



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 04:22 am GMT

PDB ID : 5TGA  
Title : Crystal structure of the *S.cerevisiae* 80S ribosome in complex with the A-site bound aminoacyl-tRNA analog ACCA-Pro  
Authors : Melnikov, S.; Mailliot, J.  
Deposited on : 2016-09-27  
Resolution : 3.30 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>.

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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

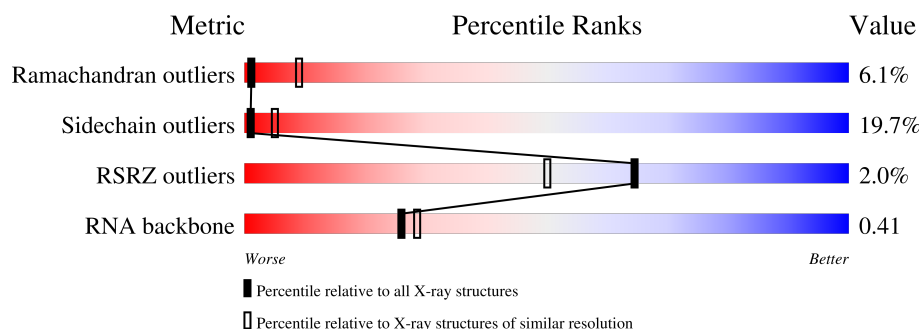
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



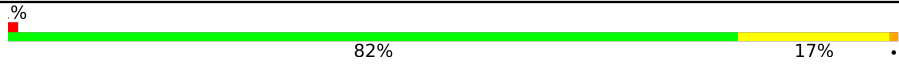

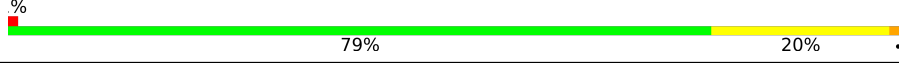

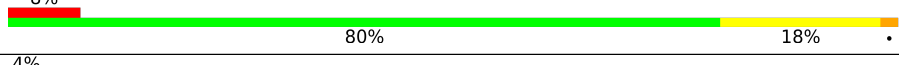
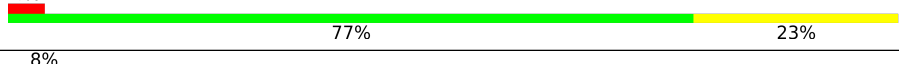
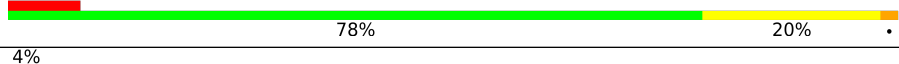

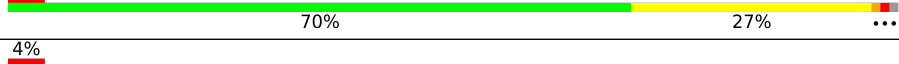


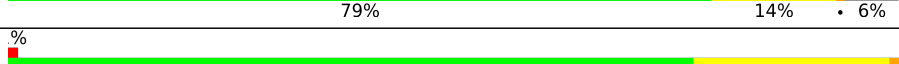
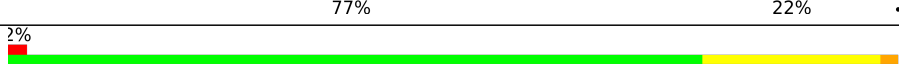
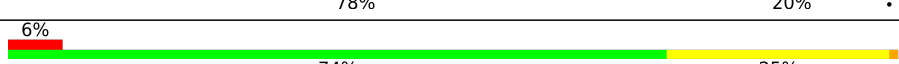

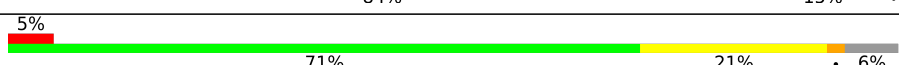
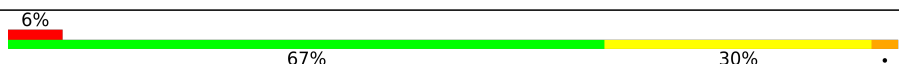
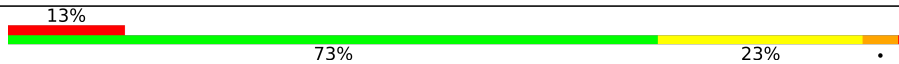
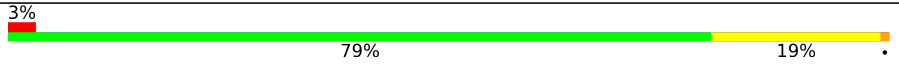


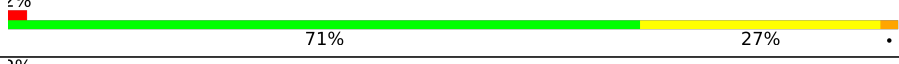
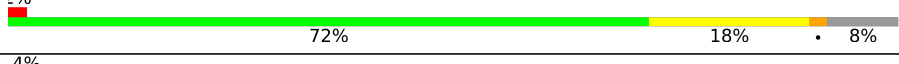


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1829	<div> <div>2%</div> <div>58% 33% 6% .</div> </div>
2	S0	206	<div> <div>4%</div> <div>77% 20% .</div> </div>
2	s0	206	<div> <div>2%</div> <div>73% 25% .</div> </div>
3	S1	216	<div> <div>6%</div> <div>73% 24% ..</div> </div>
3	s1	216	<div> <div>2%</div> <div>76% 20% .</div> </div>
4	S2	217	<div> <div>3%</div> <div>76% 22% .</div> </div>
4	s2	217	<div> <div>3%</div> <div>73% 25% .</div> </div>

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Mol	Chain	Length	Quality of chain
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	
14	c2	124	
15	C3	150	
15	c3	150	
16	C4	128	
16	c4	128	
17	C5	135	
17	c5	135	

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Mol	Chain	Length	Quality of chain
18	C6	142	<div> <div>4%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
18	c6	142	<div> <div>7%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
19	C7	125	<div> <div>2%</div> <div>74%</div> <div>18%</div> <div>.</div> </div>
19	c7	125	<div> <div>2%</div> <div>70%</div> <div>22%</div> <div>• 6%</div> </div>
20	C8	145	<div> <div>%</div> <div>75%</div> <div>20%</div> <div>5%</div> </div>
20	c8	145	<div> <div>5%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
21	C9	143	<div> <div>3%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
21	c9	143	<div> <div>3%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
22	D0	110	<div> <div>9%</div> <div>71%</div> <div>26%</div> <div>.</div> </div>
22	d0	110	<div> <div>4%</div> <div>65%</div> <div>33%</div> <div>.</div> </div>
23	D1	87	<div> <div>2%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
23	d1	87	<div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div>
24	D2	129	<div> <div>2%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
24	d2	129	<div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div>
25	D3	144	<div> <div>6%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
25	d3	144	<div> <div>3%</div> <div>85%</div> <div>15%</div> <div></div> </div>
26	D4	134	<div> <div>%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
26	d4	134	<div> <div>%</div> <div>79%</div> <div>16%</div> <div>.</div> </div>
27	D5	70	<div> <div>%</div> <div>64%</div> <div>33%</div> <div>.</div> </div>
27	d5	70	<div> <div>%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
28	D6	97	<div> <div>16%</div> <div>72%</div> <div>20%</div> <div>5%</div> <div>.</div> </div>
28	d6	97	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
29	D7	81	<div> <div>%</div> <div>84%</div> <div>16%</div> <div></div> </div>
29	d7	81	<div> <div>2%</div> <div>81%</div> <div>19%</div> <div></div> </div>
30	D8	63	<div> <div>14%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>


























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

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Mol	Chain	Length	Quality of chain
43	l6	175	
44	L7	223	
44	l7	223	
45	L8	233	
45	l8	233	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	169	
48	m1	169	
49	M3	194	
49	m3	194	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	197	
52	m6	197	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	


























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Mol	Chain	Length	Quality of chain
56	N0	172	<div> <div>2%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
56	n0	172	<div> <div>81%</div> <div>19%</div> </div>
57	N1	159	<div> <div>3%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
57	n1	159	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
58	N2	100	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
58	n2	100	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
59	N3	136	<div> <div>88%</div> <div>12%</div> </div>
59	n3	136	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
60	N4	135	<div> <div>8%</div> <div>63%</div> <div>10%</div> <div>27%</div> </div>
60	n4	135	<div> <div>5%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
61	N5	121	<div> <div>2%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
61	n5	121	<div> <div>77%</div> <div>21%</div> <div>..</div> </div>
62	N6	126	<div> <div>%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
62	n6	126	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
63	N7	135	<div> <div>%</div> <div>79%</div> <div>21%</div> <div>.</div> </div>
63	n7	135	<div> <div>77%</div> <div>21%</div> <div>.</div> </div>
64	N8	148	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
64	n8	148	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
65	N9	58	<div> <div>2%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
65	n9	58	<div> <div>3%</div> <div>67%</div> <div>26%</div> <div>7%</div> </div>
66	O0	100	<div> <div>3%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
66	o0	100	<div> <div>%</div> <div>84%</div> <div>16%</div> </div>
67	O1	109	<div> <div>2%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
67	o1	109	<div> <div>74%</div> <div>26%</div> </div>
68	O2	127	<div> <div>%</div> <div>77%</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
68	o2	127	 80% 19% .
69	O3	106	 83% 16% .
69	o3	106	 85% 13% .
70	O4	112	 4% 81% 19%
70	o4	112	 5% 86% 13% .
71	O5	119	 2% 74% 24% .
71	o5	119	 % 82% 14% .
72	O6	99	 2% 70% 28% .
72	o6	99	 % 71% 28% .
73	O7	87	 % 79% 21%
73	o7	87	 % 78% 21% .
74	O8	77	 % 75% 25%
74	o8	77	 71% 27% .
75	O9	50	 82% 14% .
75	o9	50	 88% 12%
76	Q0	52	 77% 19% .
76	q0	52	 71% 25% .
77	Q1	25	 72% 28%
77	q1	25	 64% 36%
78	Q2	105	 73% 23% . .
78	q2	105	 74% 22% .
79	Q3	91	 3% 85% 14% .
79	q3	91	 % 76% 24%
80	6	1800	 % 54% 37% 9%
81	c0	96	 7% 78% 21% .

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Mol	Chain	Length	Quality of chain
82	sM	104	
83	m2	150	
84	p0	219	
85	p1	47	
85	p2	47	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	3669	-	-	-	X
86	OHX	1	3674	-	-	-	X
86	OHX	1	3675	-	-	-	X
86	OHX	1	3683	-	-	-	X
86	OHX	1	3728	-	-	-	X
86	OHX	1	3733	-	-	-	X
86	OHX	1	3737	-	-	-	X
86	OHX	1	3739	-	-	-	X
86	OHX	1	3742	-	-	-	X
86	OHX	1	3756	-	-	-	X
86	OHX	1	3769	-	-	-	X
86	OHX	1	3772	-	-	-	X
86	OHX	1	3783	-	-	-	X
86	OHX	1	3785	-	-	-	X
86	OHX	1	3803	-	-	-	X
86	OHX	1	3806	-	-	-	X
86	OHX	1	3808	-	-	-	X
86	OHX	4	214	-	-	-	X
86	OHX	5	3636	-	-	-	X
86	OHX	5	3642	-	-	-	X
86	OHX	5	3658	-	-	-	X
86	OHX	5	3674	-	-	-	X
86	OHX	5	3688	-	-	-	X
86	OHX	5	3695	-	-	-	X
86	OHX	5	3712	-	-	-	X
86	OHX	5	3720	-	-	-	X
86	OHX	5	3730	-	-	-	X
86	OHX	5	3739	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	3741	-	-	-	X
86	OHX	5	3745	-	-	-	X
86	OHX	5	3748	-	-	-	X
86	OHX	5	3755	-	-	-	X
86	OHX	5	3756	-	-	-	X
86	OHX	5	3762	-	-	-	X
86	OHX	5	3763	-	-	-	X
86	OHX	5	3767	-	-	-	X
86	OHX	5	3768	-	-	-	X
86	OHX	5	3782	-	-	-	X
86	OHX	5	3785	-	-	-	X
86	OHX	5	3792	-	-	-	X
86	OHX	5	3797	-	-	-	X
86	OHX	5	3806	-	-	-	X
86	OHX	5	3811	-	-	-	X
86	OHX	5	3812	-	-	-	X
86	OHX	5	3818	-	-	-	X
86	OHX	6	2028	-	-	-	X
86	OHX	6	2042	-	-	-	X
86	OHX	6	2054	-	-	-	X
86	OHX	6	2060	-	-	-	X
86	OHX	6	2064	-	-	-	X
86	OHX	6	2068	-	-	-	X
86	OHX	6	2075	-	-	-	X
86	OHX	6	2087	-	-	-	X
86	OHX	6	2089	-	-	-	X
86	OHX	6	2095	-	-	-	X
86	OHX	6	2097	-	-	-	X
86	OHX	7	212	-	-	-	X
86	OHX	8	215	-	-	-	X
86	OHX	M0	303	-	-	-	X
86	OHX	m0	302	-	-	-	X
86	OHX	n3	202	-	-	-	X
86	OHX	o9	101	-	-	-	X
87	MG	1	3856	-	-	-	X
87	MG	1	3925	-	-	-	X
87	MG	1	4103	-	-	-	X
87	MG	2	2093	-	-	-	X
87	MG	2	2128	-	-	-	X
87	MG	2	2140	-	-	-	X
87	MG	2	2156	-	-	-	X
87	MG	2	2162	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	2	2173	-	-	-	X
87	MG	2	2225	-	-	-	X
87	MG	3	229	-	-	-	X
87	MG	5	4071	-	-	-	X
87	MG	5	4186	-	-	-	X
87	MG	6	2124	-	-	-	X
87	MG	6	2143	-	-	-	X
87	MG	6	2156	-	-	-	X
87	MG	6	2305	-	-	-	X
87	MG	E1	502	-	-	-	X
87	MG	M5	305	-	-	-	X

## 2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 414270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	1	0
			37970	16975	6720	12493	1782			

- 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			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	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			
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-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	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	S	0	0	0
			1105	708	203	194				
18	c6	142	Total	C	N	O	S	0	0	0
			1111	711	204	196				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Ribosome-bound 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 ribosomal RNA.

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 ribosomal RNA.

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 ribosomal RNA.

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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	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			
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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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 RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

- Molecule 81 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
81	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

- Molecule 82 is a protein called Suppressor protein STM1,Suppressor protein STM1,Ribosome-bound protein Stm1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
82	sM	104	Total	C	N	O	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 83 is a protein called 60S Ribosomal Protein L12.

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

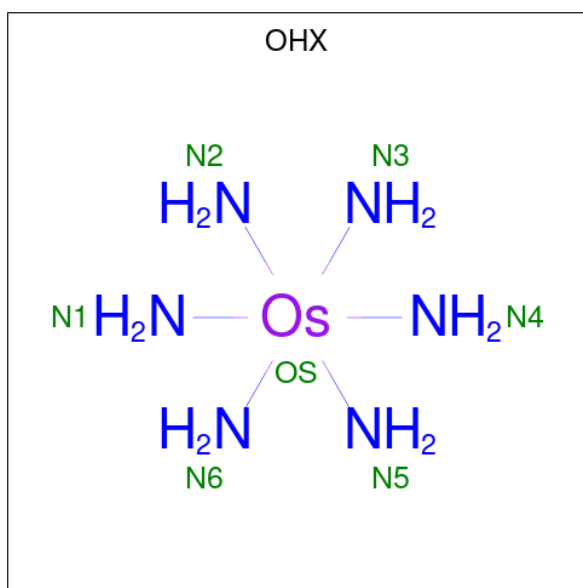
- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called 60S Ribosomal Protein P1/2.

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

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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86	S8	1	Total	N	Os	0	0
			7	6	1		
86	C3	1	Total	N	Os	0	0
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86	C5	1	Total	N	Os	0	0
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86	C8	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	3	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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			7	6	1		
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	L5	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	M0	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M8	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N8	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O1	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	Q2	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	s1	1	Total 7	N 6	Os 1	0	0
86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	c1	1	Total 7	N 6	Os 1	0	0
86	c3	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0
86	c8	1	Total 7	N 6	Os 1	0	0
86	d9	1	Total 7	N 6	Os 1	0	0
86	sR	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	2	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	0	0
86	5	1	Total 7	N 6	Os 1	1	0
86	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		
86	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	1	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	l2	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m9	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	o9	1	Total	N	Os	0	0
			7	6	1		
86	q1	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	2	170	Total	Mg	0	0
			170	170		
87	S1	1	Total	Mg	0	0
			1	1		
87	S2	1	Total	Mg	0	0
			1	1		
87	S4	2	Total	Mg	0	0
			2	2		
87	S6	1	Total	Mg	0	0
			1	1		
87	S8	1	Total	Mg	0	0
			1	1		
87	C1	2	Total	Mg	0	0
			2	2		
87	C5	1	Total	Mg	0	0
			1	1		
87	C8	1	Total	Mg	0	0
			1	1		
87	D0	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	D4	1	Total 1	Mg 1	0	0
87	D6	1	Total 1	Mg 1	0	0
87	D9	3	Total 3	Mg 3	0	0
87	E1	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	1	698	Total 698	Mg 698	0	0
87	3	18	Total 18	Mg 18	0	0
87	4	28	Total 28	Mg 28	0	0
87	L2	3	Total 3	Mg 3	0	0
87	L3	5	Total 5	Mg 5	0	0
87	L4	7	Total 7	Mg 7	0	0
87	L7	3	Total 3	Mg 3	0	0
87	L8	1	Total 1	Mg 1	0	0
87	M0	5	Total 5	Mg 5	0	0
87	M1	2	Total 2	Mg 2	0	0
87	M3	3	Total 3	Mg 3	0	0
87	M4	1	Total 1	Mg 1	0	0
87	M5	4	Total 4	Mg 4	0	0
87	M6	4	Total 4	Mg 4	0	0
87	M7	10	Total 10	Mg 10	0	0
87	M8	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	M9	2	Total 2	Mg 2	0	0
87	N0	2	Total 2	Mg 2	0	0
87	N1	1	Total 1	Mg 1	0	0
87	N3	3	Total 3	Mg 3	0	0
87	N6	2	Total 2	Mg 2	0	0
87	N8	7	Total 7	Mg 7	0	0
87	N9	1	Total 1	Mg 1	0	0
87	O1	5	Total 5	Mg 5	0	0
87	O2	4	Total 4	Mg 4	0	0
87	O3	2	Total 2	Mg 2	0	0
87	O4	1	Total 1	Mg 1	0	0
87	O5	2	Total 2	Mg 2	0	0
87	O7	6	Total 6	Mg 6	0	0
87	Q0	2	Total 2	Mg 2	0	0
87	Q2	3	Total 3	Mg 3	0	0
87	6	235	Total 235	Mg 235	0	0
87	s1	1	Total 1	Mg 1	0	0
87	s4	1	Total 1	Mg 1	0	0
87	s6	2	Total 2	Mg 2	0	0
87	s8	4	Total 4	Mg 4	0	0
87	c6	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	c7	1	Total 1	Mg 1	0	0
87	c8	4	Total 4	Mg 4	0	0
87	c9	3	Total 3	Mg 3	0	0
87	d2	1	Total 1	Mg 1	0	0
87	d3	2	Total 2	Mg 2	0	0
87	d4	2	Total 2	Mg 2	0	0
87	d5	1	Total 1	Mg 1	0	0
87	d9	2	Total 2	Mg 2	0	0
87	sM	2	Total 2	Mg 2	0	0
87	5	759	Total 759	Mg 759	0	0
87	7	28	Total 28	Mg 28	0	0
87	8	19	Total 19	Mg 19	0	0
87	l2	6	Total 6	Mg 6	0	0
87	l3	13	Total 13	Mg 13	0	0
87	l4	1	Total 1	Mg 1	0	0
87	l5	6	Total 6	Mg 6	0	0
87	l7	7	Total 7	Mg 7	0	0
87	l8	1	Total 1	Mg 1	0	0
87	l9	3	Total 3	Mg 3	0	0
87	m0	1	Total 1	Mg 1	0	0
87	m3	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	m4	1	Total 1	Mg 1	0	0
87	m5	3	Total 3	Mg 3	0	0
87	m6	4	Total 4	Mg 4	0	0
87	m7	8	Total 8	Mg 8	0	0
87	m8	4	Total 4	Mg 4	0	0
87	m9	1	Total 1	Mg 1	0	0
87	n0	5	Total 5	Mg 5	0	0
87	n1	3	Total 3	Mg 3	0	0
87	n3	3	Total 3	Mg 3	0	0
87	n6	1	Total 1	Mg 1	0	0
87	n8	7	Total 7	Mg 7	0	0
87	n9	2	Total 2	Mg 2	0	0
87	o2	3	Total 3	Mg 3	0	0
87	o3	4	Total 4	Mg 4	0	0
87	o4	1	Total 1	Mg 1	0	0
87	o6	1	Total 1	Mg 1	0	0
87	o7	1	Total 1	Mg 1	0	0
87	q0	1	Total 1	Mg 1	0	0
87	q1	2	Total 2	Mg 2	0	0
87	q2	1	Total 1	Mg 1	0	0
87	q3	1	Total 1	Mg 1	0	0

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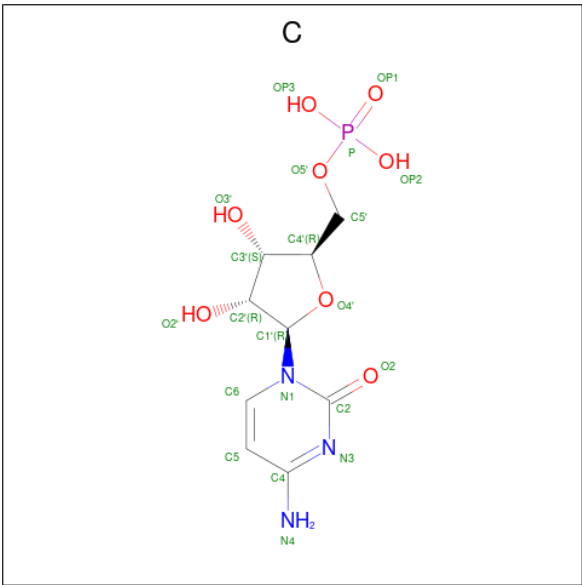
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	p0	1	Total	Mg	0	0
			1	1		

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

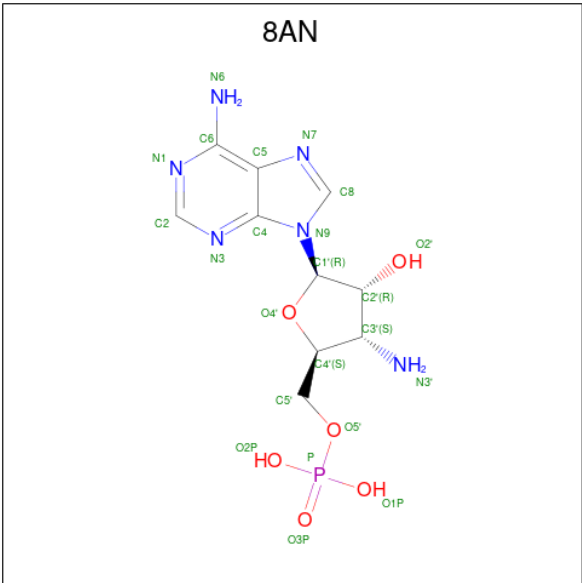
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	D6	1	Total	Zn	0	0
			1	1		
88	D7	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		
88	O7	1	Total	Zn	0	0
			1	1		
88	Q0	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	Q3	1	Total	Zn	0	0
			1	1		
88	d6	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		
88	d9	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	o7	1	Total	Zn	0	0
			1	1		
88	q0	1	Total	Zn	0	0
			1	1		
88	q2	1	Total	Zn	0	0
			1	1		
88	q3	1	Total	Zn	0	0
			1	1		

- Molecule 89 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>3</sub>O<sub>8</sub>P).



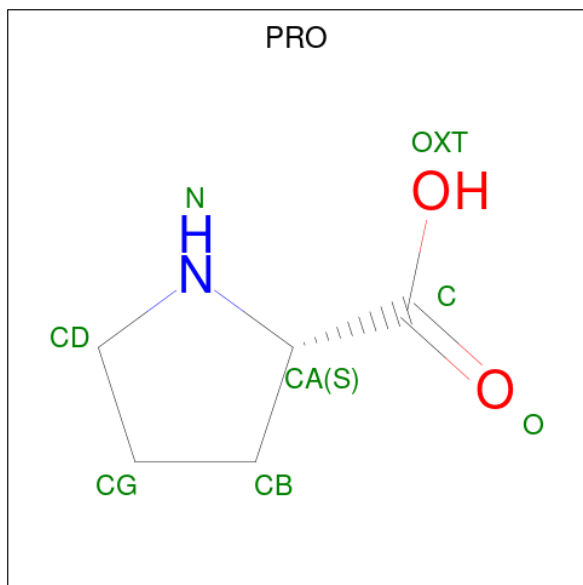
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
89	1	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
89	1	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
89	5	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
89	5	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

- Molecule 90 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>6</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
90	1	1	Total	C	N	O	P	0	0
			22	10	6	5	1		
90	5	1	Total	C	N	O	P	0	0
			22	10	6	5	1		

- Molecule 91 is PROLINE (three-letter code: PRO) (formula:  $C_5H_9NO_2$ ).

