



# wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

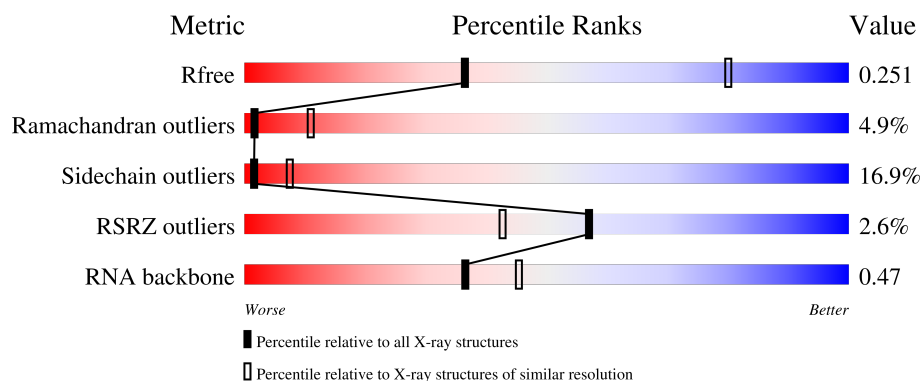
# 1 Overall quality at a glance

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  $\geq 3$ , 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>

*Continued on next page...*

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	


















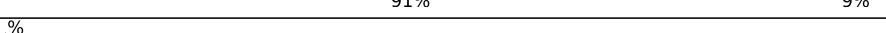







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	D8	63	<div> <div>8%</div> <div>78%</div> <div>22%</div> </div>
30	d8	63	<div> <div>8%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
31	D9	53	<div> <div>75%</div> <div>23%</div> <div>.</div> </div>
31	d9	53	<div> <div>77%</div> <div>23%</div> </div>
32	E0	62	<div> <div>8%</div> <div>84%</div> <div>10%</div> <div>.</div> <div>.</div> </div>
32	e0	62	<div> <div>5%</div> <div>73%</div> <div>23%</div> <div>5%</div> </div>
33	E1	76	<div> <div>11%</div> <div>59%</div> <div>29%</div> <div>5%</div> <div>7%</div> </div>
33	e1	76	<div> <div>14%</div> <div>61%</div> <div>32%</div> <div>.</div> <div>.</div> </div>
34	SR	318	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
35	SM	159	<div> <div>14%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
36	1	3394	<div> <div>%</div> <div>67%</div> <div>23%</div> <div>.</div> <div>7%</div> </div>
36	5	3394	<div> <div>%</div> <div>66%</div> <div>23%</div> <div>.</div> <div>7%</div> </div>
37	3	121	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
37	7	121	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
38	4	158	<div> <div>%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
38	8	158	<div> <div>%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
39	L2	252	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
39	l2	252	<div> <div>3%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
40	L3	386	<div> <div>%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
40	l3	386	<div> <div>%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
41	L4	361	<div> <div>4%</div> <div>82%</div> <div>17%</div> </div>
41	l4	361	<div> <div>5%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
42	L5	296	<div> <div>3%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
42	l5	296	<div> <div>%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
43	L6	175	<div> <div>%</div> <div>78%</div> <div>10%</div> <div>.</div> <div>11%</div> </div>

Continued on next page...

Continued from previous page...

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%.
47	m0	220	 5%79%16%.
48	M1	169	 4%80%17%
48	m1	169	 %79%19%.
49	M3	194	 5%79%19%
49	m3	194	 2%84%16%
50	M4	137	 %82%15%.
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%.
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%

Continued on next page...

Continued from previous page...

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>.</div> </div>
57	n1	159	<div> <div>2%</div> <div></div> <div>81%</div> <div>18%</div> <div>.</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>.</div> </div>
59	N3	136	<div> <div>2%</div> <div></div> <div>85%</div> <div>15%</div> </div>
59	n3	136	<div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div>
60	N4	98	<div> <div>15%</div> <div></div> <div>87%</div> <div>13%</div> </div>
61	N5	121	<div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div>
61	n5	121	<div> <div>2%</div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div>
62	N6	126	<div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div>
62	n6	126	<div> <div>2%</div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div>
63	N7	135	<div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div>
63	n7	135	<div> <div>2%</div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div>
64	N8	148	<div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div>
64	n8	148	<div> <div>2%</div> <div></div> <div>84%</div> <div>16%</div> </div>
65	N9	58	<div> <div>5%</div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div>
65	n9	58	<div> <div>3%</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>.</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>.</div> </div>
67	o1	109	<div> <div></div> <div>80%</div> <div>20%</div> </div>
68	O2	127	<div> <div>2%</div> <div></div> <div>89%</div> <div>11%</div> </div>
68	o2	127	<div> <div>2%</div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div>
69	O3	106	<div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
69	o3	106	
70	O4	112	
70	o4	112	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	c0	96	
81	c2	124	
82	c5	142	
83	sR	318	

Continued on next page...



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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			

*Continued on next page...*

*Continued from previous page...*

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			

*Continued on next page...*

*Continued from previous page...*

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			

*Continued on next page...*

*Continued from previous page...*

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			

*Continued on next page...*



*Continued from previous page...*

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		

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

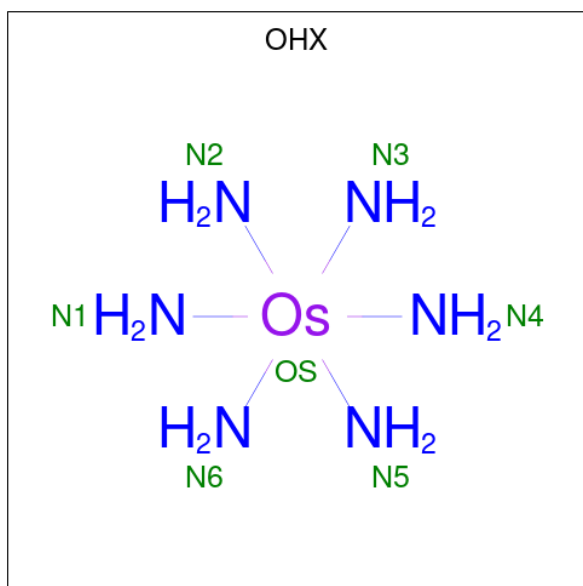
*Continued on next page...*



Continued from previous page...

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

- 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 7	N 6	Os 1	0	0
92	2	1	Total 7	N 6	Os 1	0	0
92	2	1	Total 7	N 6	Os 1	0	0
92	2	1	Total 7	N 6	Os 1	0	0

Continued on next page...

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*



*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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	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		

*Continued on next page...*

*Continued from previous page...*

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
			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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*



*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*



*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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	3	1	Total	N	Os	0	0
			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		
92	3	1	Total	N	Os	0	0
			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		
92	3	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

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
			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		
92	3	1	Total	N	Os	0	0
			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		
92	4	1	Total	N	Os	0	0
			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		
92	4	1	Total	N	Os	0	0
			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		
92	4	1	Total	N	Os	0	0
			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		
92	4	1	Total	N	Os	0	0
			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		

*Continued on next page...*

*Continued from previous page...*

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
			7	6	1		
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		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	O7	1	Total	N	Os	0	0
			7	6	1		
92	Q2	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
			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
			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
			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
			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
			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		

*Continued on next page...*

Continued from previous page...

[illegible]

*Continued on next page...*

*Continued from previous page...*

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		
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
			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
			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
			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
			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		

*Continued on next page...*

*Continued from previous page...*

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		
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
			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
			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
			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
			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
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

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		
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
			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
			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
			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
			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
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

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		
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
			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
			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
			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
			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
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

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		
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
			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
			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
			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
			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
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

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		
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
			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
			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
			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
			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
			7	6	1		

*Continued on next page...*



*Continued from previous page...*

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		
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
			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
			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
			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
			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		

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
92	d9	1	Total	N	Os	0	0
			7	6	1		
92	sR	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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*



*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*



*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		
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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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		

*Continued on next page...*

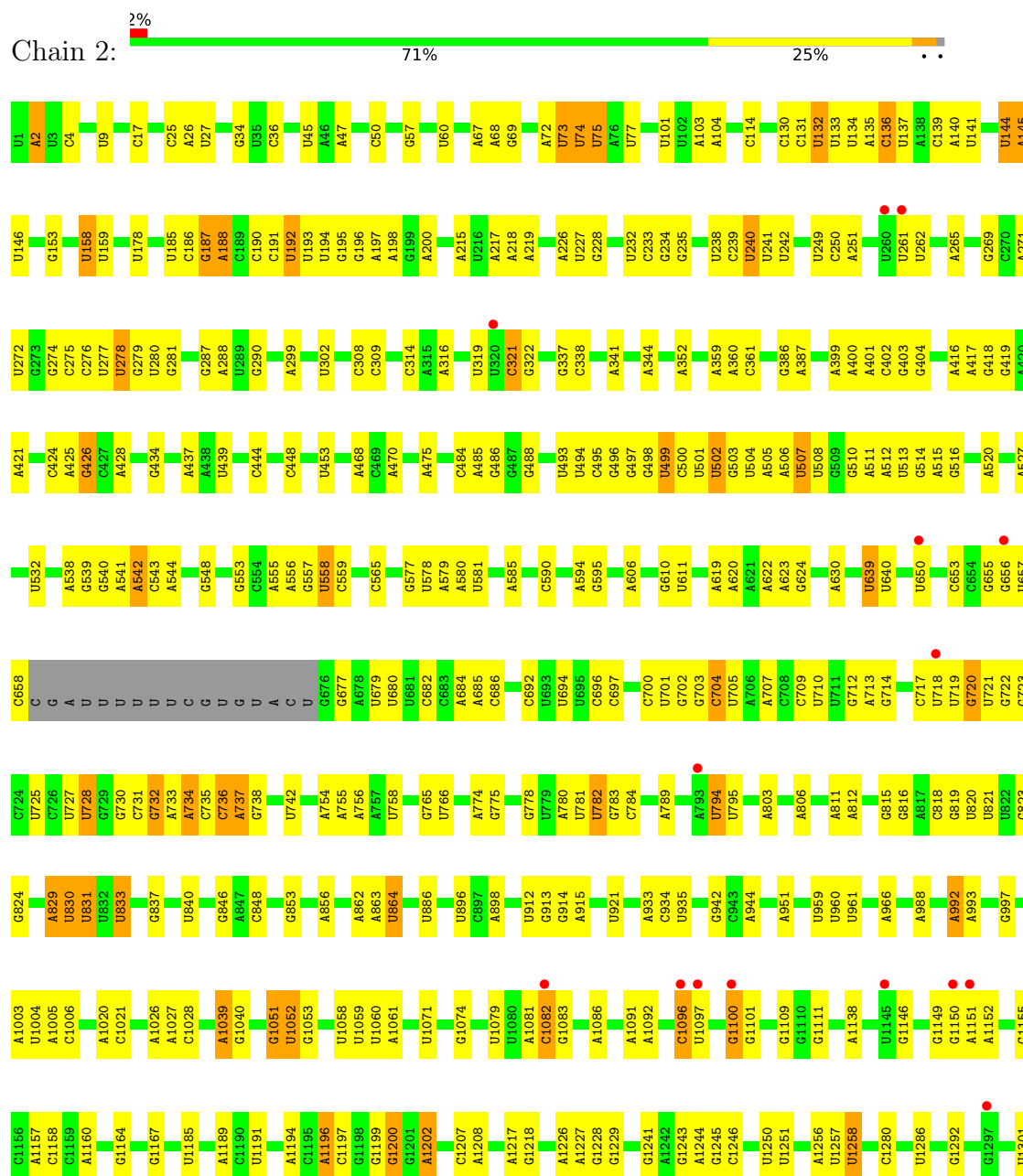
*Continued from previous page...*

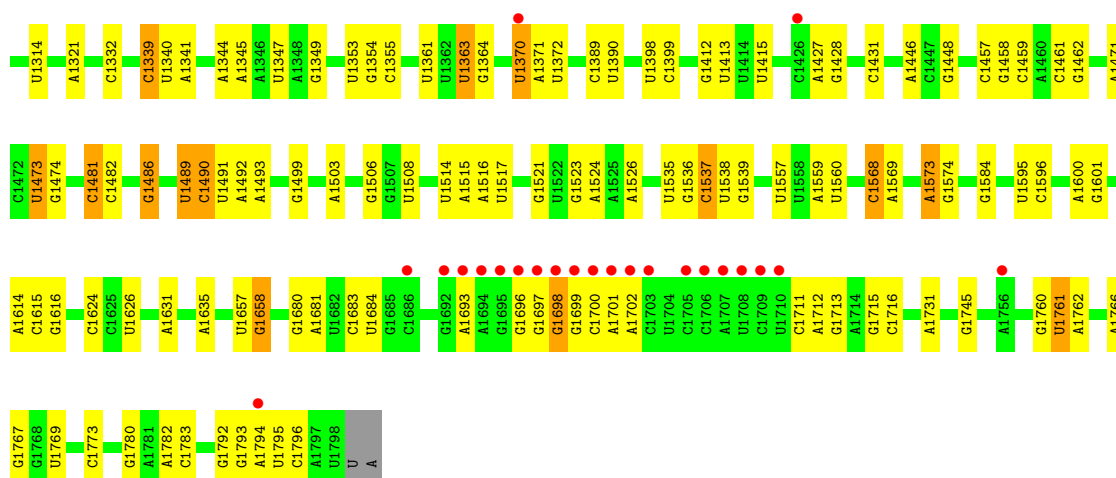
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	D7	1	Total 1	Zn 1	0	0
93	D9	1	Total 1	Zn 1	0	0
93	E1	1	Total 1	Zn 1	0	0
93	O7	1	Total 1	Zn 1	0	0
93	Q0	1	Total 1	Zn 1	0	0
93	Q2	1	Total 1	Zn 1	0	0
93	Q3	1	Total 1	Zn 1	0	0
93	d6	1	Total 1	Zn 1	0	0
93	d7	1	Total 1	Zn 1	0	0
93	d9	1	Total 1	Zn 1	0	0
93	e1	1	Total 1	Zn 1	0	0
93	o7	1	Total 1	Zn 1	0	0
93	q0	1	Total 1	Zn 1	0	0
93	q2	1	Total 1	Zn 1	0	0
93	q3	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

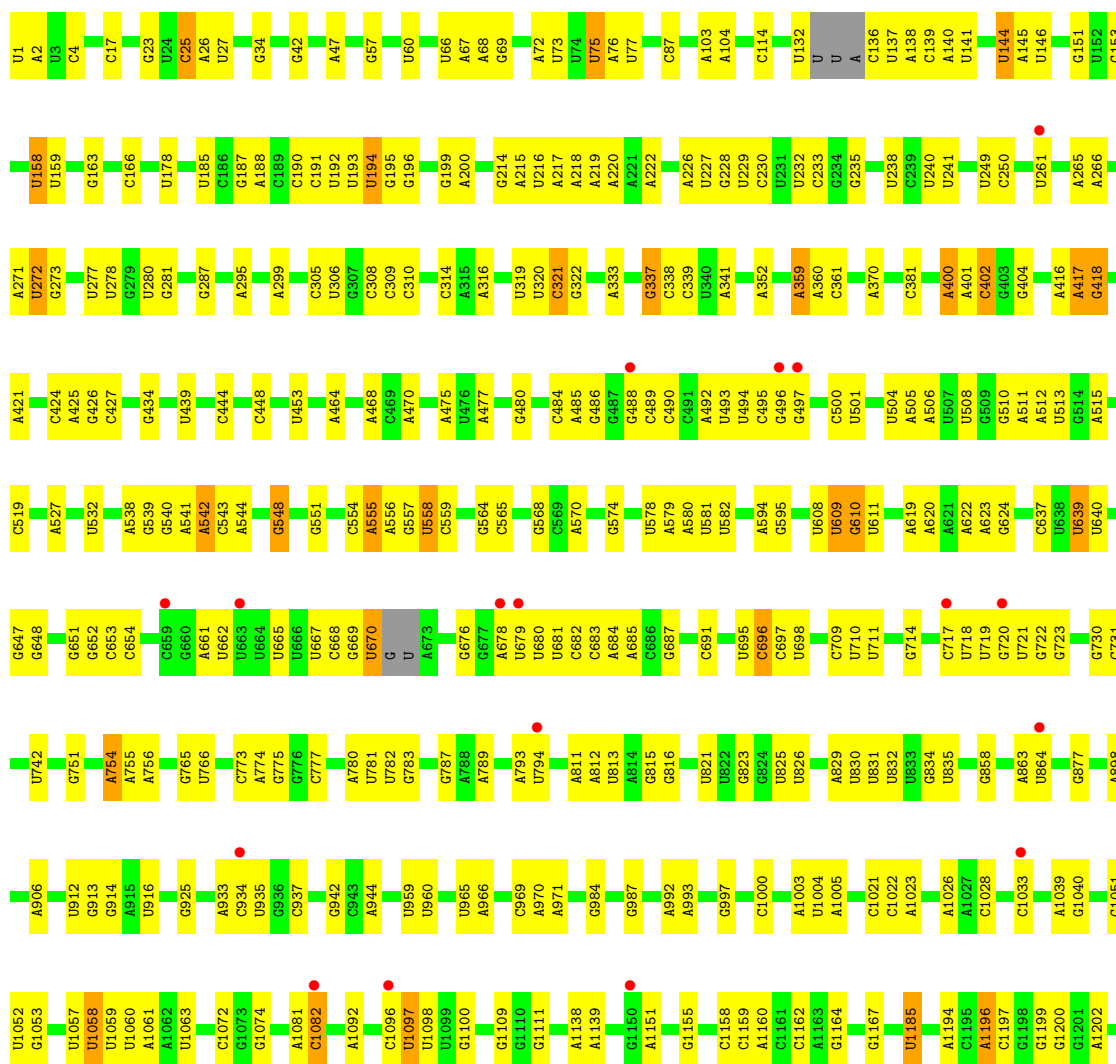
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

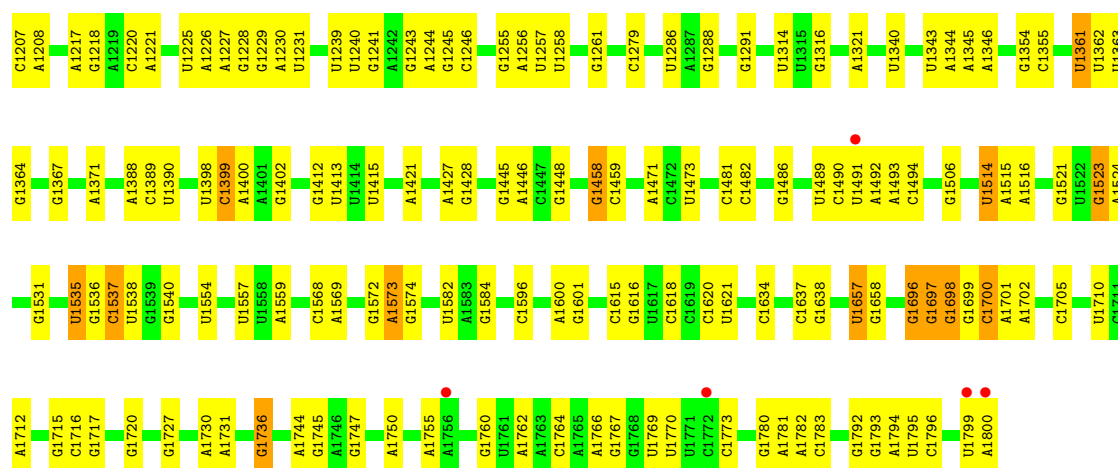
#### • Molecule 1: 18S rRNA



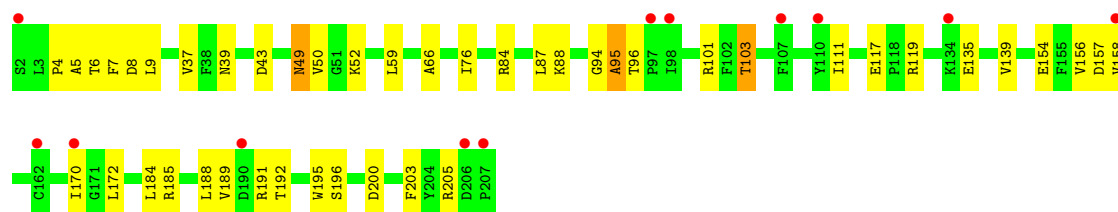
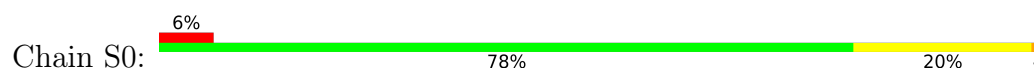


• Molecule 1: 18S rRNA

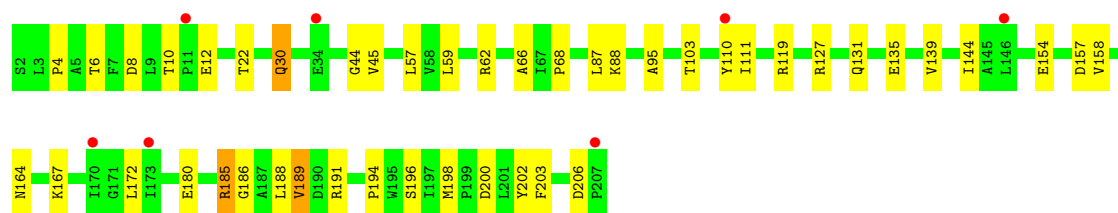
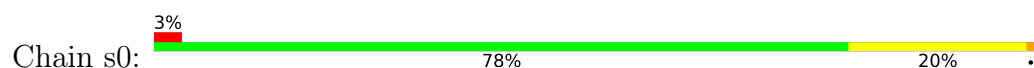




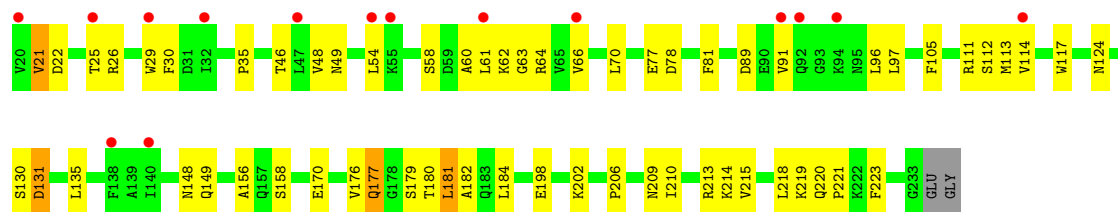
• Molecule 2: 40S ribosomal protein S0-A



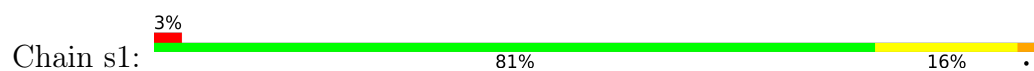
• Molecule 2: 40S ribosomal protein S0-A

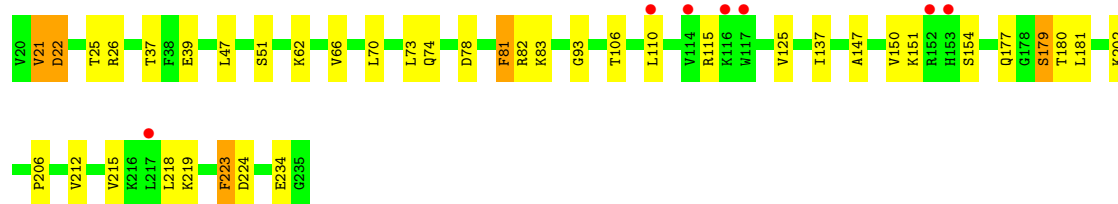


• Molecule 3: 40S ribosomal protein S1-A

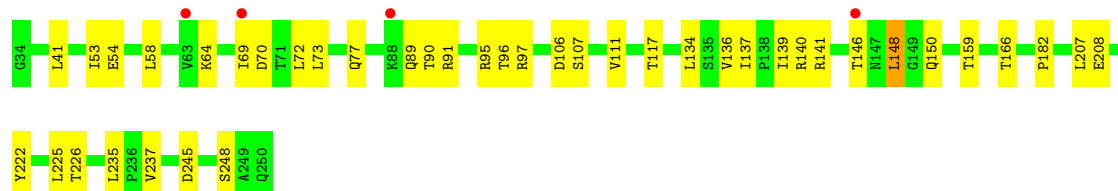
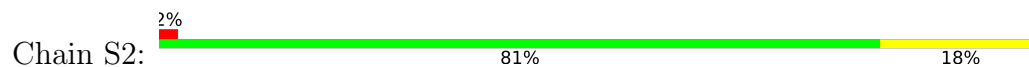


• Molecule 3: 40S ribosomal protein S1-A

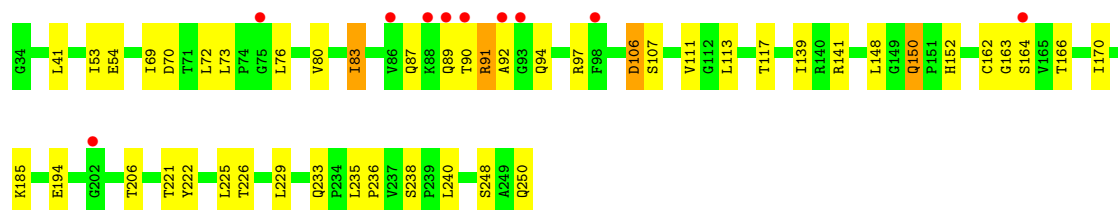
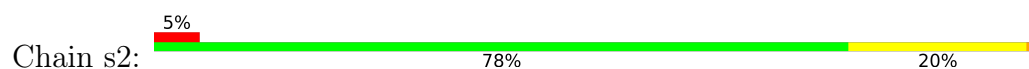




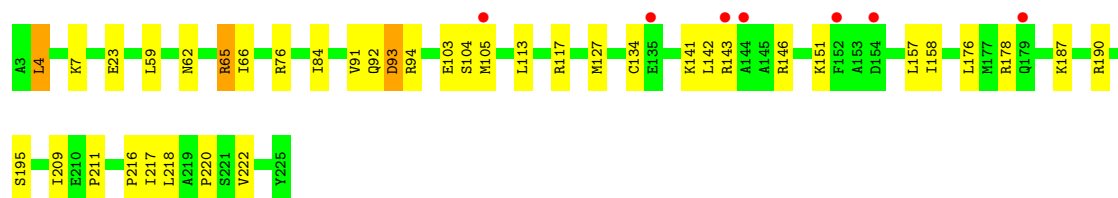
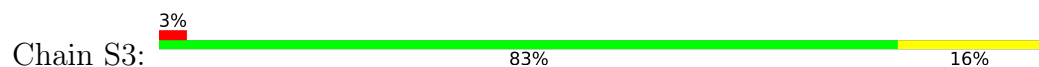
• Molecule 4: 40S ribosomal protein S2



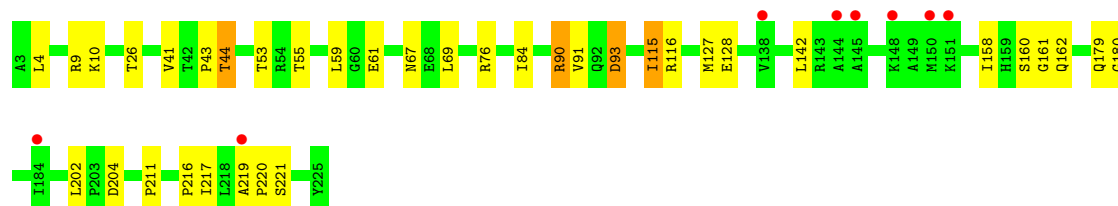
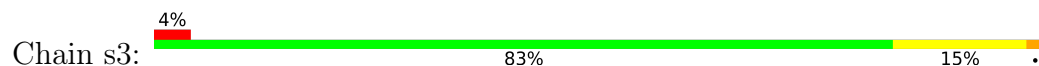
• Molecule 4: 40S ribosomal protein S2



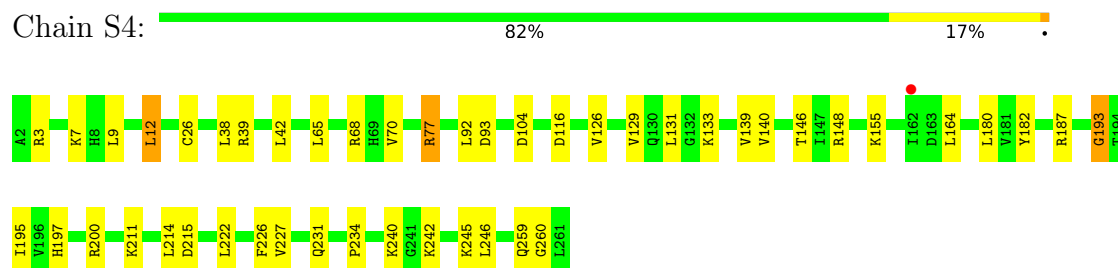
• Molecule 5: 40S ribosomal protein S3



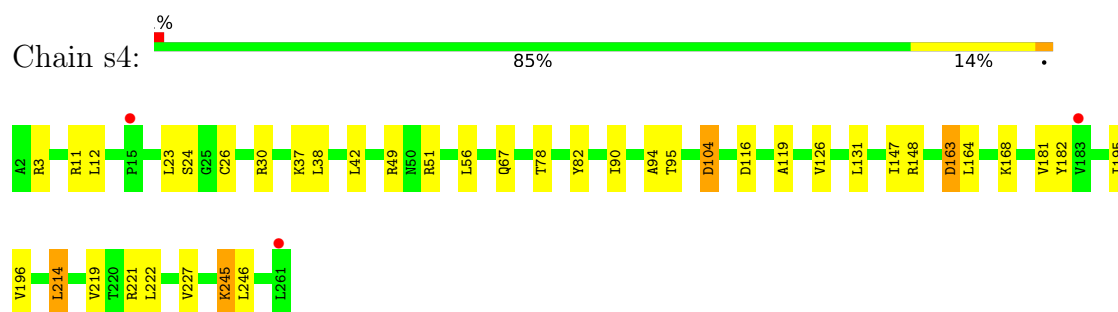
• Molecule 5: 40S ribosomal protein S3



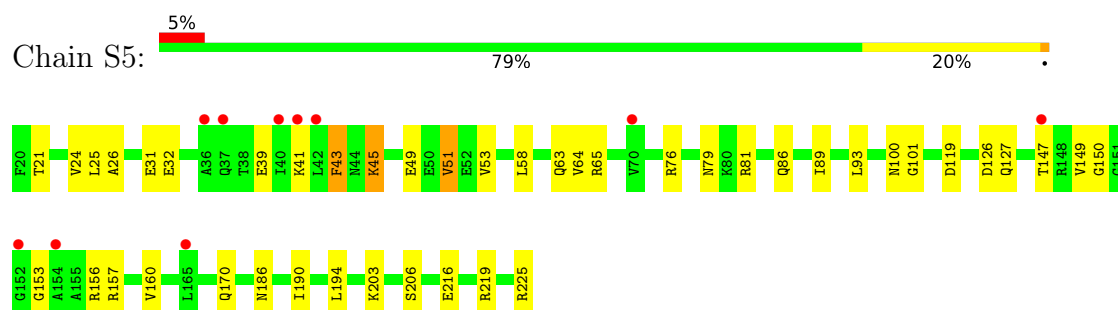
- Molecule 6: 40S ribosomal protein S4-A



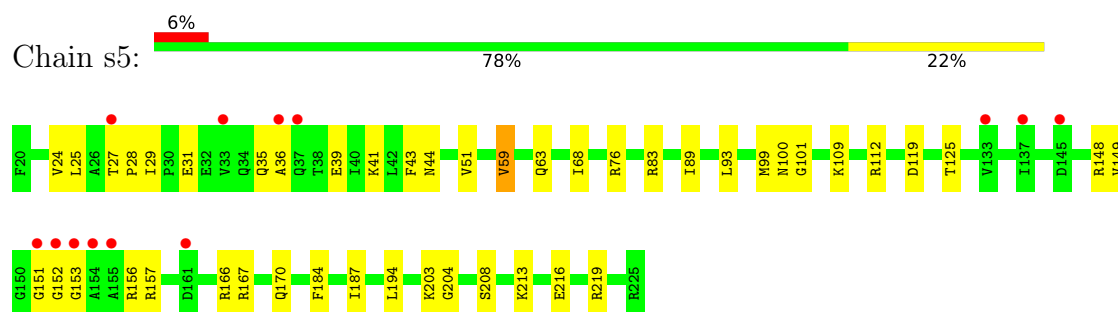
- Molecule 6: 40S ribosomal protein S4-A



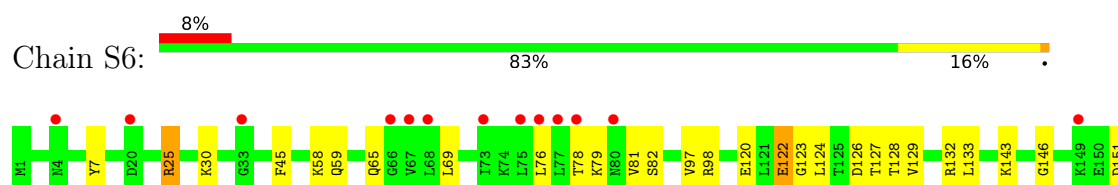
- Molecule 7: 40S ribosomal protein S5

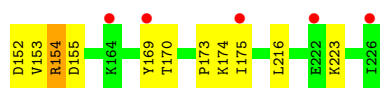


- Molecule 7: 40S ribosomal protein S5

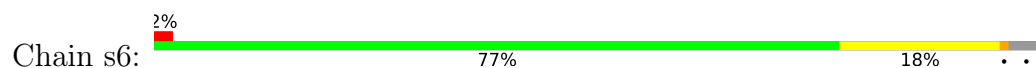


- Molecule 8: 40S ribosomal protein S6-A

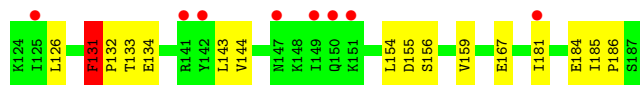
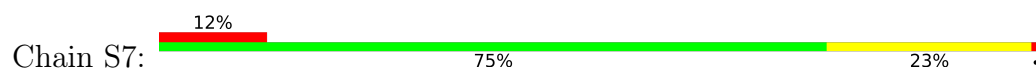




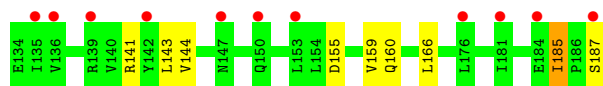
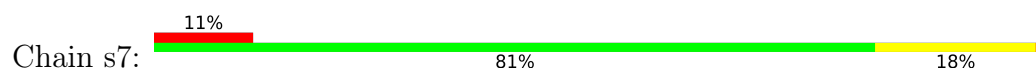
- Molecule 8: 40S ribosomal protein S6-A



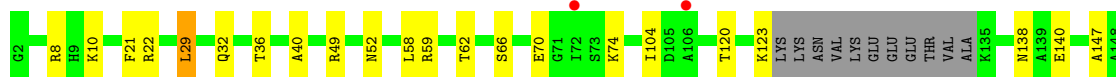
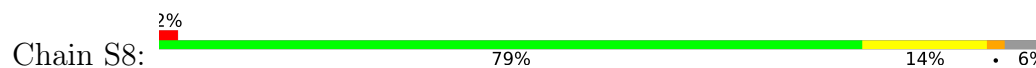
- Molecule 9: 40S ribosomal protein S7-A



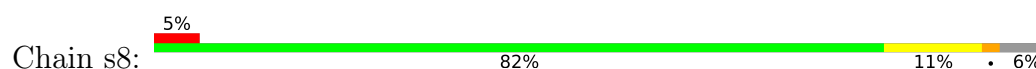
- Molecule 9: 40S ribosomal protein S7-A



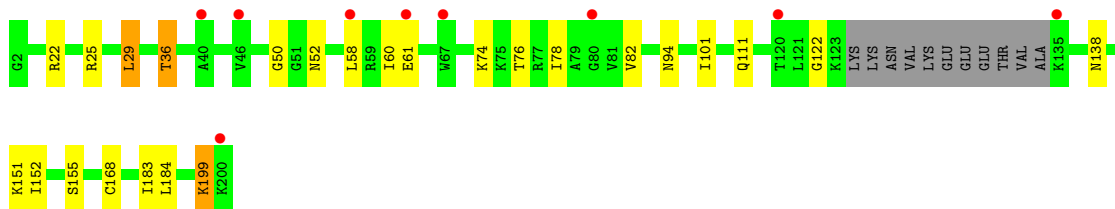
- Molecule 10: 40S ribosomal protein S8-A



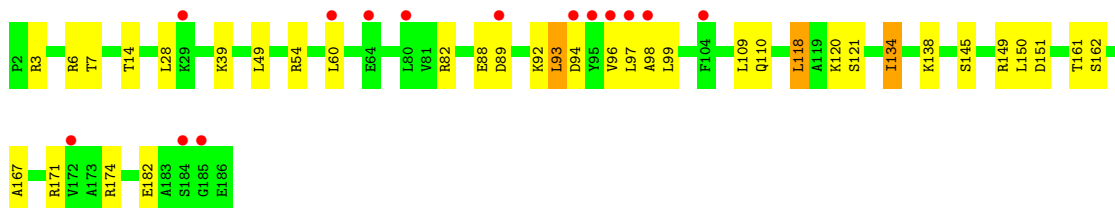
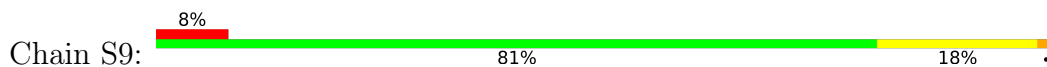
- Molecule 10: 40S ribosomal protein S8-A



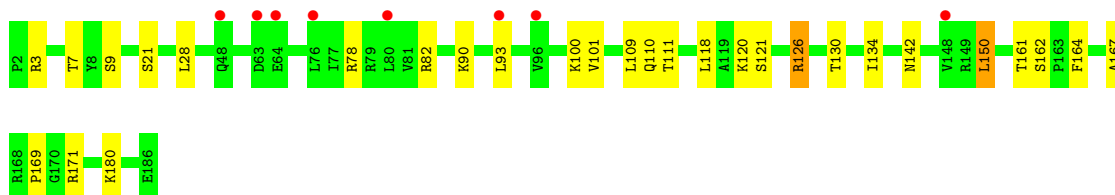
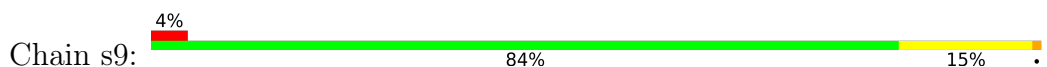




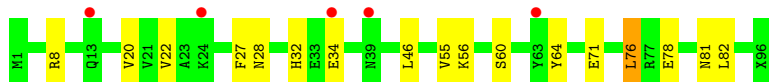
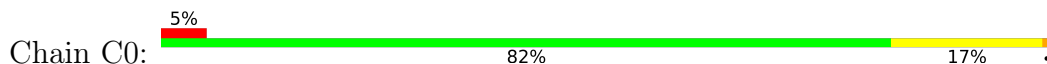
- Molecule 11: 40S ribosomal protein S9-A



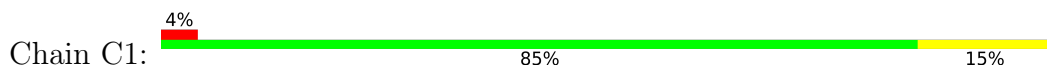
- Molecule 11: 40S ribosomal protein S9-A



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

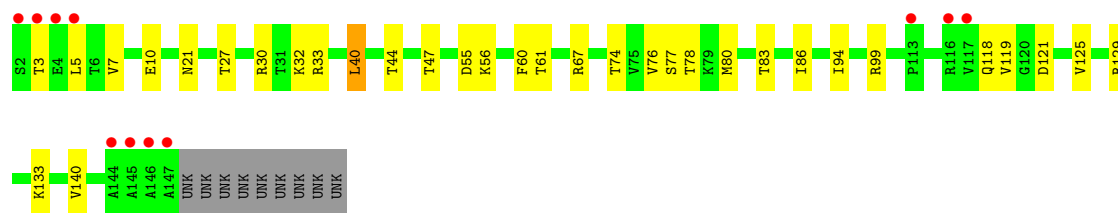


- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S Ribosomal Protein S11-A

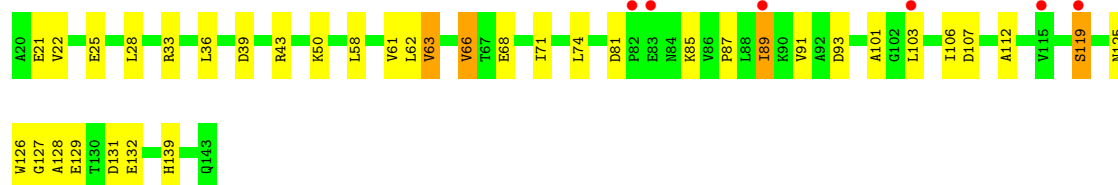


- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S Ribosomal Protein S11-A

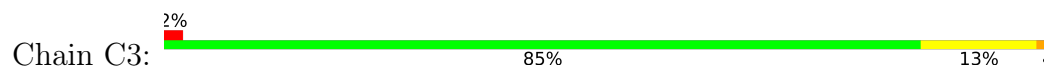




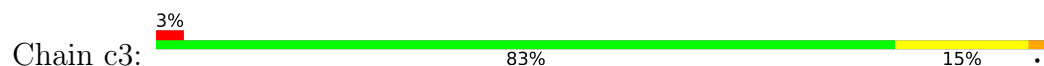
• Molecule 14: 40S Ribosomal Protein S12



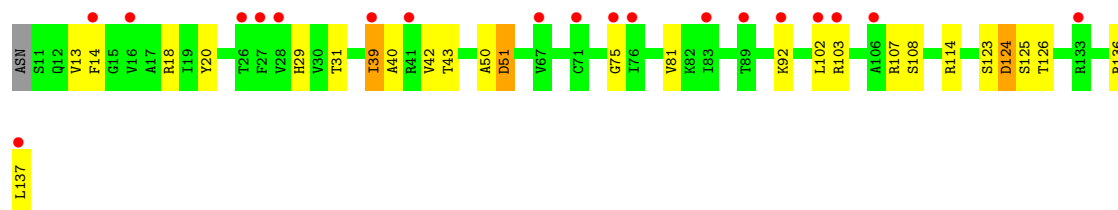
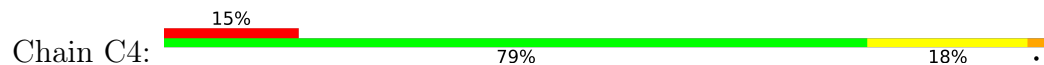
• Molecule 15: 40S ribosomal protein S13



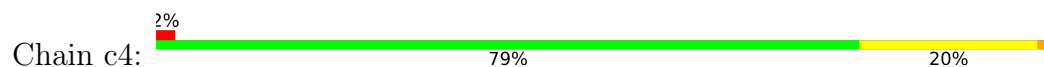
• Molecule 15: 40S ribosomal protein S13



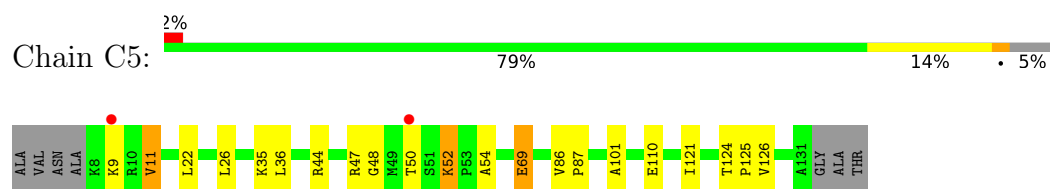
• Molecule 16: 40S Ribosomal Protein S14



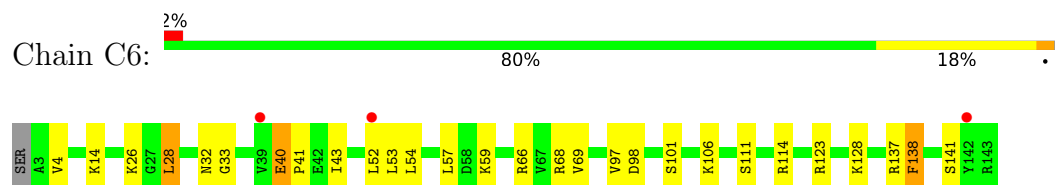
• Molecule 16: 40S Ribosomal Protein S14



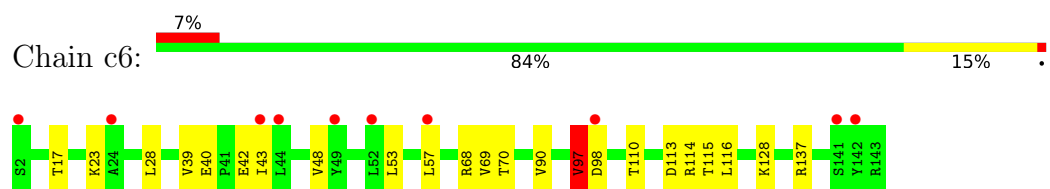
- Molecule 17: 40S ribosomal protein S15



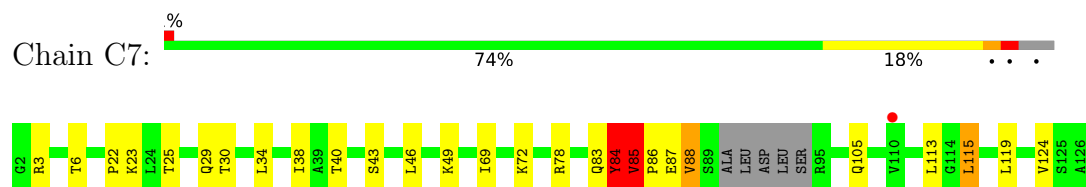
- Molecule 18: 40S ribosomal protein S16-A



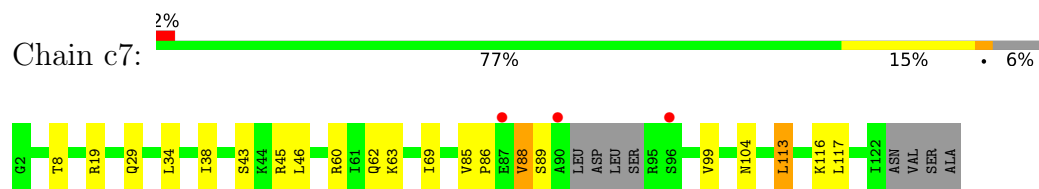
- Molecule 18: 40S ribosomal protein S16-A



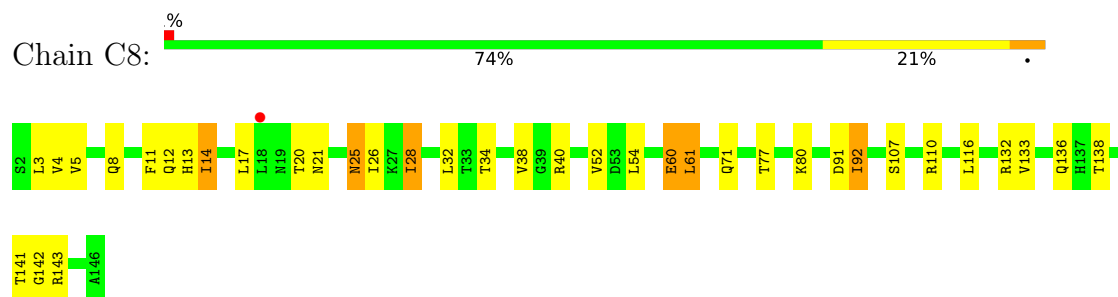
- Molecule 19: 40S ribosomal protein S17-A



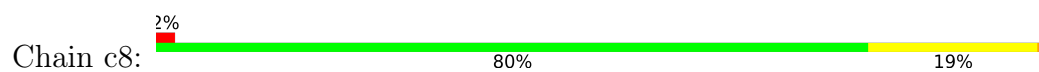
- Molecule 19: 40S ribosomal protein S17-A



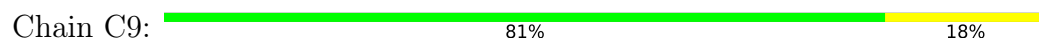
- Molecule 20: 40S ribosomal protein S18-A



