	OHX	1	4234	-	0,6,6	-	-	-		
92	OHX	1	4129	-	0,6,6	-	-	-		
92	OHX	5	4191	-	0,6,6	-	-	-		
92	OHX	C8	203	92,36	0,6,6	-	-	-		
92	OHX	5	4558	92	0,6,6	-	-	-		
92	OHX	2	2084	-	0,6,6	-	-	-		
92	OHX	1	4292	92	0,6,6	-	-	-		
92	OHX	6	2244	-	0,6,6	-	-	-		
92	OHX	5	4350	-	0,6,6	-	-	-		
92	OHX	2	2181	1	0,6,6	-	-	-		
92	OHX	1	4456	-	0,6,6	-	-	-		
92	OHX	1	4287	92	0,6,6	-	-	-		
92	OHX	5	4321	-	0,6,6	-	-	-		
92	OHX	1	4122	-	0,6,6	-	-	-		
92	OHX	2	2141	92	0,6,6	-	-	-		
92	OHX	1	4243	-	0,6,6	-	-	-		
92	OHX	5	4157	-	0,6,6	-	-	-		
92	OHX	O7	109	92	0,6,6	-	-	-		
92	OHX	2	2167	-	0,6,6	-	-	-		
92	OHX	6	2165	-	0,6,6	-	-	-		
92	OHX	1	4343	-	0,6,6	-	-	-		
92	OHX	1	4490	92	0,6,6	-	-	-		
92	OHX	2	2233	-	0,6,6	-	-	-		
92	OHX	1	4113	-	0,6,6	-	-	-		
92	OHX	1	4498	-	0,6,6	-	-	-		
92	OHX	2	2165	-	0,6,6	-	-	-		
92	OHX	2	2219	-	0,6,6	-	-	-		
92	OHX	5	4172	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2152	-	0,6,6	-	-	-		
92	OHX	5	4333	92	0,6,6	-	-	-		
92	OHX	6	2248	-	0,6,6	-	-	-		
92	OHX	1	4182	-	0,6,6	-	-	-		
92	OHX	1	4312	-	0,6,6	-	-	-		
92	OHX	1	4482	92	0,6,6	-	-	-		
92	OHX	6	2153	-	0,6,6	-	-	-		
92	OHX	1	4194	92	0,6,6	-	-	-		
92	OHX	6	2158	-	0,6,6	-	-	-		
92	OHX	6	2289	-	0,6,6	-	-	-		
92	OHX	6	2280	-	0,6,6	-	-	-		
92	OHX	7	230	-	0,6,6	-	-	-		
92	OHX	1	4436	-	0,6,6	-	-	-		
92	OHX	1	4132	-	0,6,6	-	-	-		
92	OHX	M0	306	92	0,6,6	-	-	-		
92	OHX	2	2107	-	0,6,6	-	-	-		
92	OHX	5	4249	-	0,6,6	-	-	-		
92	OHX	5	4248	-	0,6,6	-	-	-		
92	OHX	1	4144	-	0,6,6	-	-	-		
92	OHX	5	4234	92	0,6,6	-	-	-		
92	OHX	4	245	-	0,6,6	-	-	-		
92	OHX	1	4266	92	0,6,6	-	-	-		
92	OHX	1	4193	-	0,6,6	-	-	-		
92	OHX	1	4399	92	0,6,6	-	-	-		
92	OHX	5	4292	92	0,6,6	-	-	-		
92	OHX	5	4477	-	0,6,6	-	-	-		
92	OHX	1	4395	92	0,6,6	-	-	-		
92	OHX	3	226	92	0,6,6	-	-	-		
92	OHX	2	2106	-	0,6,6	-	-	-		
92	OHX	5	4409	36	0,6,6	-	-	-		
92	OHX	1	4416	-	0,6,6	-	-	-		
92	OHX	5	4337	92	0,6,6	-	-	-		
92	OHX	2	2176	92	0,6,6	-	-	-		
92	OHX	5	4338	92	0,6,6	-	-	-		
92	OHX	1	4471	36	0,6,6	-	-	-		
92	OHX	5	4256	92	0,6,6	-	-	-		
92	OHX	8	230	-	0,6,6	-	-	-		
92	OHX	6	2283	92	0,6,6	-	-	-		
92	OHX	1	4201	-	0,6,6	-	-	-		
92	OHX	6	2186	-	0,6,6	-	-	-		
92	OHX	1	4504	92	0,6,6	-	-	-		
92	OHX	6	2204	1	0,6,6	-	-	-		
92	OHX	2	2134	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	3	219	-	0,6,6	-	-	-		
92	OHX	1	4151	-	0,6,6	-	-	-		
92	OHX	m4	202	-	0,6,6	-	-	-		
92	OHX	1	4295	92	0,6,6	-	-	-		
92	OHX	6	2180	92	0,6,6	-	-	-		
92	OHX	1	4238	92	0,6,6	-	-	-		
92	OHX	1	4484	92	0,6,6	-	-	-		
92	OHX	m7	208	-	0,6,6	-	-	-		
92	OHX	6	2223	92	0,6,6	-	-	-		
92	OHX	5	4326	-	0,6,6	-	-	-		
92	OHX	5	4195	-	0,6,6	-	-	-		
92	OHX	1	4448	-	0,6,6	-	-	-		
92	OHX	5	4516	-	0,6,6	-	-	-		
92	OHX	6	2279	-	0,6,6	-	-	-		
92	OHX	2	2194	92	0,6,6	-	-	-		
92	OHX	1	4362	-	0,6,6	-	-	-		
92	OHX	6	2275	-	0,6,6	-	-	-		
92	OHX	6	2299	92	0,6,6	-	-	-		
92	OHX	5	4385	92	0,6,6	-	-	-		
92	OHX	2	2196	1	0,6,6	-	-	-		
92	OHX	2	2229	-	0,6,6	-	-	-		
92	OHX	1	4426	-	0,6,6	-	-	-		
92	OHX	5	4259	92	0,6,6	-	-	-		
92	OHX	5	4320	92	0,6,6	-	-	-		
92	OHX	8	222	92	0,6,6	-	-	-		
92	OHX	1	4446	92,36	0,6,6	-	-	-		
92	OHX	1	4418	-	0,6,6	-	-	-		
92	OHX	5	4506	92	0,6,6	-	-	-		
92	OHX	2	2227	92	0,6,6	-	-	-		
92	OHX	7	240	-	0,6,6	-	-	-		
92	OHX	5	4158	-	0,6,6	-	-	-		
92	OHX	5	4456	-	0,6,6	-	-	-		
92	OHX	O3	204	-	0,6,6	-	-	-		
92	OHX	6	2200	-	0,6,6	-	-	-		
92	OHX	1	4461	-	0,6,6	-	-	-		
92	OHX	6	2232	-	0,6,6	-	-	-		
92	OHX	5	4383	92	0,6,6	-	-	-		
92	OHX	1	4277	-	0,6,6	-	-	-		
92	OHX	1	4171	92	0,6,6	-	-	-		
92	OHX	5	4413	92	0,6,6	-	-	-		
92	OHX	1	4248	-	0,6,6	-	-	-		
92	OHX	5	4201	92	0,6,6	-	-	-		
92	OHX	2	2193	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4387	-	0,6,6	-	-	-		
92	OHX	1	4250	-	0,6,6	-	-	-		
92	OHX	5	4238	-	0,6,6	-	-	-		
92	OHX	5	4484	92	0,6,6	-	-	-		
92	OHX	1	4501	92	0,6,6	-	-	-		
92	OHX	5	4556	92,36	0,6,6	-	-	-		
92	OHX	1	4136	-	0,6,6	-	-	-		
92	OHX	2	2085	-	0,6,6	-	-	-		
92	OHX	2	2074	92	0,6,6	-	-	-		
92	OHX	1	4145	-	0,6,6	-	-	-		
92	OHX	5	4198	-	0,6,6	-	-	-		
92	OHX	5	4497	-	0,6,6	-	-	-		
92	OHX	5	4324	92	0,6,6	-	-	-		
92	OHX	5	4297	-	0,6,6	-	-	-		
92	OHX	5	4380	-	0,6,6	-	-	-		
92	OHX	2	2156	92	0,6,6	-	-	-		
92	OHX	5	4445	-	0,6,6	-	-	-		
92	OHX	5	4564	92	0,6,6	-	-	-		
92	OHX	1	4310	-	0,6,6	-	-	-		
92	OHX	1	4438	-	0,6,6	-	-	-		
92	OHX	6	2291	1	0,6,6	-	-	-		
92	OHX	1	4207	-	0,6,6	-	-	-		
92	OHX	2	2136	-	0,6,6	-	-	-		
92	OHX	1	4281	92	0,6,6	-	-	-		
92	OHX	C3	201	-	0,6,6	-	-	-		
92	OHX	1	4156	92	0,6,6	-	-	-		
92	OHX	2	2122	92	0,6,6	-	-	-		
92	OHX	1	4107	-	0,6,6	-	-	-		
92	OHX	1	4100	-	0,6,6	-	-	-		
92	OHX	2	2100	-	0,6,6	-	-	-		
92	OHX	c5	201	-	0,6,6	-	-	-		
92	OHX	6	2338	92	0,6,6	-	-	-		
92	OHX	m0	302	92	0,6,6	-	-	-		
92	OHX	2	2245	92	0,6,6	-	-	-		
92	OHX	5	4461	-	0,6,6	-	-	-		
92	OHX	1	4160	-	0,6,6	-	-	-		
92	OHX	1	4375	-	0,6,6	-	-	-		
92	OHX	2	2164	-	0,6,6	-	-	-		
92	OHX	1	4492	92	0,6,6	-	-	-		
92	OHX	1	4116	92	0,6,6	-	-	-		
92	OHX	1	4216	-	0,6,6	-	-	-		
92	OHX	6	2266	1	0,6,6	-	-	-		
92	OHX	5	4282	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4177	-	0,6,6	-	-	-		
92	OHX	1	4369	92	0,6,6	-	-	-		
92	OHX	5	4304	-	0,6,6	-	-	-		
92	OHX	5	4185	-	0,6,6	-	-	-		
92	OHX	5	4334	92	0,6,6	-	-	-		
92	OHX	5	4483	92	0,6,6	-	-	-		
92	OHX	5	4205	-	0,6,6	-	-	-		
92	OHX	5	4434	-	0,6,6	-	-	-		
92	OHX	1	4142	-	0,6,6	-	-	-		
92	OHX	1	4432	-	0,6,6	-	-	-		
92	OHX	6	2301	-	0,6,6	-	-	-		
92	OHX	n1	204	-	0,6,6	-	-	-		
92	OHX	8	233	-	0,6,6	-	-	-		
92	OHX	1	4202	36	0,6,6	-	-	-		
92	OHX	5	4209	92	0,6,6	-	-	-		
92	OHX	1	4363	-	0,6,6	-	-	-		
92	OHX	5	4392	-	0,6,6	-	-	-		
92	OHX	1	4366	-	0,6,6	-	-	-		
92	OHX	2	2086	92	0,6,6	-	-	-		
92	OHX	1	4434	-	0,6,6	-	-	-		
92	OHX	1	4488	-	0,6,6	-	-	-		
92	OHX	5	4407	-	0,6,6	-	-	-		
92	OHX	4	240	-	0,6,6	-	-	-		
92	OHX	s1	302	-	0,6,6	-	-	-		
92	OHX	1	4114	-	0,6,6	-	-	-		
92	OHX	1	4260	-	0,6,6	-	-	-		
92	OHX	2	2252	92	0,6,6	-	-	-		
92	OHX	6	2143	-	0,6,6	-	-	-		
92	OHX	8	234	38	0,6,6	-	-	-		
92	OHX	o9	102	-	0,6,6	-	-	-		
92	OHX	2	2246	-	0,6,6	-	-	-		
92	OHX	1	4244	-	0,6,6	-	-	-		
92	OHX	6	2209	-	0,6,6	-	-	-		
92	OHX	2	2113	92	0,6,6	-	-	-		
92	OHX	5	4446	-	0,6,6	-	-	-		
92	OHX	1	4500	92,36	0,6,6	-	-	-		
92	OHX	2	2128	-	0,6,6	-	-	-		
92	OHX	5	4507	-	0,6,6	-	-	-		
92	OHX	1	4415	-	0,6,6	-	-	-		
92	OHX	5	4298	-	0,6,6	-	-	-		
92	OHX	1	4254	-	0,6,6	-	-	-		
92	OHX	5	4275	92	0,6,6	-	-	-		
92	OHX	6	2149	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2203	-	0,6,6	-	-	-		
92	OHX	5	4551	92	0,6,6	-	-	-		
92	OHX	6	2242	92	0,6,6	-	-	-		
92	OHX	2	2082	-	0,6,6	-	-	-		
92	OHX	1	4379	92	0,6,6	-	-	-		
92	OHX	5	4202	-	0,6,6	-	-	-		
92	OHX	6	2311	92	0,6,6	-	-	-		
92	OHX	Q2	505	-	0,6,6	-	-	-		
92	OHX	5	4347	36	0,6,6	-	-	-		
92	OHX	5	4468	-	0,6,6	-	-	-		
92	OHX	5	4504	-	0,6,6	-	-	-		
92	OHX	1	4479	92	0,6,6	-	-	-		
92	OHX	5	4488	-	0,6,6	-	-	-		
92	OHX	5	4390	-	0,6,6	-	-	-		
92	OHX	5	4519	-	0,6,6	-	-	-		
92	OHX	1	4402	-	0,6,6	-	-	-		
92	OHX	2	2185	-	0,6,6	-	-	-		
92	OHX	1	4493	-	0,6,6	-	-	-		
92	OHX	sR	401	-	0,6,6	-	-	-		
92	OHX	6	2156	-	0,6,6	-	-	-		
92	OHX	5	4244	-	0,6,6	-	-	-		
92	OHX	1	4251	92	0,6,6	-	-	-		
92	OHX	1	4319	92	0,6,6	-	-	-		
92	OHX	5	4481	92	0,6,6	-	-	-		
92	OHX	6	2319	-	0,6,6	-	-	-		
92	OHX	5	4176	-	0,6,6	-	-	-		
92	OHX	5	4269	92	0,6,6	-	-	-		
92	OHX	6	2327	-	0,6,6	-	-	-		
92	OHX	5	4168	-	0,6,6	-	-	-		
92	OHX	5	4190	-	0,6,6	-	-	-		
92	OHX	5	4442	-	0,6,6	-	-	-		
92	OHX	6	2188	-	0,6,6	-	-	-		
92	OHX	1	4346	-	0,6,6	-	-	-		
92	OHX	1	4398	-	0,6,6	-	-	-		
92	OHX	2	2117	-	0,6,6	-	-	-		
92	OHX	1	4401	92	0,6,6	-	-	-		
92	OHX	5	4184	-	0,6,6	-	-	-		
92	OHX	1	4439	92	0,6,6	-	-	-		
92	OHX	1	4485	-	0,6,6	-	-	-		
92	OHX	5	4364	-	0,6,6	-	-	-		
92	OHX	6	2337	92,1	0,6,6	-	-	-		
92	OHX	1	4437	92	0,6,6	-	-	-		
92	OHX	5	4433	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2181	92	0,6,6	-	-	-		
92	OHX	2	2160	-	0,6,6	-	-	-		
92	OHX	1	4427	36	0,6,6	-	-	-		
92	OHX	1	4480	-	0,6,6	-	-	-		
92	OHX	6	2247	-	0,6,6	-	-	-		
92	OHX	5	4173	-	0,6,6	-	-	-		
92	OHX	1	4191	-	0,6,6	-	-	-		
92	OHX	5	4509	92	0,6,6	-	-	-		
92	OHX	1	4274	-	0,6,6	-	-	-		
92	OHX	2	2089	92	0,6,6	-	-	-		
92	OHX	1	4228	92	0,6,6	-	-	-		
92	OHX	1	4300	-	0,6,6	-	-	-		
92	OHX	5	4455	-	0,6,6	-	-	-		
92	OHX	2	2115	-	0,6,6	-	-	-		
92	OHX	1	4290	-	0,6,6	-	-	-		
92	OHX	1	4463	-	0,6,6	-	-	-		
92	OHX	5	4235	-	0,6,6	-	-	-		
92	OHX	5	4189	-	0,6,6	-	-	-		
92	OHX	1	4285	-	0,6,6	-	-	-		
92	OHX	6	2254	-	0,6,6	-	-	-		
92	OHX	5	4423	92,36	0,6,6	-	-	-		
92	OHX	5	4430	-	0,6,6	-	-	-		
92	OHX	1	4276	-	0,6,6	-	-	-		
92	OHX	5	4247	-	0,6,6	-	-	-		
92	OHX	5	4346	92	0,6,6	-	-	-		
92	OHX	8	221	-	0,6,6	-	-	-		
92	OHX	6	2257	-	0,6,6	-	-	-		
92	OHX	1	4487	92	0,6,6	-	-	-		
92	OHX	2	2212	-	0,6,6	-	-	-		
92	OHX	2	2135	-	0,6,6	-	-	-		
92	OHX	2	2247	92	0,6,6	-	-	-		
92	OHX	2	2243	92,1	0,6,6	-	-	-		
92	OHX	1	4477	-	0,6,6	-	-	-		
92	OHX	3	221	-	0,6,6	-	-	-		
92	OHX	1	4305	92	0,6,6	-	-	-		
92	OHX	6	2187	-	0,6,6	-	-	-		
92	OHX	5	4353	-	0,6,6	-	-	-		
92	OHX	5	4521	36	0,6,6	-	-	-		
92	OHX	6	2183	-	0,6,6	-	-	-		
92	OHX	1	4314	-	0,6,6	-	-	-		
92	OHX	2	2226	-	0,6,6	-	-	-		
92	OHX	2	2147	92	0,6,6	-	-	-		
92	OHX	5	4498	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2232	92	0,6,6	-	-	-		
92	OHX	2	2242	-	0,6,6	-	-	-		
92	OHX	1	4473	92	0,6,6	-	-	-		
92	OHX	6	2164	-	0,6,6	-	-	-		
92	OHX	1	4322	-	0,6,6	-	-	-		
92	OHX	1	4329	-	0,6,6	-	-	-		
92	OHX	1	4381	92,36	0,6,6	-	-	-		
92	OHX	1	4453	92	0,6,6	-	-	-		
92	OHX	L5	301	-	0,6,6	-	-	-		
92	OHX	5	4196	-	0,6,6	-	-	-		
92	OHX	2	2130	-	0,6,6	-	-	-		
92	OHX	5	4366	-	0,6,6	-	-	-		
92	OHX	1	4215	-	0,6,6	-	-	-		
92	OHX	6	2273	-	0,6,6	-	-	-		
92	OHX	1	4422	-	0,6,6	-	-	-		
92	OHX	1	4338	92	0,6,6	-	-	-		
92	OHX	5	4420	-	0,6,6	-	-	-		
92	OHX	6	2326	1	0,6,6	-	-	-		
92	OHX	5	4159	-	0,6,6	-	-	-		
92	OHX	7	233	-	0,6,6	-	-	-		
92	OHX	5	4309	-	0,6,6	-	-	-		
92	OHX	6	2151	-	0,6,6	-	-	-		
92	OHX	2	2214	1	0,6,6	-	-	-		
92	OHX	2	2070	-	0,6,6	-	-	-		
92	OHX	5	4482	92	0,6,6	-	-	-		
92	OHX	1	4389	92	0,6,6	-	-	-		
92	OHX	8	223	-	0,6,6	-	-	-		
92	OHX	1	4154	-	0,6,6	-	-	-		
92	OHX	5	4236	-	0,6,6	-	-	-		
92	OHX	1	4131	92	0,6,6	-	-	-		
92	OHX	O7	107	-	0,6,6	-	-	-		
92	OHX	1	4336	-	0,6,6	-	-	-		
92	OHX	2	2182	-	0,6,6	-	-	-		
92	OHX	1	4382	-	0,6,6	-	-	-		
92	OHX	5	4469	-	0,6,6	-	-	-		
92	OHX	5	4241	-	0,6,6	-	-	-		
92	OHX	5	4399	36	0,6,6	-	-	-		
92	OHX	6	2162	92	0,6,6	-	-	-		
92	OHX	5	4322	-	0,6,6	-	-	-		
92	OHX	6	2238	-	0,6,6	-	-	-		
92	OHX	5	4329	-	0,6,6	-	-	-		
92	OHX	2	2203	92	0,6,6	-	-	-		
92	OHX	1	4152	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	m5	304	-	0,6,6	-	-	-		
92	OHX	2	2217	-	0,6,6	-	-	-		
92	OHX	1	4177	-	0,6,6	-	-	-		
92	OHX	6	2160	-	0,6,6	-	-	-		
92	OHX	1	4141	-	0,6,6	-	-	-		
92	OHX	5	4165	-	0,6,6	-	-	-		
92	OHX	5	4287	-	0,6,6	-	-	-		
92	OHX	1	4332	-	0,6,6	-	-	-		
92	OHX	1	4468	92	0,6,6	-	-	-		
92	OHX	5	4246	-	0,6,6	-	-	-		
92	OHX	5	4327	-	0,6,6	-	-	-		
92	OHX	5	4422	92	0,6,6	-	-	-		
92	OHX	8	240	-	0,6,6	-	-	-		
92	OHX	2	2250	-	0,6,6	-	-	-		
92	OHX	6	2214	92	0,6,6	-	-	-		
92	OHX	a	101	92,90	0,6,6	-	-	-		
92	OHX	1	4181	92	0,6,6	-	-	-		
92	OHX	2	2174	-	0,6,6	-	-	-		
92	OHX	5	4426	-	0,6,6	-	-	-		
92	OHX	5	4525	-	0,6,6	-	-	-		
92	OHX	5	4217	-	0,6,6	-	-	-		
92	OHX	1	4268	-	0,6,6	-	-	-		
92	OHX	5	4361	-	0,6,6	-	-	-		
92	OHX	2	2251	92	0,6,6	-	-	-		
92	OHX	6	2333	92	0,6,6	-	-	-		
92	OHX	5	4194	-	0,6,6	-	-	-		
92	OHX	5	4263	-	0,6,6	-	-	-		
92	OHX	1	4396	-	0,6,6	-	-	-		
92	OHX	5	4550	-	0,6,6	-	-	-		
92	OHX	6	2303	-	0,6,6	-	-	-		
92	OHX	2	2198	92	0,6,6	-	-	-		
92	OHX	5	4414	-	0,6,6	-	-	-		
92	OHX	5	4473	-	0,6,6	-	-	-		
92	OHX	4	236	-	0,6,6	-	-	-		
92	OHX	1	4320	36	0,6,6	-	-	-		
92	OHX	6	2167	-	0,6,6	-	-	-		
92	OHX	1	4124	92	0,6,6	-	-	-		
92	OHX	2	2072	-	0,6,6	-	-	-		
92	OHX	6	2219	-	0,6,6	-	-	-		
92	OHX	6	2221	1	0,6,6	-	-	-		
92	OHX	2	2172	-	0,6,6	-	-	-		
92	OHX	1	4466	92	0,6,6	-	-	-		
92	OHX	5	4272	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2189	1	0,6,6	-	-	-		
92	OHX	1	4232	36	0,6,6	-	-	-		
92	OHX	15	310	-	0,6,6	-	-	-		
92	OHX	1	4503	92	0,6,6	-	-	-		
92	OHX	1	4386	92	0,6,6	-	-	-		
92	OHX	5	4522	92	0,6,6	-	-	-		
92	OHX	1	4443	-	0,6,6	-	-	-		
92	OHX	1	4294	-	0,6,6	-	-	-		
92	OHX	1	4356	-	0,6,6	-	-	-		
92	OHX	5	4438	-	0,6,6	-	-	-		
92	OHX	2	2120	1	0,6,6	-	-	-		
92	OHX	6	2193	1	0,6,6	-	-	-		
92	OHX	5	4472	-	0,6,6	-	-	-		
92	OHX	5	4295	92	0,6,6	-	-	-		
92	OHX	1	4323	-	0,6,6	-	-	-		
92	OHX	1	4358	-	0,6,6	-	-	-		
92	OHX	6	2252	-	0,6,6	-	-	-		
92	OHX	2	2171	1	0,6,6	-	-	-		
92	OHX	1	4253	92	0,6,6	-	-	-		
92	OHX	5	4375	-	0,6,6	-	-	-		
92	OHX	1	4206	92	0,6,6	-	-	-		
92	OHX	2	2225	-	0,6,6	-	-	-		
92	OHX	1	4269	-	0,6,6	-	-	-		
92	OHX	2	2096	-	0,6,6	-	-	-		
92	OHX	5	4170	-	0,6,6	-	-	-		
92	OHX	5	4424	-	0,6,6	-	-	-		
92	OHX	2	2175	-	0,6,6	-	-	-		
92	OHX	5	4535	-	0,6,6	-	-	-		
92	OHX	15	309	-	0,6,6	-	-	-		
92	OHX	5	4523	92	0,6,6	-	-	-		
92	OHX	5	4160	-	0,6,6	-	-	-		
92	OHX	1	4502	92	0,6,6	-	-	-		
92	OHX	1	4318	-	0,6,6	-	-	-		
92	OHX	7	239	-	0,6,6	-	-	-		
92	OHX	1	4470	-	0,6,6	-	-	-		
92	OHX	1	4335	-	0,6,6	-	-	-		
92	OHX	5	4313	-	0,6,6	-	-	-		
92	OHX	1	4464	-	0,6,6	-	-	-		
92	OHX	6	2272	92,1	0,6,6	-	-	-		
92	OHX	1	4421	92	0,6,6	-	-	-		
92	OHX	5	4232	-	0,6,6	-	-	-		
92	OHX	1	4138	-	0,6,6	-	-	-		
92	OHX	1	4303	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2256	1	0,6,6	-	-	-		
92	OHX	5	4491	-	0,6,6	-	-	-		
92	OHX	4	239	-	0,6,6	-	-	-		
92	OHX	2	2239	-	0,6,6	-	-	-		
92	OHX	1	4435	92	0,6,6	-	-	-		
92	OHX	6	2237	-	0,6,6	-	-	-		
92	OHX	m0	303	92	0,6,6	-	-	-		
92	OHX	5	4171	-	0,6,6	-	-	-		
92	OHX	1	4257	-	0,6,6	-	-	-		
92	OHX	5	4166	-	0,6,6	-	-	-		
92	OHX	M5	309	-	0,6,6	-	-	-		
92	OHX	2	2118	-	0,6,6	-	-	-		
92	OHX	1	4408	92	0,6,6	-	-	-		
92	OHX	6	2250	92	0,6,6	-	-	-		
92	OHX	1	4164	36	0,6,6	-	-	-		
92	OHX	6	2174	-	0,6,6	-	-	-		
92	OHX	1	4169	92	0,6,6	-	-	-		
92	OHX	1	4130	92	0,6,6	-	-	-		
92	OHX	7	238	92	0,6,6	-	-	-		
92	OHX	5	4162	-	0,6,6	-	-	-		
92	OHX	1	4236	-	0,6,6	-	-	-		
92	OHX	6	2212	-	0,6,6	-	-	-		
92	OHX	6	2251	-	0,6,6	-	-	-		
92	OHX	5	4404	92	0,6,6	-	-	-		
92	OHX	2	2095	-	0,6,6	-	-	-		
92	OHX	6	2207	92	0,6,6	-	-	-		
92	OHX	1	4286	92	0,6,6	-	-	-		
92	OHX	o2	204	-	0,6,6	-	-	-		
92	OHX	5	4486	92	0,6,6	-	-	-		
92	OHX	8	239	92	0,6,6	-	-	-		
92	OHX	5	4204	-	0,6,6	-	-	-		
92	OHX	5	4379	-	0,6,6	-	-	-		
92	OHX	14	405	-	0,6,6	-	-	-		
92	OHX	2	2213	-	0,6,6	-	-	-		
92	OHX	S8	303	-	0,6,6	-	-	-		
92	OHX	5	4441	-	0,6,6	-	-	-		
92	OHX	5	4156	-	0,6,6	-	-	-		
92	OHX	2	2154	-	0,6,6	-	-	-		
92	OHX	1	4271	-	0,6,6	-	-	-		
92	OHX	6	2300	-	0,6,6	-	-	-		
92	OHX	1	4403	-	0,6,6	-	-	-		
92	OHX	1	4447	-	0,6,6	-	-	-		
92	OHX	4	246	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2206	-	0,6,6	-	-	-		
92	OHX	6	2222	-	0,6,6	-	-	-		
92	OHX	6	2263	-	0,6,6	-	-	-		
92	OHX	6	2308	92	0,6,6	-	-	-		
92	OHX	5	4449	92	0,6,6	-	-	-		
92	OHX	6	2245	92	0,6,6	-	-	-		
92	OHX	6	2259	-	0,6,6	-	-	-		
92	OHX	1	4355	92,36	0,6,6	-	-	-		
92	OHX	5	4470	-	0,6,6	-	-	-		
92	OHX	6	2217	-	0,6,6	-	-	-		
92	OHX	6	2225	-	0,6,6	-	-	-		
92	OHX	2	2231	-	0,6,6	-	-	-		
92	OHX	5	4567	92	0,6,6	-	-	-		
92	OHX	o3	206	-	0,6,6	-	-	-		
92	OHX	2	2078	-	0,6,6	-	-	-		
92	OHX	6	2175	-	0,6,6	-	-	-		
92	OHX	2	2163	-	0,6,6	-	-	-		
92	OHX	5	4401	92	0,6,6	-	-	-		
92	OHX	1	4192	-	0,6,6	-	-	-		
92	OHX	2	2080	-	0,6,6	-	-	-		
92	OHX	5	4273	-	0,6,6	-	-	-		
92	OHX	2	2121	-	0,6,6	-	-	-		
92	OHX	6	2335	92	0,6,6	-	-	-		
92	OHX	5	4405	-	0,6,6	-	-	-		
92	OHX	2	2079	-	0,6,6	-	-	-		
92	OHX	6	2185	-	0,6,6	-	-	-		
92	OHX	5	4266	92	0,6,6	-	-	-		
92	OHX	2	2179	-	0,6,6	-	-	-		
92	OHX	6	2190	92,1	0,6,6	-	-	-		
92	OHX	6	2331	92	0,6,6	-	-	-		
92	OHX	6	2150	1	0,6,6	-	-	-		
92	OHX	5	4393	-	0,6,6	-	-	-		
92	OHX	1	4365	-	0,6,6	-	-	-		
92	OHX	1	4460	-	0,6,6	-	-	-		
92	OHX	5	4512	-	0,6,6	-	-	-		
92	OHX	4	238	-	0,6,6	-	-	-		
92	OHX	A	102	92,90	0,6,6	-	-	-		
92	OHX	5	4199	92	0,6,6	-	-	-		
92	OHX	5	4553	92,36	0,6,6	-	-	-		
92	OHX	1	4413	92	0,6,6	-	-	-		
92	OHX	2	2123	-	0,6,6	-	-	-		
92	OHX	5	4505	36	0,6,6	-	-	-		
92	OHX	1	4406	92	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4279	92	0,6,6	-	-	-		
92	OHX	2	2241	92	0,6,6	-	-	-		
92	OHX	1	4221	-	0,6,6	-	-	-		
92	OHX	5	4463	-	0,6,6	-	-	-		
92	OHX	8	228	-	0,6,6	-	-	-		
92	OHX	5	4355	-	0,6,6	-	-	-		
92	OHX	6	2317	-	0,6,6	-	-	-		
92	OHX	5	4315	92	0,6,6	-	-	-		
92	OHX	6	2220	-	0,6,6	-	-	-		
92	OHX	2	2201	-	0,6,6	-	-	-		
92	OHX	5	4299	36	0,6,6	-	-	-		
92	OHX	s4	302	-	0,6,6	-	-	-		
92	OHX	5	4192	-	0,6,6	-	-	-		
92	OHX	5	4496	36	0,6,6	-	-	-		
92	OHX	n9	103	-	0,6,6	-	-	-		
92	OHX	5	4394	92	0,6,6	-	-	-		
92	OHX	6	2260	-	0,6,6	-	-	-		
92	OHX	8	231	92	0,6,6	-	-	-		
92	OHX	1	4118	-	0,6,6	-	-	-		
92	OHX	5	4179	-	0,6,6	-	-	-		
92	OHX	2	2081	-	0,6,6	-	-	-		
92	OHX	1	4111	-	0,6,6	-	-	-		
92	OHX	8	238	-	0,6,6	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

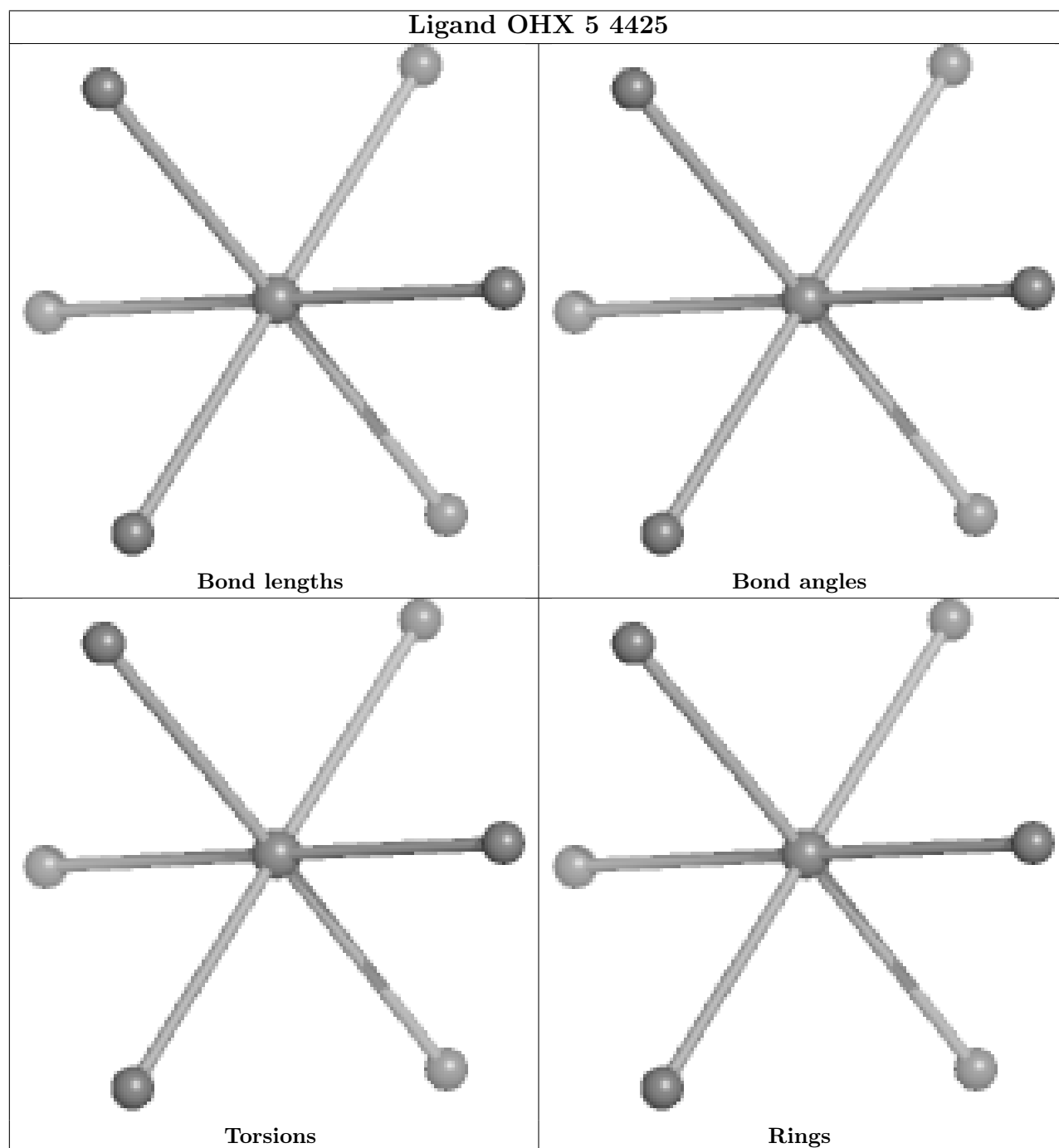
There are no ring outliers.