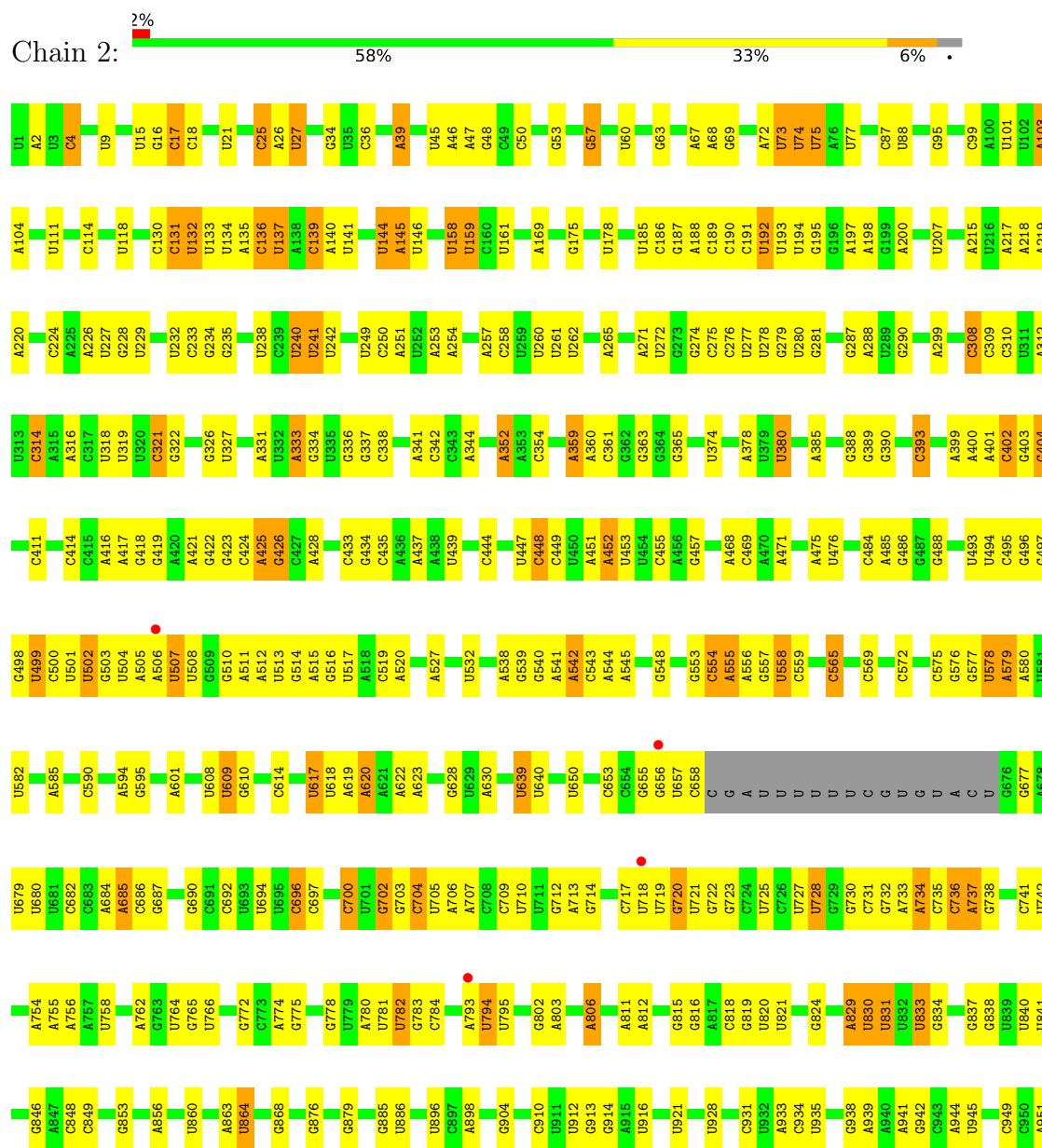


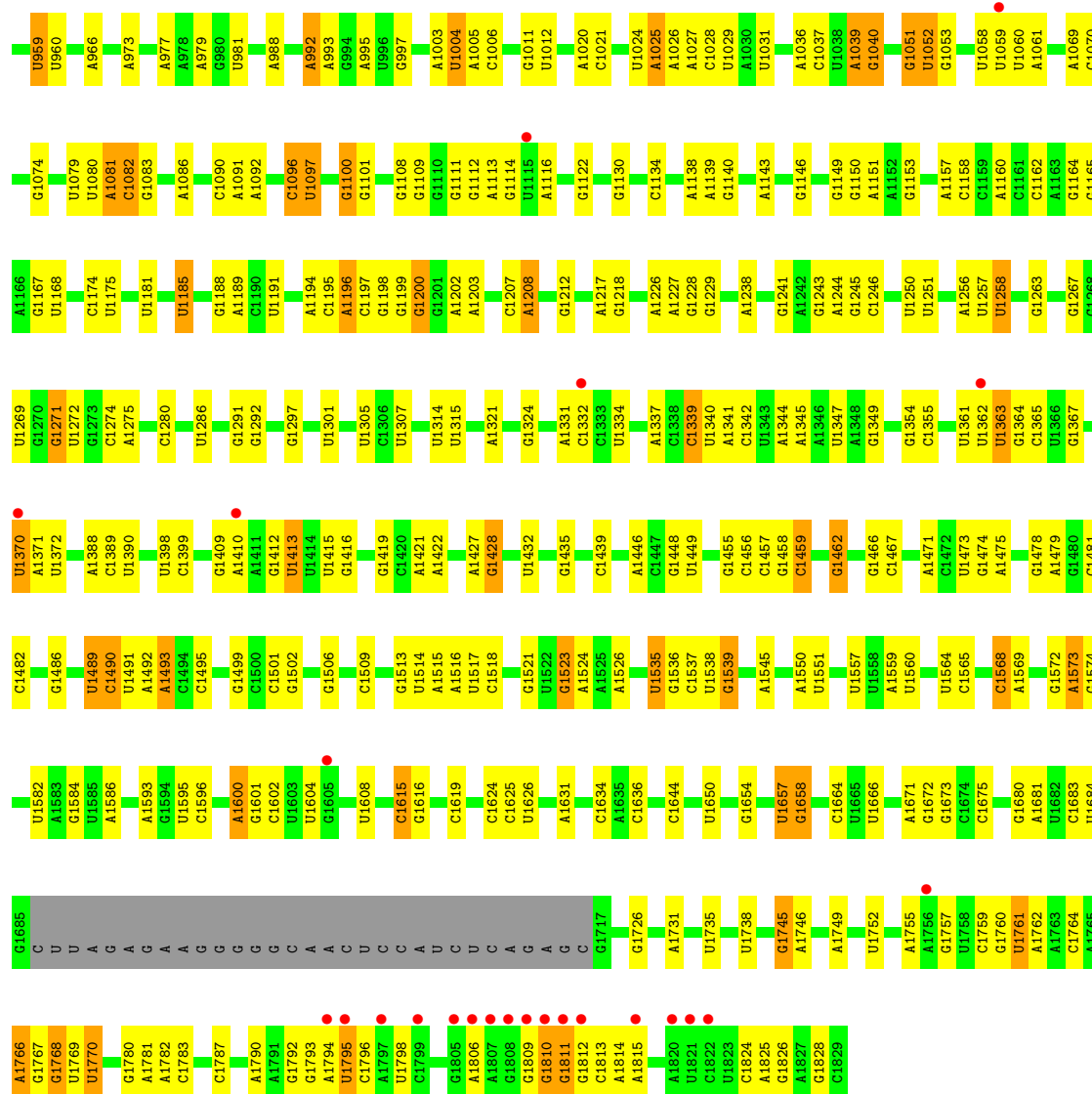
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
91	1	1	Total	C	N	O	0	0
			7	5	1	1		
91	5	1	Total	C	N	O	0	0
			7	5	1	1		

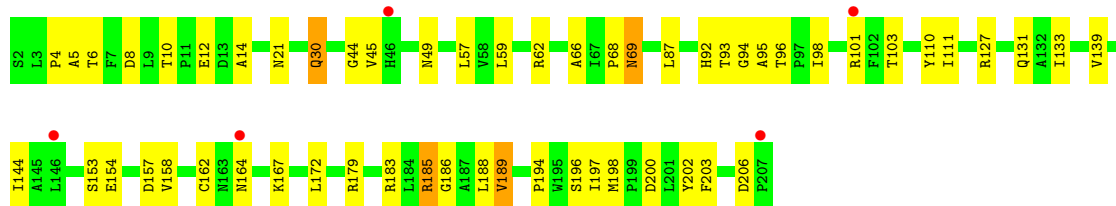
### 3 Residue-property plots

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

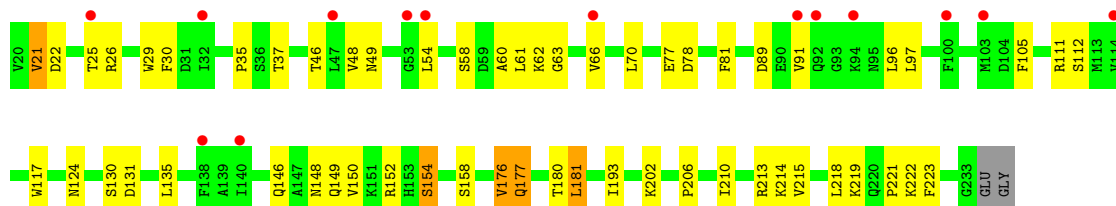
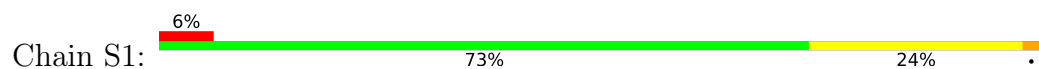
#### • Molecule 1: 18S ribosomal RNA



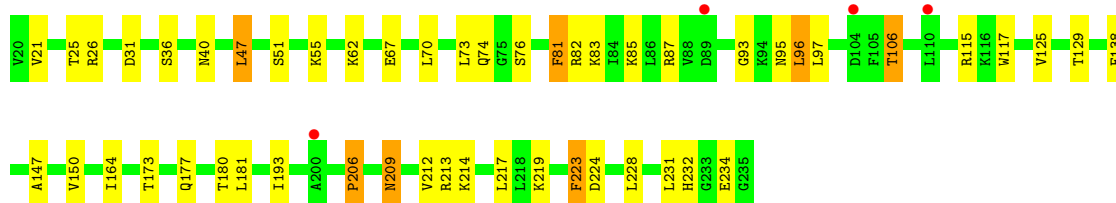
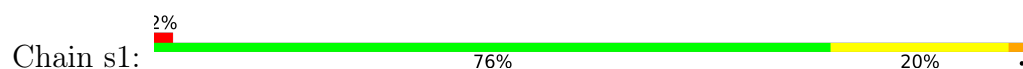




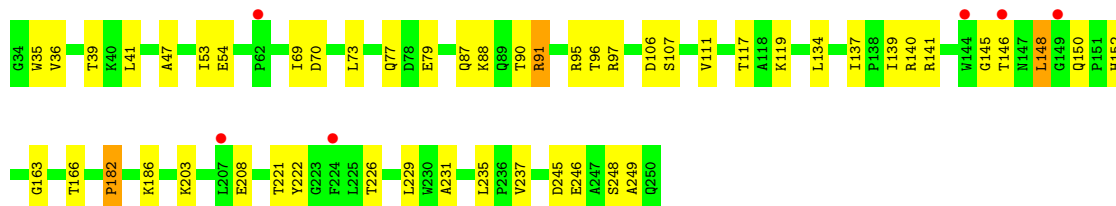
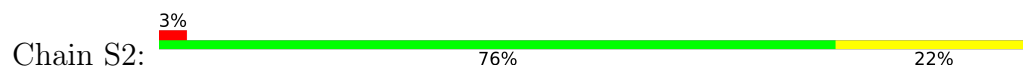
• Molecule 3: 40S ribosomal protein S1-A



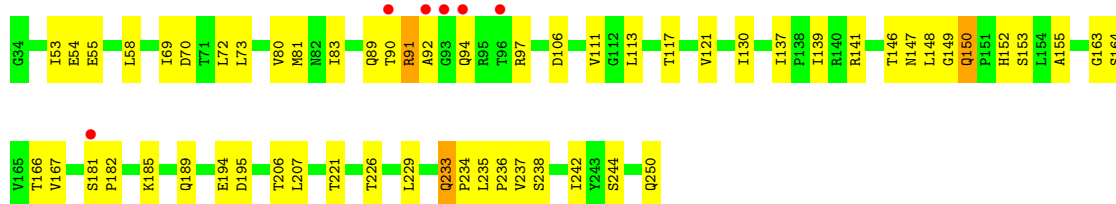
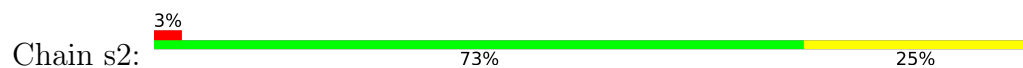
• Molecule 3: 40S ribosomal protein S1-A



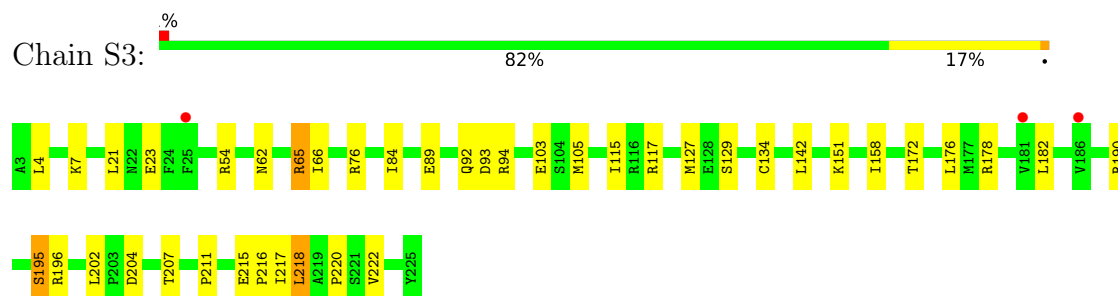
• Molecule 4: 40S ribosomal protein S2



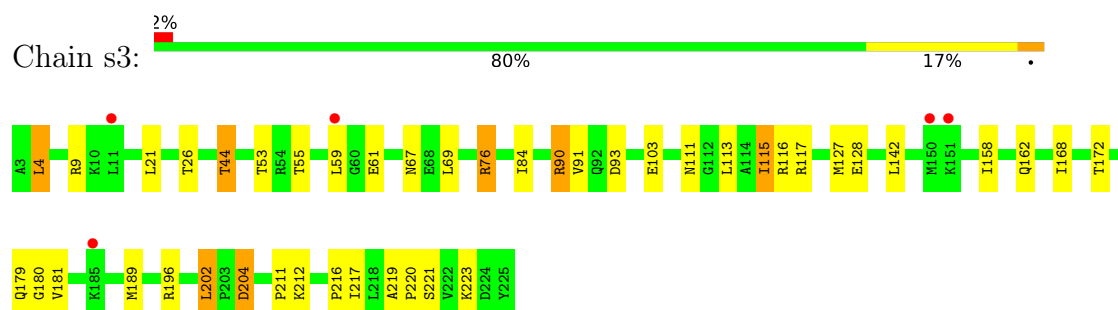
• Molecule 4: 40S ribosomal protein S2



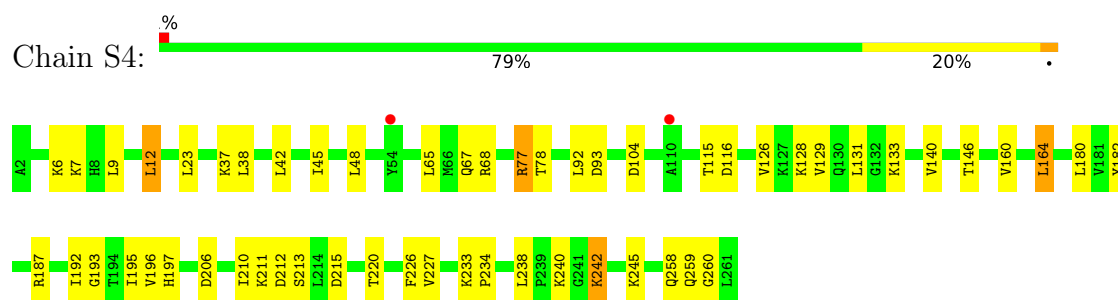
- Molecule 5: 40S ribosomal protein S3



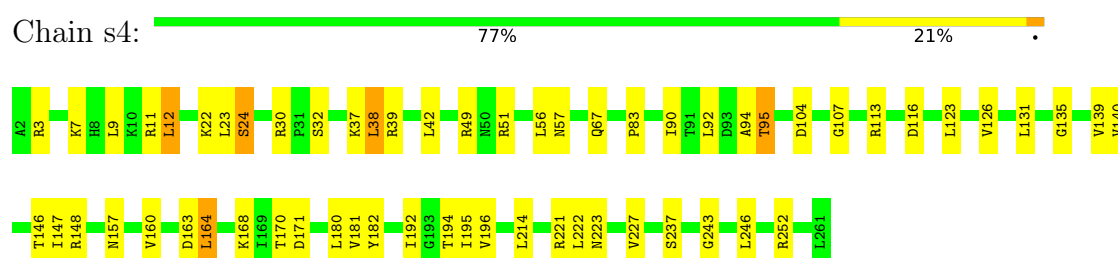
- Molecule 5: 40S ribosomal protein S3



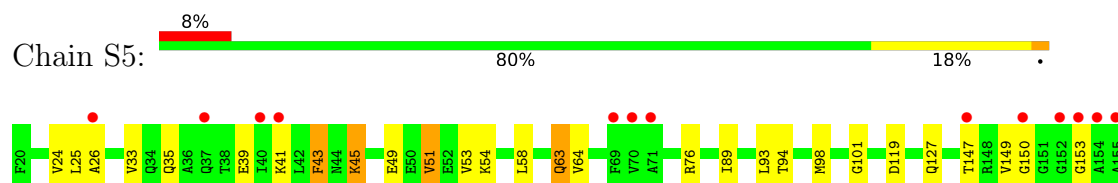
- Molecule 6: 40S ribosomal protein S4-A



- Molecule 6: 40S ribosomal protein S4-A

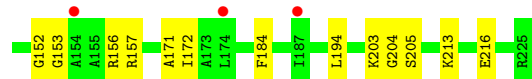
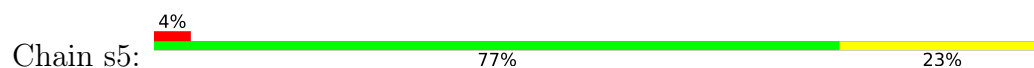


- Molecule 7: 40S ribosomal protein S5

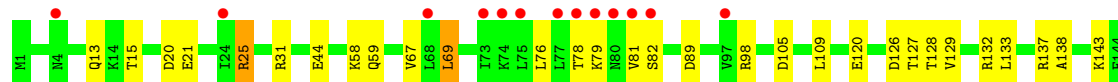
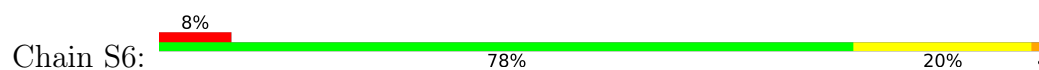




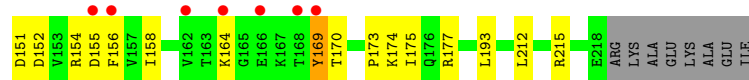
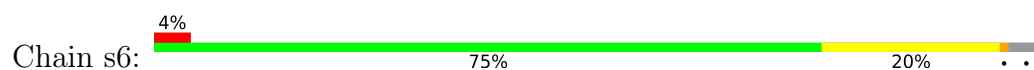
- Molecule 7: 40S ribosomal protein S5



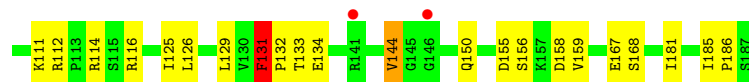
- Molecule 8: 40S ribosomal protein S6-A



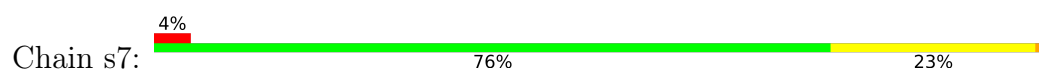
- Molecule 8: 40S ribosomal protein S6-A



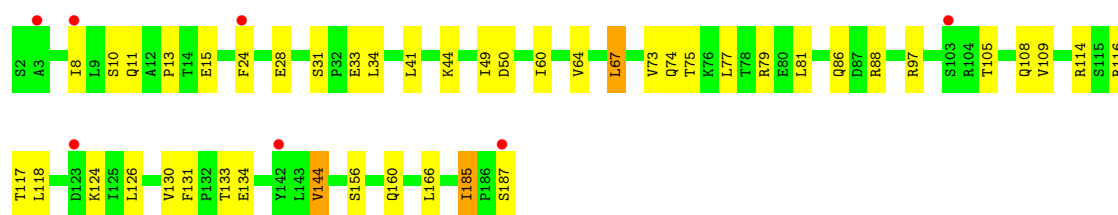
- Molecule 9: 40S ribosomal protein S7-A



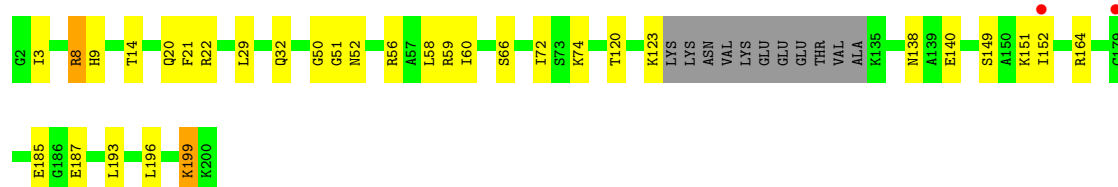
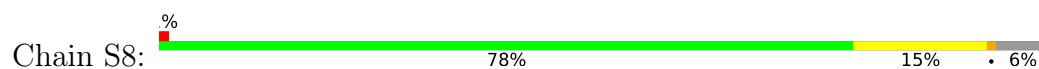
- Molecule 9: 40S ribosomal protein S7-A



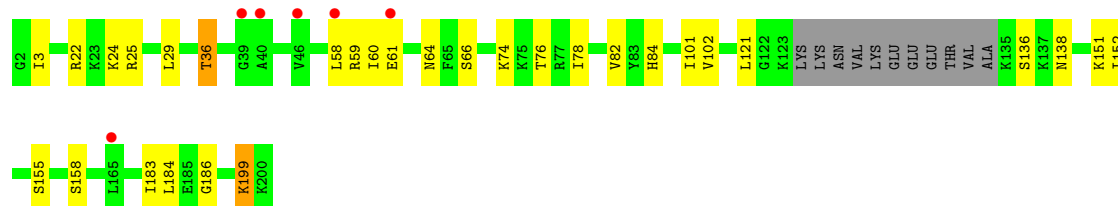
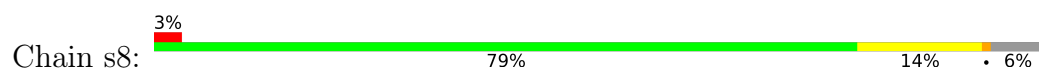




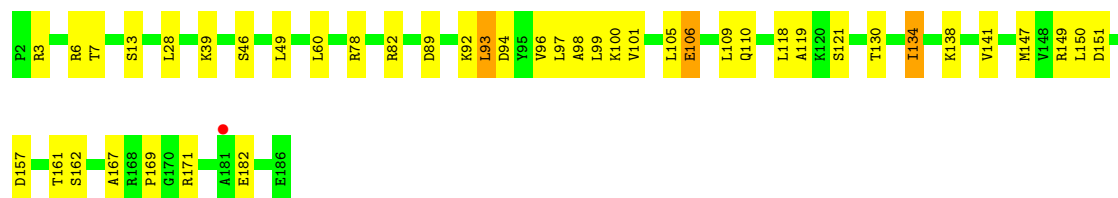
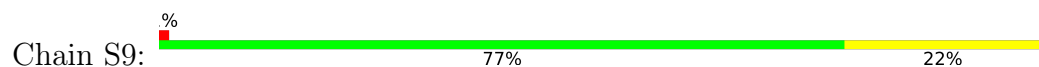
• Molecule 10: 40S ribosomal protein S8-A



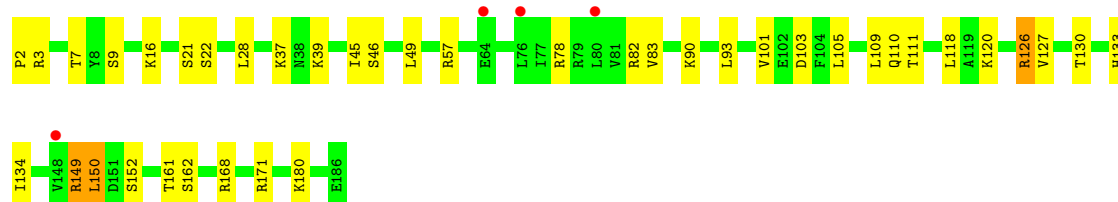
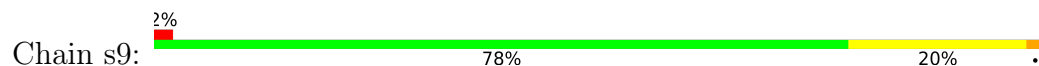
• Molecule 10: 40S ribosomal protein S8-A



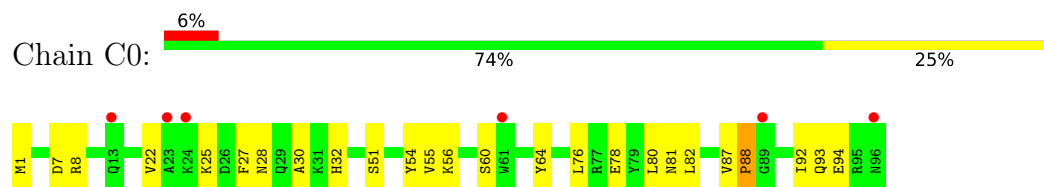
• Molecule 11: 40S ribosomal protein S9-A



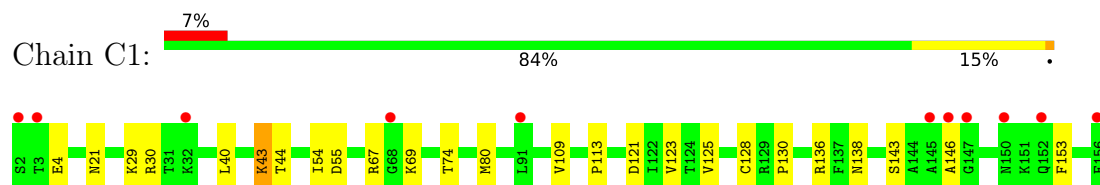
• Molecule 11: 40S ribosomal protein S9-A



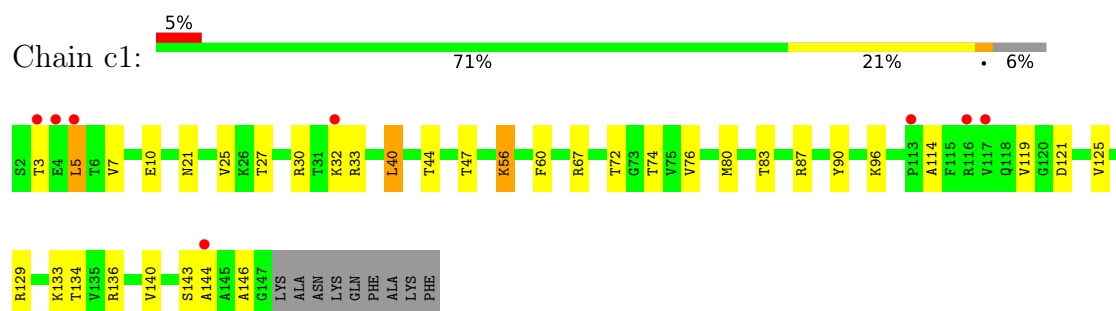
- Molecule 12: 40S ribosomal protein S10-A



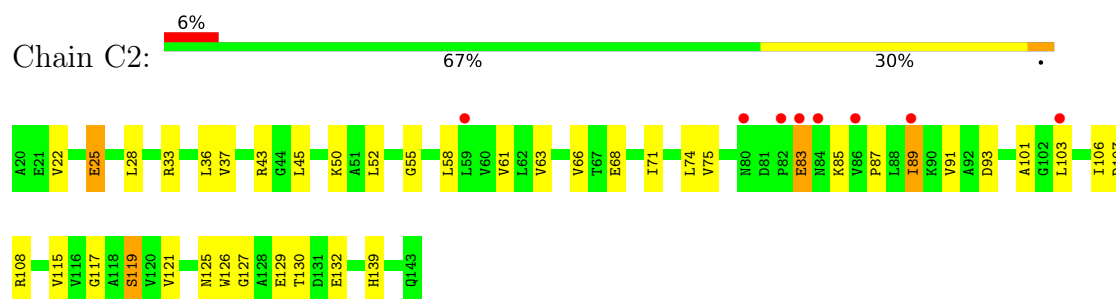
- Molecule 13: 40S ribosomal protein S11-A