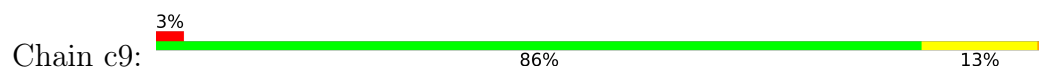
- Molecule 20: 40S ribosomal protein S18-A



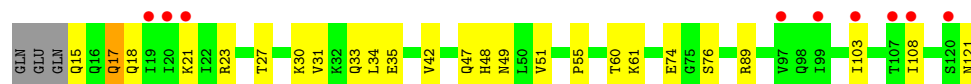
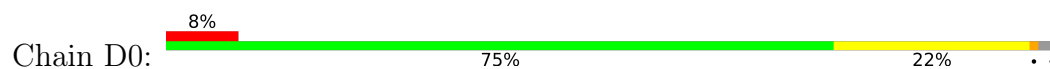
- Molecule 21: 40S ribosomal protein S19-A



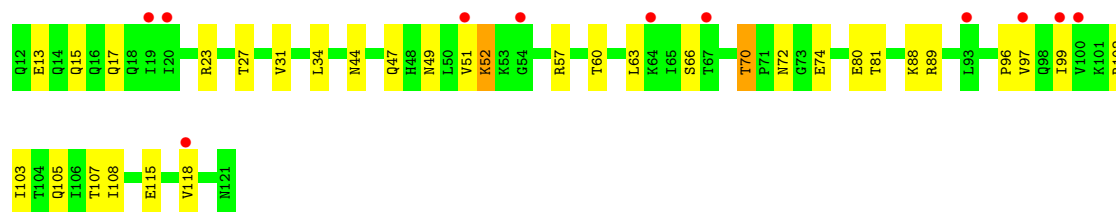
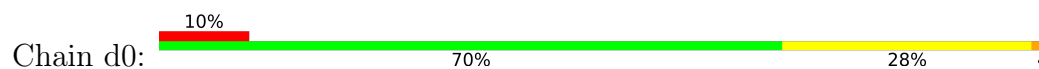
- Molecule 21: 40S ribosomal protein S19-A



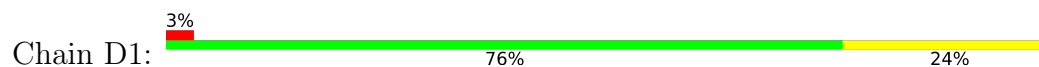
- Molecule 22: 40S ribosomal protein S20



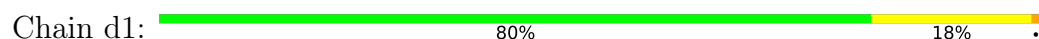
- Molecule 22: 40S ribosomal protein S20



- Molecule 23: 40S ribosomal protein S21-A

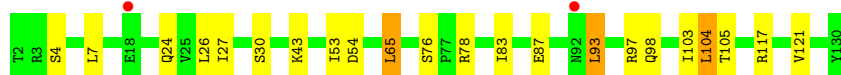
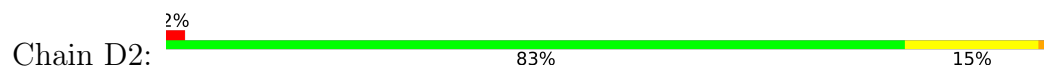


- Molecule 23: 40S ribosomal protein S21-A





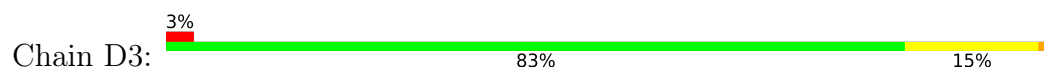
- Molecule 24: 40S ribosomal protein S22-A



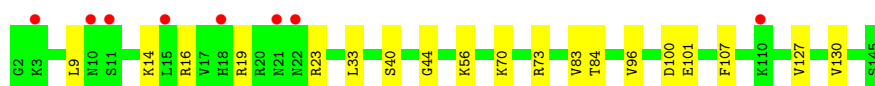
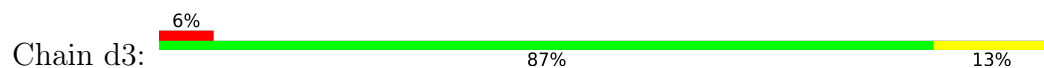
- Molecule 24: 40S ribosomal protein S22-A



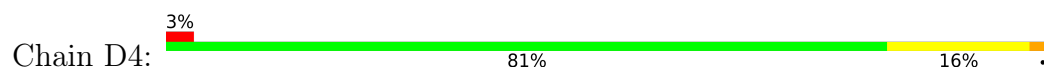
- Molecule 25: 40S ribosomal protein S23-A



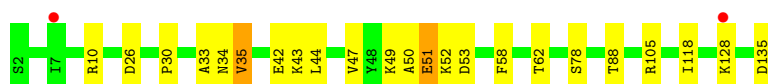
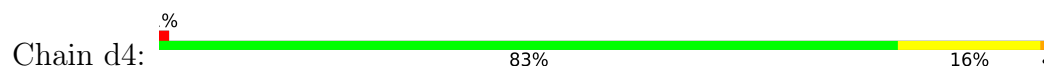
- Molecule 25: 40S ribosomal protein S23-A



- Molecule 26: 40S ribosomal protein S24-A



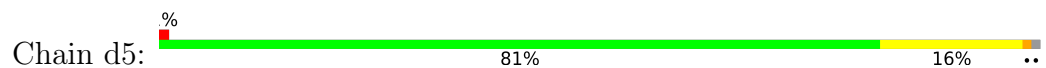
- Molecule 26: 40S ribosomal protein S24-A



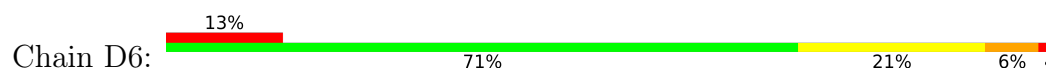
- Molecule 27: 40S ribosomal protein S25-A



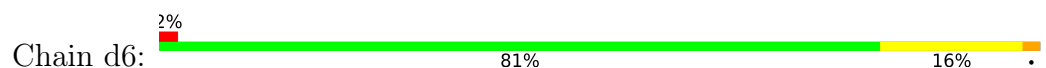
- Molecule 27: 40S ribosomal protein S25-A



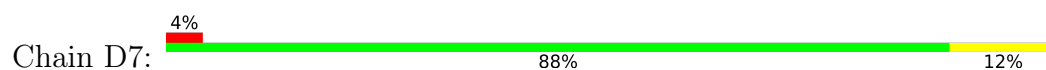
- Molecule 28: 40S ribosomal protein S26-B



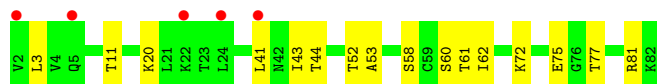
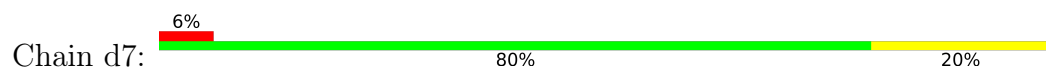
- Molecule 28: 40S ribosomal protein S26-B



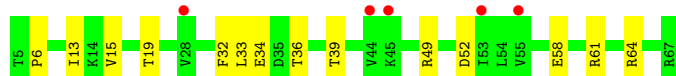
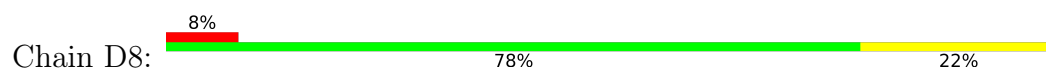
- Molecule 29: 40S ribosomal protein S27-A



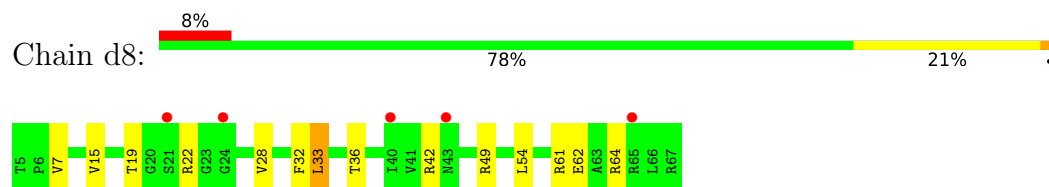
- Molecule 29: 40S ribosomal protein S27-A



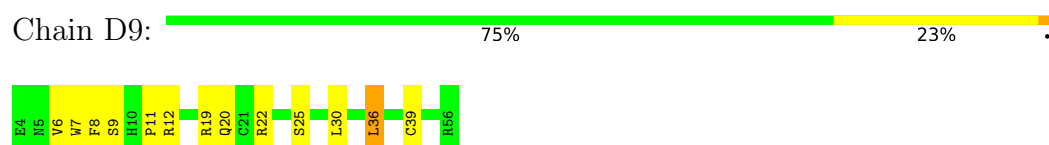
- Molecule 30: 40S ribosomal protein S28-A



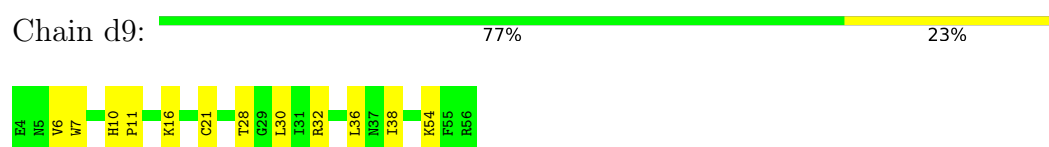
- Molecule 30: 40S ribosomal protein S28-A



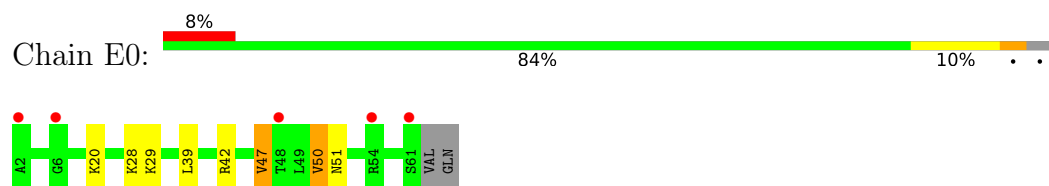
- Molecule 31: 40S ribosomal protein S29-A



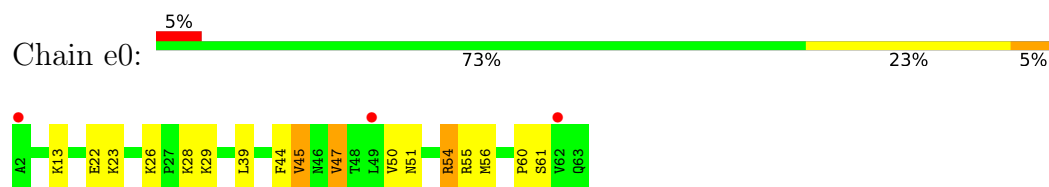
- Molecule 31: 40S ribosomal protein S29-A



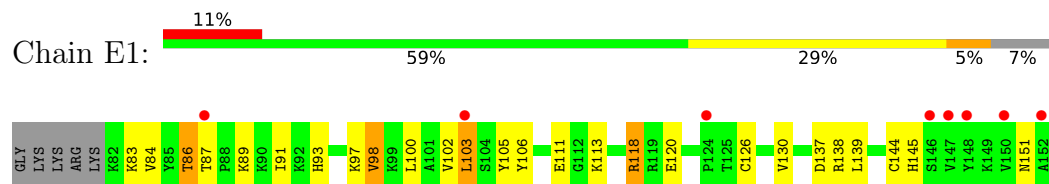
- Molecule 32: 40S ribosomal protein S30-A



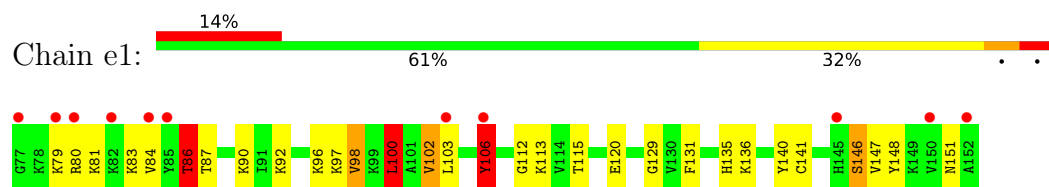
- Molecule 32: 40S ribosomal protein S30-A



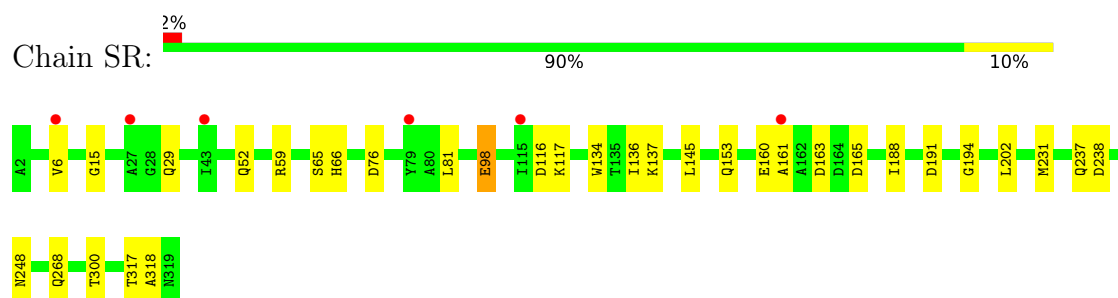
- Molecule 33: Ubiquitin-40S ribosomal protein S31



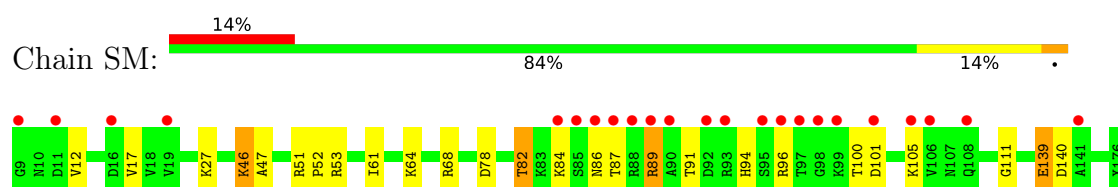
- Molecule 33: Ubiquitin-40S ribosomal protein S31



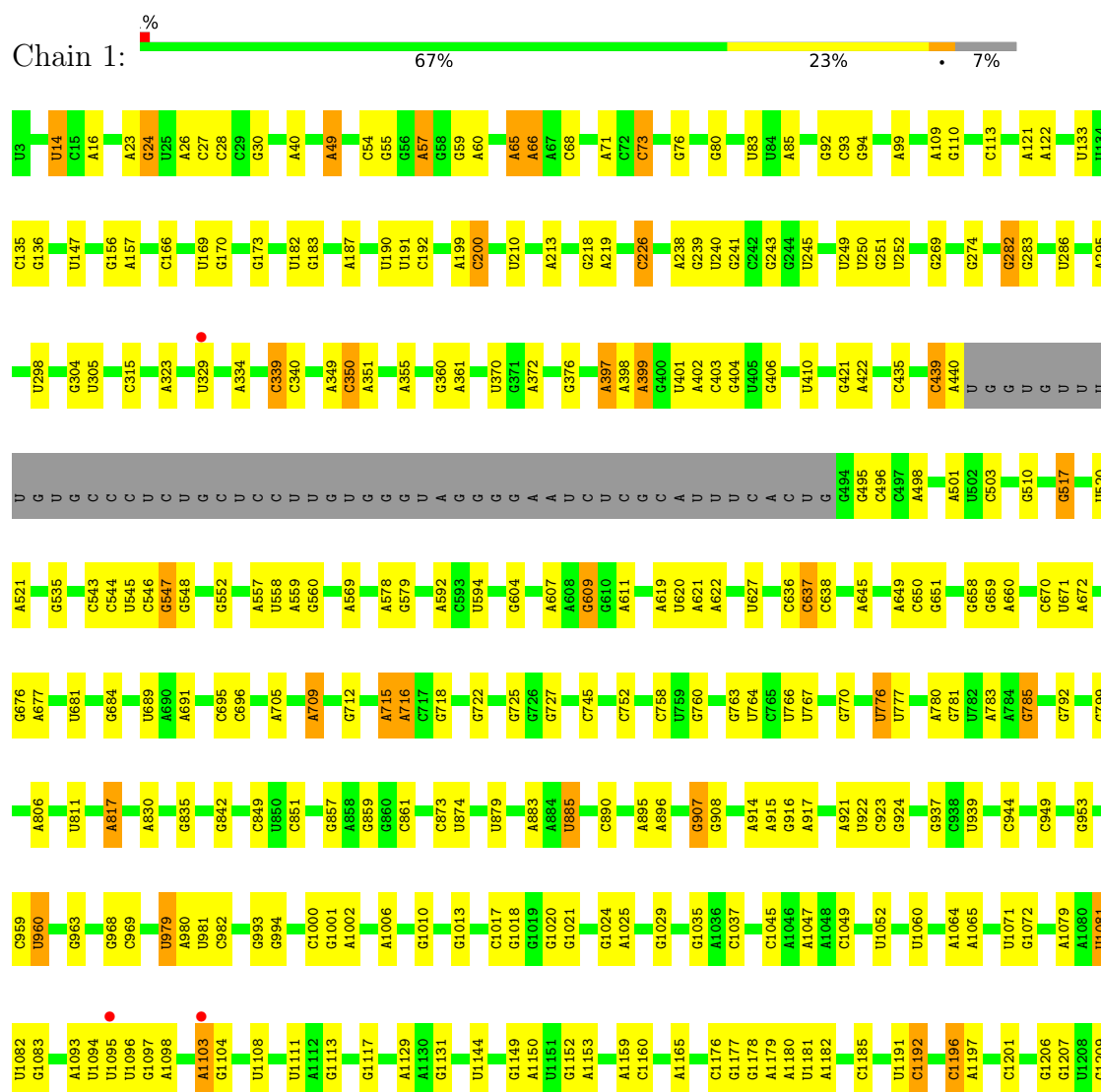
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



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

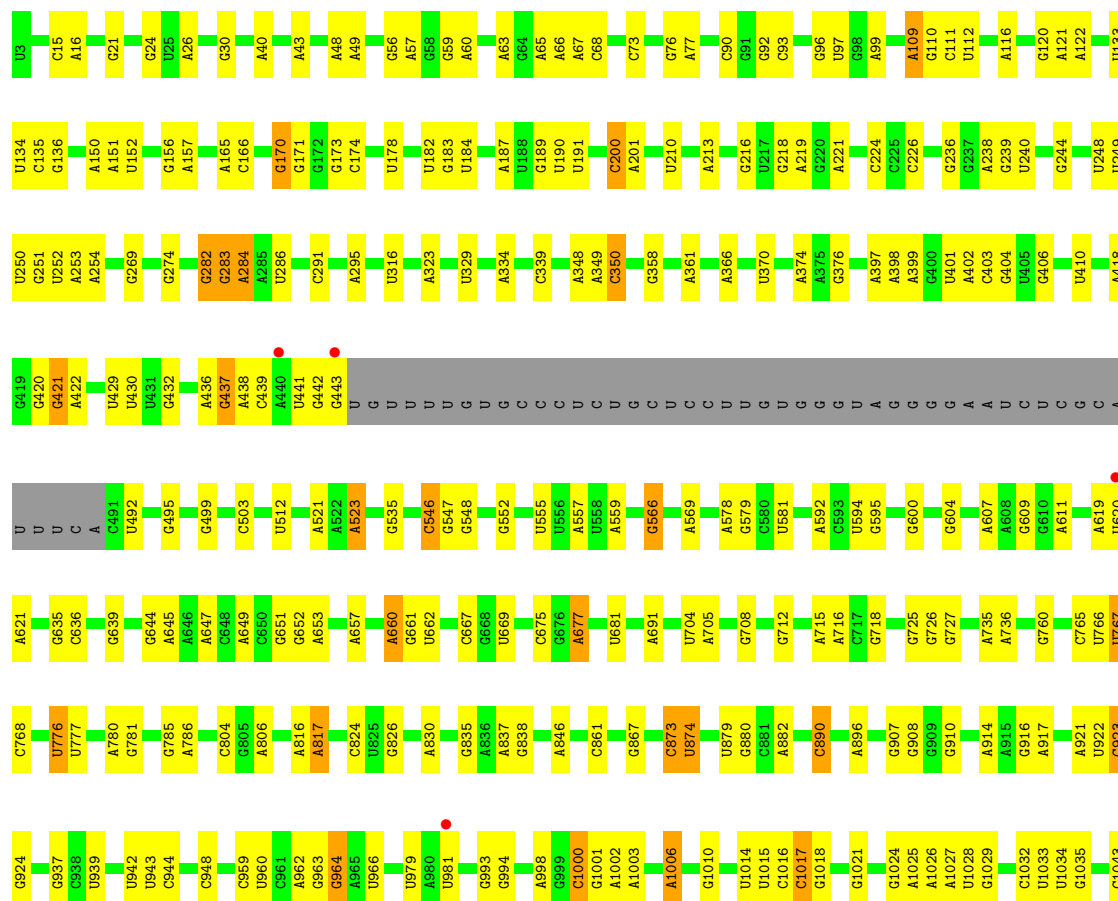


- Molecule 36: 25S rRNA

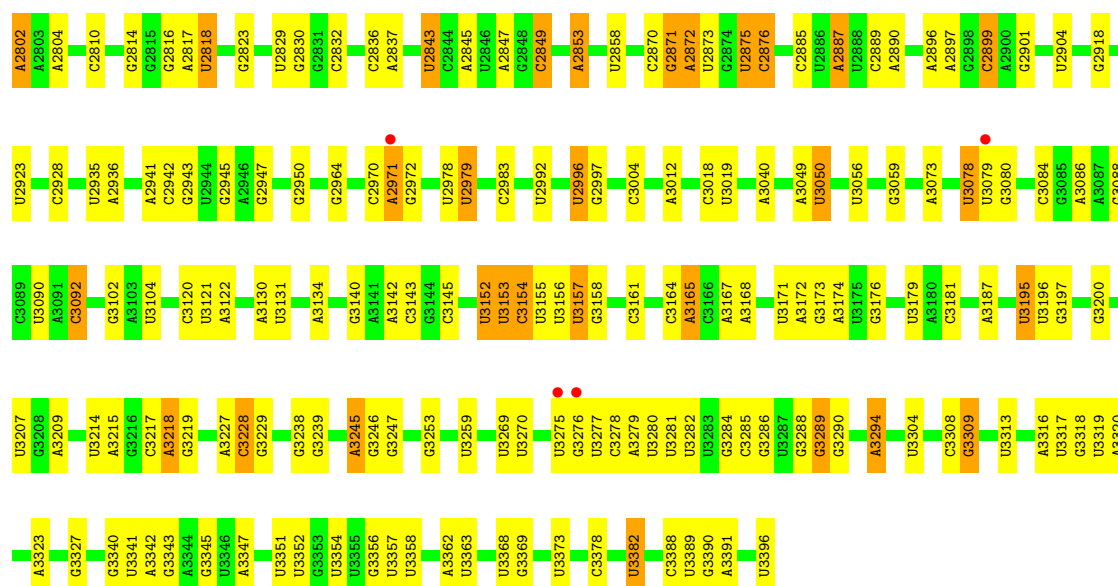




C2726	A2727	G2586	U2411	G2288	U2140	G	U	A1901	G1775	A1583	A1433	G1306	A1212
G2728	A2593	A2594	G2418	U2298	A2144	G	C	U1902	G1780	A1587	G1434	G1307	G1213
C2737	C2594	C2594	A2419	U2298	A2144	U	U	G1903	C1781	A1588	A1435	A1308	
G2745	G2603	G2603	U2426	C2306	A2147	G	G	U1904	A1797	A1589	C1437	U1309	C1216
U2752	G2606	G2607	U2434	C2307	U2148	U	U	G1905	A1797	G1590	G1443	A1217	
G2753	G2614	G2614	G2435	U2310	A2149	C	U	G1906	C1805	U1595	U1324	U1221	A1222
G2754	U2501	U2501	U2436	A2313	A2158	U	G	G1929	U1596	U1596	U1446	G1222	
C2755	A2502	A2502	G2437	U2314	G2169	C	G	G1935	G1604	G1450	U1329	A1225	A1225
A2758	G2503	G2503	U2444	U2315	U2170	U	G	U1949	A1605	U1330	A1330	G1226	G1226
U2759	U2504	U2504	A2445	G2316	G2171	U	U	U1950	U1606	A1332	A1332	C1227	C1227
G2760	C2507	C2507	U	U2334	U2172	A	U	C1951	U1607	C1333	C1333	C1232	C1232
G2761	U2513	U2513	A	U2335	U2173	U	G	G1952	U1620	G1345	G1345	G1233	G1233
A2762	U2514	U2514	G	U2336	U2174	G	G	U1953	U1620	U1346	U1346	G1236	G1236
A2626	A2515	A2515	C	C2337	U2175	C	C	G1954	U1629	U1347	U1347	G1237	G1237
U2766	G2522	G2522	G	U2341	G2187	C	U	U1955	C1639	G1484	G1484	U1241	U1241
U2771	A2523	A2523	U	A2342	C2197	U	G	A	G1640	A1350	A1350	G1242	G1242
C2772	U2524	U2524	G	C2343	A2198	C	C	U1821	U1641	U1351	U1351	G1243	G1243
G2777	G2525	G2525	U	G2355	U2205	C	A	U1818	A1643	U1494	U1494	A1244	A1244
G2778	C2526	C2526	A	U2361	G2286	U	G	U1819	C1644	U1495	U1495	G1245	G1245
A2779	U2532	U2532	G	A2362	A2207	G	G	U1820	U1645	A1355	A1355	G1246	G1246
G2788	G2533	G2533	A	A2363	U2209	C	C	C1952	C1657	U1356	U1356	U1247	U1247
G2796	U2537	U2537	U	A2364	G2210	U	U	G1954	C1663	G1357	G1357	G1248	G1248
A2799	U2538	U2538	A	C2365	U2222	C	C	U1955	U1683	G1365	G1365	G1249	G1249
G2800	C2539	C2539	G	C2366	A2223	A	U	A	U1702	U1512	U1512	U1258	U1258
A2801	U2540	U2540	U	G2369	U2224	A	A	G1844	C1527	G1367	G1367	G1262	G1262
A2802	U2542	U2542	G	U2372	U2225	U	C	U1845	U1716	U1368	U1368	A1263	A1263
A2803	U2543	U2543	A	A2373	G2226	A	U	C1846	U1717	G1371	G1371	G1264	G1264
C2808	A2547	A2547	G	C2374	C2227	C	C	U1849	U1724	G1377	G1377	U1265	U1265
G2809	G2548	G2548	C	G2375	A2228	U	G	A1850	C1725	G1380	G1380	G1266	G1266
A2810	G2549	G2549	U	G2376	C2231	C	U	G1851	C1726	U1557	U1557	U1267	U1267
A2811	C2552	C2552	C	A2385	A2244	U	C	A1858	G1727	A1557	A1557	G1268	G1268
A2812	U2553	U2553	G	A2386	G2249	C	C	A1864	G1736	A1386	A1386	A1270	A1270
A2813	A2554	A2554	C	A2387	G2280	U	U	U1865	U1741	G1392	G1392	C1271	C1271
G2814	G2555	G2555	U	C2393	A2255	G	G	C1866	A1741	U1398	U1398	A1272	A1272
A2694	A2561	A2561	G	G2394	A2256	U	C	A1874	G1736	A1399	A1399	A1273	A1273
A2696	G2568	G2568	C	G2395	A2256	U	C	G1875	A1741	G1400	G1400	A1274	A1274
G2700	A2569	A2569	U	A2397	A2262	G	U	A1879	A1750	U1564	U1564		
A2704	U2570	U2570	U	A2398	G2272	A	G	U1880	G1751	A1566	A1566	A1278	A1278
A2705	G2571	G2571	G	A2399	G2273	C	C	A1886	C1762	U1567	U1567	C1279	C1279
G2706	C2572	C2572	U	G2400	G2123	A	U	A1891	U1765	U1568	U1568	G1285	G1285
U2829	G2573	G2573	A	A2401	G2123	C	U	A1895	U1766	U1570	U1570	A1287	A1287
G2714	A2402	A2402	U	G2403	A2131	G	G	A1896	C1767	A1571	A1571	G1289	G1289
A2715	G2404	G2404	A	A2404	A2131	C	U	G1897	G1770	U1572	U1572	U1292	U1292
U2719	C2405	C2405	C	C2406	G2134	C	G	A1898		G1576	G1576	U1293	U1293
U2725	G2585	G2585	A		G2137	U	U	A1899		A1580	A1580	A1294	A1294

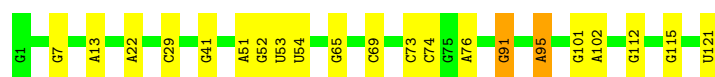


G2662	U2543	G2397	G2288	A2172	G	G1770	C1579	C1451	G1311	U1191	A1047
G2663	G2549	A2398	C2293	U2176	G	G1775	A1580	A1452	C1314	C1192	A1048
A2667	C2552	A2401	U2298	A2188	C	G1779	C1581	A1453	U1329	A1193	C1049
A2674	G2555	G2402	A2303	U2189	U	G1780	A1583	U1457	A1330	C1196	A1064
G2677	C2566	G2403	U2297	C2197	G	G1781	A1588	A1460	U1331	A1200	A1065
A2678	C2567	A2404	G2307	A2198	U	G1794	A1589	A1461	C1349	C1201	U1071
U2681	C2568	C2405	U2310	U2199	U	G1795	A1593	A1462	U1351	A1202	G1072
C2682	U2570	U2411	A2313	G2201	A	G1796	C1597	A1465	U1352	G1209	U1081
U2683	U2571	G2418	U2314	C2204	G	G1797	G1604	G1480	U1353	U1082	U1082
G2689	C2572	A2419	G2315	U2205	C	G1812	A1605	A1481	G1354	C1216	A1085
A2690	G2573	C2420	U2318	U2209	U	A1813	U1606	A1482	A1355	G1222	U1085
A2691	G2574	U2421	U2319	G2210	G	A1814	U1607	G1483	U1356	A1223	U1088
A2694	G2584	G2435	A2320	U2211	U	A1815	C1608	U1484	G1357	G1232	U1093
A2695	G2585	U2436	U2327	C2212	C	A1816	U1609	G1487	G1367	U1241	U1094
A2696	G2589	A2437	U2330	A2213	A	G1817	U1620	A1490	A1373	G1236	U1095
A2704	U2593	A2438	C2330	U2222	G	U1818	C1628	U1495	G1374	G1237	U1096
G2705	C2594	A2440	U2334	A2223	G	U1819	U1629	C1496	U1379	C1238	G1097
A2706	G2594	A2441	G2335	U2224	C	U1820	U1639	G1503	G1380	C1239	A1098
C2707	A2601	G2442	U2336	U2225	U	U1821	C1639	A1503	U1386	A1240	A1103
G2714	G2606	A2443	U2337	A2228	C	A1840	A1643	A1506	C1385	U1242	G1104
U2719	U2505	A	C2337	U2229	U	A1841	U1644	G1507	A1386	G1245	G1116
U2719	G2607	U	C2338	C2231	U	A1842	U1645	C1508	G1387	A1246	G1117
C2726	G2608	A	U2340	G2234	U	C1846	G1655	G1536	U1388	G1245	C1118
A2727	A2609	G	U2341	U2234	A	A1847	G1656	A1539	A1389	A1252	C1119
G2728	G2610	A	A2345	A2244	A2093	A1848	C1657	U1540	C1391	U1253	U1129
U2729	G2614	G	G	G2249	C2101	A1849	U1657	G1541	A1399	C1254	A1130
G2730	G2615	G	U2349	G2250	U2102	A1850	C1665	G1541	G1400	A1259	G1131
C2742	G2618	U	G	G2251	U2112	C1856	A1683	U1553	C1403	G1262	G1134
A2743	U2744	U	A	A2252	C2113	A1867	A1704	U1554	C1403	G1263	A1143
U2752	G2621	G	A	U2253	C2114	U1872	U1716	U1555	A1418	G1264	U1148
G2753	C2625	U	A	G2254	C2115	A1878	U1717	A1557	A1419	U1265	G1148
A2762	A2626	A	U2372	U2258	G2121	U1879	U1717	G1560	C1424	G1266	G1152
U2771	U2634	A	A2373	U2264	G2122	U1880	U1724	G1561	G1429	G1284	A1153
C2772	A2635	G	G2374	G2264	C2128	U1885	C1725	C1562	U1430	G1285	A1154
C2773	A2636	U	G2375	G2272	A2131	A1886	G1736	A1566	G1431	C1292	C1155
C2777	C2637	U	U2376	G2273	C2132	A1891	U1750	U1567	A1432	G1295	C1156
G2777	G2638	G	C2377	G2273	C2132	G1892	G1751	U1568	G1434	C1297	A1159
G2778	G2639	A	U2378	G2276	A2144	A1893	U1751	U1569	C1437	C1297	C1160
A2779	C2644	G	A2384	C2277	A2145	U1897	A1760	A1571	U1438	G1300	G1178
G2796	U2652	C	G2385	C2278	C2146	G1897	C1761	A1572	U1445	U1305	A1179
C2797	U2538	U	A2385	A2279	C2146	A1901	C1762	G1573	U1446	G1306	U1181
C2798	A2656	U	C2386	A2280	C2156	C1904	U1763	A1574	G1447	G1307	A1182
A2799	G2659	C	U2388	A2281	G2157	U1905	U1764	A1575	U1448	A1308	U1189
G2800	G2659	G	U2389	U2282	A2158	G1906	G1765	G1576	U1449	U1309	C1189
A2801	G2659	C	G2392	G2283	G2169	U1906	G1766	C1578	A1450	G1310	A1190



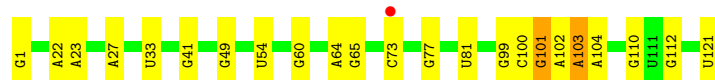
• Molecule 37: 5S rRNA

Chain 3: 83% 16%



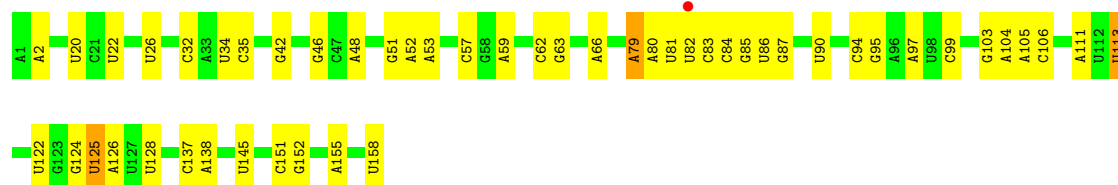
• Molecule 37: 5S rRNA

Chain 7: 81% 17%



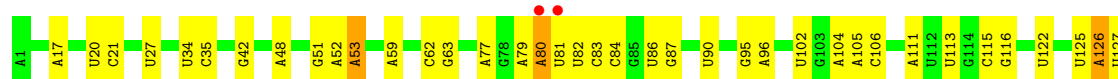
• Molecule 38: 5.8S rRNA

Chain 4: 68% 30%



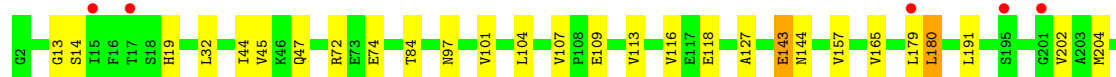
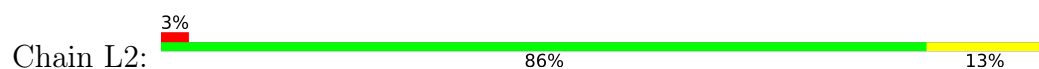
• Molecule 38: 5.8S rRNA

Chain 8: 73% 25%

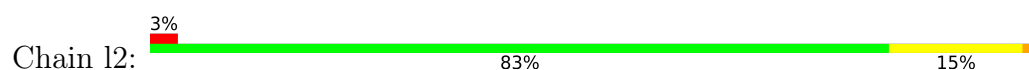




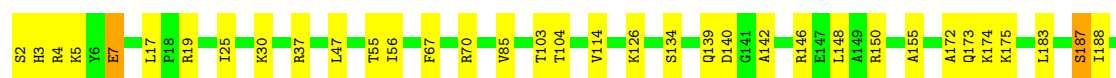
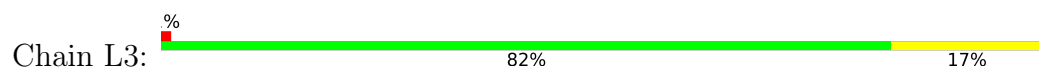
- Molecule 39: 60S ribosomal protein L2-A



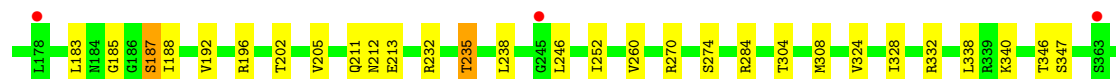
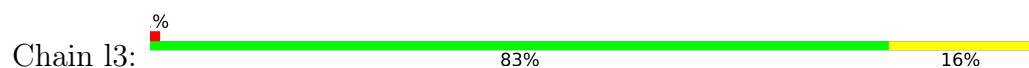
- Molecule 39: 60S ribosomal protein L2-A

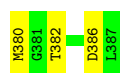


- Molecule 40: 60S ribosomal protein L3

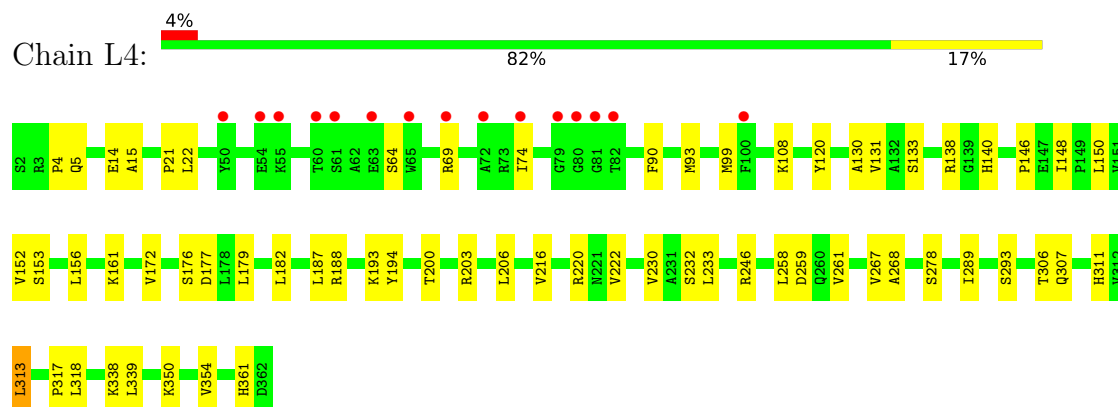


- Molecule 40: 60S ribosomal protein L3

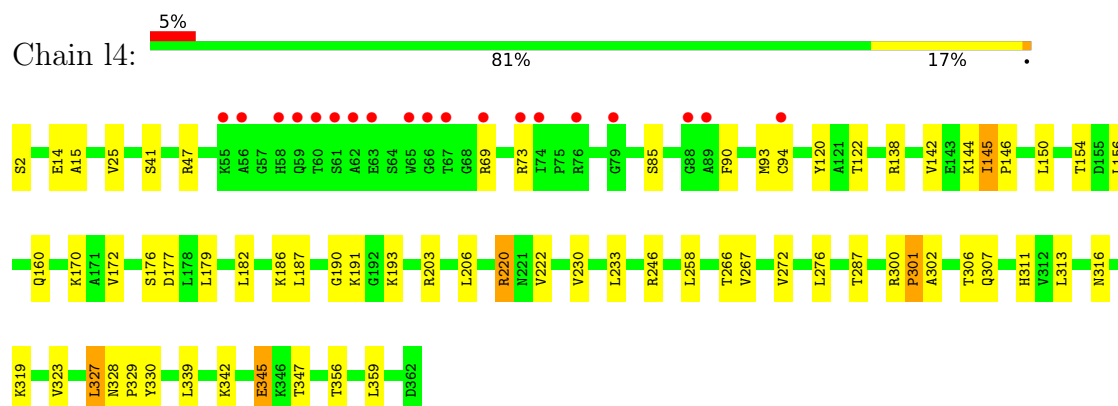




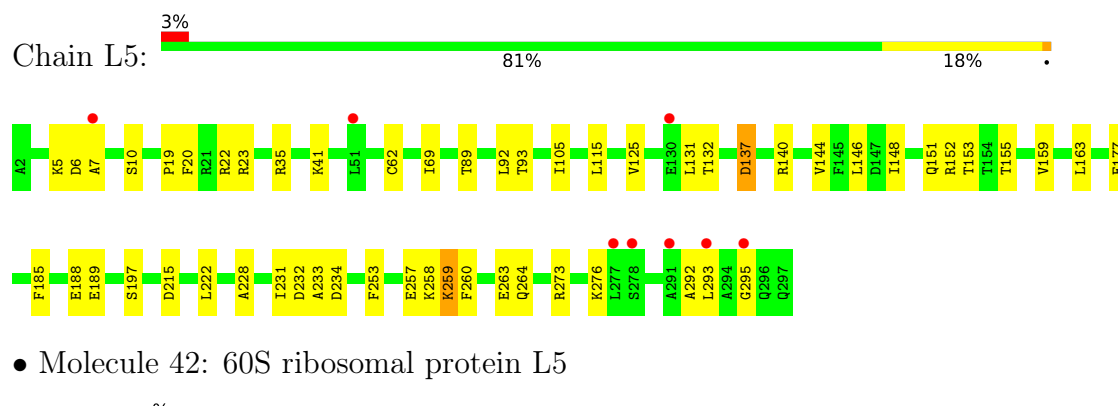
- Molecule 41: 60S ribosomal protein L4-A



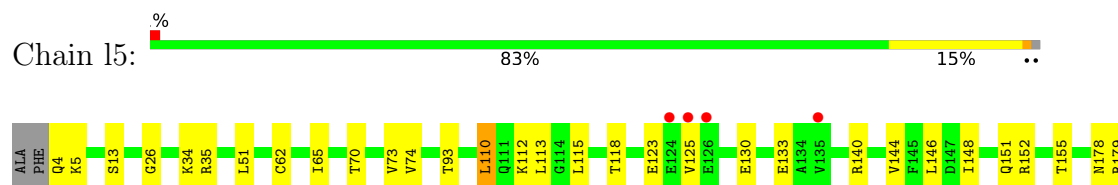
- Molecule 41: 60S ribosomal protein L4-A

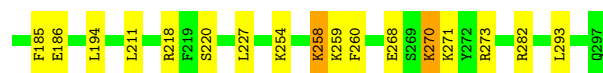


- Molecule 42: 60S ribosomal protein L5

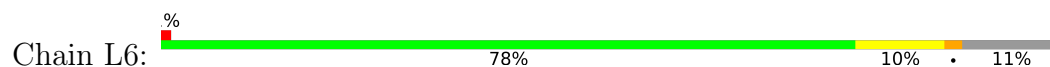


- Molecule 42: 60S ribosomal protein L5

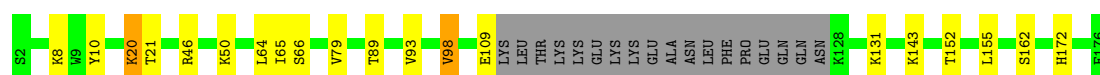
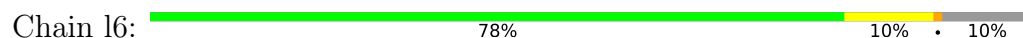




- Molecule 43: 60S ribosomal protein L6-A



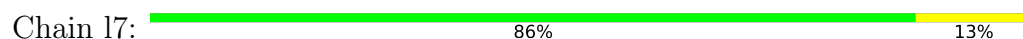
- Molecule 43: 60S ribosomal protein L6-A



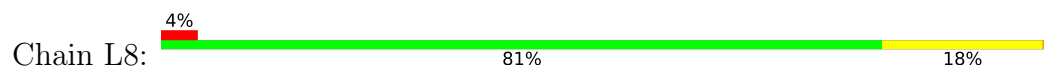
- Molecule 44: 60S ribosomal protein L7-A



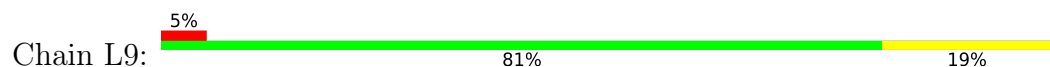
- Molecule 44: 60S ribosomal protein L7-A



- Molecule 45: 60S ribosomal protein L8-A

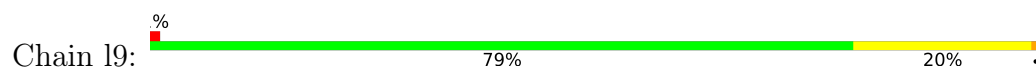


- Molecule 46: 60S ribosomal protein L9-A

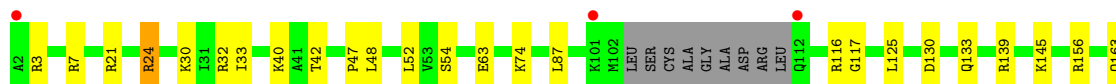
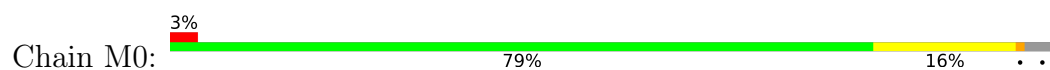




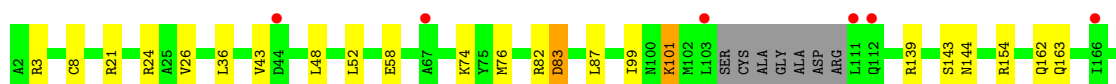
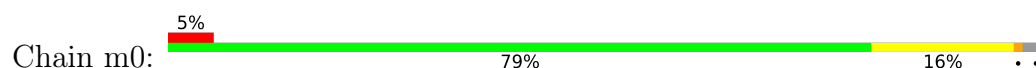
- Molecule 46: 60S ribosomal protein L9-A



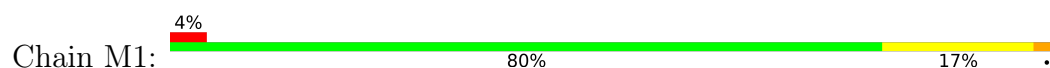
- Molecule 47: 60S ribosomal protein L10



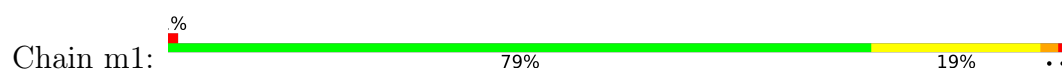
- Molecule 47: 60S ribosomal protein L10



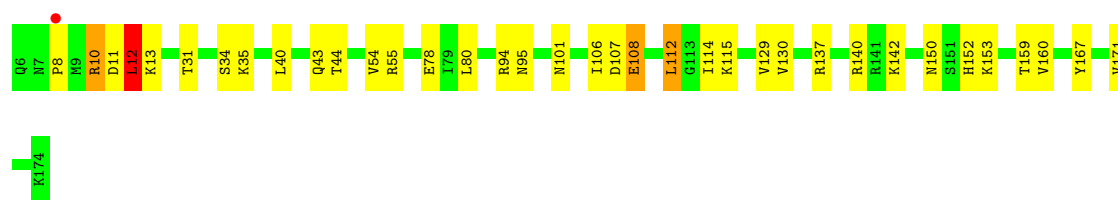
- Molecule 48: 60S ribosomal protein L11-B



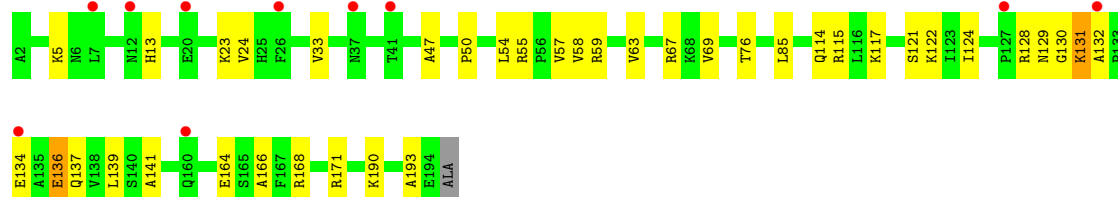
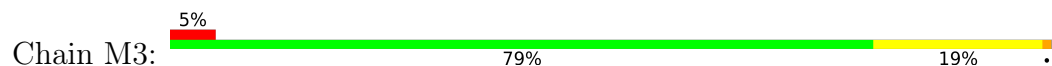
- Molecule 48: 60S ribosomal protein L11-B