1 monomer is involved in 1 short contact:

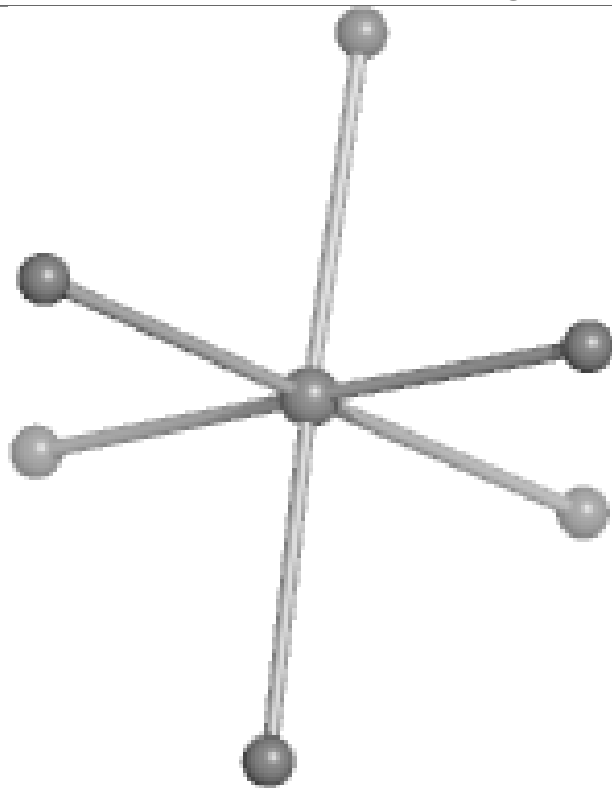
Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	l9	204	OHX	0	1

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

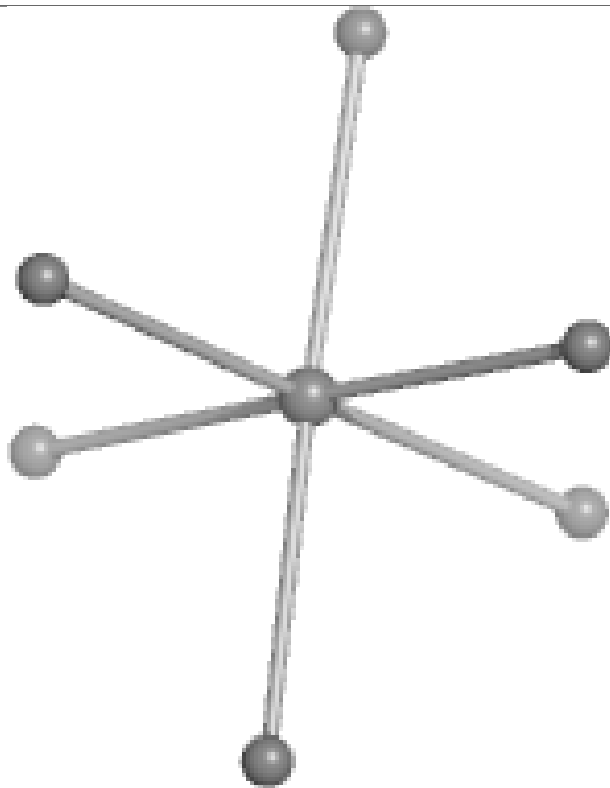
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



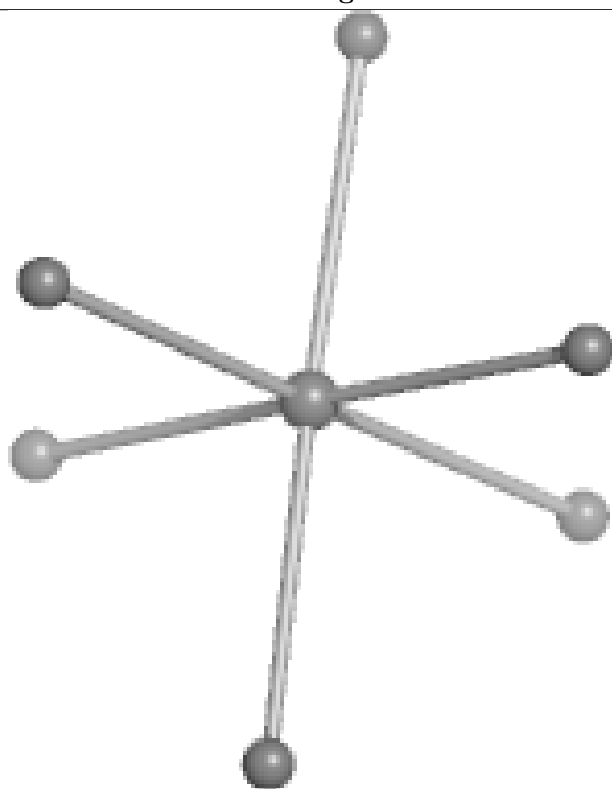
Ligand OHX 5 4533



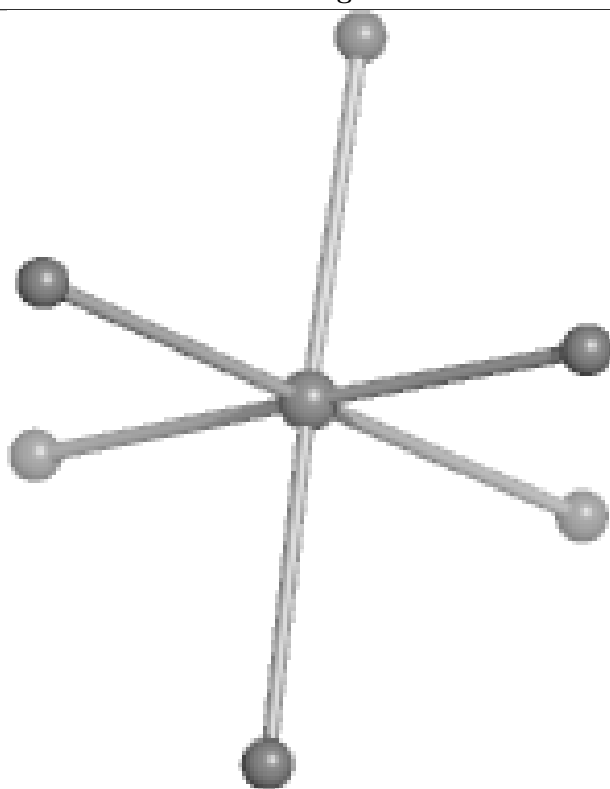
Bond lengths



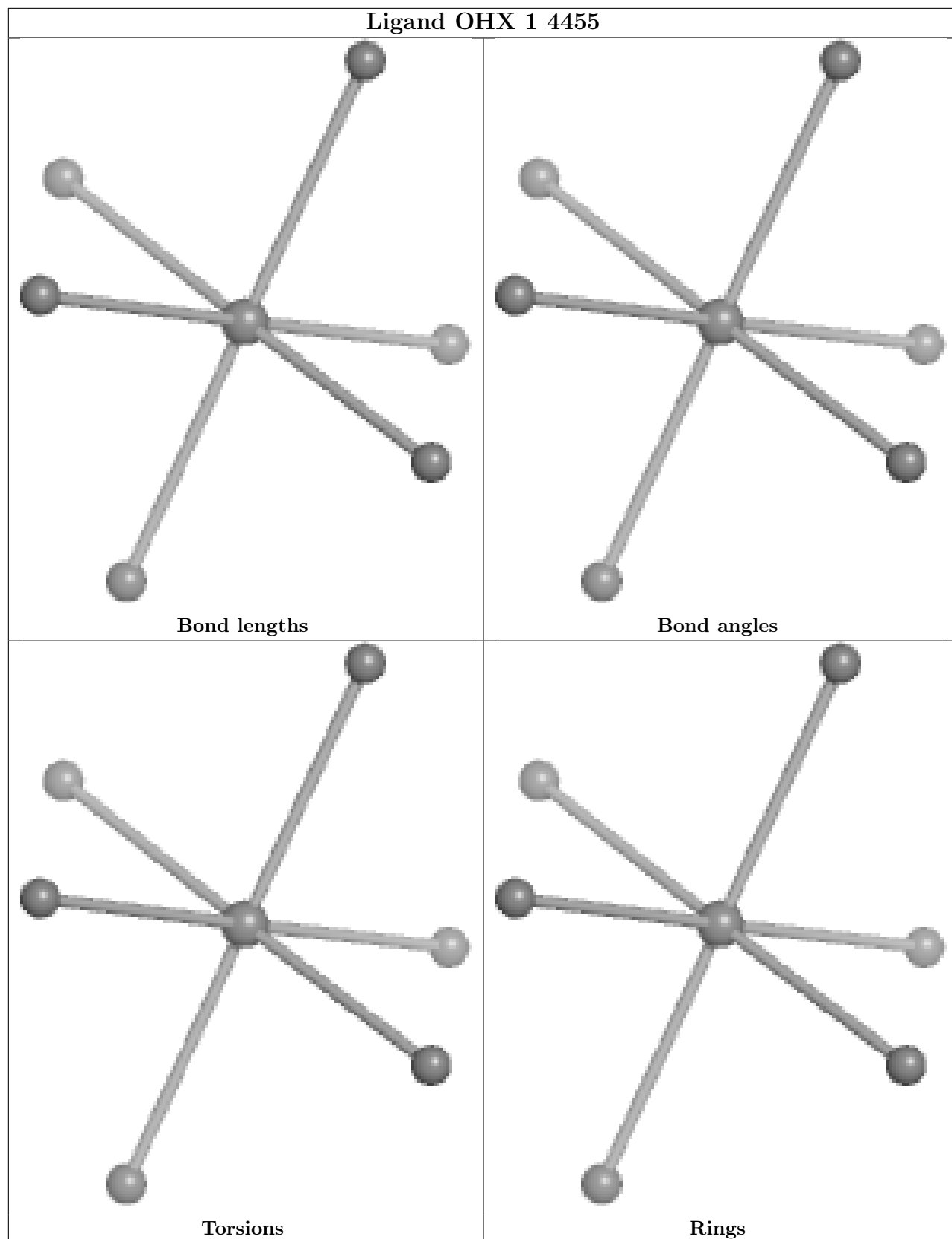
Bond angles

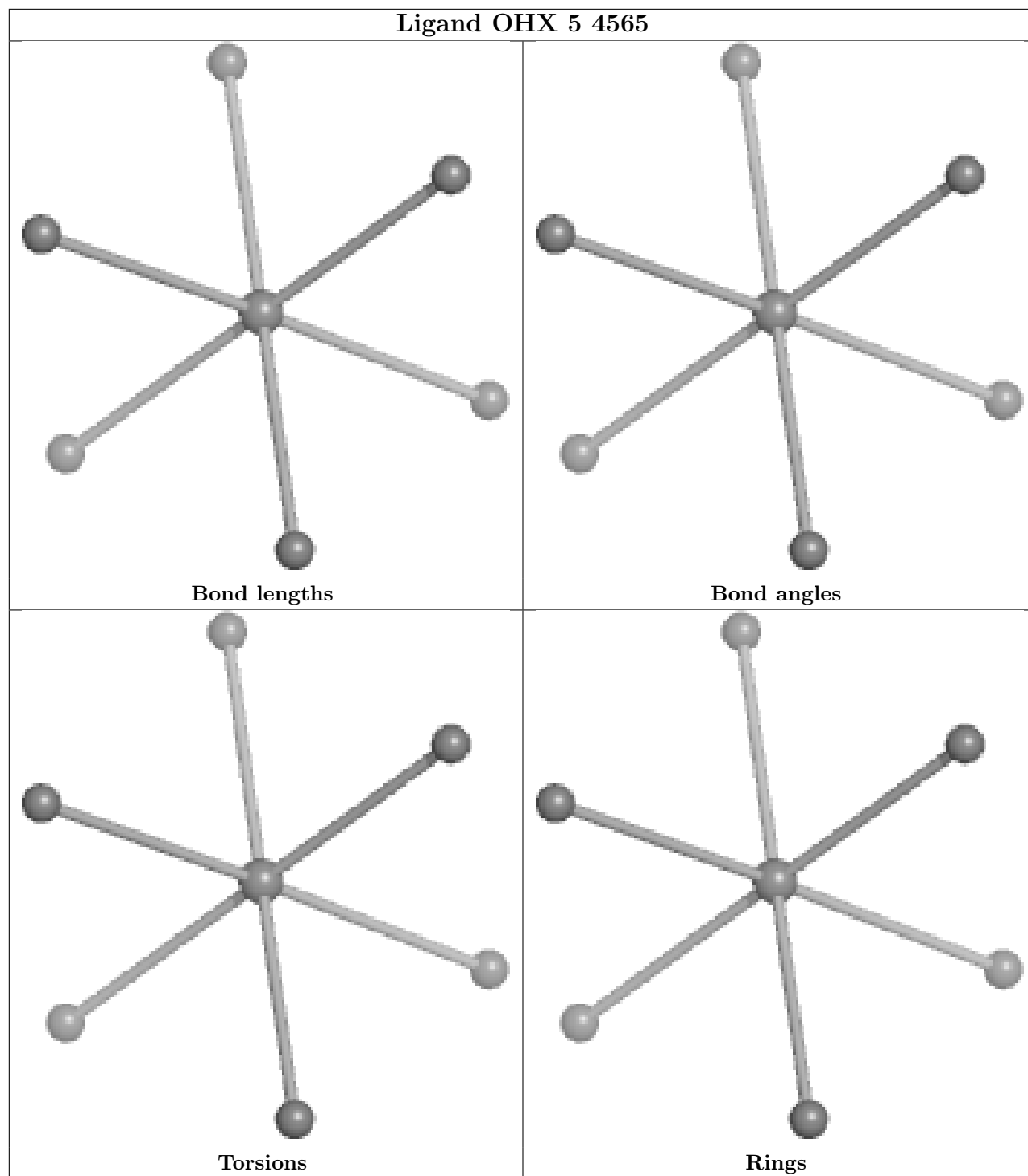


Torsions

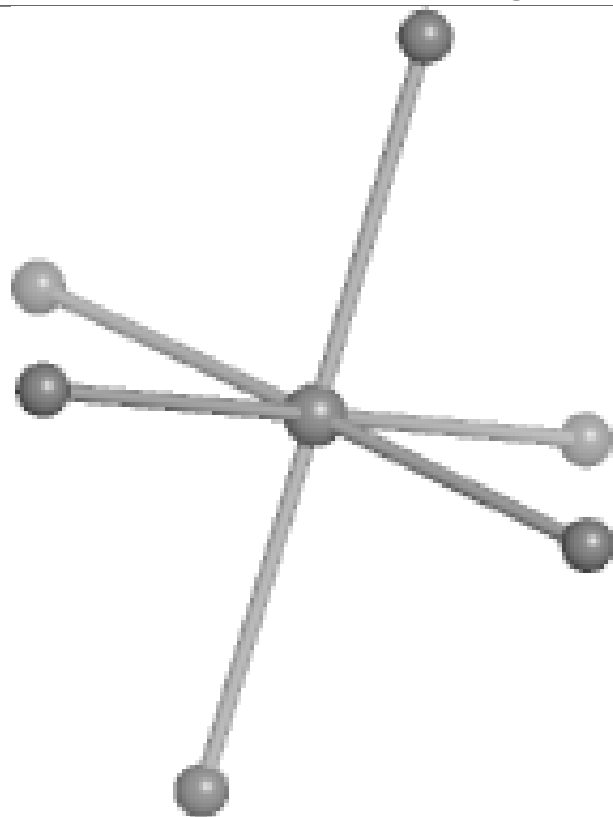


Rings

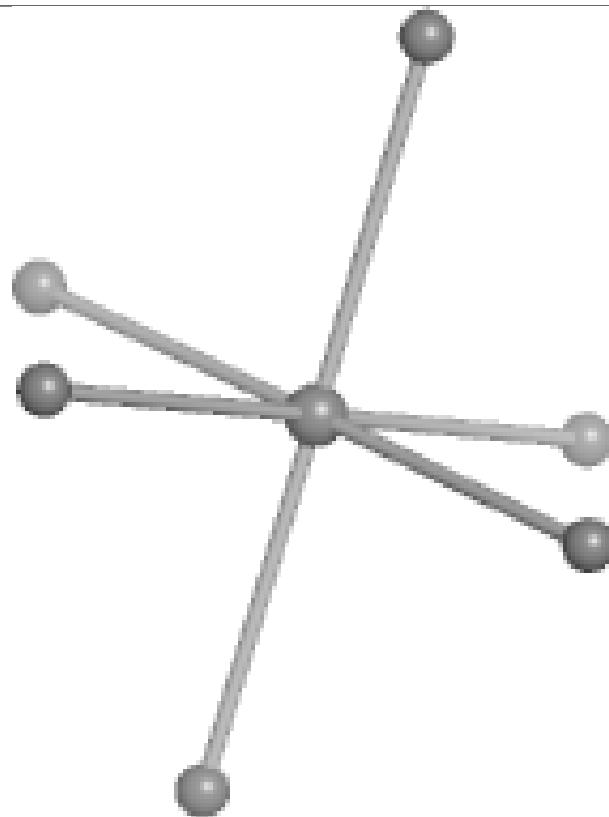




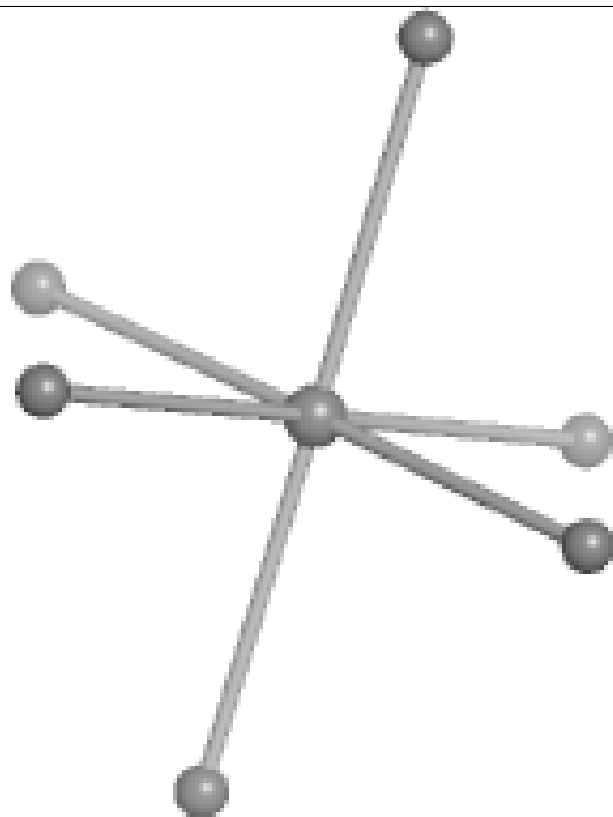
Ligand OHX 1 4465



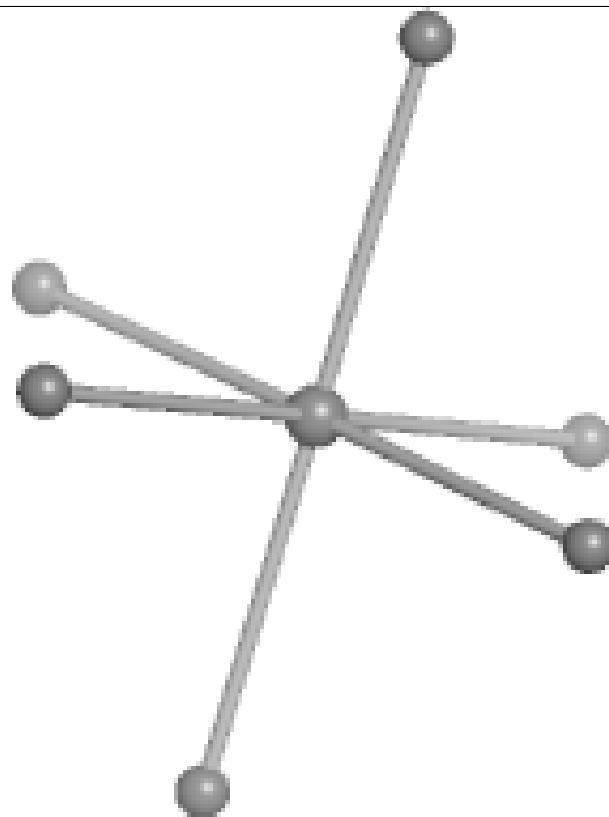
Bond lengths



Bond angles

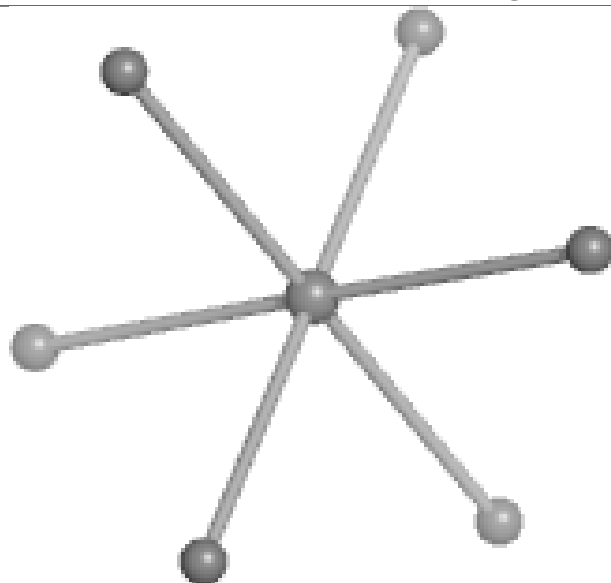


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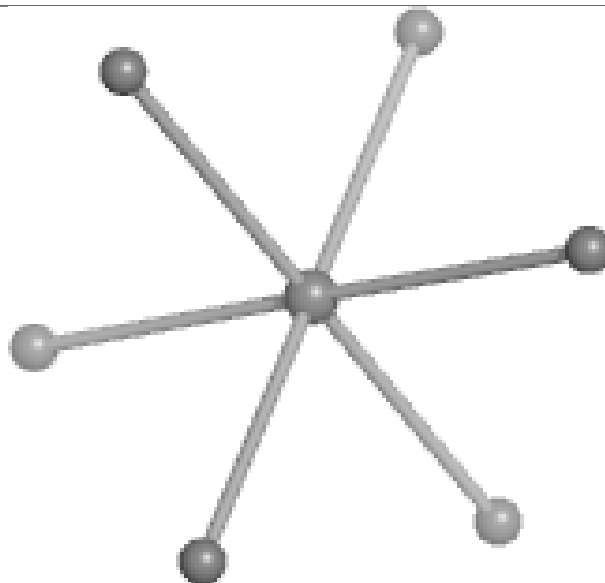


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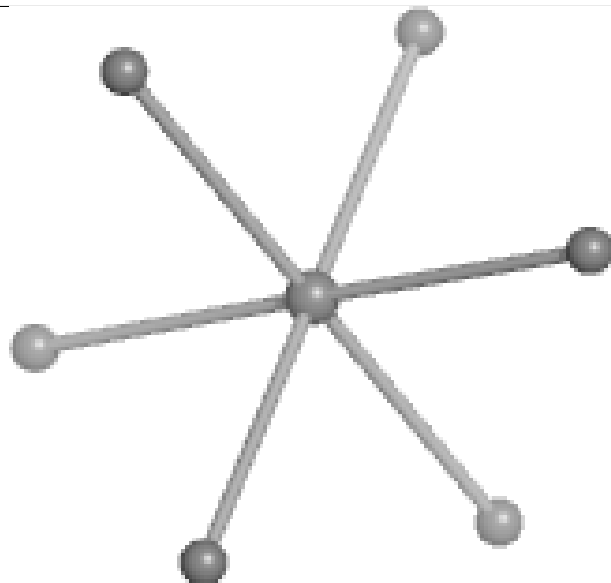
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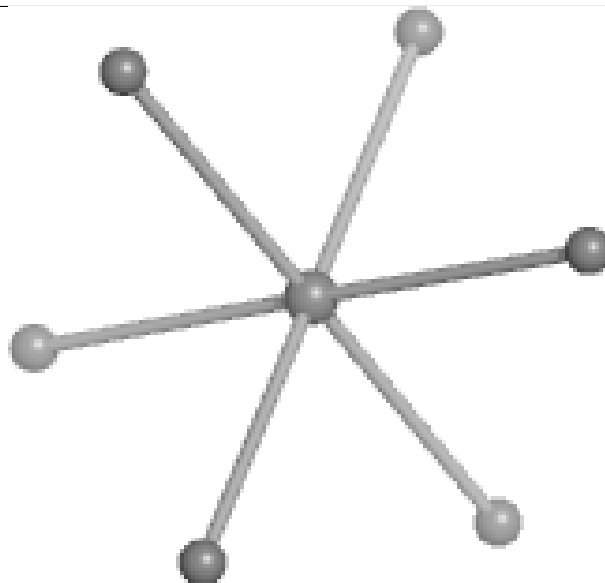
Bond lengths