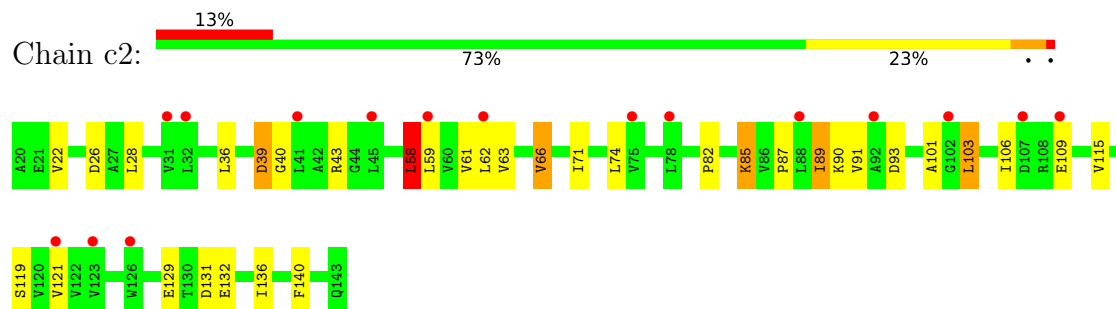
- Molecule 13: 40S ribosomal protein S11-A



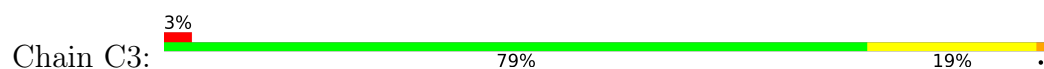
- Molecule 14: 40S ribosomal protein S12



- Molecule 14: 40S ribosomal protein S12

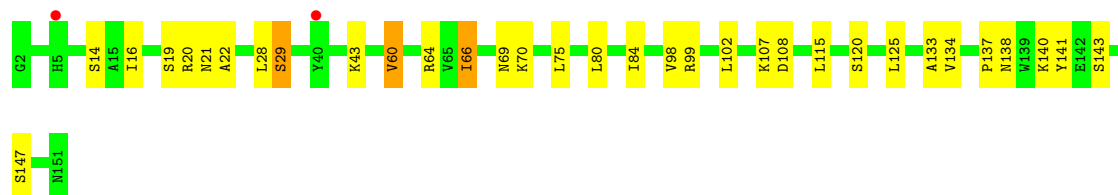
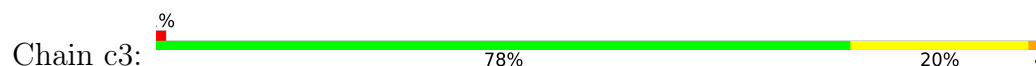


- Molecule 15: 40S ribosomal protein S13

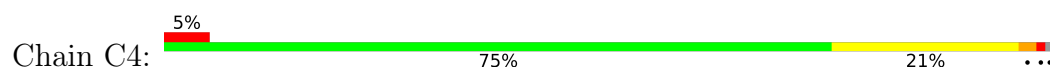




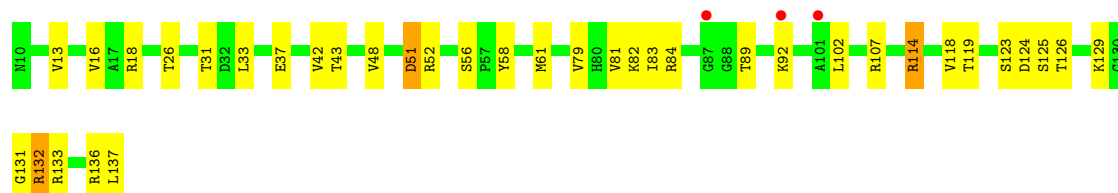
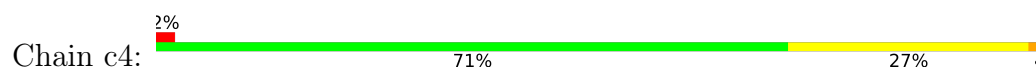
- Molecule 15: 40S ribosomal protein S13



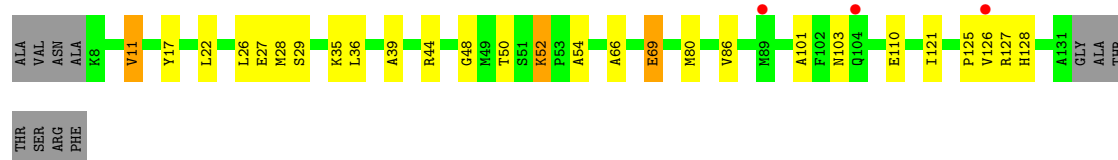
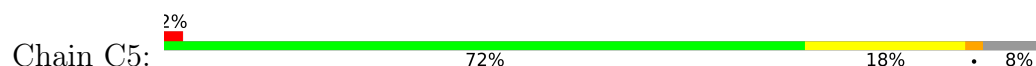
- Molecule 16: 40S ribosomal protein S14-B



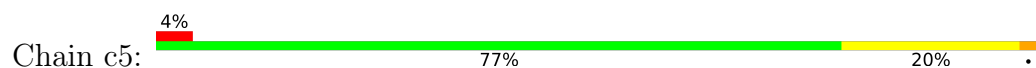
- Molecule 16: 40S ribosomal protein S14-B



- Molecule 17: 40S ribosomal protein S15

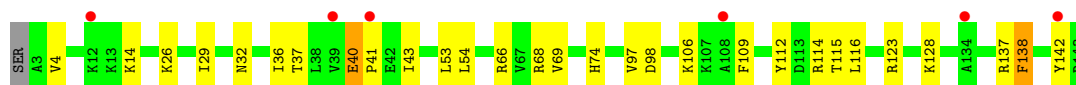
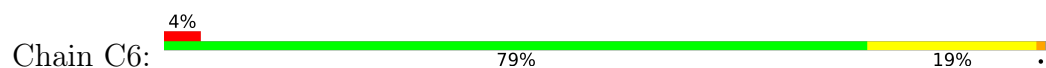


- Molecule 17: 40S ribosomal protein S15

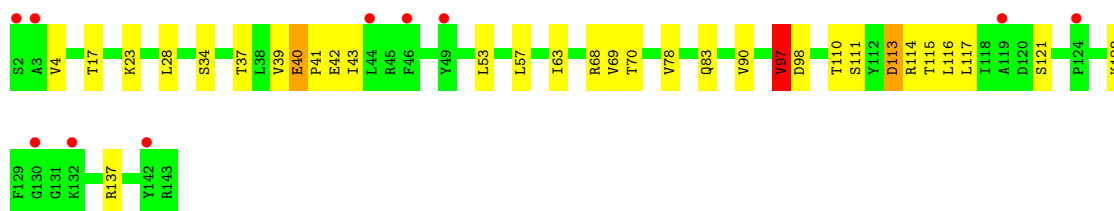
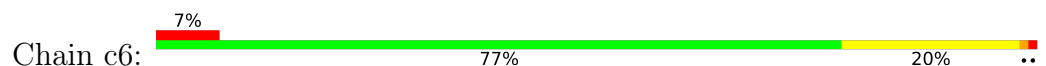




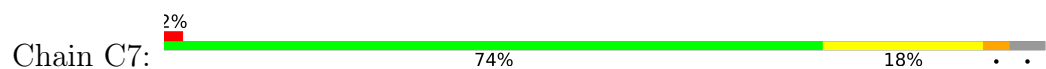
- Molecule 18: 40S ribosomal protein S16-A



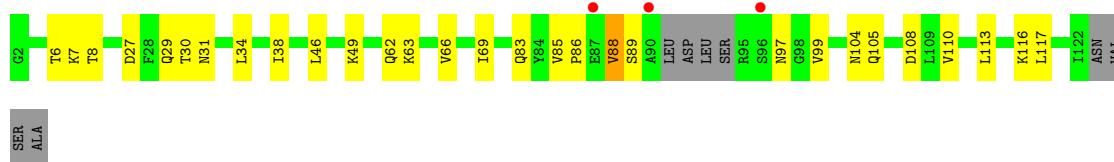
- Molecule 18: 40S ribosomal protein S16-A



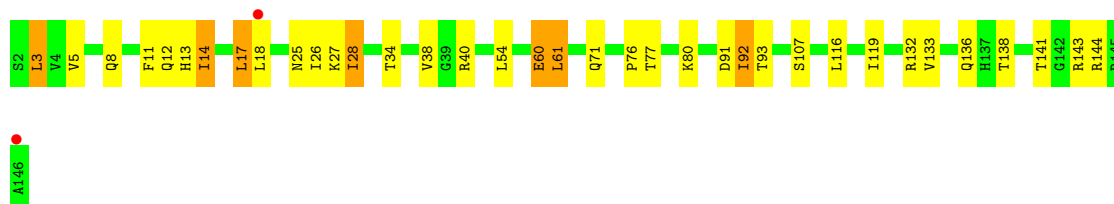
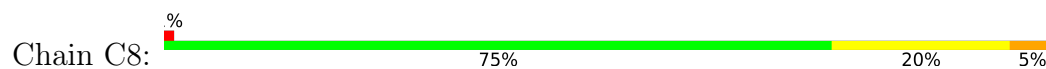
- Molecule 19: 40S ribosomal protein S17-B



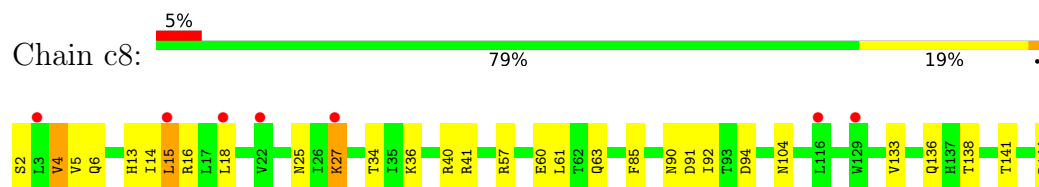
- Molecule 19: 40S ribosomal protein S17-B



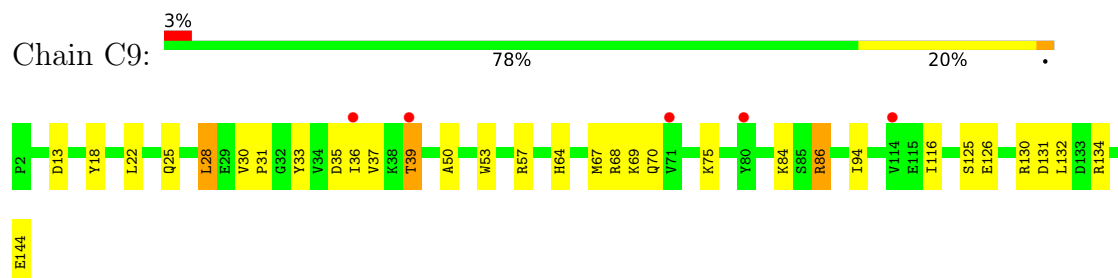
- Molecule 20: 40S ribosomal protein S18-A



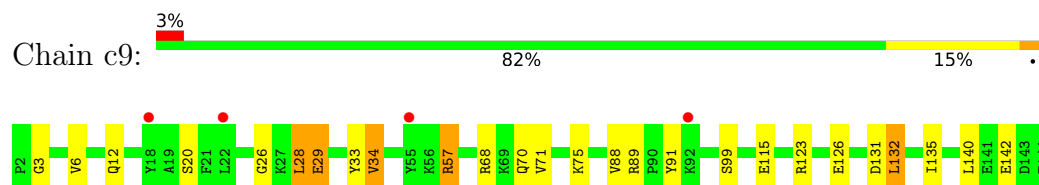
## • Molecule 20: 40S ribosomal protein S18-A



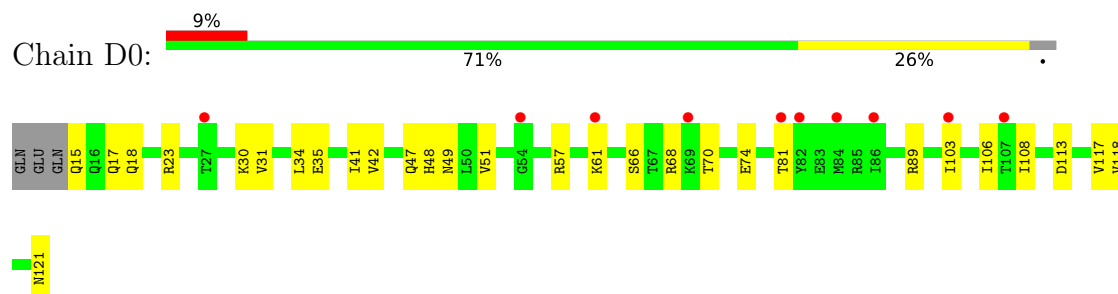
## • Molecule 21: 40S ribosomal protein S19-A



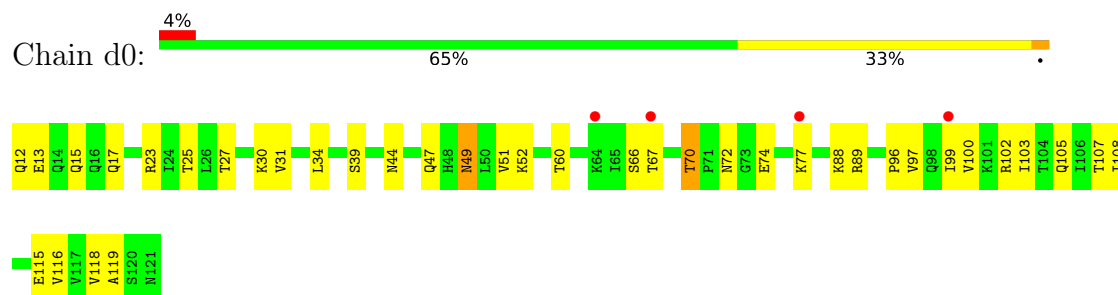
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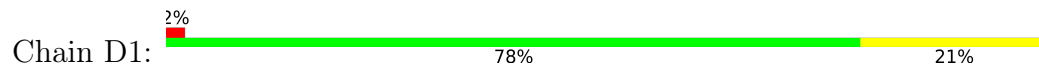
## • Molecule 22: 40S ribosomal protein S20



## • Molecule 22: 40S ribosomal protein S20

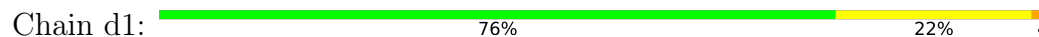


## • Molecule 23: 40S ribosomal protein S21-A

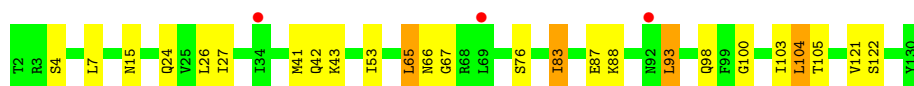
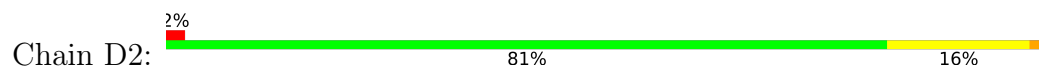




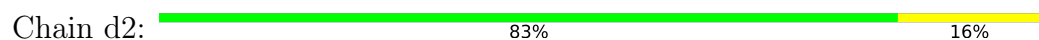
- Molecule 23: 40S ribosomal protein S21-A



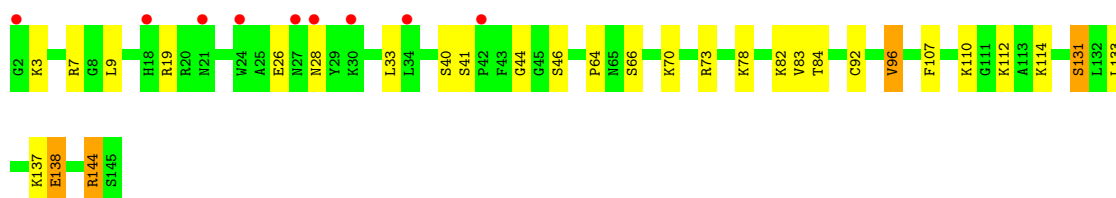
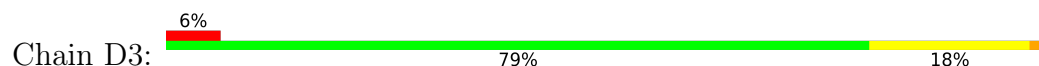
- Molecule 24: 40S ribosomal protein S22-A



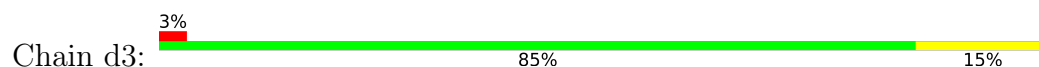
- Molecule 24: 40S ribosomal protein S22-A



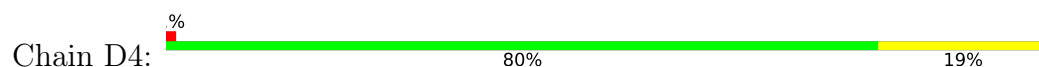
- Molecule 25: 40S ribosomal protein S23-A



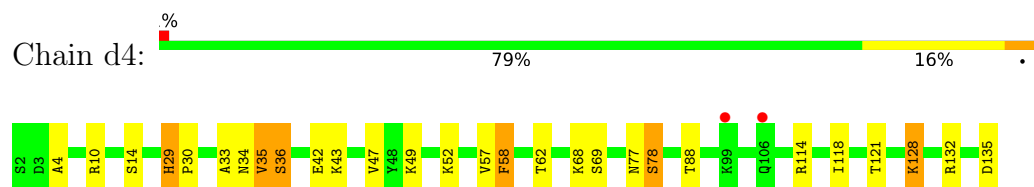
- Molecule 25: 40S ribosomal protein S23-A



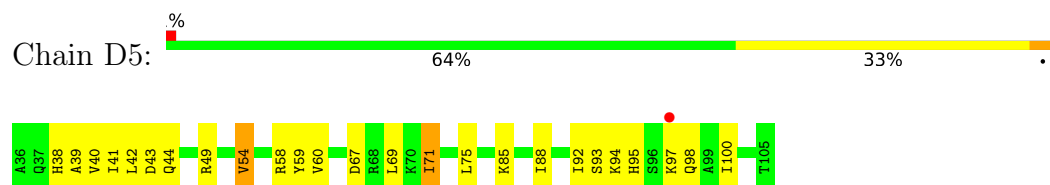
- Molecule 26: 40S ribosomal protein S24-A



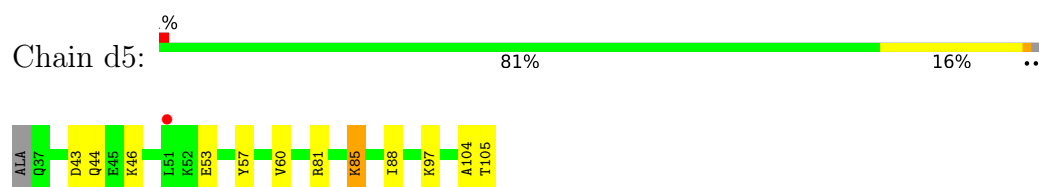
- Molecule 26: 40S ribosomal protein S24-A



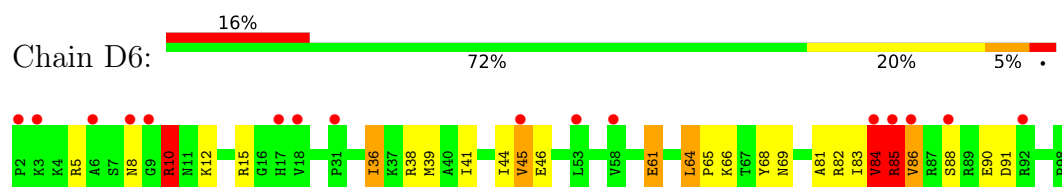
- Molecule 27: 40S ribosomal protein S25-A



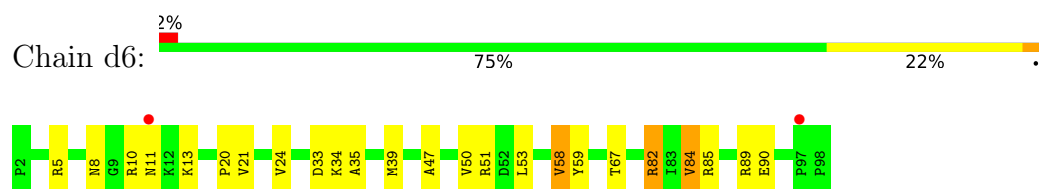
- Molecule 27: 40S ribosomal protein S25-A



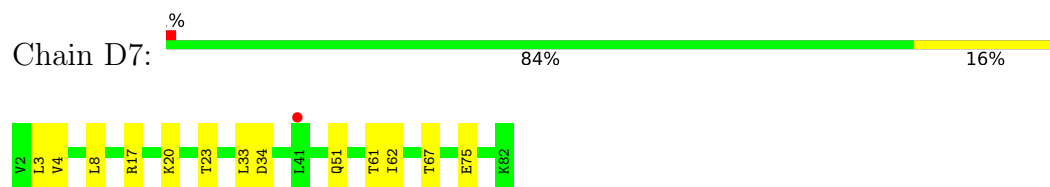
- Molecule 28: 40S ribosomal protein S26-B



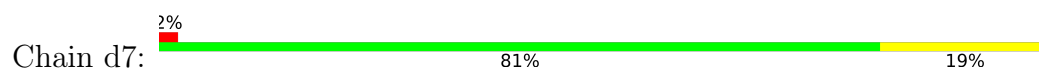
- Molecule 28: 40S ribosomal protein S26-B



- Molecule 29: 40S ribosomal protein S27-A

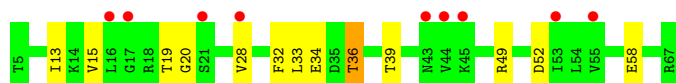
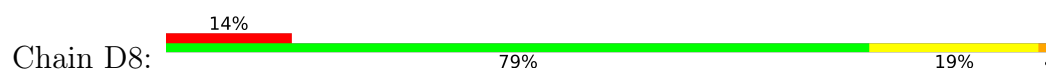


- Molecule 29: 40S ribosomal protein S27-A

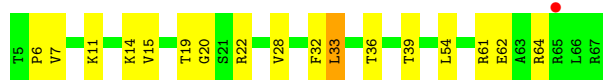
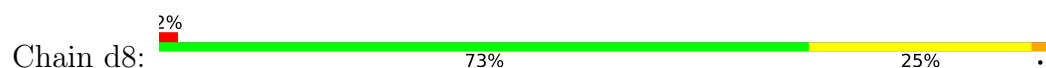




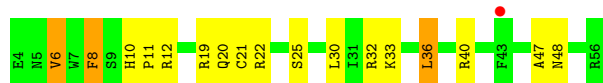
- Molecule 30: 40S ribosomal protein S28-A



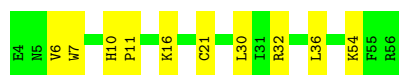
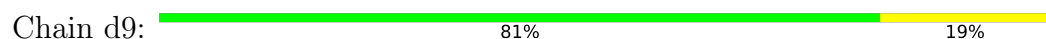
- Molecule 30: 40S ribosomal protein S28-A



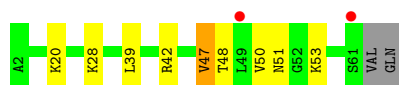
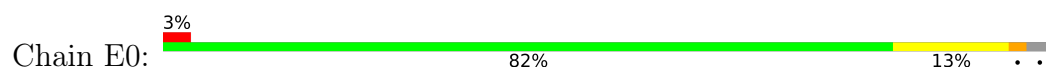
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A



- Molecule 32: 40S ribosomal protein S30-A



- Molecule 33: Ubiquitin-40S ribosomal protein S31

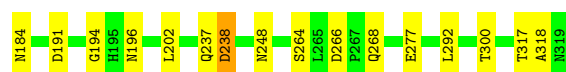
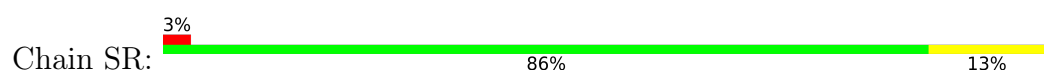




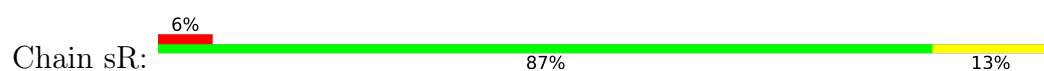
• Molecule 33: Ubiquitin-40S ribosomal protein S31



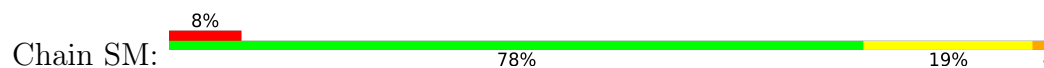
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



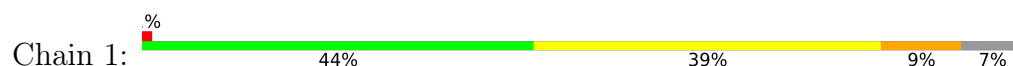
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Ribosome-bound protein Stm1