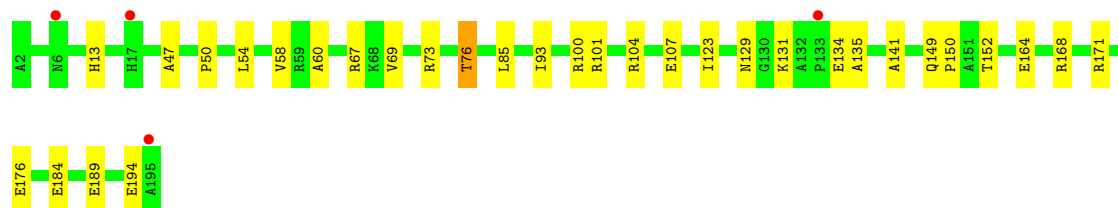
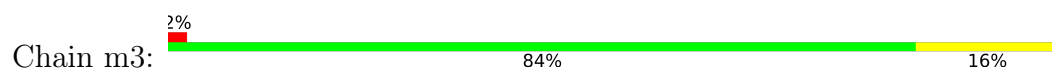




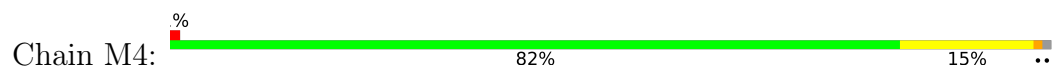
- Molecule 49: 60S ribosomal protein L13-A



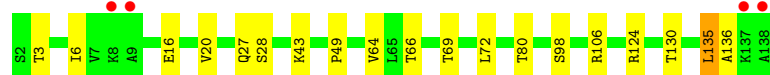
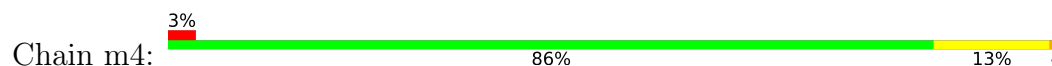
- Molecule 49: 60S ribosomal protein L13-A



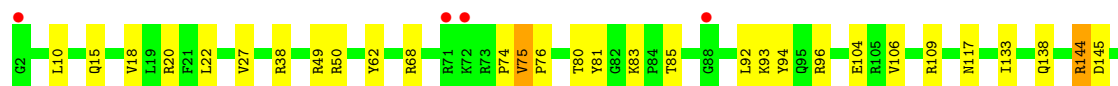
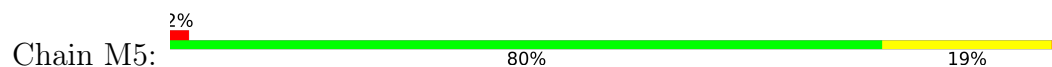
- Molecule 50: 60S ribosomal protein L14-A



- Molecule 50: 60S ribosomal protein L14-A

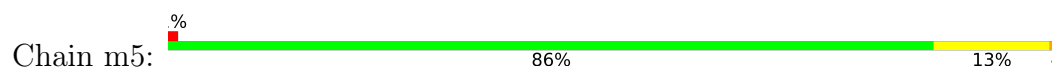


- Molecule 51: 60S ribosomal protein L15-A





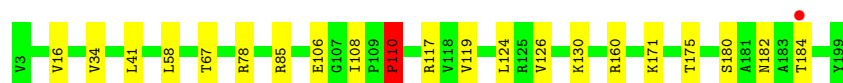
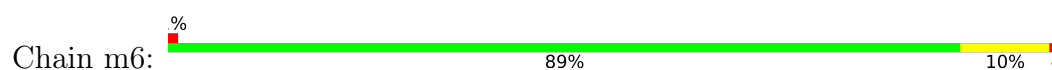
- Molecule 51: 60S ribosomal protein L15-A



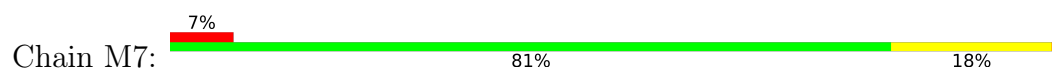
- Molecule 52: 60S ribosomal protein L16-A



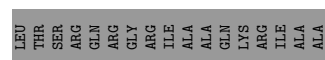
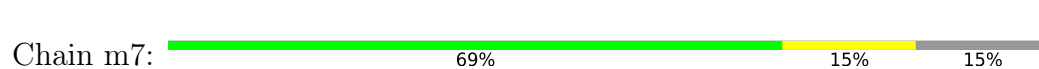
- Molecule 52: 60S ribosomal protein L16-A



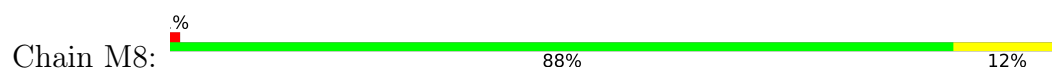
- Molecule 53: 60S ribosomal protein L17-A



- Molecule 53: 60S ribosomal protein L17-A

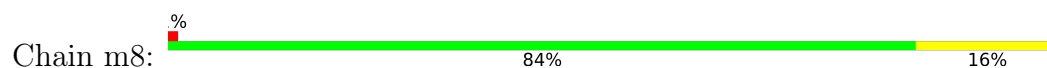


- Molecule 54: 60S ribosomal protein L18-A

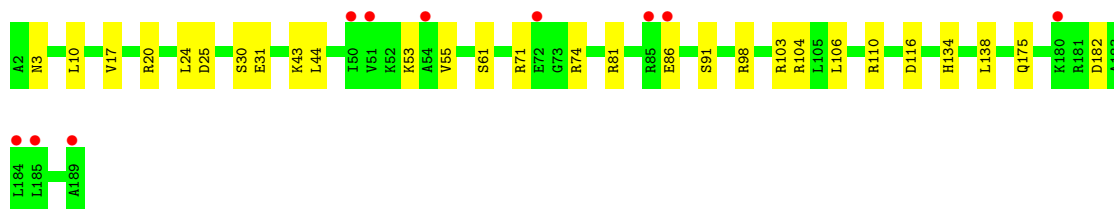
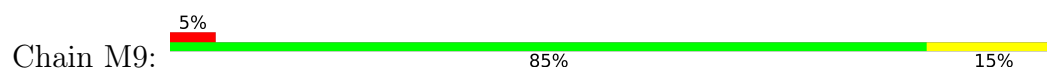




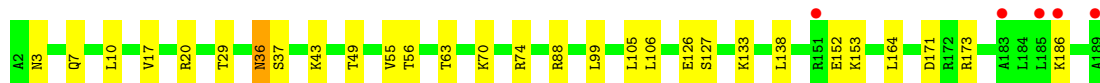
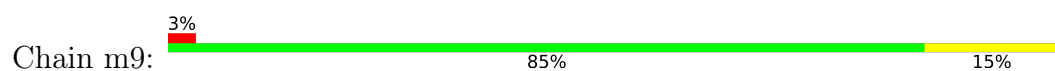
- Molecule 54: 60S ribosomal protein L18-A



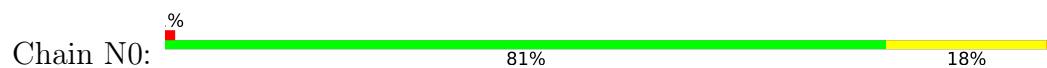
- Molecule 55: 60S ribosomal protein L19-A



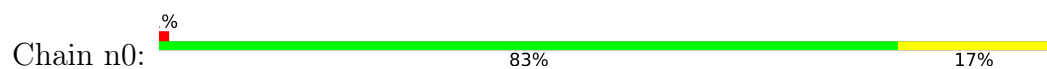
- Molecule 55: 60S ribosomal protein L19-A



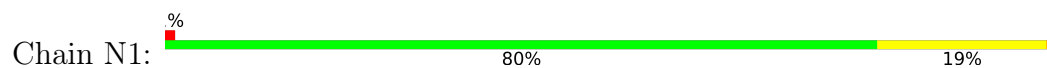
- Molecule 56: 60S ribosomal protein L20-A



- Molecule 56: 60S ribosomal protein L20-A

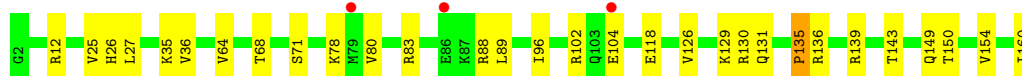
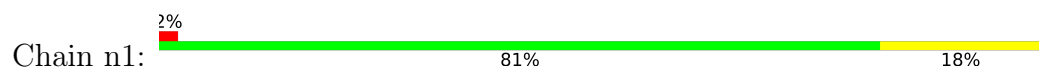


- Molecule 57: 60S ribosomal protein L21-A

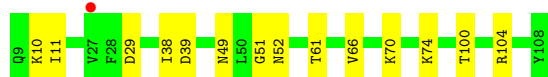
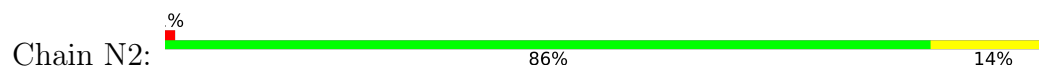




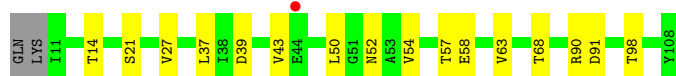
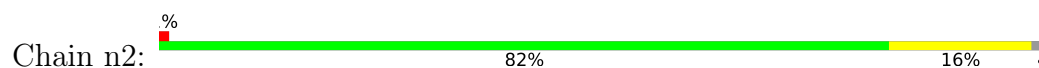
- Molecule 57: 60S ribosomal protein L21-A



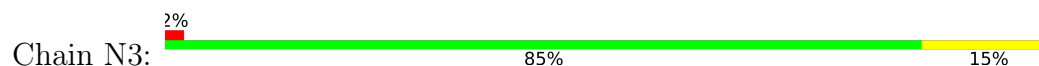
- Molecule 58: 60S ribosomal protein L22-A



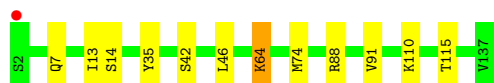
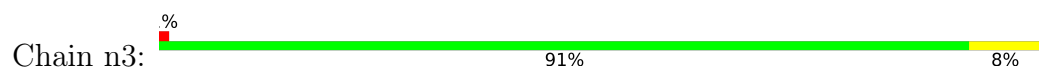
- Molecule 58: 60S ribosomal protein L22-A



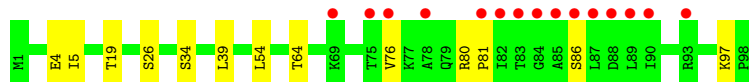
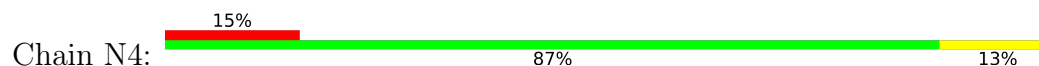
- Molecule 59: 60S ribosomal protein L23-A



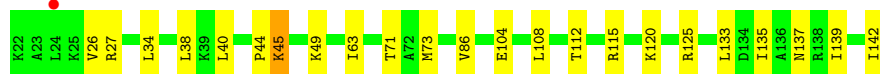
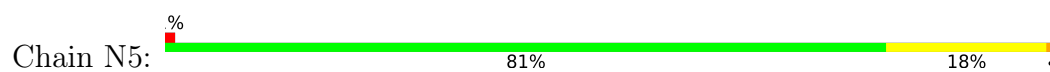
- Molecule 59: 60S ribosomal protein L23-A



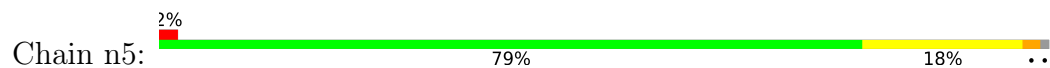
- Molecule 60: 60S ribosomal protein L24-A



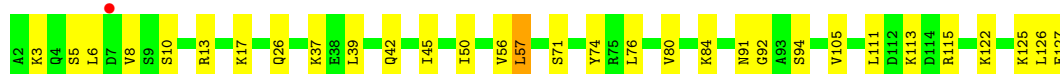
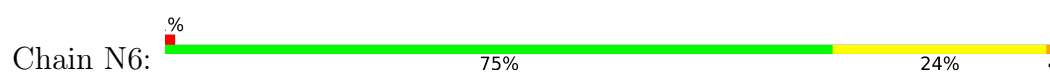
- Molecule 61: 60S ribosomal protein L25



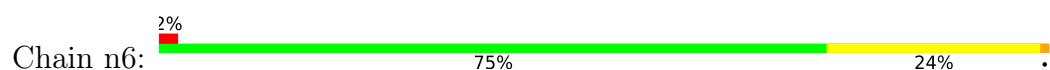
- Molecule 61: 60S ribosomal protein L25



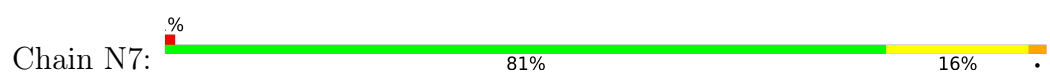
- Molecule 62: 60S ribosomal protein L26-A



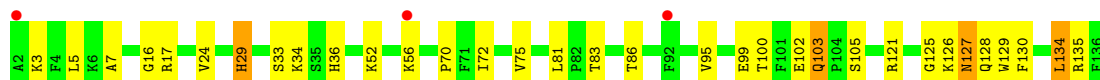
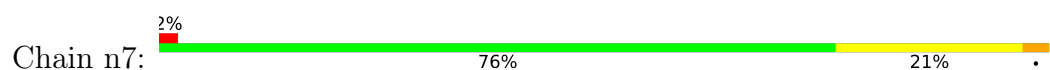
- Molecule 62: 60S ribosomal protein L26-A



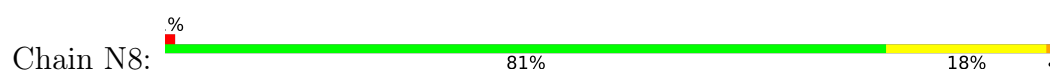
- Molecule 63: 60S ribosomal protein L27-A



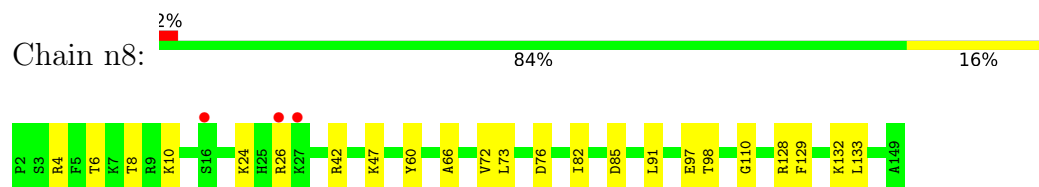
- Molecule 63: 60S ribosomal protein L27-A



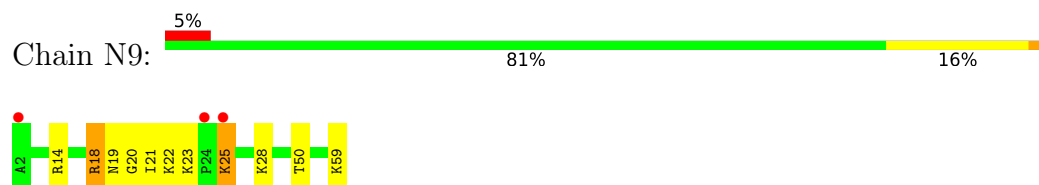
- Molecule 64: 60S ribosomal protein L28



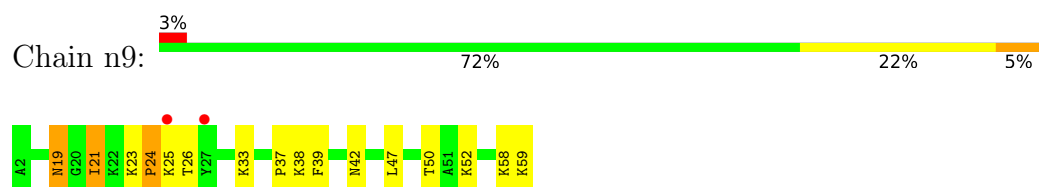
## • Molecule 64: 60S ribosomal protein L28



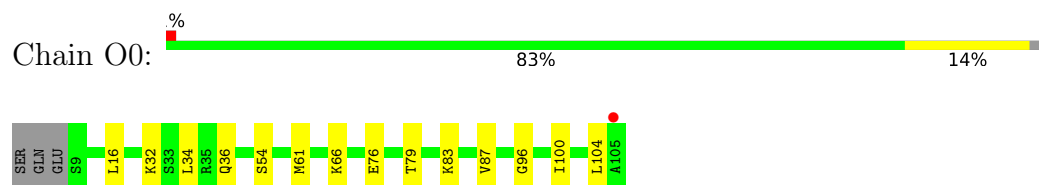
## • Molecule 65: 60S ribosomal protein L29



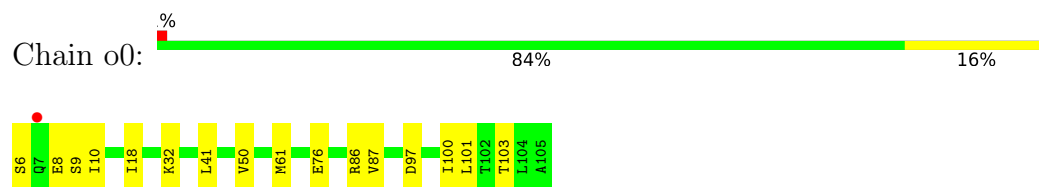
## • Molecule 65: 60S ribosomal protein L29



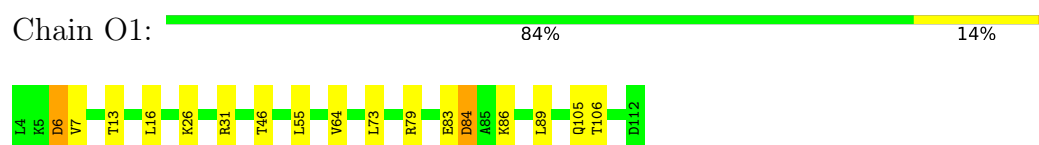
## • Molecule 66: 60S ribosomal protein L30



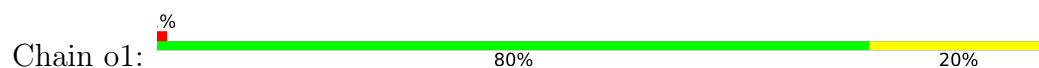
## • Molecule 66: 60S ribosomal protein L30



## • Molecule 67: 60S ribosomal protein L31-A

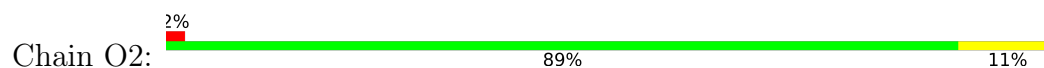


## • Molecule 67: 60S ribosomal protein L31-A

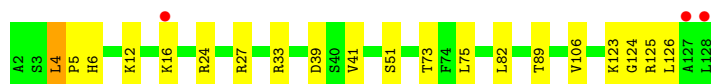
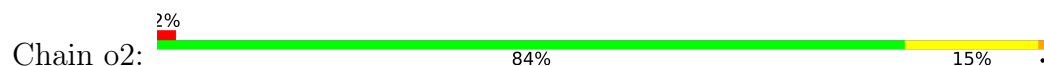




- Molecule 68: 60S ribosomal protein L32



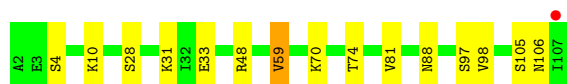
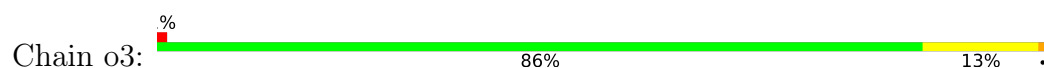
- Molecule 68: 60S ribosomal protein L32



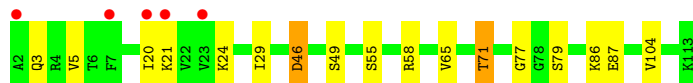
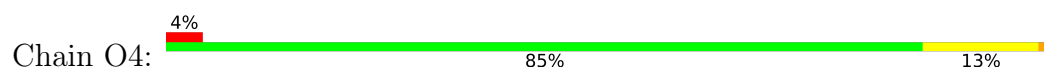
- Molecule 69: 60S ribosomal protein L33-A



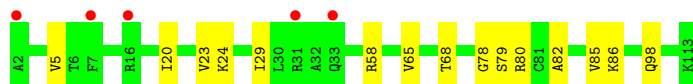
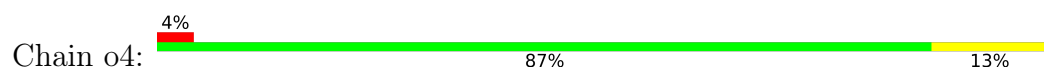
- Molecule 69: 60S ribosomal protein L33-A



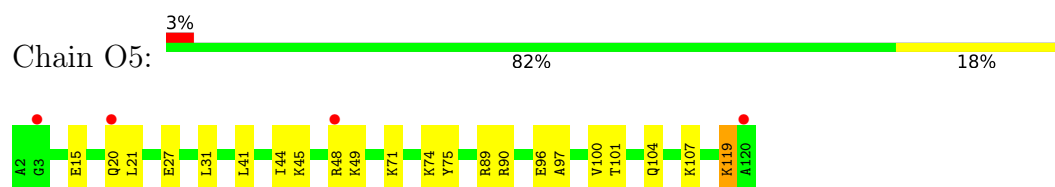
- Molecule 70: 60S ribosomal protein L34-A



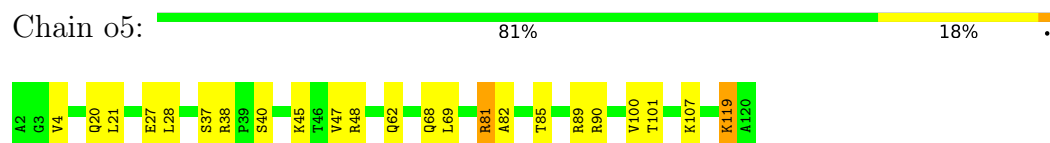
- Molecule 70: 60S ribosomal protein L34-A



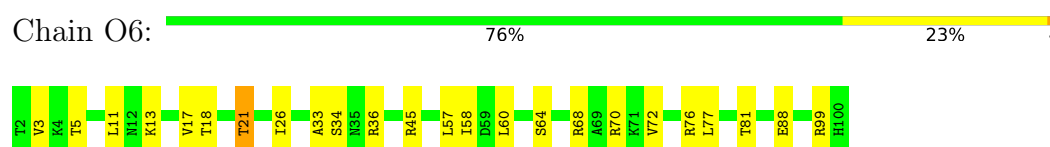
- Molecule 71: 60S ribosomal protein L35-A



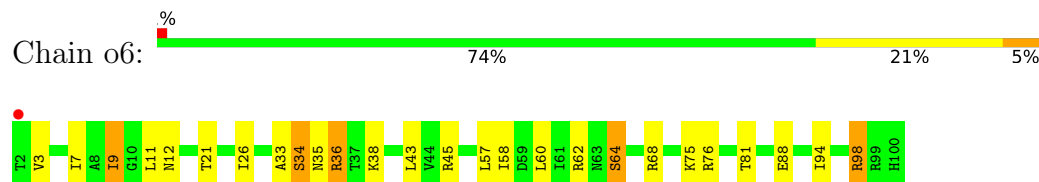
- Molecule 71: 60S ribosomal protein L35-A



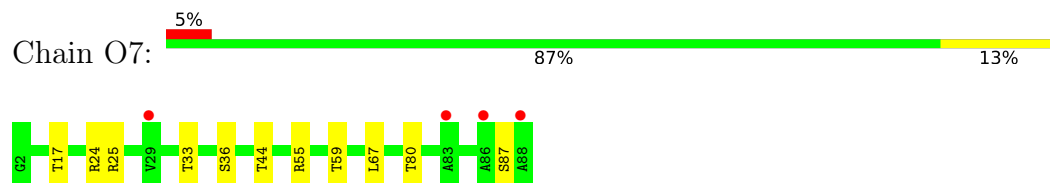
- Molecule 72: 60S ribosomal protein L36-A



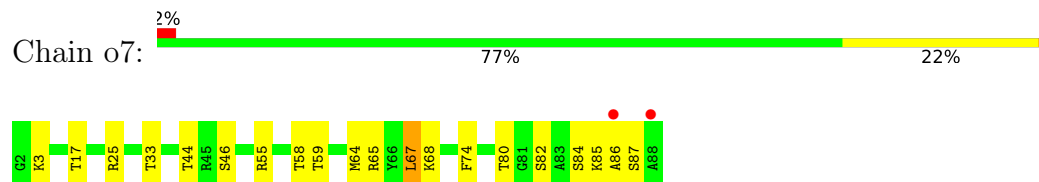
- Molecule 72: 60S ribosomal protein L36-A



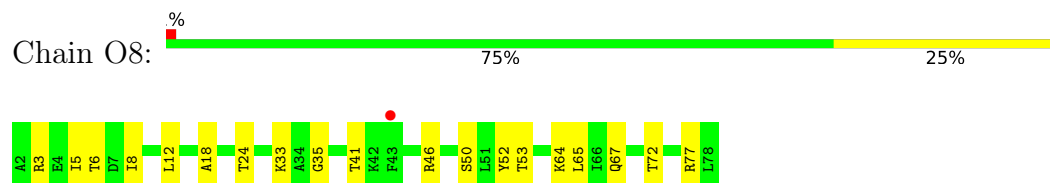
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 73: 60S ribosomal protein L37-A

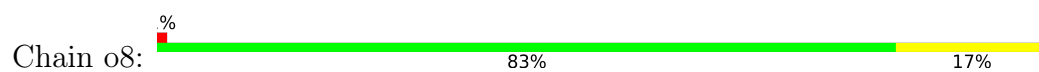


- Molecule 74: 60S ribosomal protein L38

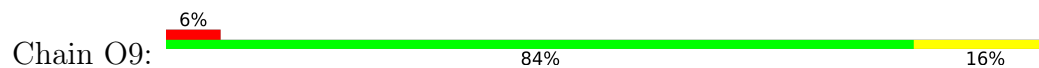


- Molecule 74: 60S ribosomal protein L38

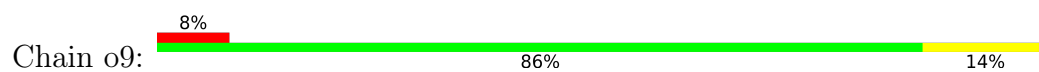




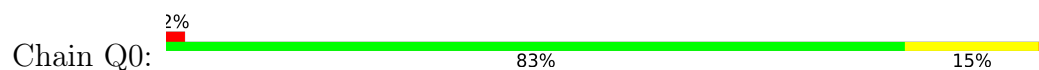
- Molecule 75: 60S ribosomal protein L39



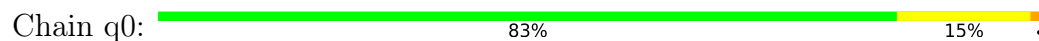
- Molecule 75: 60S ribosomal protein L39



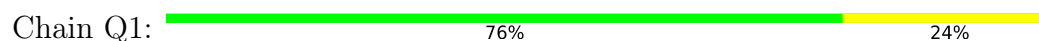
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



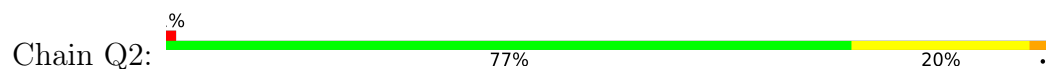
- Molecule 77: 60S ribosomal protein L41-A



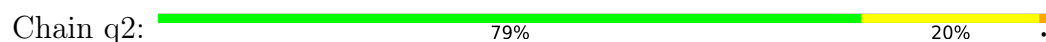
- Molecule 77: 60S ribosomal protein L41-A



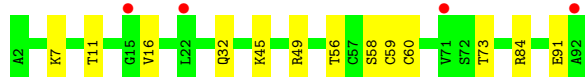
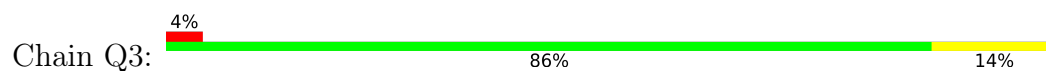
- Molecule 78: 60S ribosomal protein L42-A



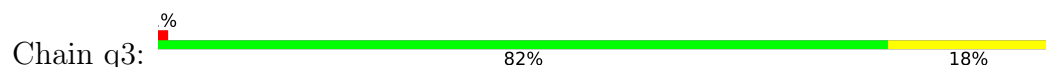
- Molecule 78: 60S ribosomal protein L42-A



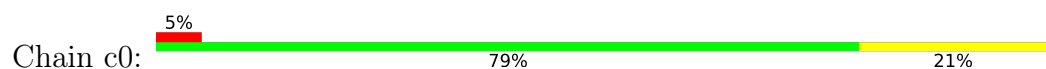
- Molecule 79: 60S ribosomal protein L43-A



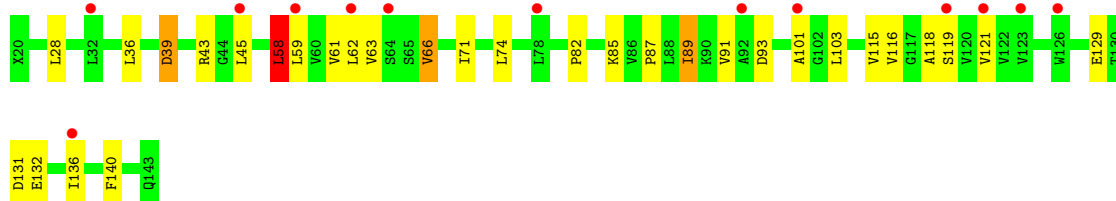
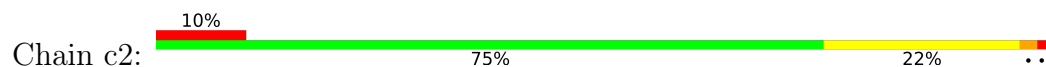
- Molecule 79: 60S ribosomal protein L43-A



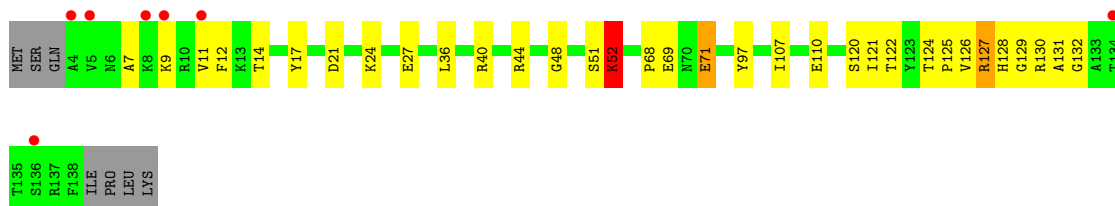
- Molecule 80: 40S ribosomal protein S10-A, 40S ribosomal protein S10-A, 40S Ribosomal Protein S10



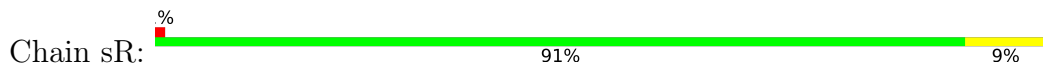
- Molecule 81: 40S Ribosomal Protein S12



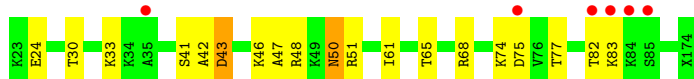
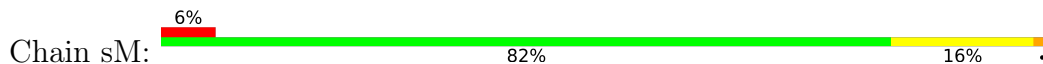
- Molecule 82: 40S ribosomal protein S15



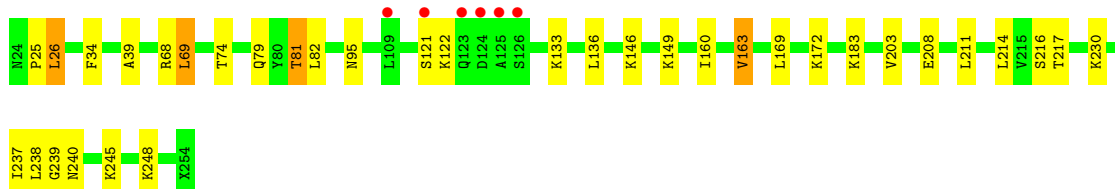
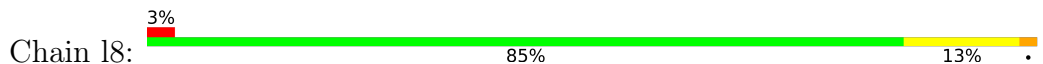
- Molecule 83: Guanine nucleotide-binding protein subunit beta-like protein



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



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

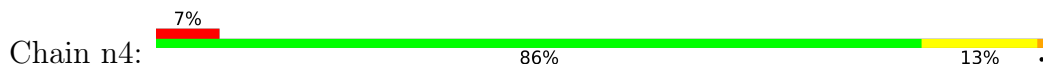


- Molecule 86: 60S Ribosomal Protein L12

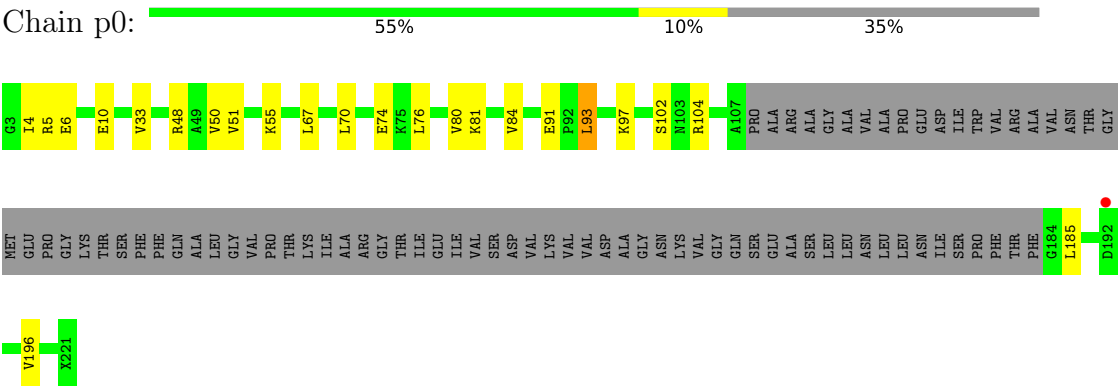


There are no outlier residues recorded for this chain.

- Molecule 87: 60S ribosomal protein L24-A



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



- Molecule 89: 60S Ribosomal Protein P1/2

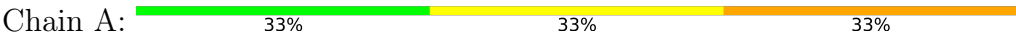


There are no outlier residues recorded for this chain.

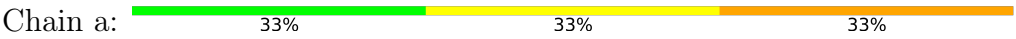
- Molecule 89: 60S Ribosomal Protein P1/2



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	90.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

*Continued on next page...*

*Continued from previous page...*

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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	22	PRO	Peptide
19	C7	85	VAL	Peptide
3	S1	131	ASP	Peptide
6	S4	193	GLY	Peptide
9	S7	131	PHE	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

5 of 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

### 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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 3173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	s8	82	VAL
39	l2	147	ARG
13	c1	47	THR
10	s8	74	LYS
22	d0	31	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
42	l5	81	HIS
64	n8	25	HIS
42	l5	264	GLN
51	m5	178	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
70	o4	3	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%)

5 of 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

5 of 275 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	1819	U
36	5	2209	U
36	5	3121	U
36	1	1751	G
36	1	1562	C

## 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
90	A	76	PPU	C5-C4	2.19	1.46	1.40

The worst 5 of 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

There are no chirality outliers.

5 of 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

*Continued on next page...*



*Continued from previous page...*

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

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 [i](#)

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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	19	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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-	-		
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.



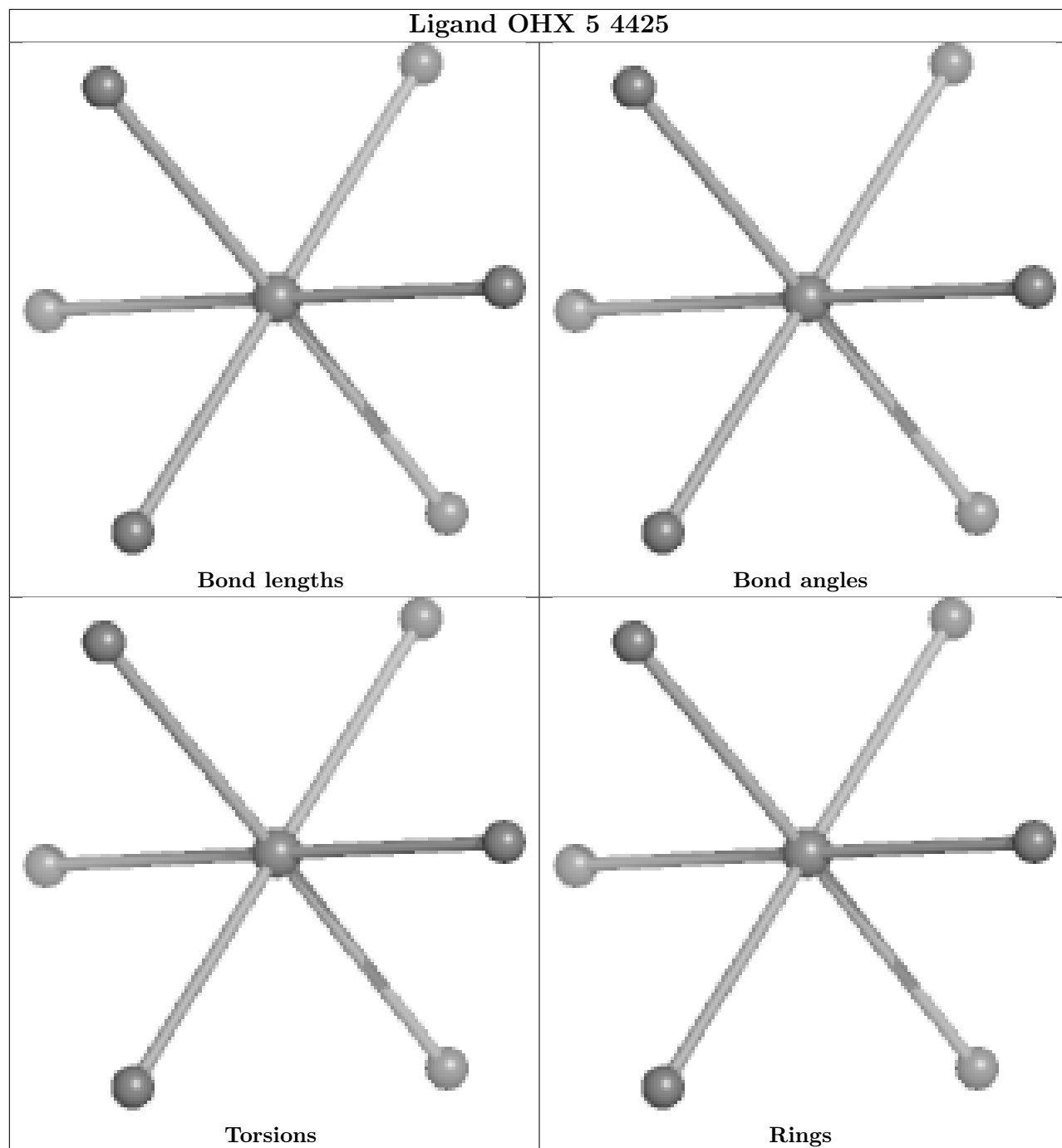
There are no torsion outliers.

There are no ring outliers.

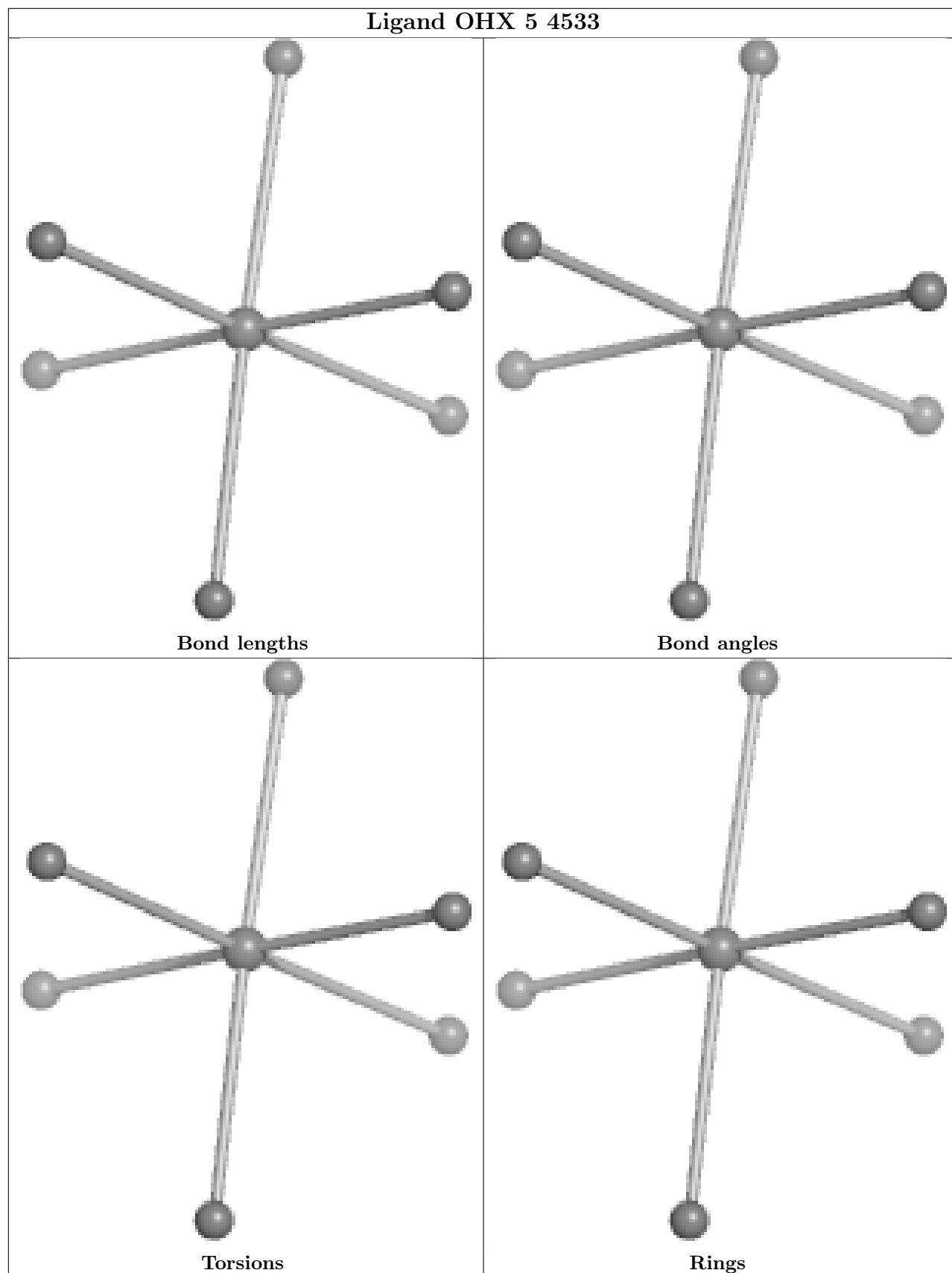
1 monomer is involved in 1 short contact:

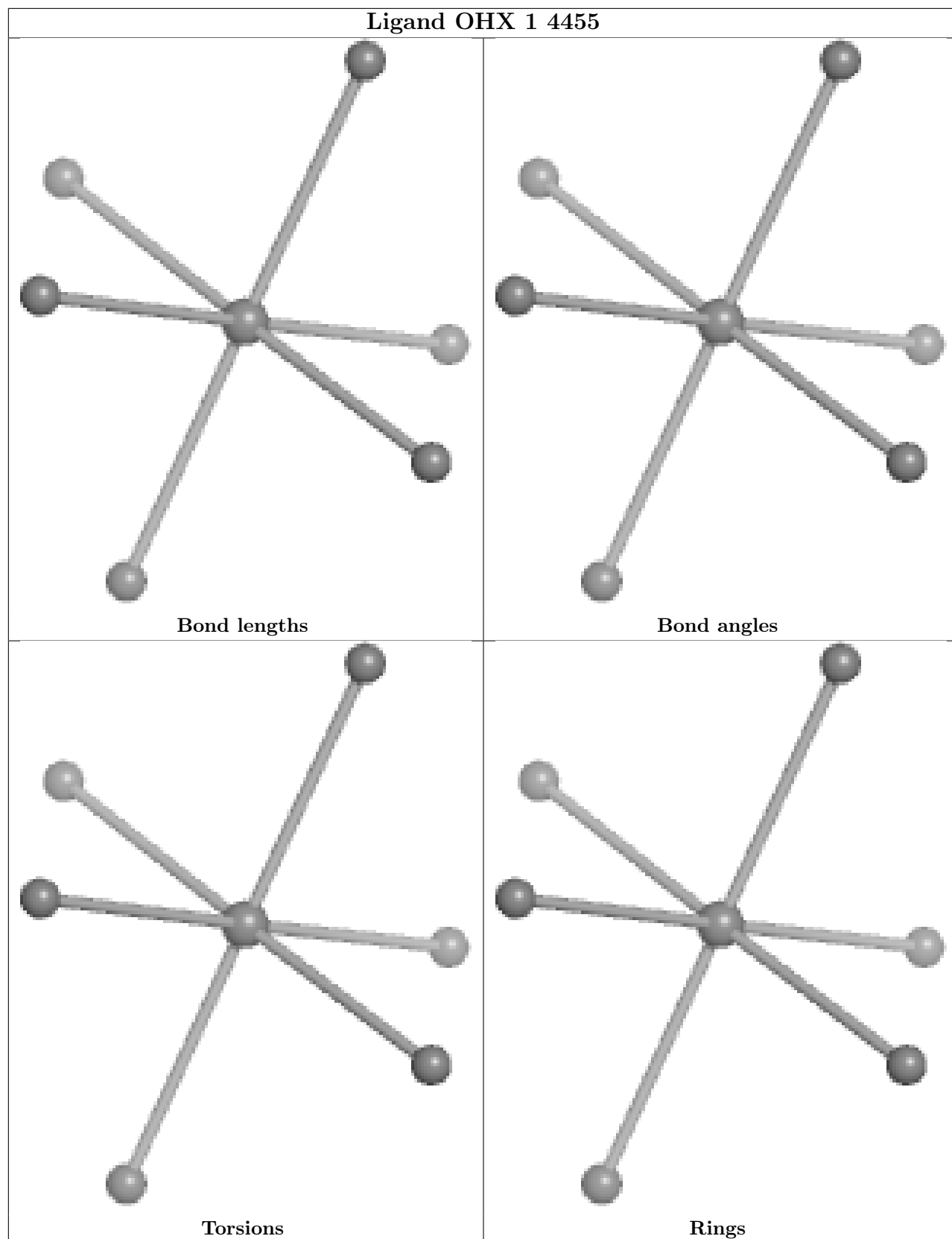
Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	19	204	OHX	0	1