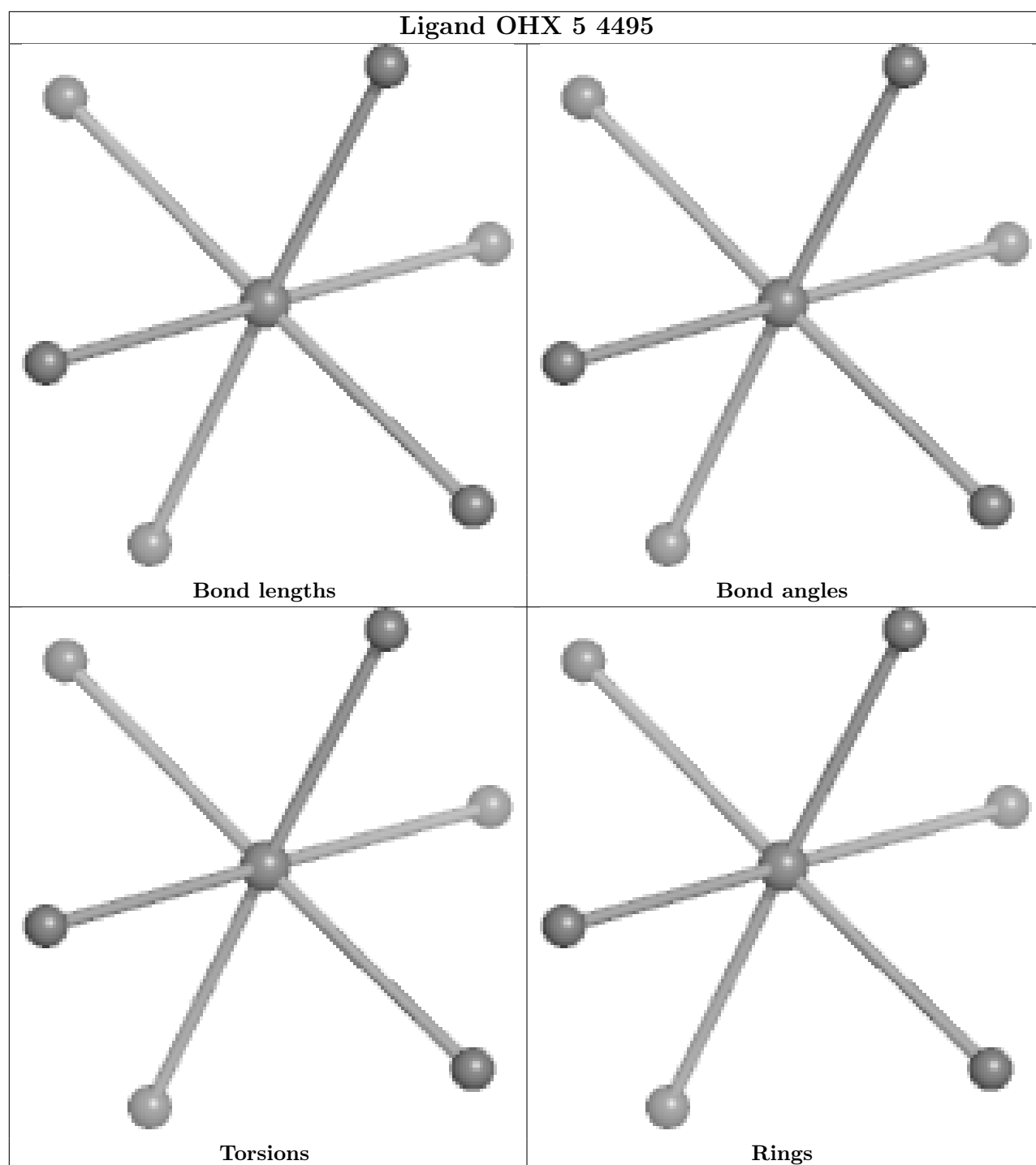
Bond angles



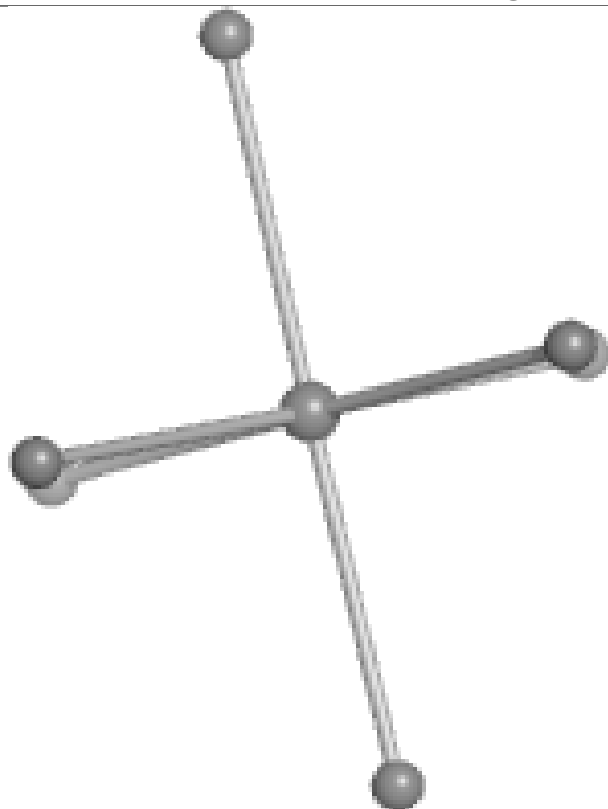
Torsions



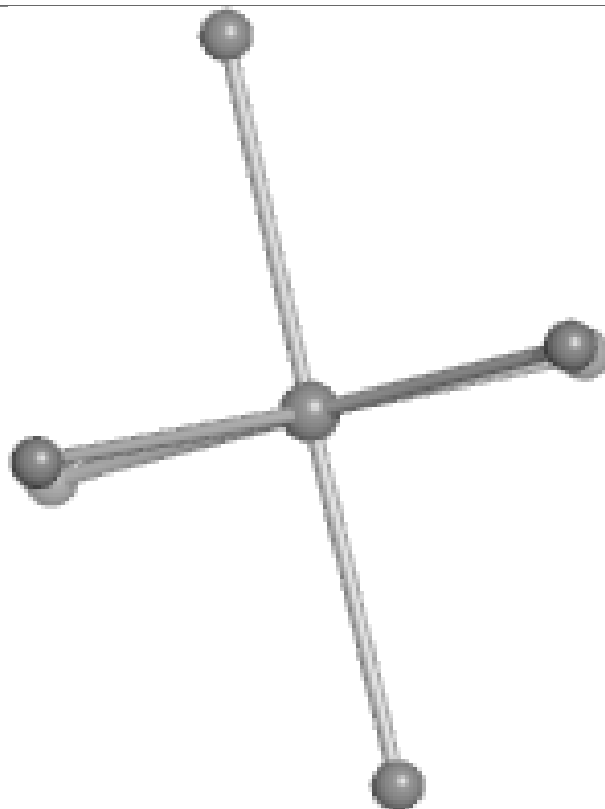
Rings



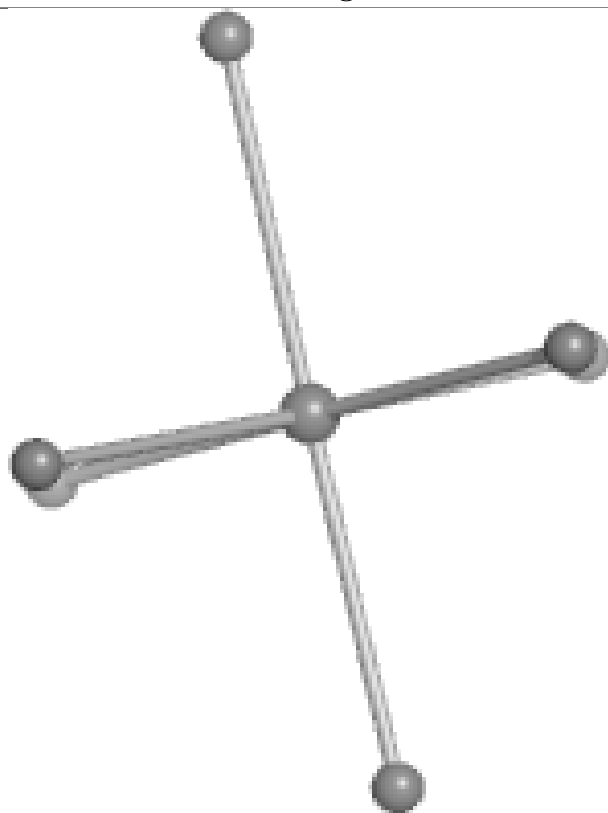
Ligand OHX 5 4391



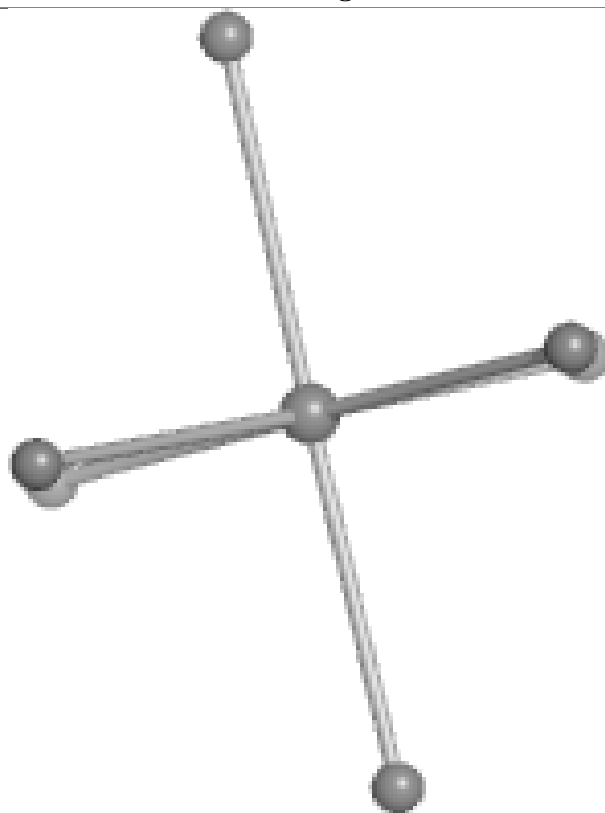
Bond lengths



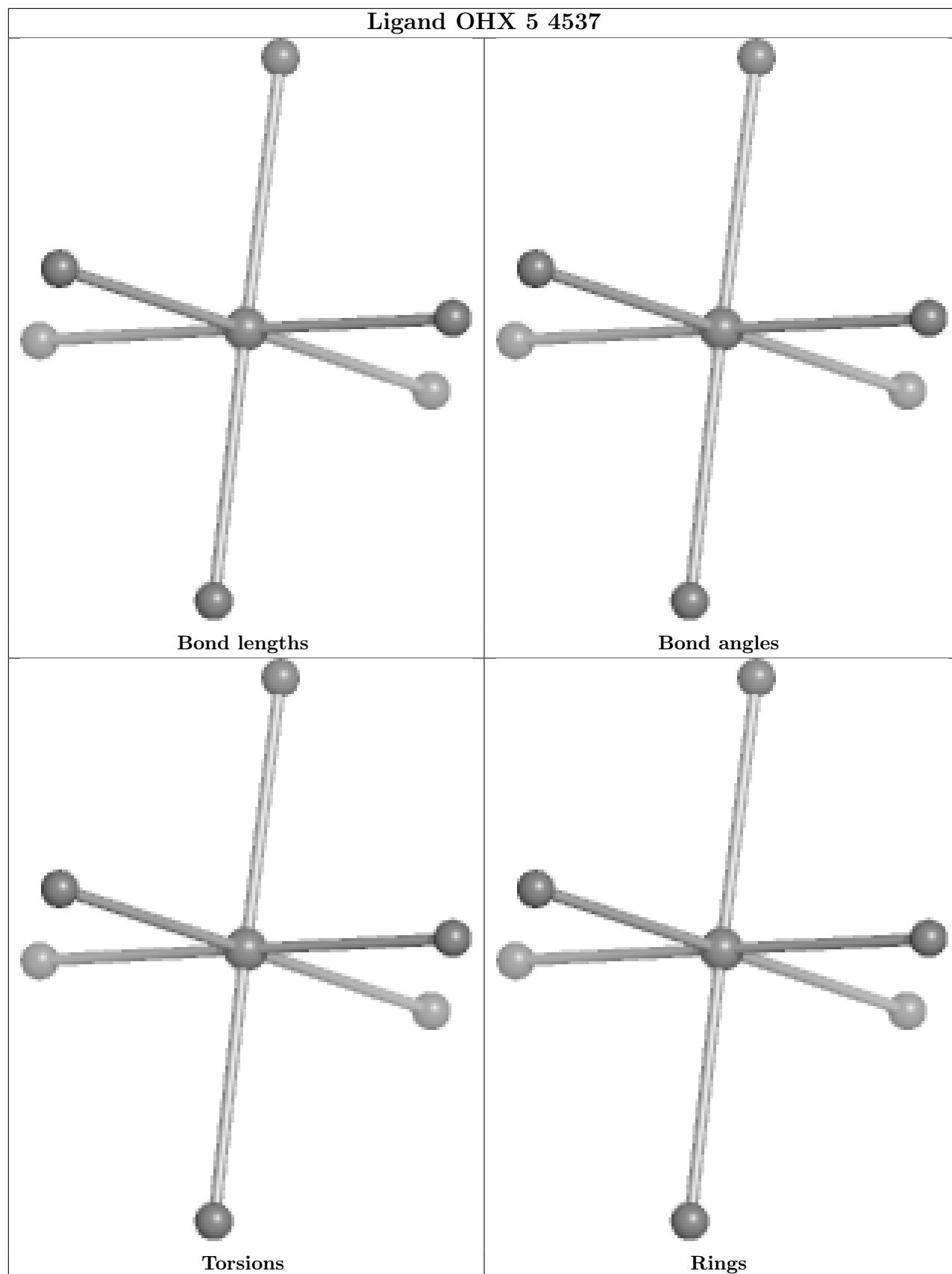
Bond angles

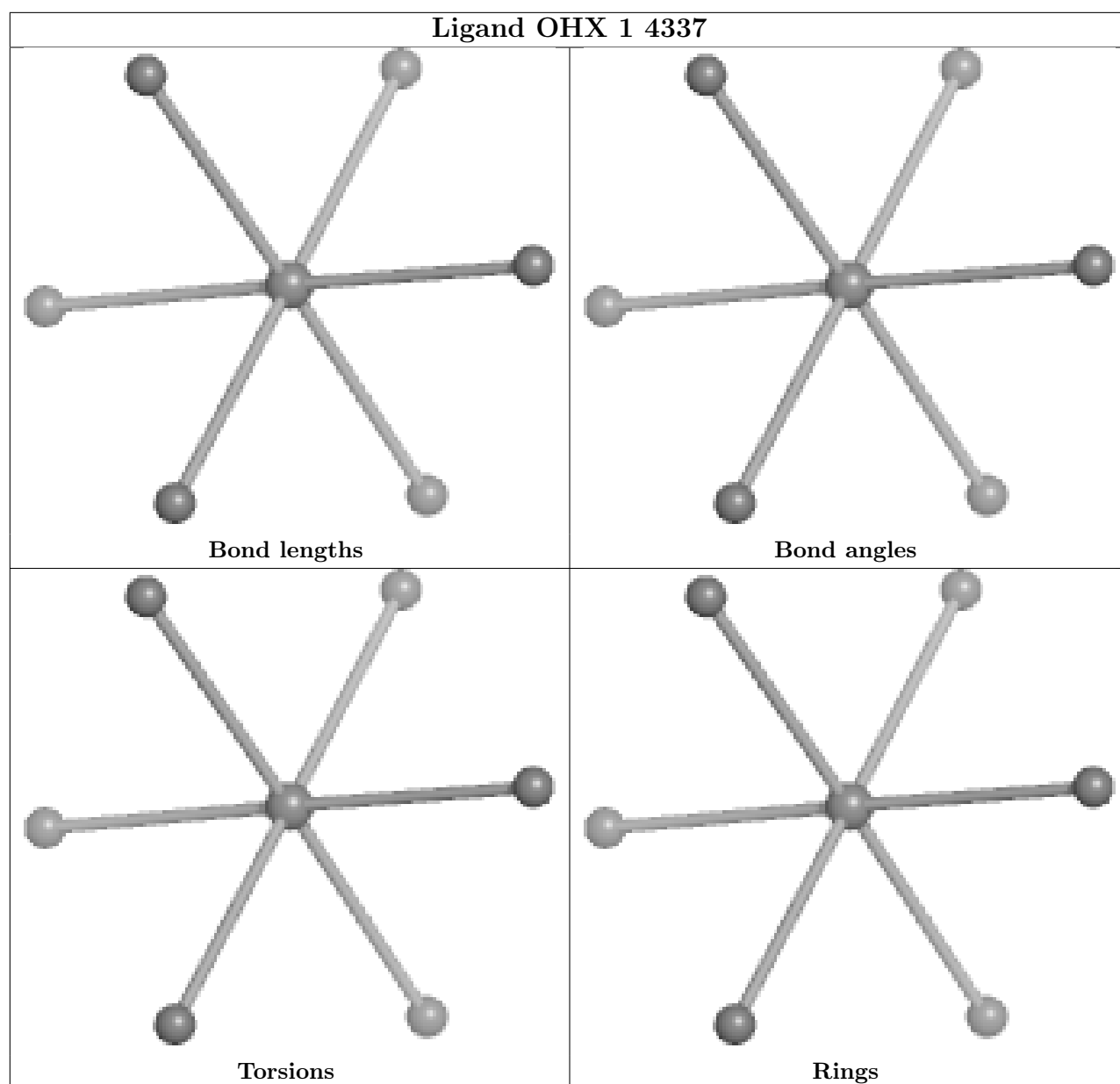


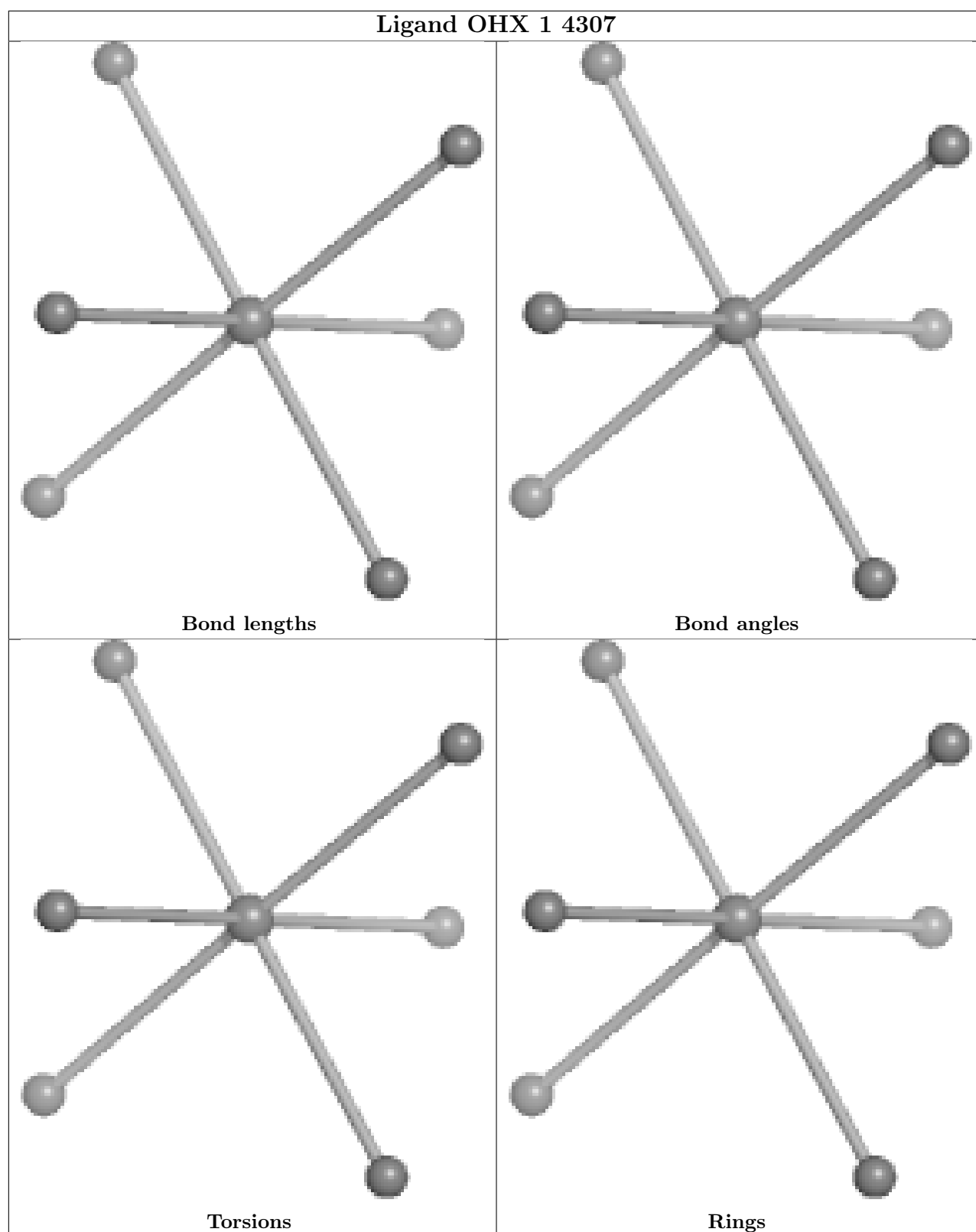
Torsions

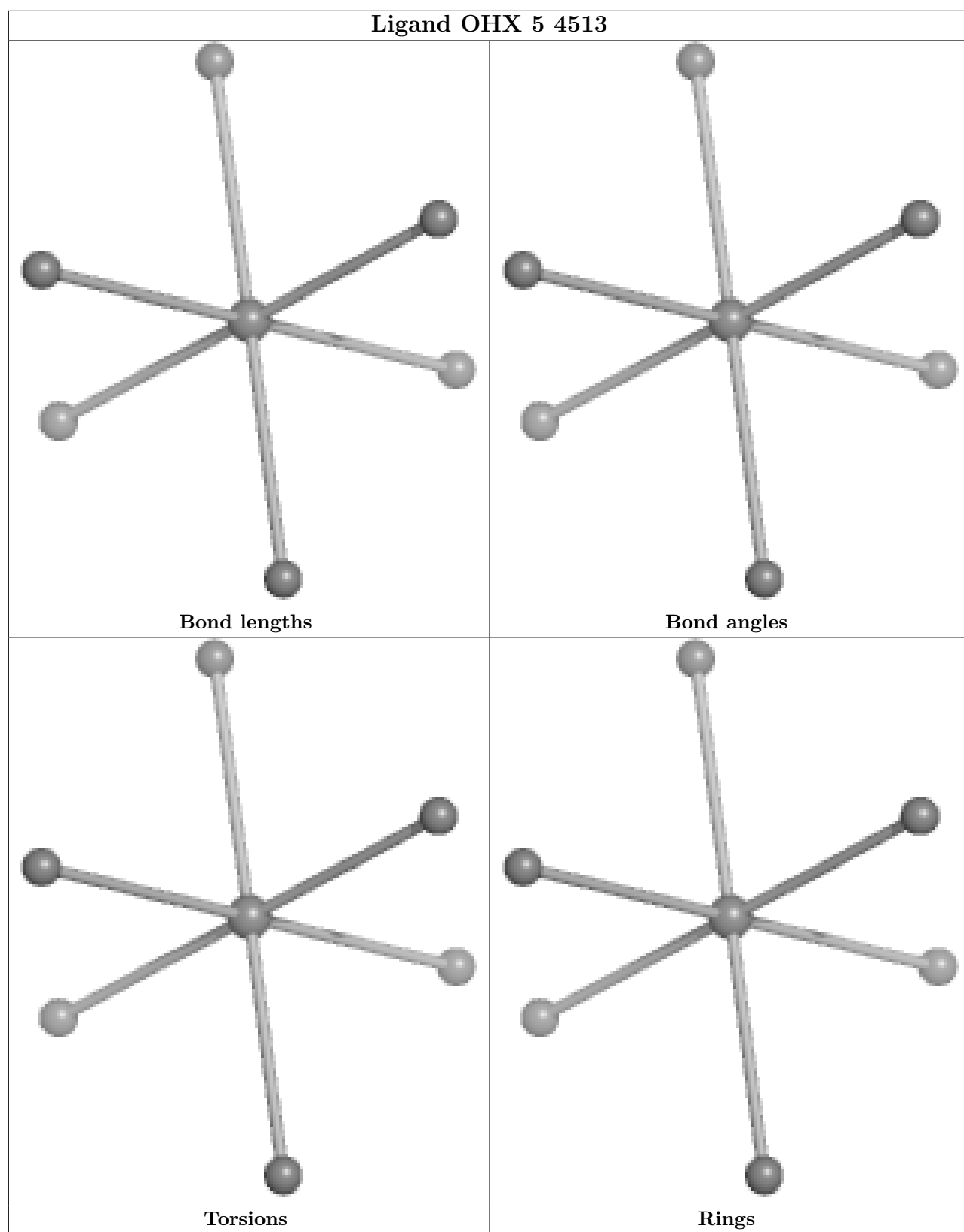


Rings

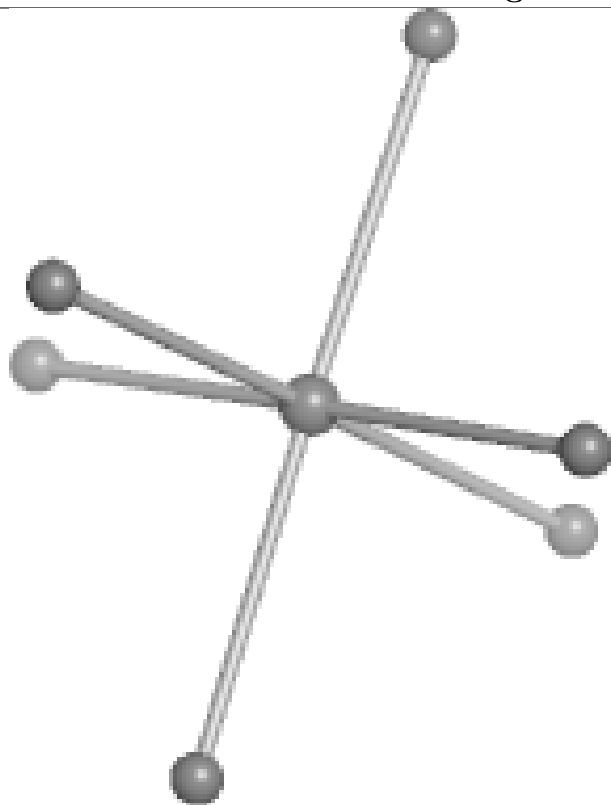




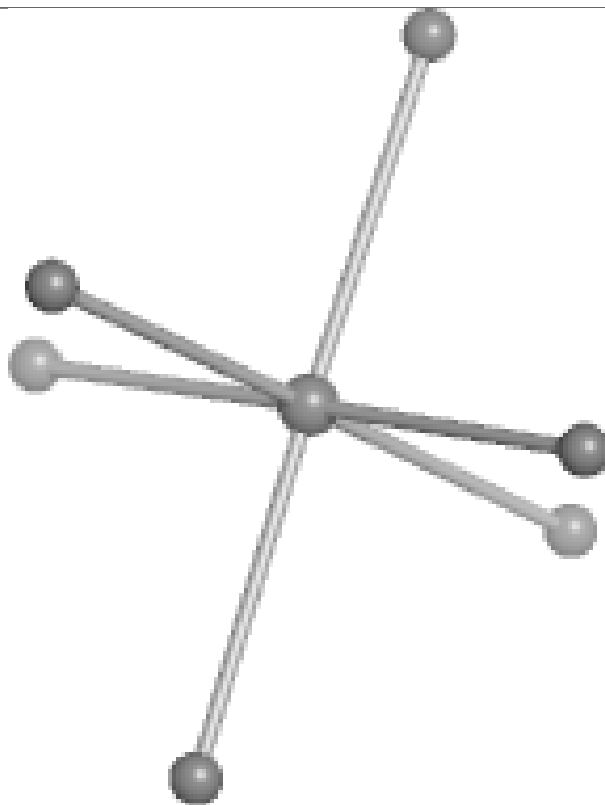




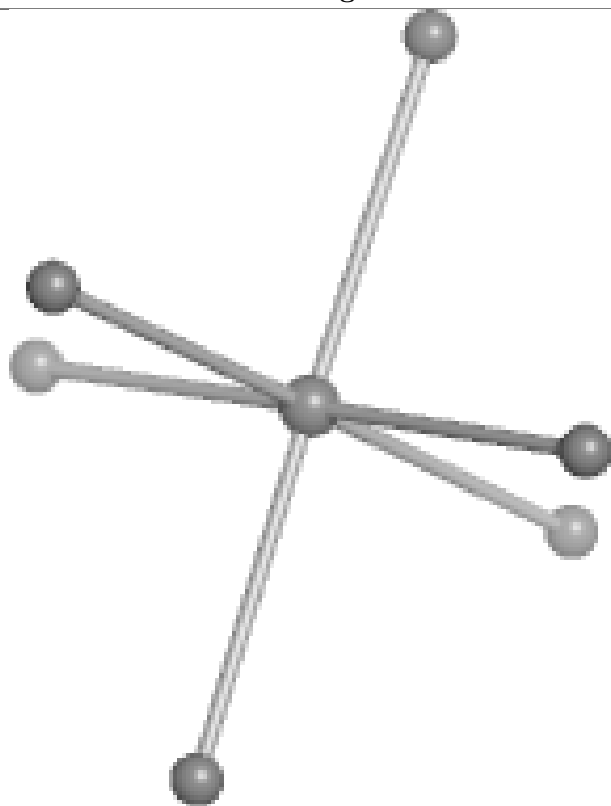
Ligand OHX 5 4548



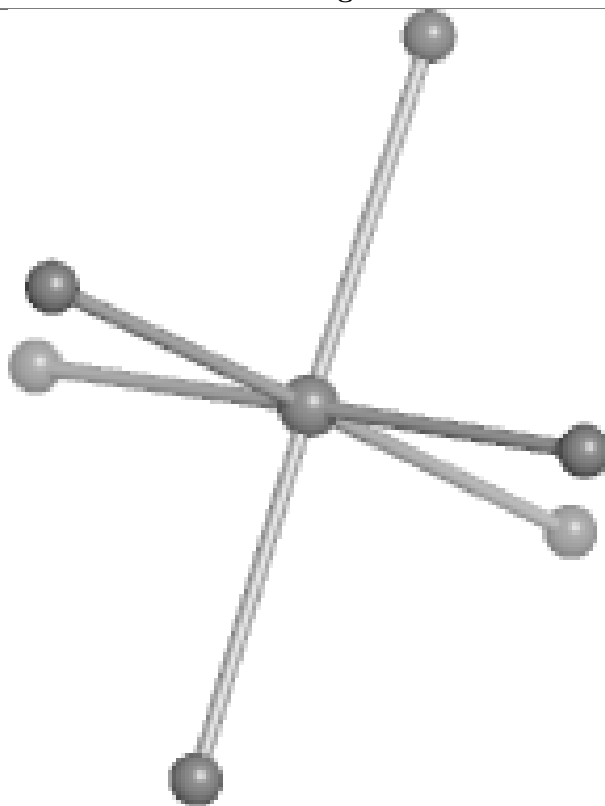
Bond lengths



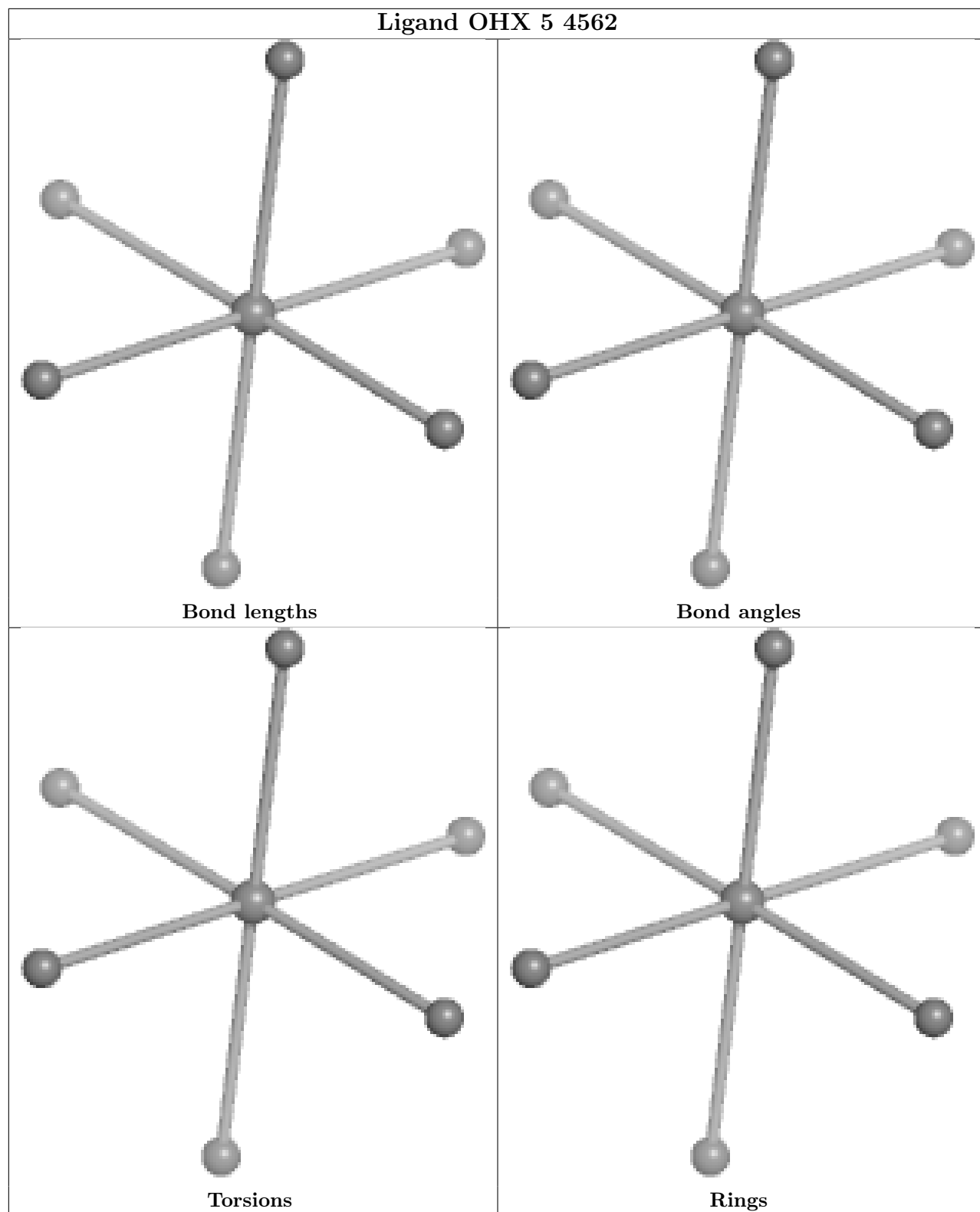
Bond angles

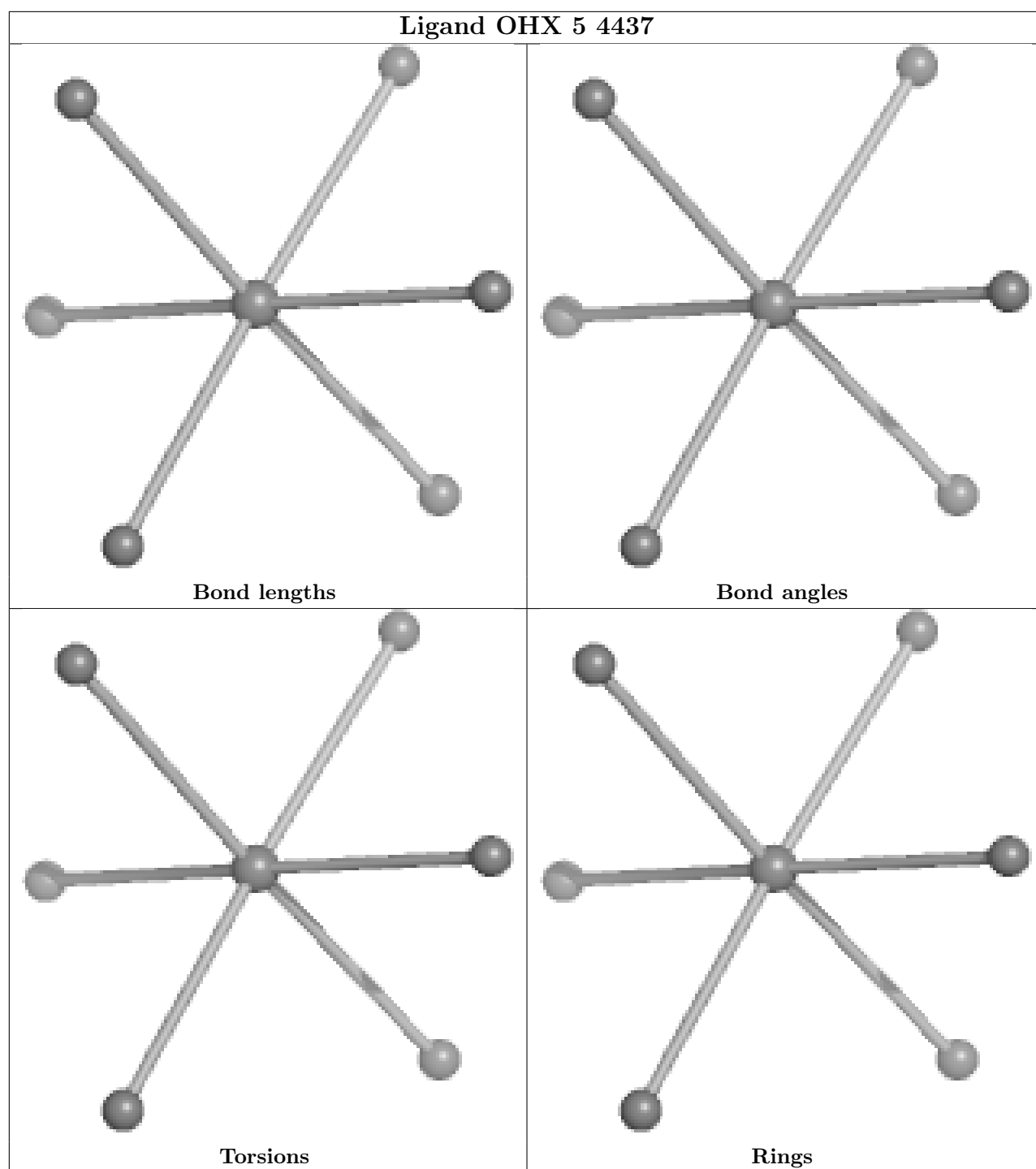


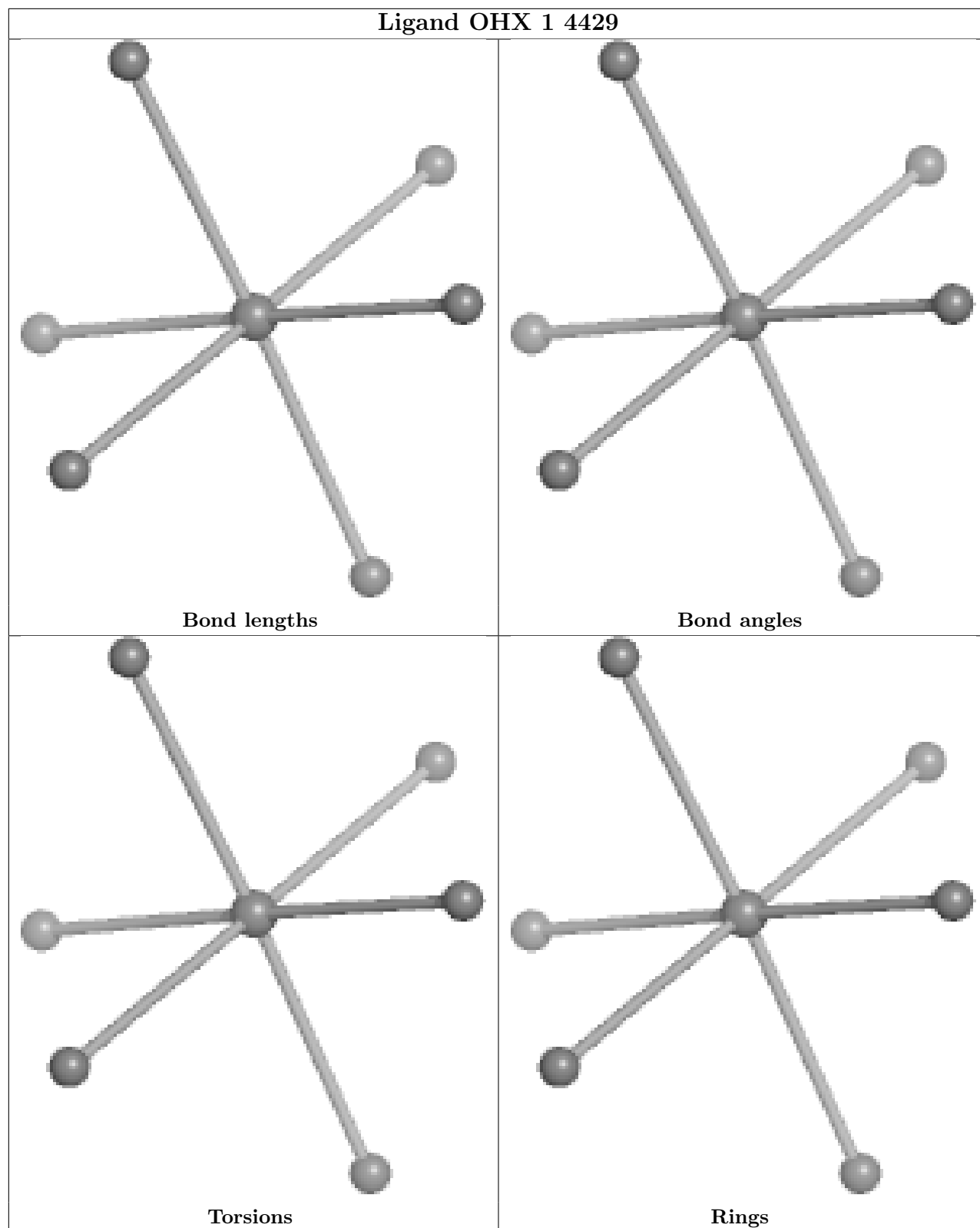
Torsions



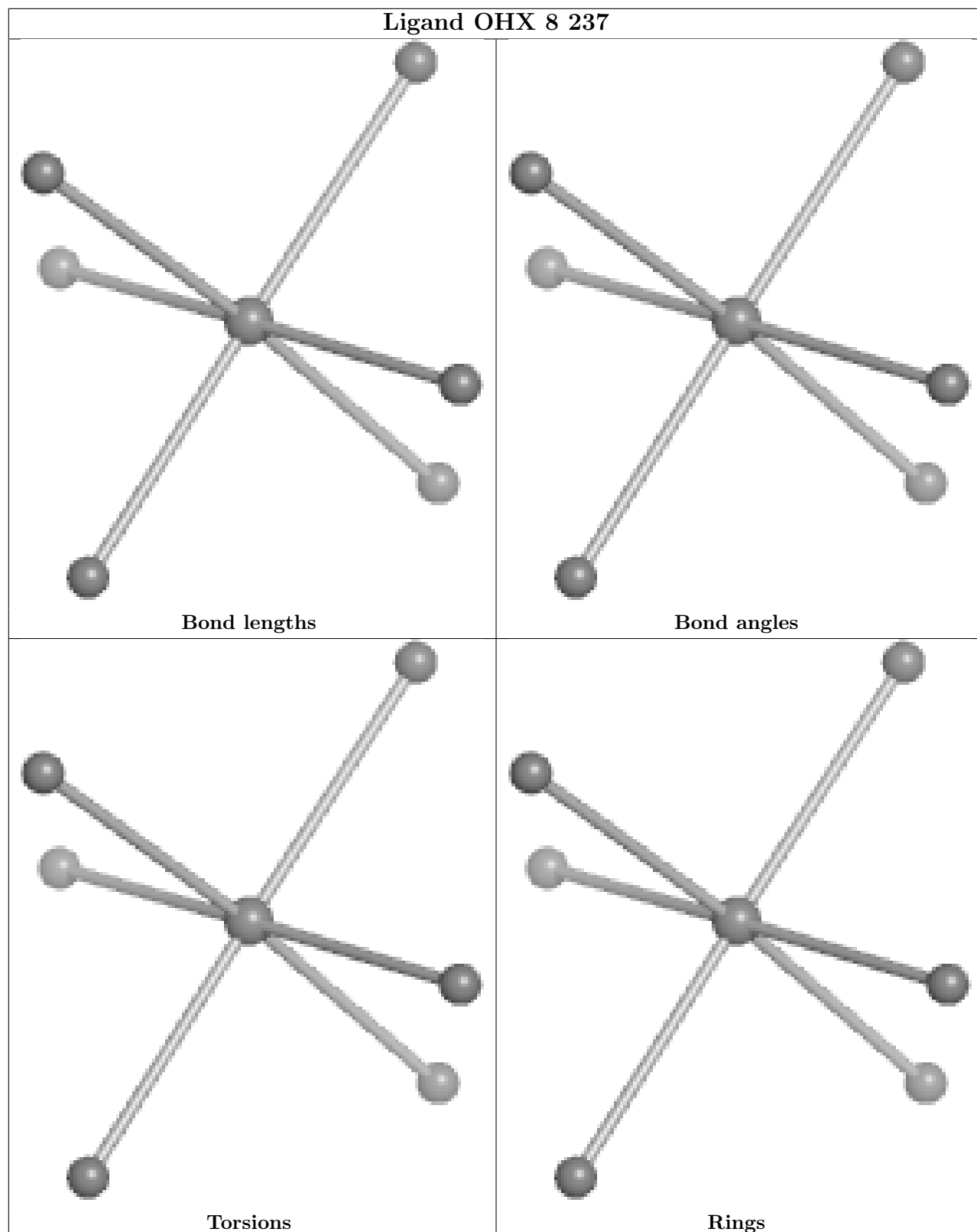
Rings

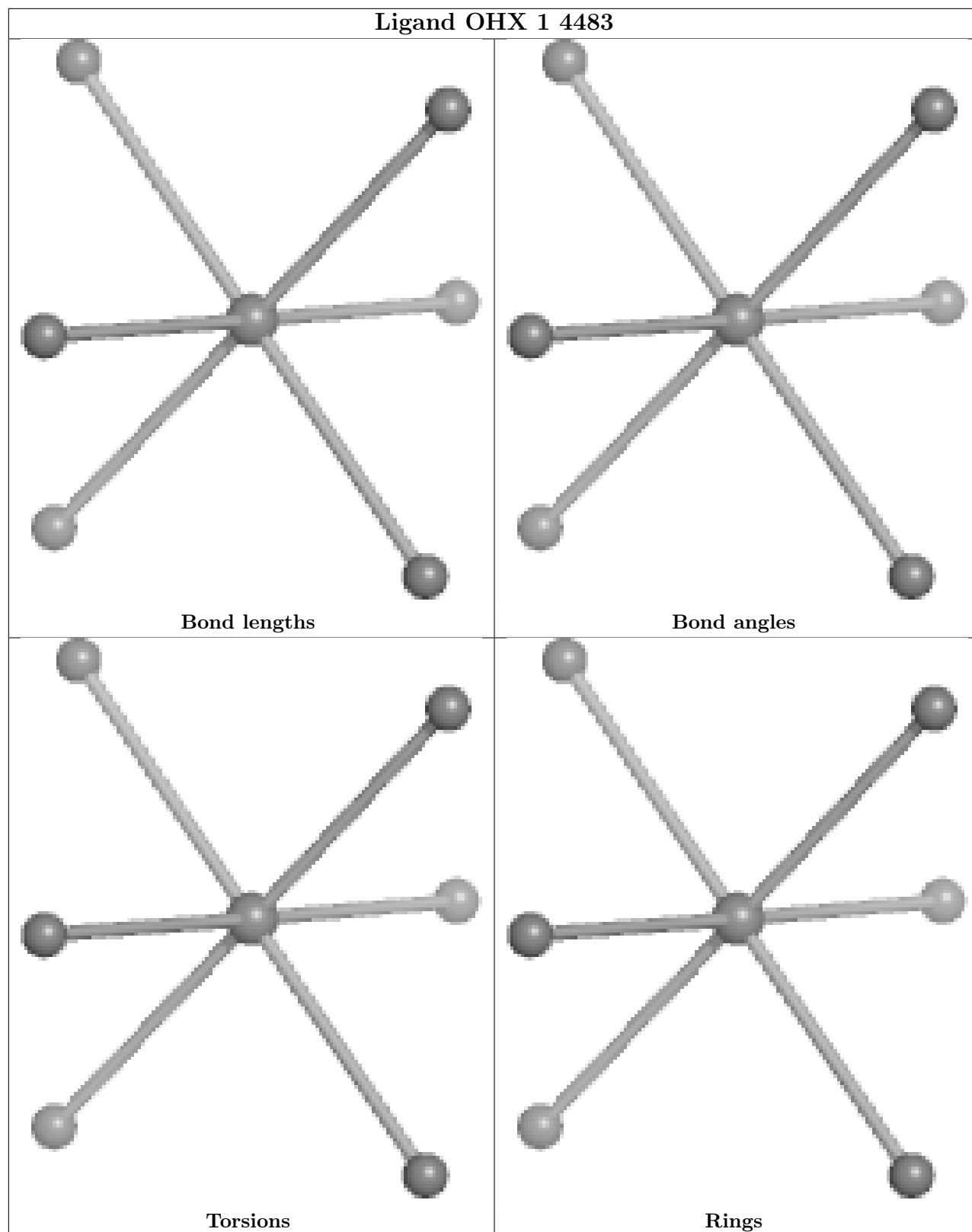




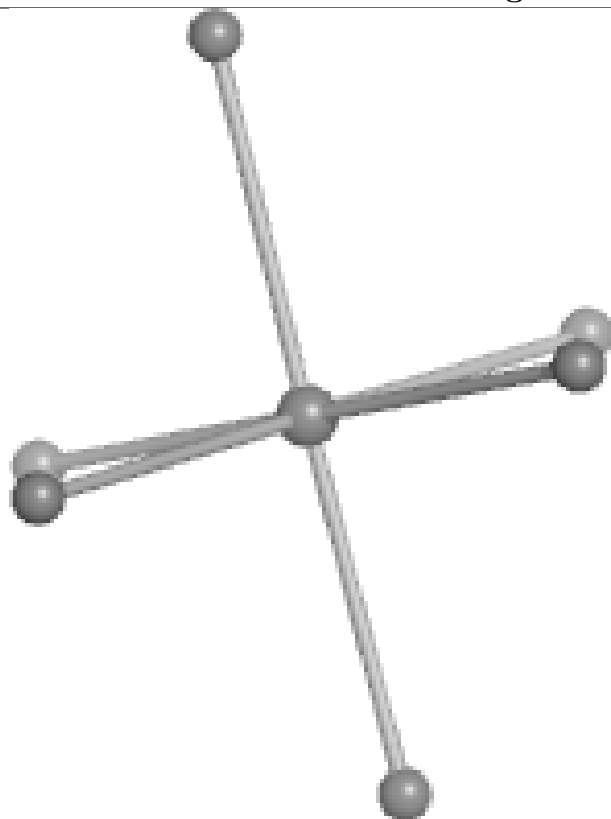


Ligand OHX 8 237

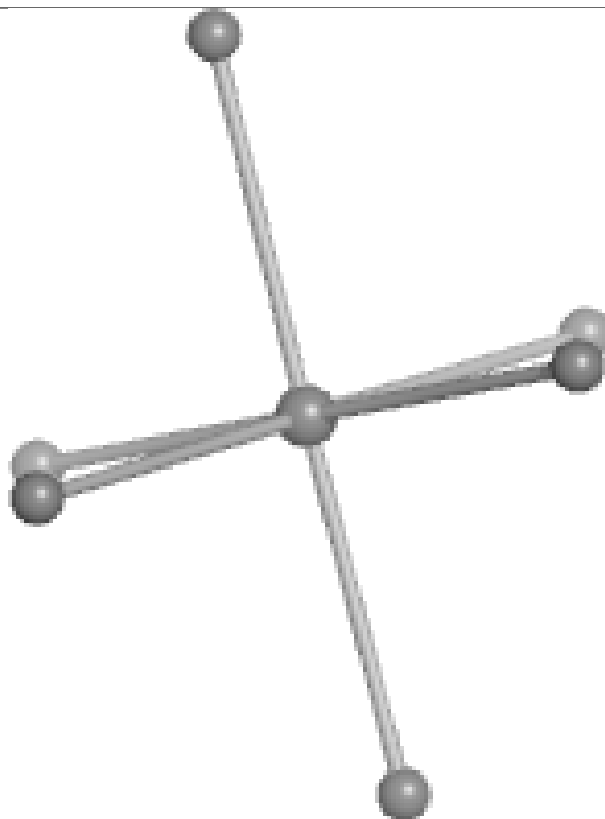




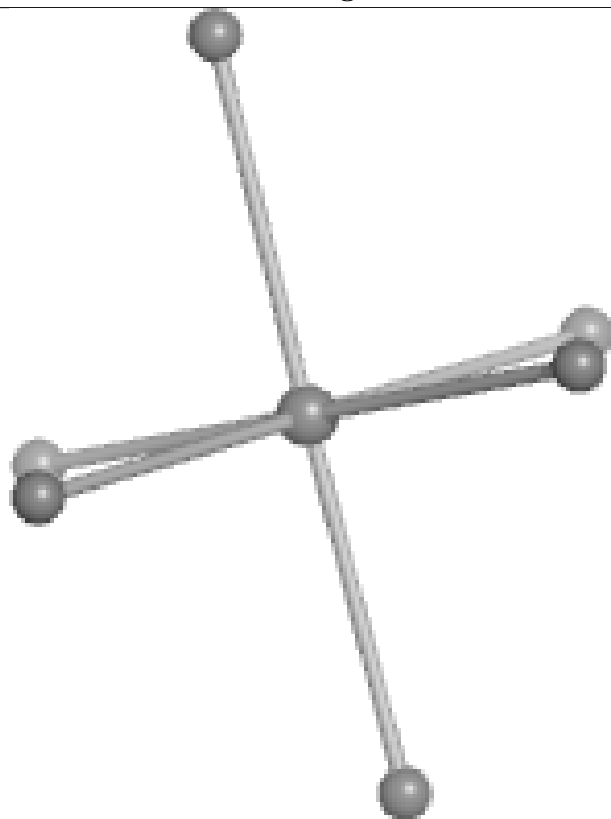
Ligand OHX 1 4361



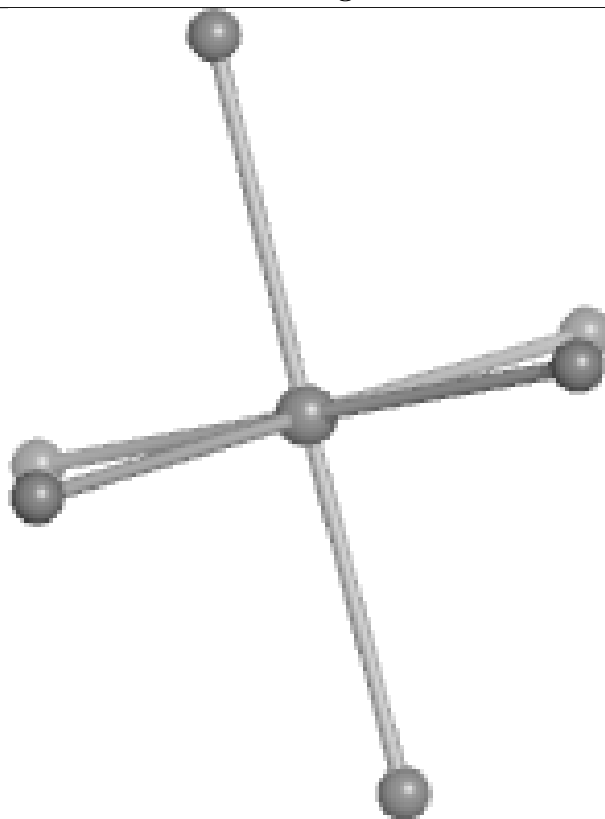
Bond lengths



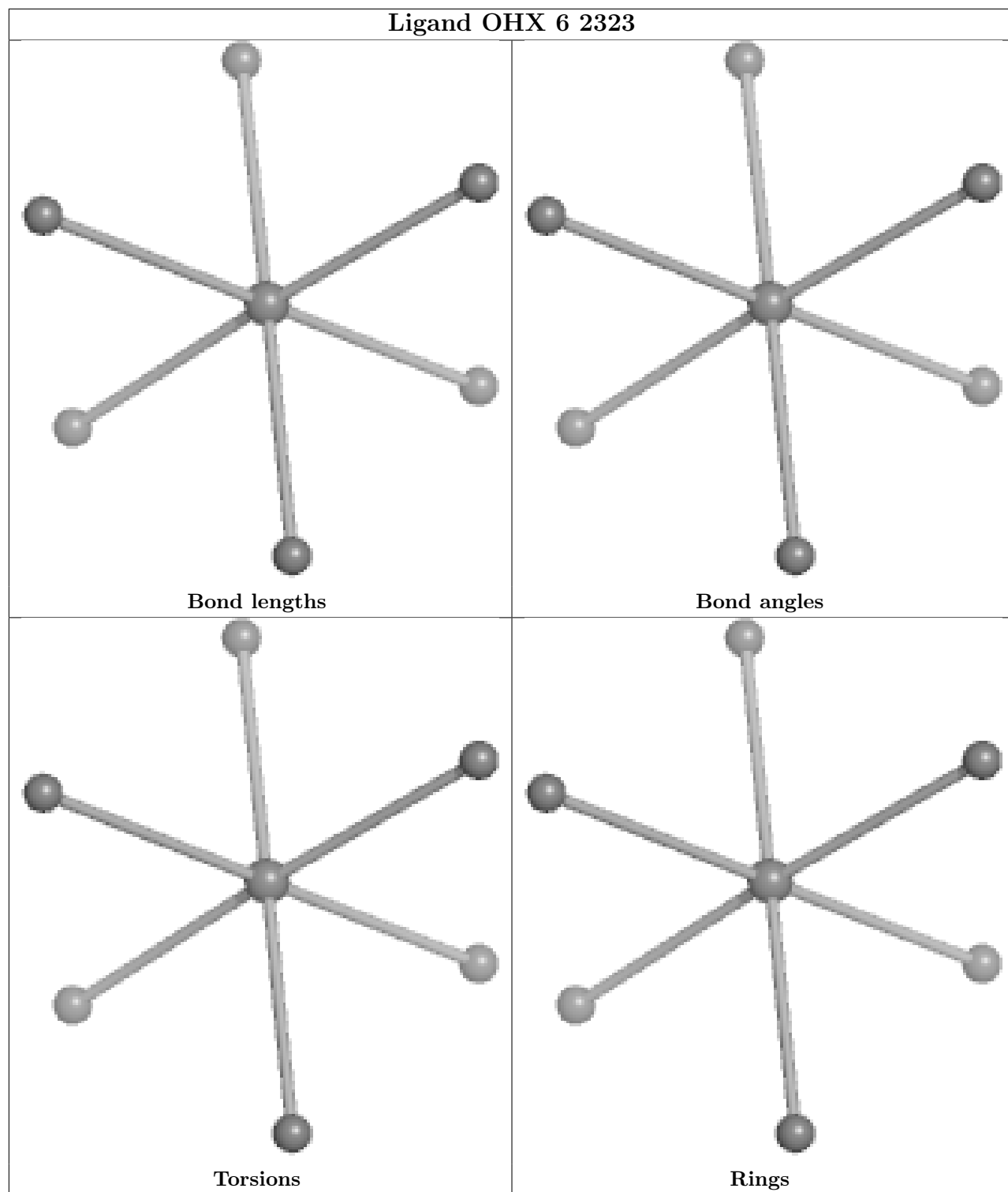
Bond angles

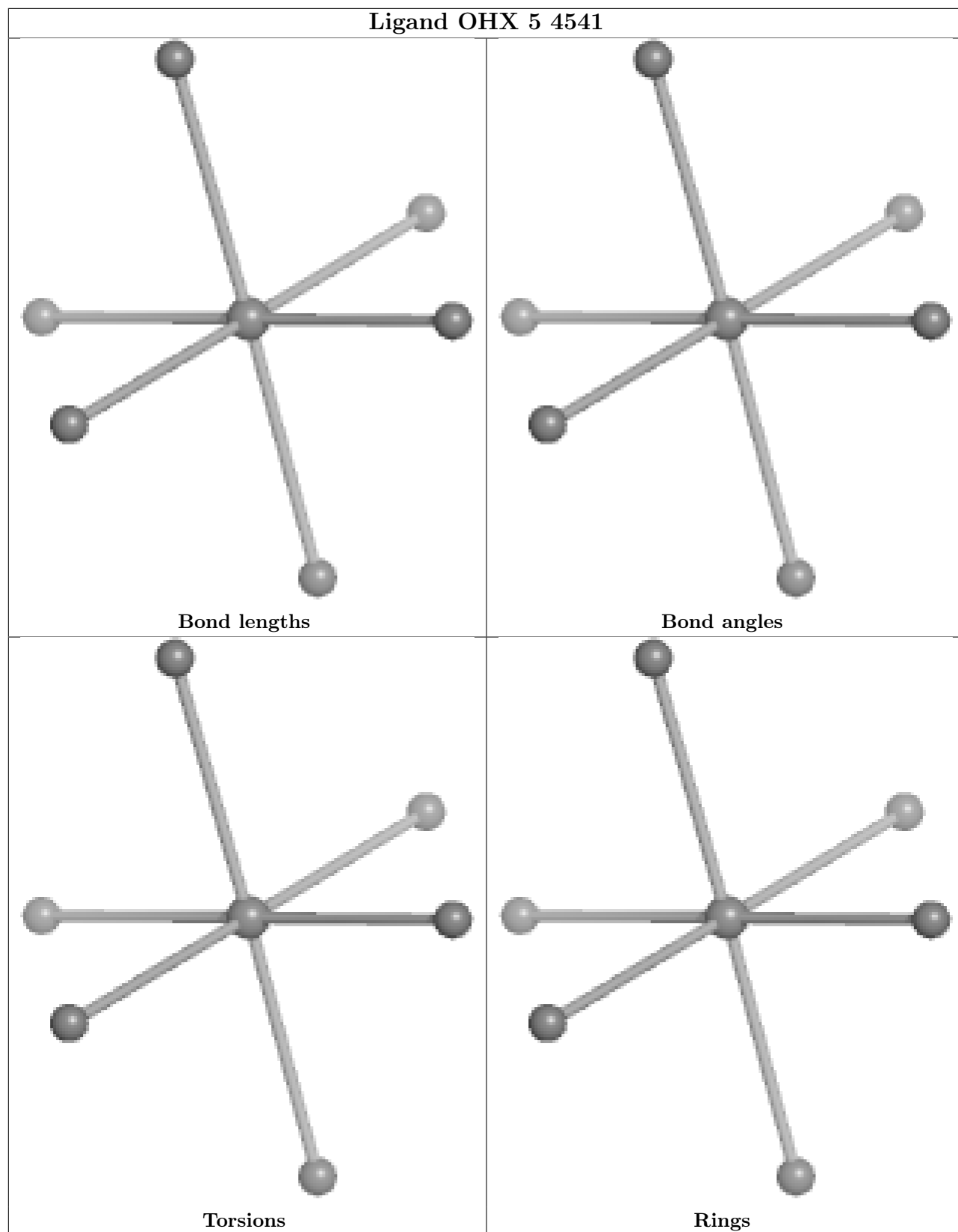


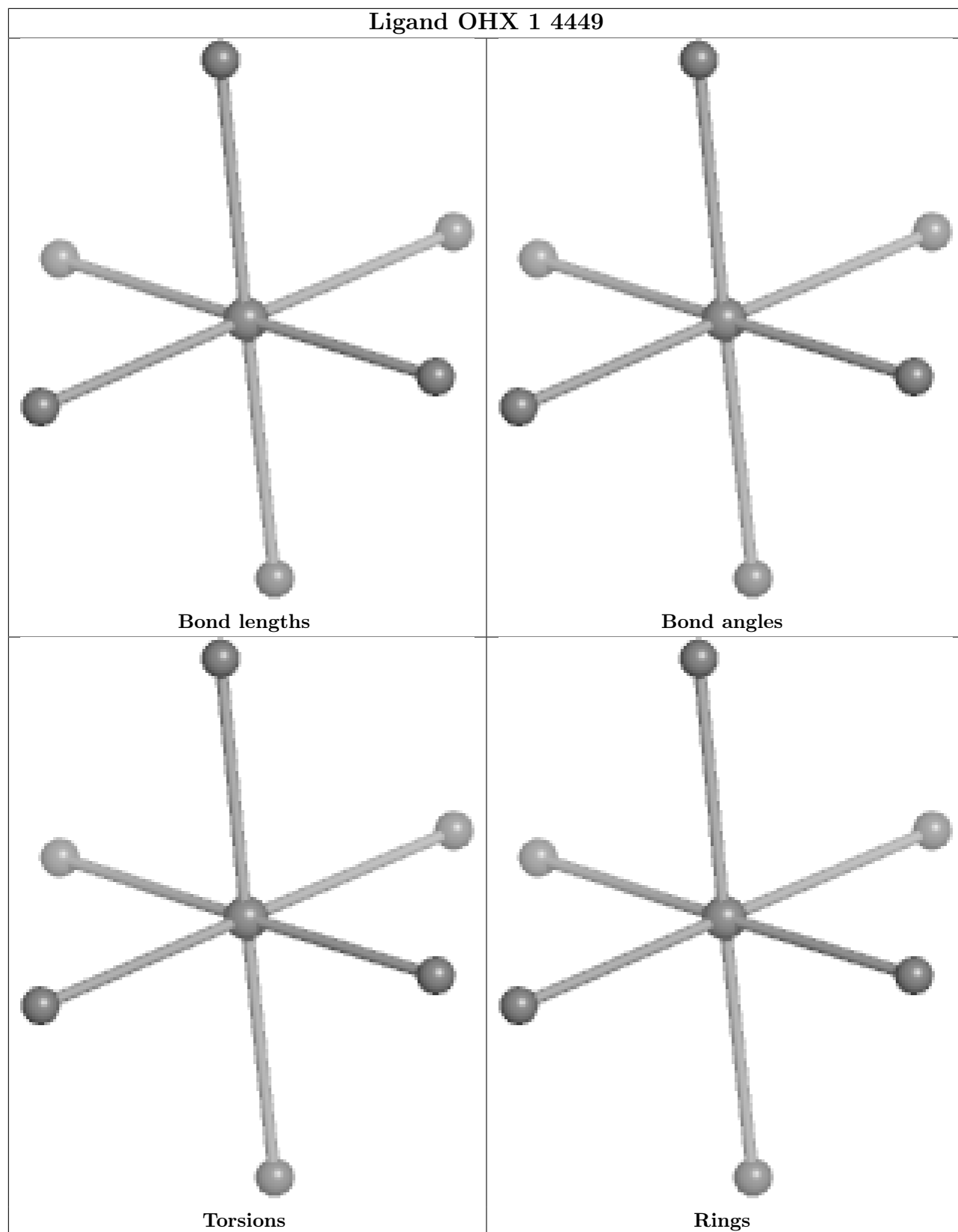
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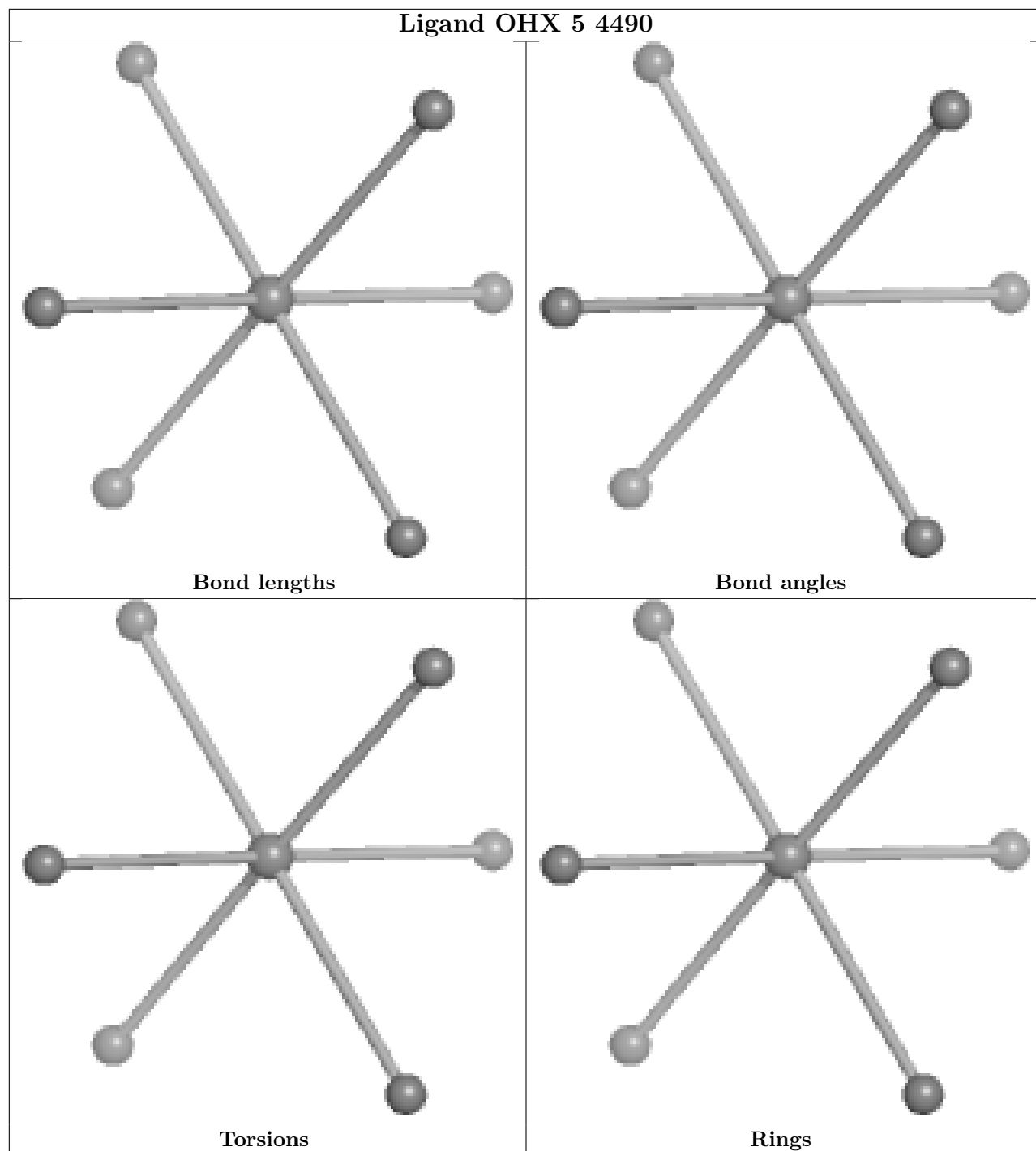