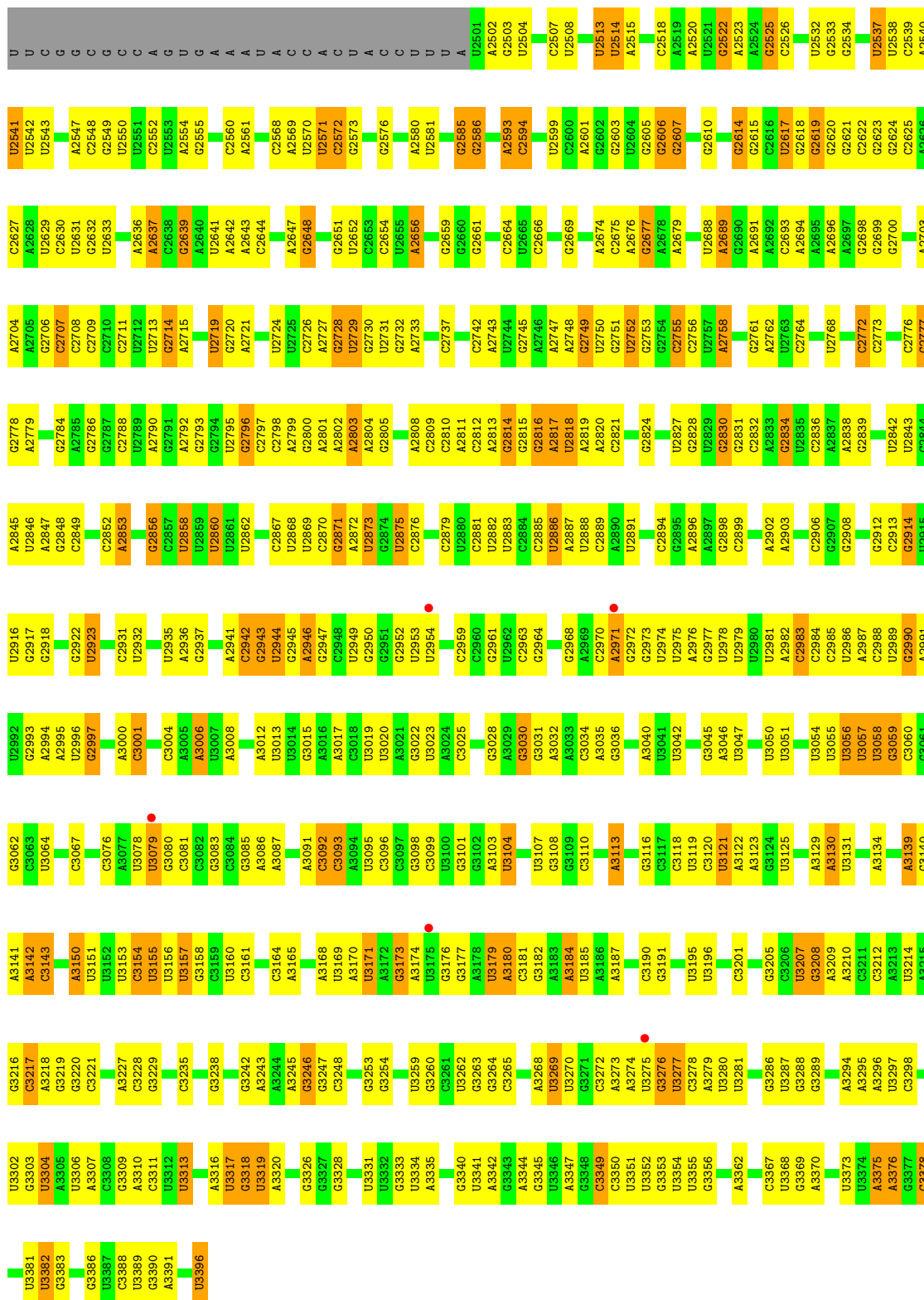


• Molecule 36: 25S ribosomal RNA

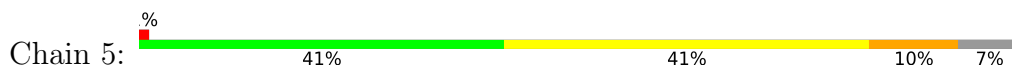


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G1174	A1103	A1025	G950	C881	A802	G718	C648	U569	U	U	A417	G345	G269	U184	G91	G18
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G1177	U1110	G953	G953	C805	G805	A720	C651	U575	C	C	G423	C348	G272	C187	G94	G21
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A1180	U1112	G1035	C958	A808	G727	G727	A656	A578	U	U	G424	C350	U278	U191	G96	G22
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A1182	U1114	C1037	U960	A810	G729	G729	C658	C580	C	C	G426	C352	G282	C193	G98	G24
G1186	G1115	U1041	C961	C893	G734	C734	C659	U576	A	A	C427	A355	G283	C194	A99	U25
C1187	G1116	U1041	C962	C894	G735	G735	C660	C577	C	C	U430	U359	G284	G196	U100	A26
A1190	G1117	C1045	G963	A895	G736	G736	C661	A585	U	U	U431	C360	A285	C197	A108	A35
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C1201	U1122	U1050	G971	U905	G741	G741	C666	C591	A498	A498	U436	C365	G290	G204	A108	A34
A1202	U1123	U1051	A972	A906	G742	G742	C667	A592	G499	G499	U437	C366	G291	A204	A109	A35
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U1211	U1131	U1060	U979	A913	G750	G750	C675	G601	U510	U510	U445	C374	G307	A221	U127	C54
C1216	U1132	A1061	U980	A914	G751	G751	C676	A611	U511	U511	U446	C375	U314	U223	U133	G55
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A1221	G1146	U1077	U982	A916	G753	G753	C678	U513	U521	U521	U448	C377	U316	C225	U135	A57
G1222	G1147	U1078	U983	A917	G754	G754	C679	U514	A521	A521	U449	C378	U317	C226	G136	G58
C1227	G1148	A1079	U984	A918	G755	G755	C680	U515	A522	A522	U450	C379	U318	G227	U147	A60
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G1233	G1150	U1081	U986	A920	G757	G757	C682	U517	A524	A524	U452	C381	U320	U229	G148	A62
C1234	G1151	U1082	U987	A921	G758	G758	C683	U518	A525	A525	U453	C382	U321	U230	U149	A63
U1235	G1152	U1083	U988	A922	G759	G759	C684	U519	A526	A526	U454	C383	U322	U231	A151	A65
G1236	A1153	G1083	U989	A923	G760	G760	C685	U520	A527	A527	U455	C384	U323	G231	U152	A66
G1237	G1154	U1084	U990	A924	G761	G761	C686	U521	A528	A528	U456	C385	U324	A152	U153	A67
U1241	G1155	C1085	U991	A925	G762	G762	C687	U522	A529	A529	U457	C386	U325	A153	U154	C68
G1242	G1156	U1085	U992	A926	G763	G763	C688	U523	A530	A530	U458	C387	U326	A154	G155	C69
A1244	G1157	C1086	U993	A927	G764	G764	C689	U524	A531	A531	U459	C388	U327	A155	G156	A70
	G1158	U1086	U994	A928	G765	G765	C690	U525	A532	A532	U460	C389	U328	A156	A157	A71
	A1159	A1087	U995	A929	G766	G766	C691	U526	A533	A533	U461	C390	U329	A157	C72	C72
	C1160	G1092	U996	A930	G767	G767	C692	U527	A534	A534	U462	C391	U330	A158	C73	C73
	G1161	A1093	U997	A931	G768	G768	C693	U528	A535	A535	U463	C392	U331	A159	C74	C74
	U1162	U1094	U998	A932	G769	G769	C694	U529	A536	A536	U464	C393	U332	A160	G161	G75
	A1163	U1095	U999	A933	G770	G770	C695	U530	A537	A537	U465	C394	U333	A161	C166	
	G1164	U1096	U999	A934	G771	G771	C696	U531	A538	A538	U466	C395	U334	A162		
				A935	G772	G772	C697	U532	A539	A539	U467	C396	U335	A163		
				A936	G773	G773	C698	U533	A540	A540	U468	C397	U336	A164		
				A937	G774	G774	C699	U534	A541	A541	U469	C398	U337	A165		
				A938	G775	G775	C700	U535	A542	A542	U470	C399	U338	A166		
				A939	G776	G776	C701	U536	A543	A543	U471	C400	U339	A167		
				A940	G777	G777	C702	U537	A544	A544	U472	C401	U340	A168		
				A941	G778	G778	C703	U538	A545	A545	U473	C402	U341	A169		
				A942	G779	G779	C704	U539	A546	A546	U474	C403	U342	A170		
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				A945	G782	G782	C707	U542	A549	A549	U477	C406	U345	A173		
				A946	G783	G783	C708	U543	A550	A550	U478	C407	U346	A174		
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				A948	G785	G785	C710	U545	A552	A552	U480	C409	U348	A176		
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				A951	G788	G788	C713	U548	A555	A555	U483	C412	U351	A179		
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				A953	G790	G790	C715	U550	A557	A557	U485	C414	U353	A181		
				A954	G791	G791	C716	U551	A558	A558	U486	C415	U354	A182		
				A955	G792	G792	C717	U552	A559	A559	U487	C416	U355	A183		
				A956	G793	G793	C718	U553	A560	A560	U488	C417	U356	A184		
				A957	G794	G794	C719	U554	A561	A561	U489	C418	U357	A185		
				A958	G795	G795	C720	U555	A562	A562	U490	C419	U358	A186		
				A959	G796	G796	C721	U556	A563	A563	U491	C420	U359	A187		
				A960	G797	G797	C722	U557	A564	A564	U492	C421	U360	A188		
				A961	G798	G798	C723	U558	A565	A565	U493	C422	U361	A189		
				A962	G799	G799	C724	U559	A566	A566	U494	C423	U362	A190		
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				A964	G801	G801	C726	U561	A568	A568	U496	C425	U364	A192		
				A965	G802	G802	C727	U562	A569	A569	U497	C426	U365	A193		
				A966	G803	G803	C728	U563	A570	A570	U498	C427	U366	A194		
				A967	G804	G804	C729	U564	A571	A571	U499	C428	U367	A195		
				A968	G805	G805	C730	U565	A572	A572	U500	C429	U368	A196		
				A969	G806	G806	C731	U566	A573	A573	U501	C430	U369	A197		
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				A972	G809	G809	C734	U569	A576	A576	U504	C433	U372	A200		
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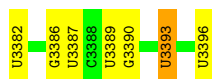
- Molecule 36: 25S ribosomal RNA



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A1046	A1046	C902	A735	C654	U582	U492	U434	A352	A266	U182	U87	A11
U1128	U1128	C901	A736	C655	U583	G493	U435	A353	G267	U183	A88	A12
A1129	A1048	U903	U824	A656	U584	C494	G436	G358	A268	U184	C90	C15
A1130	C1049	A904	U825	A657	U585	C495	A437	U359	G269	A187	G91	A16
G1131	U1050	U976	G826	G658	C586	C496	A438	G360	U270	U190	G92	A16
C1132	U1051	C977	A830	A660	U587	C503	A439	U361	G271	U191	C93	A23
A1133	U1052	U979	C743	A661	U588	A504	A440	U362	G272	U192	G94	G24
G1134	A1055	A980	C745	U662	U589	U508	U441	G364	G274	G197	G96	U25
U1137	U1056	U981	A837	C667	U592	U509	U442	A365	U279	C200	G98	C27
U1138	A1057	A914	C752	G668	C593	G510	G443	A366	U280	A201	C28	C28
G1139	U1058	A915	C753	U669	U594	G511	U	A367	G281	G202	A100	C29
C1140	U1059	G916	A755	U670	U595	U512	U	G368	G282	G203	G30	G30
U1141	U1060	A917	A756	U671	C599	C515	U	A369	G283	G204	A109	A34
A1142	A1061	C918	C768	U672	G600	A516	U	A370	A284	C205	C110	A35
A1143	A1062	C919	U769	U673	A607	G517	U	A371	A285	G206	C111	A40
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G1145	A1064	U920	G769	U675	G609	U520	U	A373	G290	G208	C113	
C1146	A1065	A921	C774	U676	U610	A521	C	A374	C291	U210	A116	U44
U1147	C1069	C923	A775	U677	A611	A522	C	A375	A295	A211	A45	A45
G1148	U1070	G924	U776	U678	U612	A523	U	A376	G297	G212	U46	U46
U1149	A1071	C927	U777	U679	C614	U524	U	A391	G300	G213	A121	C47
A1150	U1072	U932	A780	U680	G615	U531	U	A392	G301	G214	A122	A48
U1151	G1073	U933	G781	U681	U616	G535	U	A393	U302	G215	A49	A49
G1152	U1074	A933	U782	U682	A617	U536	U	A394	G303	G216	U50	U50
A1153	A1075	C934	A783	U683	U618	G542	U	G400	G304	G217	G128	G55
C1154	A1076	U935	U784	U684	U619	G547	U	U401	U321	U218	U133	G56
U1155	G1003	U936	G785	U685	A620	C548	U	A402	A221	G219	U134	A57
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G1157	G1005	C937	U787	U687	U622	U551	U	G404	U314	G221	G136	G59
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U1159	U1007	C939	U789	U689	U624	G547	U	G406	A317	A235	A61	A61
C1160	G1010	U940	A789	U690	U625	U548	U	A407	A318	G236	A62	A62
G1161	A1011	C941	U790	U691	A630	U549	U	A408	A319	G237	A63	A63
U1162	U1012	U942	C793	U692	U631	A551	U	A409	C321	A238	G64	G64
A1163	U1013	U943	U794	U693	U632	U555	U	U410	U322	U239	A65	A65
A1085	U1014	U944	U795	U694	U633	U557	U	U411	A323	U240	A66	A66
C1086	C1015	C945	U796	U695	U634	U558	U	G412	U326	G241	A67	A67
U1093	U1016	U946	U797	U696	U635	U559	U	U413	A150	G242	C68	C68
U1094	C1017	U947	U798	U697	U636	G560	U	U414	A151	G243	A70	A70
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G1021	U1019	C949	U800	U699	U638	U564	U	A416	A165	U245	G75	G75
A951	A951	A951	U801	U704	U639	G567	U	A417	C166	U246	G76	G76
A952	A952	A952	A806	U705	U640	U568	U	U418	U167	C247	G77	G77
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A1025	U1033	C953	A808	A707	U642	A570	U	U420	U169	U249	U78	U78
A1026	U1034	G963	U811	U708	U643	A571	U	G421	U170	U250	U79	U79
A1027	U1035	G964	U812	U709	U644	A572	U	A422	G171	G251	G80	G80
A1028	U1036	A965	U813	U710	U645	C576	U	A423	G172	U252	C81	C81
U1029	C958	U966	U814	U711	U646	C577	U	G424	A157	G253	C82	C82
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C961	C961	C961	U816	U713	U648	G579	U	A426	A166	C167	C174	C174
A962	A962	A962	U817	U714	U649	G580	U	U427	U167	U249	U168	U168
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U1042	U1042	U1042	U822	U719	U654	G585	U	U432	U172	U254	C173	C173
U1043	U1043	U1043	U823	U720	U655	G586	U	U433	U173	U255	U84	U84
A967	A967	A967	U824	U721	U656	G587	U	U434	U174	U256	U85	U85
G968	G968	G968	U825	U722	U657	G588	U	U435	U175	U257	U86	U86
U969	U969	U969	U826	U723	U658	G589	U	U436	U176	U258	U87	U87
C1043	C1043	C1043	U827	U724	U659	G590	U	U437	U177	U259	U88	U88
A968	A968	A968	U828	U725	U660	G591	U	U438	U178	U260	U89	U89
U1044	U1044	U1044	U829	U726	U661	G592	U	U439	U179	U261	U90	U90
C1045	C1045	C1045	U830	U727	U662	G593	U	U440	U180	U262	U91	U91
A1046	A1046	A1046	U831	U728	U663	G594	U	U441	U181	U263	U92	U92
U1047	U1047	U1047	U832	U729	U664	G595	U	U442	U182	U264	U93	U93
A1048	A1048	A1048	U833	U730	U665	G596	U	U443	U183	U265	U94	U94
C1049	C1049	C1049	U834	U731	U666	G597	U	U444	U184	U266	U95	U95
U1050	U1050	U1050	U835	U732	U667	G598	U	U445	U185	U267	U96	U96
U1051	U1051	U1051	U836	U733	U668	G599	U	U446	U186	U268	U97	U97
C977	C977	C977	U837	U734	U669	G600	U	U447	U187	U269	U98	U98
U979	U979	U979	U838	U735	U670	G601	U	U448	U188	U270	U99	U99
A980	A980	A980	U839	U736	U671	G602	U	U449	U189	U271	U100	U100
U981	U981	U981	U840	U737	U672	G603	U	U450	U190	U272	U101	U101
U985	U985	U985	U841	U738	U673	G604	U	U451	U191	U273	U102	U102
A989	A989	A989	U842	U739	U674	G605	U	U452	U192	U274	U103	U103
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G1076	G1076	G1076	U856	U753	U688	G619	U	U466	U206	U288	U117	U117
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G1083	G1083	G1083	U863	U760	U695	G626	U	U473	U213	U295	U124	U124
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U1095	U1095	U1095	U869	U766	U701	G632	U	U479	U219	U301	U130	U130
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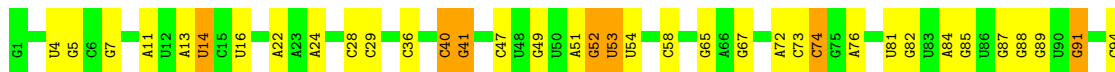
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G2329	A2166	A2166	C	G	C	U1894	A1815	C1706	A1593	G1525	U1445	G1306	G1202
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U2333	G2171	G2171	A	U	G	G1898	U1818	G1713	G1598	C1527	U1448	G1310	G1209
U2334	A2172	A2172	A	A	G	G1899	U1819	G1713	G1598	U1530	U1449	A1381	U1210
G2335	G2177	G2177	U	U	C	U1900	U1820	U1716	G1604	U1531	G1450	G1312	G1211
U2336	G2177	G2177	U	U	C	A1901	U1821	U1717	A1605	C1532	U1451	G1313	U1211
C2337	G2177	G2177	A	A	U	G1902	C1827	G1718	U1606	G1536	U1452	G1314	G1222
C2338	G2177	G2177	A	A	U	U1903	U1827	G1719	C1607	A1537	U1453	U1315	A1223
G2339	G2177	G2177	A	A	U	C1904	U1834	G1724	C1608	A1538	U1454	G1316	A1223
U2340	G2181	C2181	C	C	G	G1905	U1840	U1725	C1615	A1539	U1455	A1317	G1232
U2341	G2186	U2186	G	G	C	G1906	U1841	C1725	C1615	A1460	U1459	G1321	G1233
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U2344	U2189	U2189	U	U	C	A1911	C1846	G1736	U1629	G1542	A1385	U1324	G1238
A2345	C2192	C2192	G	G	G	U1912	C1847	G1743	U1632	G1543	A1386	U1325	C1239
U2346	U2193	U2193	U	U	G	A1914	A1847	G1748	A1632	G1547	U1466	A1326	G1240
U2347	G2194	G2194	U	U	G	U1915	G1848	G1749	G1635	U1549	A1467	C1327	U1241
U2348	A2280	A2280	U	U	G	A1916	C1849	A1750	U1635	G1554	U1475	U1329	G1242
U2349	U2282	U2282	G	G	U	C1917	A1850	A1751	C1639	U1555	A1401	A1330	G1245
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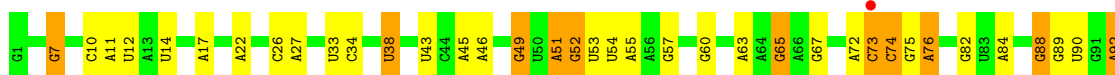
• Molecule 37: 5S ribosomal RNA

Chain 3: 61% 31% 7%



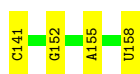
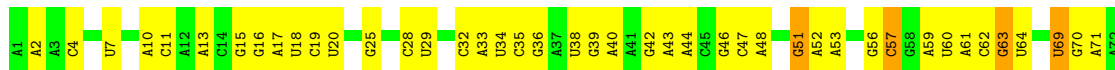
• Molecule 37: 5S ribosomal RNA

Chain 7: % 57% 31% 12%



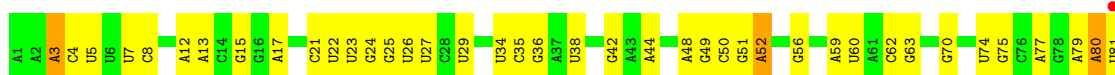
• Molecule 38: 5.8S ribosomal RNA

Chain 4: % 41% 53% 7%



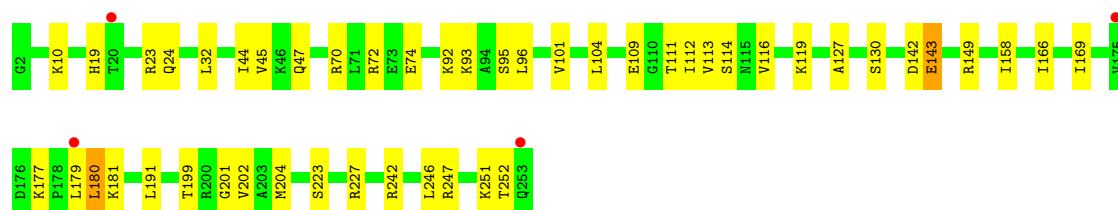
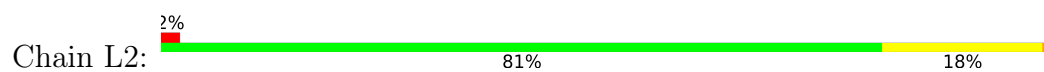
• Molecule 38: 5.8S ribosomal RNA

Chain 8: % 53% 42% 5%

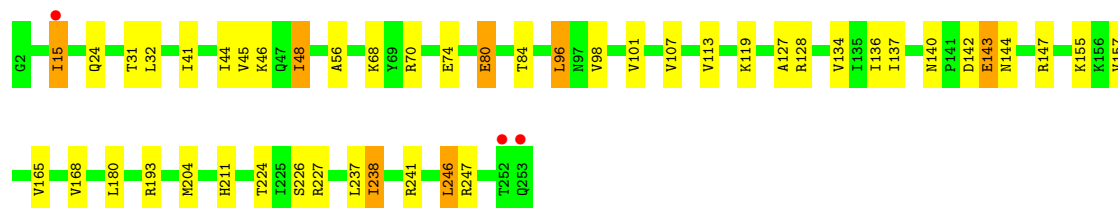
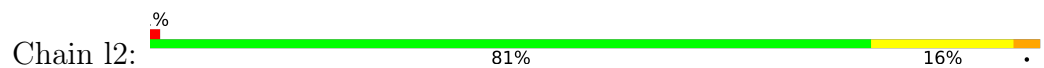


• Molecule 39: 60S ribosomal protein L2-A

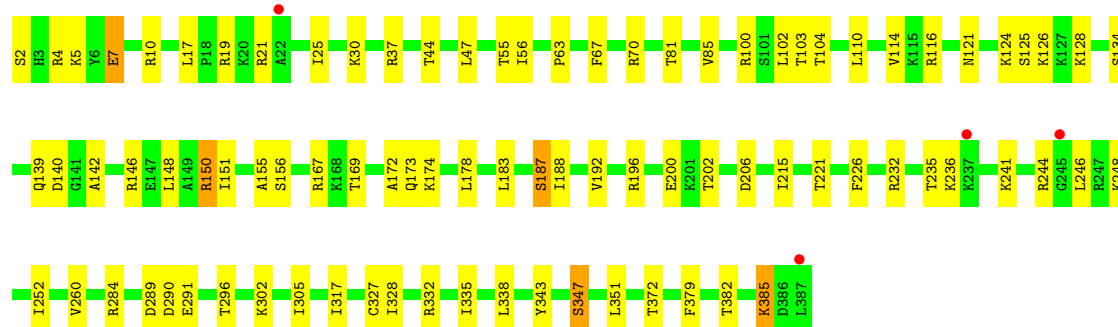
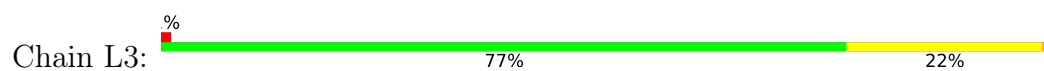




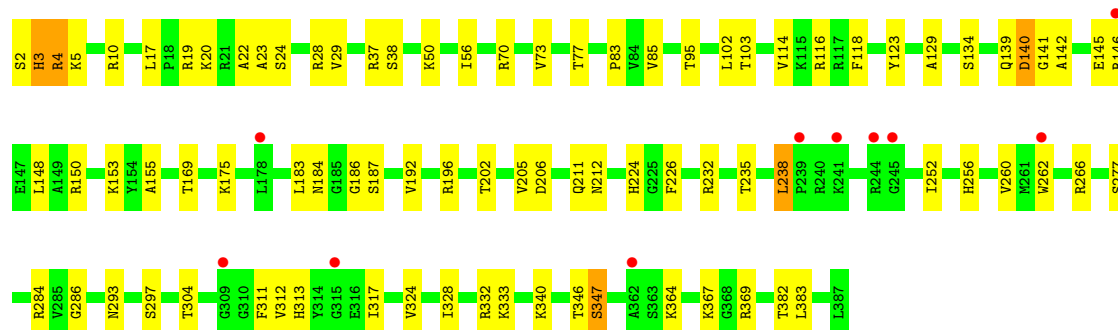
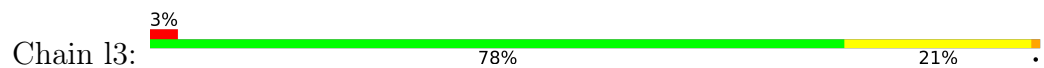
- Molecule 39: 60S ribosomal protein L2-A



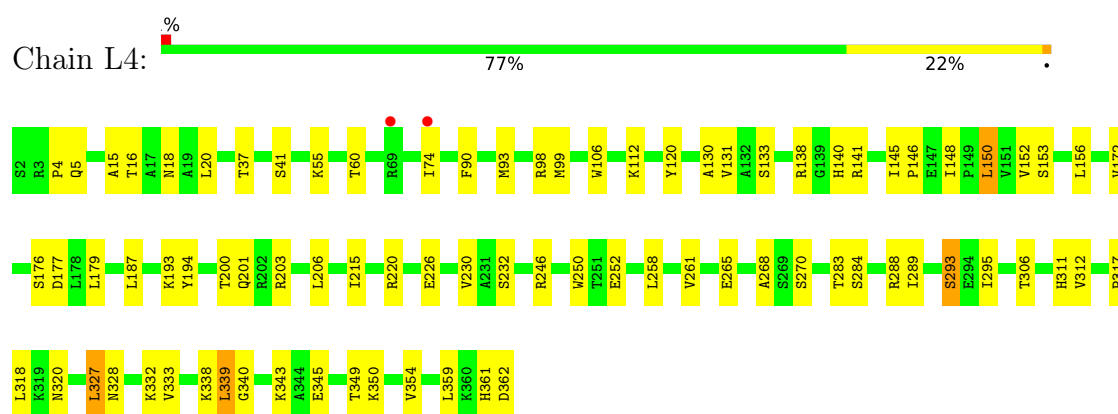
- Molecule 40: 60S ribosomal protein L3



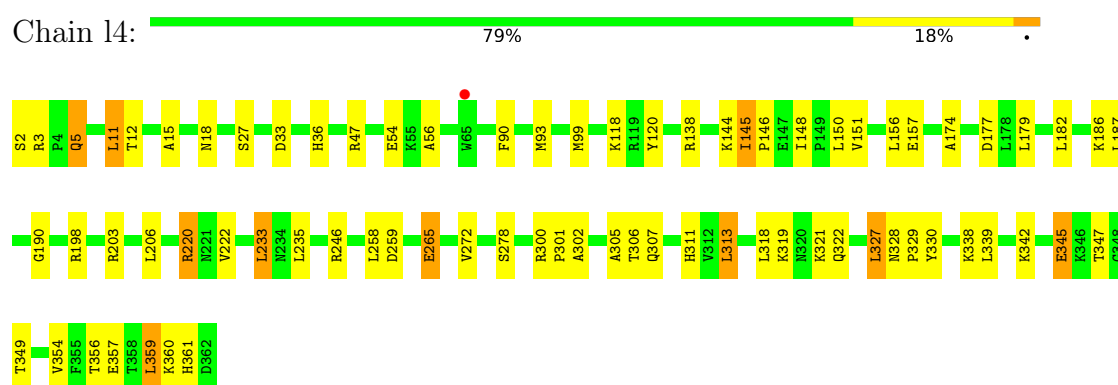
- Molecule 40: 60S ribosomal protein L3



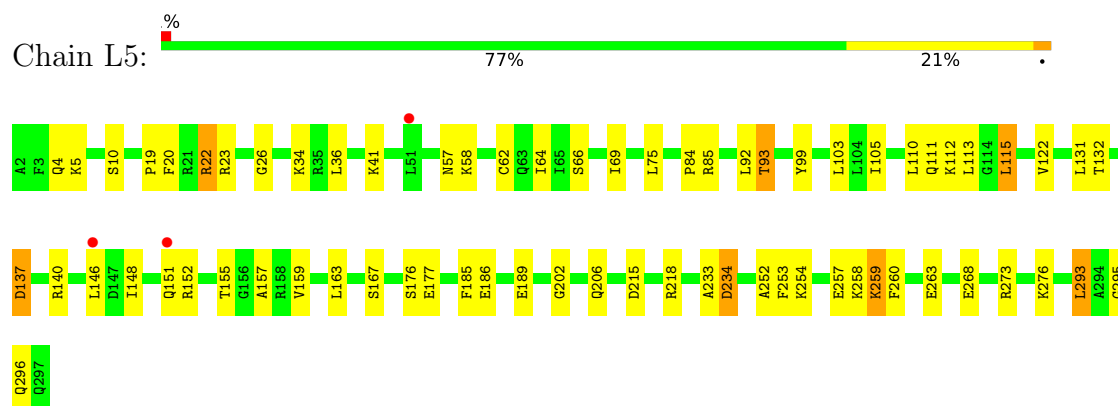
- Molecule 41: 60S ribosomal protein L4-A