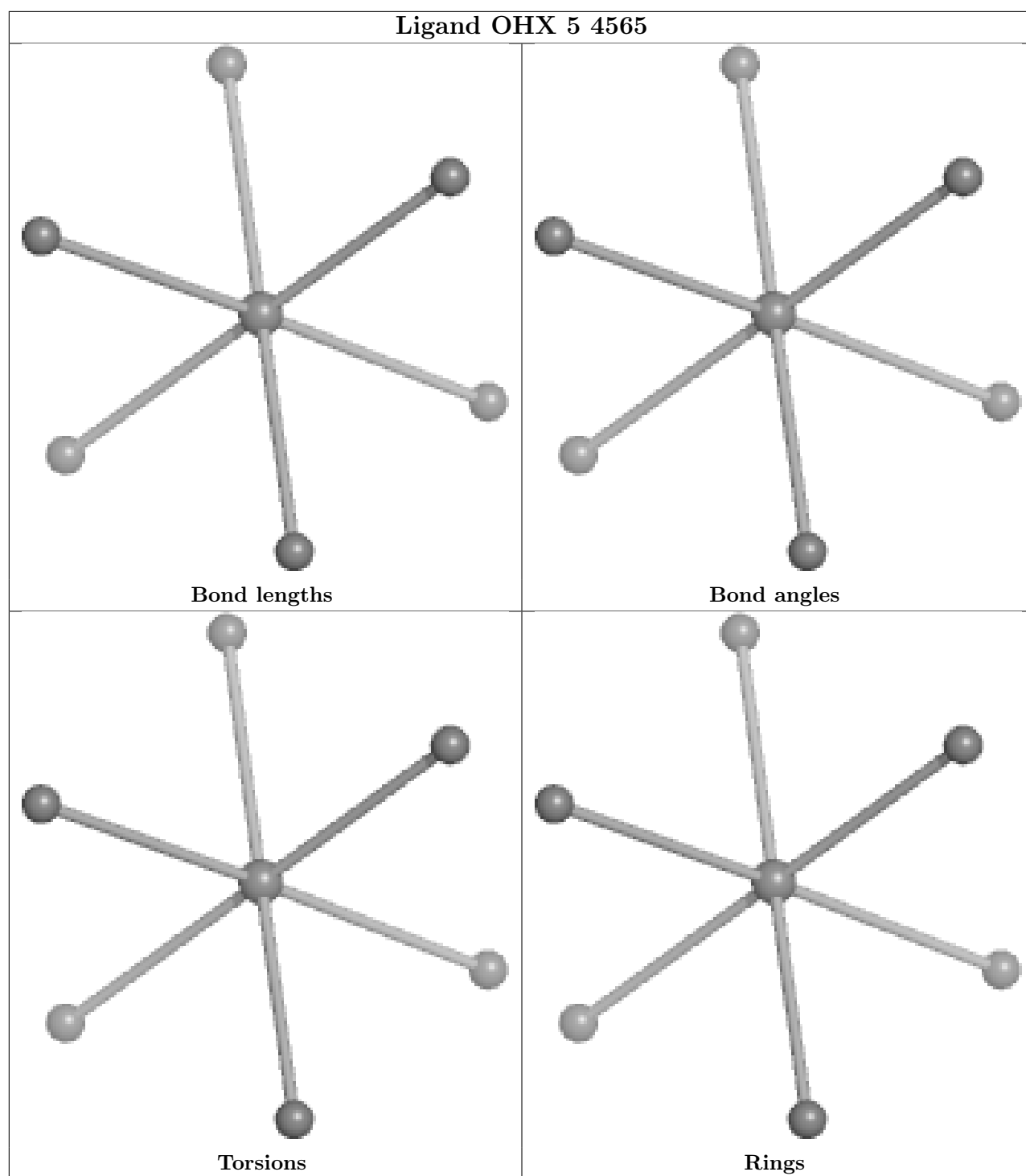
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