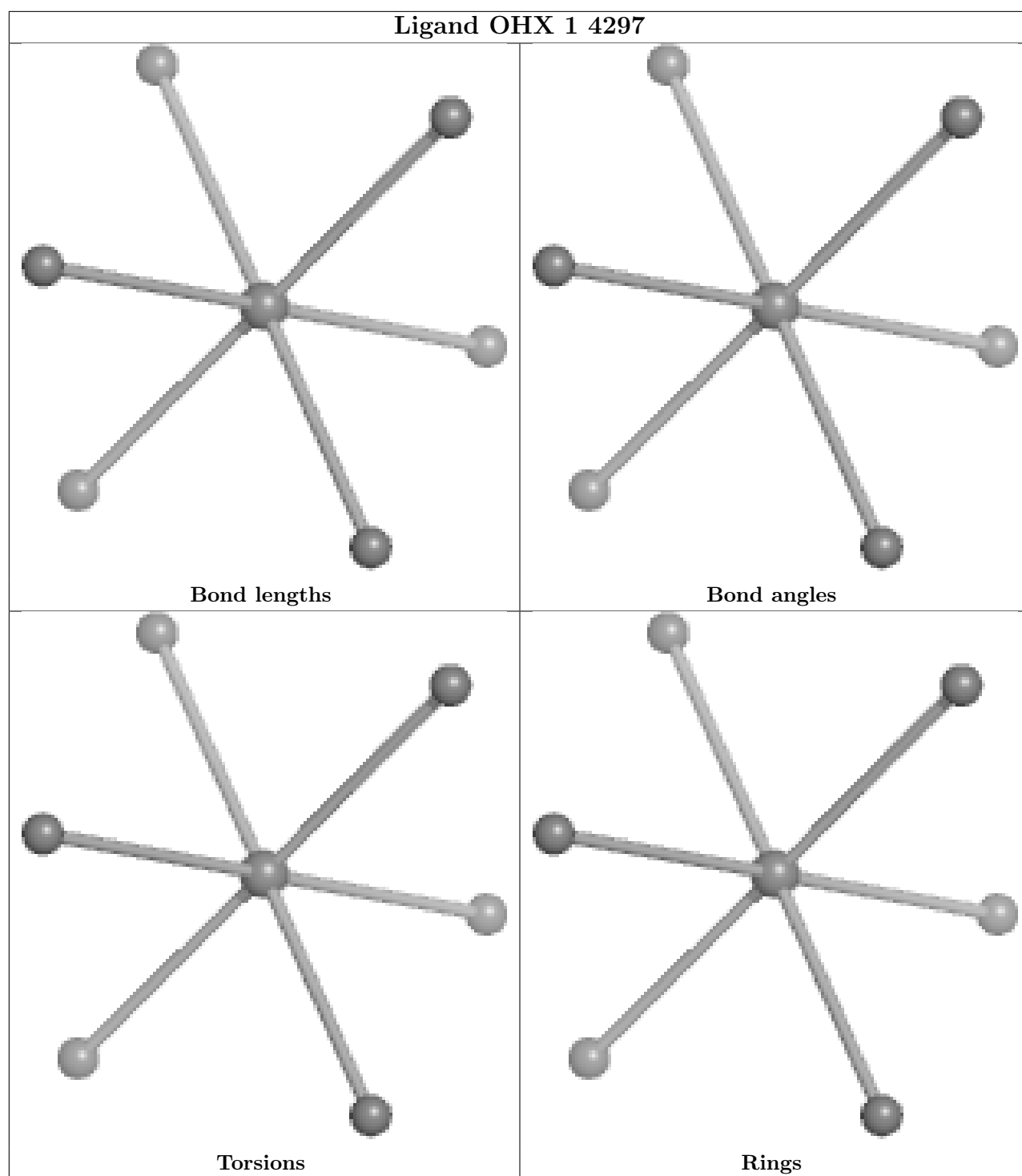
Rings



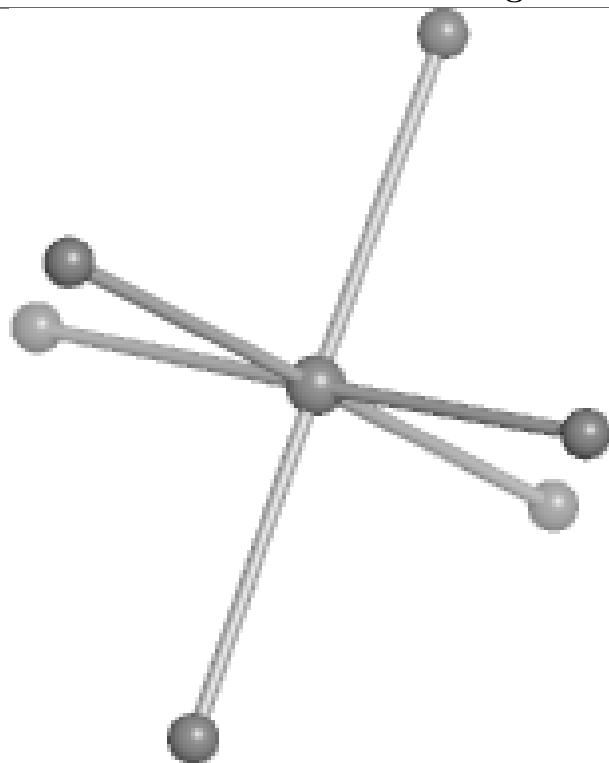




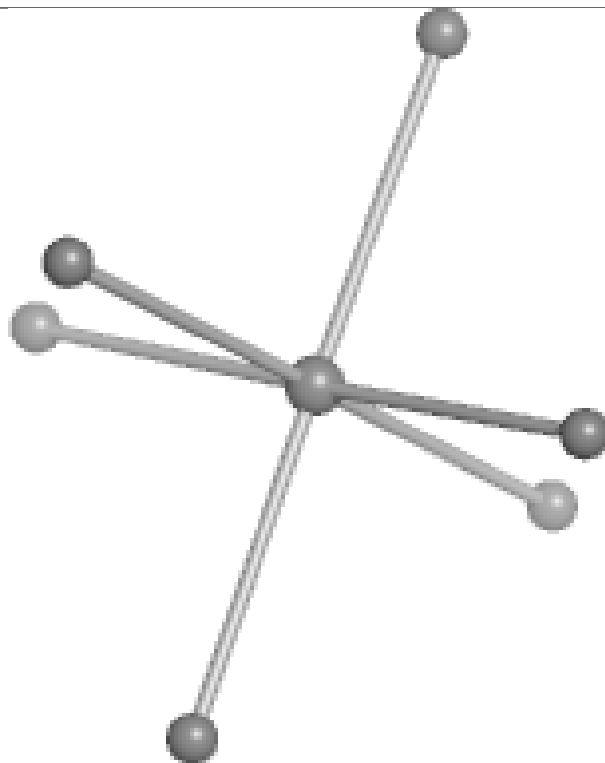




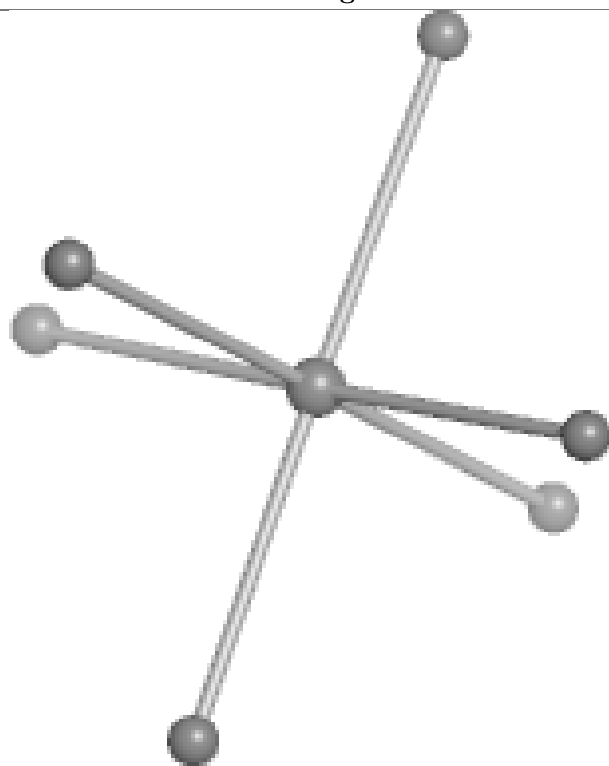
Ligand OHX 1 4385



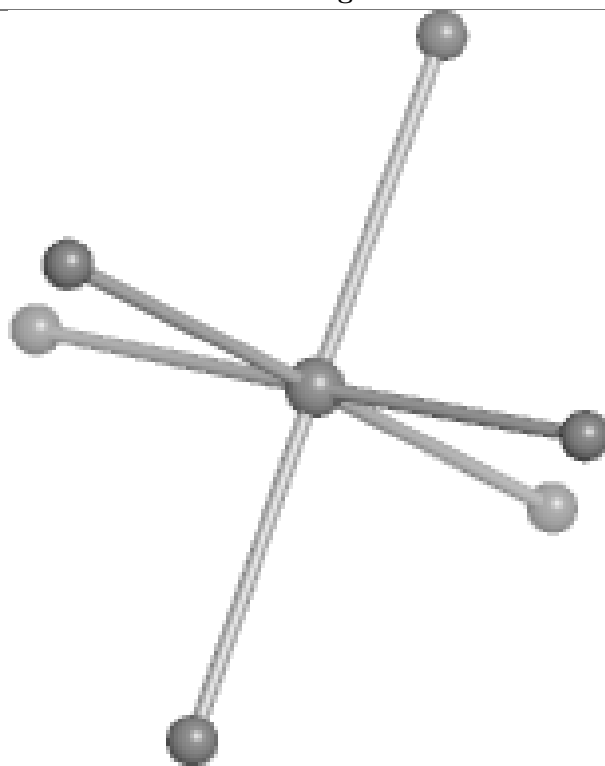
Bond lengths



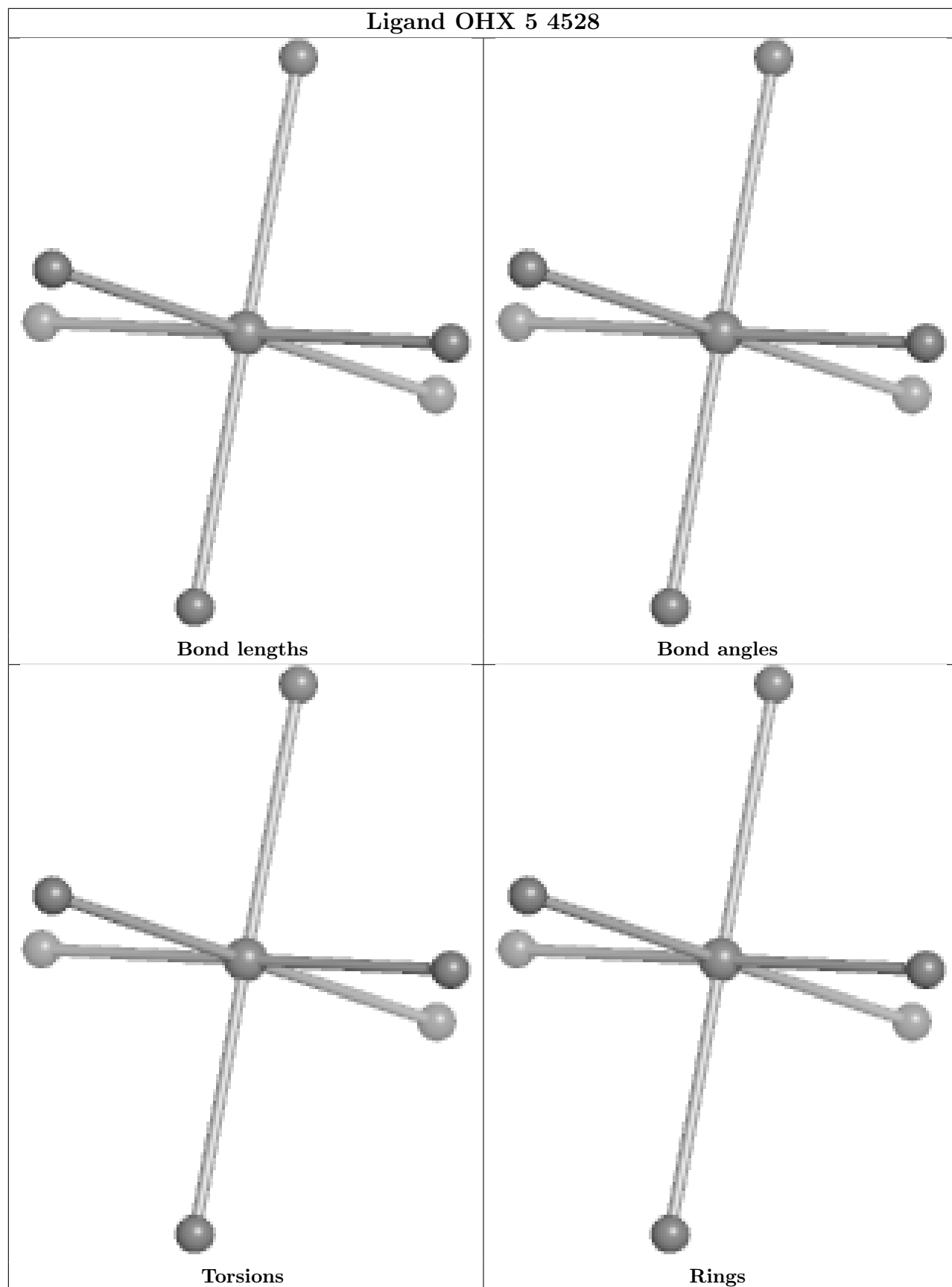
Bond angles

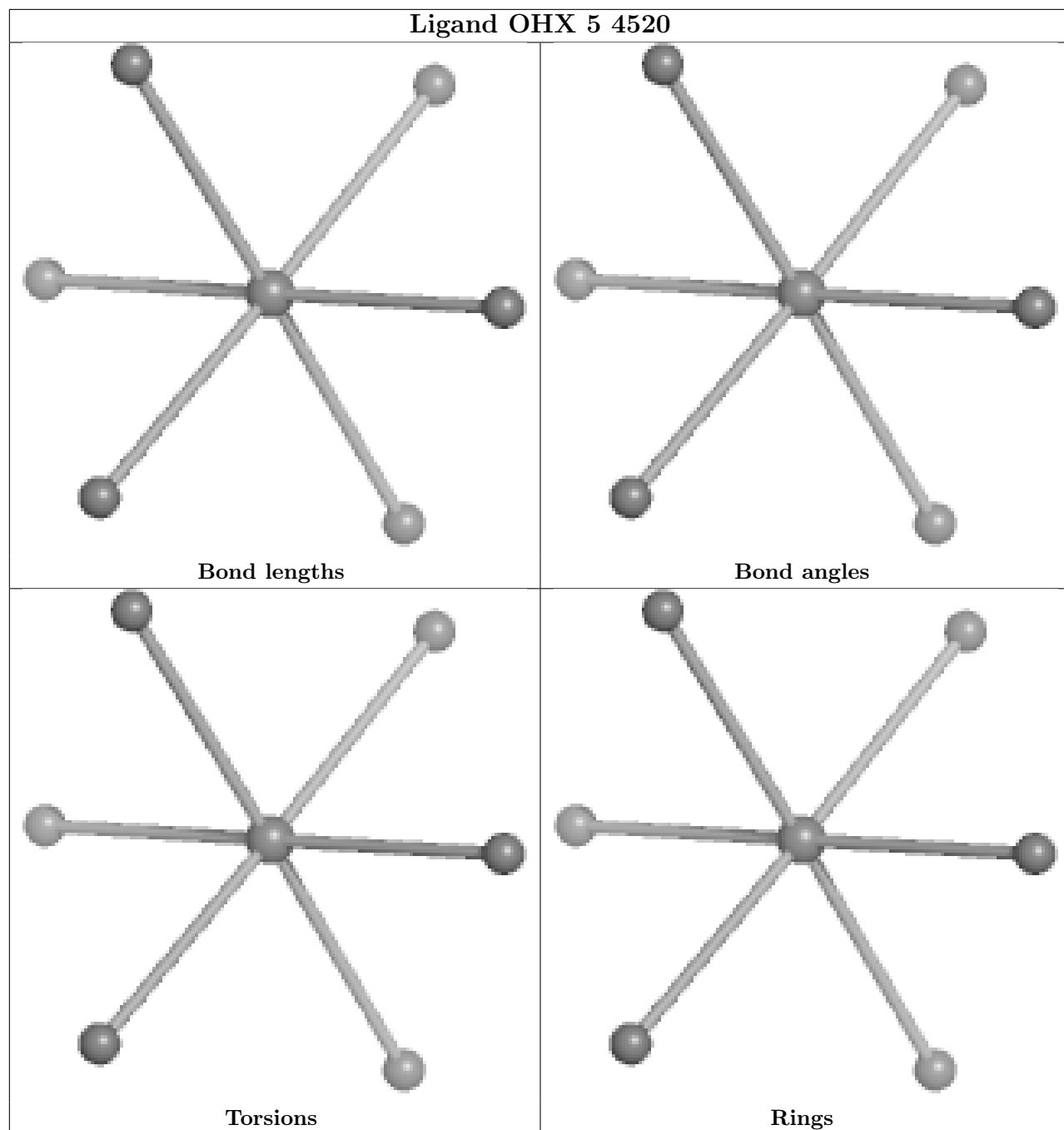


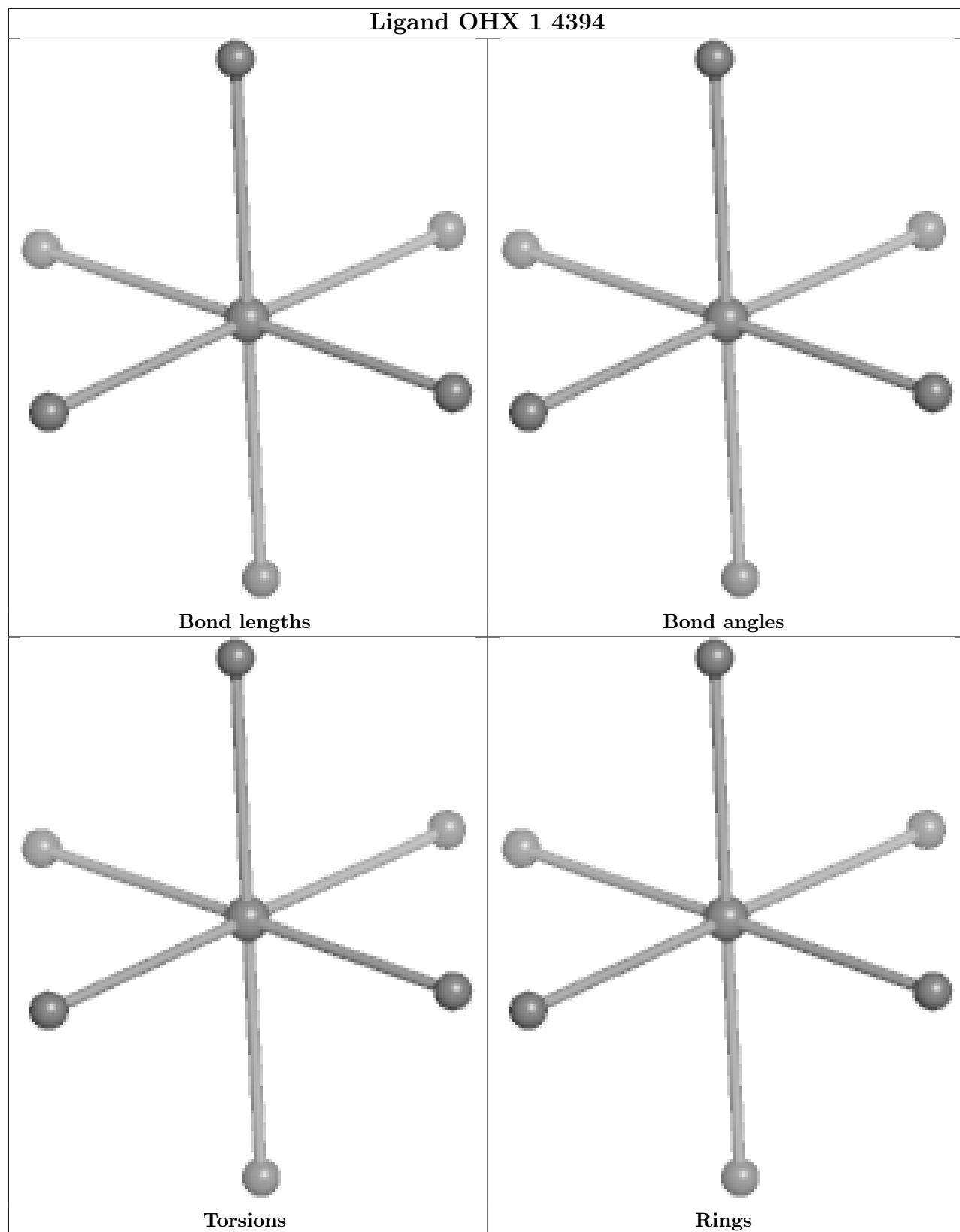
Torsions

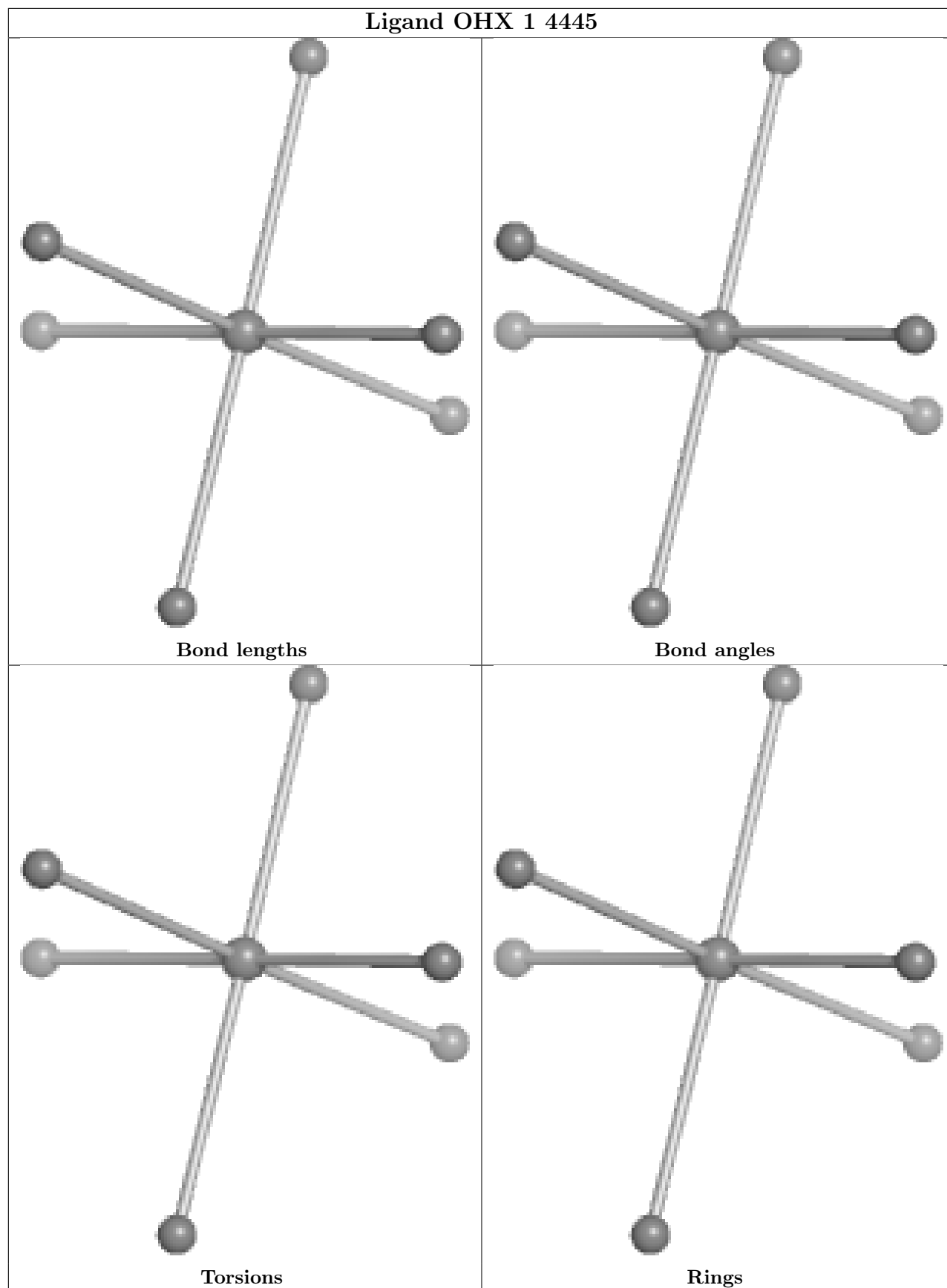


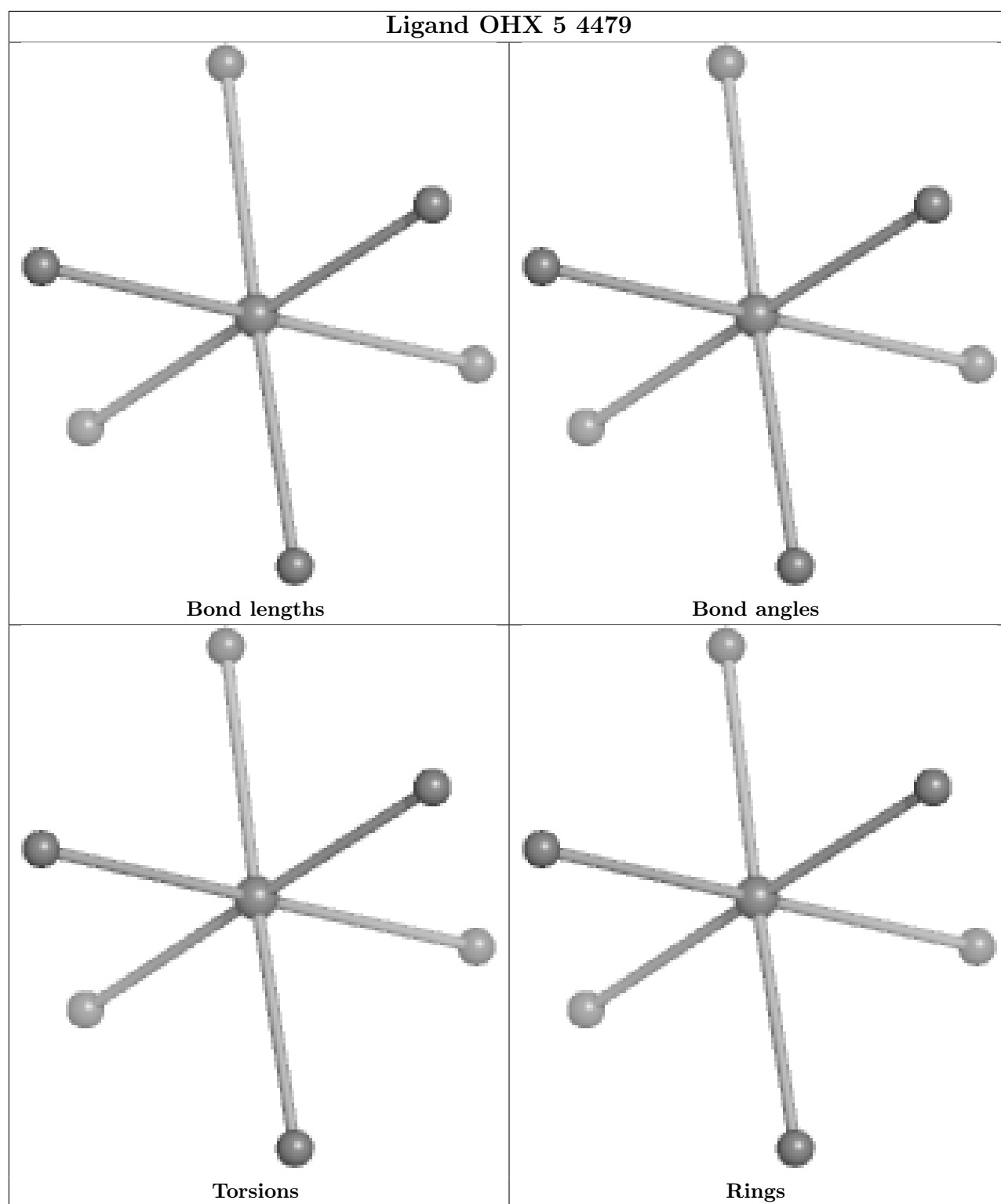
Rings

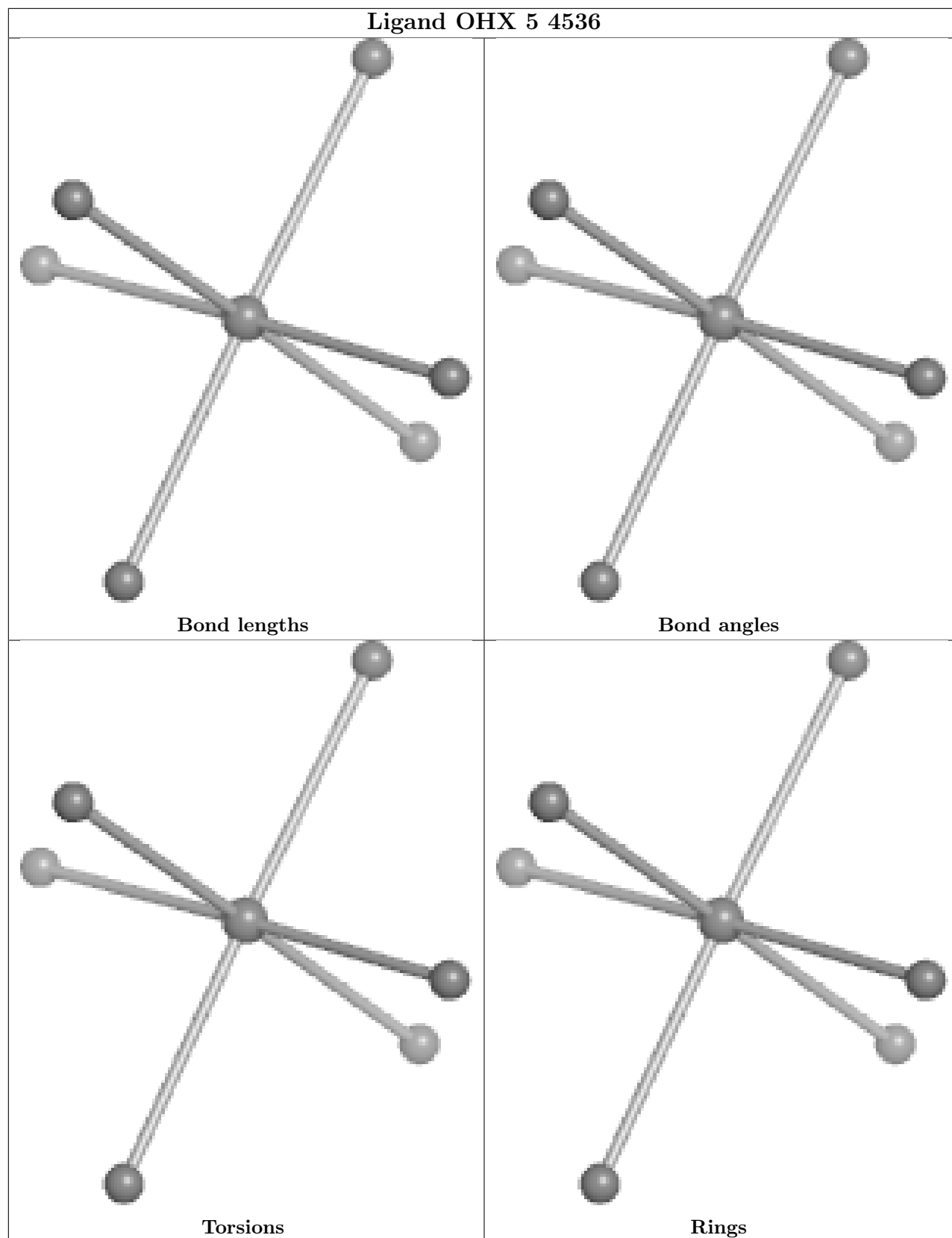


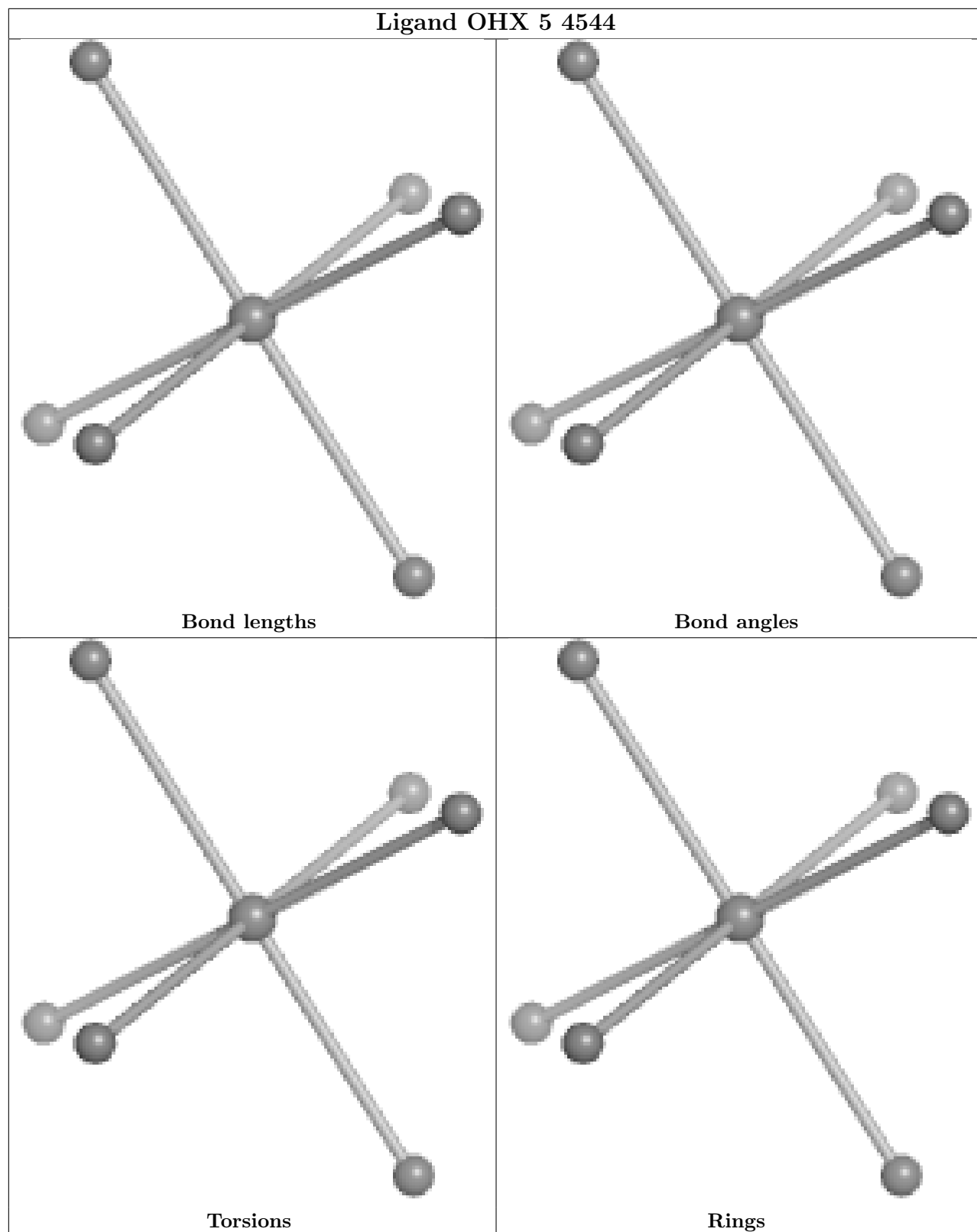


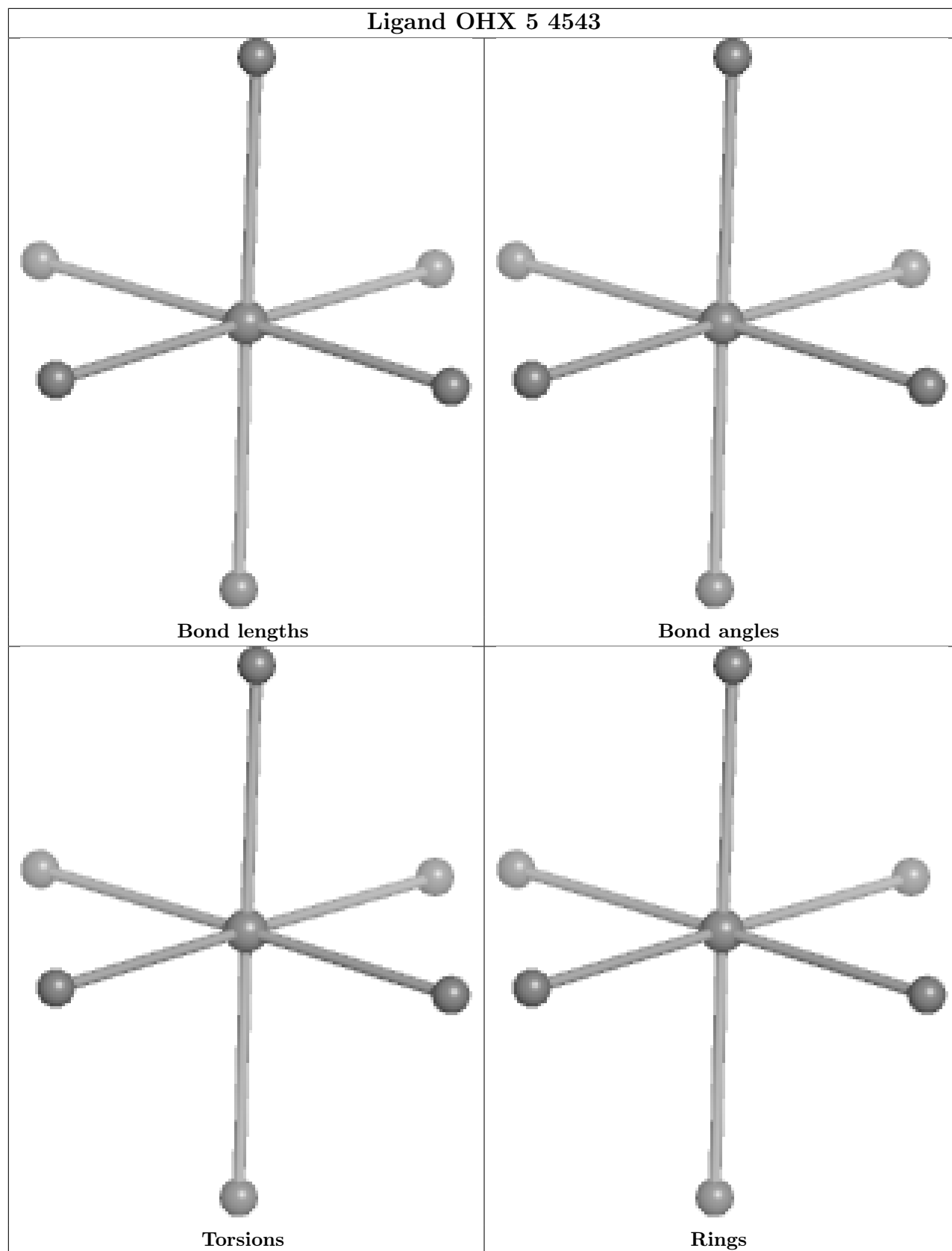




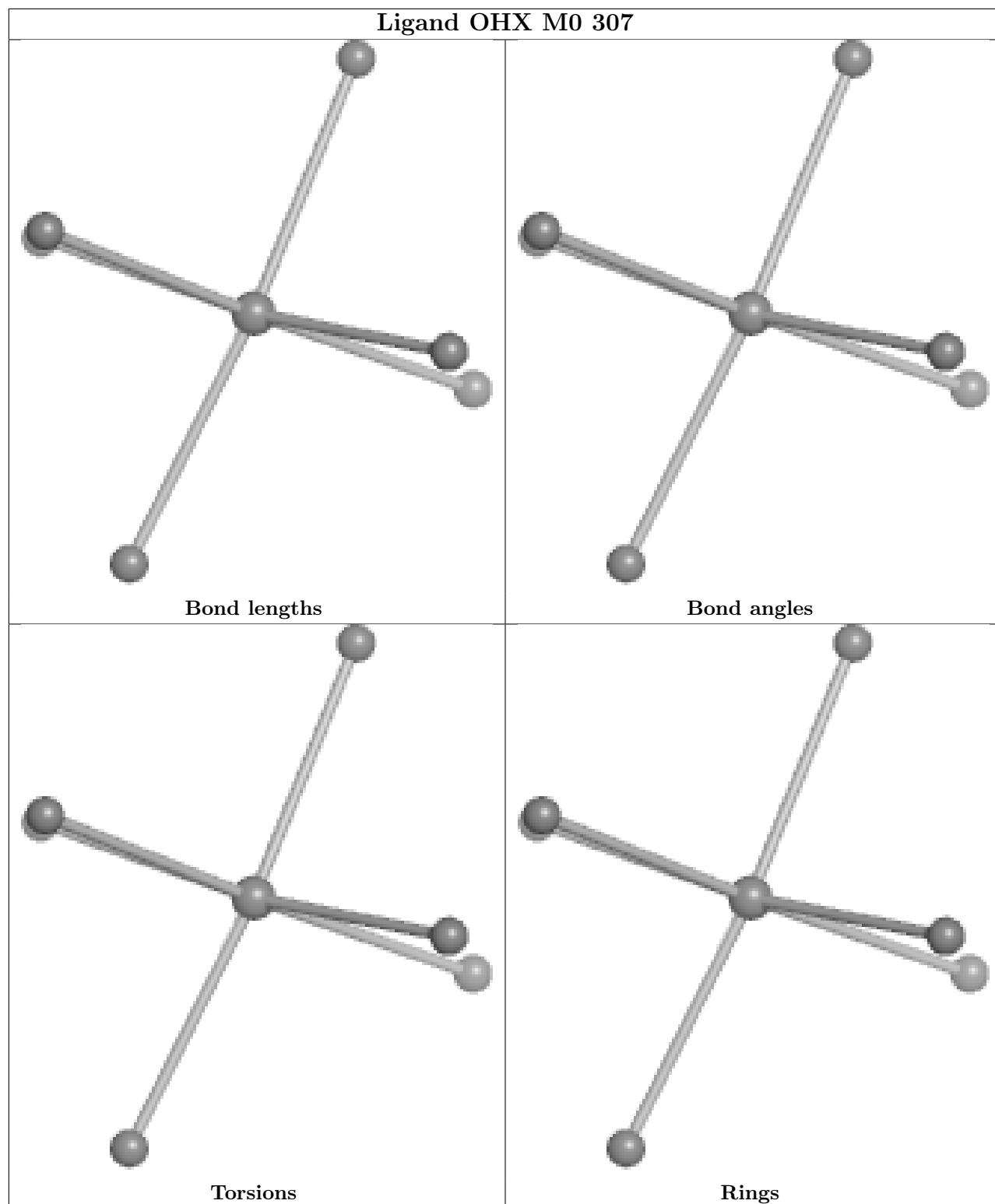


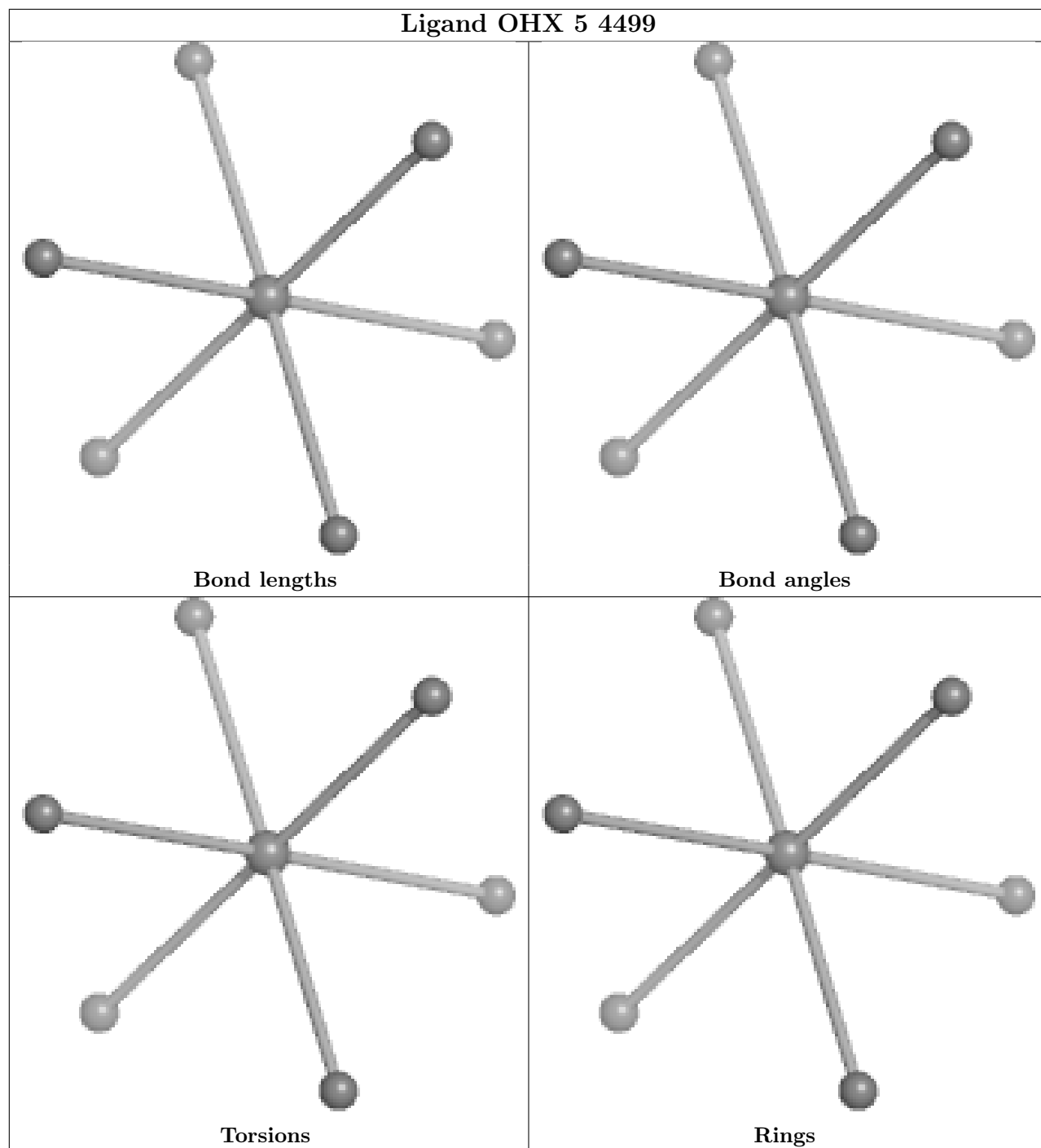


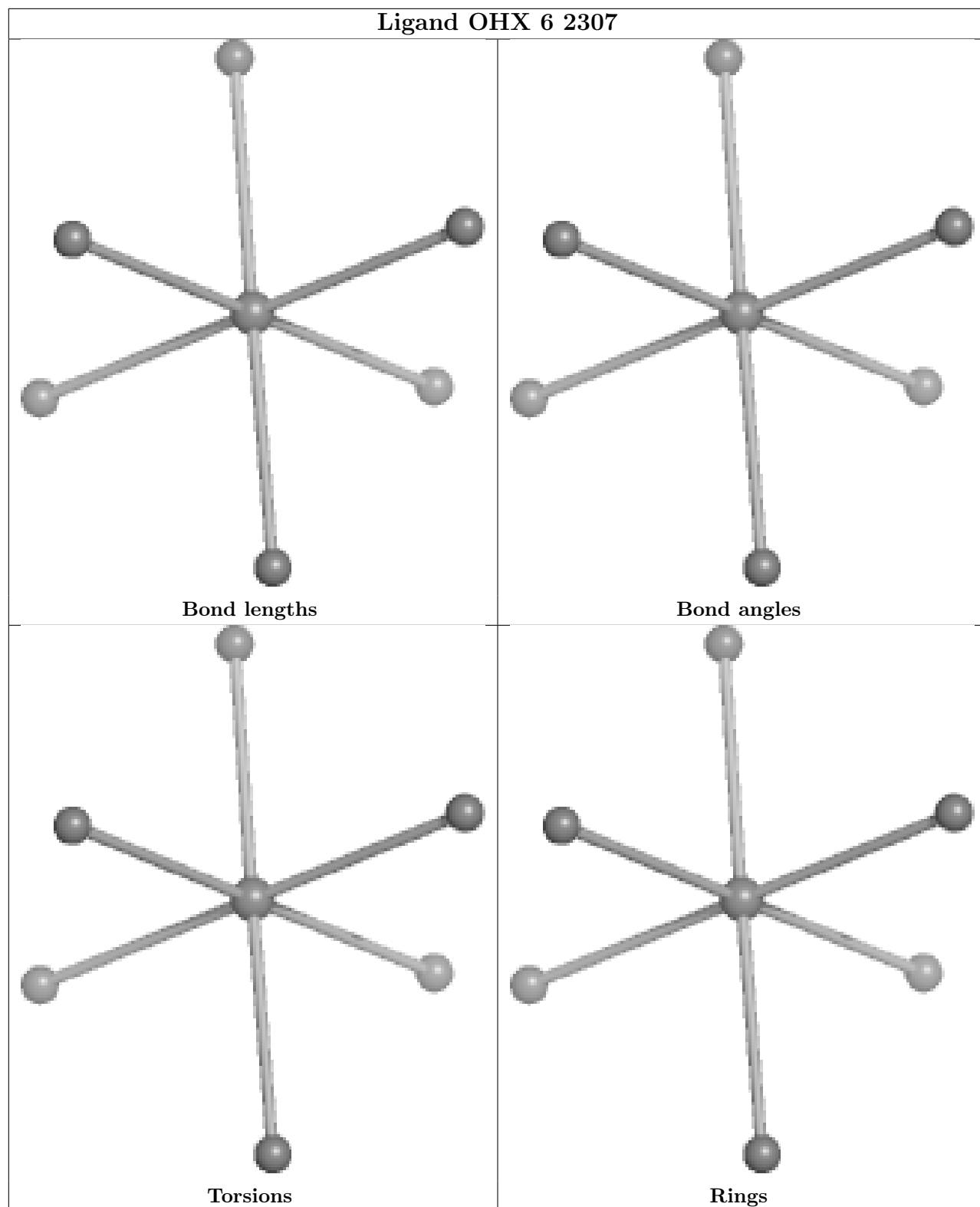


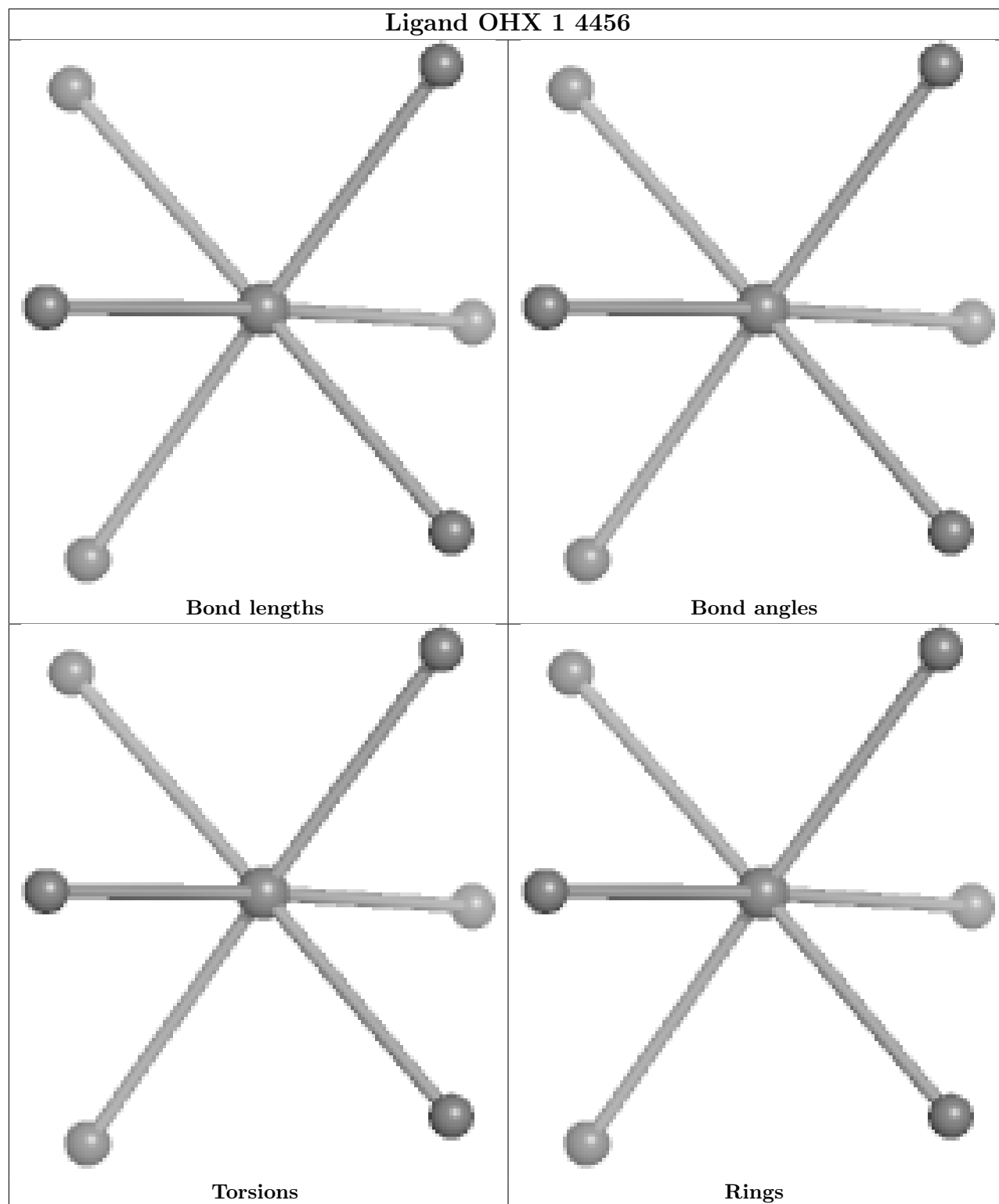


Ligand OHX M0 307

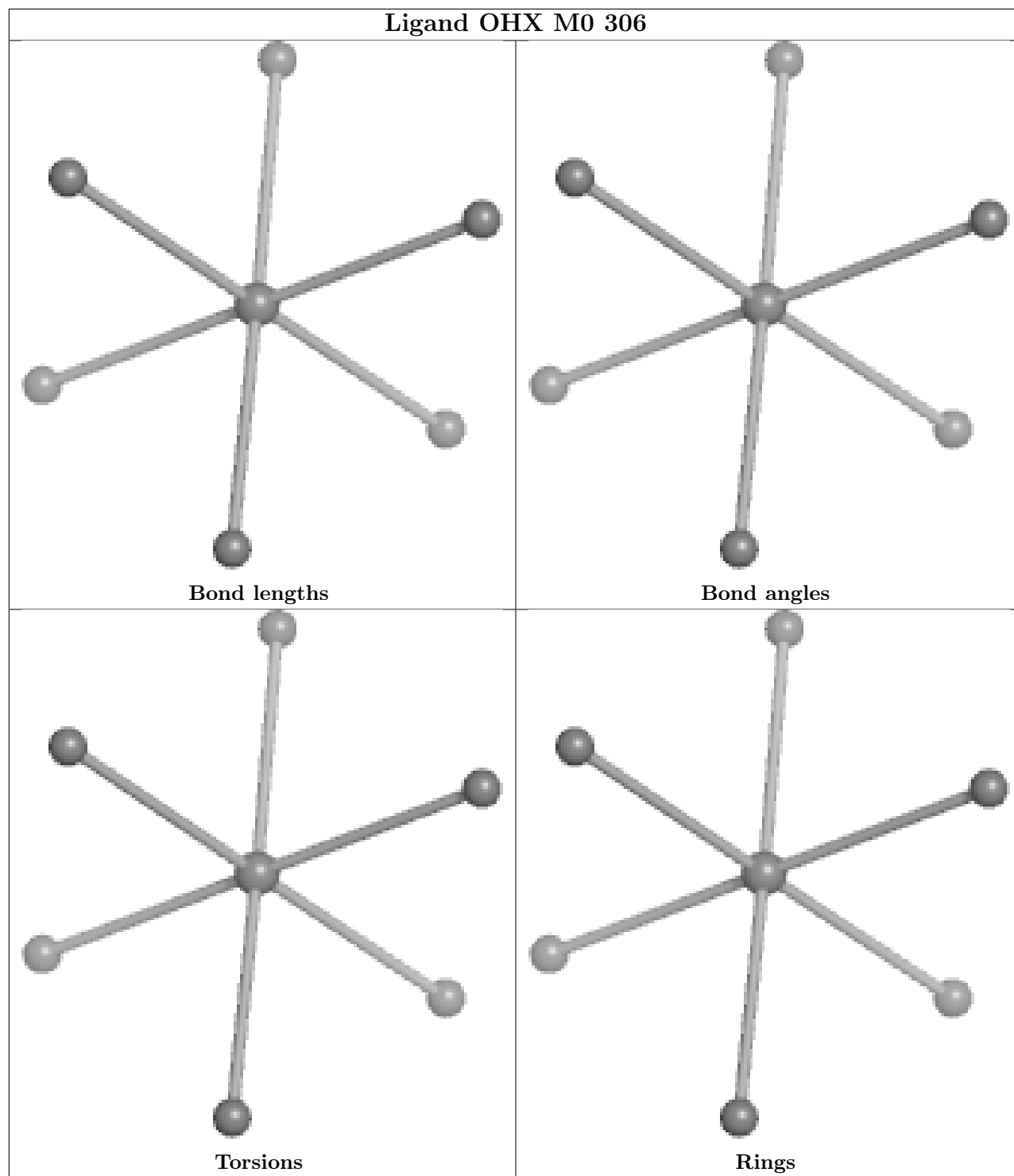


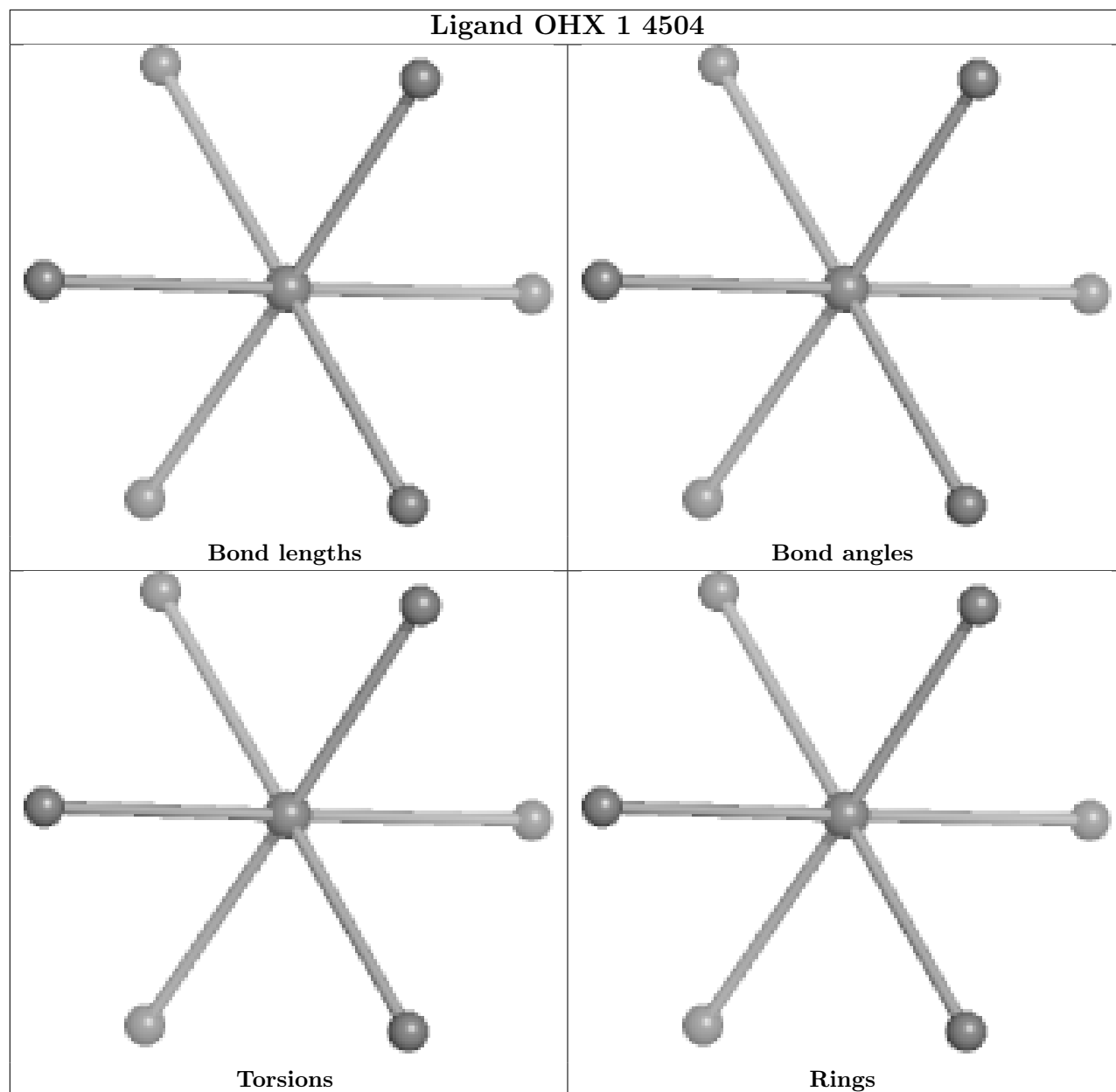


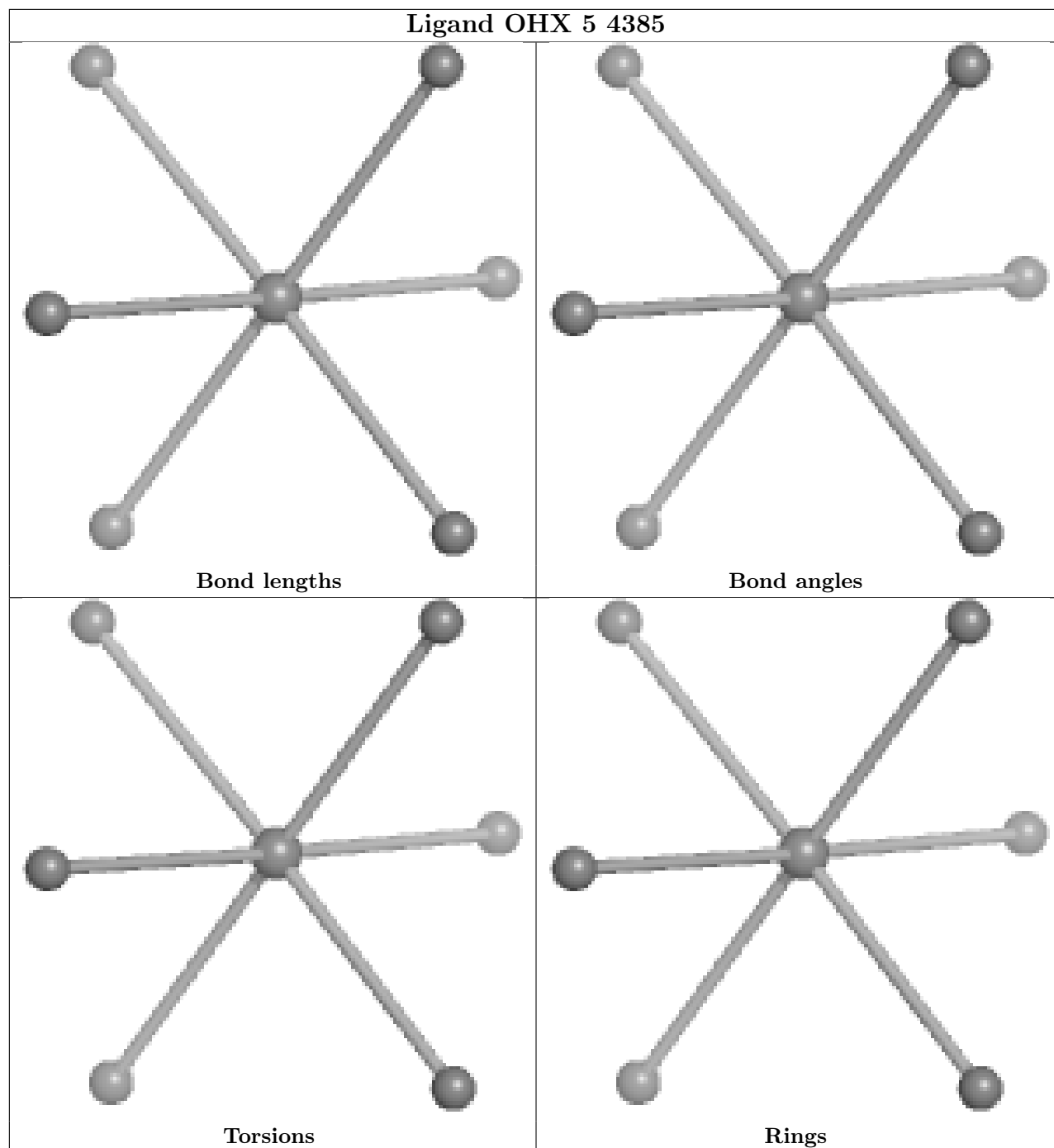


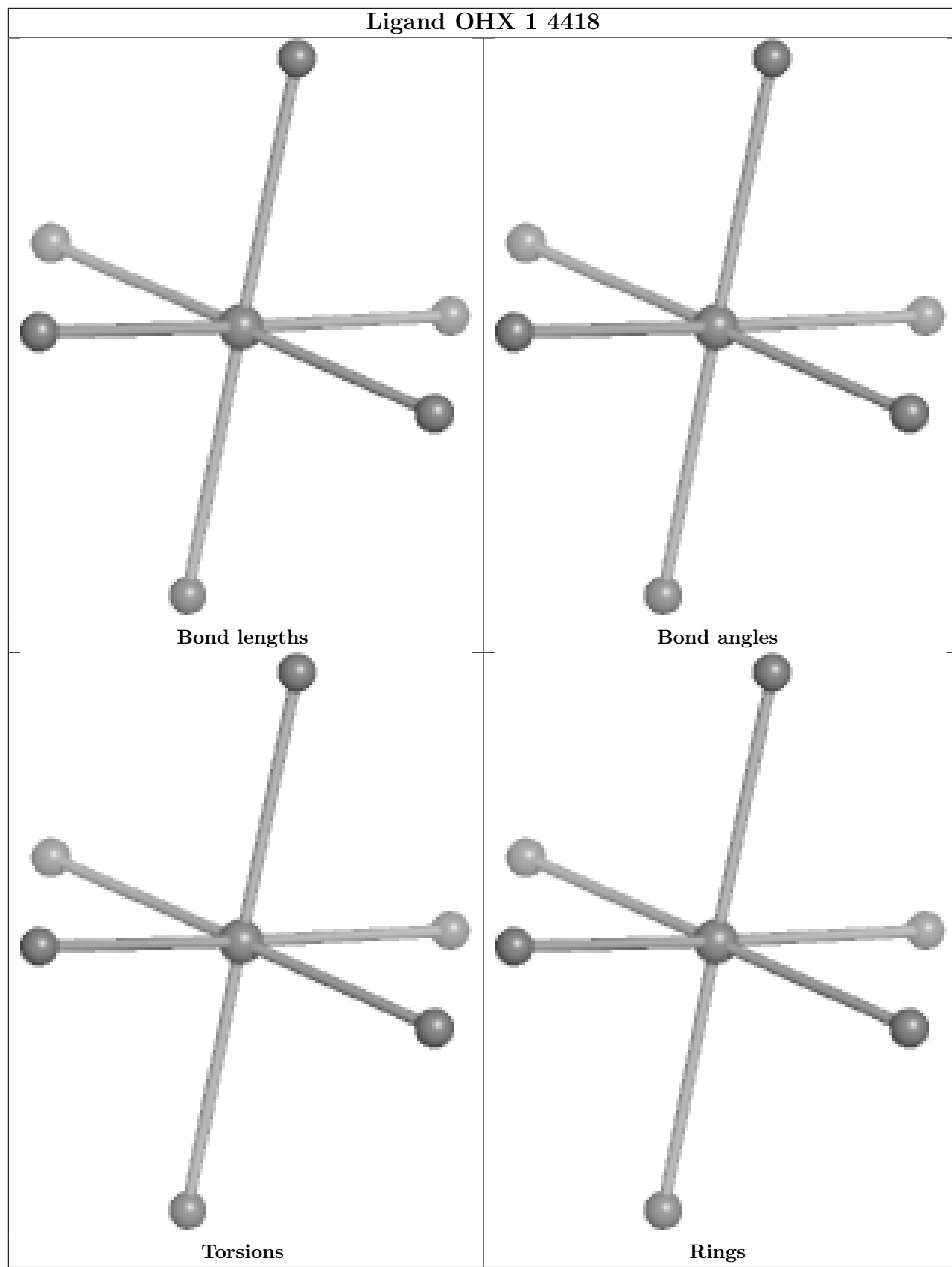


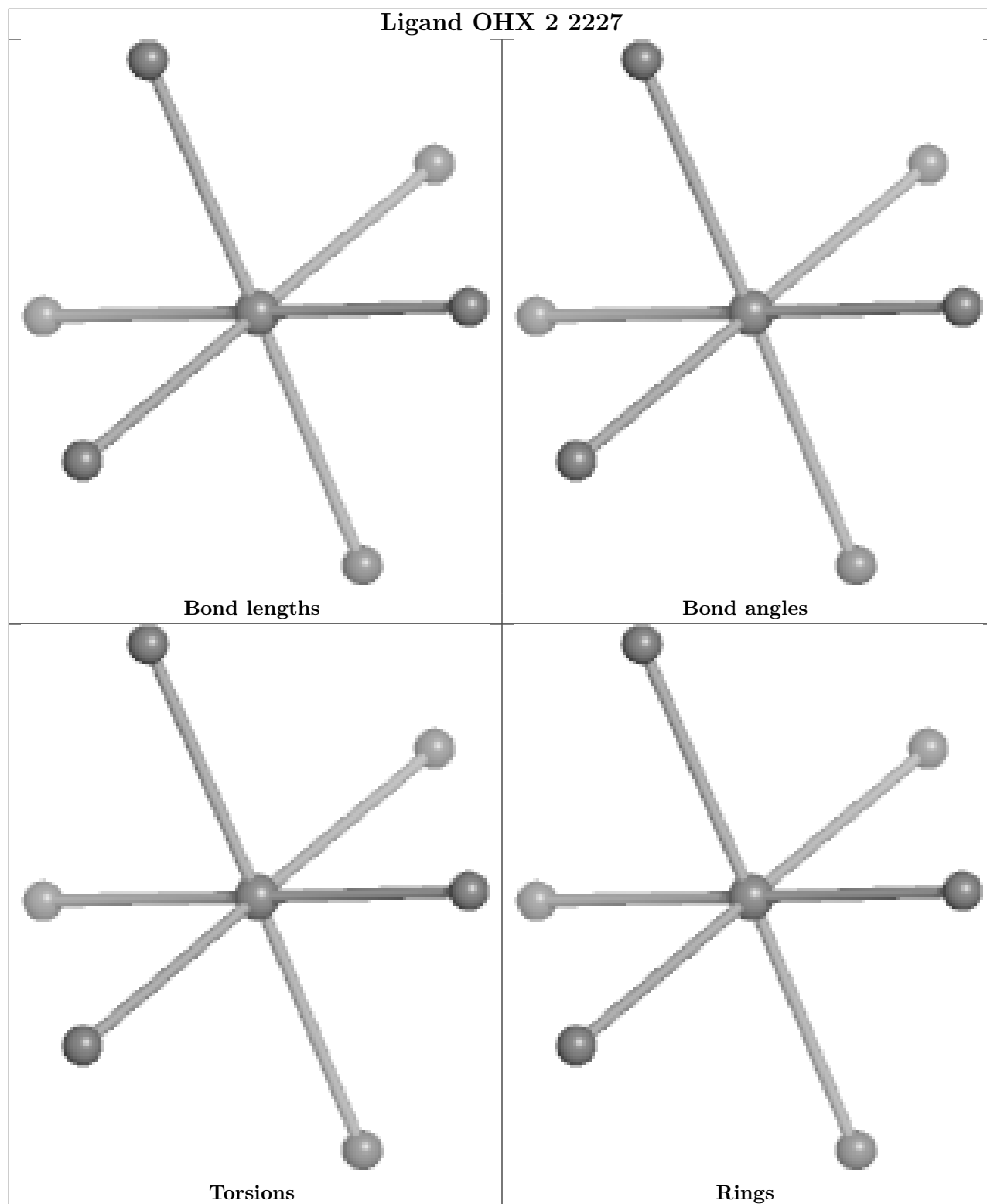
Ligand OHX M0 306

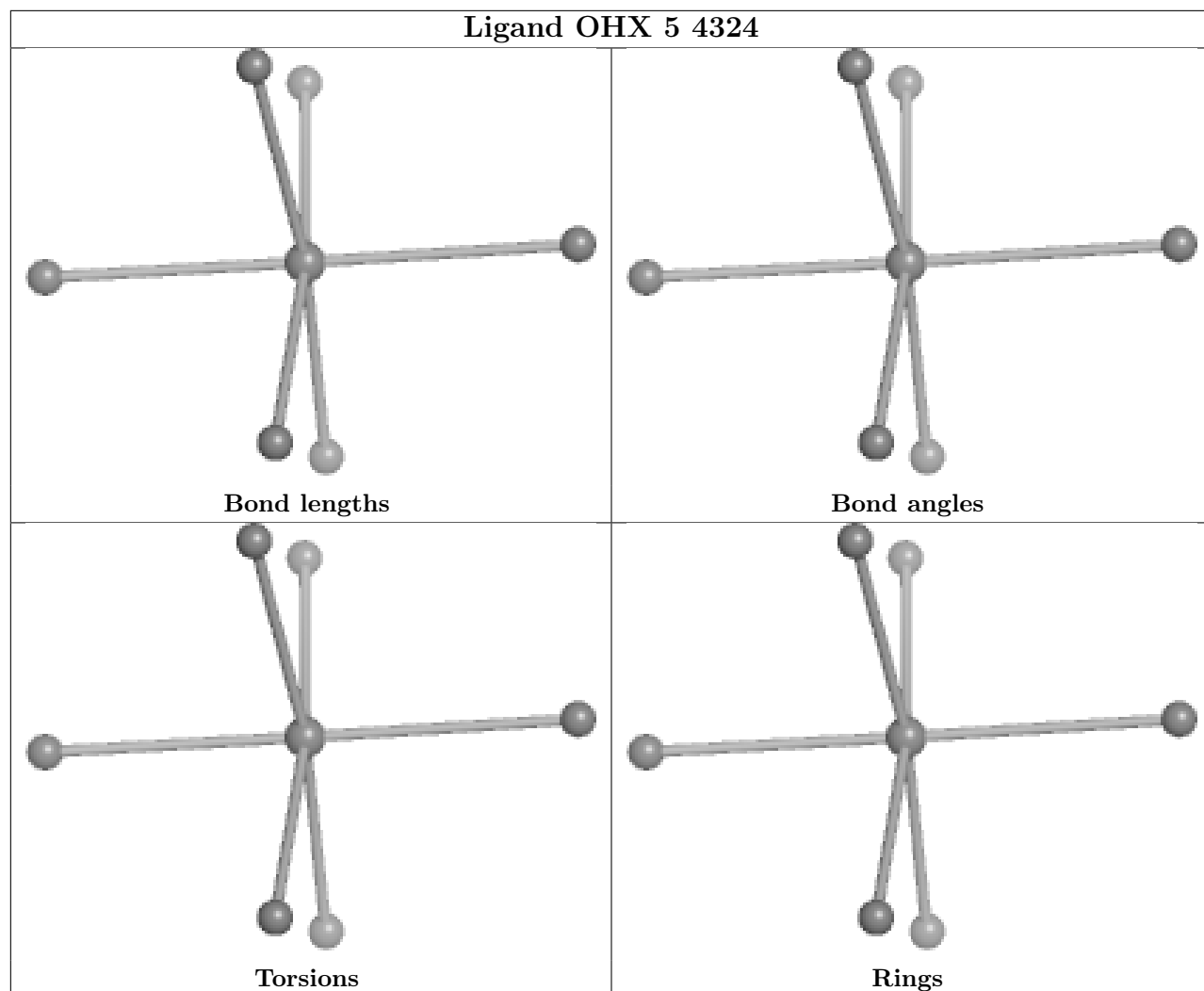


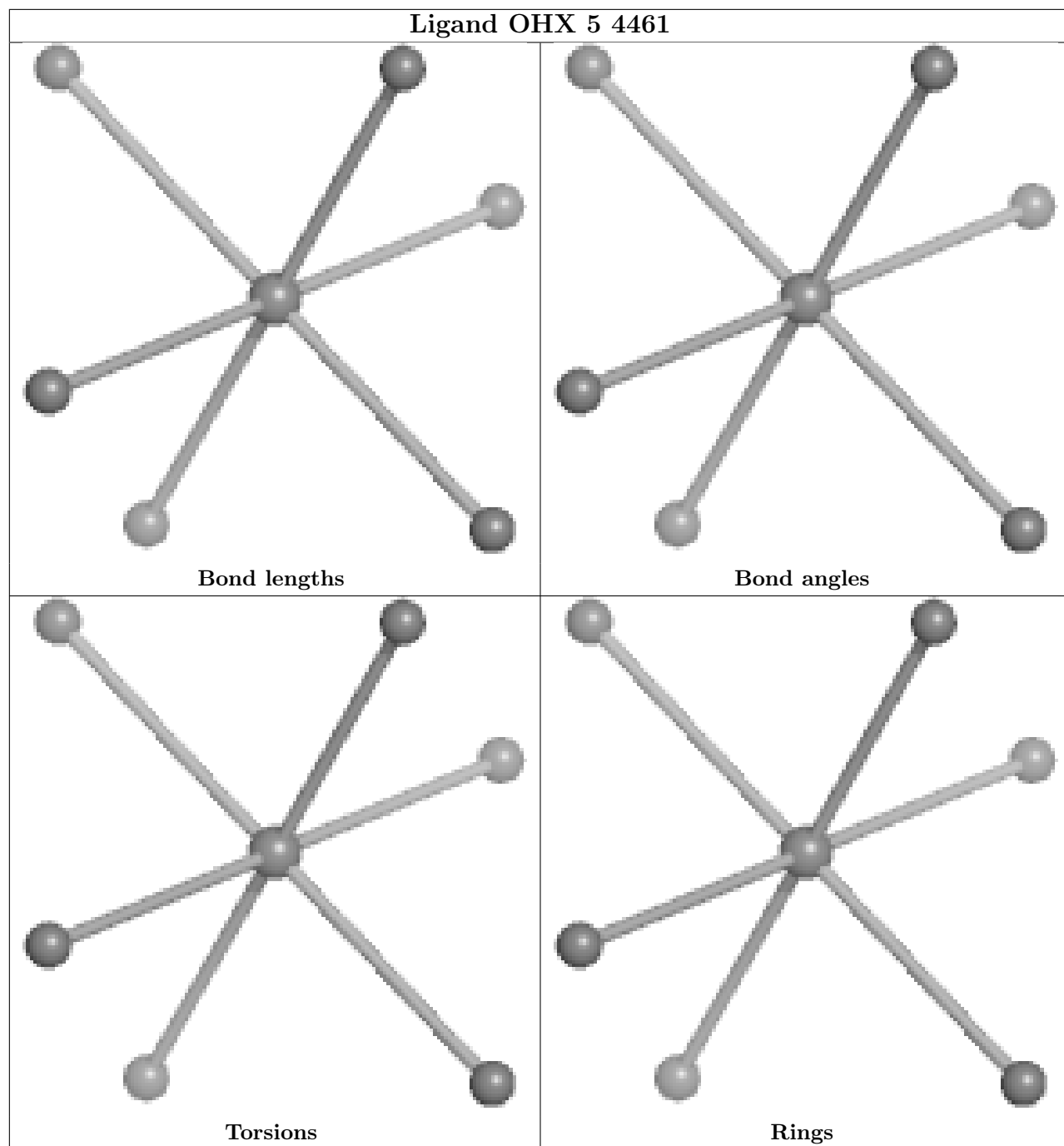


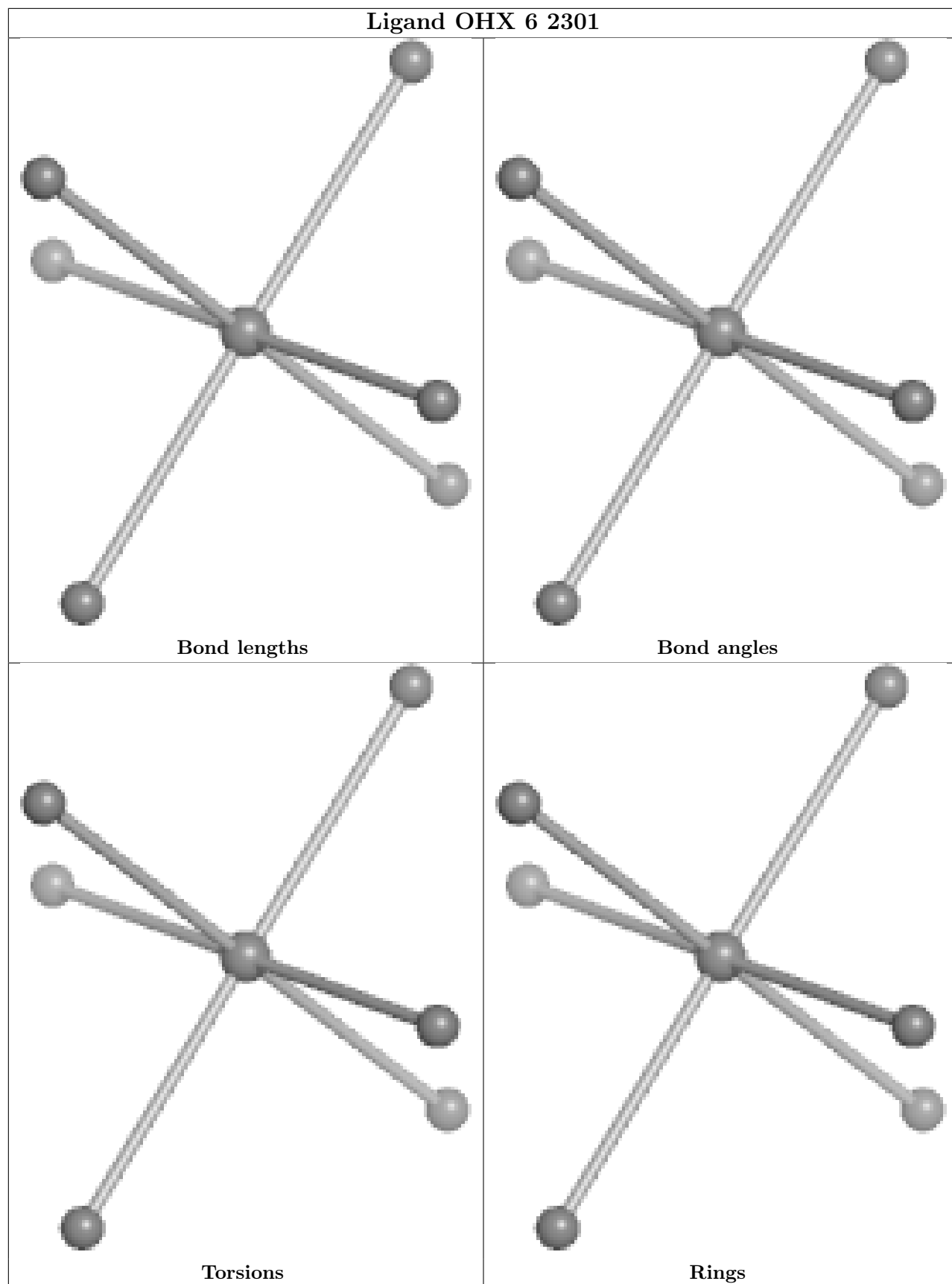


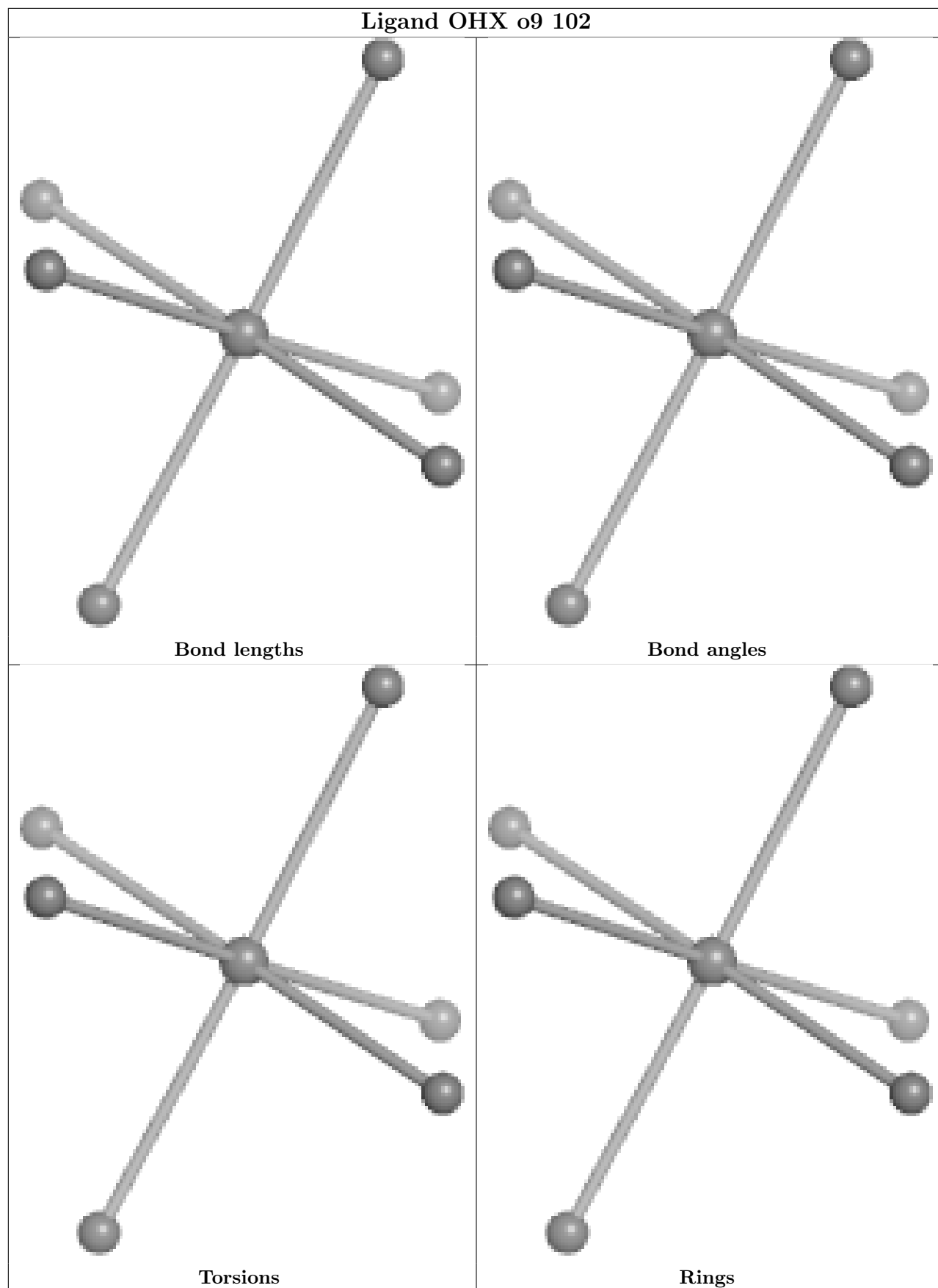


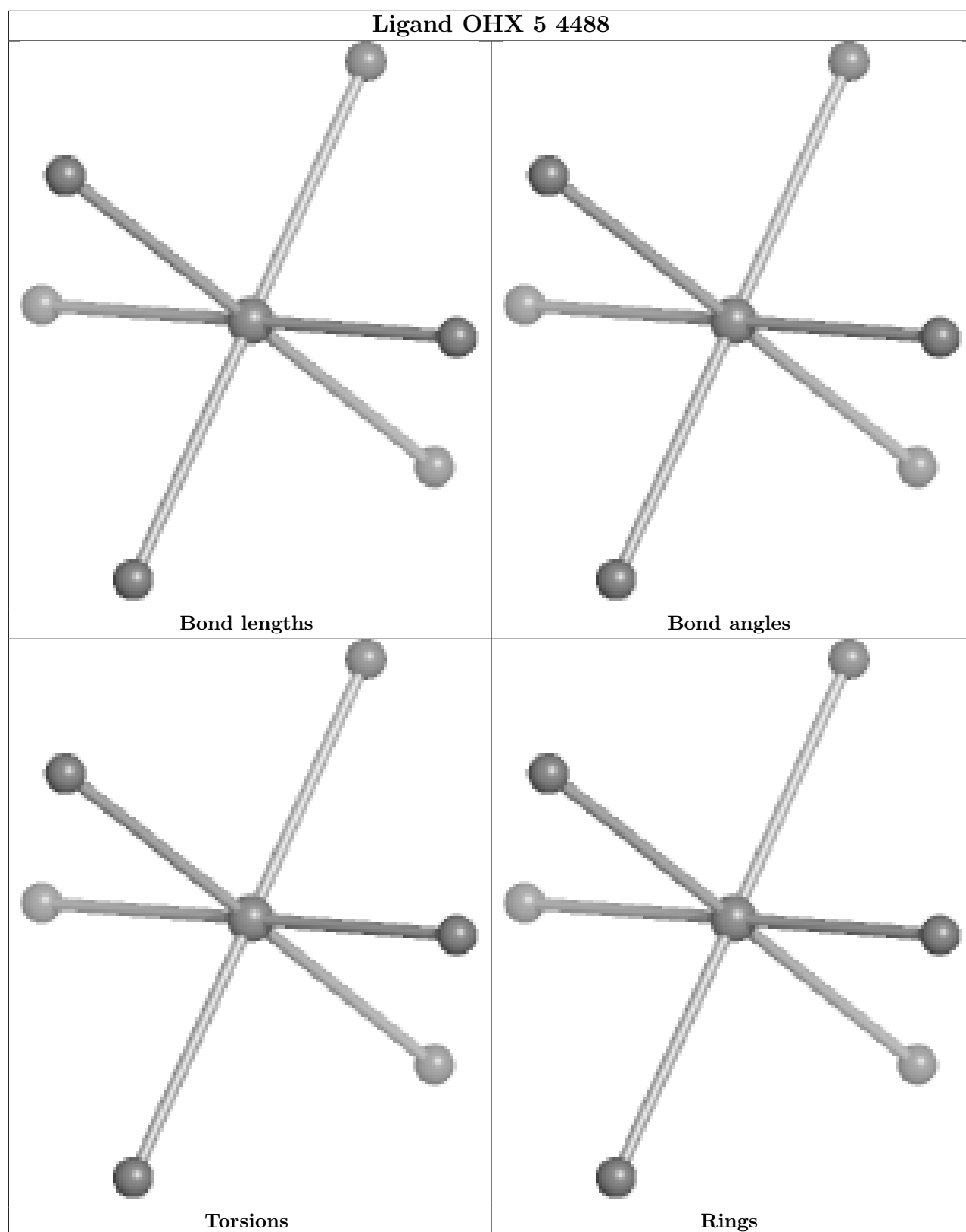


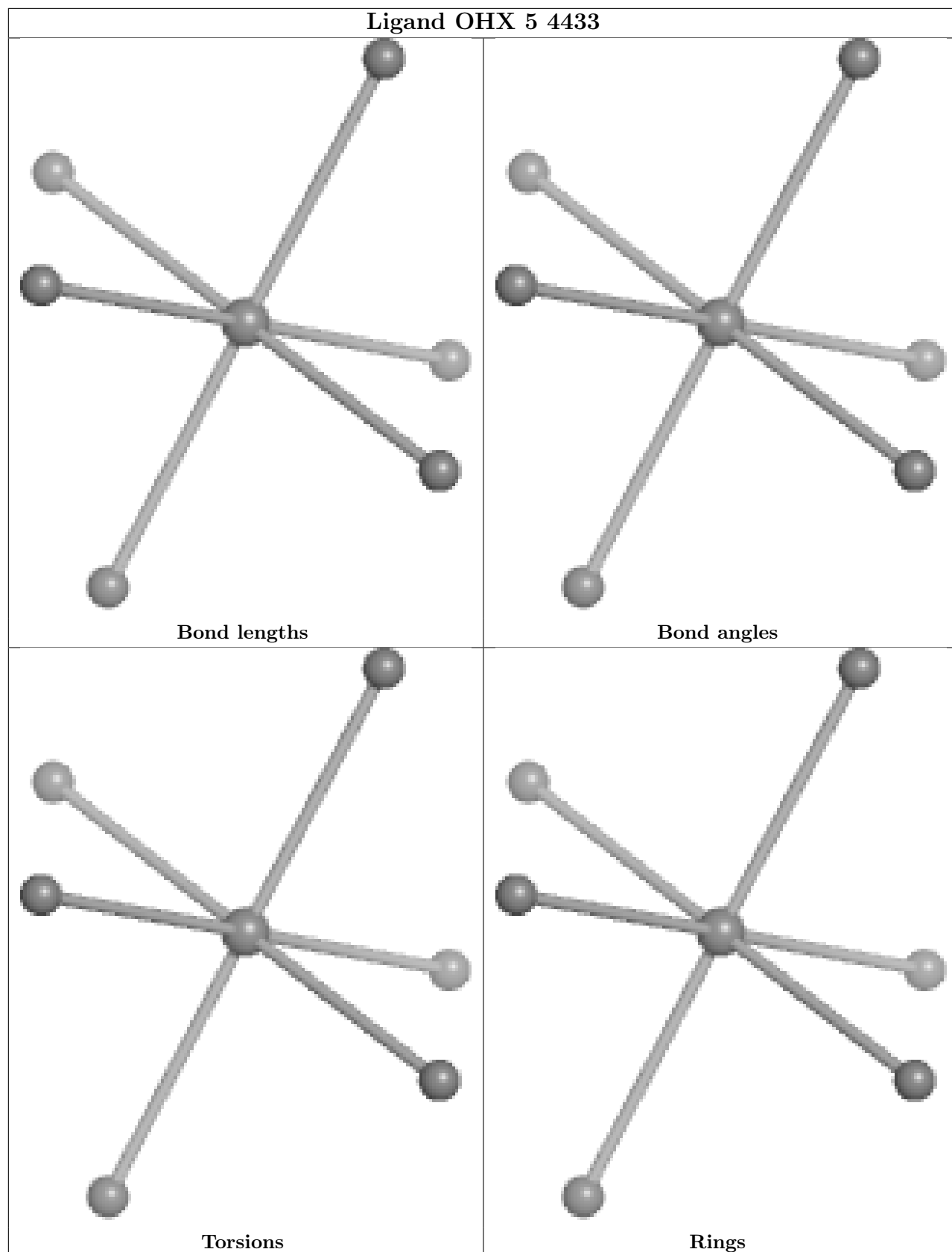


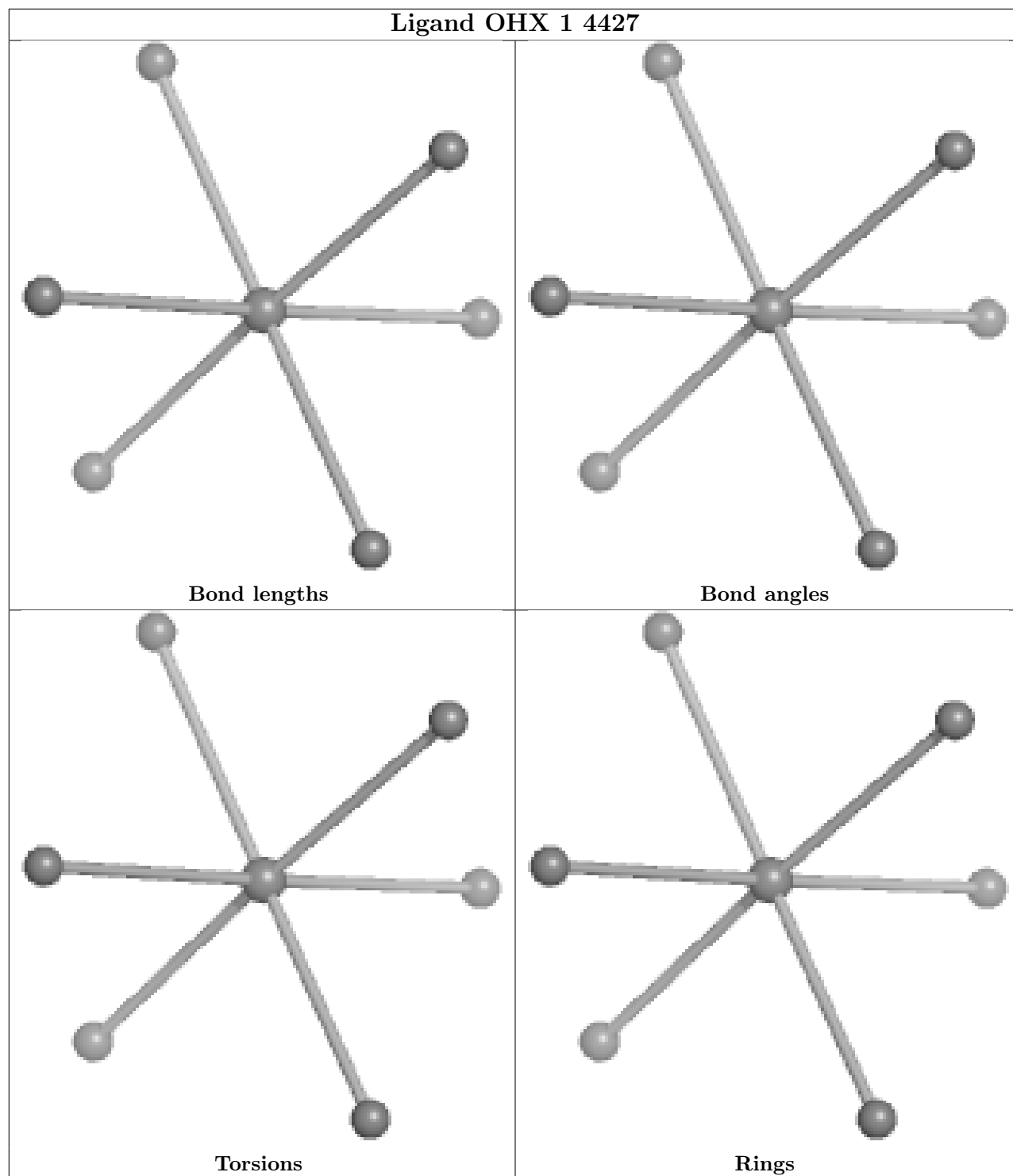


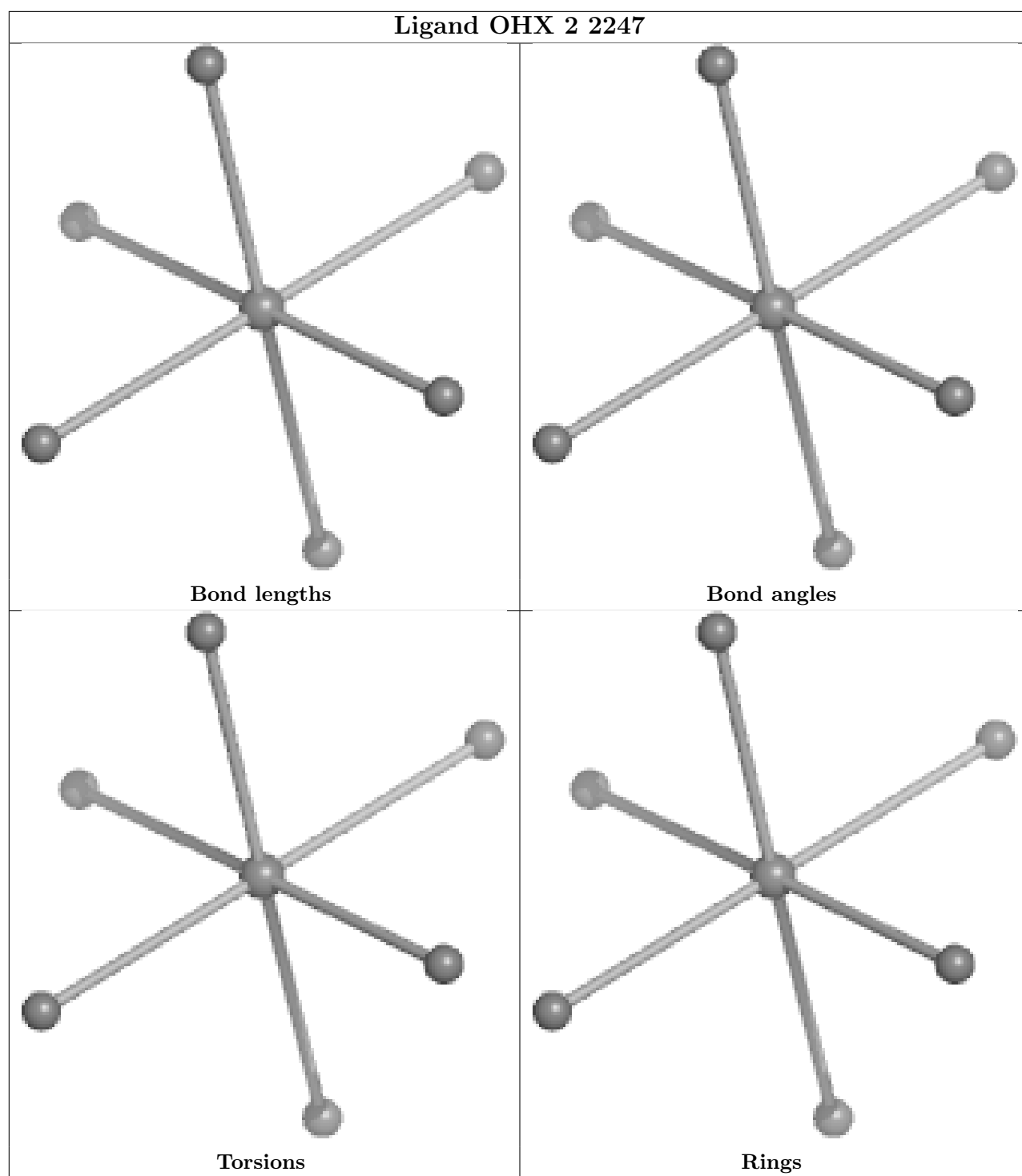


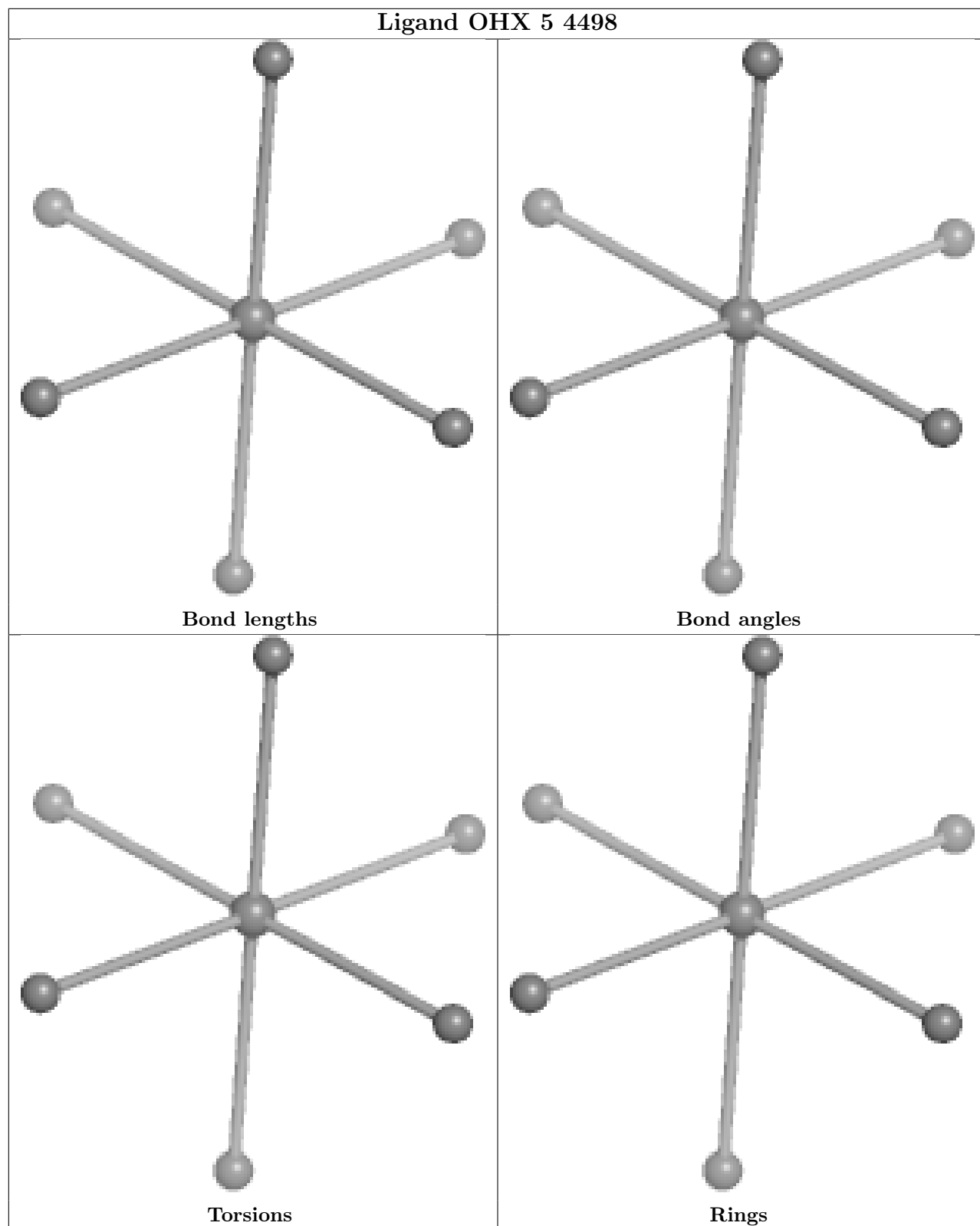


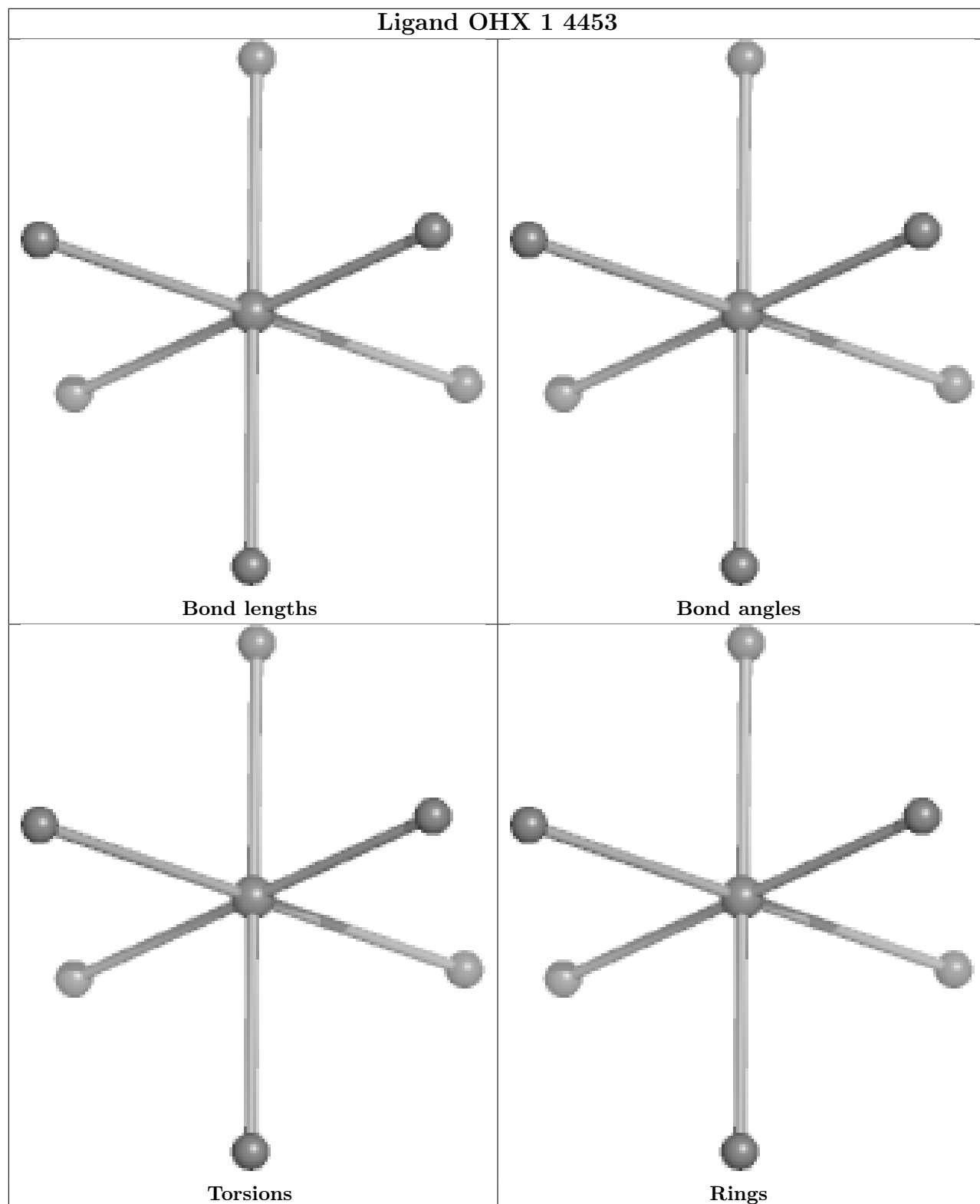


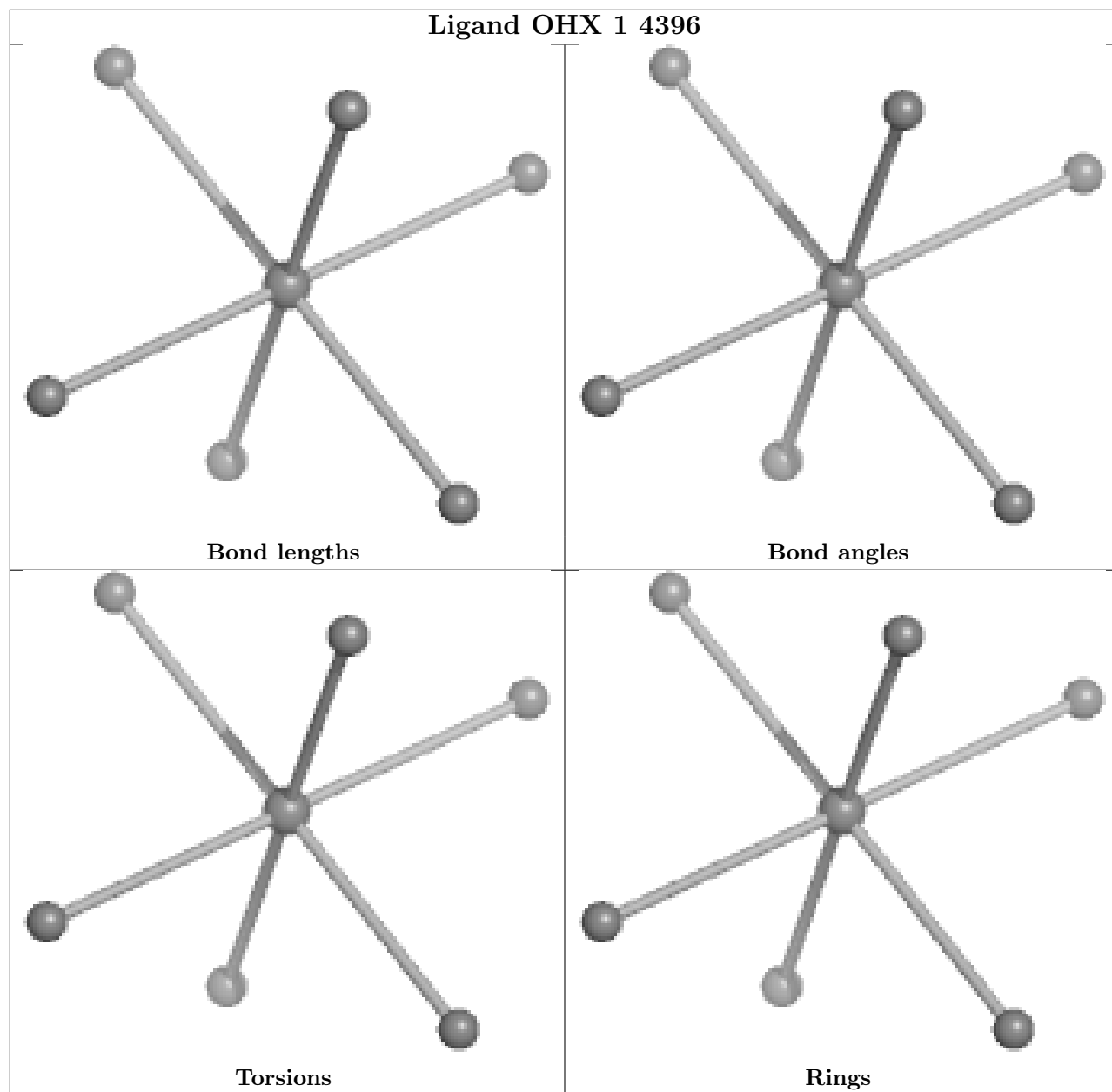


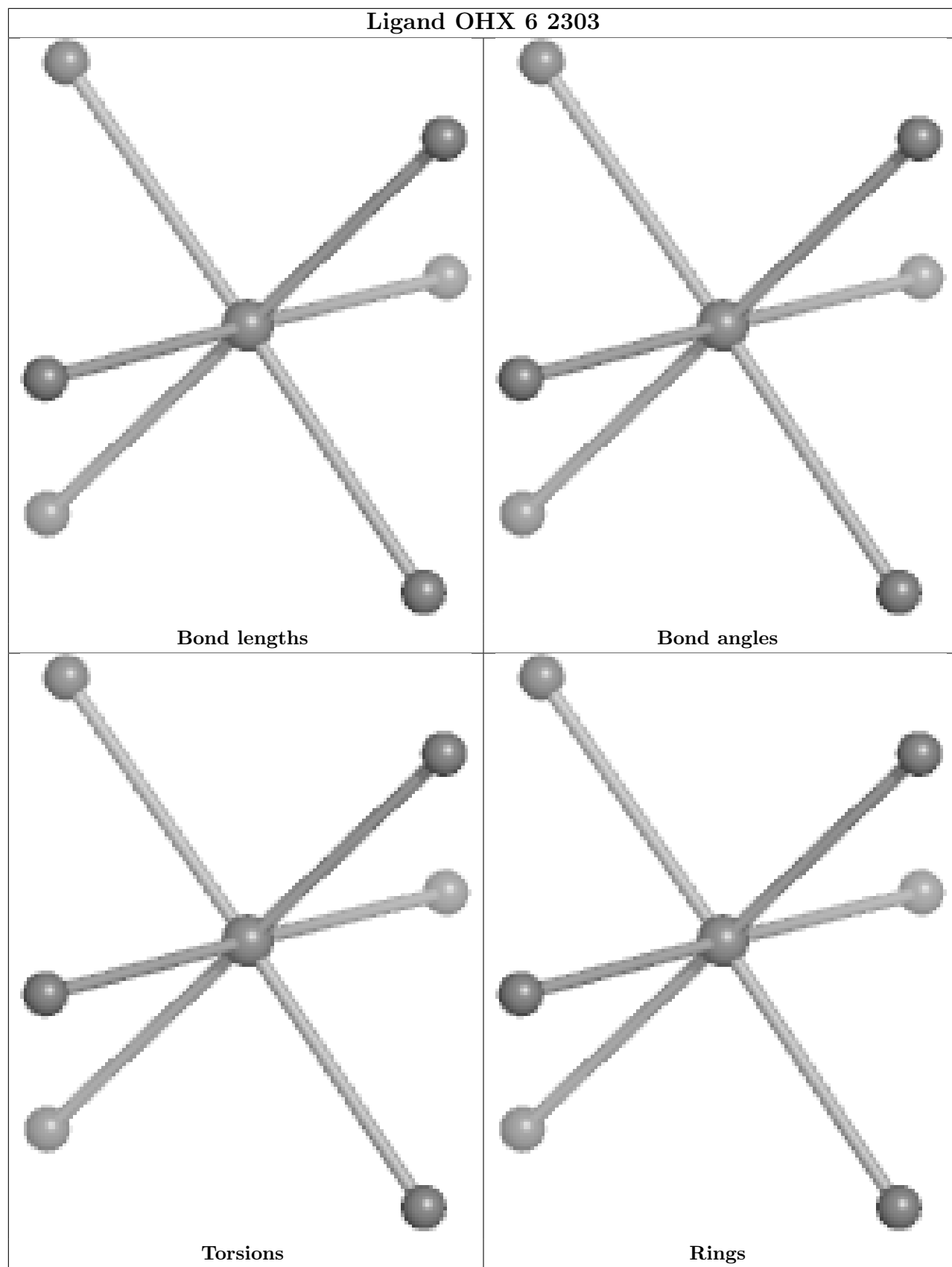


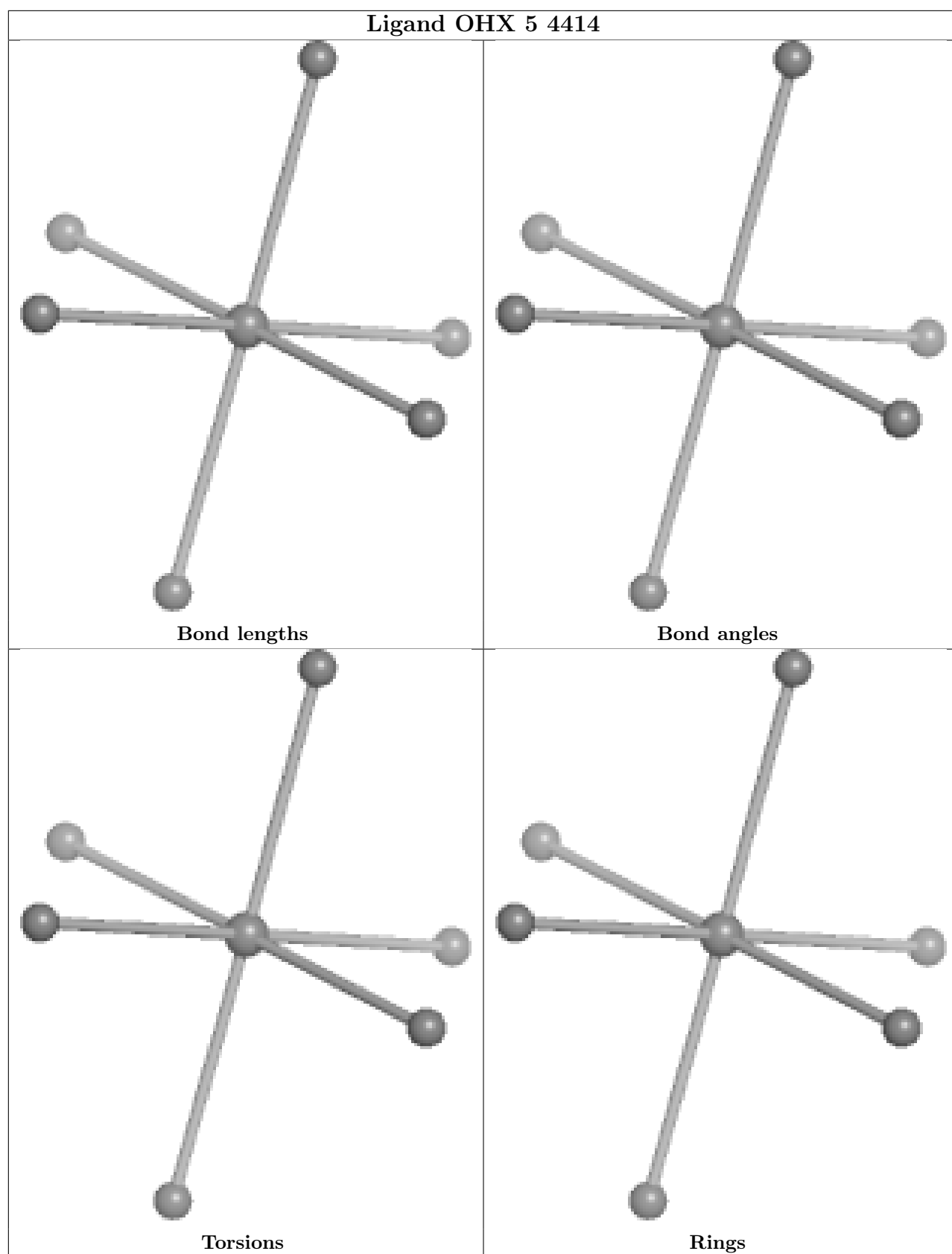


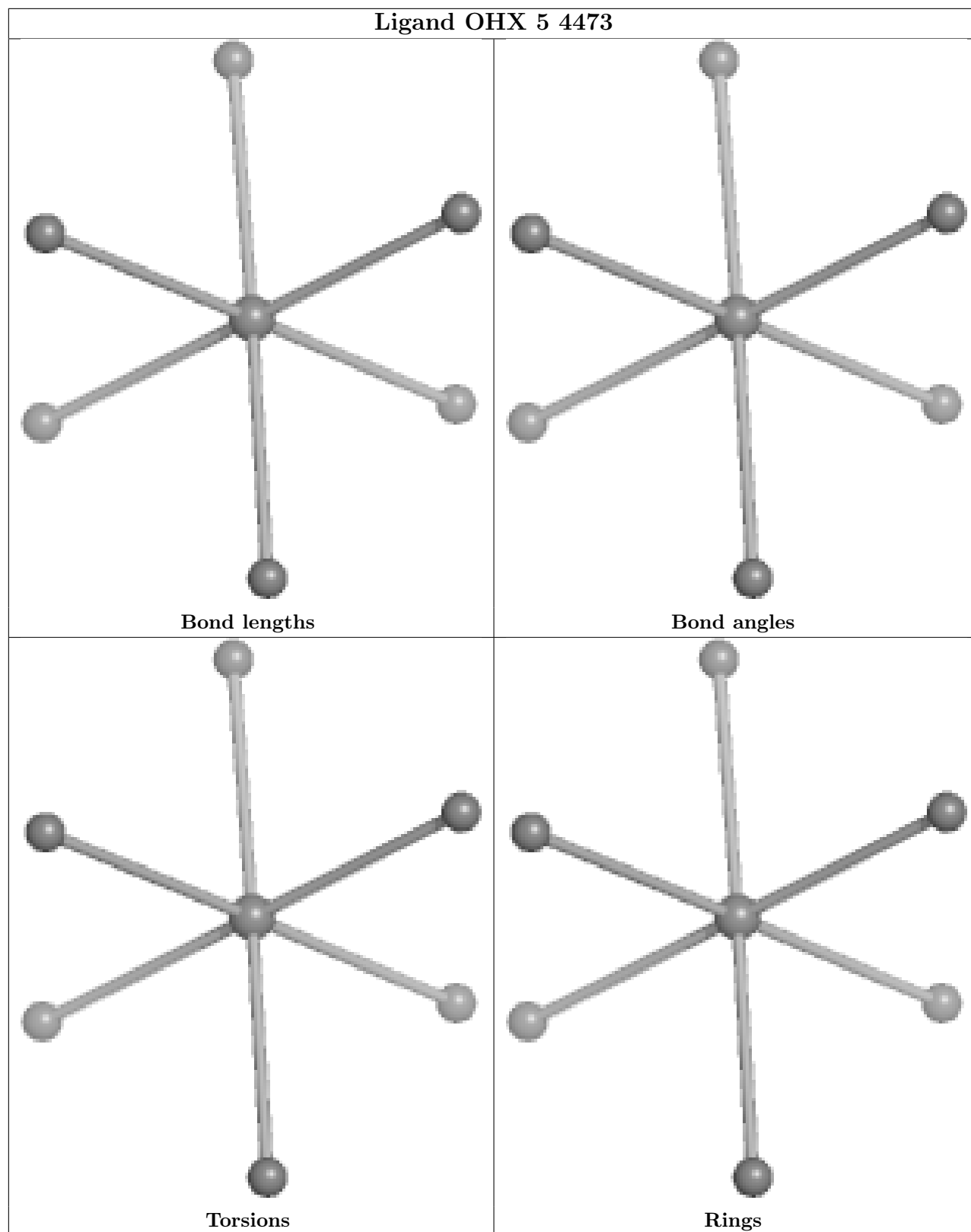


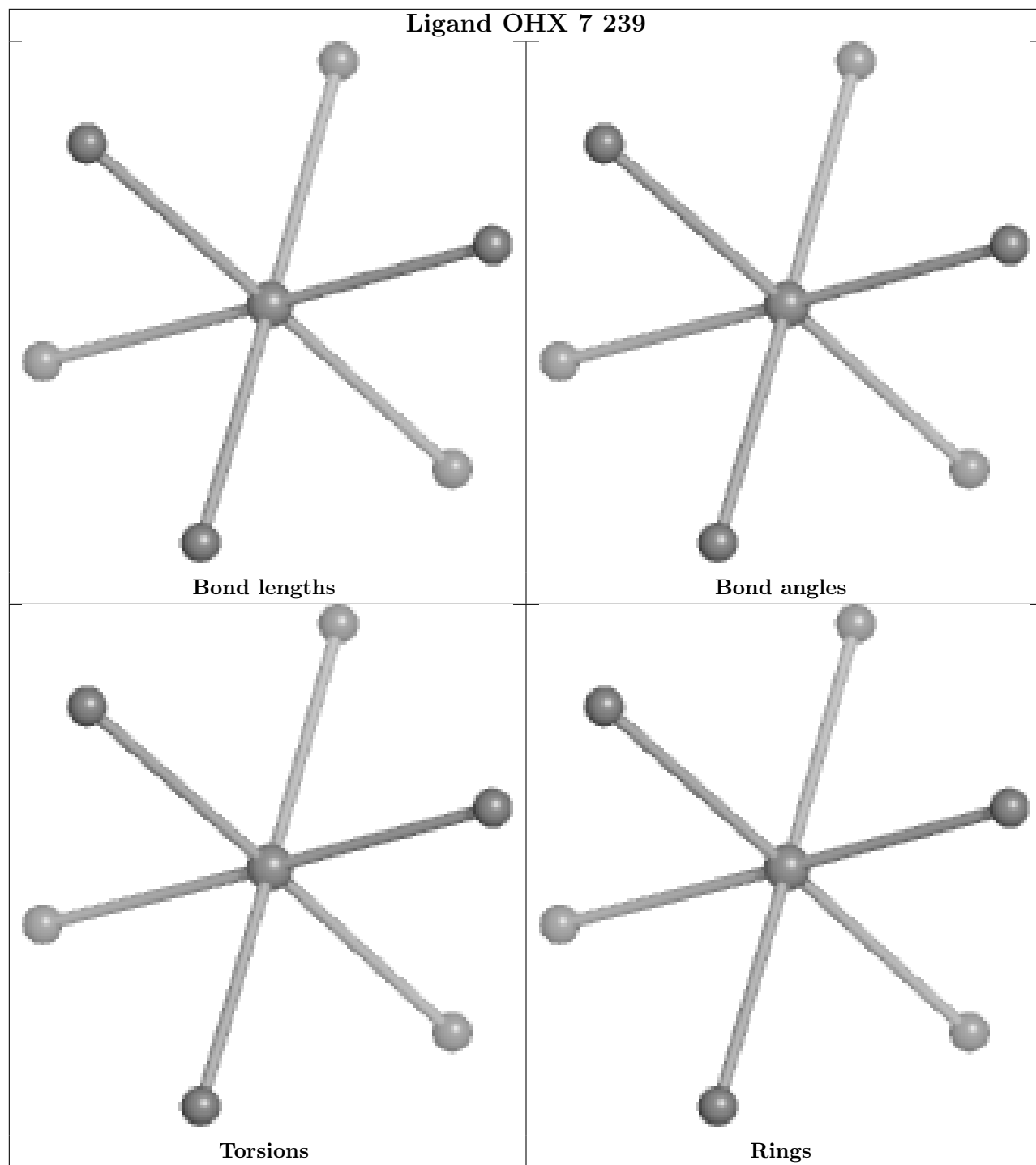


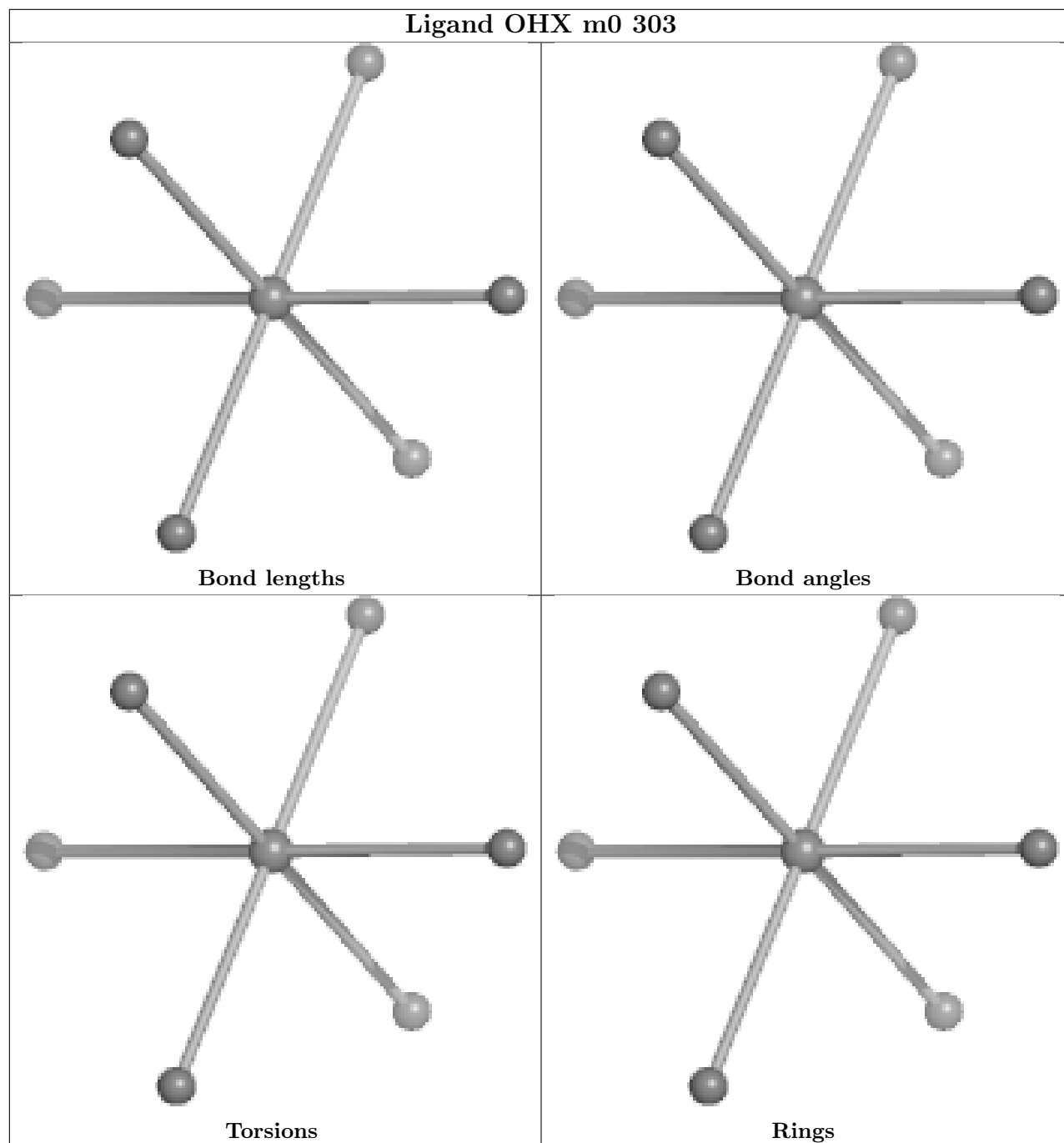


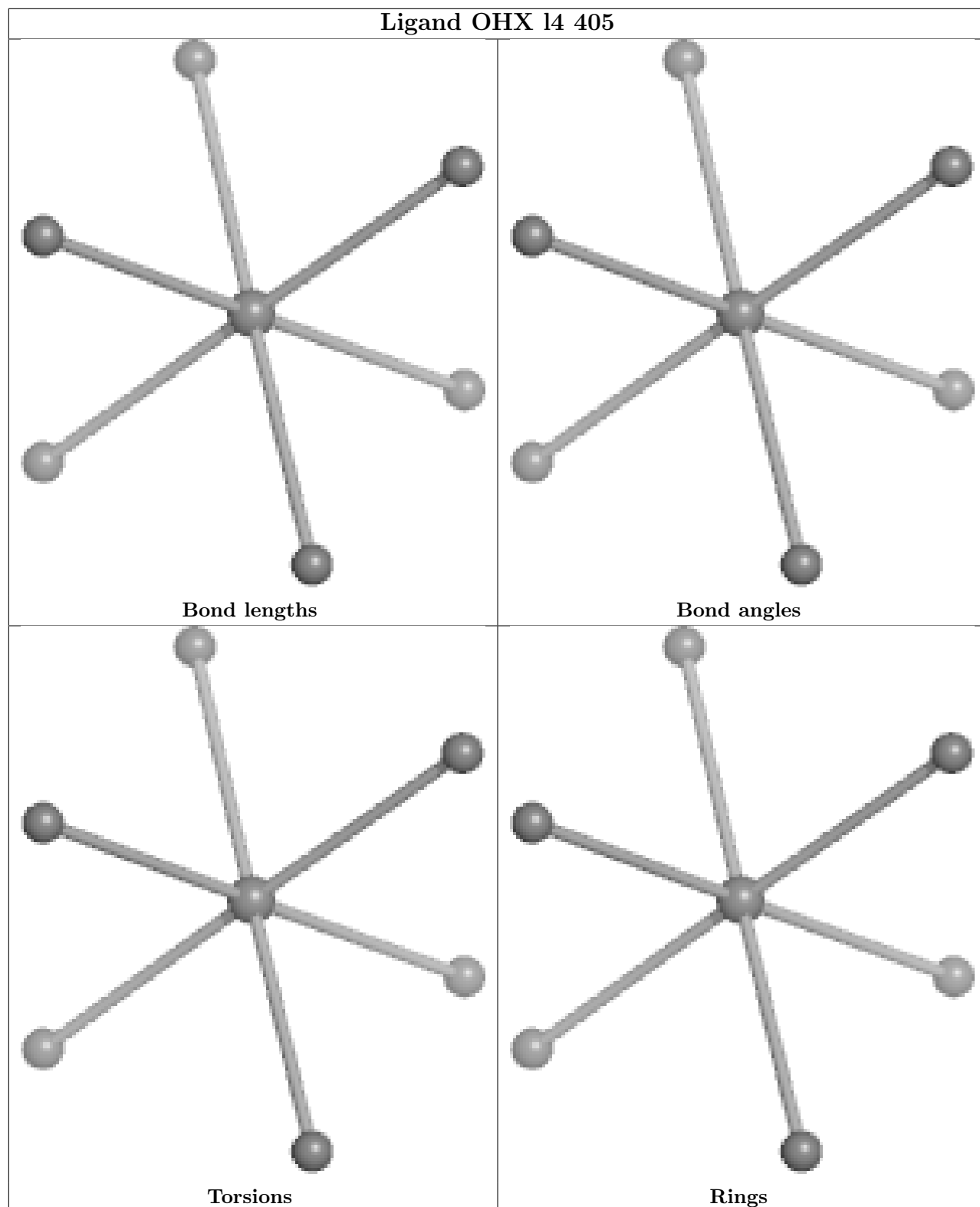


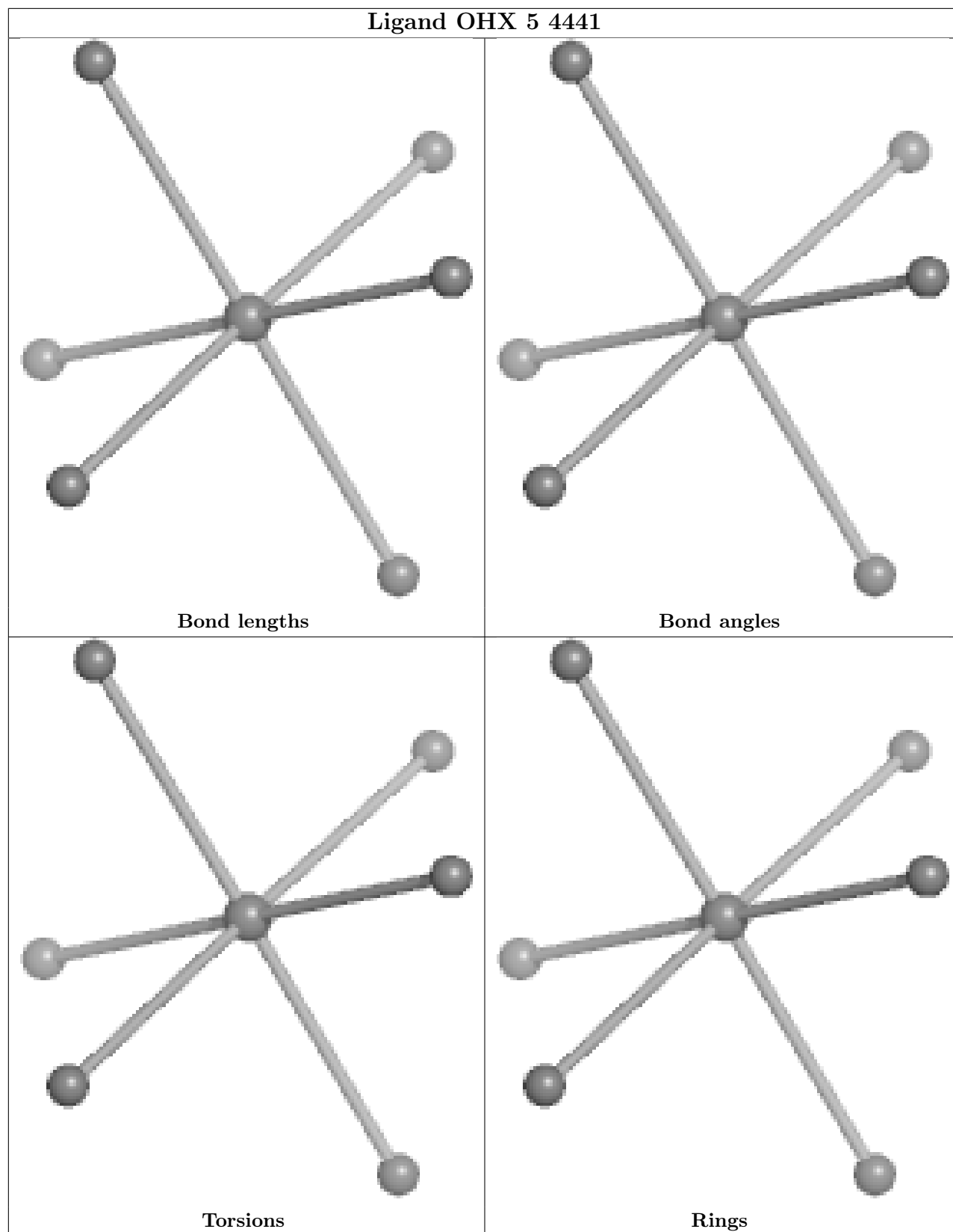


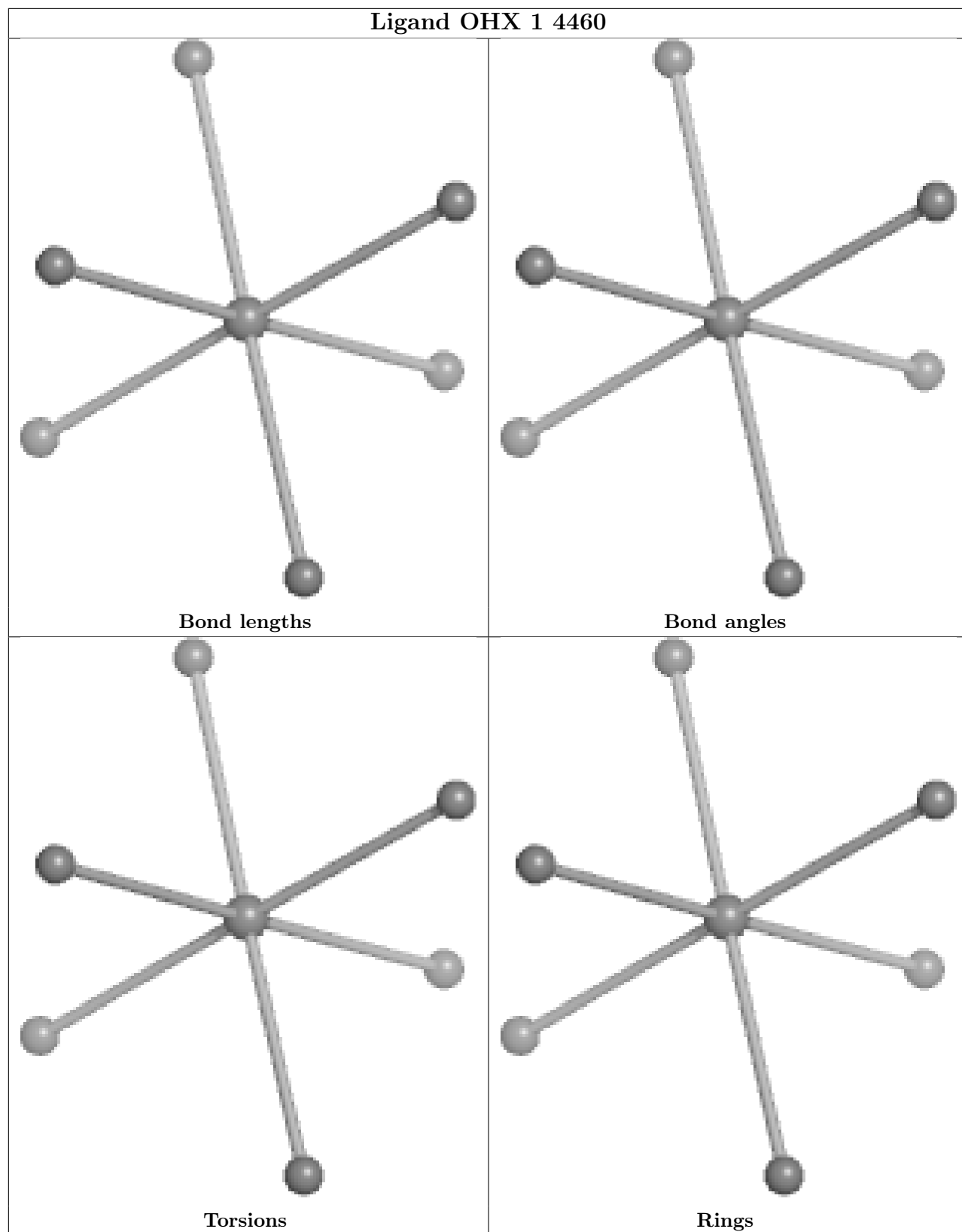


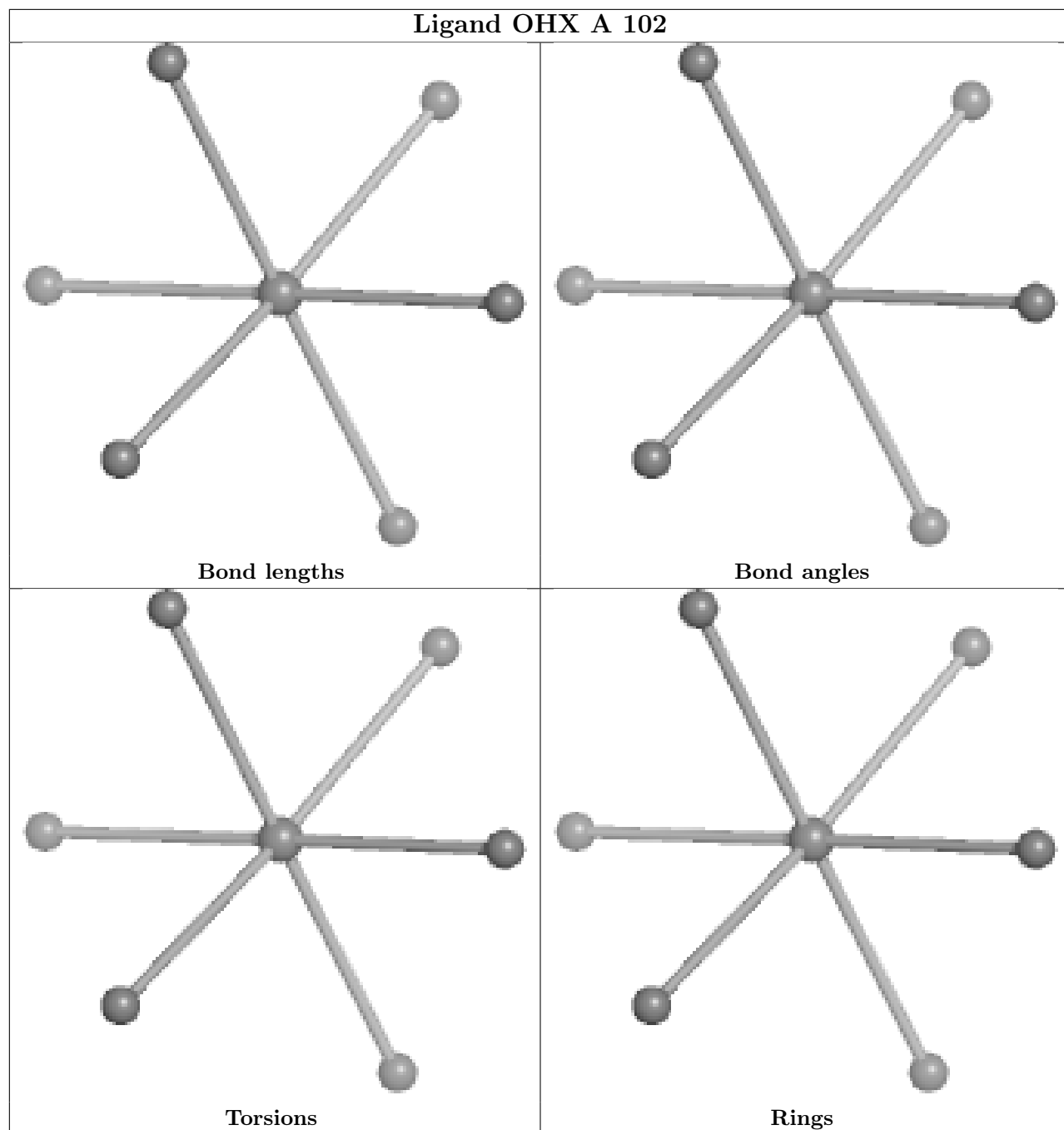


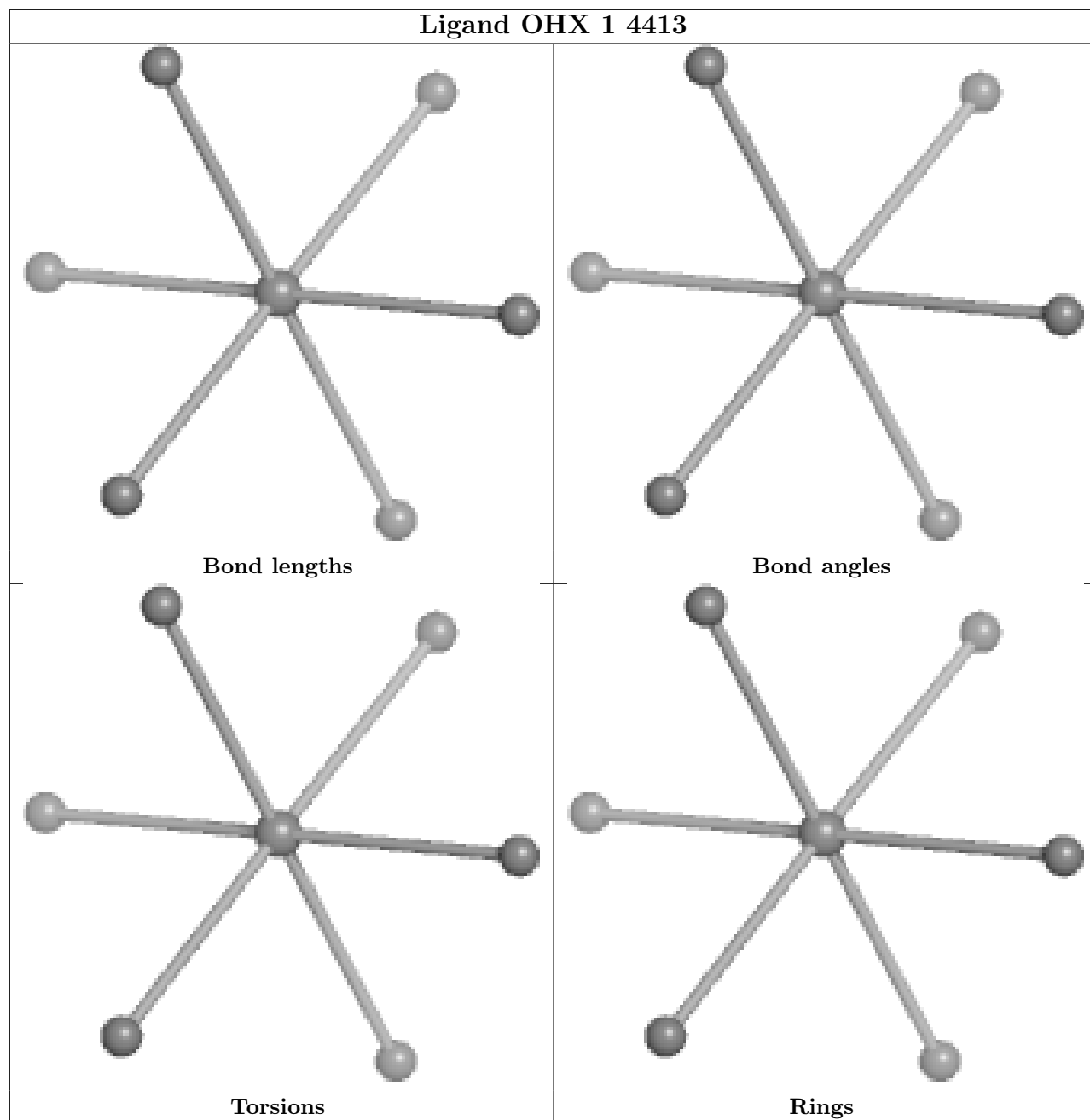


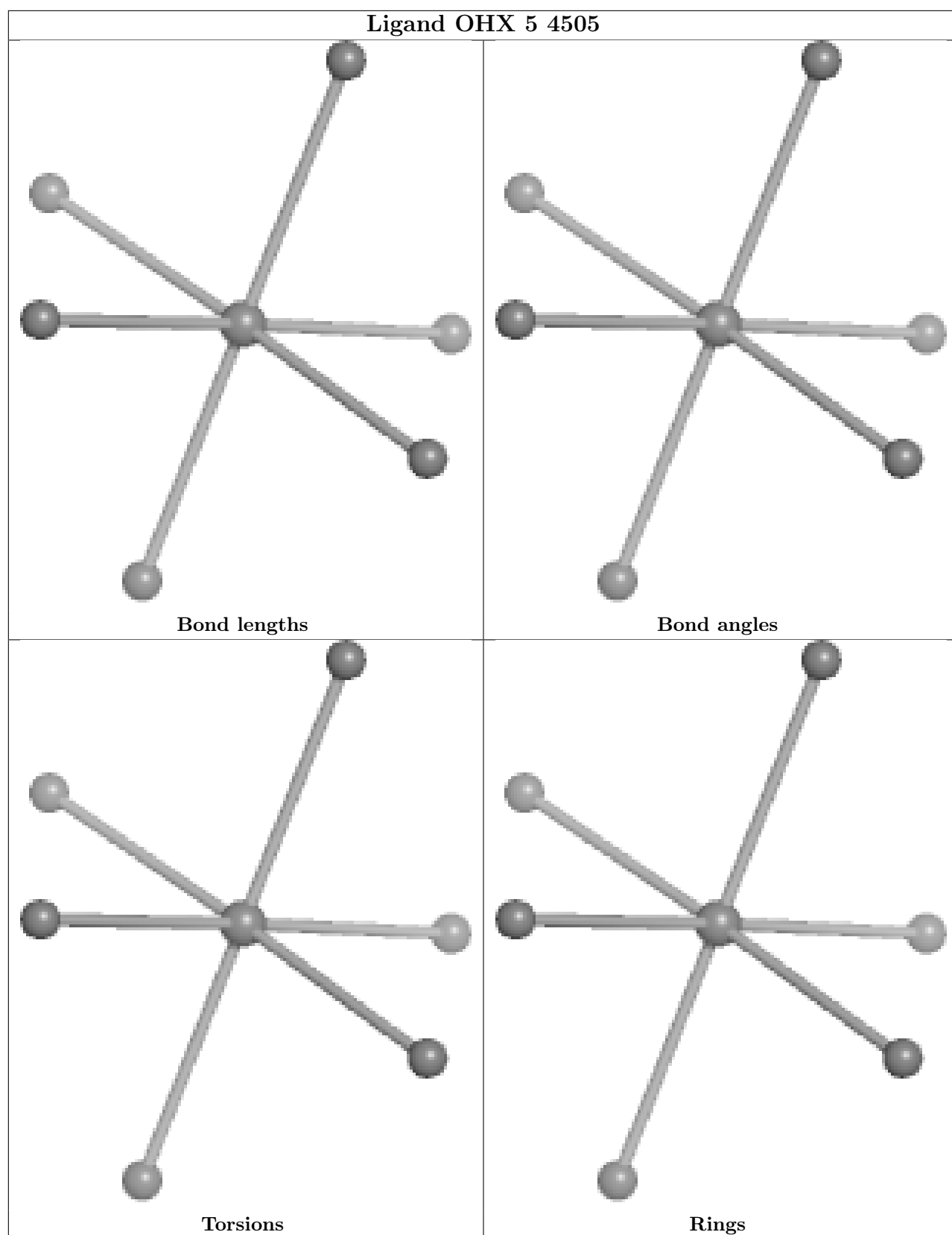












5.7 Other polymers [i](#)

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
84	sM	2
86	m2	2
35	SM	1
80	c0	1
1	2	1
6	s4	1
42	l5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	43.93
1	sM	139:UNK	C	155:UNK	N	38.21
1	SM	141:ALA	C	151:UNK	N	26.51
1	c0	84:UNK	C	87:UNK	N	7.82
1	2	1716:C	O3'	1717:G	P	3.78
1	m2	23:UNK	C	28:UNK	N	3.12
1	m2	52:UNK	C	54:UNK	N	3.12
1	s4	82:TYR	C	83:PRO	N	1.20
1	l5	179:ARG	C	180:PHE	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	2	1781/1800 (98%)	-0.12	38 (2%)	63	49	43, 101, 181, 226	1 (0%)
1	6	1795/1800 (99%)	-0.19	22 (1%)	76	63	37, 93, 167, 227	1 (0%)
2	S0	206/206 (100%)	0.48	12 (5%)	30	24	106, 120, 129, 135	0
2	s0	206/206 (100%)	0.40	7 (3%)	48	36	91, 107, 119, 120	0
3	S1	214/216 (99%)	0.72	15 (7%)	24	19	112, 144, 166, 170	0
3	s1	216/216 (100%)	0.24	7 (3%)	50	37	89, 100, 117, 126	0
4	S2	217/217 (100%)	0.35	4 (1%)	67	53	88, 100, 114, 121	0
4	s2	217/217 (100%)	0.39	10 (4%)	38	28	75, 90, 101, 110	0
5	S3	223/223 (100%)	0.50	7 (3%)	51	38	95, 105, 125, 136	0
5	s3	223/223 (100%)	0.44	8 (3%)	46	34	93, 115, 133, 138	0
6	S4	260/260 (100%)	0.10	1 (0%)	89	82	77, 102, 112, 131	0
6	s4	260/260 (100%)	0.08	3 (1%)	76	63	62, 90, 105, 125	0
7	S5	206/206 (100%)	0.47	10 (4%)	36	27	105, 121, 131, 140	0
7	s5	206/206 (100%)	0.53	13 (6%)	27	22	97, 116, 131, 137	0
8	S6	226/226 (100%)	0.69	18 (7%)	20	17	80, 112, 126, 133	0
8	s6	218/226 (96%)	0.30	5 (2%)	61	46	65, 92, 110, 121	0
9	S7	184/186 (98%)	1.01	22 (11%)	10	9	100, 124, 149, 154	0
9	s7	186/186 (100%)	0.85	21 (11%)	11	10	84, 115, 139, 144	0
10	S8	188/199 (94%)	0.25	4 (2%)	63	49	74, 89, 121, 132	0
10	s8	188/199 (94%)	0.41	9 (4%)	36	27	61, 83, 121, 139	0
11	S9	185/185 (100%)	0.65	14 (7%)	21	18	92, 109, 138, 156	0
11	s9	185/185 (100%)	0.55	8 (4%)	40	30	77, 95, 122, 136	0
12	C0	83/96 (86%)	0.40	5 (6%)	29	23	98, 116, 126, 129	0
13	C1	146/155 (94%)	0.34	6 (4%)	42	31	76, 86, 106, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	c1	146/155 (94%)	0.60	11 (7%) 22 18	66, 81, 109, 129	0
14	C2	124/124 (100%)	0.74	6 (4%) 36 27	142, 150, 160, 162	0
15	C3	150/150 (100%)	0.45	3 (2%) 64 51	84, 99, 113, 118	0
15	c3	150/150 (100%)	0.38	4 (2%) 56 42	75, 88, 104, 107	0
16	C4	127/128 (99%)	0.95	19 (14%) 6 6	87, 145, 156, 158	0
16	c4	128/128 (100%)	0.39	2 (1%) 70 57	72, 104, 112, 117	0
17	C5	124/131 (94%)	0.32	2 (1%) 70 57	92, 105, 122, 138	0
18	C6	141/142 (99%)	0.42	3 (2%) 63 49	94, 114, 118, 121	0
18	c6	142/142 (100%)	0.62	10 (7%) 24 19	91, 111, 122, 135	0
19	C7	120/125 (96%)	0.27	1 (0%) 82 72	103, 116, 136, 138	0
19	c7	117/125 (93%)	0.35	3 (2%) 57 43	98, 111, 126, 134	0
20	C8	145/145 (100%)	0.10	1 (0%) 84 75	89, 109, 134, 139	0
20	c8	145/145 (100%)	0.18	3 (2%) 63 49	91, 105, 125, 130	0
21	C9	143/143 (100%)	0.33	0 100 100	97, 109, 123, 130	0
21	c9	143/143 (100%)	0.35	5 (3%) 47 35	93, 105, 119, 128	0
22	D0	107/110 (97%)	0.93	9 (8%) 18 16	90, 117, 134, 136	0
22	d0	110/110 (100%)	0.74	11 (10%) 14 13	91, 121, 142, 148	0
23	D1	87/87 (100%)	0.28	3 (3%) 48 36	102, 110, 125, 131	0
23	d1	87/87 (100%)	0.05	0 100 100	87, 96, 116, 122	0
24	D2	129/129 (100%)	0.54	2 (1%) 70 57	86, 97, 103, 115	0
24	d2	129/129 (100%)	0.14	0 100 100	72, 82, 90, 98	0
25	D3	144/144 (100%)	0.31	4 (2%) 55 41	76, 81, 92, 104	0
25	d3	144/144 (100%)	0.28	8 (5%) 31 24	64, 69, 78, 90	0
26	D4	134/134 (100%)	0.41	4 (2%) 52 39	90, 110, 120, 125	0
26	d4	134/134 (100%)	0.36	2 (1%) 71 58	71, 94, 104, 110	0
27	D5	70/70 (100%)	0.29	1 (1%) 73 60	118, 130, 136, 138	0
27	d5	69/70 (98%)	0.30	1 (1%) 73 60	108, 121, 130, 131	0