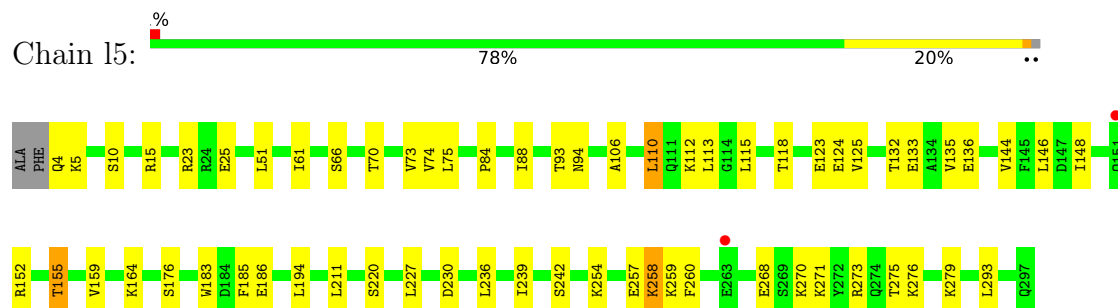
• Molecule 41: 60S ribosomal protein L4-A



• Molecule 42: 60S ribosomal protein L5



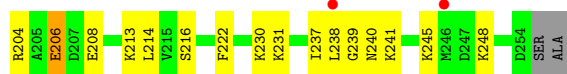
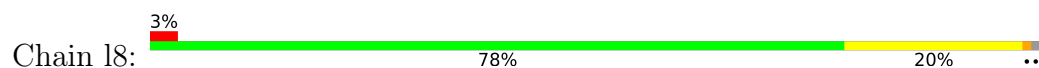
• Molecule 42: 60S ribosomal protein L5



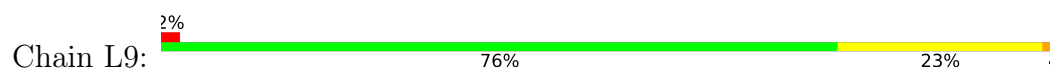
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N95	10
E118	10
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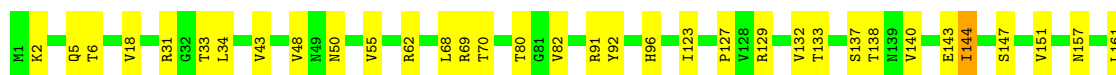
• Molecule 45: 60S ribosomal protein L8-A



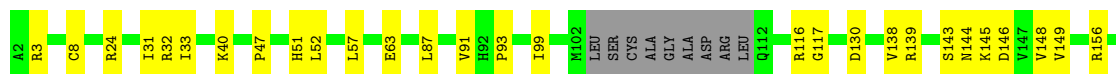
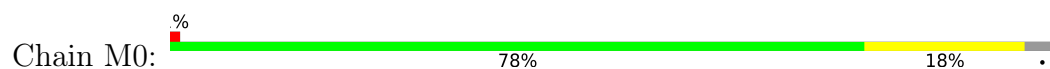
• Molecule 46: 60S ribosomal protein L9-A



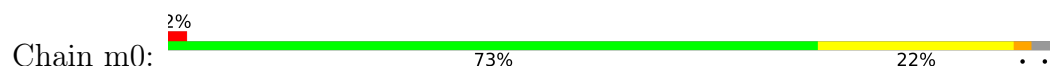
• Molecule 46: 60S ribosomal protein L9-A

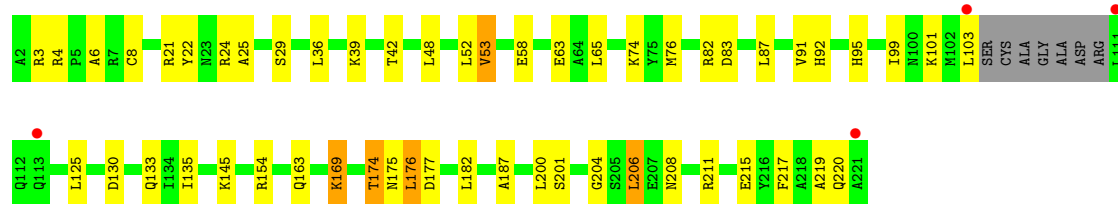


• Molecule 47: 60S ribosomal protein L10

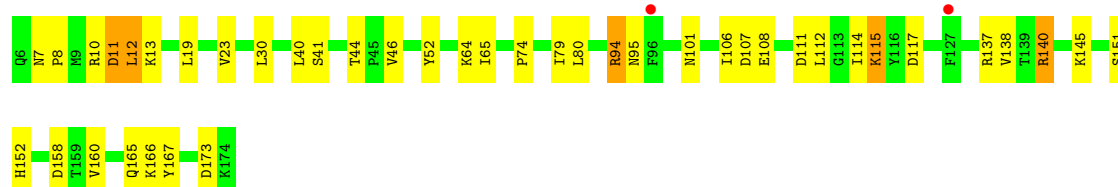
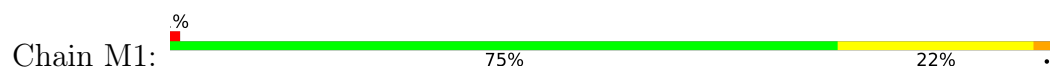


• Molecule 47: 60S ribosomal protein L10

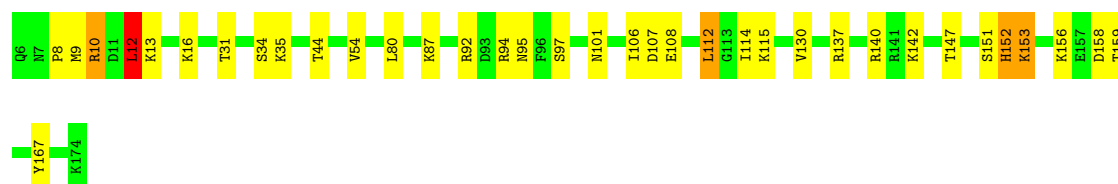
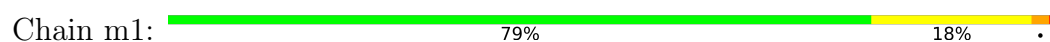




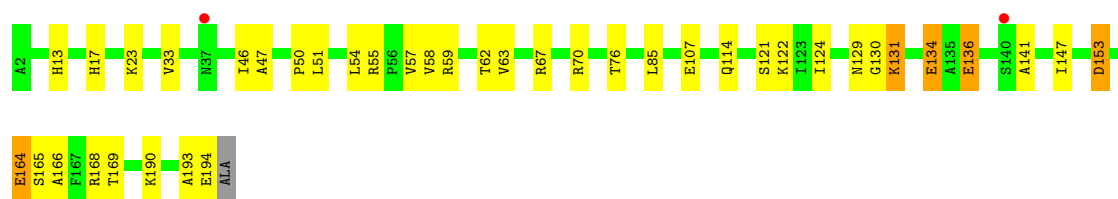
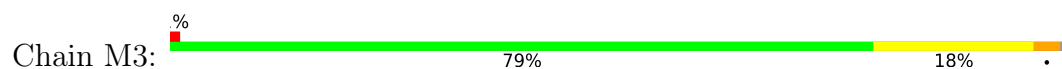
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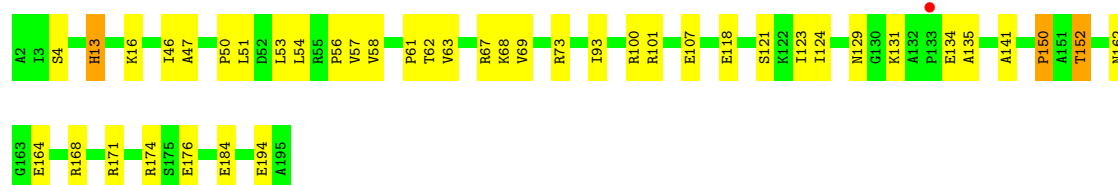
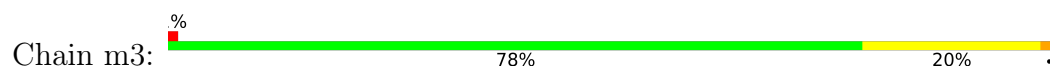
• Molecule 48: 60S ribosomal protein L11-B



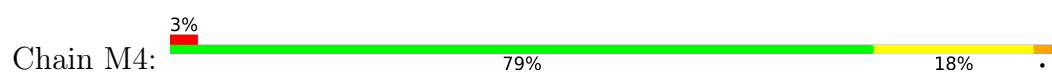
• Molecule 49: 60S ribosomal protein L13-A



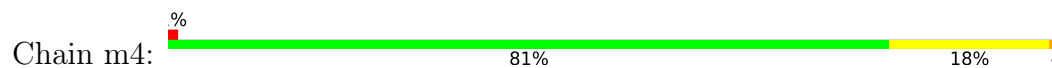
• Molecule 49: 60S ribosomal protein L13-A



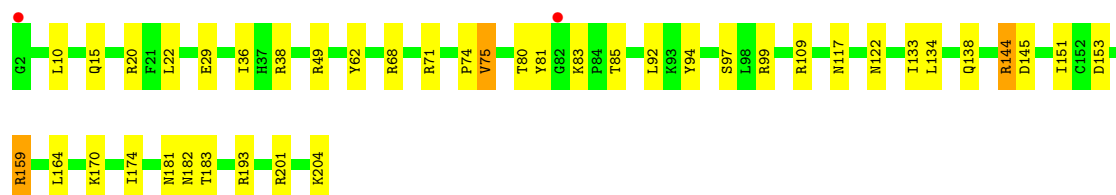
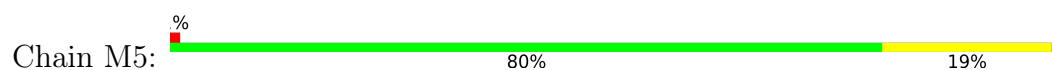
• Molecule 50: 60S ribosomal protein L14-A



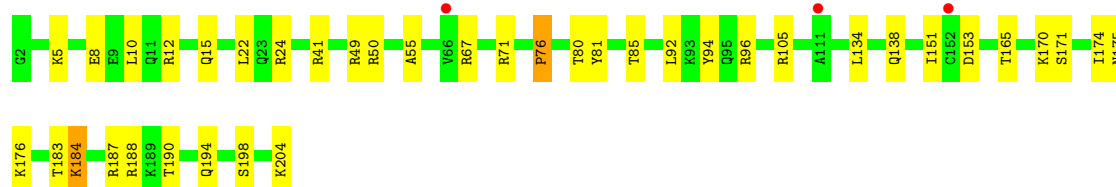
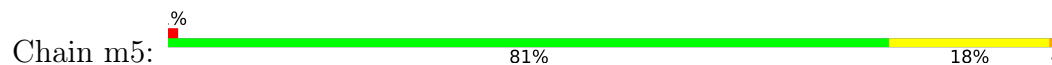
- Molecule 50: 60S ribosomal protein L14-A



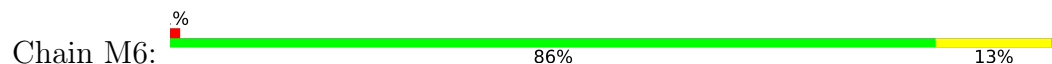
- Molecule 51: 60S ribosomal protein L15-A



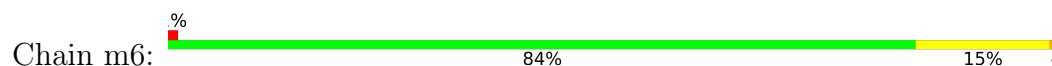
- Molecule 51: 60S ribosomal protein L15-A



- Molecule 52: 60S ribosomal protein L16-A

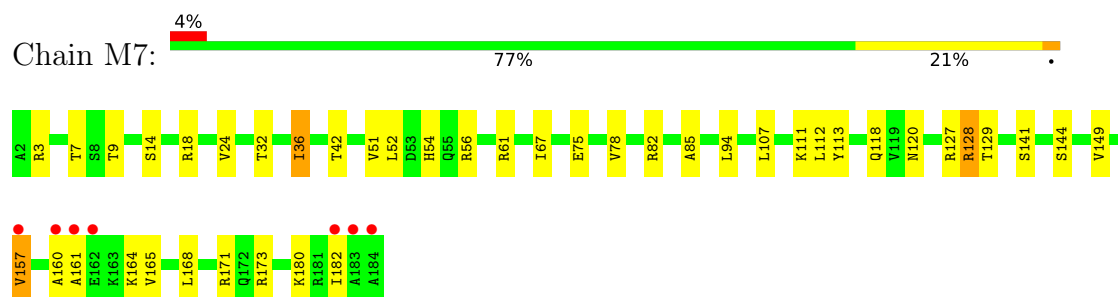


- Molecule 52: 60S ribosomal protein L16-A

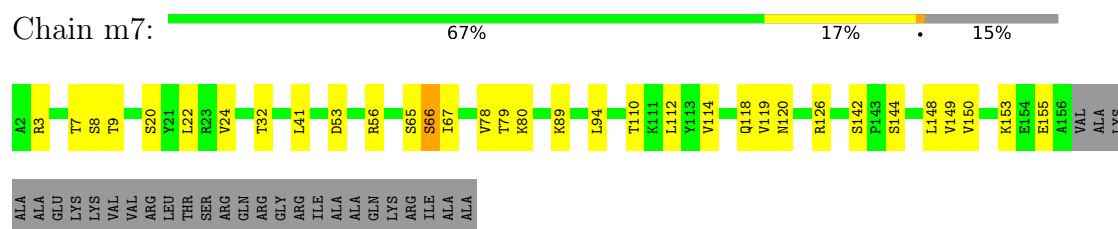


Y199

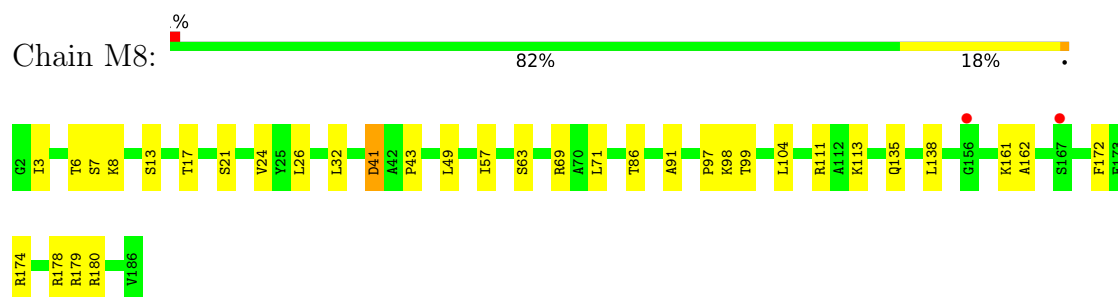
- Molecule 53: 60S ribosomal protein L17-A



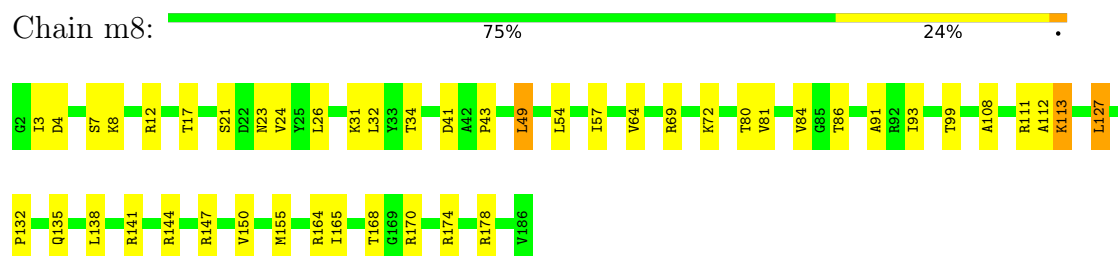
- Molecule 53: 60S ribosomal protein L17-A



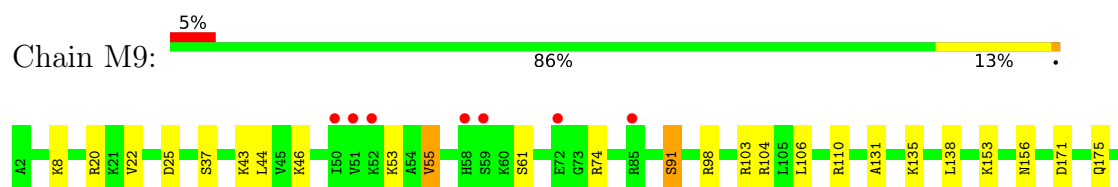
- Molecule 54: 60S ribosomal protein L18-A

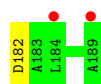


- Molecule 54: 60S ribosomal protein L18-A

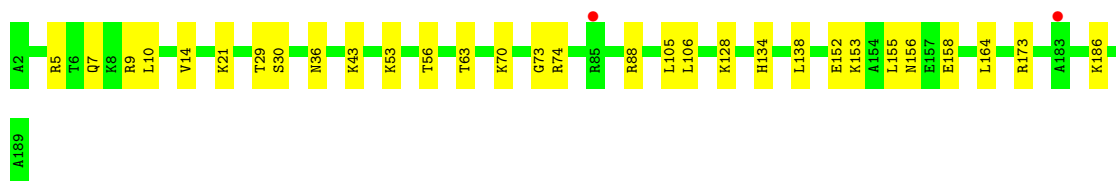
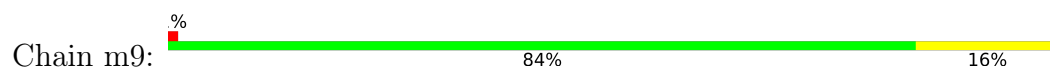


- Molecule 55: 60S ribosomal protein L19-A

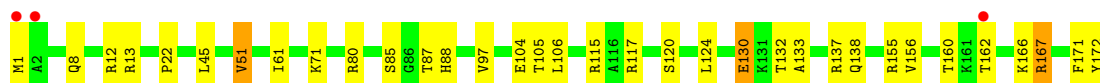
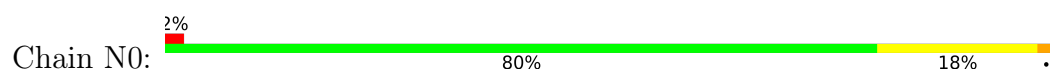




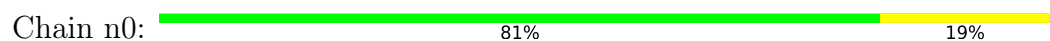
• Molecule 55: 60S ribosomal protein L19-A



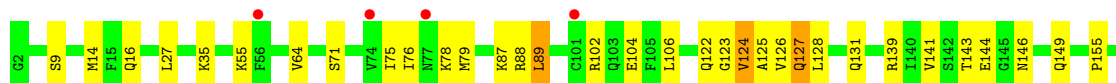
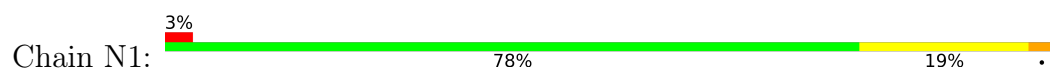
• Molecule 56: 60S ribosomal protein L20-A



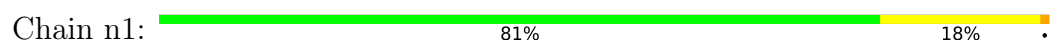
• Molecule 56: 60S ribosomal protein L20-A



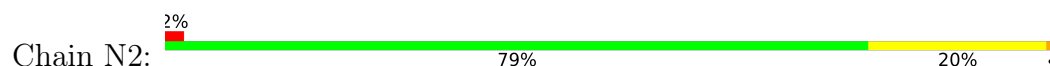
• Molecule 57: 60S ribosomal protein L21-A



• Molecule 57: 60S ribosomal protein L21-A



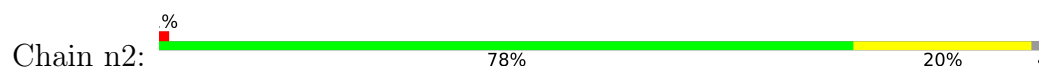
• Molecule 58: 60S ribosomal protein L22-A







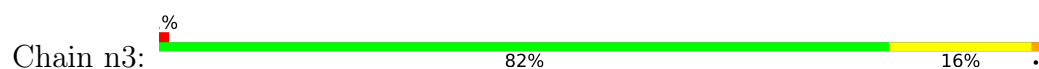
- Molecule 58: 60S ribosomal protein L22-A



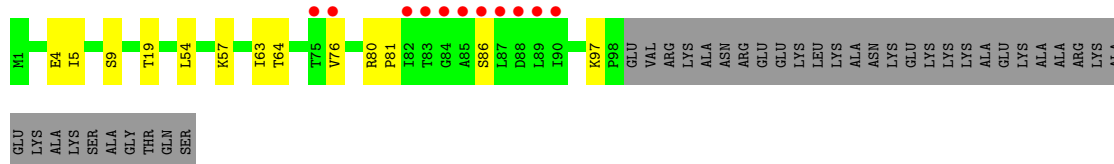
- Molecule 59: 60S ribosomal protein L23-A



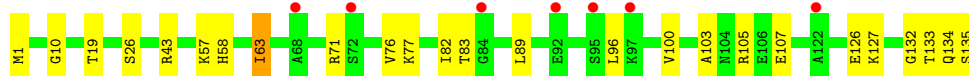
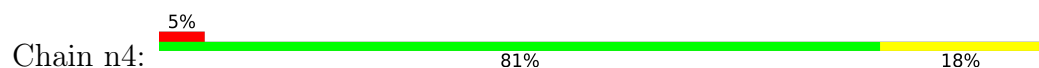
- Molecule 59: 60S ribosomal protein L23-A



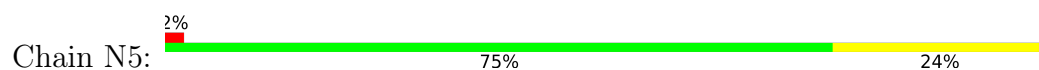
- Molecule 60: 60S ribosomal protein L24-A



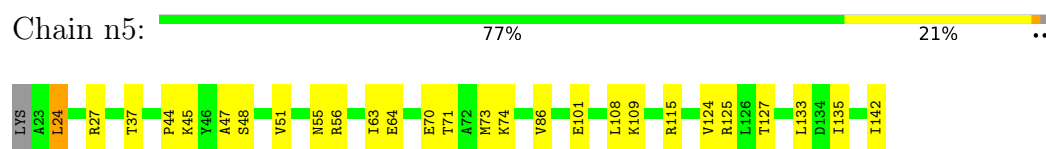
- Molecule 60: 60S ribosomal protein L24-A



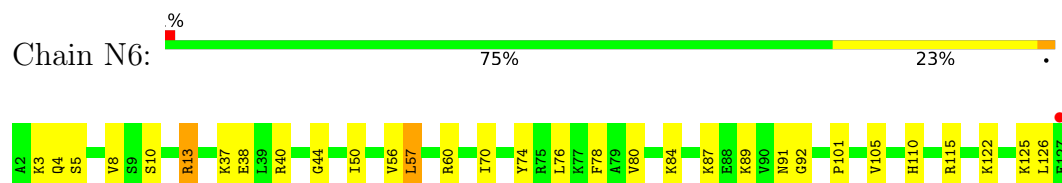
- Molecule 61: 60S ribosomal protein L25



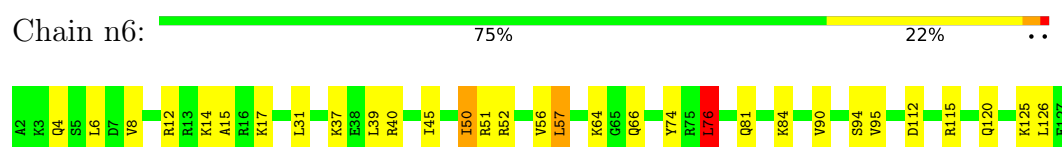
- Molecule 61: 60S ribosomal protein L25



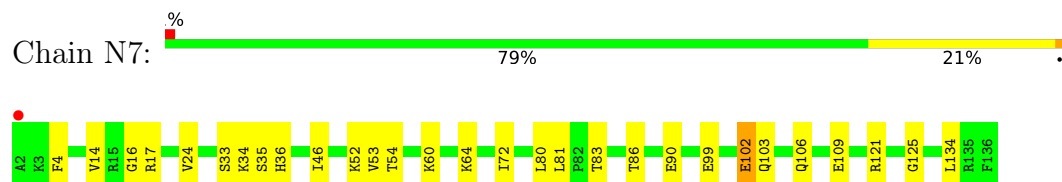
- Molecule 62: 60S ribosomal protein L26-A



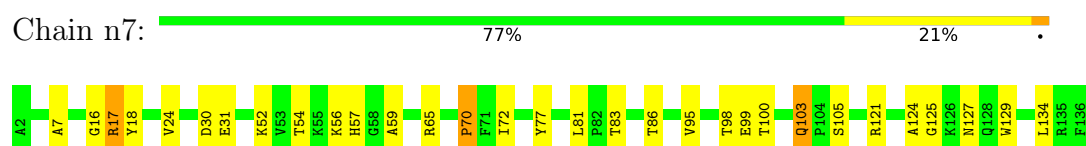
- Molecule 62: 60S ribosomal protein L26-A