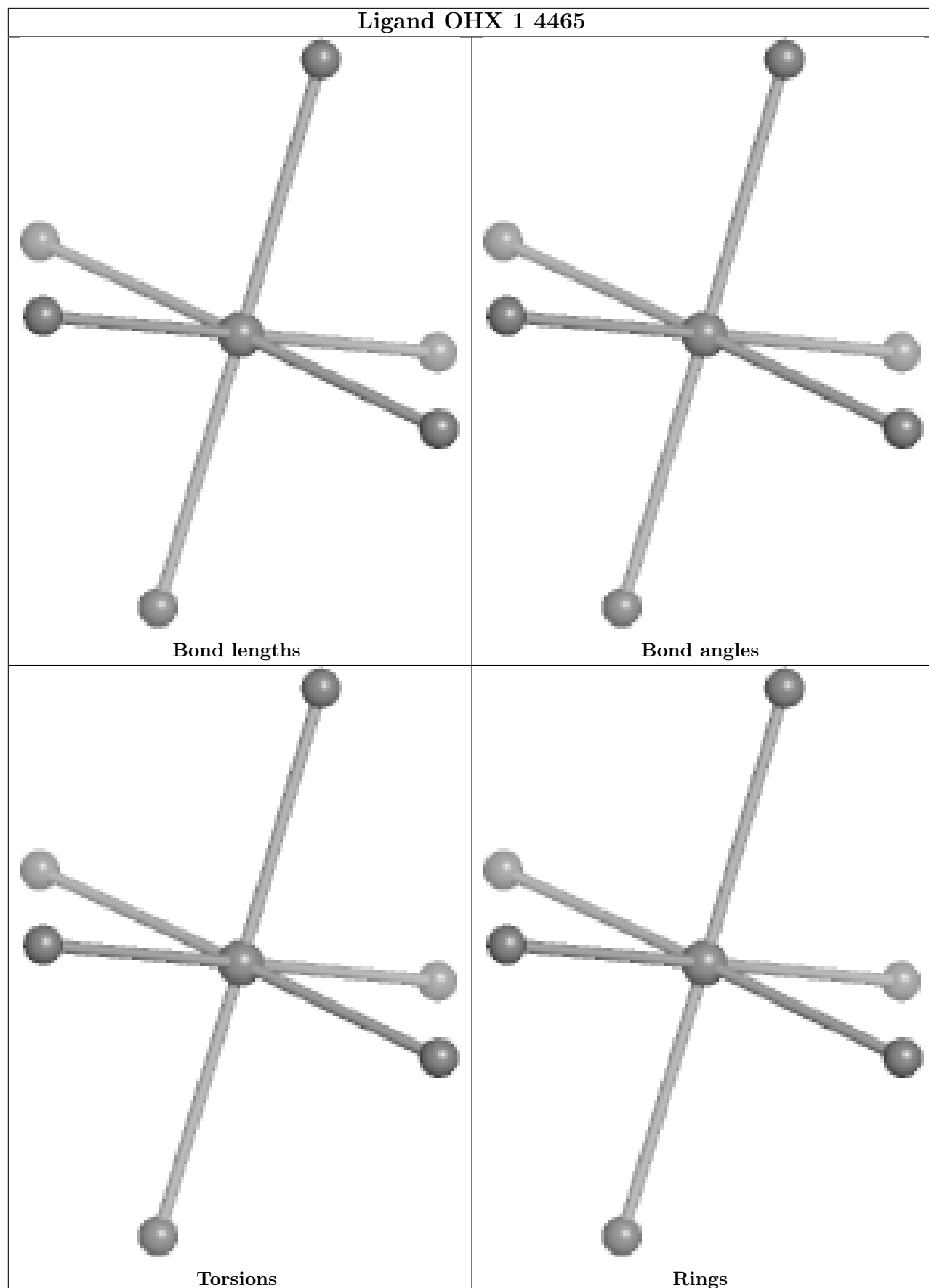
## Ligand OHX 5 4533



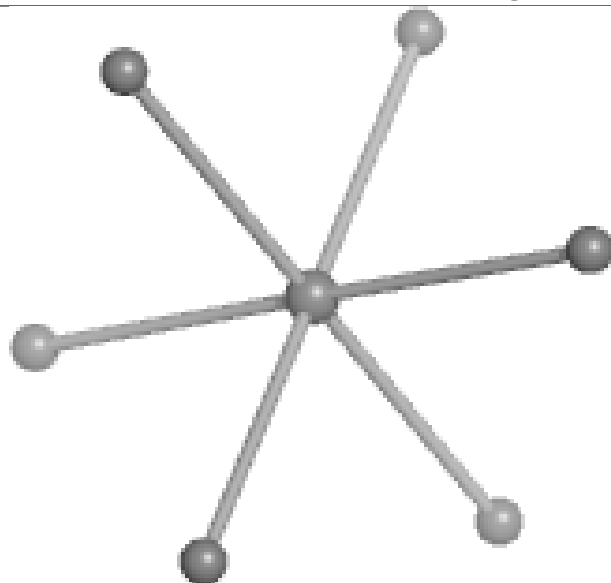




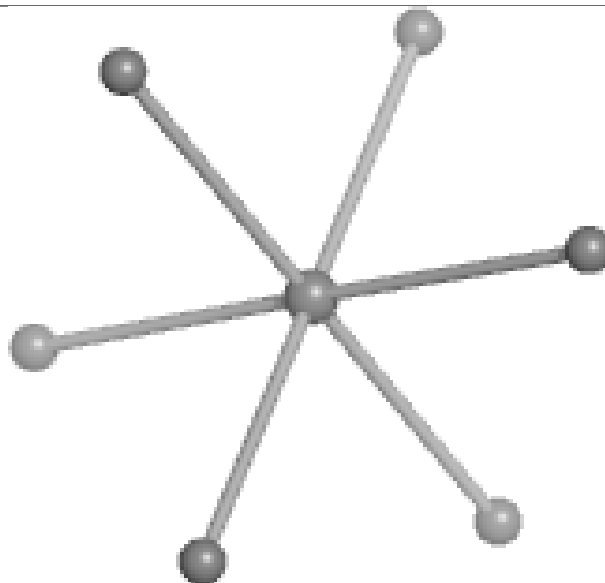
## Ligand OHX 1 4465



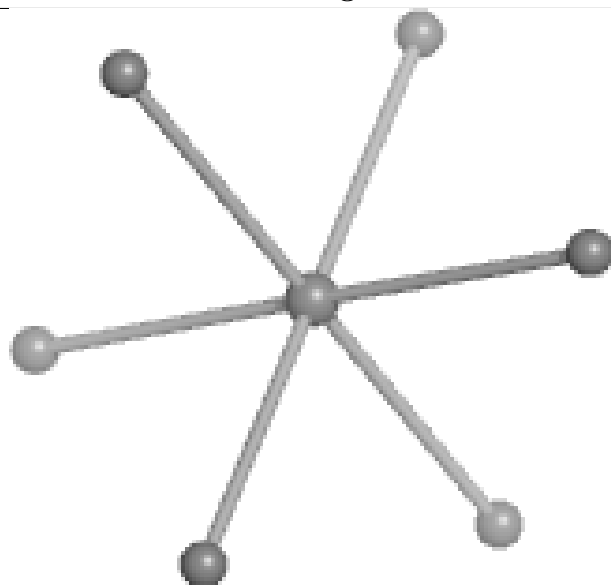
## Ligand OHX 1 4423



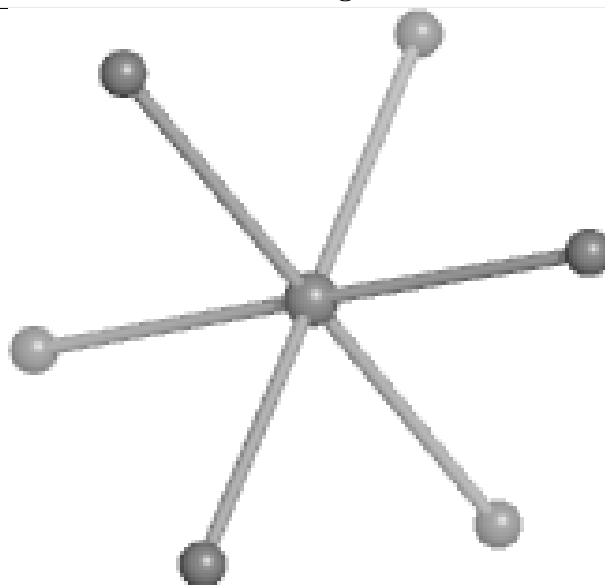
Bond lengths



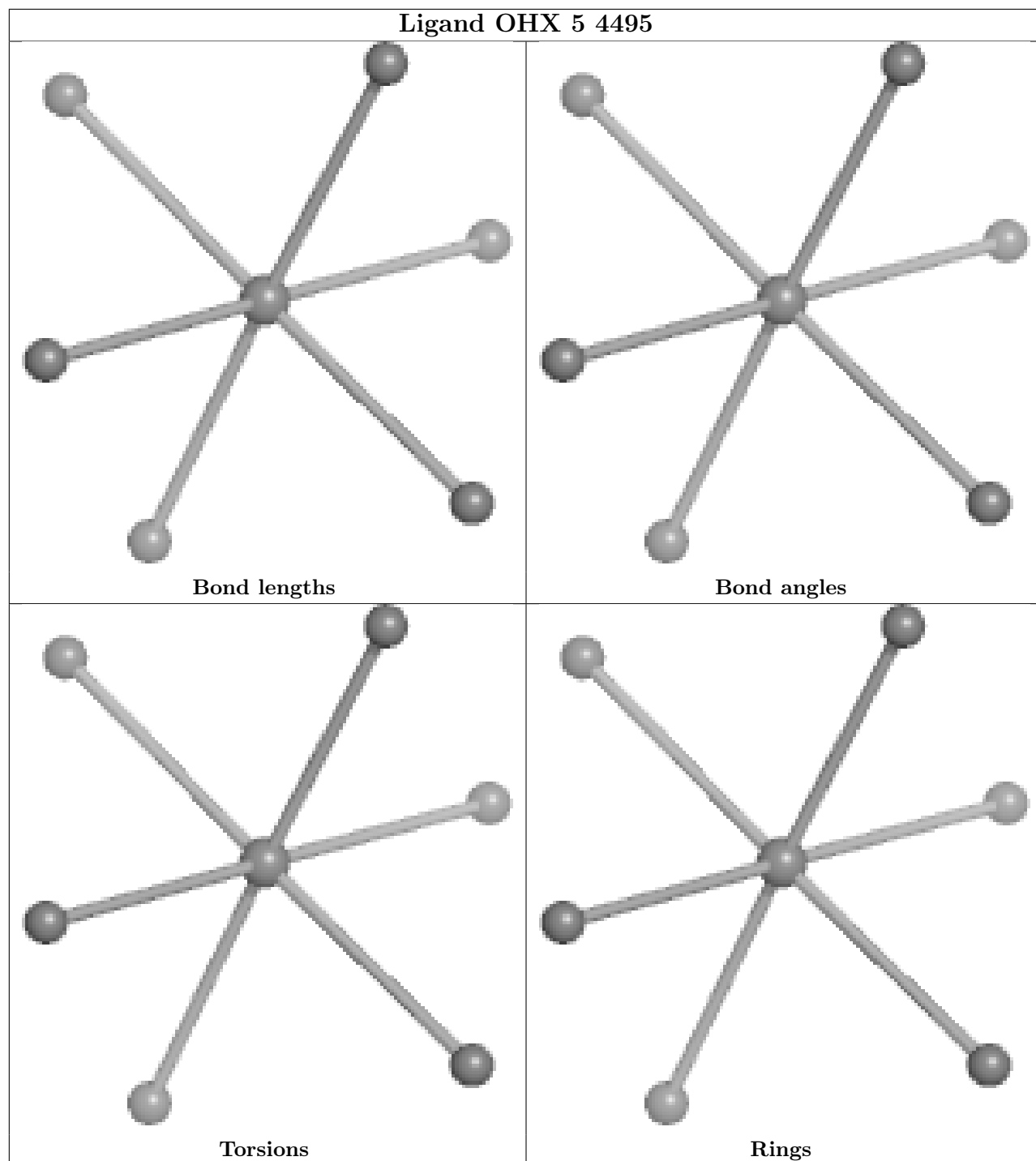
Bond angles



Torsions

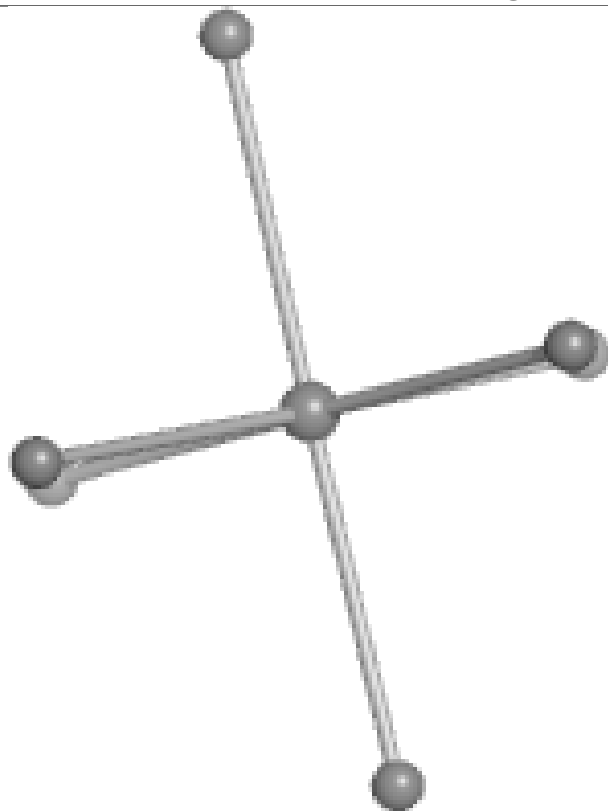


Rings

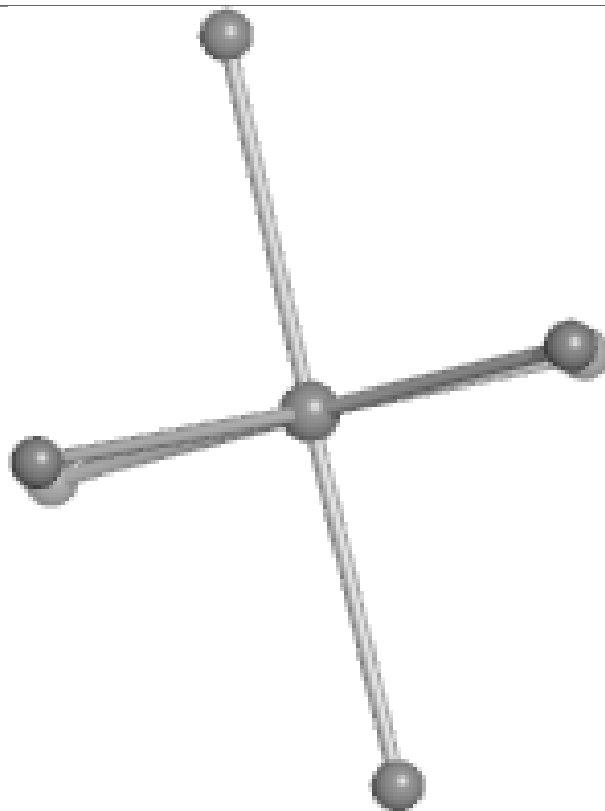




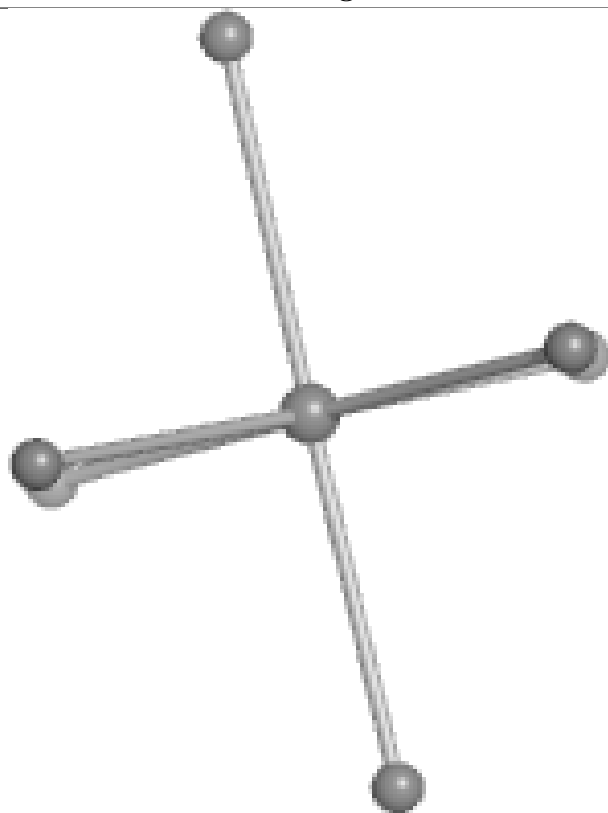
## Ligand OHX 5 4391



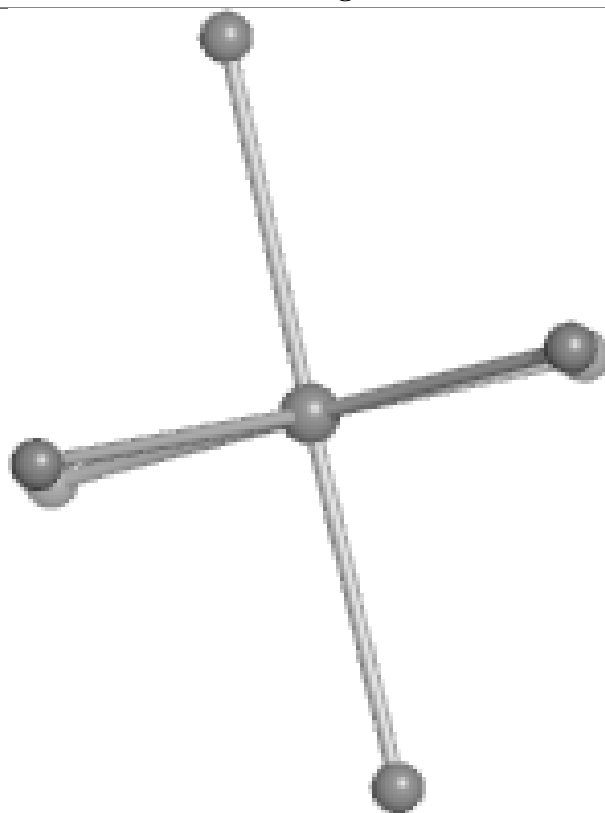
Bond lengths



Bond angles

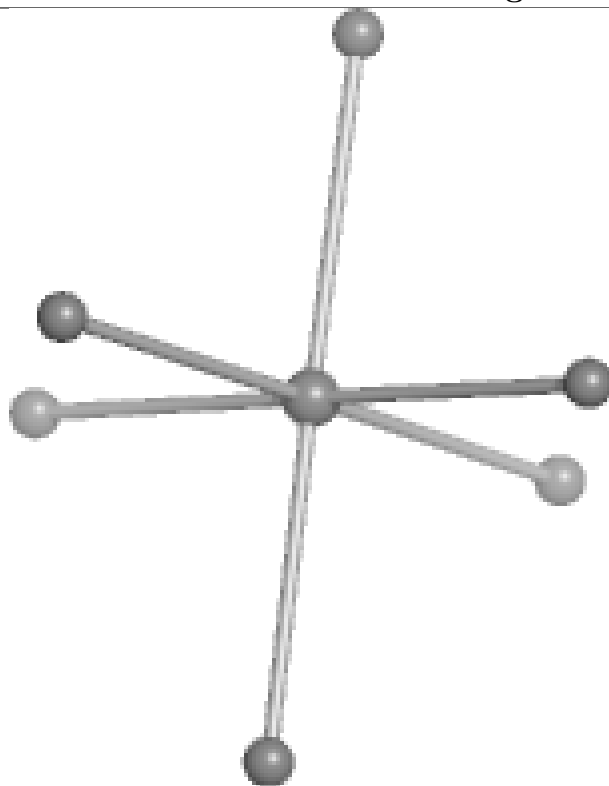


Torsions

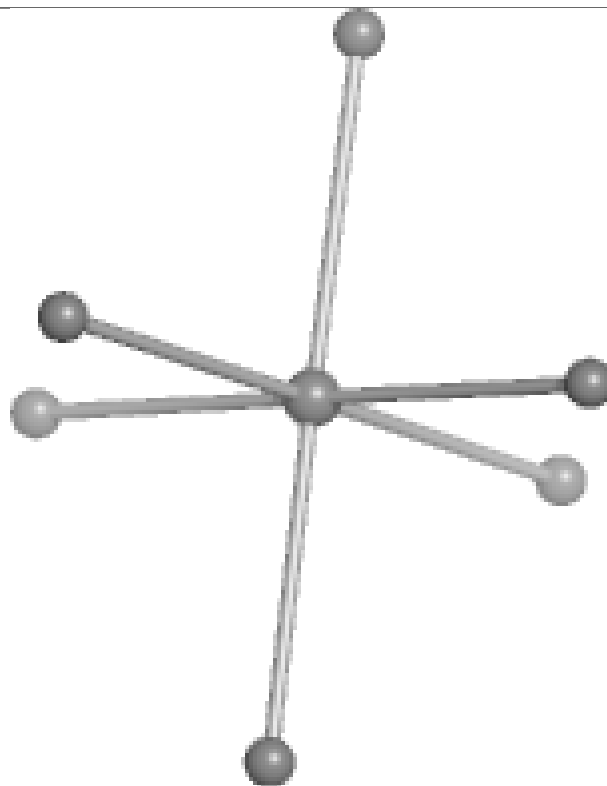


Rings

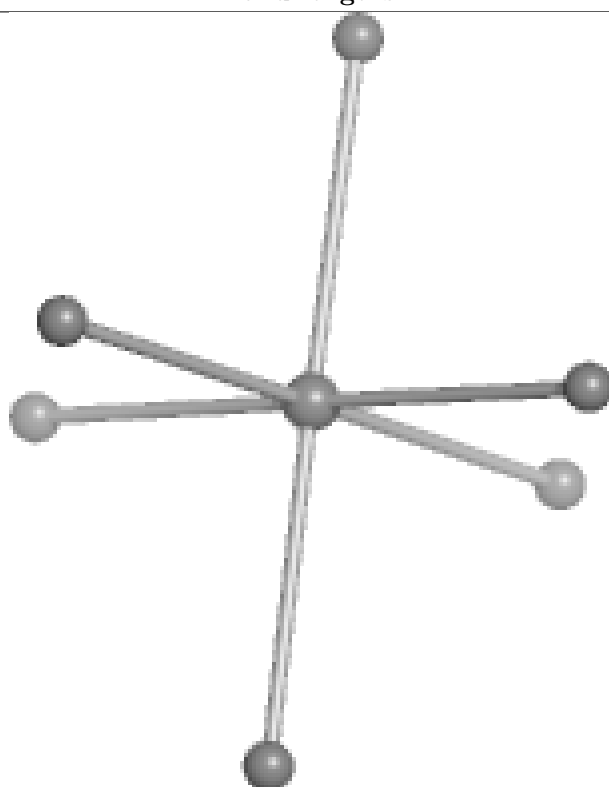
## Ligand OHX 5 4537



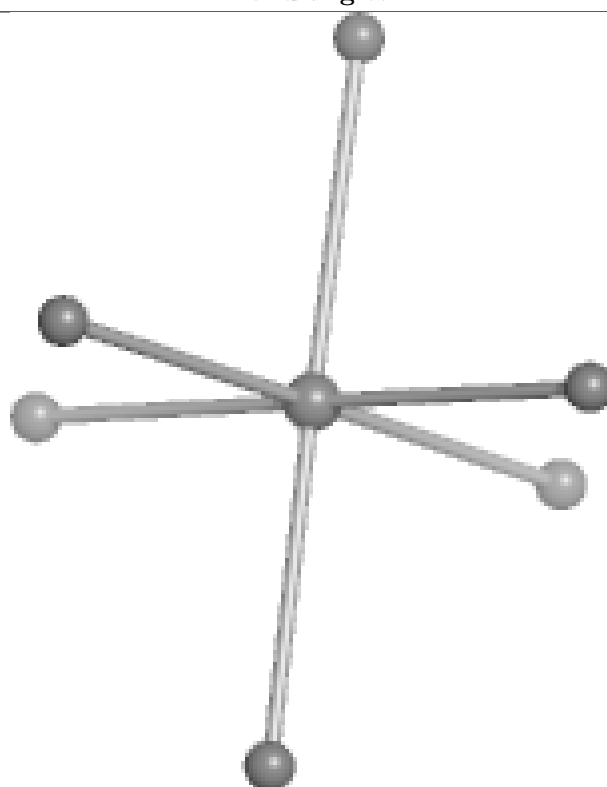
Bond lengths



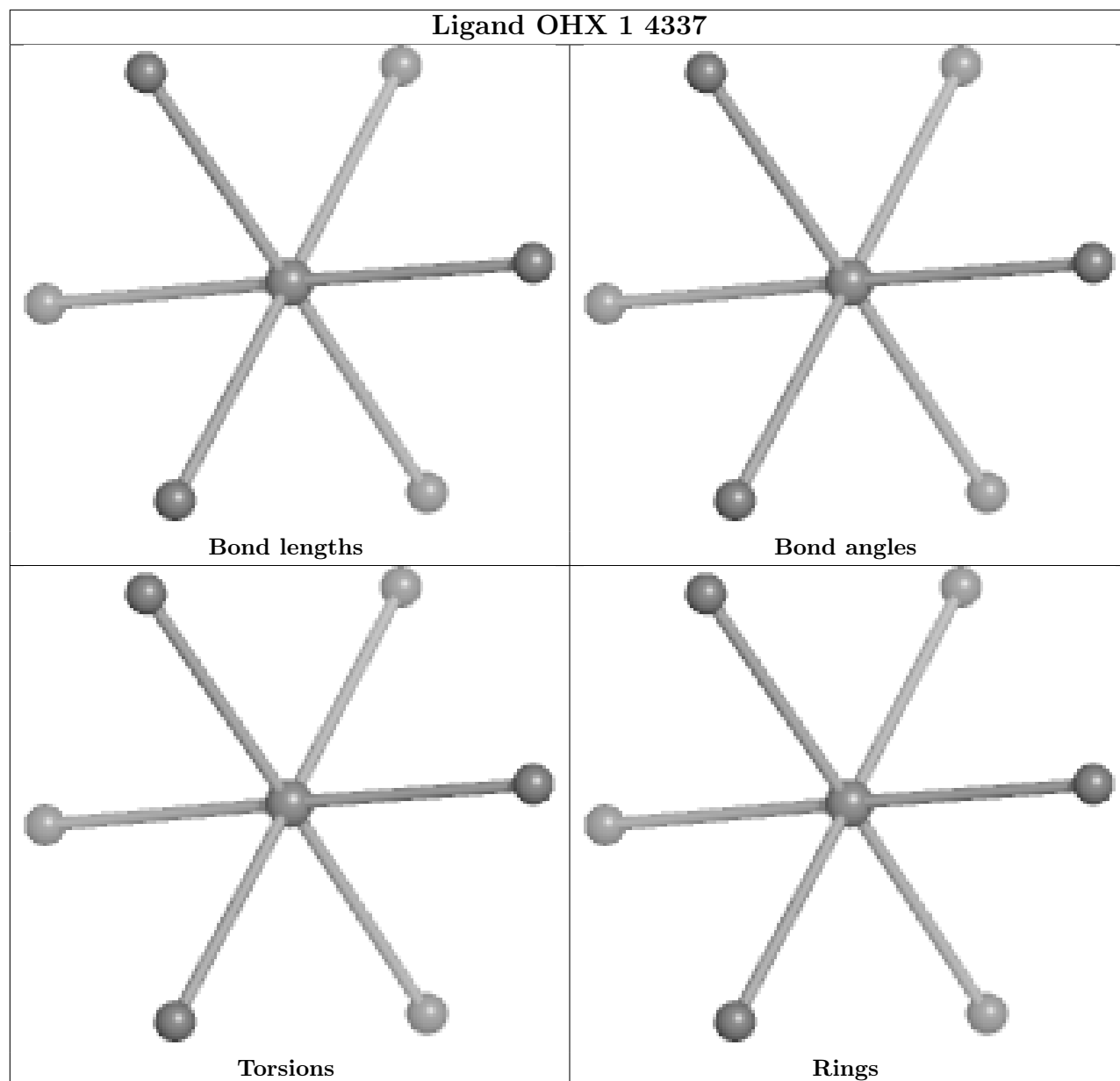
Bond angles

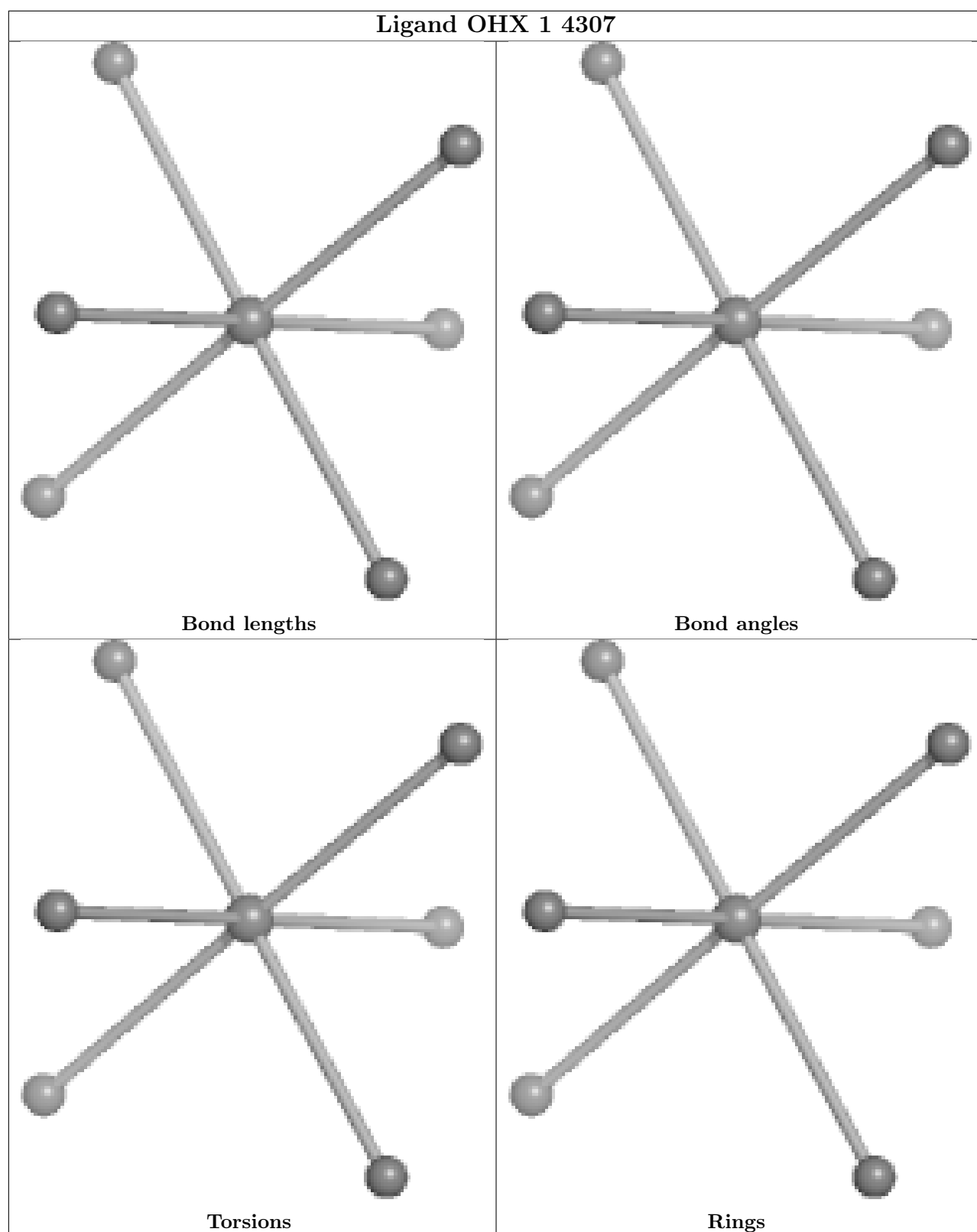


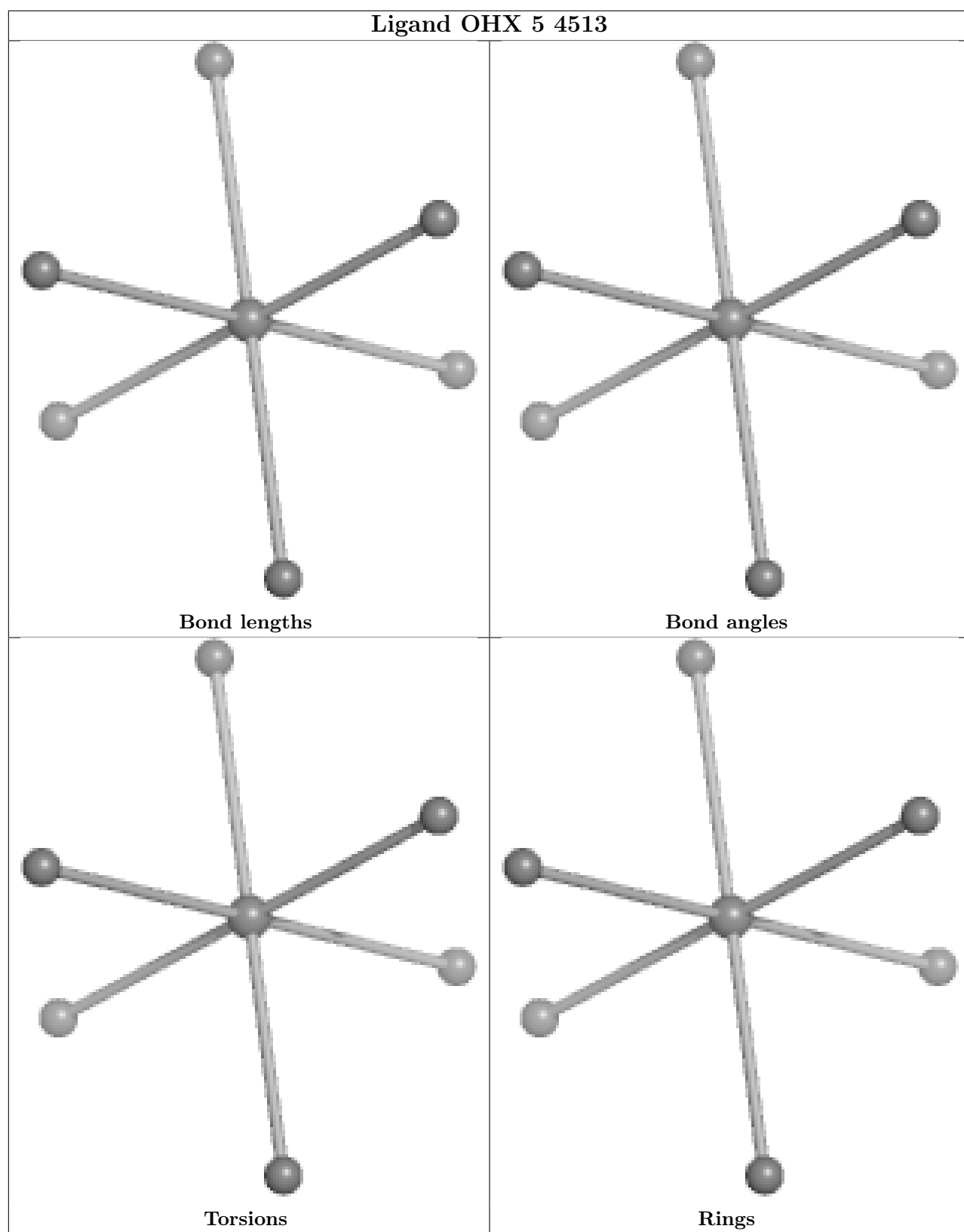
Torsions



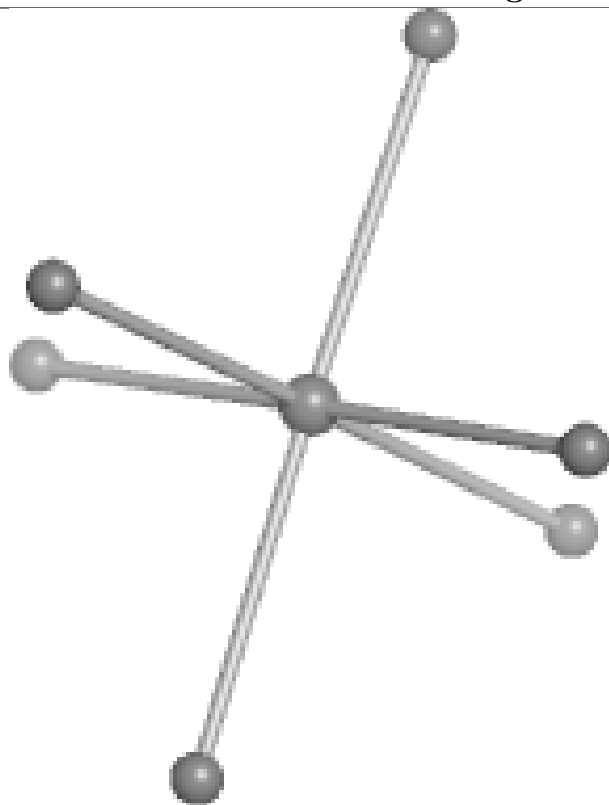
Rings



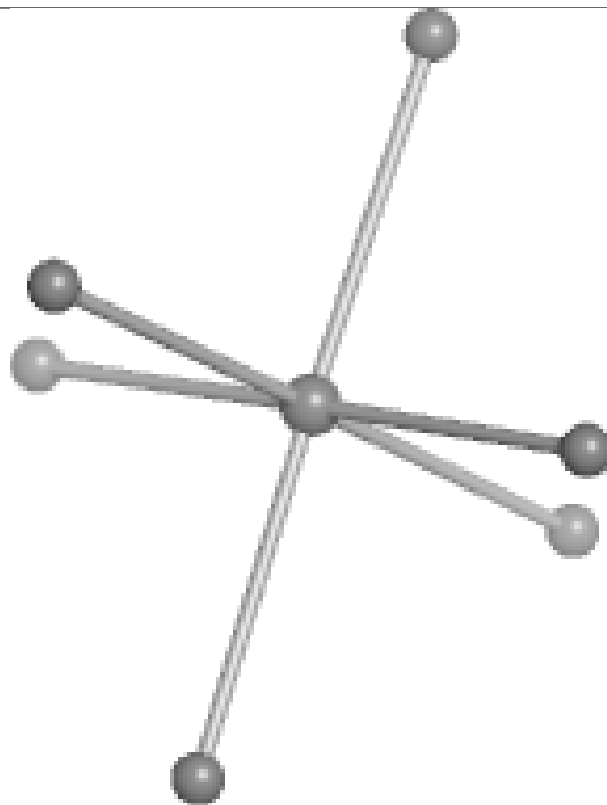




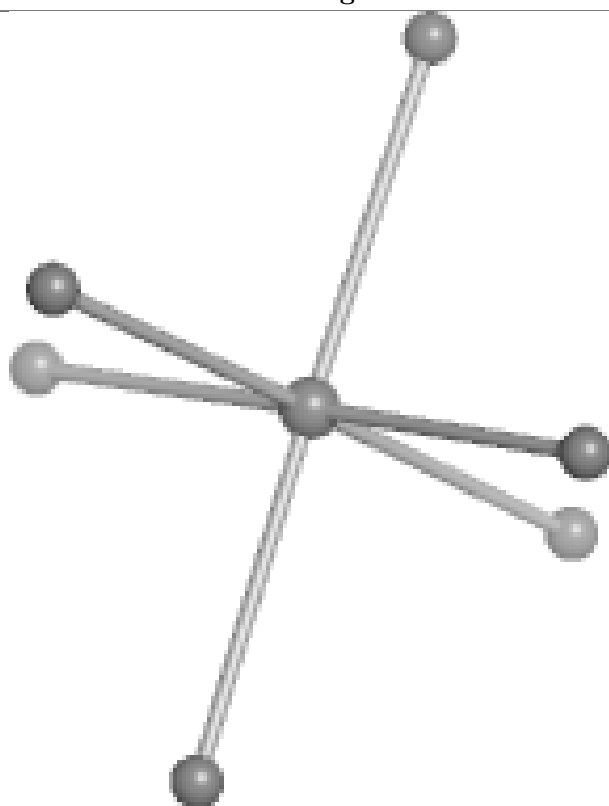
## Ligand OHX 5 4548



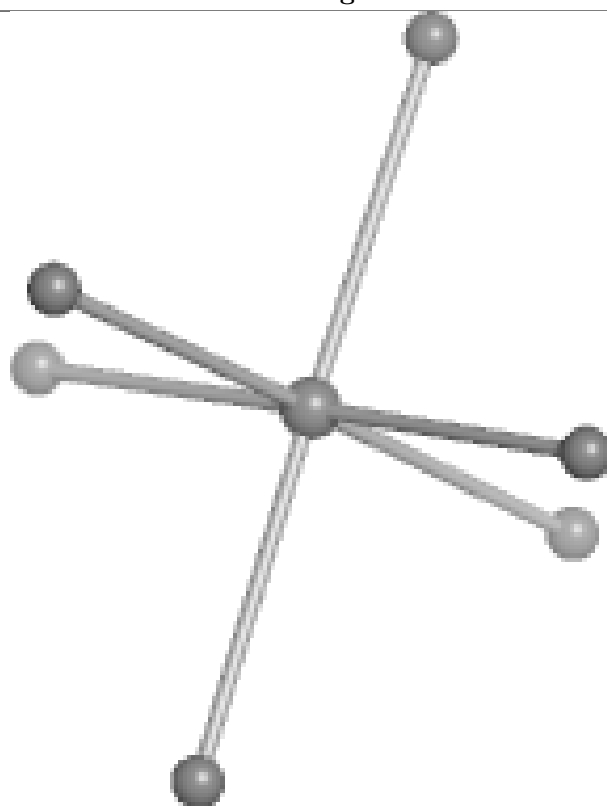