28	D6	97/97 (100%)	1.14	13 (13%) 8 8	94, 110, 156, 157	0
28	d6	97/97 (100%)	0.51	2 (2%) 63 49	79, 92, 115, 120	0
29	D7	81/81 (100%)	0.63	3 (3%) 45 34	100, 113, 138, 141	0
29	d7	81/81 (100%)	0.63	5 (6%) 28 22	86, 100, 133, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
30	D8	63/63 (100%)	0.84	5 (7%)	20 17	115, 130, 137, 140	0
30	d8	63/63 (100%)	0.83	5 (7%)	20 17	111, 126, 132, 136	0
31	D9	53/53 (100%)	0.10	0	100 100	89, 93, 112, 118	0
31	d9	53/53 (100%)	0.19	0	100 100	90, 98, 126, 138	0
32	E0	60/62 (96%)	0.47	5 (8%)	19 16	82, 110, 134, 137	0
32	e0	62/62 (100%)	0.54	3 (4%)	36 27	73, 97, 118, 122	0
33	E1	71/76 (93%)	0.80	8 (11%)	11 10	111, 138, 149, 152	0
33	e1	76/76 (100%)	0.90	11 (14%)	7 7	115, 163, 180, 182	0
34	SR	318/318 (100%)	0.09	6 (1%)	66 52	110, 122, 134, 155	0
35	SM	133/159 (83%)	0.65	23 (17%)	5 4	70, 100, 131, 138	0
36	1	3149/3394 (92%)	-0.36	23 (0%)	84 75	44, 66, 136, 228	0
36	5	3150/3394 (92%)	-0.42	23 (0%)	84 75	43, 64, 129, 201	0
37	3	121/121 (100%)	-0.46	0	100 100	52, 83, 98, 103	0
37	7	121/121 (100%)	-0.52	1 (0%)	82 72	48, 67, 79, 86	0
38	4	158/158 (100%)	-0.52	1 (0%)	85 77	51, 67, 103, 140	0
38	8	158/158 (100%)	-0.49	2 (1%)	74 61	53, 73, 107, 132	0
39	L2	252/252 (100%)	0.20	7 (2%)	55 41	51, 67, 83, 90	0
39	l2	252/252 (100%)	0.23	8 (3%)	50 37	52, 69, 84, 93	0
40	L3	386/386 (100%)	-0.01	2 (0%)	87 80	49, 70, 82, 98	0
40	l3	386/386 (100%)	-0.19	5 (1%)	74 61	44, 58, 71, 88	0
41	L4	361/361 (100%)	0.03	15 (4%)	41 31	46, 62, 78, 81	0
41	l4	361/361 (100%)	0.26	19 (5%)	33 25	49, 66, 81, 90	0
42	L5	296/296 (100%)	0.19	8 (2%)	56 42	66, 90, 106, 125	0
42	l5	294/296 (99%)	-0.00	4 (1%)	73 60	56, 70, 91, 107	0
43	L6	156/175 (89%)	-0.12	1 (0%)	85 77	58, 66, 81, 92	0
43	l6	157/175 (89%)	-0.10	0	100 100	59, 66, 86, 97	0
44	L7	222/223 (99%)	-0.24	0	100 100	50, 58, 85, 115	0
44	l7	223/223 (100%)	-0.20	0	100 100	49, 58, 91, 116	0
45	L8	233/233 (100%)	0.48	10 (4%)	40 30	74, 88, 117, 122	0
46	L9	191/191 (100%)	0.37	10 (5%)	34 26	68, 78, 88, 98	0
46	l9	191/191 (100%)	-0.02	2 (1%)	79 68	54, 63, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	M0	211/220 (95%)	0.23	6 (2%) 55 41	55, 70, 100, 113	0
47	m0	213/220 (96%)	0.52	10 (4%) 37 28	51, 69, 89, 101	0
48	M1	169/169 (100%)	0.36	7 (4%) 42 31	78, 94, 104, 110	0
48	m1	169/169 (100%)	0.00	1 (0%) 85 77	61, 76, 85, 88	0
49	M3	193/194 (99%)	0.29	10 (5%) 34 26	49, 71, 105, 128	0
49	m3	194/194 (100%)	0.13	4 (2%) 63 49	52, 78, 112, 125	0
50	M4	136/137 (99%)	-0.04	1 (0%) 84 75	62, 69, 79, 88	0
50	m4	137/137 (100%)	-0.07	4 (2%) 54 40	57, 64, 81, 88	0
51	M5	203/203 (100%)	0.06	5 (2%) 58 44	50, 63, 74, 77	0
51	m5	203/203 (100%)	0.09	2 (0%) 79 68	54, 71, 82, 87	0
52	M6	197/197 (100%)	-0.11	3 (1%) 71 58	50, 58, 77, 81	0
52	m6	197/197 (100%)	-0.14	1 (0%) 87 80	44, 51, 77, 82	0
53	M7	183/183 (100%)	0.05	12 (6%) 26 21	53, 61, 108, 127	0
53	m7	155/183 (84%)	-0.31	0 100 100	49, 55, 67, 93	0
54	M8	185/185 (100%)	-0.12	1 (0%) 87 80	51, 62, 78, 93	0
54	m8	185/185 (100%)	-0.03	1 (0%) 87 80	51, 66, 77, 81	0
55	M9	188/188 (100%)	0.41	10 (5%) 33 25	70, 84, 147, 155	0
55	m9	188/188 (100%)	0.28	5 (2%) 56 42	63, 76, 134, 143	0
56	N0	172/172 (100%)	0.07	2 (1%) 76 63	59, 65, 77, 83	0
56	n0	172/172 (100%)	-0.10	2 (1%) 76 63	52, 59, 70, 79	0
57	N1	159/159 (100%)	0.04	2 (1%) 74 61	51, 65, 104, 111	0
57	n1	159/159 (100%)	-0.08	3 (1%) 66 52	51, 57, 95, 99	0
58	N2	100/100 (100%)	0.32	1 (1%) 79 68	100, 111, 117, 125	0
58	n2	98/100 (98%)	0.38	1 (1%) 79 68	88, 98, 103, 106	0
59	N3	136/136 (100%)	0.21	3 (2%) 62 48	57, 67, 77, 83	0
59	n3	136/136 (100%)	-0.02	1 (0%) 84 75	45, 55, 65, 70	0
60	N4	98/98 (100%)	1.07	15 (15%) 6 6	66, 78, 138, 139	0
61	N5	121/121 (100%)	0.04	1 (0%) 82 72	63, 75, 90, 110	0
61	n5	120/121 (99%)	0.07	2 (1%) 69 55	66, 79, 95, 105	0
62	N6	126/126 (100%)	0.05	1 (0%) 82 72	56, 72, 81, 90	0
62	n6	126/126 (100%)	0.21	3 (2%) 59 45	60, 76, 88, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
63	N7	135/135 (100%)	0.17	1 (0%) 84 75	88, 100, 110, 115	0
63	n7	135/135 (100%)	0.33	3 (2%) 62 48	93, 104, 116, 122	0
64	N8	148/148 (100%)	-0.13	2 (1%) 73 60	44, 64, 84, 94	0
64	n8	148/148 (100%)	-0.06	3 (2%) 64 51	44, 67, 84, 87	0
65	N9	58/58 (100%)	-0.01	3 (5%) 34 26	48, 70, 103, 114	0
65	n9	58/58 (100%)	-0.06	2 (3%) 48 36	48, 67, 86, 92	0
66	O0	97/100 (97%)	0.14	1 (1%) 79 68	87, 95, 113, 117	0
66	o0	100/100 (100%)	0.30	1 (1%) 79 68	84, 95, 111, 117	0
67	O1	109/109 (100%)	-0.03	0 100 100	67, 79, 99, 105	0
67	o1	109/109 (100%)	-0.01	1 (0%) 81 70	57, 69, 96, 109	0
68	O2	127/127 (100%)	-0.12	3 (2%) 59 45	46, 58, 72, 82	0
68	o2	127/127 (100%)	-0.06	3 (2%) 59 45	46, 62, 75, 82	0
69	O3	106/106 (100%)	-0.14	0 100 100	49, 57, 77, 86	0
69	o3	106/106 (100%)	-0.13	1 (0%) 81 70	49, 56, 80, 90	0
70	O4	112/112 (100%)	0.44	5 (4%) 39 29	63, 80, 115, 124	0
70	o4	112/112 (100%)	0.51	5 (4%) 39 29	62, 82, 116, 121	0
71	O5	119/119 (100%)	0.44	4 (3%) 48 36	61, 78, 86, 93	0
71	o5	119/119 (100%)	0.11	0 100 100	68, 83, 96, 106	0
72	O6	99/99 (100%)	0.10	0 100 100	68, 77, 102, 116	0
72	o6	99/99 (100%)	0.05	1 (1%) 79 68	76, 85, 101, 114	0
73	O7	87/87 (100%)	0.18	4 (4%) 38 28	51, 57, 76, 86	0
73	o7	87/87 (100%)	-0.04	2 (2%) 61 46	49, 58, 85, 99	0
74	O8	77/77 (100%)	0.24	1 (1%) 74 61	89, 100, 114, 117	0
74	o8	77/77 (100%)	0.28	1 (1%) 74 61	88, 99, 108, 110	0
75	O9	50/50 (100%)	0.32	3 (6%) 29 23	60, 64, 69, 69	0
75	o9	50/50 (100%)	0.12	4 (8%) 20 17	59, 65, 72, 74	0
76	Q0	52/52 (100%)	0.15	1 (1%) 66 52	62, 67, 82, 91	0
76	q0	52/52 (100%)	-0.41	0 100 100	50, 54, 65, 68	0
77	Q1	25/25 (100%)	-0.13	0 100 100	69, 74, 78, 79	0
77	q1	25/25 (100%)	-0.07	0 100 100	62, 63, 65, 66	0