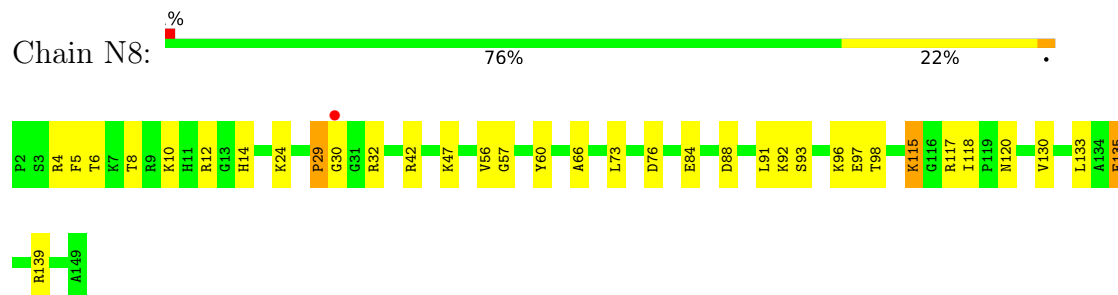
- Molecule 63: 60S ribosomal protein L27-A



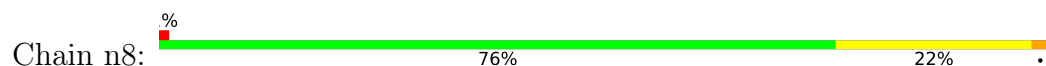
- Molecule 63: 60S ribosomal protein L27-A

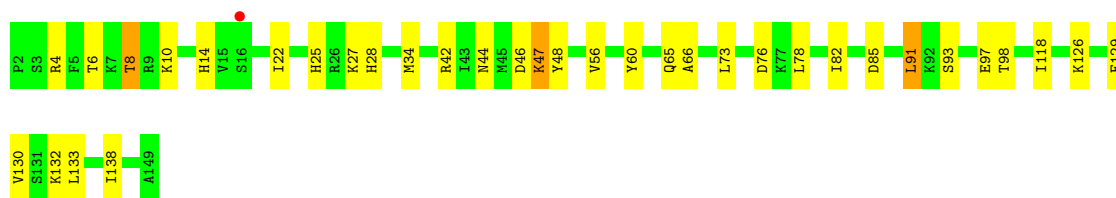


- Molecule 64: 60S ribosomal protein L28

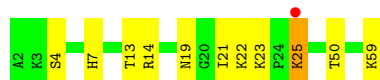
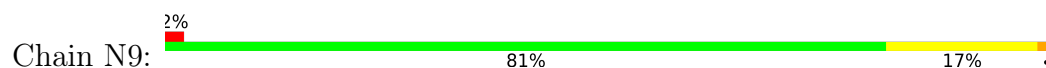


- Molecule 64: 60S ribosomal protein L28

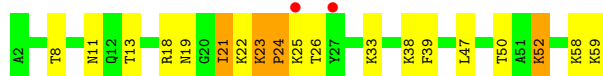




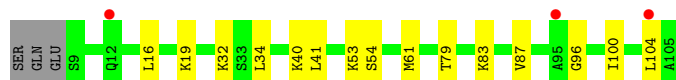
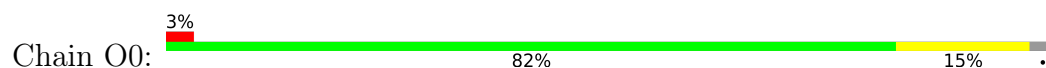
- Molecule 65: 60S ribosomal protein L29



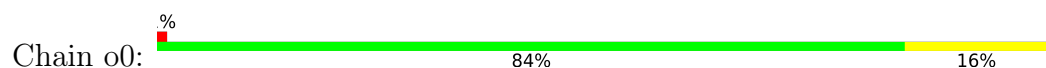
- Molecule 65: 60S ribosomal protein L29



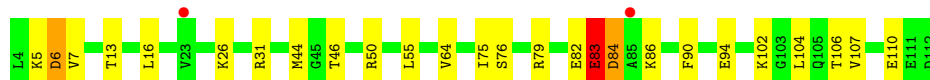
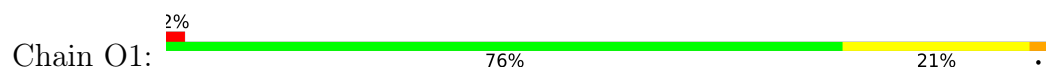
- Molecule 66: 60S ribosomal protein L30



- Molecule 66: 60S ribosomal protein L30



- Molecule 67: 60S ribosomal protein L31-A

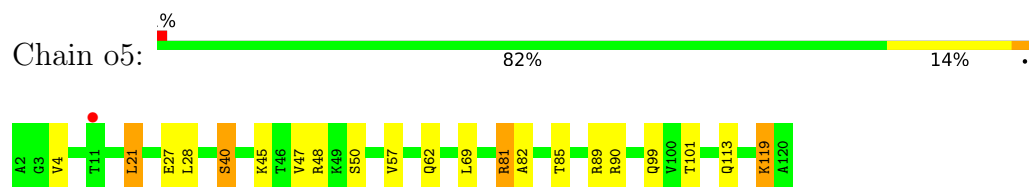


- Molecule 67: 60S ribosomal protein L31-A

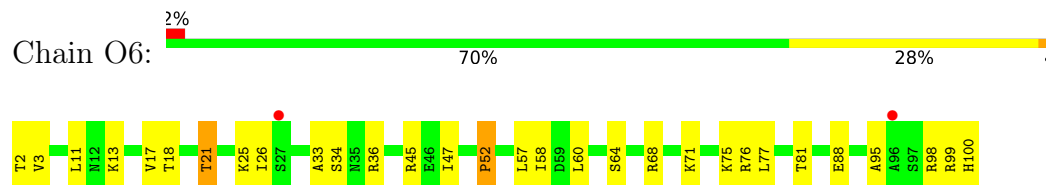


- 
- | Category | Count |
|----------|-------|
| A2       | 10    |
| A3       | 10    |
| V4       | 10    |
| G3       | 10    |
| S13      | 10    |
| K14      | 10    |
| E15      | 10    |
| Q20      | 10    |
| L21      | 10    |
| V22      | 10    |
| E27      | 10    |
| L31      | 10    |
| K35      | 10    |
| L36      | 10    |
| S40      | 10    |
| L41      | 10    |
| P42      | 10    |
| K43      | 10    |
| R48      | 10    |
| K49      | 10    |
| E64      | 10    |
| L69      | 10    |
| K74      | 10    |
| Y75      | 10    |
| Q76      | 10    |
| K84      | 10    |
| T85      | 10    |
| R89      | 10    |
| R90      | 10    |
| A91      | 10    |
| F95      | 10    |
| E96      | 10    |
| A97      | 10    |
| E102     | 10    |
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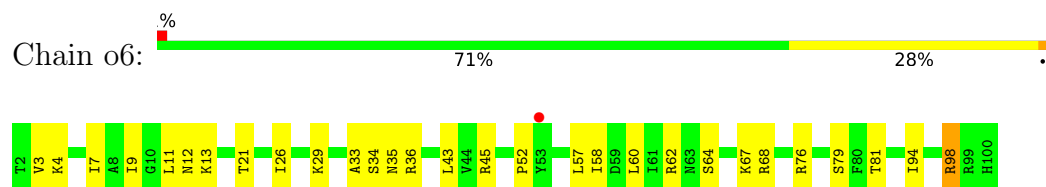
- Molecule 71: 60S ribosomal protein L35-A



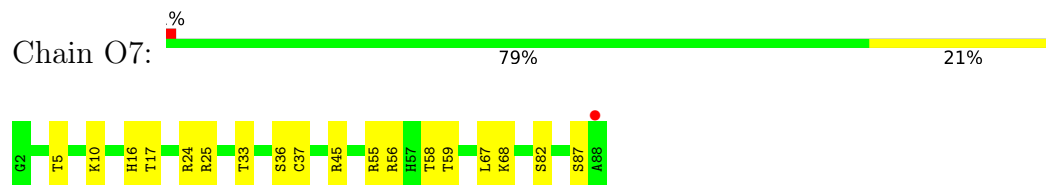
- Molecule 72: 60S ribosomal protein L36-A



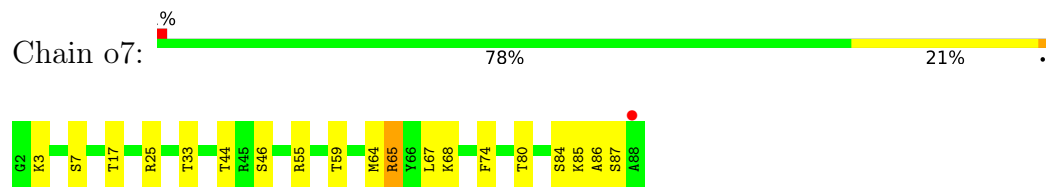
- Molecule 72: 60S ribosomal protein L36-A



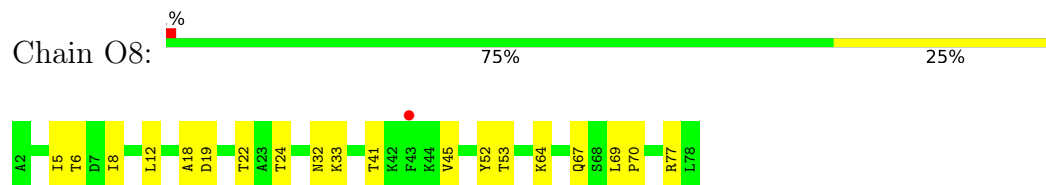
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38

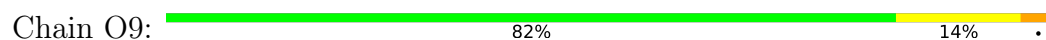


- Molecule 74: 60S ribosomal protein L38

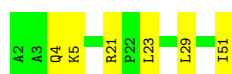
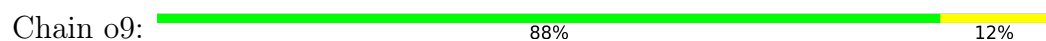




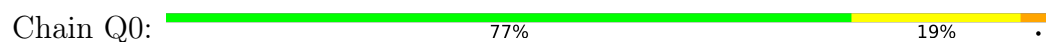
- Molecule 75: 60S ribosomal protein L39



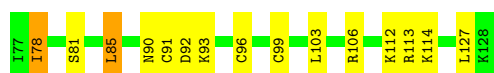
- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 77: 60S ribosomal protein L41-A

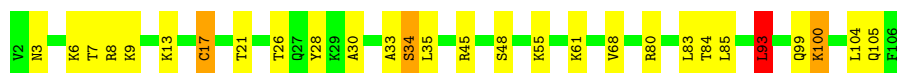


- Molecule 77: 60S ribosomal protein L41-A

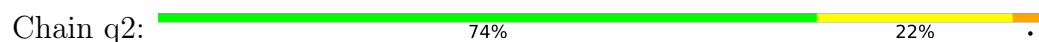


- Molecule 78: 60S ribosomal protein L42-A

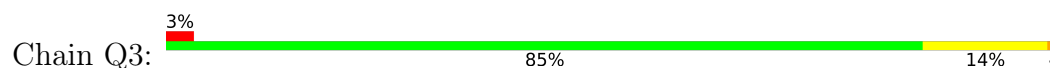




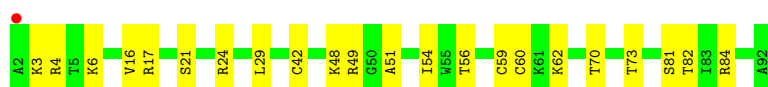
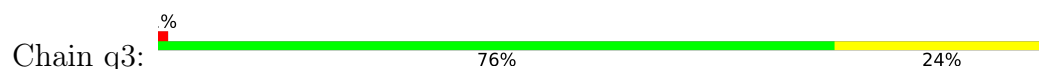
- Molecule 78: 60S ribosomal protein L42-A



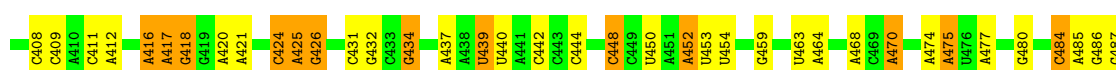
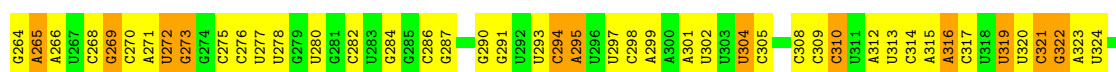
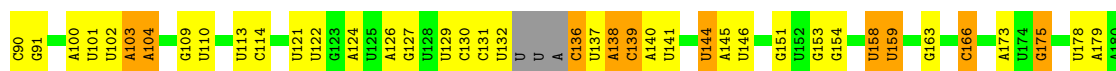
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A




- Molecule 80: 18S ribosomal RNA



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U983	U983	U983	A985	A986	A987	U988	C989	A970	G972	C975	A978	A979	G980	U981	U982	A983	G984	G985	U989	C990	G991	A992	A993	G994	A995	U996	U999	C1000	G1003	U1004	A1005	G1008	U1009	U1015	A1019	A1020	C1021	C1022	A1023	U1024	A1025	A1026	A1027	C1028	U1029	G1035	A1036	C1037	U1038																						
A755	U756	A757	U758	U759	A760	G761	G765	A766	G767	C768	C773	A774	G775	U779	A780	U781	U782	G783	C784	G787	A788	A789	U792	A793	U794	A795	A796	U800	G801	G802	A803	A804	U805	A806	A811	A812	U813	A814	G815	G816	U821	U822	G823	G824	U825	U826	C827	U828	A829	U830	U831																				
U832	U833	G834	U835	A850	G858	A859	U860	U861	A862	A863	U864	G871	G876	G877	G878	G879	C880	A881	U882	C883	A884	U886	U894	A898	G901	G904	A905	A906	U911	U912	G913	G914	G925	U932	A933	U935	G938	A939	G942	C943	U944	U945	A952																												
G574	A661	G577	U578	A579	A580	U581	U582	C583	C584	C590	A591	A592	U593	A594	G595	C596	G597	U608	U609	A511	A512	C683	U611	U612	G613	G616	U617	U618	A619	A620	A621	A622	A623	G624	A638	U639	U640	G651	G652	C653	G654	G655	G656	U657	C658	U659	C660																								




- Molecule 81: 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10-A

Chain c0:  7% 78% 21%



- Molecule 82: Suppressor protein STM1,Suppressor protein STM1,Ribosome-bound protein Stm1

Chain sM:  5% 80% 19%



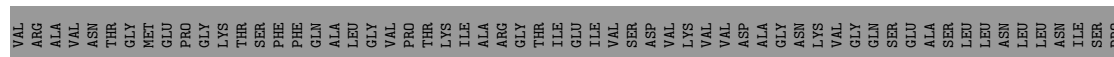
- Molecule 83: 60S Ribosomal Protein L12

Chain m2:  100%

There are no outlier residues recorded for this chain.

- Molecule 84: 60S acidic ribosomal protein P0

Chain p0:  2% 53% 11% 35%

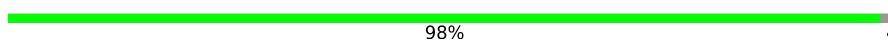


- Molecule 85: 60S Ribosomal Protein P1/2

Chain p1:  100%

There are no outlier residues recorded for this chain.

- Molecule 85: 60S Ribosomal Protein P1/2

Chain p2:  98%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	435.45Å 288.14Å 304.16Å 90.00° 99.11° 90.00°	Depositor
Resolution (Å)	149.31 – 3.30 149.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.3 (149.31-3.30) 92.3 (149.31-3.30)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.211 , 0.265 0.213 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 74.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	414270	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: 8AN, OHX, MG, ZN

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	0.75	7/42467 (0.0%)	1.40	452/66169 (0.7%)
2	S0	0.54	1/1617 (0.1%)	0.63	0/2215
2	s0	0.51	0/1623	0.70	0/2222
3	S1	0.37	0/1735	0.62	1/2335 (0.0%)
3	s1	0.48	0/1748	0.67	3/2352 (0.1%)
4	S2	0.46	0/1665	0.69	0/2263
4	s2	0.61	0/1665	0.78	2/2263 (0.1%)
5	S3	0.46	0/1759	0.63	1/2368 (0.0%)
5	s3	0.48	0/1759	0.64	1/2368 (0.0%)
6	S4	0.45	0/2109	0.71	0/2839
6	s4	0.55	0/2109	0.78	3/2839 (0.1%)
7	S5	0.39	0/1629	0.59	0/2202
7	s5	0.46	0/1629	0.63	0/2202
8	S6	0.47	0/1823	0.64	0/2439
8	s6	0.56	0/1779	0.77	2/2379 (0.1%)
9	S7	0.44	0/1506	0.66	0/2028
9	s7	0.51	0/1516	0.69	1/2043 (0.0%)
10	S8	0.50	0/1514	0.67	0/2021
10	s8	0.59	0/1514	0.74	0/2021
11	S9	0.48	0/1519	0.65	0/2035
11	s9	0.55	0/1519	0.74	1/2035 (0.0%)
12	C0	0.41	0/789	0.69	1/1067 (0.1%)
13	C1	0.52	0/1239	0.65	0/1673
13	c1	0.60	0/1194	0.78	1/1610 (0.1%)
14	C2	0.40	0/898	0.67	0/1220
14	c2	0.33	0/898	0.61	1/1220 (0.1%)
15	C3	0.48	0/1215	0.66	1/1638 (0.1%)
15	c3	0.53	0/1215	0.70	0/1638
16	C4	0.37	0/901	0.62	0/1217
16	c4	0.50	0/960	0.66	0/1290
17	C5	0.48	0/998	0.65	0/1341
17	c5	0.51	0/1060	0.68	0/1426

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	C6	0.43	0/1125	0.68	2/1510 (0.1%)
18	c6	0.55	1/1131 (0.1%)	0.69	1/1518 (0.1%)
19	C7	0.43	0/935	0.67	0/1254
19	c7	0.48	0/914	0.66	0/1224
20	C8	0.48	0/1211	0.69	2/1628 (0.1%)
20	c8	0.46	0/1211	0.67	1/1628 (0.1%)
21	C9	0.45	0/1130	0.64	0/1517
21	c9	0.50	0/1130	0.66	3/1517 (0.2%)
22	D0	0.47	0/865	0.68	0/1169
22	d0	0.45	0/892	0.65	0/1205
23	D1	0.44	0/693	0.65	0/935
23	d1	0.64	0/693	0.75	1/935 (0.1%)
24	D2	0.49	0/1038	0.74	3/1395 (0.2%)
24	d2	0.59	0/1038	0.77	1/1395 (0.1%)
25	D3	0.57	0/1139	0.72	1/1518 (0.1%)
25	d3	0.63	0/1139	0.83	0/1518
26	D4	0.46	0/1087	0.63	0/1449
26	d4	0.55	0/1087	0.74	0/1449
27	D5	0.42	0/571	0.68	0/768
27	d5	0.45	0/566	0.60	0/761
28	D6	0.43	0/782	0.70	1/1047 (0.1%)
28	d6	0.58	0/782	0.68	0/1047
29	D7	0.44	0/620	0.64	0/838
29	d7	0.48	0/620	0.70	0/838
30	D8	0.40	0/499	0.60	0/670
30	d8	0.43	0/499	0.63	0/670
31	D9	0.59	0/452	0.71	1/600 (0.2%)
31	d9	0.52	0/452	0.64	0/600
32	E0	0.45	0/483	0.61	0/643
32	e0	0.55	0/499	0.72	0/665
33	E1	0.43	0/577	0.73	0/770
33	e1	0.40	0/619	0.72	2/822 (0.2%)
34	SR	0.40	0/2490	0.61	1/3389 (0.0%)
34	sR	0.41	0/2495	0.61	0/3395
35	SM	0.49	0/984	0.67	0/1323
36	1	1.08	150/75394 (0.2%)	1.76	2353/117545 (2.0%)
36	5	1.16	238/75414 (0.3%)	1.85	2720/117575 (2.3%)
37	3	0.96	4/2883 (0.1%)	1.60	55/4491 (1.2%)
37	7	1.09	5/2883 (0.2%)	1.77	83/4491 (1.8%)
38	4	1.01	3/3746 (0.1%)	1.72	114/5832 (2.0%)
38	8	0.95	2/3746 (0.1%)	1.62	75/5832 (1.3%)
39	L2	0.58	0/1948	0.77	0/2617
39	l2	0.61	0/1946	0.82	2/2614 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	L3	0.65	2/3146 (0.1%)	0.81	3/4228 (0.1%)
40	l3	0.73	0/3146	0.84	4/4228 (0.1%)
41	L4	0.67	1/2800 (0.0%)	0.84	4/3790 (0.1%)
41	l4	0.68	1/2800 (0.0%)	0.81	2/3790 (0.1%)
42	L5	0.59	0/2425	0.71	2/3271 (0.1%)
42	l5	0.73	2/2408 (0.1%)	0.77	1/3248 (0.0%)
43	L6	0.65	1/1260 (0.1%)	0.77	0/1694
43	l6	0.68	0/1269	0.79	0/1705
44	L7	0.66	0/1821	0.80	4/2451 (0.2%)
44	l7	0.71	0/1828	0.86	3/2461 (0.1%)
45	L8	0.49	0/1836	0.64	1/2481 (0.0%)
45	l8	0.48	0/1795	0.65	1/2429 (0.0%)
46	L9	0.58	0/1539	0.74	0/2073
46	l9	0.70	0/1539	0.77	0/2073
47	M0	0.72	1/1741 (0.1%)	0.77	0/2335
47	m0	0.85	2/1758 (0.1%)	0.83	0/2358
48	M1	0.52	0/1374	0.70	0/1842
48	m1	0.66	0/1374	0.80	2/1842 (0.1%)
49	M3	0.63	0/1568	0.78	0/2106
49	m3	0.59	0/1573	0.76	0/2113
50	M4	0.61	0/1068	0.72	0/1438
50	m4	0.66	0/1074	0.79	2/1446 (0.1%)
51	M5	0.63	0/1757	0.77	0/2354
51	m5	0.57	0/1757	0.73	0/2354
52	M6	0.74	0/1585	0.83	4/2128 (0.2%)
52	m6	0.83	1/1585 (0.1%)	0.84	2/2128 (0.1%)
53	M7	0.69	0/1443	0.82	2/1944 (0.1%)
53	m7	0.77	0/1250	0.84	0/1683
54	M8	0.66	1/1465 (0.1%)	0.84	2/1965 (0.1%)
54	m8	0.64	0/1465	0.84	2/1965 (0.1%)
55	M9	0.49	0/1538	0.66	0/2050
55	m9	0.58	0/1538	0.67	0/2050
56	N0	0.65	0/1481	0.78	1/1990 (0.1%)
56	n0	0.68	0/1481	0.78	0/1990
57	N1	0.66	0/1300	0.78	1/1743 (0.1%)
57	n1	0.69	1/1300 (0.1%)	0.74	0/1743
58	N2	0.44	0/812	0.62	0/1099
58	n2	0.54	0/794	0.67	0/1076
59	N3	0.66	0/1018	0.82	0/1369
59	n3	0.78	2/1018 (0.2%)	0.90	2/1369 (0.1%)
60	N4	0.54	0/712	0.68	0/958
60	n4	0.61	0/1052	0.71	0/1398
61	N5	0.57	0/979	0.75	3/1321 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	n5	0.56	0/974	0.74	0/1314
62	N6	0.62	0/1004	0.84	3/1341 (0.2%)
62	n6	0.62	0/1004	0.80	2/1341 (0.1%)
63	N7	0.48	0/1118	0.61	0/1497
63	n7	0.49	0/1118	0.61	0/1497
64	N8	0.68	1/1204 (0.1%)	0.84	2/1612 (0.1%)
64	n8	0.72	1/1204 (0.1%)	0.90	3/1612 (0.2%)
65	N9	0.64	0/473	0.78	0/629
65	n9	0.68	0/473	0.89	0/629
66	O0	0.42	0/751	0.59	0/1008
66	o0	0.50	0/775	0.72	0/1040
67	O1	0.60	0/890	0.74	0/1196
67	o1	0.74	0/897	0.76	0/1205
68	O2	0.68	0/1041	0.81	0/1394
68	o2	0.70	0/1041	0.82	1/1394 (0.1%)
69	O3	0.81	0/868	0.85	1/1168 (0.1%)
69	o3	0.77	0/868	0.82	0/1168
70	O4	0.54	0/890	0.70	2/1189 (0.2%)
70	o4	0.55	0/890	0.69	0/1189
71	O5	0.60	1/978 (0.1%)	0.70	0/1301
71	o5	0.58	0/974	0.69	1/1297 (0.1%)
72	O6	0.57	0/778	0.72	0/1034
72	o6	0.51	0/777	0.76	0/1033
73	O7	0.58	0/696	0.77	1/923 (0.1%)
73	o7	0.62	0/696	0.89	1/923 (0.1%)
74	O8	0.48	0/618	0.62	0/826
74	o8	0.47	0/614	0.63	0/822
75	O9	0.70	0/443	0.88	2/588 (0.3%)
75	o9	0.69	0/443	0.86	0/588
76	Q0	0.70	0/423	0.85	2/562 (0.4%)
76	q0	0.86	1/423 (0.2%)	1.00	3/562 (0.5%)
77	Q1	0.61	0/234	0.76	0/300
77	q1	0.68	0/234	0.84	0/300
78	Q2	0.91	1/860 (0.1%)	0.85	1/1136 (0.1%)
78	q2	0.81	1/860 (0.1%)	0.83	1/1136 (0.1%)
79	Q3	0.64	1/701 (0.1%)	0.77	0/934
79	q3	0.69	0/701	0.81	2/934 (0.2%)
80	6	0.97	84/42790 (0.2%)	1.64	980/66673 (1.5%)
81	c0	0.40	0/718	0.60	1/968 (0.1%)
82	sM	0.51	0/481	0.62	0/644
84	p0	0.42	0/1092	0.62	1/1474 (0.1%)
All	All	0.87	517/430468 (0.1%)	1.41	6951/632045 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	2
19	C7	0	2
19	c7	0	1
22	d0	0	1
24	d2	0	1
25	D3	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	3
33	E1	0	3
33	e1	0	1
39	L2	0	1
39	l2	0	3
40	L3	0	1
40	l3	0	1
41	l4	0	1
42	L5	0	2
42	l5	0	2
43	L6	0	1
44	l7	0	2
45	L8	0	1
47	M0	0	1
48	m1	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
55	m9	0	1
56	N0	0	2
56	n0	0	2
59	n3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
62	N6	0	1
64	N8	0	1
64	n8	0	1
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
68	o2	0	2
70	o4	0	1
78	Q2	0	1
78	q2	0	1
All	All	0	67

The worst 5 of 517 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	2707	C	C4-N4	22.02	1.53	1.33
78	Q2	17	CYS	CB-SG	16.14	2.09	1.82
47	m0	92	HIS	C-N	-13.33	1.08	1.34
80	6	89	G	C6-O6	13.07	1.35	1.24
36	5	2606	G	N7-C5	12.96	1.47	1.39

The worst 5 of 6951 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3144	G	O5'-P-OP1	-41.01	61.49	110.70
36	5	2707	C	N3-C4-C5	-37.89	106.74	121.90
36	5	2707	C	C6-N1-C2	-27.23	109.41	120.30
36	5	1779	C	C2-N3-C4	-24.43	107.69	119.90
36	5	1134	G	C5-N7-C8	-21.53	93.53	104.30