Bond lengths



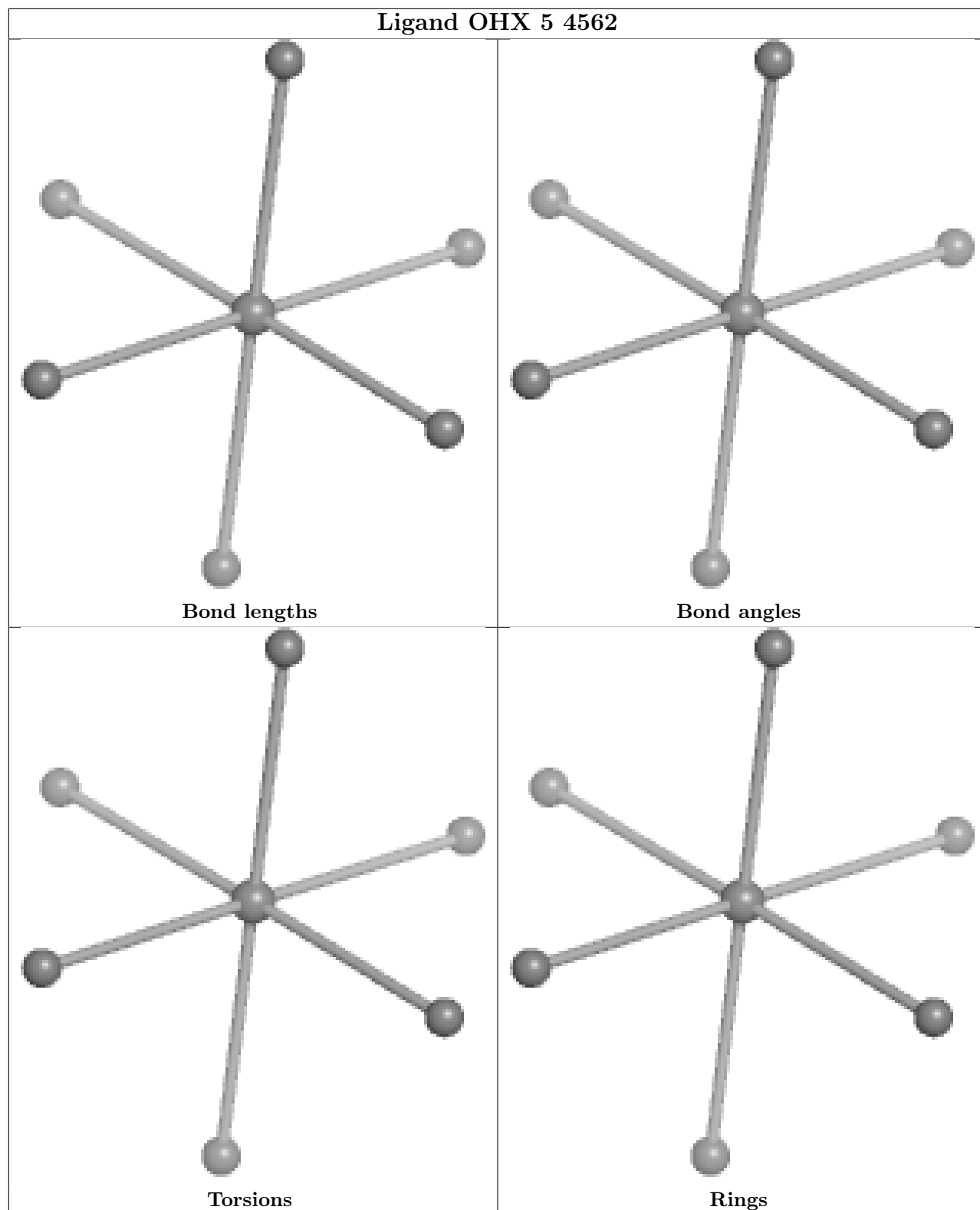
Bond angles

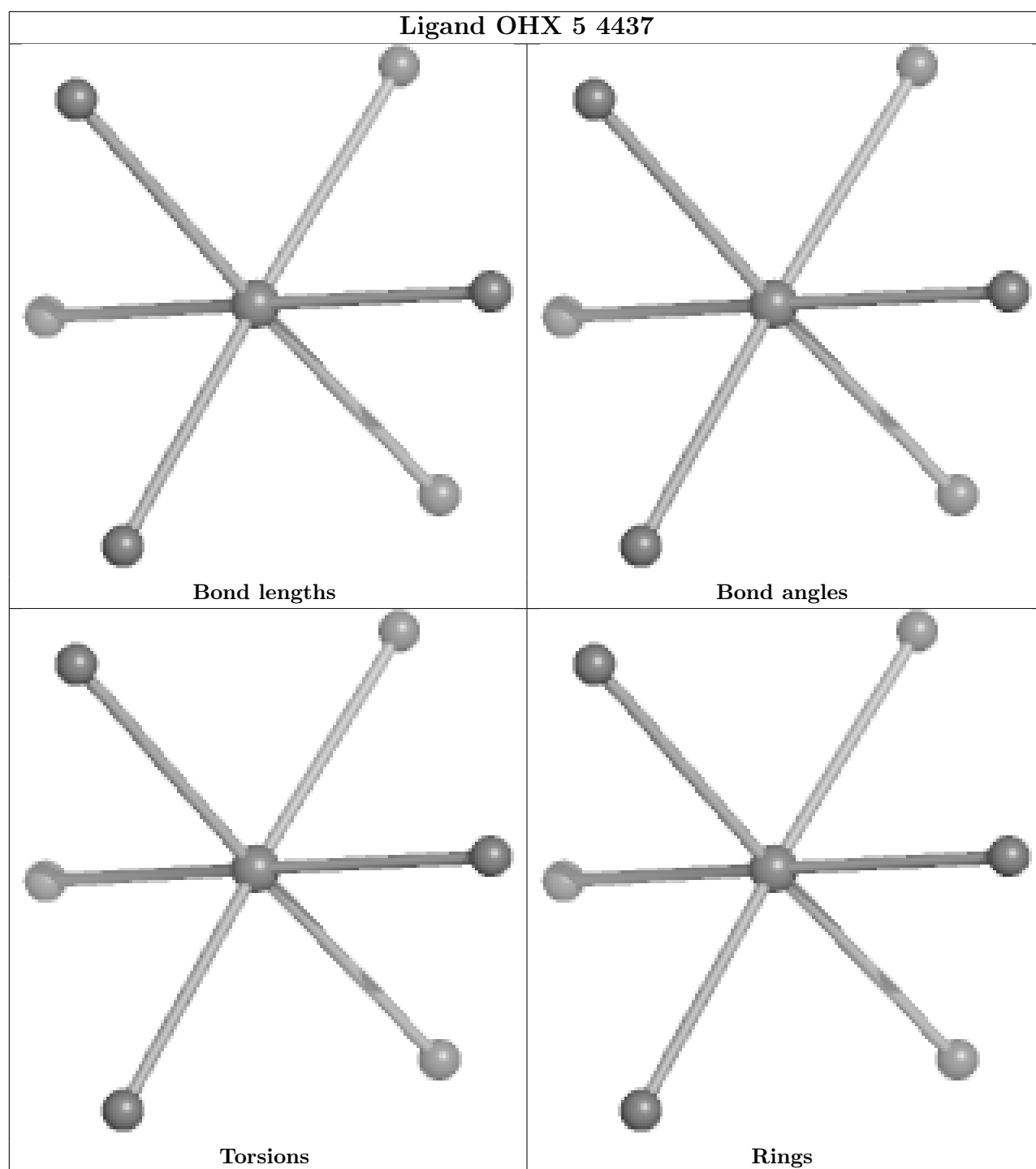


Torsions

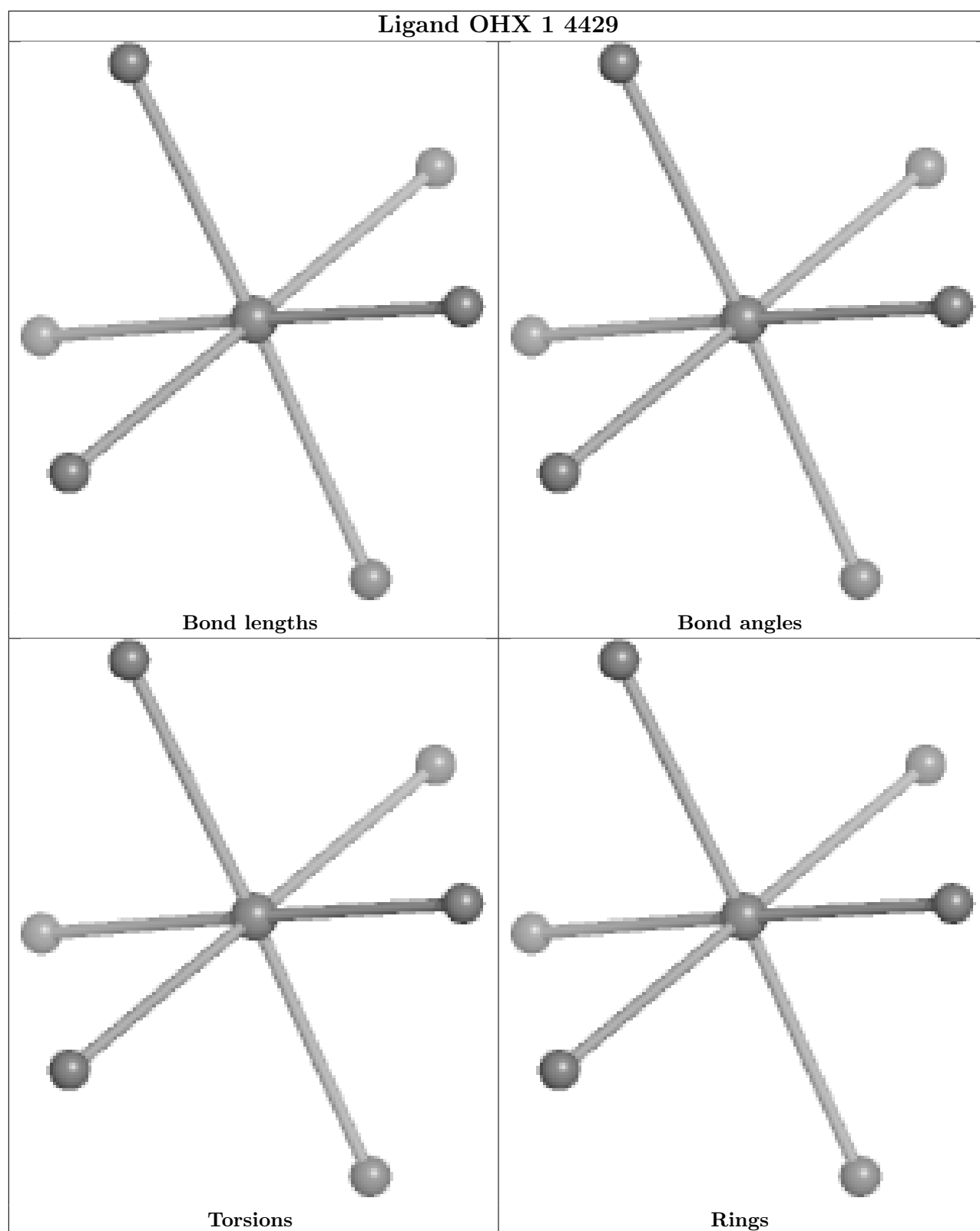


Rings

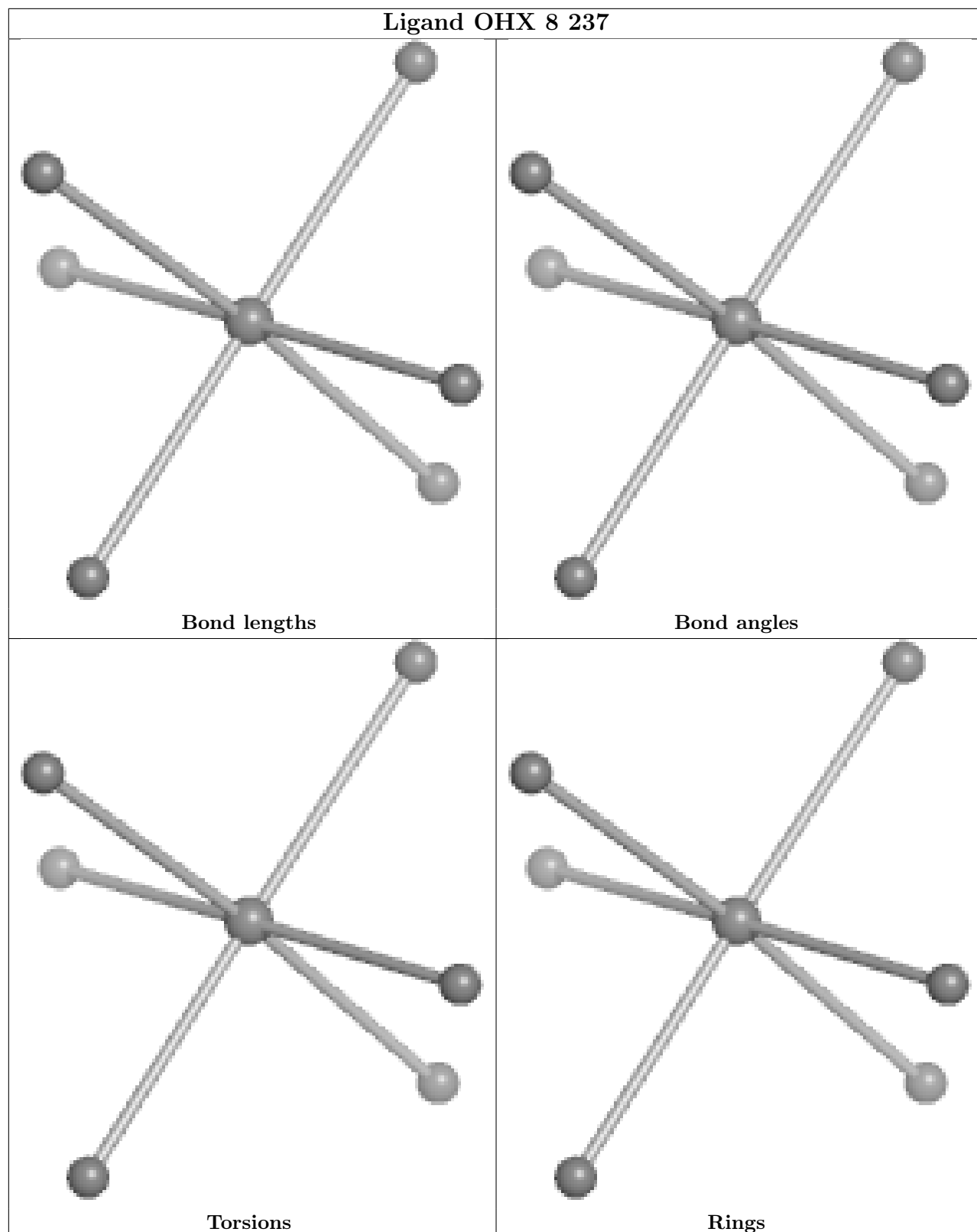


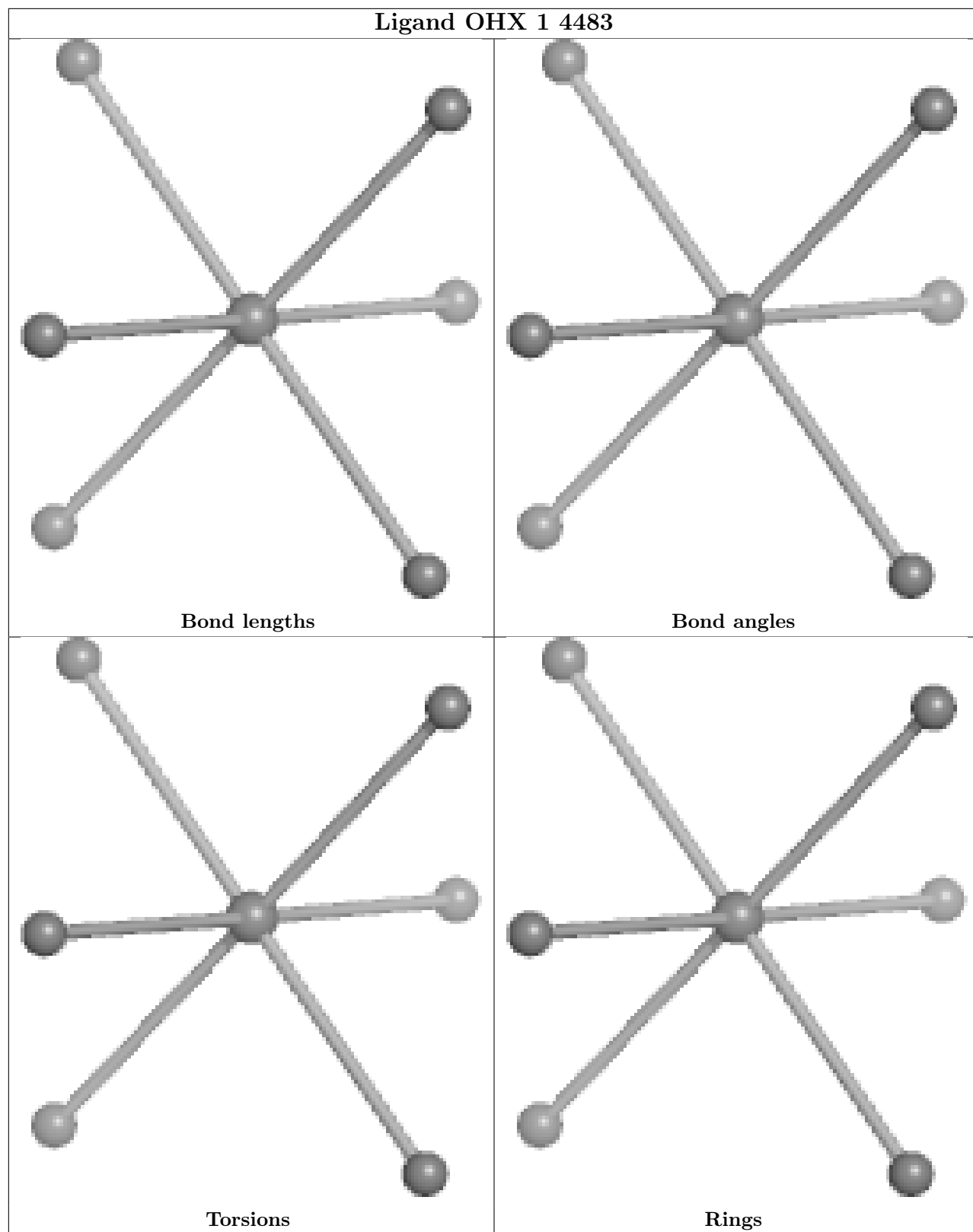




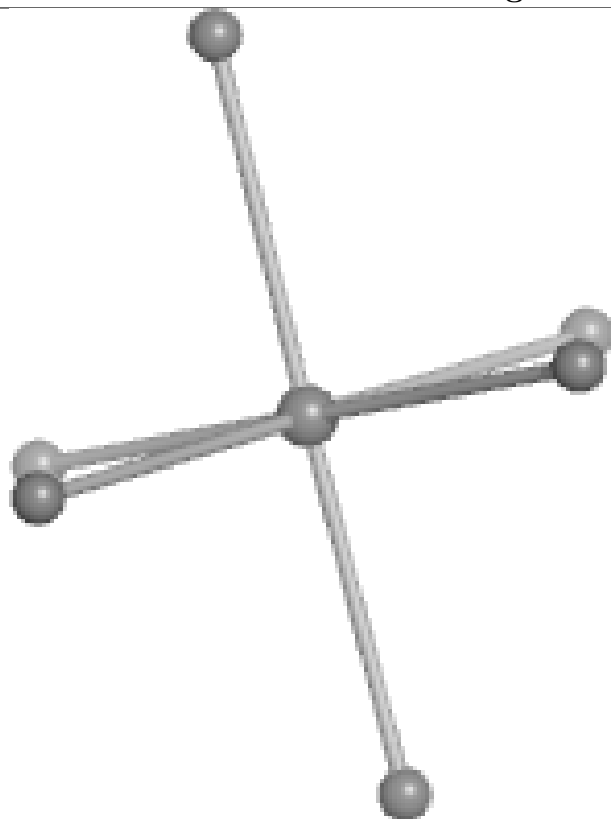


## Ligand OHX 8 237

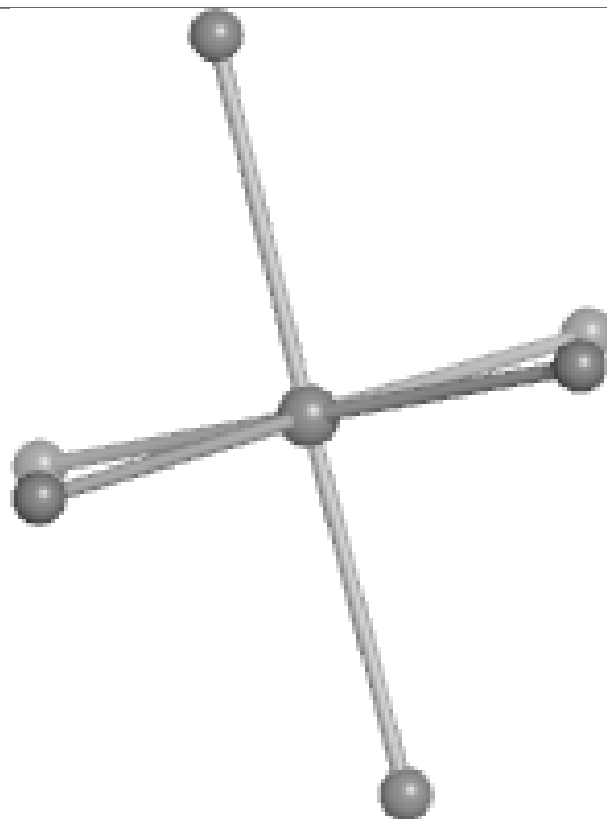




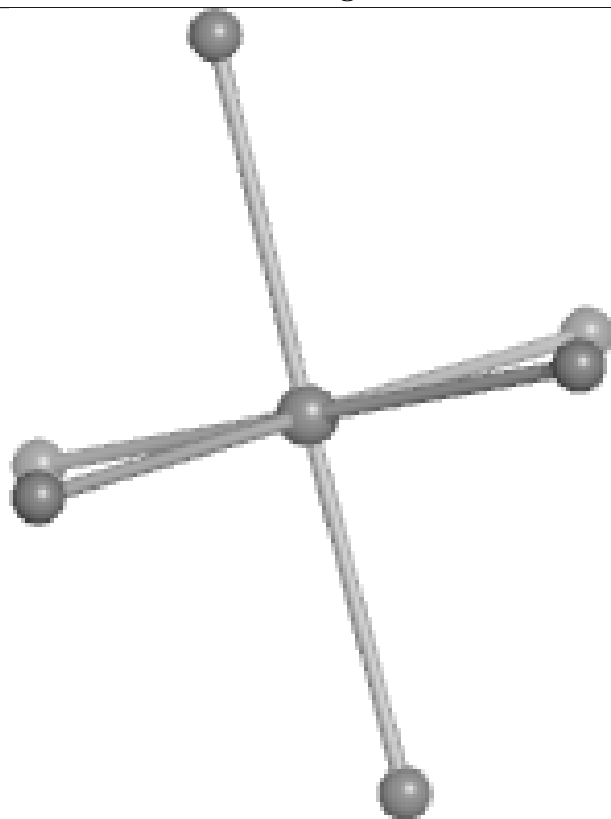
## Ligand OHX 1 4361



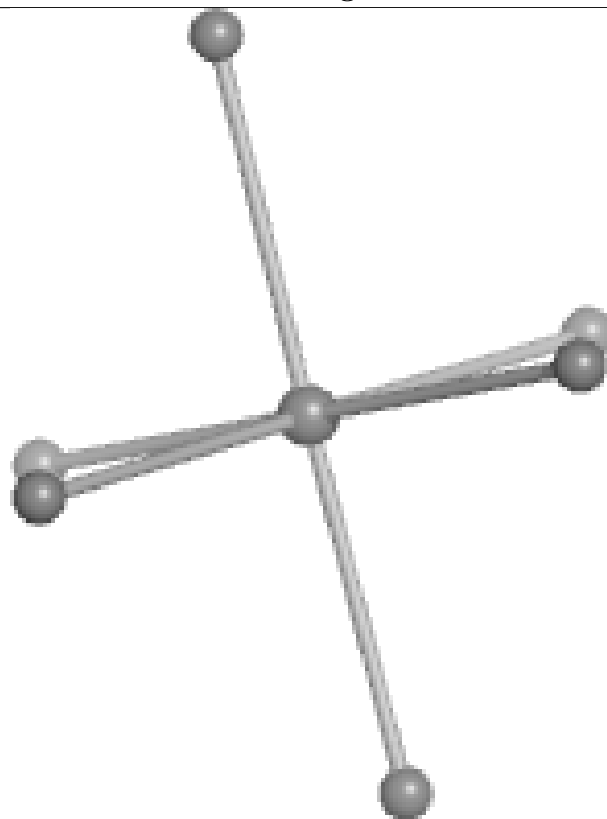
Bond lengths



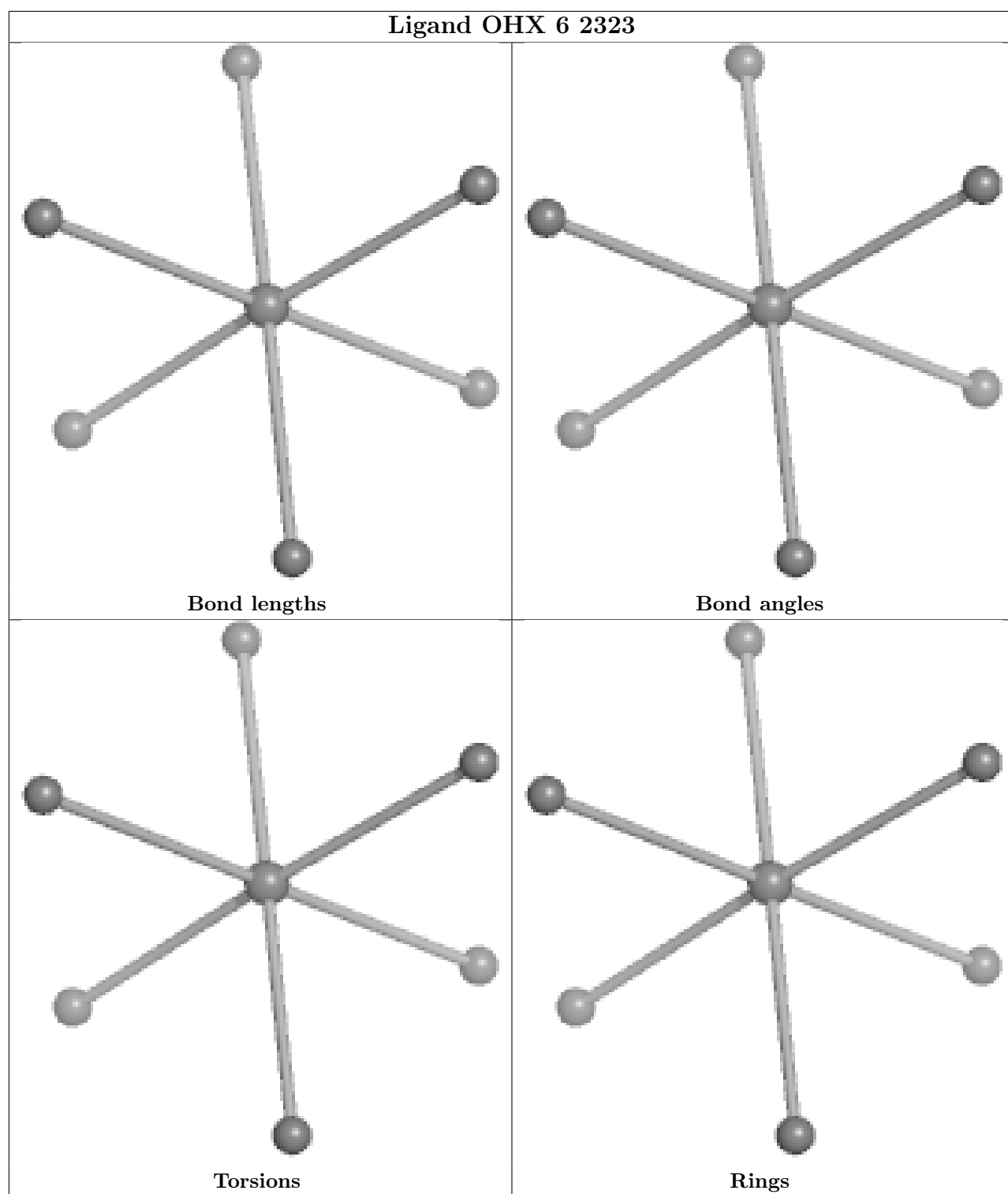
Bond angles

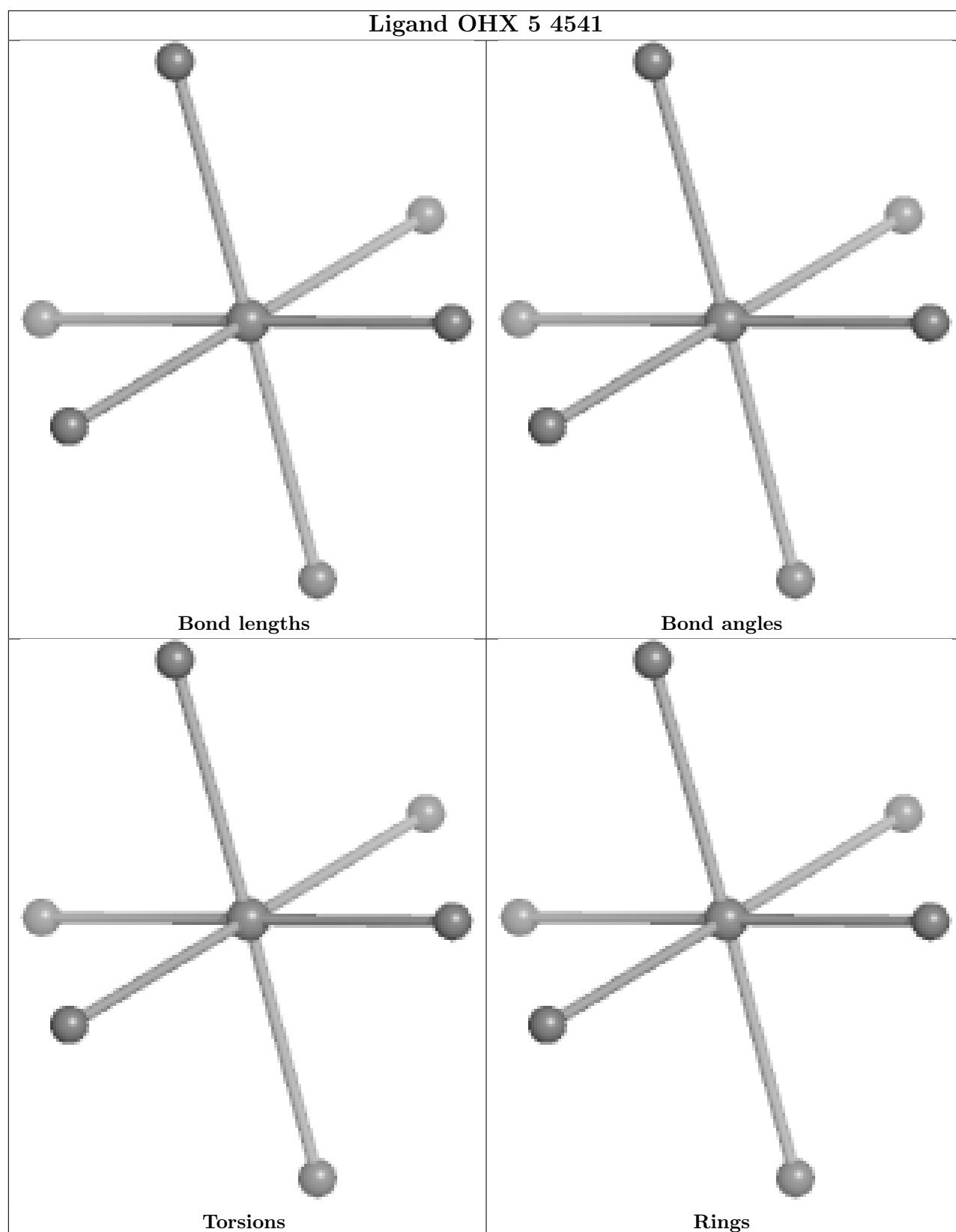


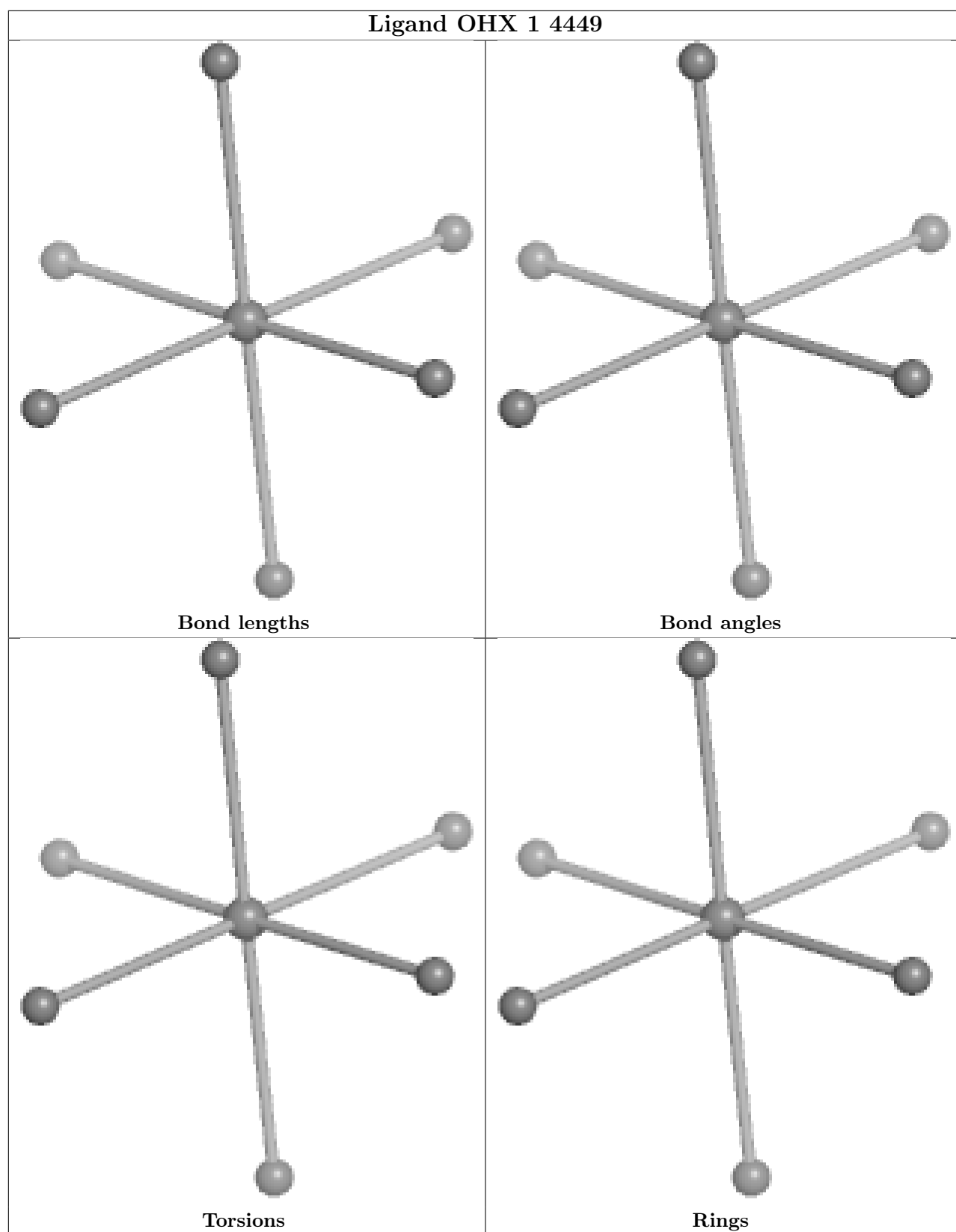
Torsions

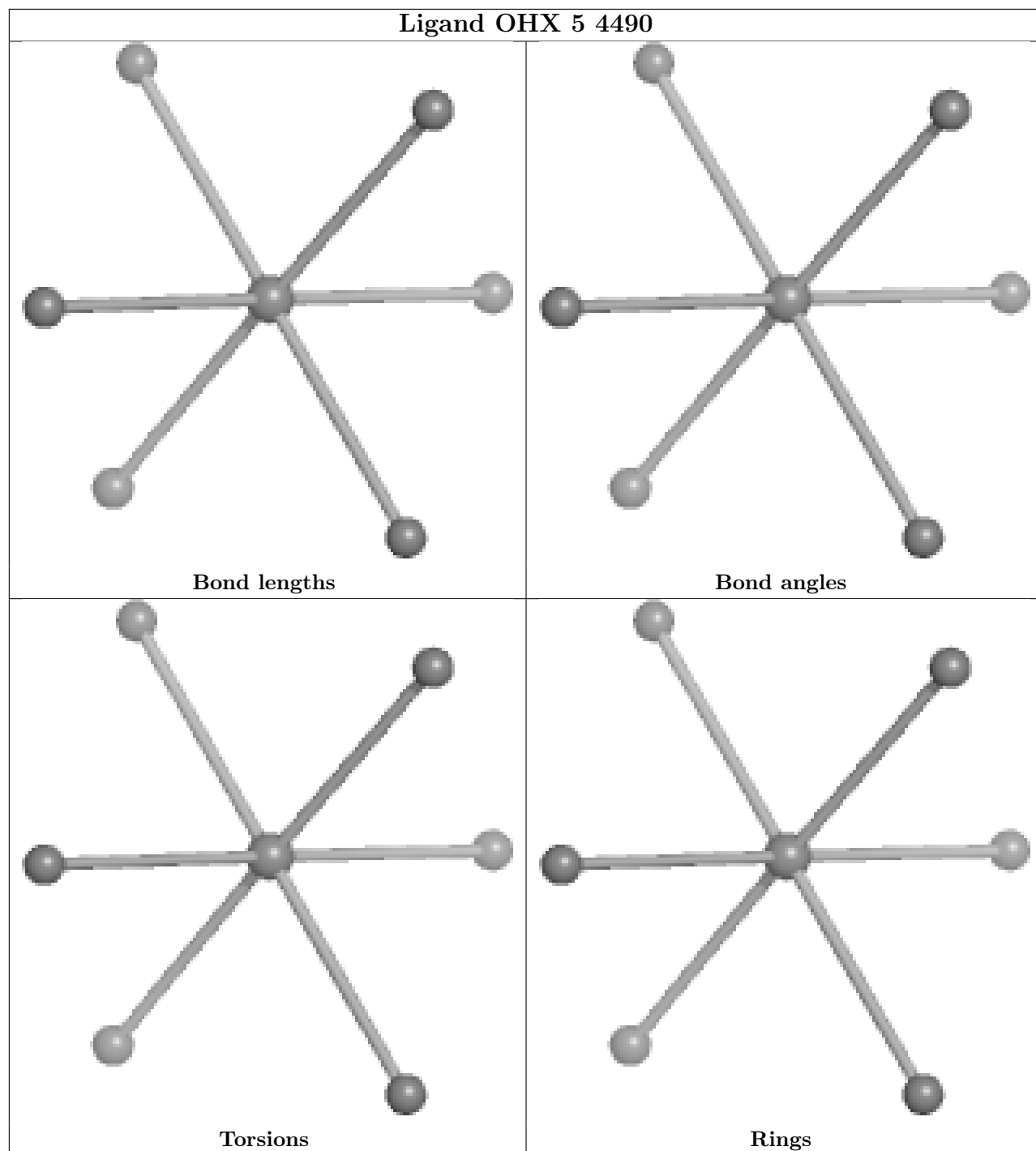


Rings

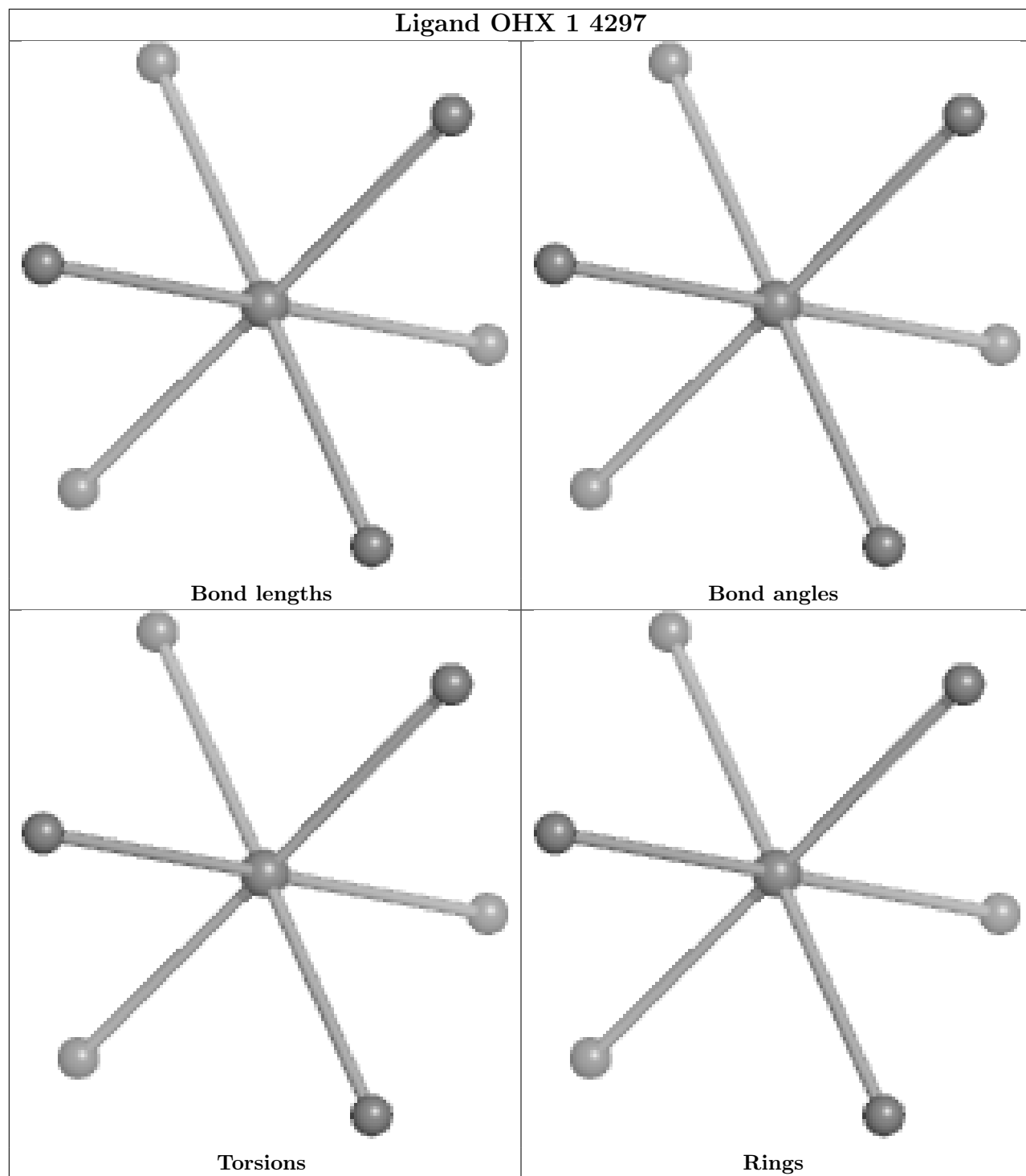


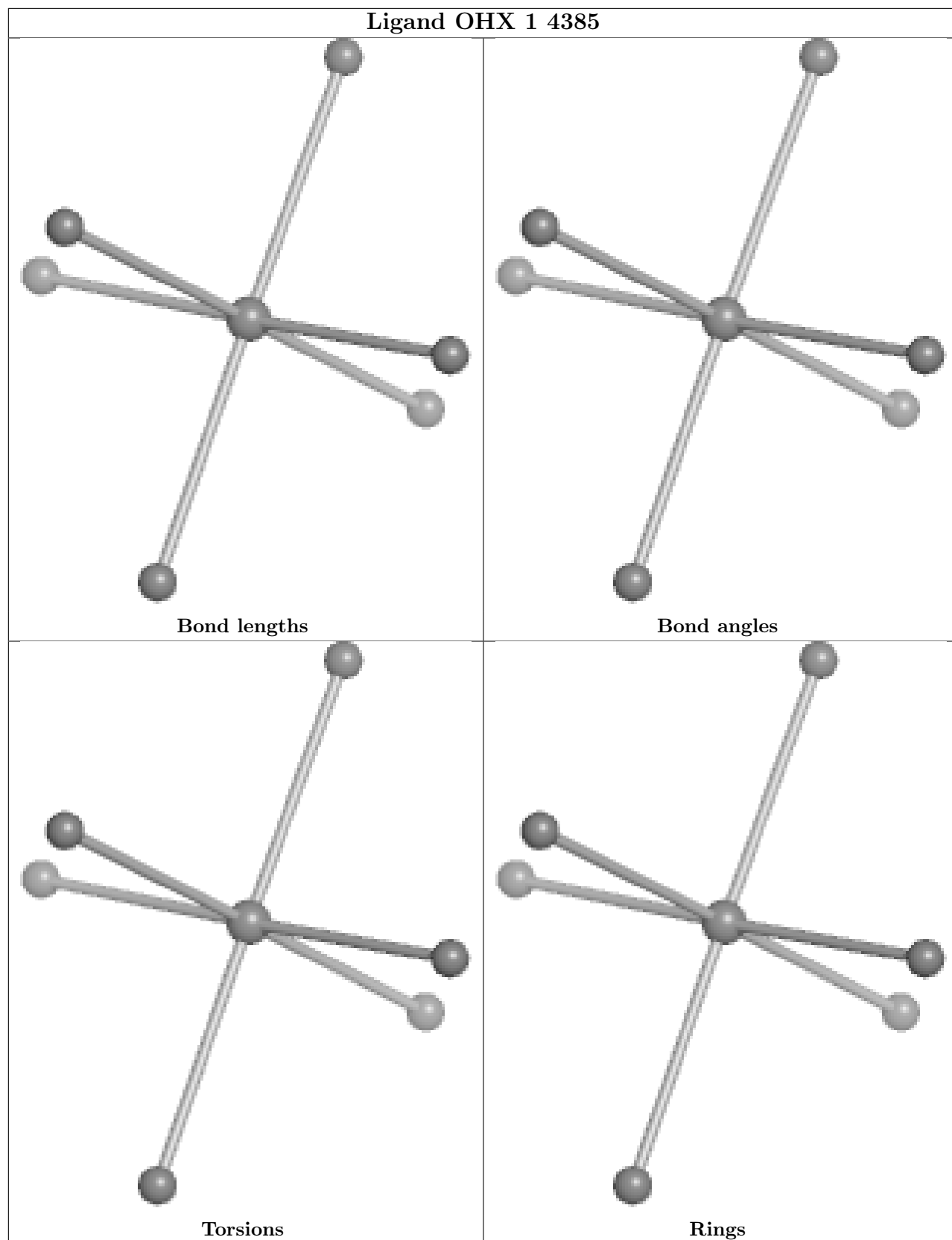




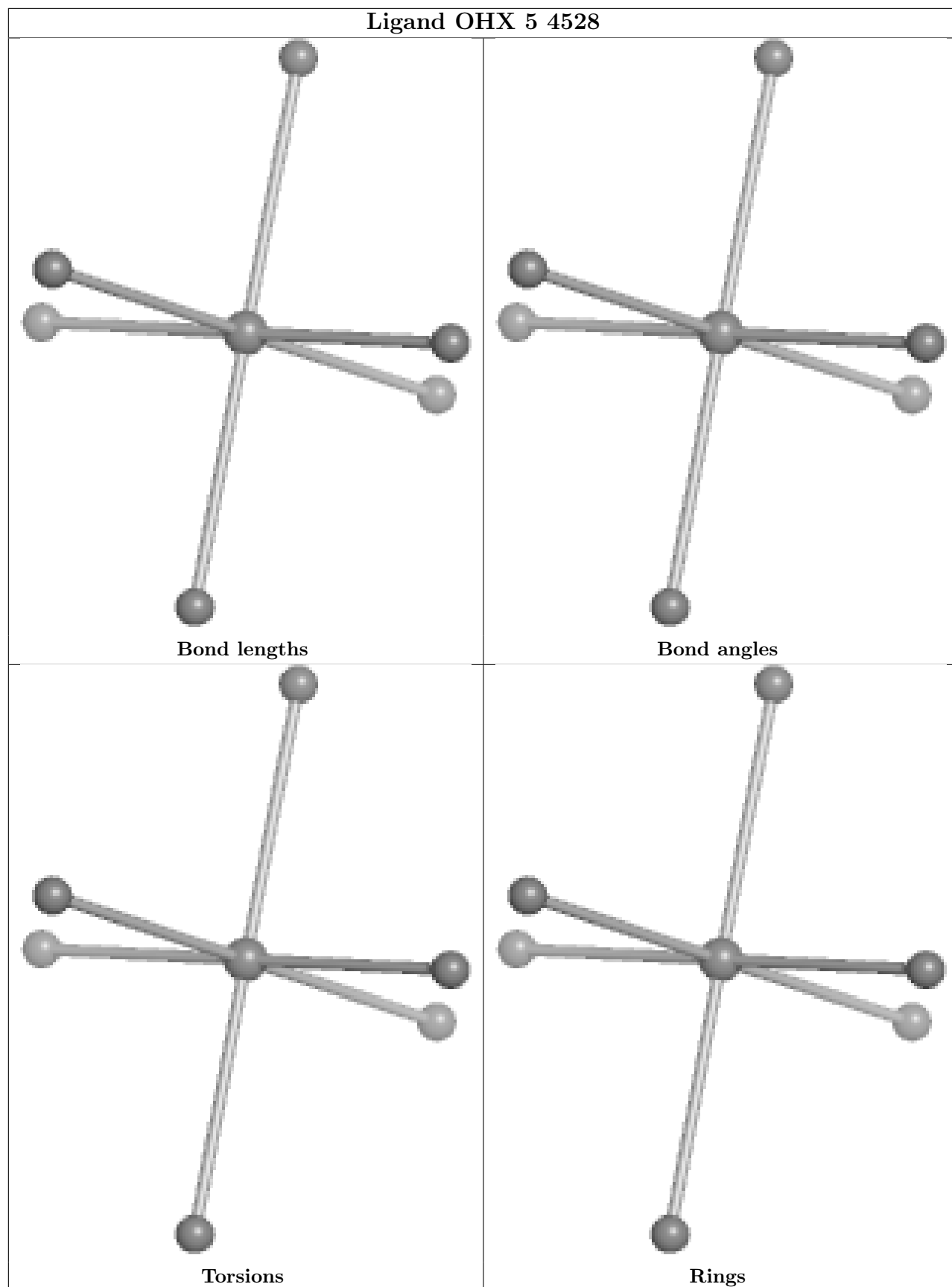


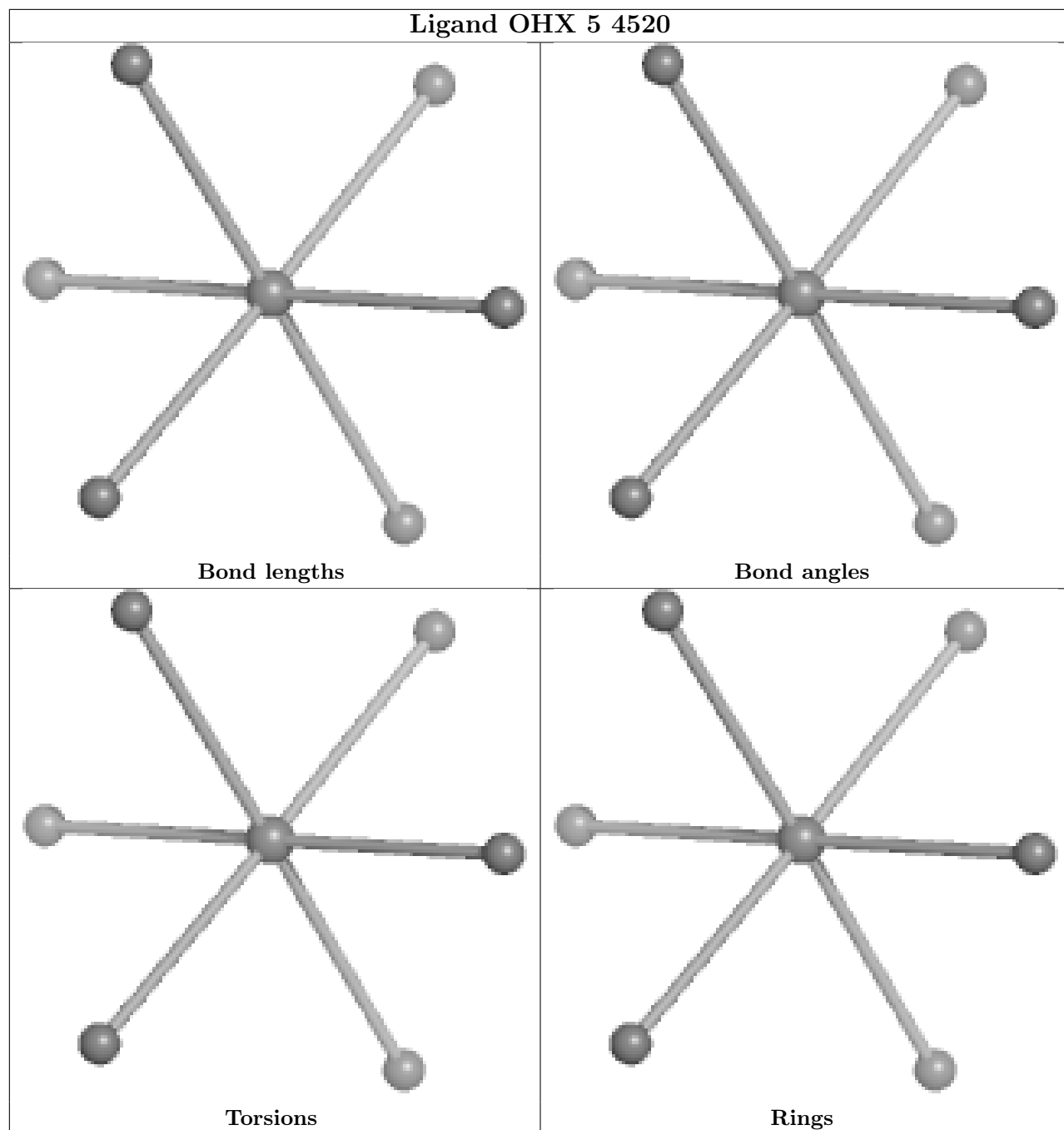


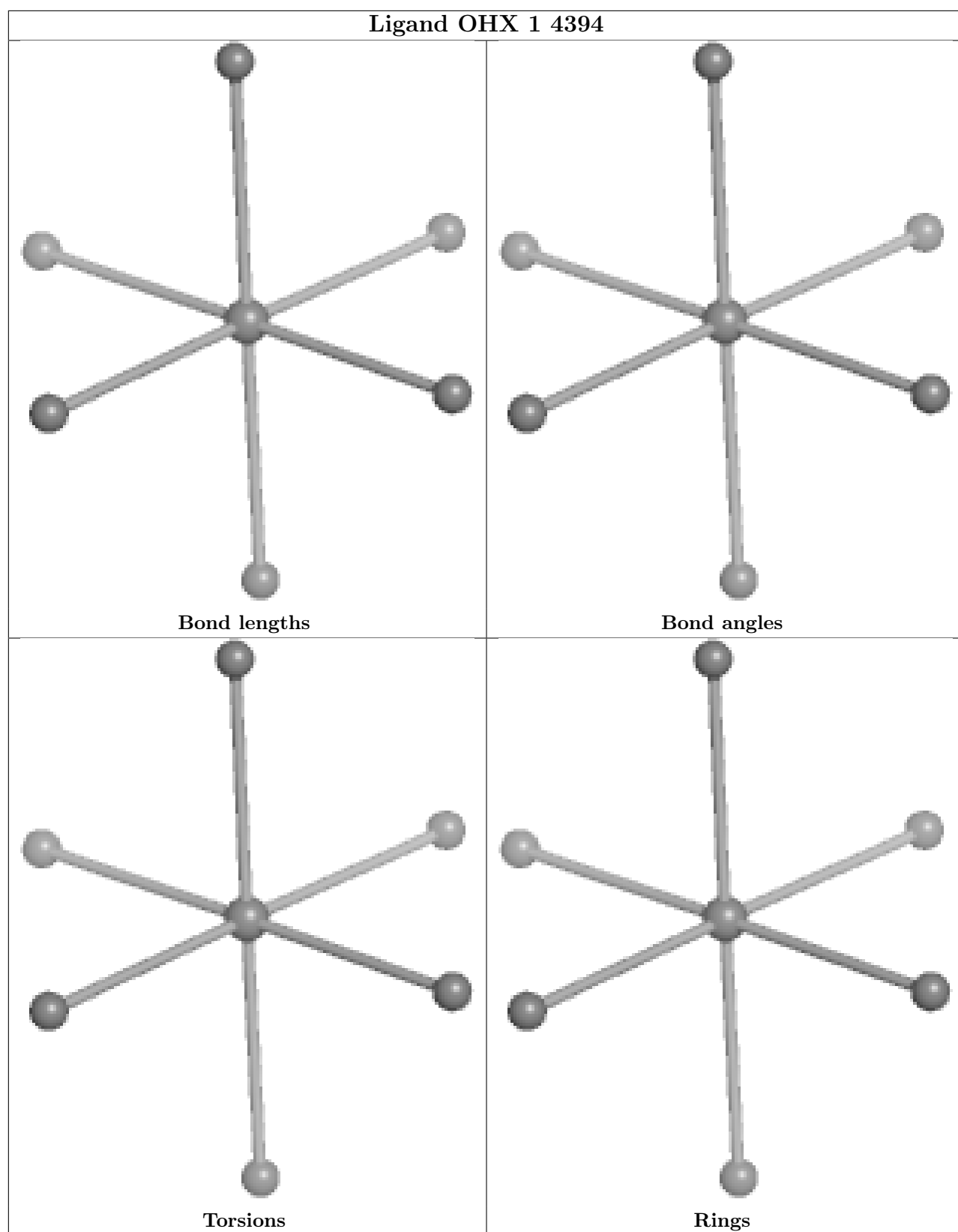


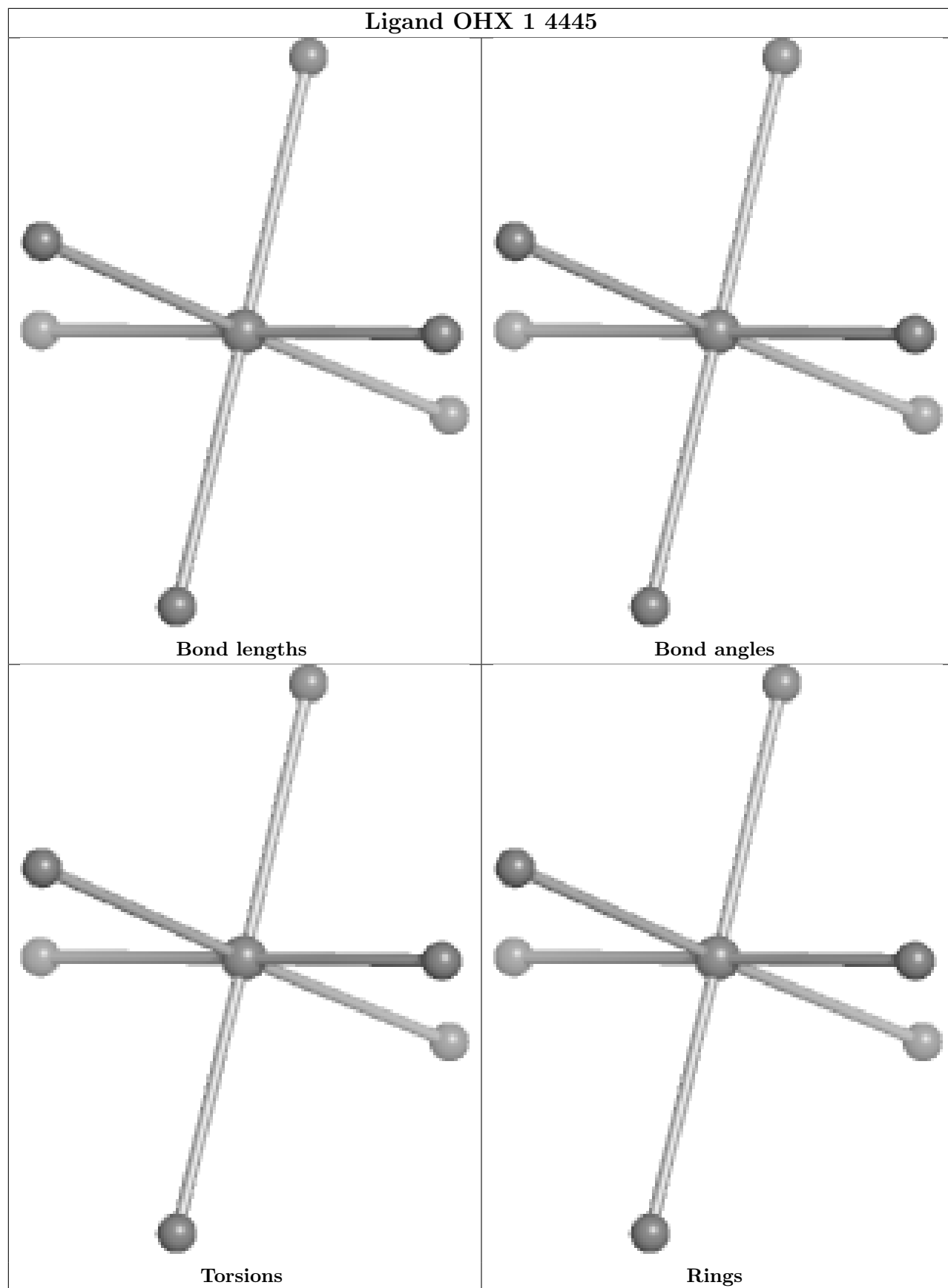


## Ligand OHX 5 4528

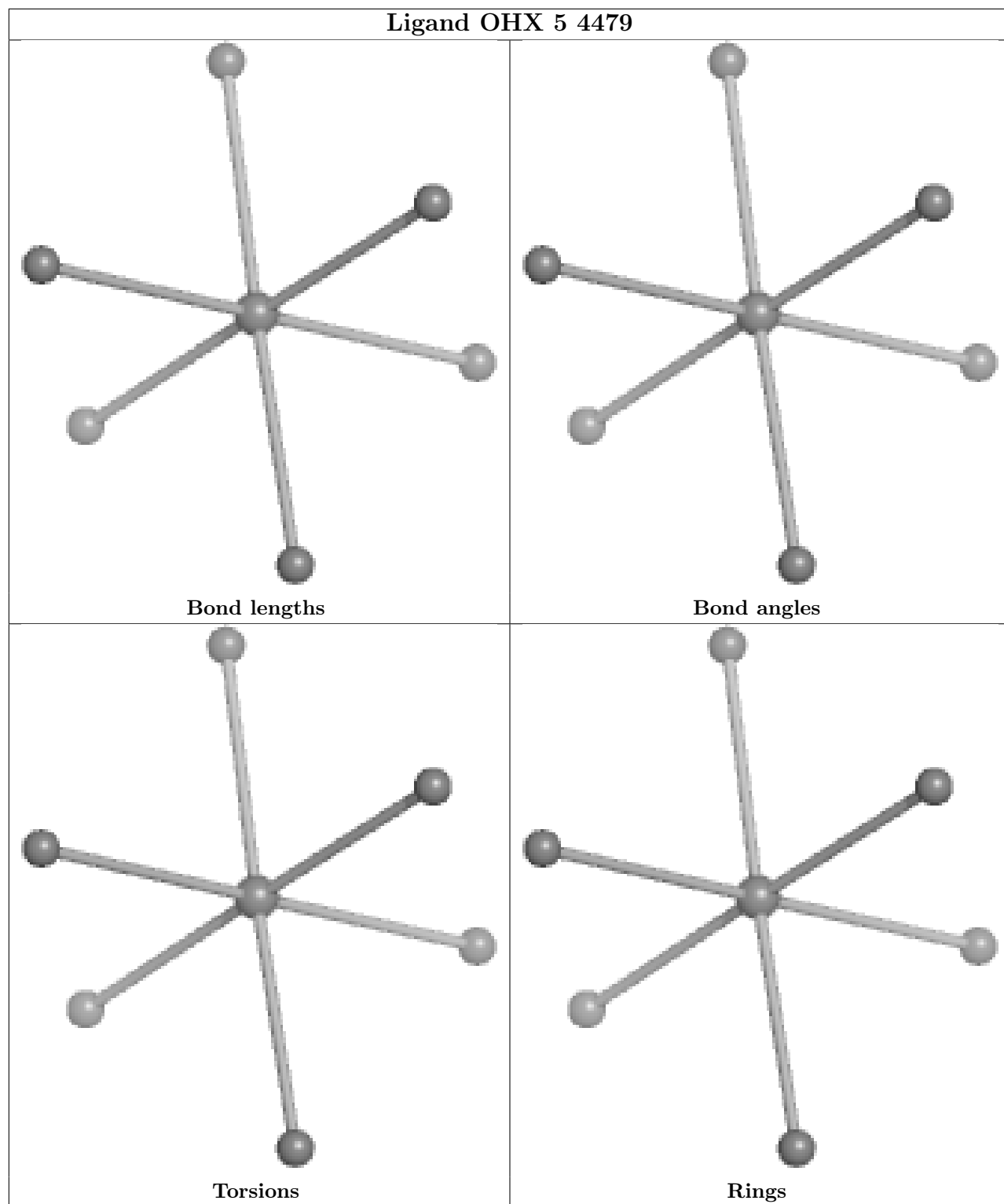


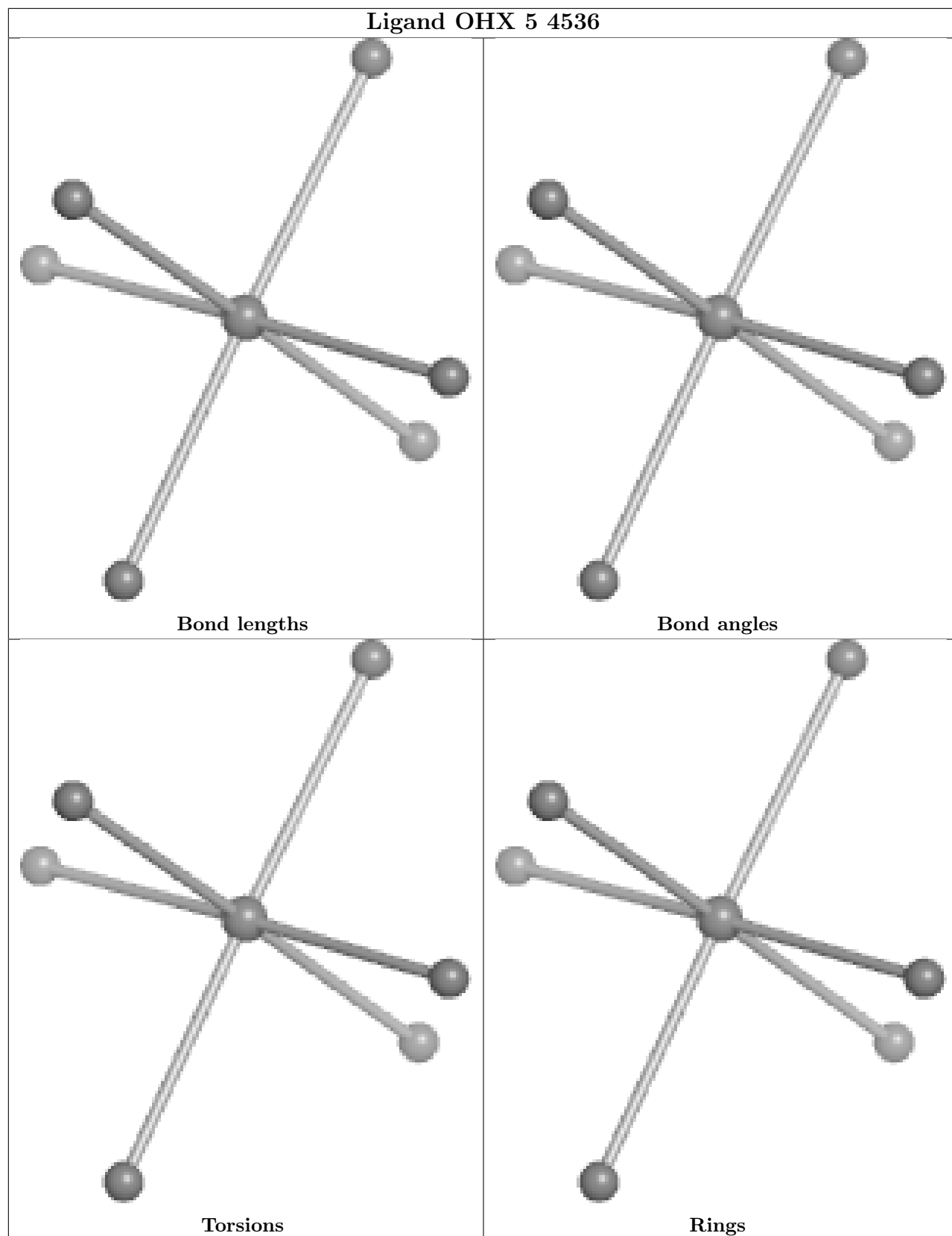




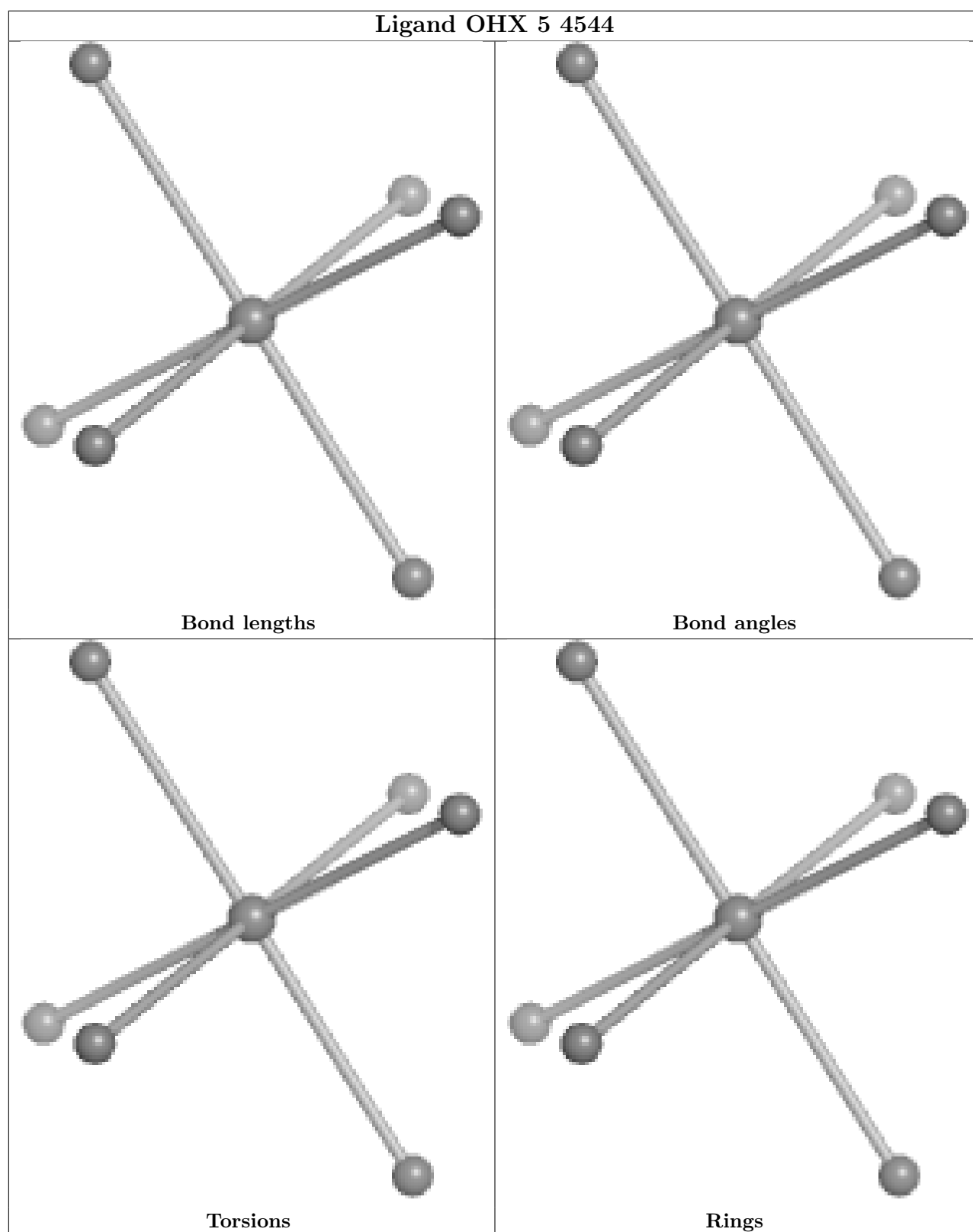