78	Q2	105/105 (100%)	-0.19	1 (0%) 79 68	54, 67, 86, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
78	q2	105/105 (100%)	-0.26	0 100 100	54, 66, 80, 100	0
79	Q3	91/91 (100%)	0.16	4 (4%) 39 30	58, 71, 85, 91	0
79	q3	91/91 (100%)	0.01	1 (1%) 77 66	54, 69, 81, 89	0
80	c0	79/96 (82%)	0.65	5 (6%) 27 22	108, 133, 143, 145	0
81	c2	109/124 (87%)	0.94	13 (11%) 10 9	173, 185, 191, 194	0
82	c5	135/142 (95%)	0.46	7 (5%) 34 26	84, 110, 123, 125	0
83	sR	318/318 (100%)	0.33	2 (0%) 85 77	117, 131, 143, 156	0
84	sM	63/104 (60%)	0.29	6 (9%) 15 14	61, 111, 117, 122	0
85	l8	225/231 (97%)	0.50	6 (2%) 56 42	83, 95, 118, 123	0
86	m2	0/150	-	-	-	-
87	n4	135/135 (100%)	0.62	10 (7%) 22 18	54, 97, 121, 135	0
88	p0	120/219 (54%)	0.34	1 (0%) 82 72	103, 120, 135, 142	0
89	p1	0/47	-	-	-	-
89	p2	0/47	-	-	-	-
90	A	2/3 (66%)	1.08	0 100 100	106, 106, 106, 107	0
90	a	2/3 (66%)	1.08	0 100 100	100, 100, 100, 102	0
All	All	32948/34108 (96%)	0.07	848 (2%) 57 43	37, 82, 136, 228	2 (0%)

All (848) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	86	SER	11.6
13	c1	3	THR	10.1
60	N4	88	ASP	7.0
28	D6	2	PRO	6.1
60	N4	89	LEU	6.1
37	7	73	C	5.8
33	e1	80	ARG	5.7
47	m0	111	LEU	5.6
73	O7	88	ALA	5.6
60	N4	85	ALA	5.5
60	N4	87	LEU	5.5
56	N0	1	MET	5.5
13	c1	2	SER	5.5
21	c9	55	TYR	5.4
60	N4	84	GLY	5.4
29	d7	24	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
80	c0	25	LYS	5.2
60	N4	83	THR	5.1
13	C1	145	ALA	4.9
1	6	1799	U	4.9
22	D0	19	ILE	4.8
82	c5	4	ALA	4.8
9	s7	8	ILE	4.7
40	L3	387	LEU	4.6
36	1	3275	U	4.6
85	l8	124	ASP	4.6
7	s5	37	GLN	4.6
1	2	1699	G	4.6
52	m6	184	THR	4.5
79	q3	2	ALA	4.5
41	L4	81	GLY	4.5
1	2	1696	G	4.5
30	d8	21	SER	4.5
8	S6	80	ASN	4.4
13	C1	146	ALA	4.4
13	c1	4	GLU	4.4
9	s7	142	TYR	4.4
1	2	1702	A	4.4
24	D2	92	ASN	4.4
41	l4	65	TRP	4.4
11	s9	64	GLU	4.4
87	n4	68	ALA	4.3
10	s8	61	GLU	4.3
35	SM	89	ARG	4.3
8	S6	73	ILE	4.3
60	N4	76	VAL	4.3
28	D6	58	VAL	4.2
25	d3	21	ASN	4.2
41	L4	54	GLU	4.2
41	L4	63	GLU	4.2
4	s2	90	THR	4.2
55	M9	189	ALA	4.1
1	2	1698	G	4.1
15	C3	14	SER	4.1
25	d3	18	HIS	4.1
35	SM	87	THR	4.1
13	c1	5	LEU	4.0
30	d8	65	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
32	e0	2	ALA	4.0
41	L4	69	ARG	4.0
60	N4	90	ILE	4.0
41	l4	62	ALA	4.0
50	m4	138	ALA	4.0
60	N4	75	THR	4.0
36	5	2401	A	4.0
1	2	1686	C	4.0
55	M9	184	LEU	4.0
33	E1	124	PRO	3.9
9	s7	4	PRO	3.9
22	d0	64	LYS	3.9
33	E1	87	THR	3.9
79	Q3	92	ALA	3.9
81	c2	126	TRP	3.9
48	M1	127	PHE	3.9
7	S5	37	GLN	3.9
1	6	794	U	3.9
1	2	1693	A	3.9
73	o7	88	ALA	3.9
41	l4	61	SER	3.8
53	M7	161	ALA	3.8
10	S8	152	ILE	3.8
9	S7	151	LYS	3.8
21	c9	19	ALA	3.8
56	n0	1	MET	3.8
9	S7	150	GLN	3.8
23	D1	10	GLU	3.8
41	l4	67	THR	3.8
35	SM	101	ASP	3.7
11	S9	95	TYR	3.7
70	O4	23	VAL	3.7
82	c5	8	LYS	3.7
9	S7	8	ILE	3.7
46	L9	14	GLU	3.7
18	c6	49	TYR	3.7
82	c5	9	LYS	3.7
7	S5	152	GLY	3.7
75	O9	2	ALA	3.7
40	l3	146	ARG	3.7
8	S6	77	LEU	3.7
9	s7	176	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
26	D4	117	LYS	3.7
28	D6	3	LYS	3.6
60	N4	82	ILE	3.6
41	L4	65	TRP	3.6
85	l8	109	LEU	3.6
85	l8	121	SER	3.6
5	S3	152	PHE	3.6
21	c9	22	LEU	3.6
18	c6	142	TYR	3.6
1	6	1082	C	3.6
4	s2	92	ALA	3.6
13	c1	145	ALA	3.6
64	n8	16	SER	3.6
47	m0	103	LEU	3.6
84	sM	83	LYS	3.6
62	N6	7	ASP	3.5
35	SM	85	SER	3.5
39	L2	195	SER	3.5
57	N1	160	ILE	3.5
1	2	1694	A	3.5
42	l5	125	VAL	3.5
35	SM	84	LYS	3.5
13	c1	144	ALA	3.5
20	c8	18	LEU	3.5
22	d0	118	VAL	3.5
22	D0	20	ILE	3.5
84	sM	84	LYS	3.5
55	M9	72	GLU	3.5
1	6	679	U	3.5
36	5	1567	U	3.5
9	S7	38	LEU	3.5
53	M7	184	ALA	3.5
41	l4	66	GLY	3.5
9	s7	123	ASP	3.5
13	c1	116	ARG	3.5
41	l4	63	GLU	3.5
10	S8	179	CYS	3.5
30	D8	53	ILE	3.5
9	S7	4	PRO	3.4
36	5	1349	G	3.4
22	d0	93	LEU	3.4
35	SM	106	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
55	M9	51	VAL	3.4
12	C0	24	LYS	3.4
16	C4	14	PHE	3.4
70	O4	7	PHE	3.4
36	1	2404	A	3.4
56	N0	2	ALA	3.4
48	M1	83	GLY	3.4
47	M0	112	GLN	3.4
11	S9	97	LEU	3.4
9	S7	142	TYR	3.4
13	c1	146	ALA	3.3
13	c1	113	PRO	3.3
9	s7	127	GLU	3.3
80	c0	64	TYR	3.3
1	2	1709	C	3.3
9	S7	98	ILE	3.3
5	s3	151	LYS	3.3
9	s7	150	GLN	3.3
36	5	1103	A	3.3
9	s7	3	ALA	3.3
1	2	1695	G	3.3
9	S7	115	SER	3.3
66	o0	7	GLN	3.3
87	n4	67	VAL	3.3
36	5	2971	A	3.3
18	c6	43	ILE	3.3
41	l4	60	THR	3.3
70	O4	2	ALA	3.3
81	c2	123	VAL	3.3
36	5	3275	U	3.3
7	s5	151	GLY	3.3
3	S1	114	VAL	3.3
41	L4	74	ILE	3.3
53	M7	182	ILE	3.3
11	s9	148	VAL	3.2
5	s3	219	ALA	3.2
22	D0	120	SER	3.2
47	m0	166	ILE	3.2
7	s5	153	GLY	3.2
36	1	1556	C	3.2
22	D0	97	VAL	3.2
73	o7	86	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	6	678	A	3.2
22	d0	99	ILE	3.2
9	S7	141	ARG	3.2
35	SM	88	ARG	3.2
1	2	1426	C	3.2
5	s3	148	LYS	3.2
1	2	1697	G	3.2
32	E0	6	GLY	3.2
9	s7	184	GLU	3.2
33	E1	150	VAL	3.2
3	s1	117	TRP	3.2
3	S1	92	GLN	3.2
9	s7	2	SER	3.2
28	D6	86	VAL	3.2
22	D0	103	ILE	3.2
2	s0	207	PRO	3.1
32	e0	62	VAL	3.1
19	c7	90	ALA	3.1
2	S0	98	ILE	3.1
39	l2	15	ILE	3.1
36	5	1350	A	3.1
88	p0	192	ASP	3.1
3	s1	110	LEU	3.1
18	c6	57	LEU	3.1
5	S3	143	ARG	3.1
3	S1	66	VAL	3.1
79	Q3	71	VAL	3.1
71	O5	120	ALA	3.1
81	c2	92	ALA	3.1
35	SM	86	ASN	3.1
15	c3	5	HIS	3.1
14	C2	89	ILE	3.1
47	m0	112	GLN	3.1
9	S7	109	VAL	3.1
10	s8	46	VAL	3.1
11	S9	184	SER	3.0
82	c5	136	SER	3.0
28	d6	11	ASN	3.0
1	2	1708	U	3.0
42	L5	293	LEU	3.0
55	M9	85	ARG	3.0
83	sR	136	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
46	L9	190	ASP	3.0
70	O4	21	LYS	3.0
10	s8	58	LEU	3.0
22	d0	19	ILE	3.0
55	m9	189	ALA	3.0
3	s1	152	ARG	3.0
11	S9	60	LEU	3.0
42	L5	277	LEU	3.0
49	m3	6	ASN	3.0
55	m9	183	ALA	3.0
2	S0	158	VAL	3.0
39	l2	14	SER	3.0
25	d3	10	ASN	3.0
2	S0	207	PRO	2.9
40	l3	245	GLY	2.9
81	c2	32	LEU	2.9
36	5	2404	A	2.9
39	l2	252	THR	2.9
82	c5	134	THR	2.9
41	l4	79	GLY	2.9
34	SR	115	ILE	2.9
55	M9	54	ALA	2.9
20	c8	17	LEU	2.9