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
19	C7	22	PRO	Peptide
3	S1	131	ASP	Peptide
9	S7	131	PHE	Peptide
10	S8	8	ARG	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%)	150 (74%)	34 (17%)	20 (10%)	0	3
2	s0	204/206 (99%)	151 (74%)	30 (15%)	23 (11%)	0	2
3	S1	212/216 (98%)	149 (70%)	42 (20%)	21 (10%)	0	3
3	s1	214/216 (99%)	174 (81%)	29 (14%)	11 (5%)	1	11
4	S2	215/217 (99%)	176 (82%)	22 (10%)	17 (8%)	1	5
4	s2	215/217 (99%)	177 (82%)	23 (11%)	15 (7%)	1	7
5	S3	221/223 (99%)	177 (80%)	34 (15%)	10 (4%)	2	13
5	s3	221/223 (99%)	172 (78%)	31 (14%)	18 (8%)	1	5
6	S4	258/260 (99%)	204 (79%)	40 (16%)	14 (5%)	1	10
6	s4	258/260 (99%)	207 (80%)	30 (12%)	21 (8%)	1	5
7	S5	204/206 (99%)	168 (82%)	21 (10%)	15 (7%)	1	6
7	s5	204/206 (99%)	156 (76%)	30 (15%)	18 (9%)	0	4
8	S6	224/226 (99%)	194 (87%)	18 (8%)	12 (5%)	1	10
8	s6	216/226 (96%)	186 (86%)	18 (8%)	12 (6%)	1	10
9	S7	182/186 (98%)	133 (73%)	25 (14%)	24 (13%)	0	1
9	s7	184/186 (99%)	147 (80%)	23 (12%)	14 (8%)	1	6
10	S8	184/199 (92%)	146 (79%)	29 (16%)	9 (5%)	2	12
10	s8	184/199 (92%)	150 (82%)	27 (15%)	7 (4%)	2	17
11	S9	183/185 (99%)	143 (78%)	28 (15%)	12 (7%)	1	7
11	s9	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	3	19
12	C0	94/96 (98%)	67 (71%)	16 (17%)	11 (12%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	C1	153/155 (99%)	128 (84%)	18 (12%)	7 (5%)	2	13
13	c1	144/155 (93%)	114 (79%)	19 (13%)	11 (8%)	1	6
14	C2	122/124 (98%)	73 (60%)	27 (22%)	22 (18%)	0	1
14	c2	122/124 (98%)	70 (57%)	31 (25%)	21 (17%)	0	1
15	C3	148/150 (99%)	120 (81%)	23 (16%)	5 (3%)	3	19
15	c3	148/150 (99%)	115 (78%)	20 (14%)	13 (9%)	0	4
16	C4	125/128 (98%)	97 (78%)	16 (13%)	12 (10%)	0	3
16	c4	126/128 (98%)	98 (78%)	20 (16%)	8 (6%)	1	8
17	C5	122/135 (90%)	90 (74%)	18 (15%)	14 (12%)	0	2
17	c5	133/135 (98%)	100 (75%)	13 (10%)	20 (15%)	0	1
18	C6	139/142 (98%)	115 (83%)	18 (13%)	6 (4%)	2	14
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	1	9
19	C7	116/125 (93%)	90 (78%)	18 (16%)	8 (7%)	1	7
19	c7	113/125 (90%)	92 (81%)	11 (10%)	10 (9%)	0	4
20	C8	143/145 (99%)	109 (76%)	25 (18%)	9 (6%)	1	8
20	c8	143/145 (99%)	120 (84%)	15 (10%)	8 (6%)	1	10
21	C9	141/143 (99%)	114 (81%)	19 (14%)	8 (6%)	1	9
21	c9	141/143 (99%)	120 (85%)	15 (11%)	6 (4%)	2	14
22	D0	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	12
22	d0	108/110 (98%)	82 (76%)	14 (13%)	12 (11%)	0	2
23	D1	85/87 (98%)	65 (76%)	11 (13%)	9 (11%)	0	2
23	d1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	7
24	D2	127/129 (98%)	102 (80%)	21 (16%)	4 (3%)	3	21
24	d2	127/129 (98%)	100 (79%)	25 (20%)	2 (2%)	8	32
25	D3	142/144 (99%)	109 (77%)	22 (16%)	11 (8%)	1	5
25	d3	142/144 (99%)	119 (84%)	20 (14%)	3 (2%)	5	27
26	D4	132/134 (98%)	108 (82%)	16 (12%)	8 (6%)	1	9
26	d4	132/134 (98%)	100 (76%)	19 (14%)	13 (10%)	0	3
27	D5	68/70 (97%)	49 (72%)	11 (16%)	8 (12%)	0	1
27	d5	67/70 (96%)	51 (76%)	13 (19%)	3 (4%)	2	13
28	D6	95/97 (98%)	62 (65%)	18 (19%)	15 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	d6	95/97 (98%)	71 (75%)	13 (14%)	11 (12%)	0	2
29	D7	79/81 (98%)	62 (78%)	13 (16%)	4 (5%)	1	11
29	d7	79/81 (98%)	58 (73%)	15 (19%)	6 (8%)	1	6
30	D8	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	3	19
30	d8	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	5
31	D9	51/53 (96%)	36 (71%)	8 (16%)	7 (14%)	0	1
31	d9	51/53 (96%)	42 (82%)	6 (12%)	3 (6%)	1	9
32	E0	58/62 (94%)	47 (81%)	7 (12%)	4 (7%)	1	7
32	e0	60/62 (97%)	43 (72%)	10 (17%)	7 (12%)	0	1
33	E1	69/76 (91%)	39 (56%)	15 (22%)	15 (22%)	0	0
33	e1	74/76 (97%)	38 (51%)	19 (26%)	17 (23%)	0	0
34	SR	316/318 (99%)	275 (87%)	31 (10%)	10 (3%)	3	20
34	sR	316/318 (99%)	259 (82%)	44 (14%)	13 (4%)	2	15
35	SM	131/159 (82%)	95 (72%)	18 (14%)	18 (14%)	0	1
39	L2	250/252 (99%)	222 (89%)	17 (7%)	11 (4%)	2	14
39	l2	250/252 (99%)	201 (80%)	39 (16%)	10 (4%)	2	16
40	L3	384/386 (100%)	323 (84%)	44 (12%)	17 (4%)	2	14
40	l3	384/386 (100%)	331 (86%)	35 (9%)	18 (5%)	2	13
41	L4	359/361 (99%)	284 (79%)	50 (14%)	25 (7%)	1	7
41	l4	359/361 (99%)	275 (77%)	57 (16%)	27 (8%)	1	6
42	L5	294/296 (99%)	225 (76%)	43 (15%)	26 (9%)	0	4
42	l5	292/296 (99%)	243 (83%)	42 (14%)	7 (2%)	5	25
43	L6	152/175 (87%)	131 (86%)	18 (12%)	3 (2%)	6	28
43	l6	153/175 (87%)	123 (80%)	25 (16%)	5 (3%)	3	19
44	L7	220/223 (99%)	185 (84%)	26 (12%)	9 (4%)	2	15
44	l7	221/223 (99%)	195 (88%)	18 (8%)	8 (4%)	3	18
45	L8	231/233 (99%)	180 (78%)	35 (15%)	16 (7%)	1	7
45	l8	229/233 (98%)	179 (78%)	33 (14%)	17 (7%)	1	6
46	L9	189/191 (99%)	159 (84%)	22 (12%)	8 (4%)	2	15
46	l9	189/191 (99%)	156 (82%)	25 (13%)	8 (4%)	2	15
47	M0	207/220 (94%)	166 (80%)	30 (14%)	11 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	m0	209/220 (95%)	164 (78%)	30 (14%)	15 (7%)	1	6
48	M1	167/169 (99%)	132 (79%)	16 (10%)	19 (11%)	0	2
48	m1	167/169 (99%)	137 (82%)	18 (11%)	12 (7%)	1	6
49	M3	191/194 (98%)	148 (78%)	28 (15%)	15 (8%)	1	5
49	m3	192/194 (99%)	153 (80%)	26 (14%)	13 (7%)	1	7
50	M4	134/137 (98%)	109 (81%)	14 (10%)	11 (8%)	1	5
50	m4	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	8	33
51	M5	201/203 (99%)	171 (85%)	21 (10%)	9 (4%)	2	13
51	m5	201/203 (99%)	169 (84%)	26 (13%)	6 (3%)	3	21
52	M6	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	13	42
52	m6	195/197 (99%)	179 (92%)	13 (7%)	3 (2%)	8	33
53	M7	181/183 (99%)	144 (80%)	26 (14%)	11 (6%)	1	9
53	m7	153/183 (84%)	127 (83%)	24 (16%)	2 (1%)	10	36
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	3	19
54	m8	183/185 (99%)	151 (82%)	18 (10%)	14 (8%)	1	5
55	M9	186/188 (99%)	159 (86%)	23 (12%)	4 (2%)	5	26
55	m9	186/188 (99%)	165 (89%)	20 (11%)	1 (0%)	25	56
56	N0	170/172 (99%)	149 (88%)	16 (9%)	5 (3%)	3	22
56	n0	170/172 (99%)	150 (88%)	17 (10%)	3 (2%)	7	30
57	N1	157/159 (99%)	133 (85%)	16 (10%)	8 (5%)	1	11
57	n1	157/159 (99%)	132 (84%)	21 (13%)	4 (2%)	4	24
58	N2	98/100 (98%)	70 (71%)	23 (24%)	5 (5%)	1	11
58	n2	96/100 (96%)	82 (85%)	10 (10%)	4 (4%)	2	15
59	N3	134/136 (98%)	118 (88%)	14 (10%)	2 (2%)	8	33
59	n3	134/136 (98%)	120 (90%)	9 (7%)	5 (4%)	2	17
60	N4	96/135 (71%)	73 (76%)	17 (18%)	6 (6%)	1	8
60	n4	133/135 (98%)	103 (77%)	19 (14%)	11 (8%)	0	5
61	N5	119/121 (98%)	99 (83%)	14 (12%)	6 (5%)	1	12
61	n5	118/121 (98%)	103 (87%)	9 (8%)	6 (5%)	1	11
62	N6	124/126 (98%)	100 (81%)	19 (15%)	5 (4%)	2	16
62	n6	124/126 (98%)	108 (87%)	7 (6%)	9 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	N7	133/135 (98%)	109 (82%)	16 (12%)	8 (6%)	1	9
63	n7	133/135 (98%)	105 (79%)	16 (12%)	12 (9%)	0	4
64	N8	146/148 (99%)	109 (75%)	28 (19%)	9 (6%)	1	9
64	n8	146/148 (99%)	114 (78%)	22 (15%)	10 (7%)	1	7
65	N9	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	3	18
65	n9	56/58 (97%)	37 (66%)	11 (20%)	8 (14%)	0	1
66	O0	95/100 (95%)	85 (90%)	8 (8%)	2 (2%)	5	27
66	o0	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	6	28
67	O1	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	2	13
67	o1	107/109 (98%)	91 (85%)	11 (10%)	5 (5%)	2	13
68	O2	125/127 (98%)	94 (75%)	22 (18%)	9 (7%)	1	6
68	o2	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	12
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	3	22
69	o3	104/106 (98%)	92 (88%)	6 (6%)	6 (6%)	1	9
70	O4	110/112 (98%)	94 (86%)	12 (11%)	4 (4%)	3	18
70	o4	110/112 (98%)	91 (83%)	16 (14%)	3 (3%)	4	22
71	O5	117/119 (98%)	98 (84%)	11 (9%)	8 (7%)	1	7
71	o5	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	3	19
72	O6	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	0	2
72	o6	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	5
73	O7	85/87 (98%)	67 (79%)	17 (20%)	1 (1%)	11	38
73	o7	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	3	19
74	O8	75/77 (97%)	61 (81%)	12 (16%)	2 (3%)	4	22
74	o8	75/77 (97%)	60 (80%)	9 (12%)	6 (8%)	1	5
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	5	27
75	o9	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
76	Q0	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	2	16
76	q0	50/52 (96%)	41 (82%)	8 (16%)	1 (2%)	6	28
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	3 (13%)	1 (4%)	2	14
78	Q2	103/105 (98%)	79 (77%)	19 (18%)	5 (5%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	q2	103/105 (98%)	90 (87%)	8 (8%)	5 (5%)	2	12
79	Q3	89/91 (98%)	76 (85%)	7 (8%)	6 (7%)	1	7
79	q3	89/91 (98%)	78 (88%)	8 (9%)	3 (3%)	3	19
81	c0	82/96 (85%)	63 (77%)	11 (13%)	8 (10%)	0	3
82	sM	61/104 (59%)	38 (62%)	15 (25%)	8 (13%)	0	1
84	p0	139/219 (64%)	115 (83%)	17 (12%)	7 (5%)	1	12
All	All	22262/22948 (97%)	17987 (81%)	2915 (13%)	1360 (6%)	1	9

5 of 1360 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	5	ALA
2	S0	30	GLN
2	S0	36	TYR
2	S0	95	ALA

### 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%)	133 (81%)	31 (19%)	1	6
2	s0	165/173 (95%)	128 (78%)	37 (22%)	1	3
3	S1	191/192 (100%)	152 (80%)	39 (20%)	1	4
3	s1	192/192 (100%)	148 (77%)	44 (23%)	0	3
4	S2	176/176 (100%)	139 (79%)	37 (21%)	1	4
4	s2	176/176 (100%)	132 (75%)	44 (25%)	0	2
5	S3	182/182 (100%)	149 (82%)	33 (18%)	1	6
5	s3	182/182 (100%)	150 (82%)	32 (18%)	1	7
6	S4	221/221 (100%)	176 (80%)	45 (20%)	1	4
6	s4	221/221 (100%)	179 (81%)	42 (19%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	S5	173/173 (100%)	143 (83%)	30 (17%)	1	7
7	s5	173/173 (100%)	146 (84%)	27 (16%)	2	10
8	S6	188/193 (97%)	147 (78%)	41 (22%)	1	3
8	s6	187/193 (97%)	149 (80%)	38 (20%)	1	4
9	S7	165/166 (99%)	132 (80%)	33 (20%)	1	5
9	s7	165/166 (99%)	132 (80%)	33 (20%)	1	5
10	S8	150/160 (94%)	126 (84%)	24 (16%)	2	9
10	s8	150/160 (94%)	125 (83%)	25 (17%)	2	8
11	S9	158/158 (100%)	124 (78%)	34 (22%)	1	4
11	s9	158/158 (100%)	122 (77%)	36 (23%)	0	3
12	C0	77/89 (86%)	63 (82%)	14 (18%)	1	6
13	C1	129/136 (95%)	110 (85%)	19 (15%)	2	11
13	c1	129/136 (95%)	102 (79%)	27 (21%)	1	4
14	C2	88/100 (88%)	65 (74%)	23 (26%)	0	2
14	c2	88/100 (88%)	69 (78%)	19 (22%)	1	3
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	4
15	c3	127/127 (100%)	104 (82%)	23 (18%)	1	6
16	C4	81/97 (84%)	58 (72%)	23 (28%)	0	1
16	c4	97/97 (100%)	65 (67%)	32 (33%)	0	1
17	C5	101/111 (91%)	85 (84%)	16 (16%)	2	10
17	c5	103/111 (93%)	88 (85%)	15 (15%)	2	12
18	C6	117/118 (99%)	93 (80%)	24 (20%)	1	4
18	c6	118/118 (100%)	94 (80%)	24 (20%)	1	4
19	C7	94/113 (83%)	73 (78%)	21 (22%)	1	3
19	c7	92/113 (81%)	73 (79%)	19 (21%)	1	4
20	C8	128/128 (100%)	96 (75%)	32 (25%)	0	2
20	c8	128/128 (100%)	104 (81%)	24 (19%)	1	6
21	C9	115/115 (100%)	88 (76%)	27 (24%)	0	3
21	c9	115/115 (100%)	92 (80%)	23 (20%)	1	5
22	D0	100/103 (97%)	76 (76%)	24 (24%)	0	3
22	d0	103/103 (100%)	76 (74%)	27 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	D1	74/74 (100%)	63 (85%)	11 (15%)	2	11
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	3
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	5
24	d2	110/110 (100%)	90 (82%)	20 (18%)	1	6
25	D3	119/119 (100%)	98 (82%)	21 (18%)	1	7
25	d3	119/119 (100%)	100 (84%)	19 (16%)	2	9
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1	6
26	d4	112/112 (100%)	91 (81%)	21 (19%)	1	6
27	D5	61/61 (100%)	44 (72%)	17 (28%)	0	1
27	d5	61/61 (100%)	52 (85%)	9 (15%)	2	11
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	3
28	d6	83/83 (100%)	67 (81%)	16 (19%)	1	5
29	D7	70/70 (100%)	61 (87%)	9 (13%)	3	15
29	d7	70/70 (100%)	61 (87%)	9 (13%)	3	15
30	D8	56/56 (100%)	44 (79%)	12 (21%)	1	4
30	d8	56/56 (100%)	43 (77%)	13 (23%)	0	3
31	D9	47/47 (100%)	35 (74%)	12 (26%)	0	2
31	d9	47/47 (100%)	40 (85%)	7 (15%)	2	11
32	E0	51/53 (96%)	45 (88%)	6 (12%)	4	17
32	e0	53/53 (100%)	37 (70%)	16 (30%)	0	1
33	E1	62/66 (94%)	50 (81%)	12 (19%)	1	5
33	e1	66/66 (100%)	50 (76%)	16 (24%)	0	2
34	SR	259/261 (99%)	226 (87%)	33 (13%)	3	15
34	sR	260/261 (100%)	231 (89%)	29 (11%)	5	19
35	SM	97/107 (91%)	76 (78%)	21 (22%)	1	3
39	L2	193/194 (100%)	155 (80%)	38 (20%)	1	5
39	l2	192/194 (99%)	153 (80%)	39 (20%)	1	4
40	L3	319/322 (99%)	249 (78%)	70 (22%)	1	3
40	l3	321/322 (100%)	252 (78%)	69 (22%)	1	4
41	L4	288/288 (100%)	232 (81%)	56 (19%)	1	5
41	l4	288/288 (100%)	234 (81%)	54 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	L5	244/244 (100%)	198 (81%)	46 (19%)	1	6
42	l5	243/244 (100%)	189 (78%)	54 (22%)	1	3
43	L6	134/152 (88%)	114 (85%)	20 (15%)	2	11
43	l6	135/152 (89%)	111 (82%)	24 (18%)	1	7
44	L7	186/187 (100%)	160 (86%)	26 (14%)	3	13
44	l7	187/187 (100%)	155 (83%)	32 (17%)	1	8
45	L8	187/191 (98%)	157 (84%)	30 (16%)	2	9
45	l8	177/191 (93%)	142 (80%)	35 (20%)	1	5
46	L9	171/171 (100%)	130 (76%)	41 (24%)	0	3
46	l9	171/171 (100%)	132 (77%)	39 (23%)	0	3
47	M0	177/186 (95%)	151 (85%)	26 (15%)	2	11
47	m0	179/186 (96%)	138 (77%)	41 (23%)	0	3
48	M1	147/147 (100%)	119 (81%)	28 (19%)	1	5
48	m1	147/147 (100%)	120 (82%)	27 (18%)	1	6
49	M3	154/154 (100%)	124 (80%)	30 (20%)	1	5
49	m3	154/154 (100%)	123 (80%)	31 (20%)	1	4
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	6
50	m4	108/108 (100%)	85 (79%)	23 (21%)	1	4
51	M5	175/175 (100%)	140 (80%)	35 (20%)	1	5
51	m5	175/175 (100%)	140 (80%)	35 (20%)	1	5
52	M6	160/160 (100%)	139 (87%)	21 (13%)	3	14
52	m6	160/160 (100%)	135 (84%)	25 (16%)	2	10
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	3
53	m7	125/145 (86%)	94 (75%)	31 (25%)	0	2
54	M8	150/150 (100%)	124 (83%)	26 (17%)	1	7
54	m8	150/150 (100%)	116 (77%)	34 (23%)	0	3
55	M9	153/153 (100%)	129 (84%)	24 (16%)	2	10
55	m9	153/153 (100%)	125 (82%)	28 (18%)	1	6
56	N0	156/156 (100%)	127 (81%)	29 (19%)	1	6
56	n0	156/156 (100%)	128 (82%)	28 (18%)	1	7
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	n1	136/136 (100%)	109 (80%)	27 (20%)	1	5
58	N2	87/87 (100%)	70 (80%)	17 (20%)	1	5
58	n2	85/87 (98%)	69 (81%)	16 (19%)	1	6
59	N3	104/104 (100%)	89 (86%)	15 (14%)	2	12
59	n3	104/104 (100%)	89 (86%)	15 (14%)	2	12
60	N4	57/114 (50%)	50 (88%)	7 (12%)	4	16
60	n4	100/114 (88%)	85 (85%)	15 (15%)	2	11
61	N5	104/105 (99%)	82 (79%)	22 (21%)	1	4
61	n5	104/105 (99%)	82 (79%)	22 (21%)	1	4
62	N6	109/109 (100%)	85 (78%)	24 (22%)	1	3
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1	3
63	N7	115/115 (100%)	93 (81%)	22 (19%)	1	5
63	n7	115/115 (100%)	93 (81%)	22 (19%)	1	5
64	N8	118/118 (100%)	93 (79%)	25 (21%)	1	4
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	4
65	N9	46/46 (100%)	37 (80%)	9 (20%)	1	5
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	1
66	O0	81/84 (96%)	68 (84%)	13 (16%)	2	9
66	o0	84/84 (100%)	70 (83%)	14 (17%)	2	8
67	O1	92/96 (96%)	68 (74%)	24 (26%)	0	2
67	o1	94/96 (98%)	72 (77%)	22 (23%)	0	3
68	O2	109/109 (100%)	89 (82%)	20 (18%)	1	6
68	o2	109/109 (100%)	90 (83%)	19 (17%)	1	7
69	O3	90/90 (100%)	75 (83%)	15 (17%)	2	8
69	o3	90/90 (100%)	78 (87%)	12 (13%)	3	14
70	O4	95/95 (100%)	80 (84%)	15 (16%)	2	10
70	o4	95/95 (100%)	82 (86%)	13 (14%)	3	13
71	O5	104/104 (100%)	79 (76%)	25 (24%)	0	3
71	o5	103/104 (99%)	83 (81%)	20 (19%)	1	5
72	O6	81/81 (100%)	59 (73%)	22 (27%)	0	1
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	O7	70/70 (100%)	54 (77%)	16 (23%)	0	3
73	o7	70/70 (100%)	54 (77%)	16 (23%)	0	3
74	O8	68/68 (100%)	51 (75%)	17 (25%)	0	2
74	o8	67/68 (98%)	50 (75%)	17 (25%)	0	2
75	O9	45/45 (100%)	37 (82%)	8 (18%)	1	7
75	o9	45/45 (100%)	39 (87%)	6 (13%)	3	14
76	Q0	47/47 (100%)	37 (79%)	10 (21%)	1	4
76	q0	47/47 (100%)	34 (72%)	13 (28%)	0	1
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
78	Q2	90/90 (100%)	65 (72%)	25 (28%)	0	1
78	q2	90/90 (100%)	66 (73%)	24 (27%)	0	2
79	Q3	71/71 (100%)	63 (89%)	8 (11%)	4	18
79	q3	71/71 (100%)	54 (76%)	17 (24%)	0	3
81	c0	73/78 (94%)	60 (82%)	13 (18%)	1	7
82	sM	54/54 (100%)	40 (74%)	14 (26%)	0	2
84	p0	105/186 (56%)	82 (78%)	23 (22%)	1	3
All	All	18727/19202 (98%)	15037 (80%)	3690 (20%)	1	5

5 of 3690 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	s1	62	LYS
72	o6	11	LEU
17	c5	124	THR
69	o3	86	ARG
54	m8	135	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
47	M0	144	ASN
56	n0	8	GLN
68	O2	104	ASN
55	m9	7	GLN

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Mol	Chain	Res	Type
75	o9	33	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1829 (97%)	519 (29%)	70 (3%)
36	1	3145/3394 (92%)	765 (24%)	87 (2%)
36	5	3145/3394 (92%)	772 (24%)	92 (2%)
37	3	120/121 (99%)	22 (18%)	3 (2%)
37	7	120/121 (99%)	23 (19%)	1 (0%)
38	4	157/158 (99%)	42 (26%)	4 (2%)
38	8	157/158 (99%)	40 (25%)	3 (1%)
80	6	1792/1800 (99%)	489 (27%)	67 (3%)
All	All	10412/10975 (94%)	2672 (25%)	327 (3%)

5 of 2672 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 327 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	65	A
36	5	2372	A
36	5	374	A
36	5	1284	C
36	5	2801	A