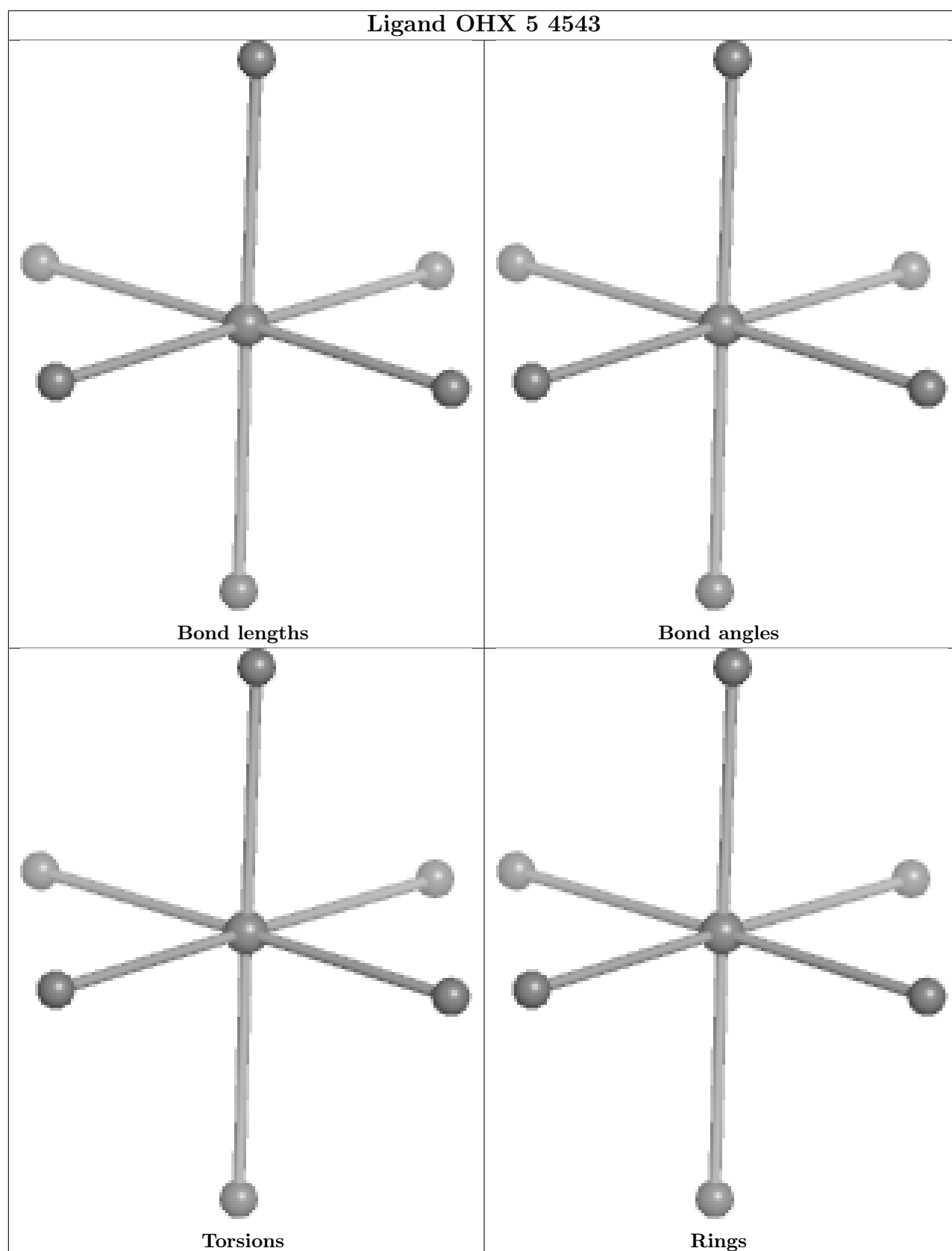
## Ligand OHX 5 4479



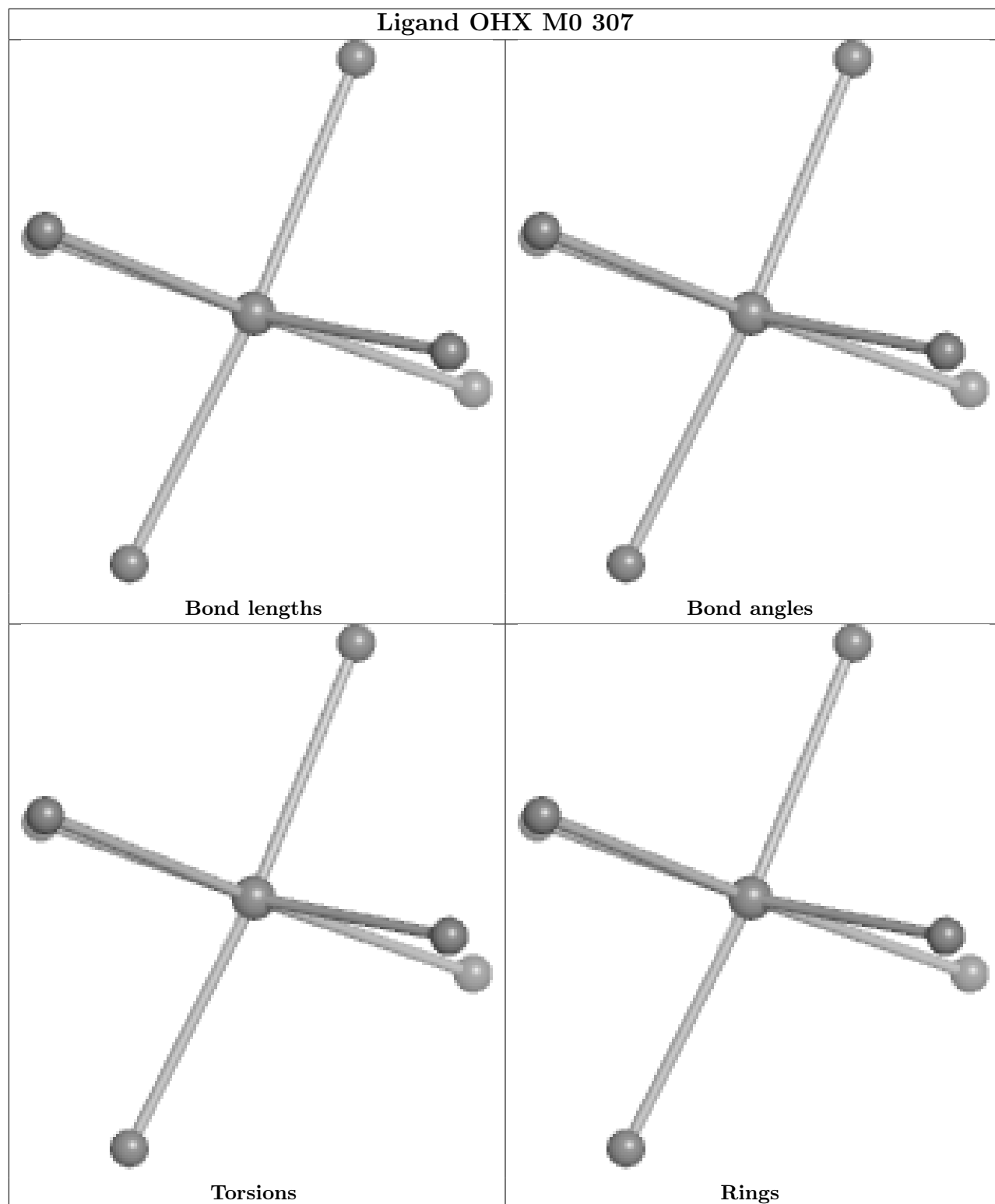


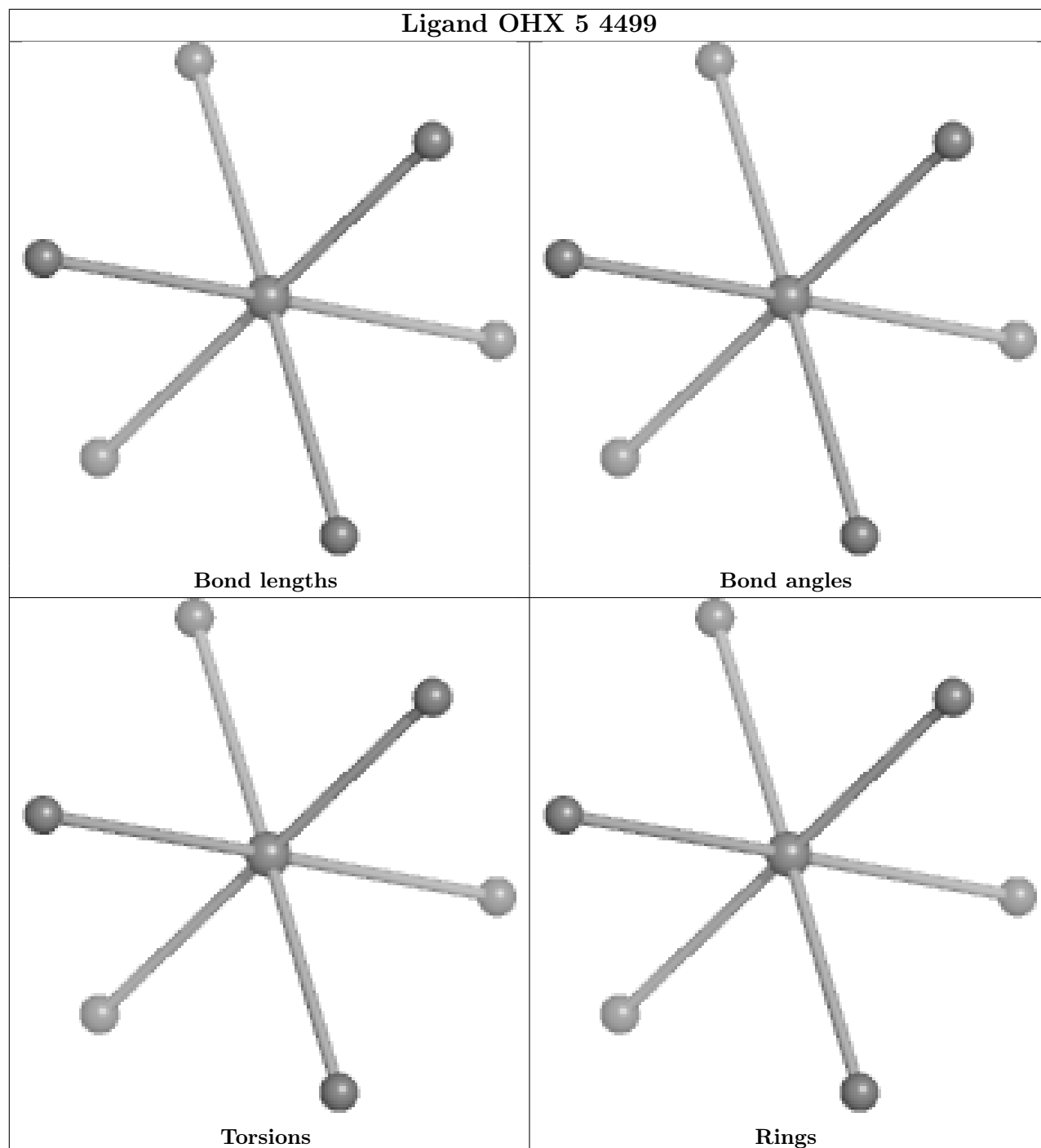


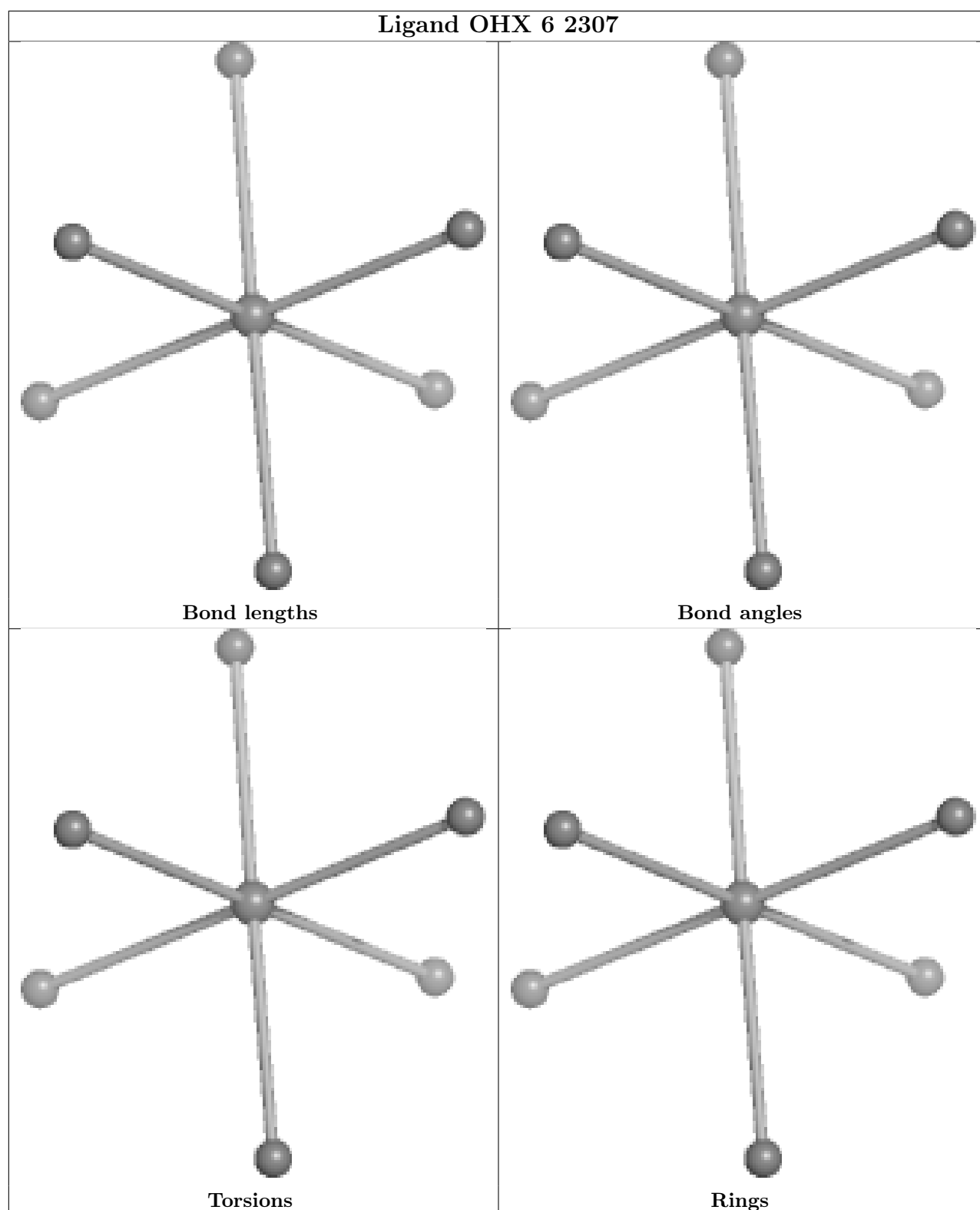


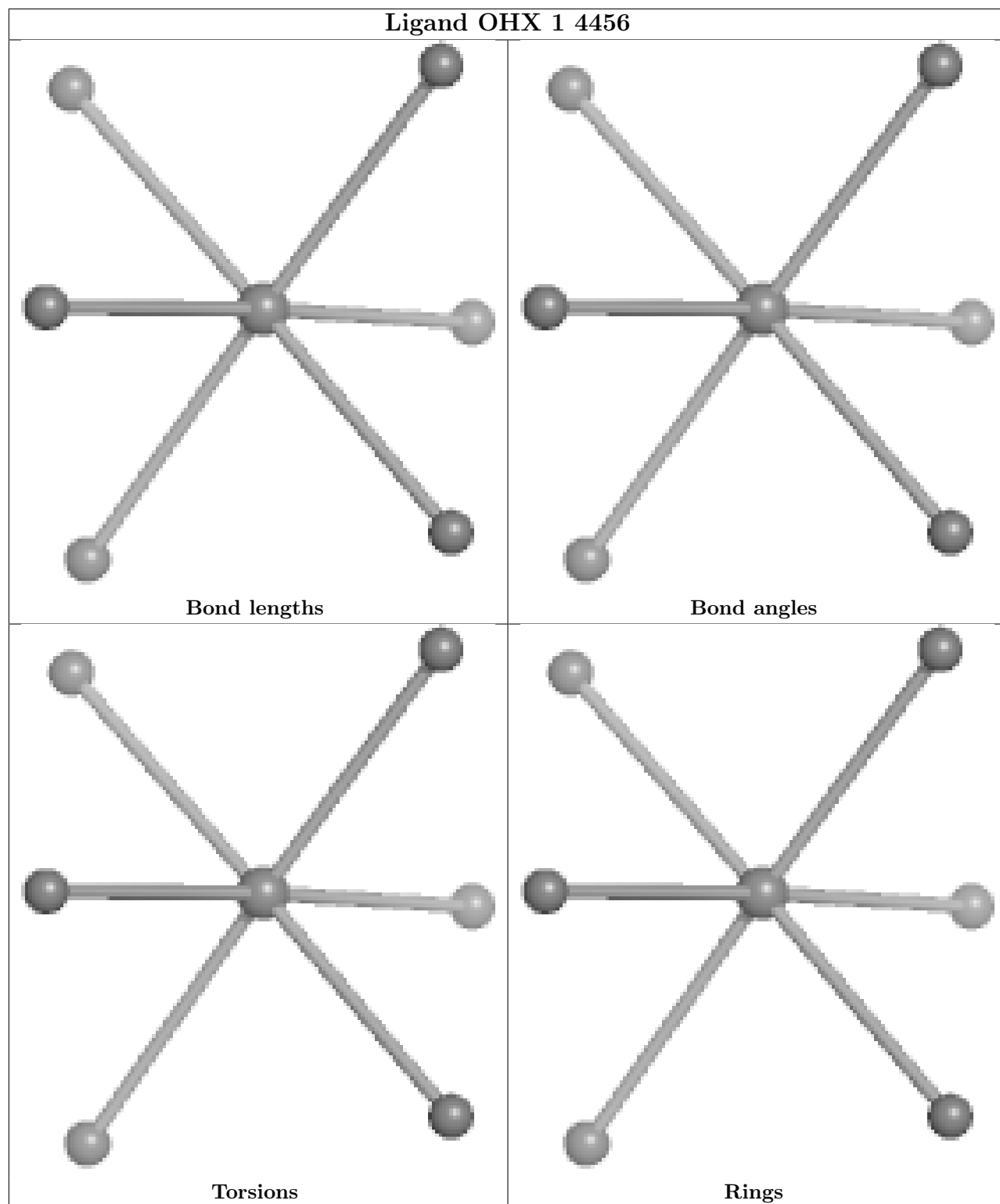


## Ligand OHX M0 307

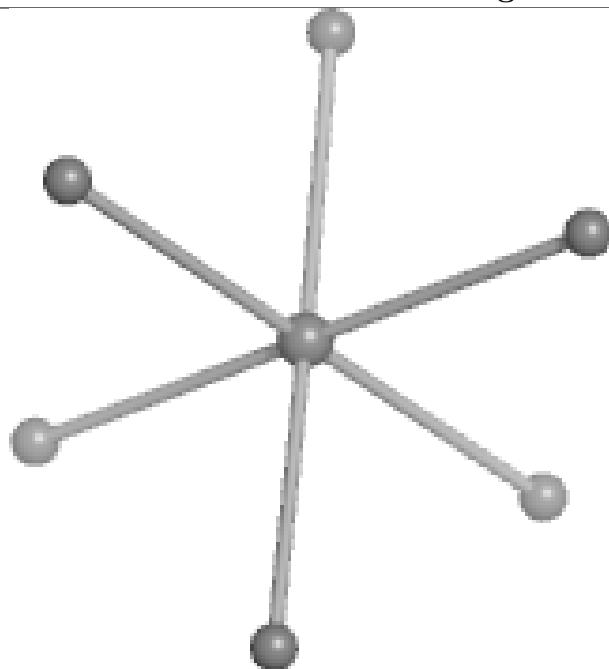




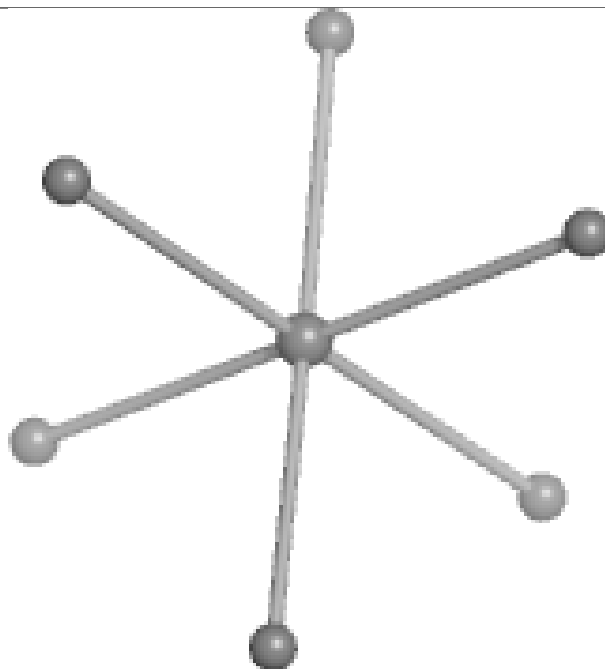




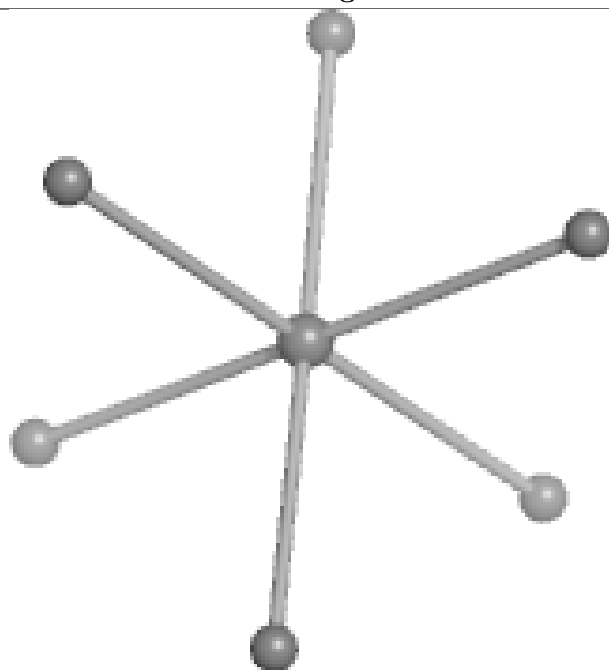
## Ligand OHX M0 306



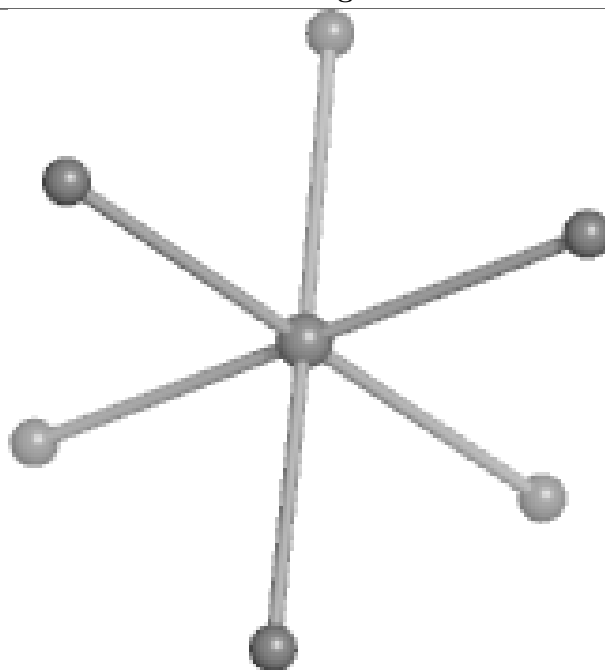
Bond lengths



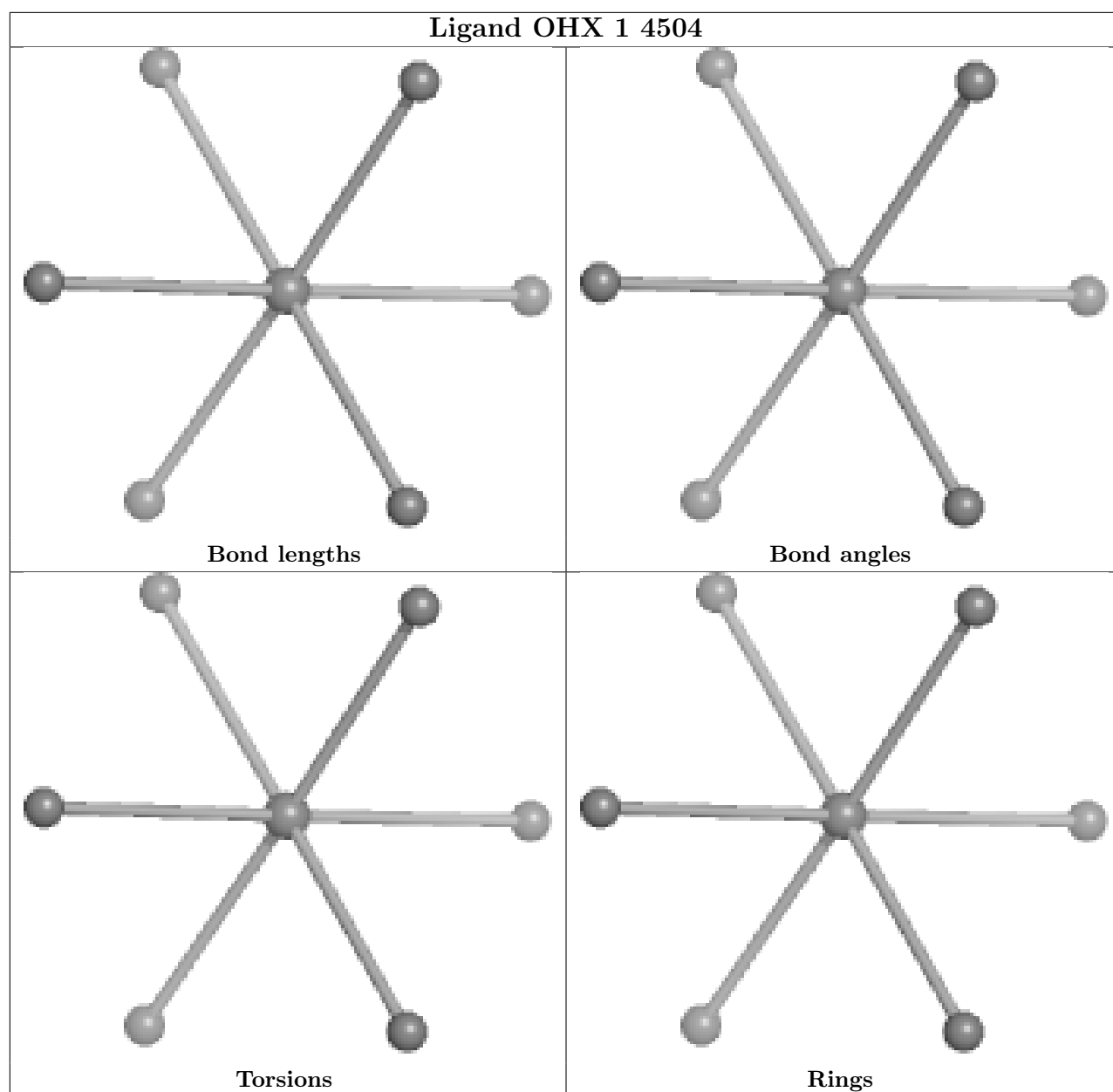
Bond angles



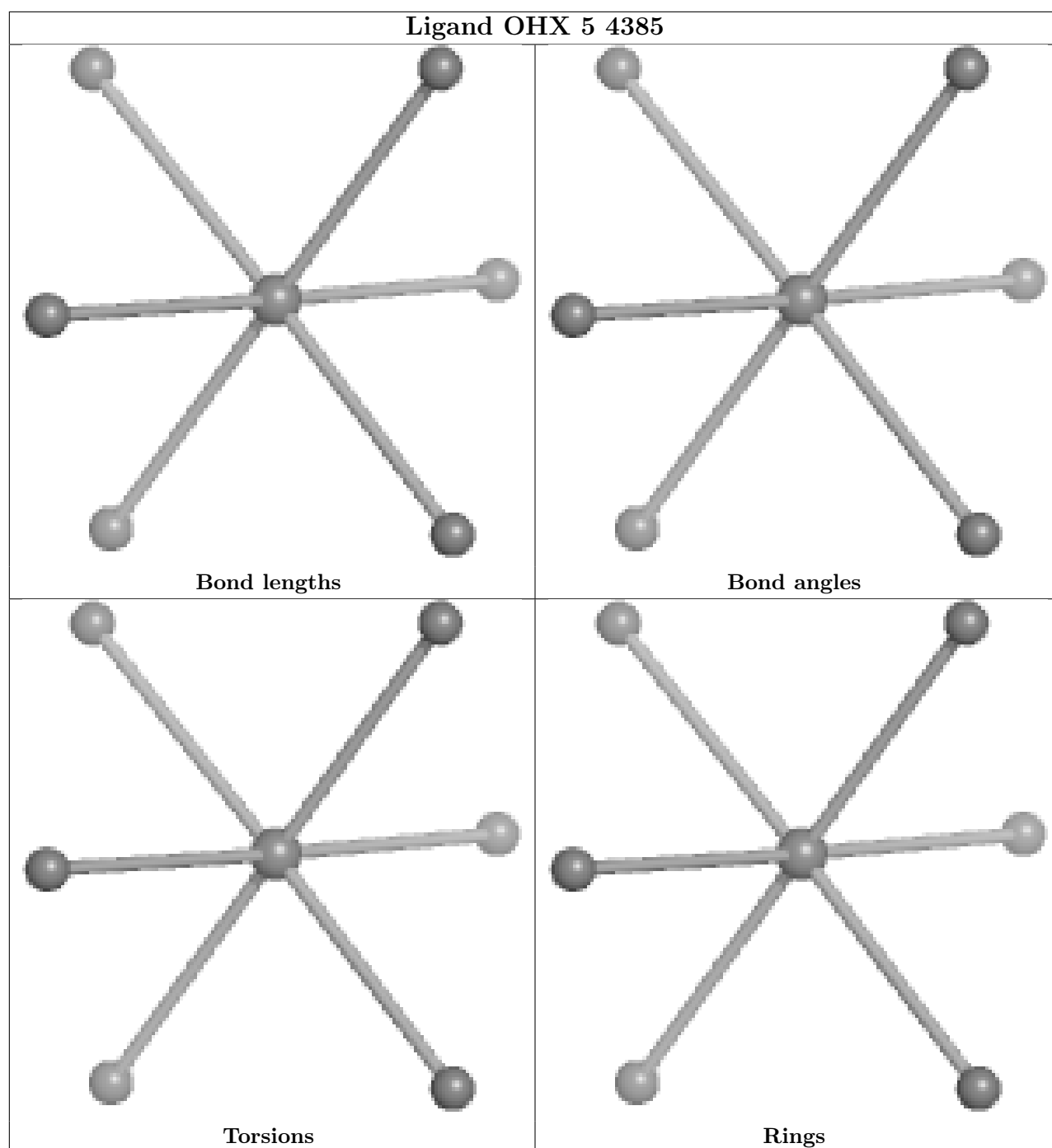
Torsions

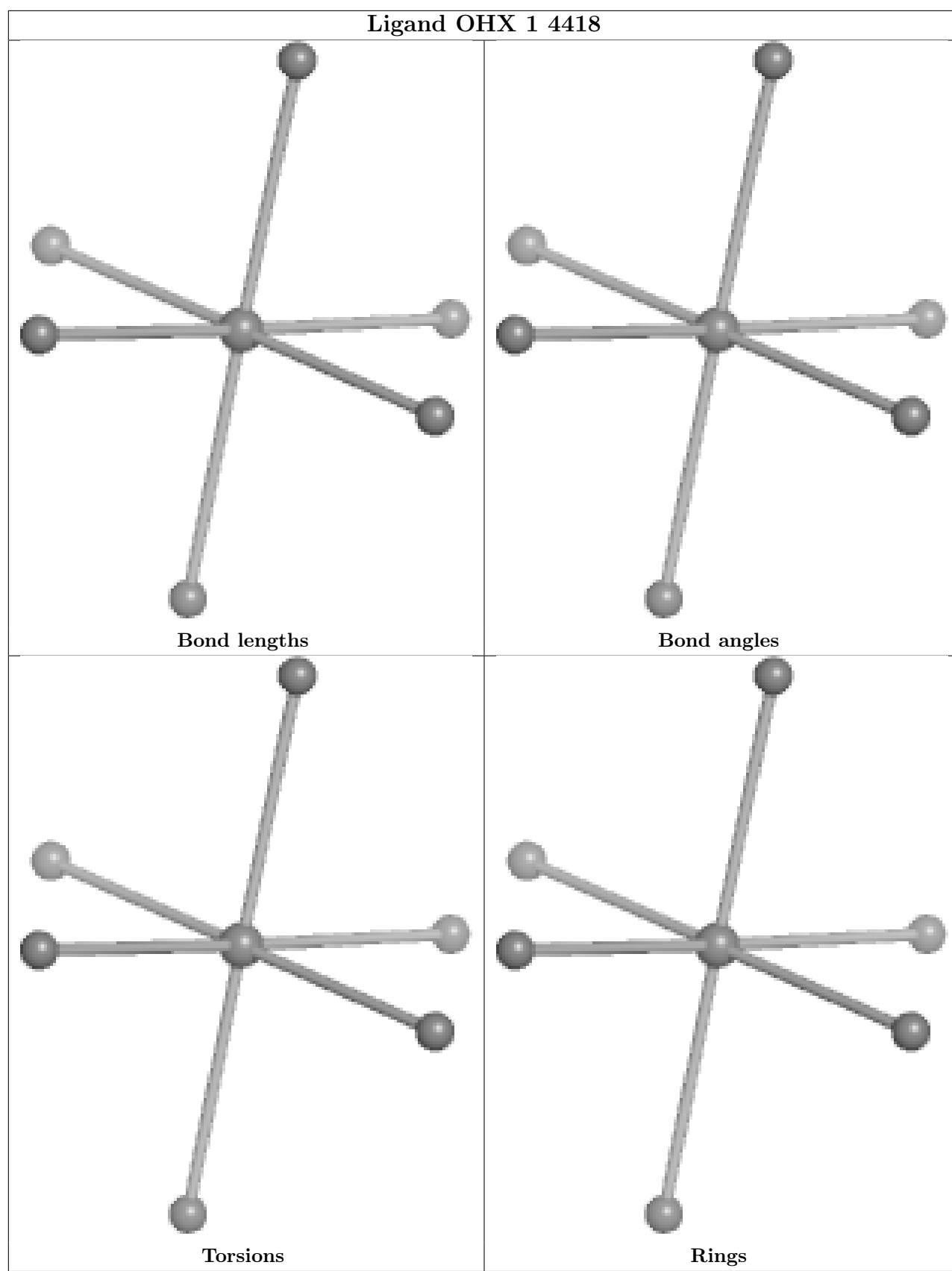


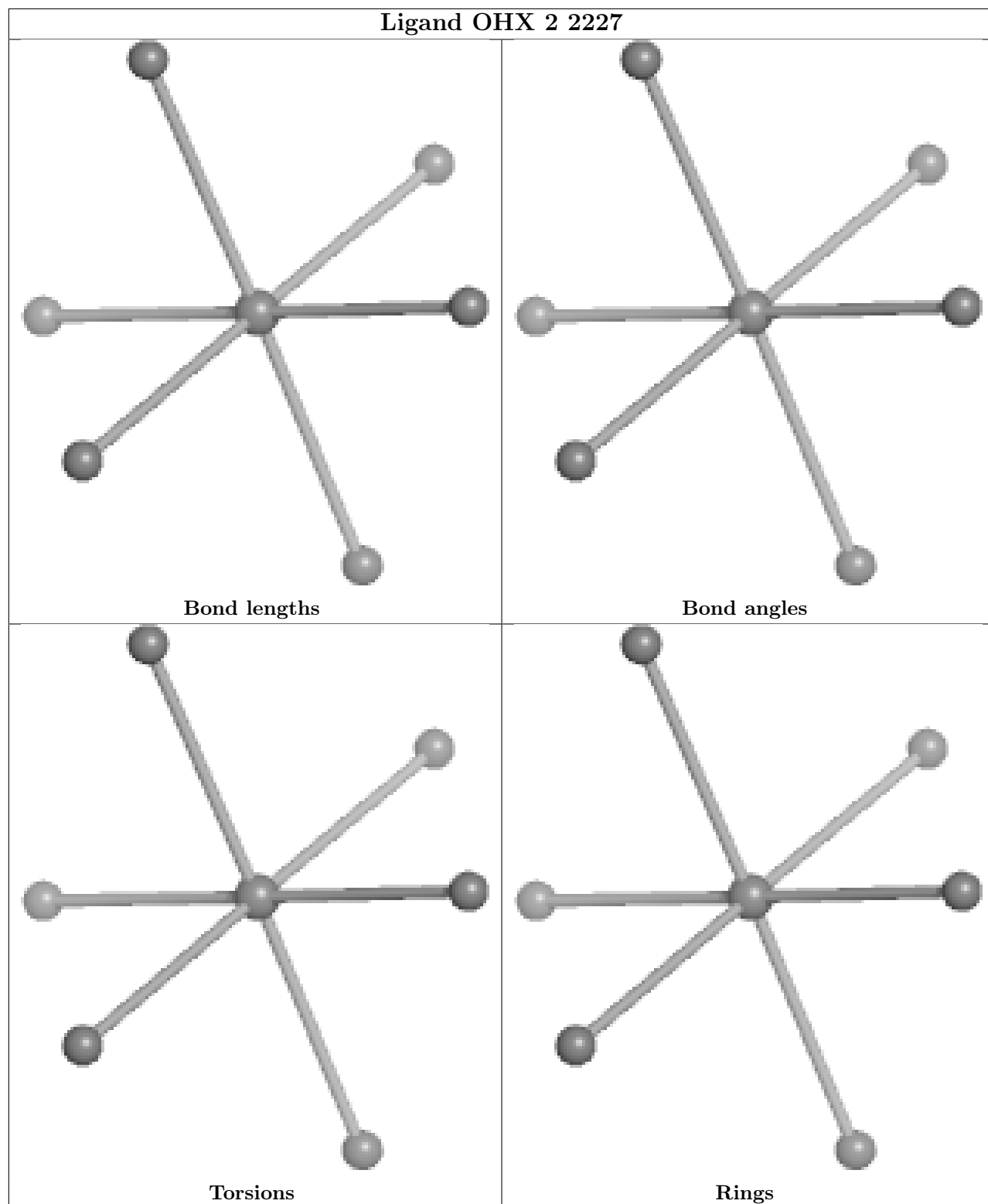
Rings

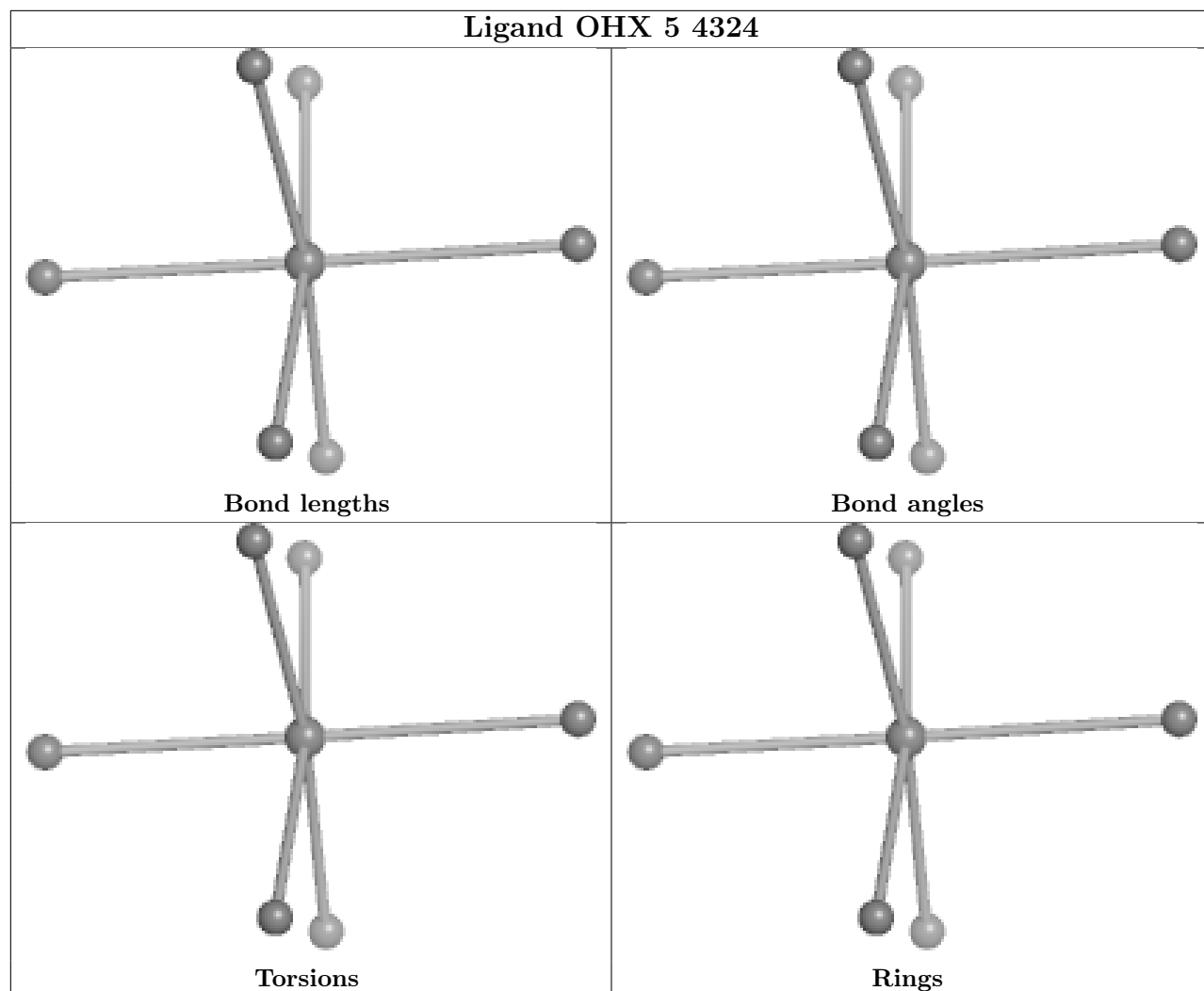


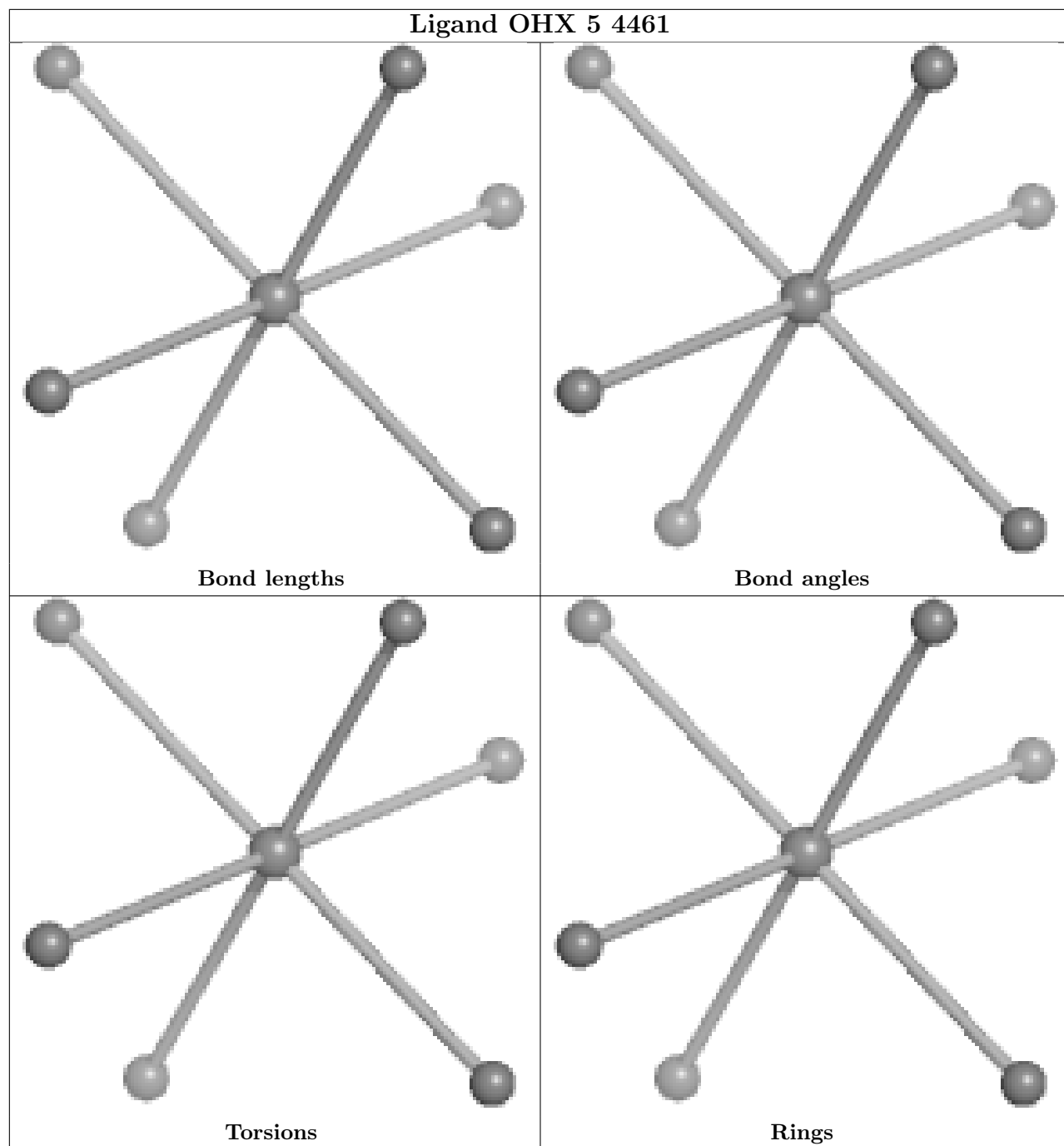


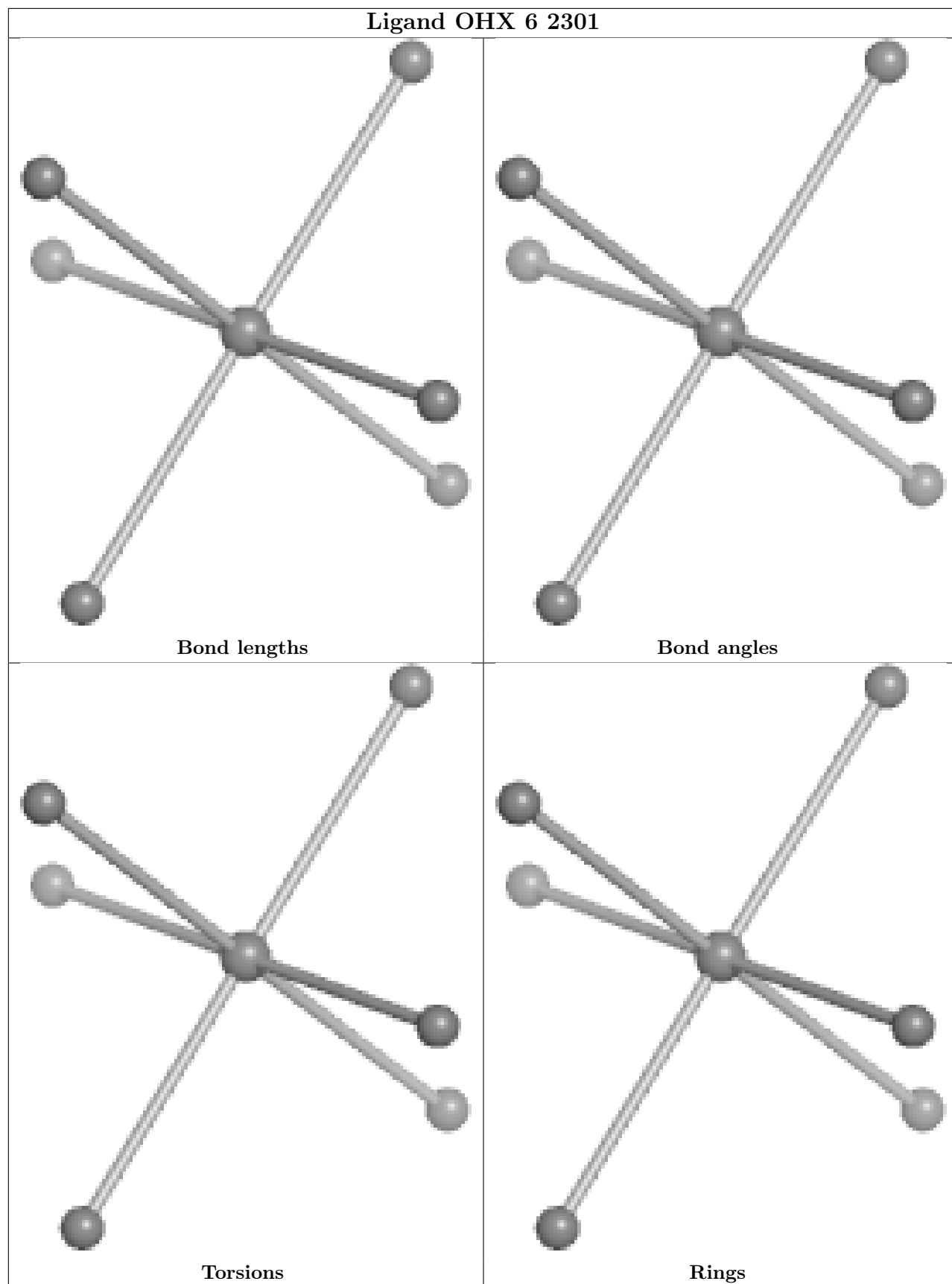


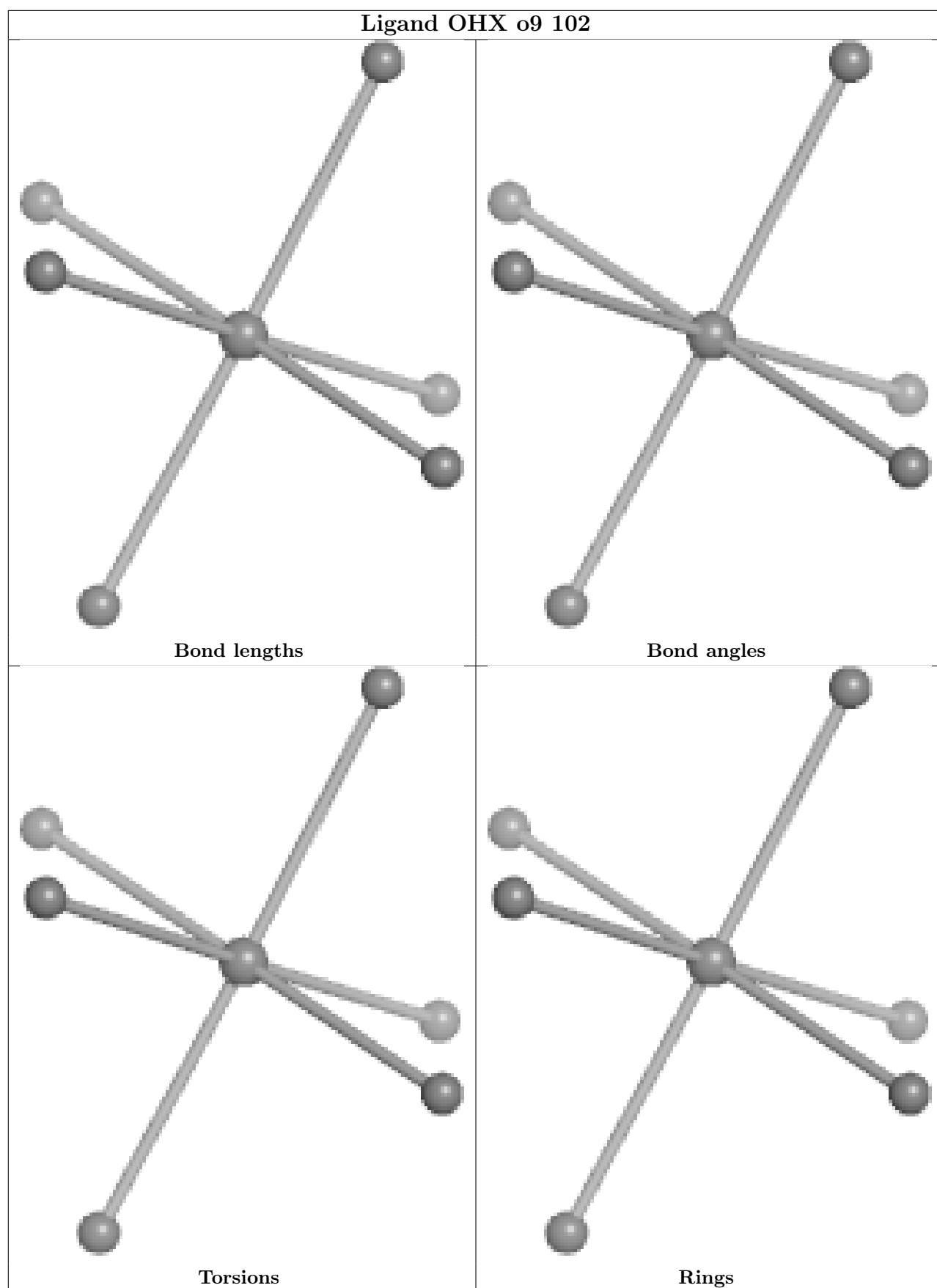


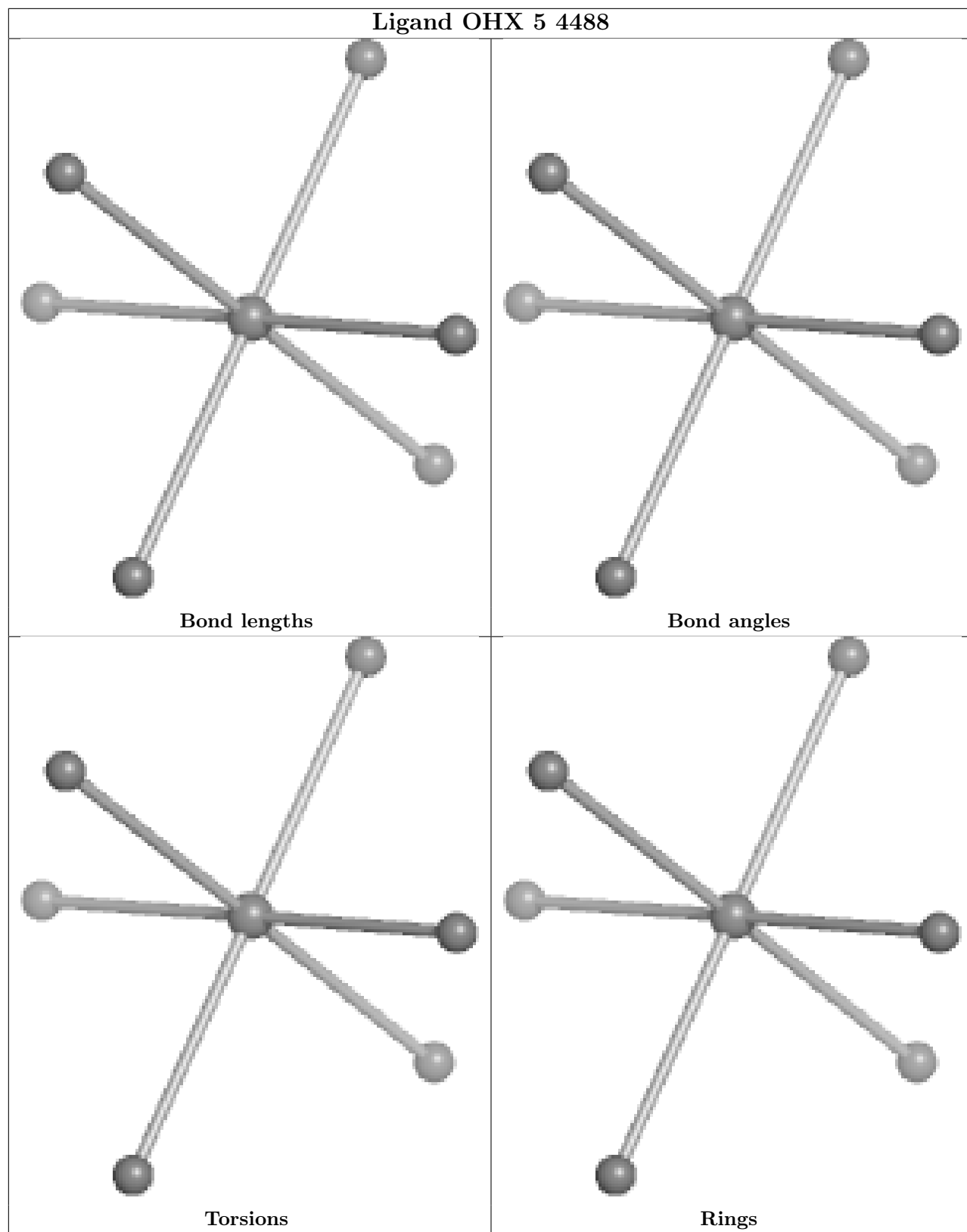




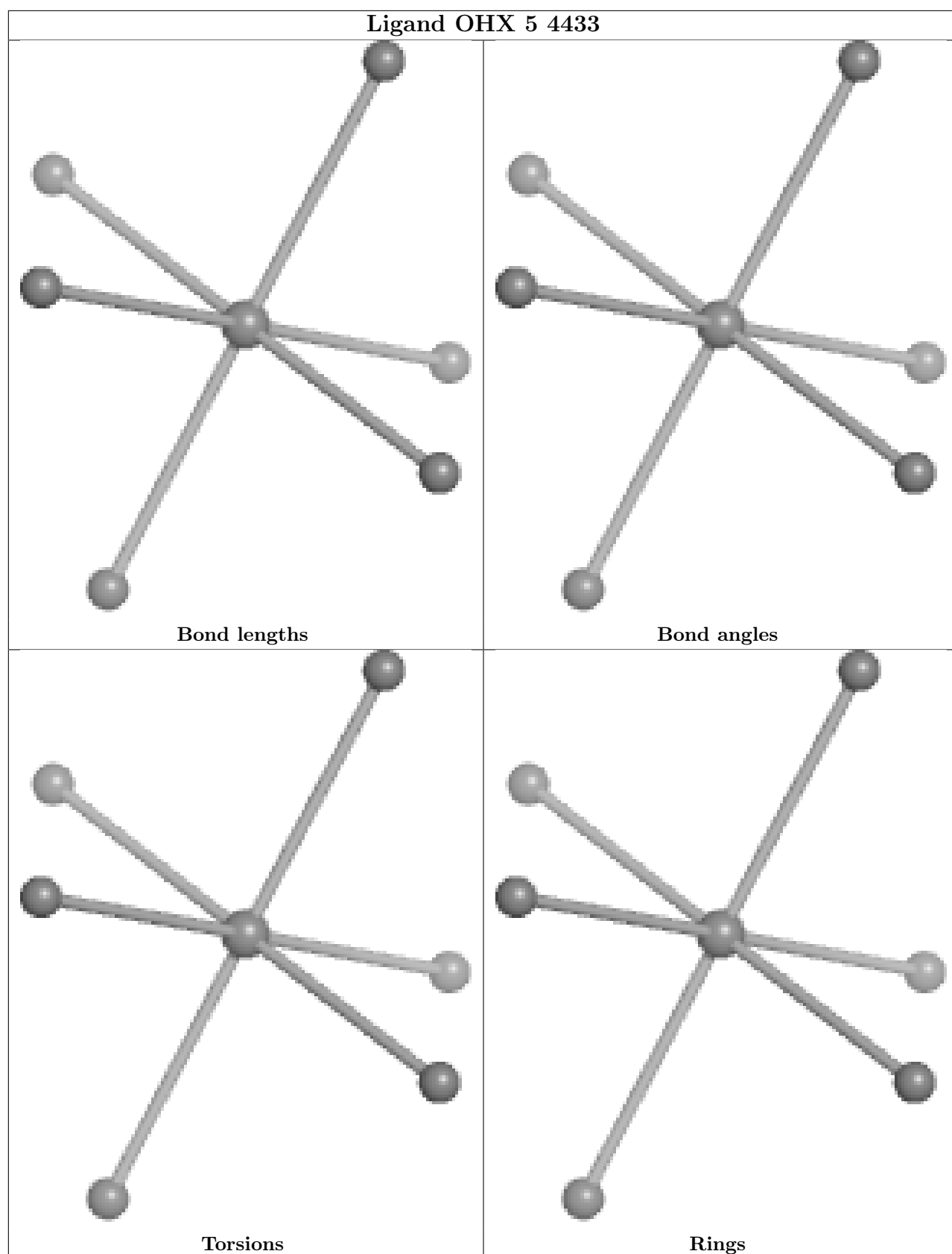




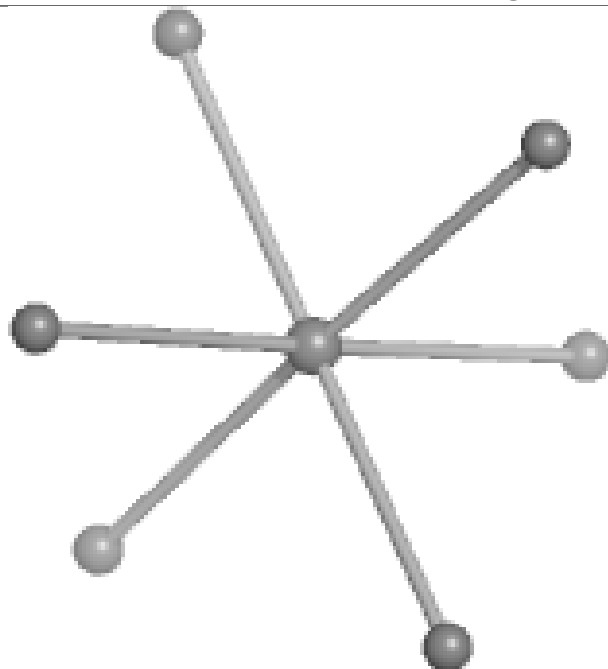




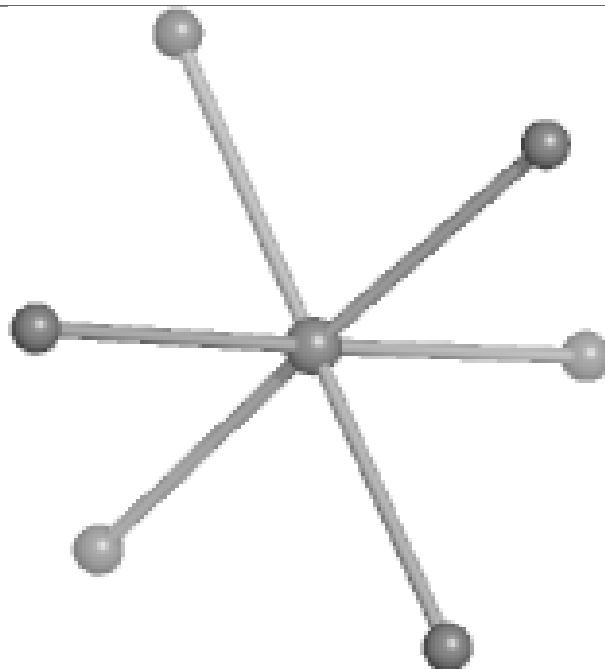




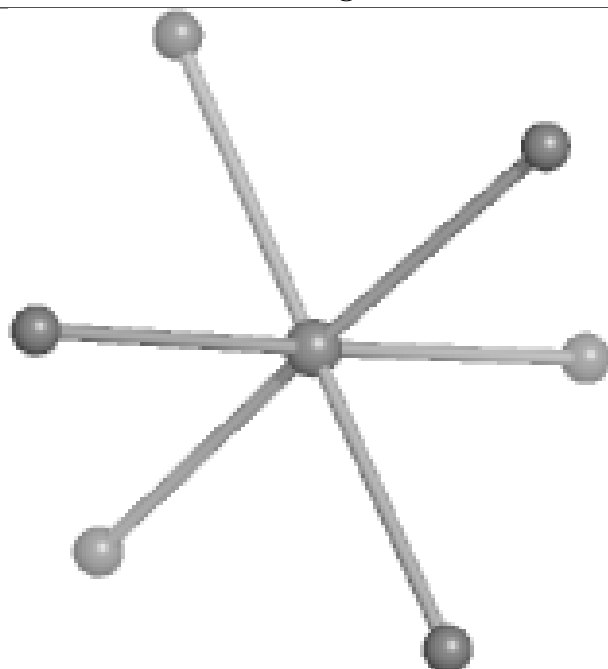
## Ligand OHX 1 4427



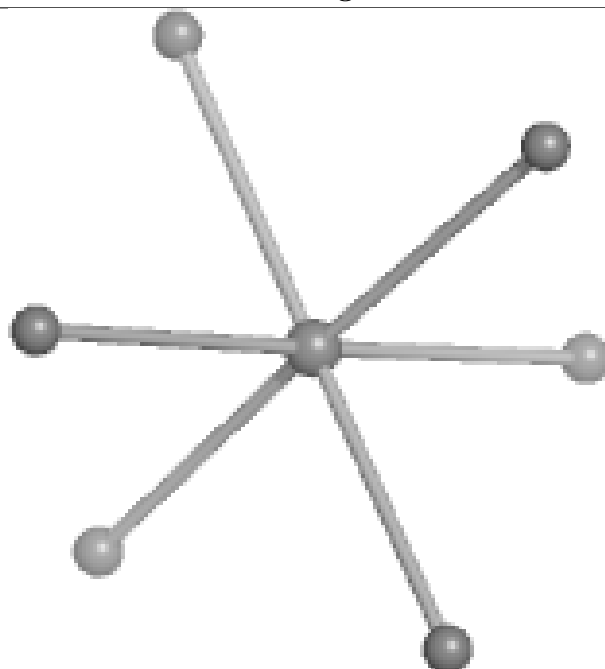
Bond lengths



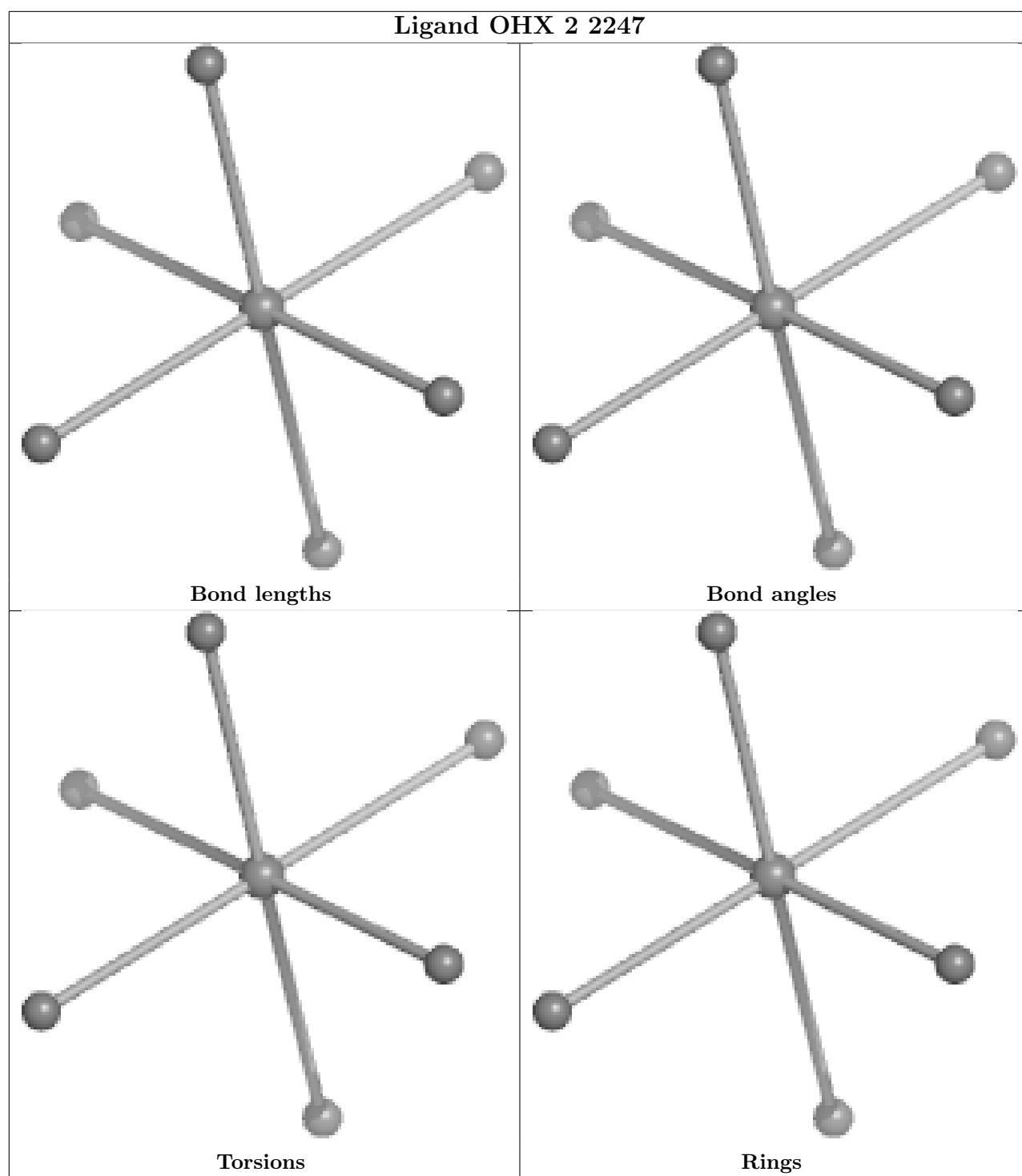