22	d0	97	VAL	2.9
30	d8	24	GLY	2.9
42	l5	124	GLU	2.9
55	M9	180	LYS	2.9
16	C4	83	ILE	2.9
13	C1	3	THR	2.9
11	S9	94	ASP	2.9
1	2	1707	A	2.9
1	6	496	G	2.9
16	C4	102	LEU	2.9
18	c6	44	LEU	2.9
4	s2	93	GLY	2.9
33	e1	77	GLY	2.9
9	S7	149	ILE	2.9
11	S9	64	GLU	2.9
70	o4	7	PHE	2.9
53	M7	160	ALA	2.9
39	l2	253	GLN	2.9
59	N3	3	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
36	1	329	U	2.9
1	2	1096	C	2.9
36	5	1582	C	2.9
1	6	497	G	2.8
29	d7	5	GLN	2.8
18	c6	141	SER	2.8
33	e1	79	LYS	2.8
41	l4	55	LYS	2.8
14	C2	82	PRO	2.8
6	S4	162	ILE	2.8
15	C3	15	ALA	2.8
36	1	2875	U	2.8
40	l3	178	LEU	2.8
1	2	1150	G	2.8
80	c0	22	VAL	2.8
11	S9	89	ASP	2.8
41	L4	79	GLY	2.8
9	s7	91	ILE	2.8
53	M7	162	GLU	2.8
33	E1	103	LEU	2.8
49	M3	7	LEU	2.8
8	S6	78	THR	2.8
36	1	1581	C	2.8
58	N2	27	VAL	2.8
16	C4	133	ARG	2.8
9	S7	12	ALA	2.8
34	SR	79	TYR	2.8
70	o4	2	ALA	2.8
55	M9	185	LEU	2.8
35	SM	141	ALA	2.8
49	M3	12	ASN	2.8
3	S1	54	LEU	2.8
3	s1	116	LYS	2.8
16	c4	92	LYS	2.8
39	L2	179	LEU	2.8
53	M7	165	VAL	2.8
22	D0	107	THR	2.8
39	L2	253	GLN	2.7
75	O9	46	ARG	2.7
53	M7	183	ALA	2.7
85	l8	125	ALA	2.7
13	C1	2	SER	2.7

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Mol	Chain	Res	Type	RSRZ
81	c2	64	SER	2.7
3	s1	217	LEU	2.7
1	6	717	C	2.7
26	D4	100	VAL	2.7
41	l4	73	ARG	2.7
60	N4	81	PRO	2.7
41	l4	89	ALA	2.7
47	m0	221	ALA	2.7
1	2	261	U	2.7
11	s9	76	LEU	2.7
21	c9	18	TYR	2.7
33	e1	103	LEU	2.7
5	s3	150	MET	2.7
28	D6	90	GLU	2.7
57	n1	86	GLU	2.7
1	2	793	A	2.7
41	l4	88	GLY	2.7
41	L4	100	PHE	2.7
28	D6	47	ALA	2.7
65	N9	25	LYS	2.7
8	s6	169	TYR	2.7
36	5	1356	U	2.7
41	l4	76	ARG	2.7
46	L9	10	ILE	2.7
35	SM	90	ALA	2.7
45	L8	141	ALA	2.7
45	L8	116	VAL	2.7
18	c6	98	ASP	2.7
32	E0	61	SER	2.7
2	s0	170	ILE	2.7
28	D6	83	ILE	2.7
36	5	3079	U	2.7
3	S1	25	THR	2.7
36	1	1349	G	2.7
47	M0	218	ALA	2.7
36	1	2207	A	2.7
36	5	440	A	2.7
11	S9	172	VAL	2.7
1	2	1705	C	2.7
11	S9	104	PHE	2.6
39	l2	13	GLY	2.6
51	M5	88	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
7	s5	154	ALA	2.6
7	s5	155	ALA	2.6
20	C8	18	LEU	2.6
8	s6	162	VAL	2.6
33	E1	148	TYR	2.6
1	6	1800	A	2.6
11	S9	29	LYS	2.6
2	S0	162	CYS	2.6
41	L4	80	GLY	2.6
67	o1	82	GLU	2.6
87	n4	66	GLU	2.6
46	l9	42	ASP	2.6
59	n3	2	SER	2.6
32	e0	49	LEU	2.6
10	s8	40	ALA	2.6
48	m1	8	PRO	2.6
1	2	320	U	2.6
1	2	1145	U	2.6
11	S9	96	VAL	2.6
18	C6	39	VAL	2.6
85	l8	123	GLN	2.6
71	O5	3	GLY	2.6
18	c6	2	SER	2.6
84	sM	85	SER	2.6
41	L4	82	THR	2.6
3	S1	91	VAL	2.6
9	s7	181	ILE	2.6
33	E1	152	ALA	2.6
33	e1	152	ALA	2.6
47	M0	219	ALA	2.6
87	n4	122	ALA	2.6
7	s5	161	ASP	2.6
30	d8	43	ASN	2.6
41	L4	60	THR	2.6
81	c2	121	VAL	2.6
1	6	1772	C	2.6
29	D7	7	LEU	2.6
55	M9	86	GLU	2.6
4	s2	86	VAL	2.6
19	c7	96	SER	2.6
41	L4	61	SER	2.6
8	S6	4	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	6	1756[A]	A	2.5
11	s9	80	LEU	2.5
40	l3	47	LEU	2.5
54	m8	156	GLY	2.5
5	s3	145	ALA	2.5
71	O5	48	ARG	2.5
7	S5	70	VAL	2.5
3	S1	32	ILE	2.5
11	s9	48	GLN	2.5
8	s6	76	LEU	2.5
16	C4	27	PHE	2.5
8	S6	66	GLY	2.5
55	m9	151	ARG	2.5
5	s3	144	ALA	2.5
60	N4	78	ALA	2.5
36	1	2401	A	2.5
43	L6	129	GLU	2.5
46	L9	13	PRO	2.5
51	M5	192	LYS	2.5
28	d6	58	VAL	2.5
30	D8	55	VAL	2.5
1	2	1370	U	2.5
3	s1	153	HIS	2.5
22	D0	108	ILE	2.5
25	D3	18	HIS	2.5
36	5	1569	U	2.5
7	s5	145	ASP	2.5
3	S1	29	TRP	2.5
75	o9	11	GLN	2.5
5	S3	144	ALA	2.5
51	M5	72	LYS	2.5
13	c1	117	VAL	2.5
24	D2	18	GLU	2.5
1	2	1756[A]	A	2.5
36	1	1103	A	2.5
8	S6	175	ILE	2.5
81	c2	136	ILE	2.5
62	n6	126	LEU	2.5
35	SM	93	ARG	2.5
59	N3	32	ARG	2.5
39	L2	201	GLY	2.5
10	s8	135	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
13	c1	147	ALA	2.5
16	C4	92	LYS	2.5
25	d3	3	LYS	2.5
47	M0	2	ALA	2.5
5	s3	138	VAL	2.5
22	d0	100	VAL	2.5
49	m3	133	PRO	2.5
75	O9	51	ILE	2.5
76	Q0	77	ILE	2.5
27	d5	51	LEU	2.5
39	l2	22	LEU	2.5
9	s7	139	ARG	2.5
3	S1	55	LYS	2.5
7	s5	152	GLY	2.5
26	d4	128	LYS	2.5
47	m0	220	GLN	2.5
63	n7	56	LYS	2.5
25	D3	27	ASN	2.5
10	S8	106	ALA	2.5
45	L8	256	ALA	2.5
46	L9	189	GLU	2.5
2	S0	170	ILE	2.4
5	s3	184	ILE	2.4
2	s0	146	LEU	2.4
81	c2	78	LEU	2.4
1	2	1100	G	2.4
9	s7	24	PHE	2.4
36	5	443	G	2.4
9	S7	111	LYS	2.4
10	s8	200	LYS	2.4
65	n9	25	LYS	2.4
4	s2	202	GLY	2.4
48	M1	6	GLN	2.4
28	D6	63	ALA	2.4
56	n0	2	ALA	2.4
36	1	1605	A	2.4
1	2	718	U	2.4
1	2	1710	U	2.4
13	C1	4	GLU	2.4
28	D6	85	ARG	2.4
32	E0	54	ARG	2.4
70	o4	16	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
83	sR	252	LEU	2.4
2	S0	107	PHE	2.4
7	S5	41	LYS	2.4
8	S6	164	LYS	2.4
55	m9	186	LYS	2.4
16	C4	89	THR	2.4
22	d0	54	GLY	2.4
51	m5	2	GLY	2.4
5	S3	179	GLN	2.4
9	S7	108	GLN	2.4
2	S0	2	SER	2.4
41	L4	50	TYR	2.4
53	M7	157	VAL	2.4
85	l8	126	SER	2.4
5	S3	154	ASP	2.4
14	C2	103	LEU	2.4
26	D4	125	LEU	2.4
36	1	2971	A	2.4
36	1	3079	U	2.4
16	C4	26	THR	2.4
35	SM	97	THR	2.4
7	S5	154	ALA	2.4
42	L5	291	ALA	2.4
19	C7	110	VAL	2.4
2	S0	110	TYR	2.4
35	SM	95	SER	2.4
9	S7	147	ASN	2.4
61	N5	24	LEU	2.4
1	2	656	G	2.4
8	S6	222	GLU	2.4
36	5	1352	A	2.4
49	m3	17	HIS	2.4
5	S3	105	MET	2.4
39	l2	248	GLY	2.4
7	s5	27	THR	2.4
10	s8	67	TRP	2.4
84	sM	82	THR	2.4
7	s5	133	VAL	2.4
35	SM	19	VAL	2.4
4	s2	89	GLN	2.4
33	e1	85	TYR	2.4
3	S1	140	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
11	s9	93	LEU	2.4
23	D1	78	LEU	2.4
54	M8	167	SER	2.4
81	c2	45	LEU	2.4
2	S0	190	ASP	2.4
5	S3	135	GLU	2.4
48	M1	98	ALA	2.4
68	O2	127	ALA	2.4
20	c8	22	VAL	2.4
1	6	1150	G	2.4
2	s0	173	ILE	2.3
18	c6	52	LEU	2.3
22	D0	99	ILE	2.3
50	m4	8	LYS	2.3
14	C2	119	SER	2.3
40	l3	363	SER	2.3
1	6	934	C	2.3
49	M3	37	ASN	2.3
33	E1	147	VAL	2.3
45	L8	114	ALA	2.3
63	N7	124	ALA	2.3
9	S7	34	LEU	2.3
25	d3	110	LYS	2.3
87	n4	115	LYS	2.3
4	s2	164	SER	2.3
47	m0	207	GLU	2.3
8	s6	146	GLY	2.3
15	c3	7	ALA	2.3
16	C4	103	ARG	2.3
60	N4	93	ARG	2.3
7	S5	42	LEU	2.3
8	S6	76	LEU	2.3
60	N4	69	LYS	2.3
46	L9	188	THR	2.3
61	n5	24	LEU	2.3