Bond angles

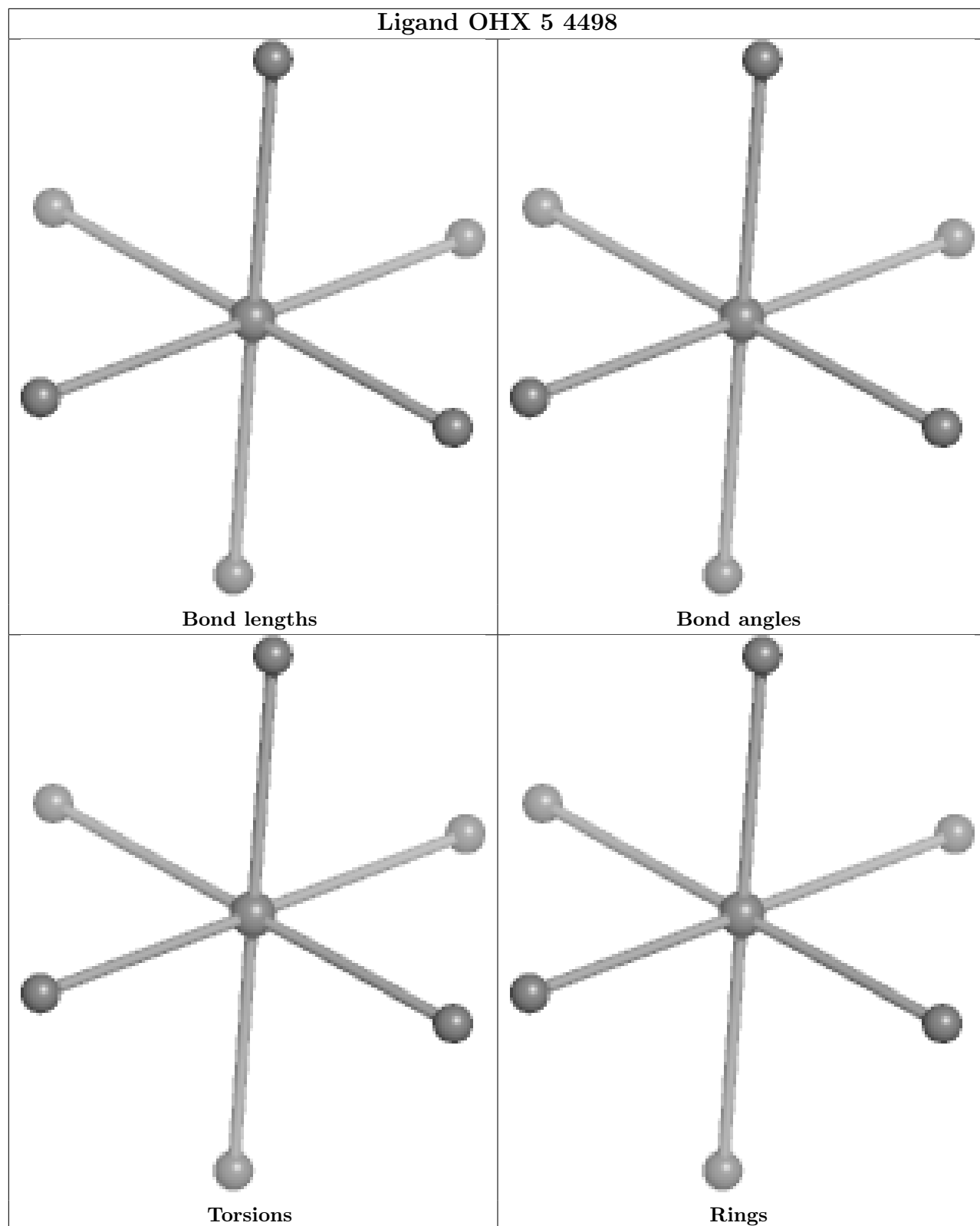


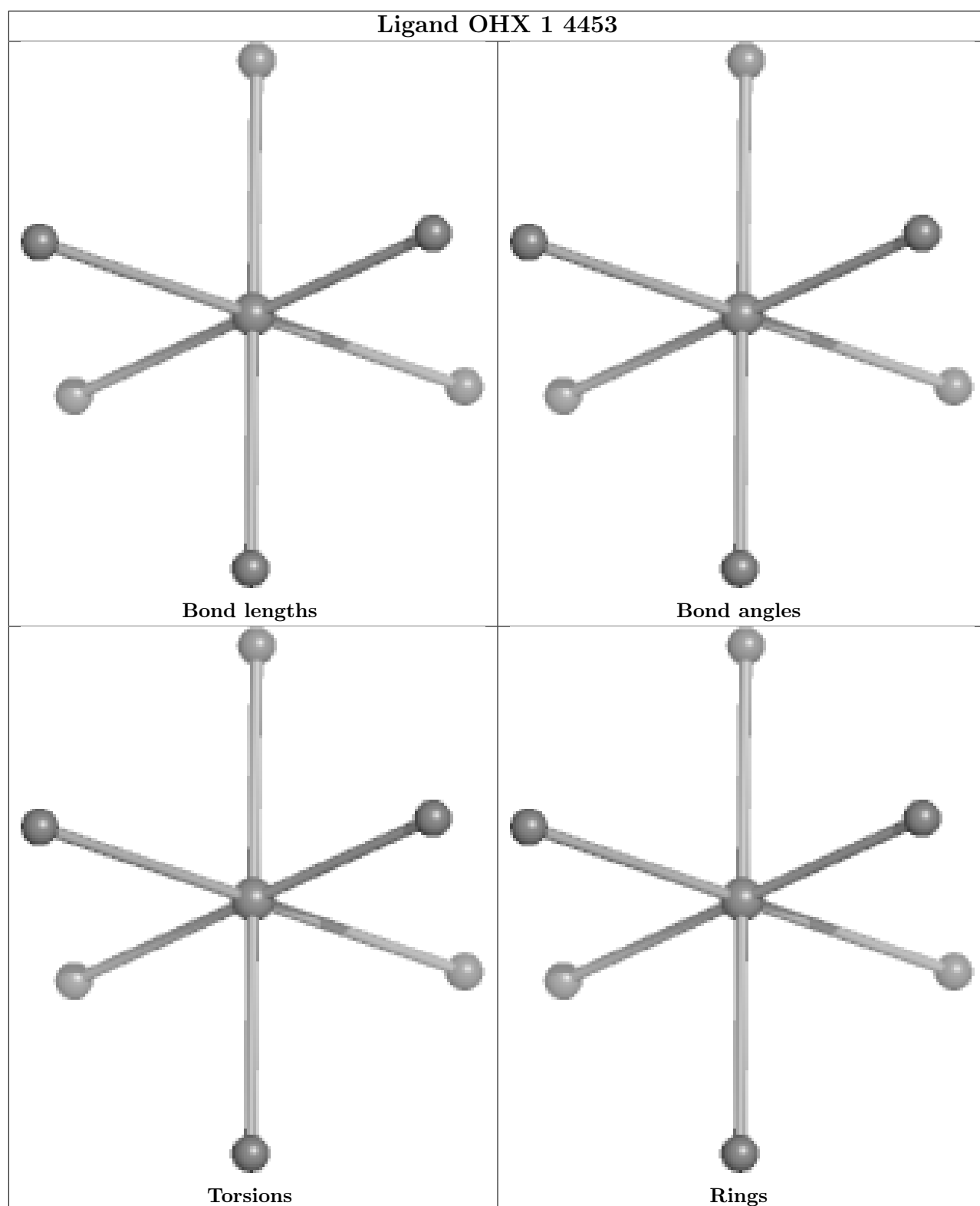
Torsions

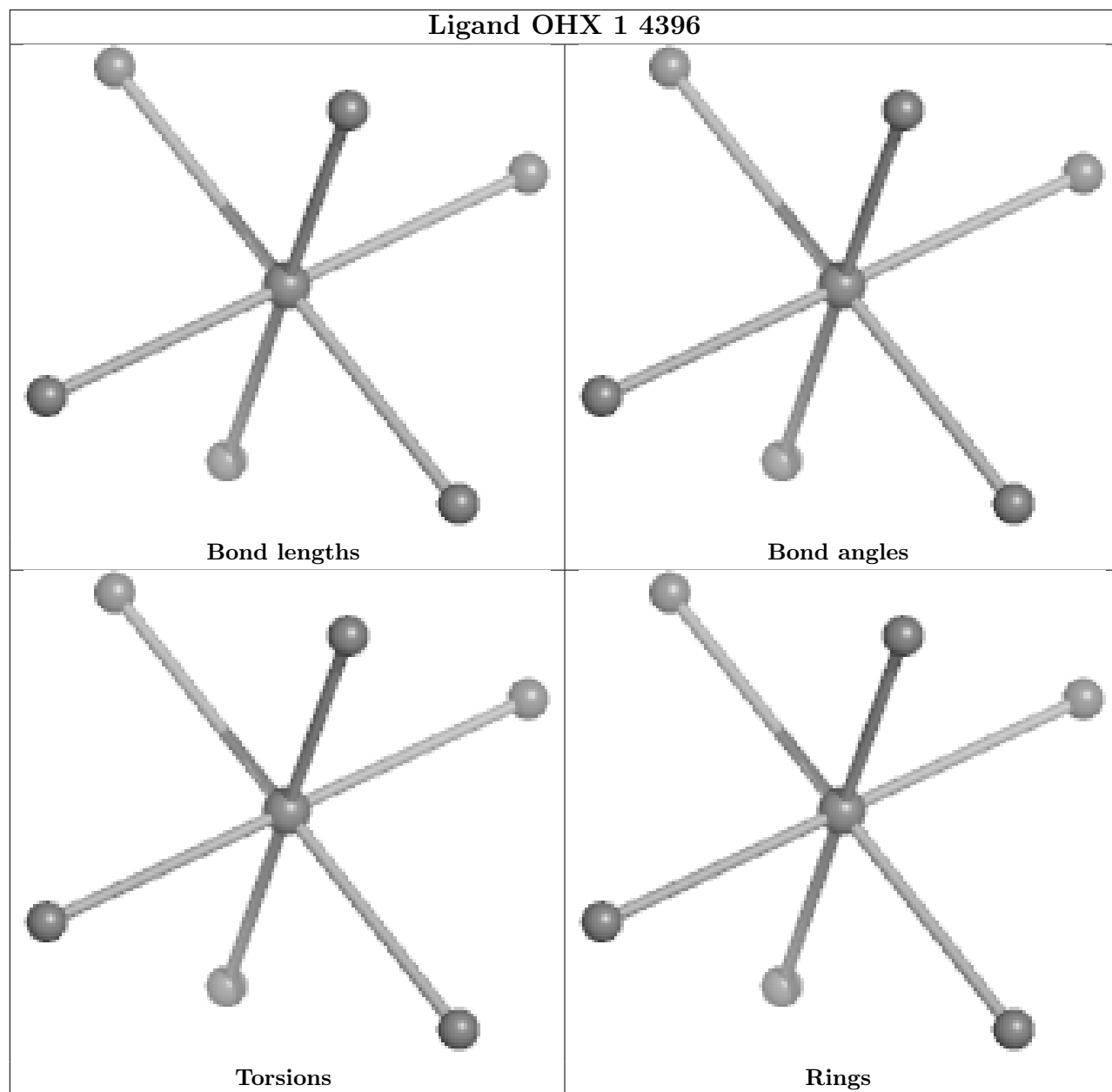


Rings

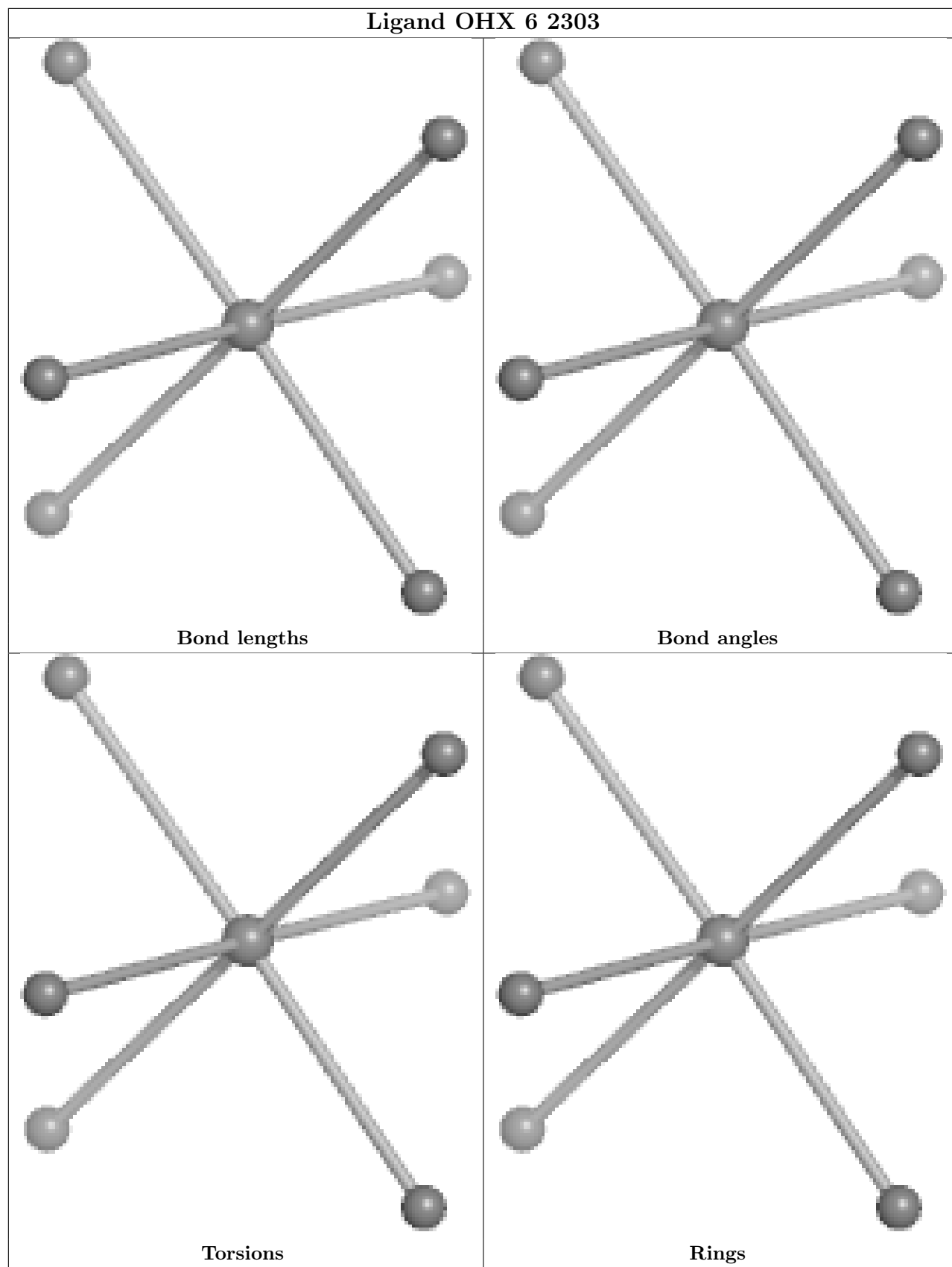


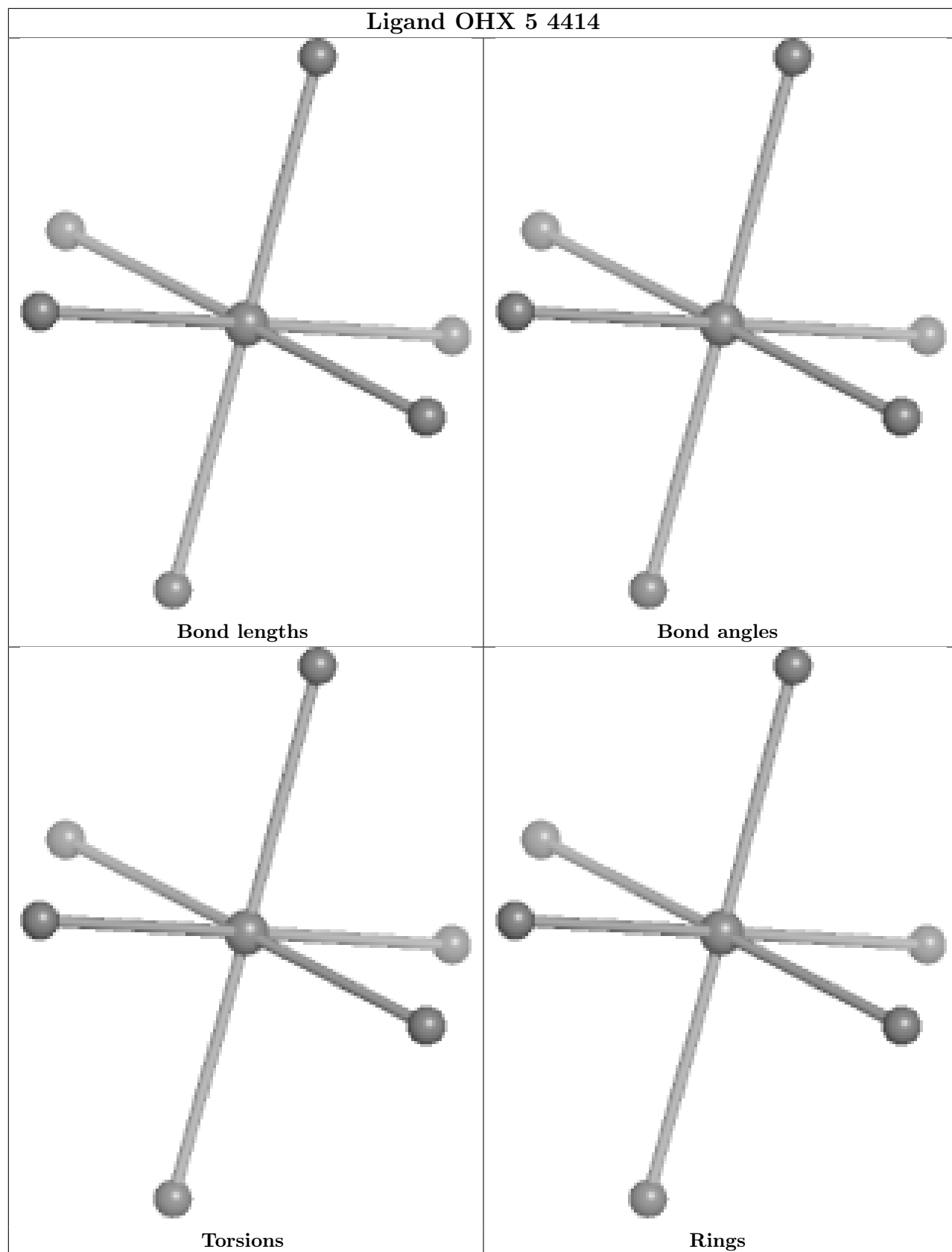




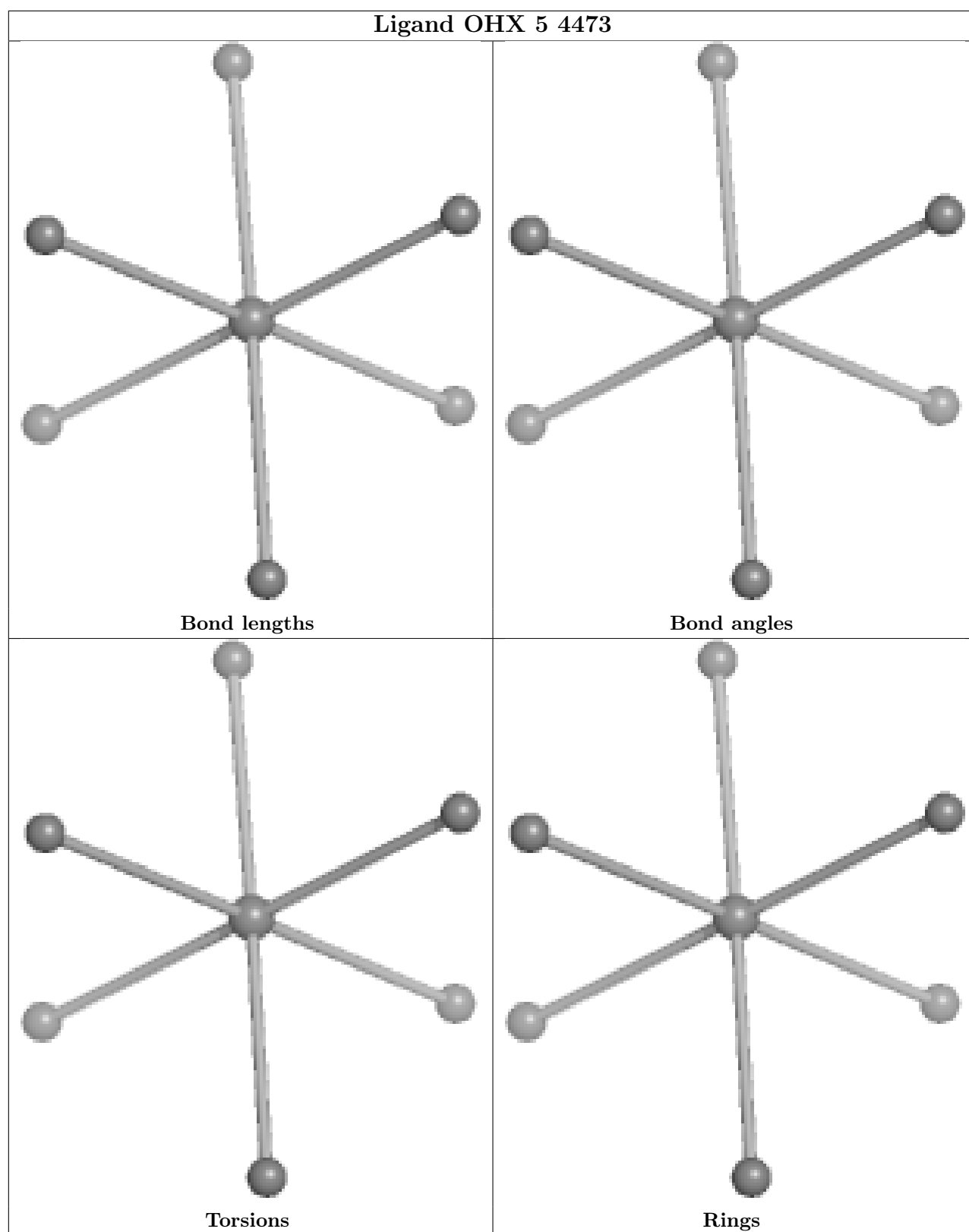


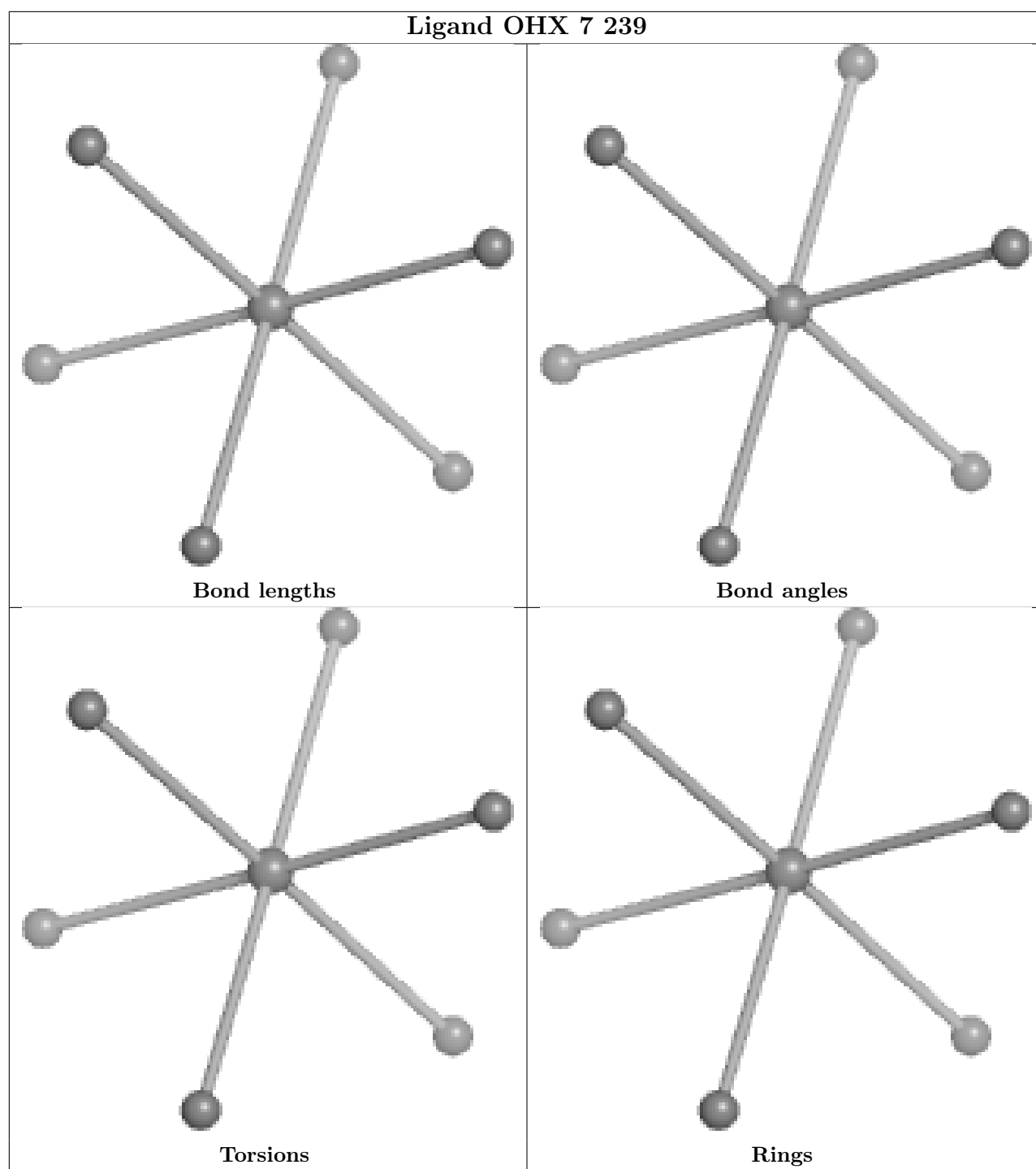
## Ligand OHX 6 2303

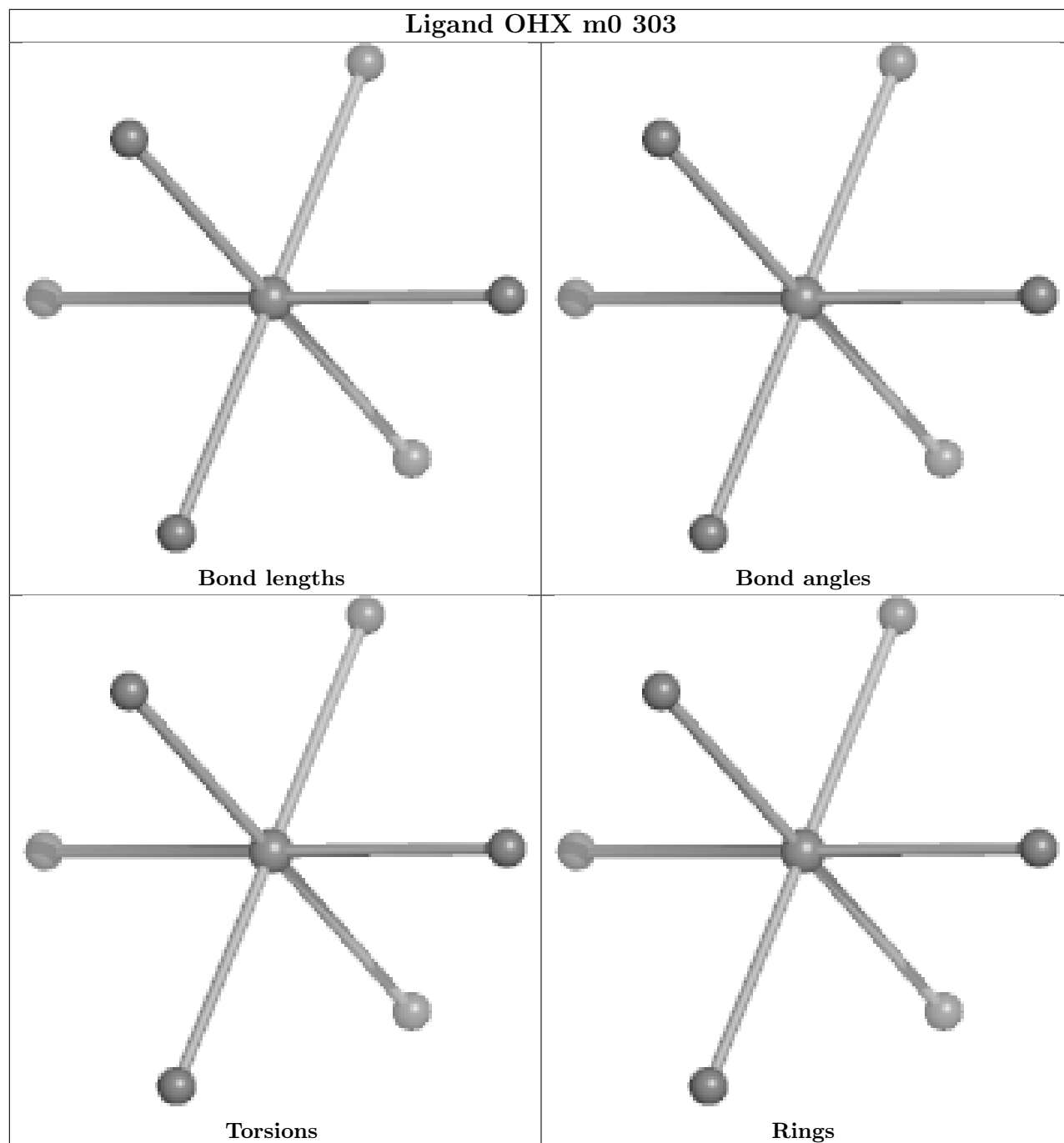


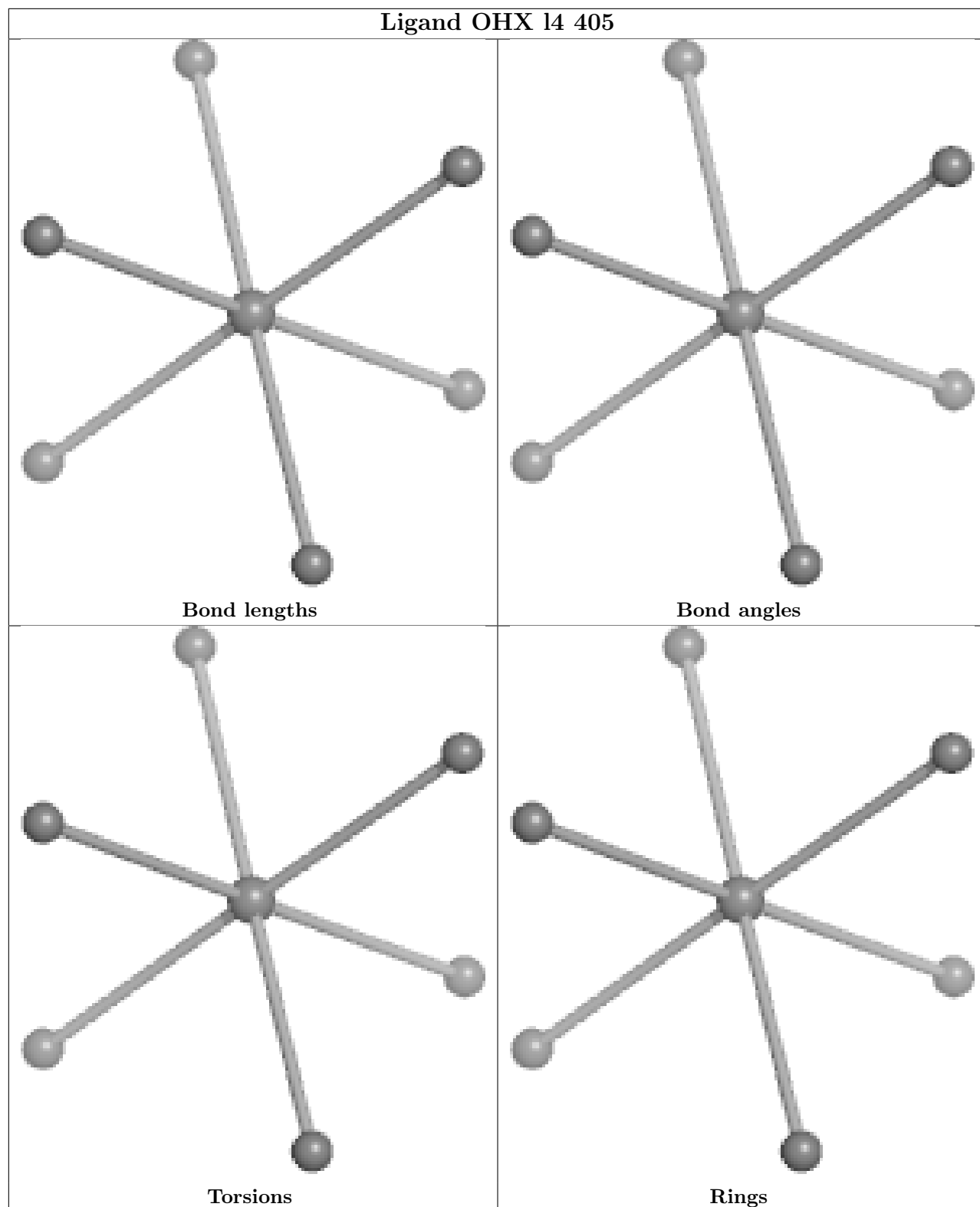




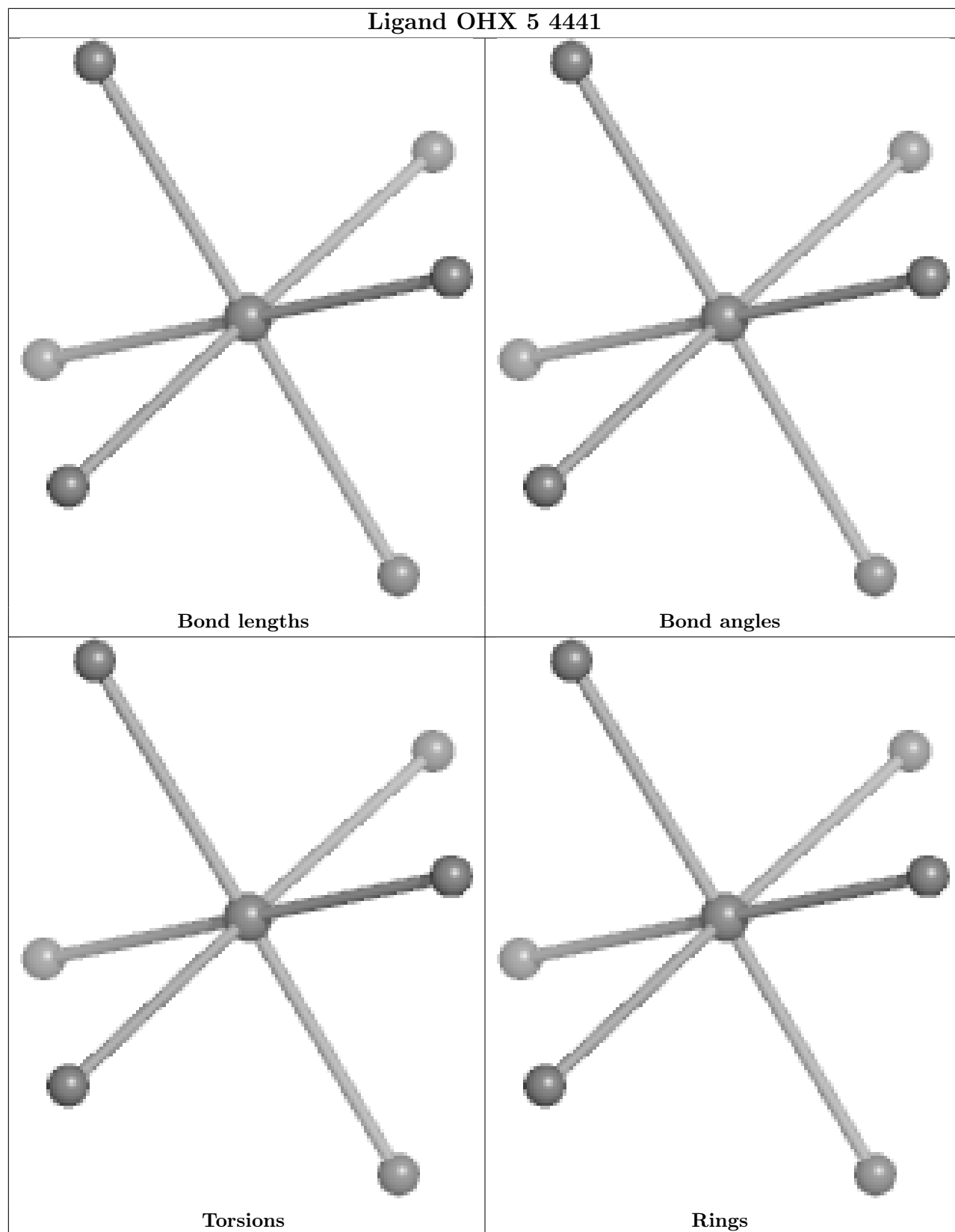


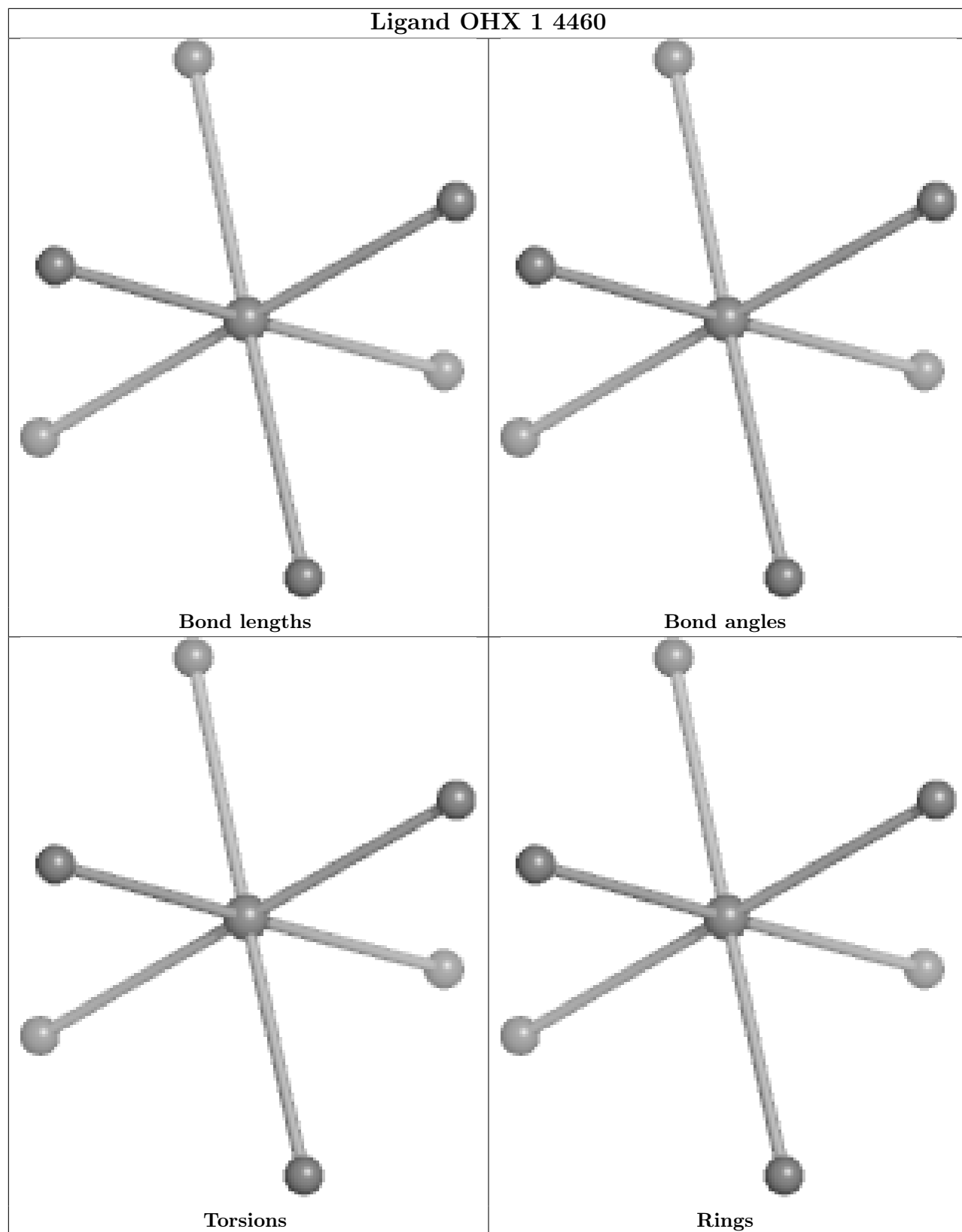


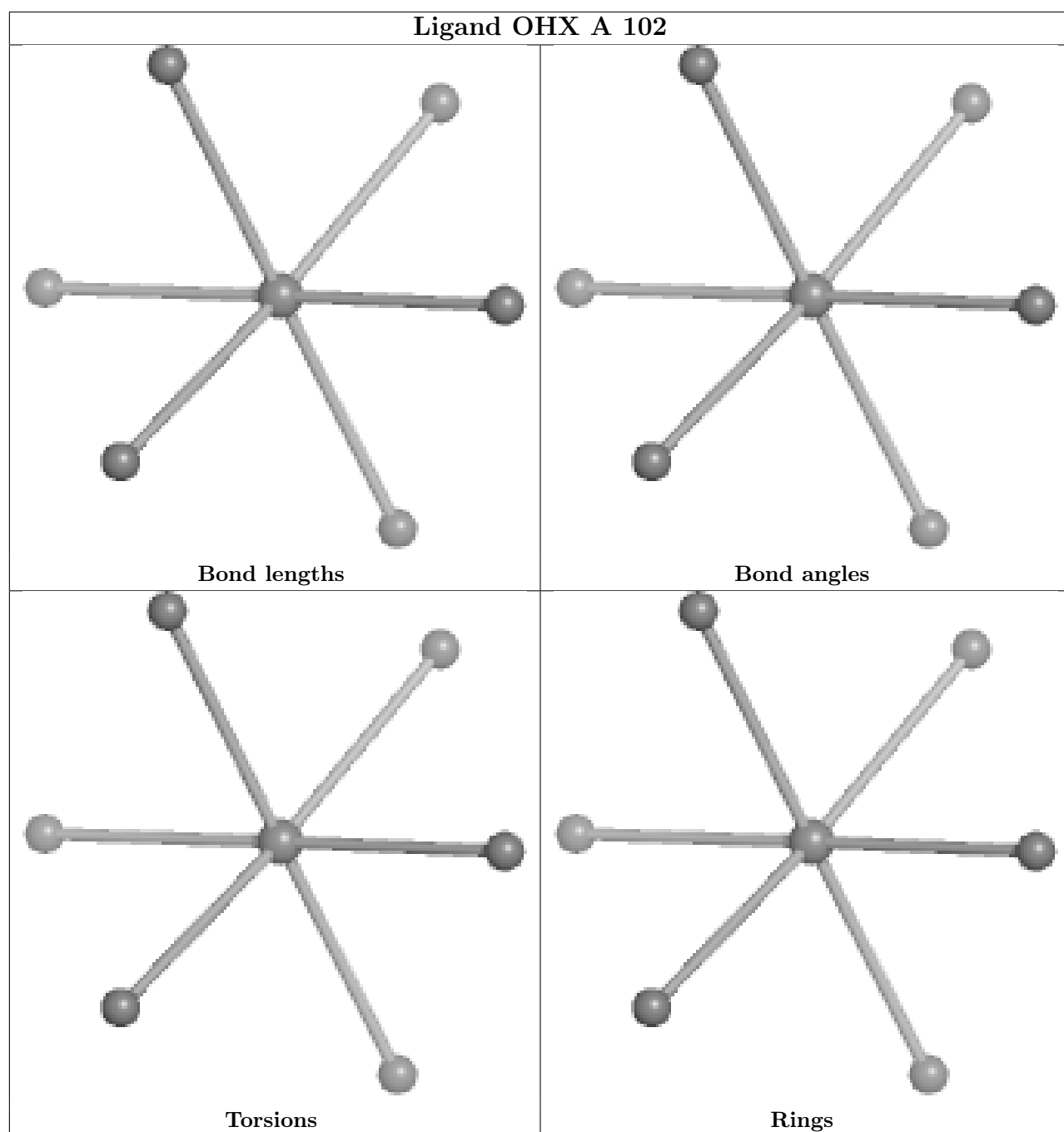


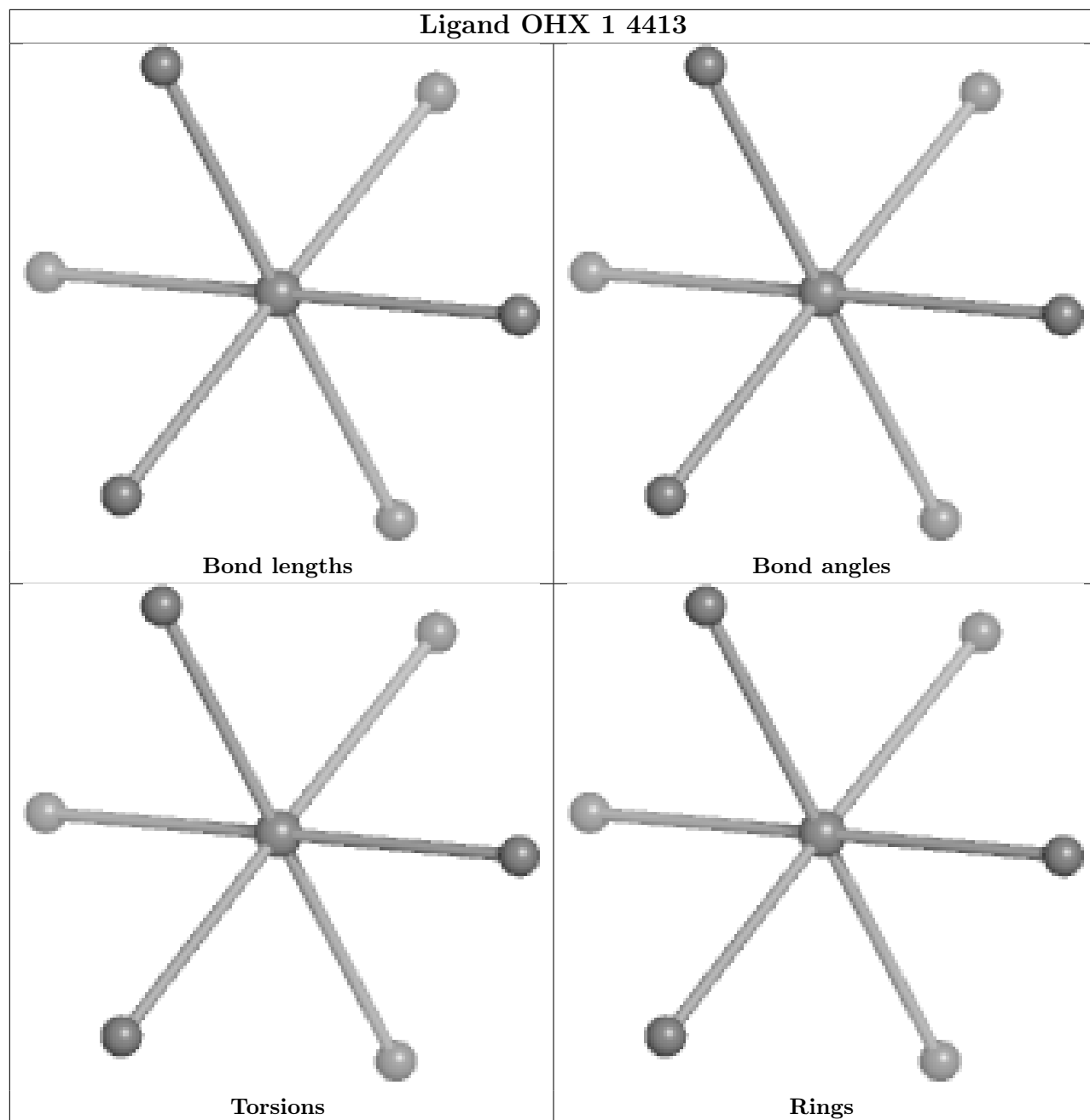


## Ligand OHX 5 4441

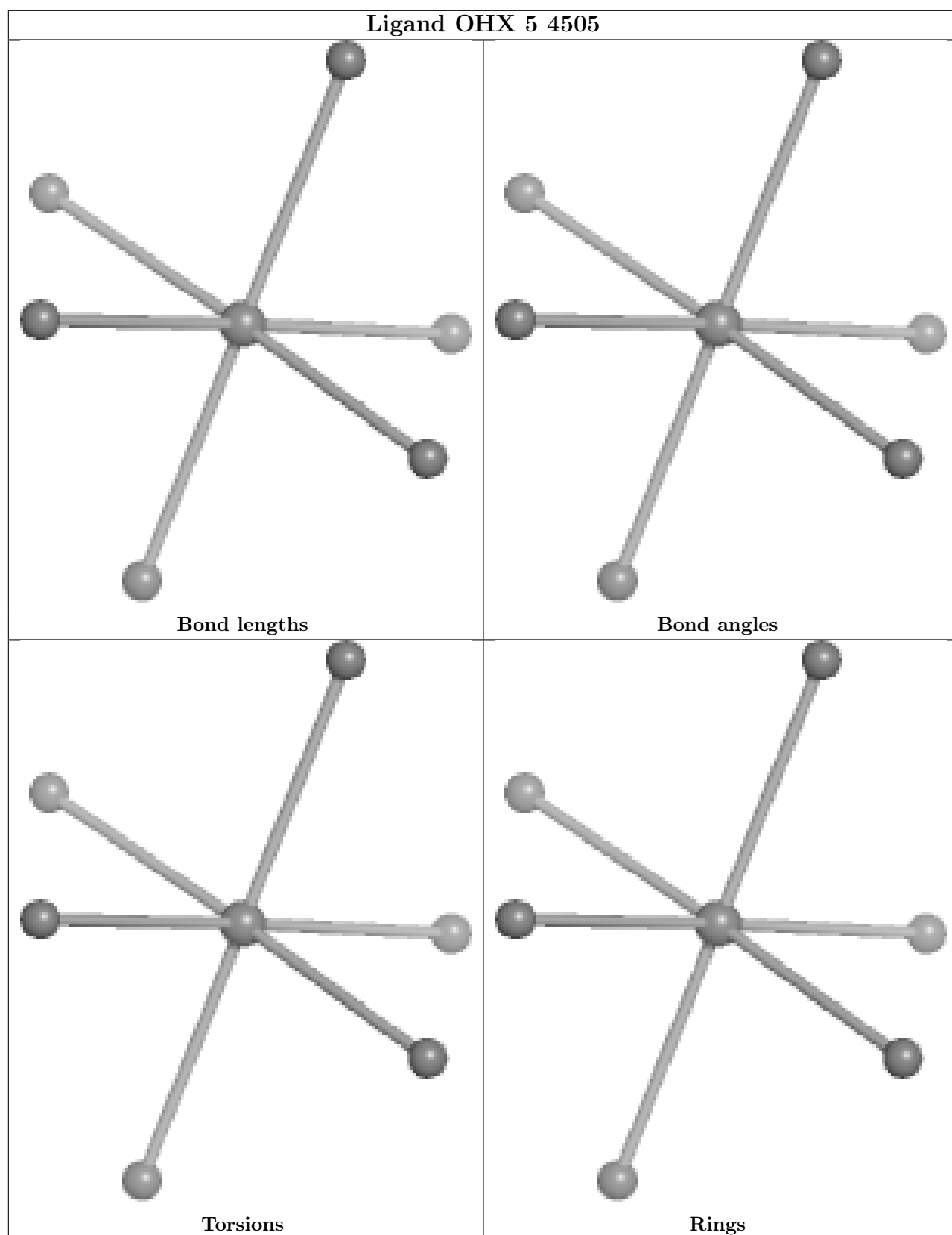












## 5.7 Other polymers [i](#)

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

The worst 5 of 9 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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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%)

The worst 5 of 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

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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.