70	O4	20	ILE	2.3
12	C0	13	GLN	2.3
1	2	260	U	2.3
36	1	2205	U	2.3
42	L5	278	SER	2.3
8	S6	20	ASP	2.3
36	5	1566	A	2.3

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Mol	Chain	Res	Type	RSRZ
40	L3	200	GLU	2.3
34	SR	27	ALA	2.3
41	l4	69	ARG	2.3
45	L8	240	ASN	2.3
9	s7	136	VAL	2.3
57	N1	124	VAL	2.3
64	N8	37	GLY	2.3
35	SM	105	LYS	2.3
36	5	3276	G	2.3
39	L2	251	LYS	2.3
1	2	1703	C	2.3
4	S2	146	THR	2.3
9	S7	13	PRO	2.3
4	s2	98	PHE	2.3
3	s1	114	VAL	2.3
4	s2	75	GLY	2.3
8	S6	67	VAL	2.3
30	D8	28	VAL	2.3
30	D8	44	VAL	2.3
34	SR	161	ALA	2.3
63	n7	2	ALA	2.3
87	n4	95	SER	2.3
46	L9	15	GLY	2.3
1	6	663	U	2.3
1	6	864	U	2.3
1	6	1491	U	2.3
3	S1	47	LEU	2.3
15	c3	125	LEU	2.3
79	Q3	22	LEU	2.3
10	S8	72	ILE	2.3
36	1	1350	A	2.3
38	8	80	A	2.3
9	s7	102	PRO	2.3
39	L2	17	THR	2.3
35	SM	108	GLN	2.3
48	M1	104	PHE	2.3
63	n7	92	PHE	2.3
78	Q2	106	PHE	2.3
16	C4	41	ARG	2.3
64	n8	26	ARG	2.3
6	s4	183	VAL	2.3
9	s7	6	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
34	SR	6	VAL	2.3
42	l5	135	VAL	2.3
82	c5	11	VAL	2.3
3	S1	61	LEU	2.3
81	c2	62	LEU	2.3
35	SM	16	ASP	2.2
35	SM	92	ASP	2.2
36	1	1570	U	2.2
1	2	1151	A	2.2
1	2	1794	A	2.2
47	M0	220	GLN	2.2
29	d7	22	LYS	2.2
41	L4	55	LYS	2.2
4	S2	63	VAL	2.2
48	M1	171	VAL	2.2
6	s4	261	LEU	2.2
7	S5	36	ALA	2.2
7	S5	165	LEU	2.2
10	s8	80	GLY	2.2
49	m3	195	ALA	2.2
1	2	1297	G	2.2
16	c4	125	SER	2.2
30	d8	40	ILE	2.2
41	l4	74	ILE	2.2
59	N3	2	SER	2.2
21	c9	127	ASN	2.2
8	s6	144	PHE	2.2
28	D6	60	PRO	2.2
49	M3	160	GLN	2.2
53	M7	130	TYR	2.2
70	o4	33	GLN	2.2
22	D0	21	LYS	2.2
47	M0	101	LYS	2.2
25	d3	15	LEU	2.2
65	N9	2	ALA	2.2
45	L8	119	GLY	2.2
8	S6	226	ILE	2.2
23	D1	23	ILE	2.2
15	c3	83	GLU	2.2
33	e1	145	HIS	2.2
81	c2	119	SER	2.2
1	2	1706	C	2.2

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Mol	Chain	Res	Type	RSRZ
11	s9	63	ASP	2.2
15	C3	138	ASN	2.2
1	2	1692	G	2.2
68	o2	16	LYS	2.2
41	l4	94	CYS	2.2
48	M1	167	TYR	2.2
22	d0	51	VAL	2.2
8	S6	75	LEU	2.2
81	c2	59	LEU	2.2
13	C1	147	ALA	2.2
32	E0	2	ALA	2.2
36	1	1095	U	2.2
36	1	1555	U	2.2
36	1	1764	U	2.2
38	4	82	U	2.2
41	l4	56	ALA	2.2
49	M3	132	ALA	2.2
73	O7	86	ALA	2.2
16	C4	76	ILE	2.2
55	M9	50	ILE	2.2
49	M3	20	GLU	2.2
52	M6	40	GLU	2.2
2	s0	11	PRO	2.2
3	S1	94	LYS	2.2
22	d0	67	THR	2.2
1	6	1096	C	2.2
29	d7	2	VAL	2.2
36	1	2772	C	2.2
62	n6	76	LEU	2.2
7	s5	36	ALA	2.2
47	m0	67	ALA	2.2
51	M5	2	GLY	2.2
36	5	1351	U	2.2
14	C2	83	GLU	2.2
19	c7	87	GLU	2.2
42	L5	130	GLU	2.2
46	L9	11	GLU	2.2
4	S2	88	LYS	2.2
49	M3	26	PHE	2.2
33	E1	146	SER	2.2
7	s5	33	VAL	2.2
28	D6	53	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
32	E0	48	THR	2.2
41	l4	59	GLN	2.2
42	L5	7	ALA	2.1
34	SR	43	ILE	2.1
75	o9	51	ILE	2.1
75	o9	46	ARG	2.1
4	s2	88	LYS	2.1
25	D3	123	LYS	2.1
30	D8	45	LYS	2.1
52	M6	80	PHE	2.1
2	S0	97	PRO	2.1
57	n1	79	MET	2.1
14	C2	115	VAL	2.1
45	L8	66	SER	2.1
2	s0	110	TYR	2.1
84	sM	75	ASP	2.1
9	S7	7	LYS	2.1
28	D6	4	LYS	2.1
50	m4	137	LYS	2.1
3	S1	138	PHE	2.1
2	s0	34	GLU	2.1
58	n2	44	GLU	2.1
1	2	1700	C	2.1
8	S6	68	LEU	2.1
9	s7	153	LEU	2.1
29	d7	41	LEU	2.1
42	L5	51	LEU	2.1
16	C4	16	VAL	2.1
16	C4	67	VAL	2.1
26	D4	70	VAL	2.1
51	m5	25	VAL	2.1
1	6	261	U	2.1
36	5	981	U	2.1
38	8	81	U	2.1
25	d3	11	SER	2.1
49	M3	41	THR	2.1
1	6	488	G	2.1
1	6	720	G	2.1
2	S0	206	ASP	2.1
7	s5	137	ILE	2.1
8	S6	33	GLY	2.1
9	s7	135	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
16	C4	75	GLY	2.1
26	d4	7	ILE	2.1
80	c0	65	TYR	2.1
33	e1	82	LYS	2.1
35	SM	96	ARG	2.1
35	SM	99	LYS	2.1
64	n8	27	LYS	2.1
36	5	1580	A	2.1
6	s4	15	PRO	2.1
49	M3	134	GLU	2.1
16	C4	137	LEU	2.1
55	m9	185	LEU	2.1
1	2	1082	C	2.1
36	1	1866	C	2.1
41	L4	72	ALA	2.1
61	n5	30	ALA	2.1
68	o2	127	ALA	2.1
10	s8	120	THR	2.1
27	D5	50	ILE	2.1
2	S0	134	LYS	2.1
33	e1	106	TYR	2.1
35	SM	9	GLY	2.1
35	SM	98	GLY	2.1
36	5	620	U	2.1
36	5	1094	U	2.1
53	M7	164	LYS	2.1
71	O5	20	GLN	2.1
87	n4	27	LYS	2.1
45	L8	156	ASP	2.1
47	m0	44	ASP	2.1
64	N8	46	ASP	2.1
12	C0	34	GLU	2.1
25	D3	42	PRO	2.1
29	D7	3	LEU	2.1
52	M6	100	GLU	2.1
65	N9	24	PRO	2.1
68	O2	26	HIS	2.1
33	e1	84	VAL	2.1
16	C4	106	ALA	2.1
28	D6	6	ALA	2.1
50	m4	9	ALA	2.1
75	o9	16	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
81	c2	101	ALA	2.1
84	sM	35	ALA	2.1
7	S5	40	ILE	2.1
17	C5	9	LYS	2.1
45	L8	120	LYS	2.1
51	M5	71	ARG	2.1
12	C0	63	TYR	2.1
17	C5	50	THR	2.1
79	Q3	15	GLY	2.1
9	s7	147	ASN	2.1
1	6	659	C	2.1
1	2	650	U	2.1
1	2	1097	U	2.1
46	l9	191	LEU	2.1
74	o8	69	LEU	2.1
87	n4	109	LEU	2.1
29	D7	19	HIS	2.1
49	M3	127	PRO	2.1
4	S2	69	ILE	2.0
8	S6	149	LYS	2.0
9	S7	181	ILE	2.0
16	C4	39	ILE	2.0
22	d0	20	ILE	2.0
45	L8	125	ALA	2.0
47	m0	195	ALA	2.0
73	O7	83	ALA	2.0
1	2	1701	A	2.0
11	S9	185	GLY	2.0
36	1	2169	G	2.0
18	C6	142	TYR	2.0
39	l2	17	THR	2.0
46	L9	83	THR	2.0
9	S7	99	LEU	2.0
11	S9	80	LEU	2.0
35	SM	11	ASP	2.0
46	L9	191	LEU	2.0
68	o2	128	LEU	2.0
11	s9	96	VAL	2.0
16	C4	28	VAL	2.0
33	e1	150	VAL	2.0
82	c5	5	VAL	2.0
1	6	1033	C	2.0

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Mol	Chain	Res	Type	RSRZ
41	l4	58	HIS	2.0
42	l5	126	GLU	2.0
70	o4	31	ARG	2.0
16	C4	71	CYS	2.0
53	M7	156	ALA	2.0
66	O0	105	ALA	2.0
69	o3	107	ILE	2.0
87	n4	50	ALA	2.0
42	L5	295	GLY	2.0
7	S5	147	THR	2.0
8	S6	169	TYR	2.0
65	n9	27	TYR	2.0
72	o6	2	THR	2.0
74	O8	43	PHE	2.0
80	c0	62	GLN	2.0
9	s7	187	SER	2.0
36	5	1355	A	2.0
18	C6	52	LEU	2.0
68	O2	128	LEU	2.0
12	C0	39	ASN	2.0
25	d3	22	ASN	2.0
3	S1	20	VAL	2.0
9	S7	123	ASP	2.0
73	O7	29	VAL	2.0
53	M7	159	LYS	2.0
9	S7	125	ILE	2.0
11	S9	98	ALA	2.0
18	c6	24	ALA	2.0
36	1	1351	U	2.0
39	L2	15	ILE	2.0
50	M4	9	ALA	2.0
57	n1	104	GLU	2.0
62	n6	127	GLU	2.0
87	n4	63	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
90	PPU	A	76	37/38	0.85	0.21	47,88,147,147	0
90	PPU	a	76	37/38	0.90	0.20	44,80,139,139	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.