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 3561 ligands modelled in this entry, 2208 are monoatomic - leaving 1353 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
86	OHX	6	2077	86	0,6,6	-	-	-		
86	OHX	5	3712	-	0,6,6	-	-	-		
86	OHX	2	2028	1	0,6,6	-	-	-		
86	OHX	1	3417	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	4	201	-	0,6,6	-	-	-		
86	OHX	5	3407	36	0,6,6	-	-	-		
86	OHX	1	3549	-	0,6,6	-	-	-		
86	OHX	2	1976	86	0,6,6	-	-	-		
86	OHX	2	1901	-	0,6,6	-	-	-		
86	OHX	1	3516	-	0,6,6	-	-	-		
86	OHX	5	3701	36	0,6,6	-	-	-		
86	OHX	5	3753	86,36	0,6,6	-	-	-		
86	OHX	1	3432	-	0,6,6	-	-	-		
86	OHX	1	3597	-	0,6,6	-	-	-		
86	OHX	5	3799	-	0,6,6	-	-	-		
86	OHX	8	204	-	0,6,6	-	-	-		
86	OHX	5	3794	86	0,6,6	-	-	-		
86	OHX	1	3653	-	0,6,6	-	-	-		
86	OHX	5	3527	86,36	0,6,6	-	-	-		
86	OHX	5	3447	86	0,6,6	-	-	-		
86	OHX	5	3675	36	0,6,6	-	-	-		
86	OHX	1	3794	86	0,6,6	-	-	-		
86	OHX	5	3512	86	0,6,6	-	-	-		
86	OHX	1	3478	86	0,6,6	-	-	-		
86	OHX	5	3526	-	0,6,6	-	-	-		
86	OHX	5	3735	86	0,6,6	-	-	-		
86	OHX	1	3558	-	0,6,6	-	-	-		
86	OHX	L3	402	-	0,6,6	-	-	-		
86	OHX	L5	301	-	0,6,6	-	-	-		
86	OHX	1	3723	86	0,6,6	-	-	-		
86	OHX	5	3756	36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	1905	-	0,6,6	-	-	-		
86	OHX	2	2009	-	0,6,6	-	-	-		
86	OHX	1	3487	-	0,6,6	-	-	-		
89	C	1	3402	90	18,21,22	0.57	0	26,30,33	0.78	1 (3%)
86	OHX	5	3589	-	0,6,6	-	-	-		
86	OHX	1	3485	-	0,6,6	-	-	-		
86	OHX	2	1980	86	0,6,6	-	-	-		
86	OHX	5	3537	36	0,6,6	-	-	-		
86	OHX	6	2039	-	0,6,6	-	-	-		
86	OHX	5	3435	-	0,6,6	-	-	-		
86	OHX	2	1975	86	0,6,6	-	-	-		
86	OHX	2	1948	86	0,6,6	-	-	-		
86	OHX	1	3600	86	0,6,6	-	-	-		
86	OHX	5	3765	86	0,6,6	-	-	-		
86	OHX	6	1979	80	0,6,6	-	-	-		
86	OHX	1	3762	-	0,6,6	-	-	-		
86	OHX	6	2088	86	0,6,6	-	-	-		
86	OHX	5	3602	86	0,6,6	-	-	-		
86	OHX	5	3709	36	0,6,6	-	-	-		
86	OHX	5	3792	86	0,6,6	-	-	-		
86	OHX	N8	201	-	0,6,6	-	-	-		
86	OHX	5	3518	36	0,6,6	-	-	-		
86	OHX	1	3724	86	0,6,6	-	-	-		
86	OHX	6	1916	-	0,6,6	-	-	-		
86	OHX	5	3696	36	0,6,6	-	-	-		
86	OHX	1	3715	86	0,6,6	-	-	-		
86	OHX	2	1965	86	0,6,6	-	-	-		
86	OHX	1	3409	36	0,6,6	-	-	-		
86	OHX	5	3725	86,36	0,6,6	-	-	-		
86	OHX	2	2003	1	0,6,6	-	-	-		
86	OHX	5	3532	-	0,6,6	-	-	-		
86	OHX	1	3589	-	0,6,6	-	-	-		
86	OHX	5	3566	-	0,6,6	-	-	-		
86	OHX	1	3501	-	0,6,6	-	-	-		
86	OHX	6	1940	-	0,6,6	-	-	-		
86	OHX	5	3480	86	0,6,6	-	-	-		
86	OHX	1	3507	-	0,6,6	-	-	-		
86	OHX	5	3708	86	0,6,6	-	-	-		
86	OHX	2	2062	1	0,6,6	-	-	-		
86	OHX	1	3759	-	0,6,6	-	-	-		
86	OHX	1	3502	86,36	0,6,6	-	-	-		
86	OHX	6	2041	80	0,6,6	-	-	-		
86	OHX	1	3564	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3505	86	0,6,6	-	-	-		
86	OHX	1	3700	86	0,6,6	-	-	-		
86	OHX	2	2013	1	0,6,6	-	-	-		
86	OHX	1	3780	-	0,6,6	-	-	-		
86	OHX	3	209	86	0,6,6	-	-	-		
86	OHX	5	3704	86	0,6,6	-	-	-		
86	OHX	5	3509	86	0,6,6	-	-	-		
86	OHX	5	3445	-	0,6,6	-	-	-		
86	OHX	1	3438	86	0,6,6	-	-	-		
86	OHX	4	208	38	0,6,6	-	-	-		
86	OHX	6	2050	80	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	5	3593	86,36	0,6,6	-	-	-		
86	OHX	1	3617	86,36	0,6,6	-	-	-		
86	OHX	1	3611	-	0,6,6	-	-	-		
86	OHX	Q2	502	-	0,6,6	-	-	-		
86	OHX	2	1951	-	0,6,6	-	-	-		
86	OHX	5	3738	-	0,6,6	-	-	-		
86	OHX	1	3444	-	0,6,6	-	-	-		
86	OHX	5	3587	86,36	0,6,6	-	-	-		
86	OHX	1	3641	-	0,6,6	-	-	-		
86	OHX	1	3786	86	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	1	3692	-	0,6,6	-	-	-		
86	OHX	1	3756	86,36	0,6,6	-	-	-		
86	OHX	1	3690	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	1	3623	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	1	3652	-	0,6,6	-	-	-		
86	OHX	1	3479	86	0,6,6	-	-	-		
86	OHX	1	3477	86	0,6,6	-	-	-		
86	OHX	1	3773	-	0,6,6	-	-	-		
86	OHX	5	3732	86	0,6,6	-	-	-		
86	OHX	6	1975	86,80	0,6,6	-	-	-		
86	OHX	1	3469	86	0,6,6	-	-	-		
86	OHX	5	3790	-	0,6,6	-	-	-		
86	OHX	1	3749	-	0,6,6	-	-	-		
86	OHX	1	3621	-	0,6,6	-	-	-		
86	OHX	m0	303	86	0,6,6	-	-	-		
86	OHX	1	3415	-	0,6,6	-	-	-		
86	OHX	5	3787	-	0,6,6	-	-	-		
86	OHX	1	3466	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	2	2019	-	0,6,6	-	-	-		
86	OHX	2	1927	-	0,6,6	-	-	-		
86	OHX	1	3573	-	0,6,6	-	-	-		
86	OHX	5	3572	86	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	5	3747	36	0,6,6	-	-	-		
86	OHX	6	1942	80	0,6,6	-	-	-		
86	OHX	1	3777	86	0,6,6	-	-	-		
86	OHX	5	3789	-	0,6,6	-	-	-		
86	OHX	1	3783	86	0,6,6	-	-	-		
86	OHX	1	3499	-	0,6,6	-	-	-		
86	OHX	5	3437	36	0,6,6	-	-	-		
86	OHX	M8	201	-	0,6,6	-	-	-		
86	OHX	5	3758	36	0,6,6	-	-	-		
86	OHX	5	3804	86,36	0,6,6	-	-	-		
86	OHX	1	3510	36	0,6,6	-	-	-		
86	OHX	1	3594	-	0,6,6	-	-	-		
86	OHX	6	1938	86,80	0,6,6	-	-	-		
86	OHX	5	3483	86	0,6,6	-	-	-		
86	OHX	1	3665	-	0,6,6	-	-	-		
86	OHX	6	1977	-	0,6,6	-	-	-		
86	OHX	1	3678	86	0,6,6	-	-	-		
86	OHX	2	2081	86	0,6,6	-	-	-		
86	OHX	1	3574	-	0,6,6	-	-	-		
86	OHX	1	3781	-	0,6,6	-	-	-		
86	OHX	6	1901	80	0,6,6	-	-	-		
86	OHX	1	3808	86	0,6,6	-	-	-		
86	OHX	1	3763	86	0,6,6	-	-	-		
86	OHX	5	3490	-	0,6,6	-	-	-		
86	OHX	5	3431	-	0,6,6	-	-	-		
86	OHX	1	3557	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	1	3533	-	0,6,6	-	-	-		
86	OHX	6	1912	-	0,6,6	-	-	-		
86	OHX	5	3745	-	0,6,6	-	-	-		
86	OHX	5	3698	-	0,6,6	-	-	-		
86	OHX	1	3553	86	0,6,6	-	-	-		
86	OHX	5	3654	86	0,6,6	-	-	-		
86	OHX	1	3684	-	0,6,6	-	-	-		
86	OHX	7	204	-	0,6,6	-	-	-		
86	OHX	2	2088	86,1	0,6,6	-	-	-		
86	OHX	1	3714	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3674	86,36	0,6,6	-	-	-		
86	OHX	5	3796	86,36	0,6,6	-	-	-		
86	OHX	7	208	-	0,6,6	-	-	-		
86	OHX	1	3490	-	0,6,6	-	-	-		
86	OHX	1	3461	86	0,6,6	-	-	-		
86	OHX	1	3420	-	0,6,6	-	-	-		
86	OHX	1	3560	36	0,6,6	-	-	-		
86	OHX	m9	201	-	0,6,6	-	-	-		
86	OHX	5	3559	-	0,6,6	-	-	-		
86	OHX	5	3684	-	0,6,6	-	-	-		
86	OHX	1	3578	-	0,6,6	-	-	-		
86	OHX	5	3523	86	0,6,6	-	-	-		
86	OHX	2	1920	-	0,6,6	-	-	-		
86	OHX	1	3646	-	0,6,6	-	-	-		
86	OHX	6	2001	-	0,6,6	-	-	-		
86	OHX	1	3716	86	0,6,6	-	-	-		
86	OHX	5	3764	-	0,6,6	-	-	-		
86	OHX	5	3535	-	0,6,6	-	-	-		
86	OHX	1	3796	-	0,6,6	-	-	-		
86	OHX	2	2053	86	0,6,6	-	-	-		
86	OHX	1	3582	36	0,6,6	-	-	-		
86	OHX	6	1970	-	0,6,6	-	-	-		
86	OHX	5	3645	86	0,6,6	-	-	-		
86	OHX	6	1980	80	0,6,6	-	-	-		
86	OHX	2	2071	86	0,6,6	-	-	-		
86	OHX	8	216	38	0,6,6	-	-	-		
86	OHX	5	3710	86	0,6,6	-	-	-		
86	OHX	5	3544	-	0,6,6	-	-	-		
86	OHX	2	1914	1	0,6,6	-	-	-		
86	OHX	1	3592	-	0,6,6	-	-	-		
86	OHX	2	1986	-	0,6,6	-	-	-		
86	OHX	1	3628	-	0,6,6	-	-	-		
86	OHX	1	3613	-	0,6,6	-	-	-		
86	OHX	6	2007	80	0,6,6	-	-	-		
86	OHX	1	3520	-	0,6,6	-	-	-		
86	OHX	5	3522	36	0,6,6	-	-	-		
86	OHX	M5	301	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	4	209	-	0,6,6	-	-	-		
86	OHX	1	3584	36	0,6,6	-	-	-		
86	OHX	6	2031	-	0,6,6	-	-	-		
86	OHX	5	3600	-	0,6,6	-	-	-		
86	OHX	5	3506	86,36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	7	203	86	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	1	3550	-	0,6,6	-	-	-		
86	OHX	5	3702	36	0,6,6	-	-	-		
86	OHX	5	3497	-	0,6,6	-	-	-		
86	OHX	1	3629	36	0,6,6	-	-	-		
86	OHX	2	1912	-	0,6,6	-	-	-		
86	OHX	6	2067	86	0,6,6	-	-	-		
86	OHX	1	3695	86	0,6,6	-	-	-		
86	OHX	1	3811	86	0,6,6	-	-	-		
86	OHX	6	2014	-	0,6,6	-	-	-		
86	OHX	1	3738	86	0,6,6	-	-	-		
86	OHX	6	1941	80	0,6,6	-	-	-		
86	OHX	5	3605	36	0,6,6	-	-	-		
86	OHX	5	3519	36	0,6,6	-	-	-		
86	OHX	1	3616	86	0,6,6	-	-	-		
86	OHX	5	3481	-	0,6,6	-	-	-		
86	OHX	5	3681	-	0,6,6	-	-	-		
86	OHX	3	208	-	0,6,6	-	-	-		
86	OHX	m1	201	-	0,6,6	-	-	-		
86	OHX	2	2070	86	0,6,6	-	-	-		
86	OHX	l5	302	-	0,6,6	-	-	-		
86	OHX	1	3776	86	0,6,6	-	-	-		
86	OHX	6	1989	80	0,6,6	-	-	-		
86	OHX	2	1911	-	0,6,6	-	-	-		
86	OHX	1	3519	36	0,6,6	-	-	-		
86	OHX	1	3702	-	0,6,6	-	-	-		
86	OHX	5	3507	86	0,6,6	-	-	-		
86	OHX	1	3462	-	0,6,6	-	-	-		
86	OHX	8	209	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	1	3722	86	0,6,6	-	-	-		
86	OHX	2	1993	1	0,6,6	-	-	-		
86	OHX	6	1919	86,80	0,6,6	-	-	-		
86	OHX	6	1955	80	0,6,6	-	-	-		
86	OHX	5	3620	86	0,6,6	-	-	-		
86	OHX	8	213	-	0,6,6	-	-	-		
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	7	211	86	0,6,6	-	-	-		
86	OHX	6	2058	86	0,6,6	-	-	-		
86	OHX	1	3491	-	0,6,6	-	-	-		
86	OHX	5	3417	-	0,6,6	-	-	-		
86	OHX	2	1936	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3549	-	0,6,6	-	-	-		
86	OHX	5	3760	86	0,6,6	-	-	-		
86	OHX	5	3432	-	0,6,6	-	-	-		
86	OHX	m0	302	86	0,6,6	-	-	-		
86	OHX	1	3769	-	0,6,6	-	-	-		
86	OHX	1	3809	86,36	0,6,6	-	-	-		
86	OHX	6	2017	80	0,6,6	-	-	-		
86	OHX	5	3746	36	0,6,6	-	-	-		
86	OHX	6	1954	86	0,6,6	-	-	-		
86	OHX	6	2083	86	0,6,6	-	-	-		
86	OHX	2	2022	86	0,6,6	-	-	-		
86	OHX	5	3601	-	0,6,6	-	-	-		
86	OHX	6	1904	80	0,6,6	-	-	-		
86	OHX	8	219	38	0,6,6	-	-	-		
86	OHX	5	3688	86	0,6,6	-	-	-		
86	OHX	5	3534	36	0,6,6	-	-	-		
86	OHX	2	2082	86,1	0,6,6	-	-	-		
86	OHX	1	3806	-	0,6,6	-	-	-		
86	OHX	5	3785	-	0,6,6	-	-	-		
86	OHX	1	3575	86	0,6,6	-	-	-		
86	OHX	5	3612	36	0,6,6	-	-	-		
86	OHX	1	3719	-	0,6,6	-	-	-		
86	OHX	5	3633	36	0,6,6	-	-	-		
86	OHX	1	3579	36	0,6,6	-	-	-		
86	OHX	L3	401	-	0,6,6	-	-	-		
86	OHX	5	3798	36	0,6,6	-	-	-		
86	OHX	6	1945	80	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	5	3550	-	0,6,6	-	-	-		
86	OHX	5	3673	86,36	0,6,6	-	-	-		
86	OHX	1	3554	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	1	3685	86,36	0,6,6	-	-	-		
86	OHX	1	3701	-	0,6,6	-	-	-		
86	OHX	1	3747	36	0,6,6	-	-	-		
86	OHX	5	3592	-	0,6,6	-	-	-		
86	OHX	5	3762	36	0,6,6	-	-	-		
86	OHX	1	3465	86	0,6,6	-	-	-		
86	OHX	6	2097	86	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	6	2027	-	0,6,6	-	-	-		
86	OHX	14	401	-	0,6,6	-	-	-		
86	OHX	1	3437	86	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3770	-	0,6,6	-	-	-		
86	OHX	2	2078	86	0,6,6	-	-	-		
86	OHX	19	201	-	0,6,6	-	-	-		
86	OHX	1	3421	-	0,6,6	-	-	-		
86	OHX	m5	502	-	0,6,6	-	-	-		
86	OHX	C8	201	86	0,6,6	-	-	-		
86	OHX	1	3433	-	0,6,6	-	-	-		
86	OHX	6	2068	86,80	0,6,6	-	-	-		
86	OHX	2	1973	86	0,6,6	-	-	-		
86	OHX	4	203	-	0,6,6	-	-	-		
86	OHX	n9	101	-	0,6,6	-	-	-		
86	OHX	5	3574	-	0,6,6	-	-	-		
86	OHX	2	2052	1	0,6,6	-	-	-		
86	OHX	1	3515	-	0,6,6	-	-	-		
86	OHX	1	3567	-	0,6,6	-	-	-		
86	OHX	1	3492	-	0,6,6	-	-	-		
86	OHX	6	2070	86,80	0,6,6	-	-	-		
86	OHX	1	3798	-	0,6,6	-	-	-		
86	OHX	1	3734	86	0,6,6	-	-	-		
86	OHX	1	3615	86	0,6,6	-	-	-		
86	OHX	s8	301	-	0,6,6	-	-	-		
86	OHX	5	3406	36	0,6,6	-	-	-		
86	OHX	5	3759	-	0,6,6	-	-	-		
86	OHX	1	3541	-	0,6,6	-	-	-		
86	OHX	5	3482	86	0,6,6	-	-	-		
86	OHX	2	2005	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	3626	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	6	1988	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	1	3408	-	0,6,6	-	-	-		
86	OHX	5	3722	86	0,6,6	-	-	-		
86	OHX	2	2035	86	0,6,6	-	-	-		
86	OHX	5	3617	-	0,6,6	-	-	-		
86	OHX	5	3640	-	0,6,6	-	-	-		
86	OHX	2	1989	86	0,6,6	-	-	-		
86	OHX	5	3637	36	0,6,6	-	-	-		
86	OHX	1	3793	-	0,6,6	-	-	-		
86	OHX	2	2001	-	0,6,6	-	-	-		
86	OHX	1	3532	-	0,6,6	-	-	-		
86	OHX	1	3667	86,36	0,6,6	-	-	-		
86	OHX	2	1930	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3458	-	0,6,6	-	-	-		
86	OHX	5	3713	86,36	0,6,6	-	-	-		
86	OHX	5	3690	-	0,6,6	-	-	-		
86	OHX	6	2028	80	0,6,6	-	-	-		
86	OHX	1	3449	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	4	215	86	0,6,6	-	-	-		
86	OHX	2	1991	86,1	0,6,6	-	-	-		
86	OHX	5	3625	36	0,6,6	-	-	-		
86	OHX	6	2020	80	0,6,6	-	-	-		
90	8AN	5	3403	89	19,24,25	8.24	3 (15%)	13,35,38	1.64	3 (23%)
86	OHX	1	3548	-	0,6,6	-	-	-		
86	OHX	1	3660	-	0,6,6	-	-	-		
86	OHX	5	3415	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	1	3649	-	0,6,6	-	-	-		
86	OHX	1	3590	86	0,6,6	-	-	-		
86	OHX	1	3658	-	0,6,6	-	-	-		
86	OHX	5	3428	-	0,6,6	-	-	-		
86	OHX	7	202	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	1	3661	86	0,6,6	-	-	-		
86	OHX	1	3624	36	0,6,6	-	-	-		
86	OHX	6	2037	80	0,6,6	-	-	-		
86	OHX	5	3783	36	0,6,6	-	-	-		
86	OHX	2	1995	-	0,6,6	-	-	-		
86	OHX	1	3435	-	0,6,6	-	-	-		
86	OHX	2	2021	-	0,6,6	-	-	-		
86	OHX	2	2046	1	0,6,6	-	-	-		
86	OHX	6	1994	-	0,6,6	-	-	-		
86	OHX	6	2011	-	0,6,6	-	-	-		
86	OHX	1	3679	-	0,6,6	-	-	-		
86	OHX	7	209	86,37	0,6,6	-	-	-		
86	OHX	1	3650	-	0,6,6	-	-	-		
86	OHX	1	3486	-	0,6,6	-	-	-		
86	OHX	6	1921	-	0,6,6	-	-	-		
86	OHX	1	3577	-	0,6,6	-	-	-		
86	OHX	6	1944	80	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	2	1969	1	0,6,6	-	-	-		
86	OHX	1	3603	-	0,6,6	-	-	-		
86	OHX	1	3517	86	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	1960	-	0,6,6	-	-	-		
86	OHX	5	3763	-	0,6,6	-	-	-		
86	OHX	2	1956	-	0,6,6	-	-	-		
86	OHX	3	201	-	0,6,6	-	-	-		
86	OHX	5	3778	-	0,6,6	-	-	-		
86	OHX	1	3475	-	0,6,6	-	-	-		
86	OHX	5	3652	86	0,6,6	-	-	-		
86	OHX	6	1908	-	0,6,6	-	-	-		
86	OHX	5	3478	86	0,6,6	-	-	-		
86	OHX	2	1959	-	0,6,6	-	-	-		
86	OHX	4	205	-	0,6,6	-	-	-		
86	OHX	c8	201	-	0,6,6	-	-	-		
86	OHX	6	1949	86	0,6,6	-	-	-		
86	OHX	5	3475	36	0,6,6	-	-	-		
86	OHX	6	1971	86	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	1	3581	86	0,6,6	-	-	-		
86	OHX	5	3466	36	0,6,6	-	-	-		
86	OHX	5	3716	86	0,6,6	-	-	-		
86	OHX	5	3573	86	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	5	3813	36	0,6,6	-	-	-		
86	OHX	1	3713	-	0,6,6	-	-	-		
86	OHX	5	3494	-	0,6,6	-	-	-		
86	OHX	2	1904	-	0,6,6	-	-	-		
86	OHX	2	2000	-	0,6,6	-	-	-		
86	OHX	1	3778	-	0,6,6	-	-	-		
86	OHX	5	3699	36	0,6,6	-	-	-		
86	OHX	1	3470	-	0,6,6	-	-	-		
86	OHX	2	1999	-	0,6,6	-	-	-		
86	OHX	6	1917	80	0,6,6	-	-	-		
86	OHX	5	3418	-	0,6,6	-	-	-		
86	OHX	2	1925	-	0,6,6	-	-	-		
86	OHX	1	3755	36	0,6,6	-	-	-		
86	OHX	5	3495	-	0,6,6	-	-	-		
86	OHX	6	2005	86	0,6,6	-	-	-		
86	OHX	5	3815	86	0,6,6	-	-	-		
86	OHX	5	3408	-	0,6,6	-	-	-		
86	OHX	5	3689	36	0,6,6	-	-	-		
86	OHX	5	3774	-	0,6,6	-	-	-		
86	OHX	6	2009	86	0,6,6	-	-	-		
86	OHX	6	2056	80	0,6,6	-	-	-		
86	OHX	6	1935	80	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	1958	80	0,6,6	-	-	-		
86	OHX	5	3666	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	5	3551	36	0,6,6	-	-	-		
86	OHX	2	1934	-	0,6,6	-	-	-		
86	OHX	1	3561	-	0,6,6	-	-	-		
86	OHX	5	3817	86	0,6,6	-	-	-		
86	OHX	2	2085	86	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		
86	OHX	5	3616	-	0,6,6	-	-	-		
86	OHX	1	3416	-	0,6,6	-	-	-		
86	OHX	5	3565	-	0,6,6	-	-	-		
86	OHX	1	3810	86	0,6,6	-	-	-		
86	OHX	O7	103	-	0,6,6	-	-	-		
86	OHX	5	3521	-	0,6,6	-	-	-		
86	OHX	5	3649	36	0,6,6	-	-	-		
86	OHX	5	3662	-	0,6,6	-	-	-		
86	OHX	2	1984	86	0,6,6	-	-	-		
86	OHX	1	3418	-	0,6,6	-	-	-		
86	OHX	1	3580	-	0,6,6	-	-	-		
86	OHX	2	1918	86	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	C5	201	17	0,6,6	-	-	-		
86	OHX	1	3644	-	0,6,6	-	-	-		
86	OHX	6	1982	86	0,6,6	-	-	-		
86	OHX	5	3611	-	0,6,6	-	-	-		
86	OHX	l5	301	-	0,6,6	-	-	-		
86	OHX	4	206	-	0,6,6	-	-	-		
86	OHX	1	3565	-	0,6,6	-	-	-		
86	OHX	5	3462	36	0,6,6	-	-	-		
86	OHX	1	3530	36	0,6,6	-	-	-		
86	OHX	1	3774	-	0,6,6	-	-	-		
86	OHX	5	3818	86,36	0,6,6	-	-	-		
86	OHX	5	3624	86,36	0,6,6	-	-	-		
86	OHX	5	3623	-	0,6,6	-	-	-		
86	OHX	1	3405	-	0,6,6	-	-	-		
86	OHX	1	3424	-	0,6,6	-	-	-		
86	OHX	1	3569	-	0,6,6	-	-	-		
86	OHX	5	3621	-	0,6,6	-	-	-		
86	OHX	1	3765	-	0,6,6	-	-	-		
86	OHX	5	3797	36	0,6,6	-	-	-		
86	OHX	1	3587	36	0,6,6	-	-	-		
86	OHX	5	3642	86,36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	1906	86	0,6,6	-	-	-		
86	OHX	5	3562	-	0,6,6	-	-	-		
86	OHX	4	212	38	0,6,6	-	-	-		
86	OHX	1	3537	-	0,6,6	-	-	-		
86	OHX	5	3731	86	0,6,6	-	-	-		
86	OHX	5	3459	36	0,6,6	-	-	-		
86	OHX	1	3779	86	0,6,6	-	-	-		
86	OHX	1	3748	86	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	L4	401	-	0,6,6	-	-	-		
86	OHX	5	3477	36	0,6,6	-	-	-		
86	OHX	5	3773	36	0,6,6	-	-	-		
86	OHX	6	1983	80	0,6,6	-	-	-		
86	OHX	5	3486	86	0,6,6	-	-	-		
86	OHX	1	3686	-	0,6,6	-	-	-		
86	OHX	1	3463	-	0,6,6	-	-	-		
86	OHX	5	3695	-	0,6,6	-	-	-		
86	OHX	6	1993	80	0,6,6	-	-	-		
86	OHX	M0	302	86	0,6,6	-	-	-		
86	OHX	1	3448	-	0,6,6	-	-	-		
86	OHX	5	3663	-	0,6,6	-	-	-		
86	OHX	2	1944	-	0,6,6	-	-	-		
86	OHX	2	1924	-	0,6,6	-	-	-		
86	OHX	5	3463	-	0,6,6	-	-	-		
86	OHX	6	2094	86,80	0,6,6	-	-	-		
86	OHX	5	3791	-	0,6,6	-	-	-		
86	OHX	5	3452	-	0,6,6	-	-	-		
86	OHX	2	1923	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	6	1976	80	0,6,6	-	-	-		
86	OHX	6	2026	80	0,6,6	-	-	-		
86	OHX	5	3472	-	0,6,6	-	-	-		
86	OHX	6	2025	-	0,6,6	-	-	-		
86	OHX	1	3707	-	0,6,6	-	-	-		
86	OHX	1	3599	36	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	1	3563	-	0,6,6	-	-	-		
86	OHX	6	2046	86	0,6,6	-	-	-		
86	OHX	6	1933	-	0,6,6	-	-	-		
86	OHX	1	3474	-	0,6,6	-	-	-		
86	OHX	1	3442	-	0,6,6	-	-	-		
86	OHX	1	3598	86	0,6,6	-	-	-		
86	OHX	5	3429	36	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3682	-	0,6,6	-	-	-		
86	OHX	5	3786	-	0,6,6	-	-	-		
86	OHX	6	1913	80	0,6,6	-	-	-		
86	OHX	2	2007	-	0,6,6	-	-	-		
86	OHX	5	3476	-	0,6,6	-	-	-		
86	OHX	6	2000	-	0,6,6	-	-	-		
86	OHX	2	1939	-	0,6,6	-	-	-		
86	OHX	2	1967	-	0,6,6	-	-	-		
86	OHX	5	3721	36	0,6,6	-	-	-		
86	OHX	6	1962	80	0,6,6	-	-	-		
86	OHX	1	3593	-	0,6,6	-	-	-		
86	OHX	1	3784	-	0,6,6	-	-	-		
86	OHX	1	3536	86	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	5	3809	86	0,6,6	-	-	-		
86	OHX	6	2085	80	0,6,6	-	-	-		
86	OHX	5	3446	-	0,6,6	-	-	-		
86	OHX	5	3560	86,36	0,6,6	-	-	-		
86	OHX	5	3730	36	0,6,6	-	-	-		
86	OHX	5	3540	86	0,6,6	-	-	-		
86	OHX	n1	201	-	0,6,6	-	-	-		
86	OHX	1	3559	86	0,6,6	-	-	-		
86	OHX	5	3455	86	0,6,6	-	-	-		
86	OHX	6	1968	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	7	212	-	0,6,6	-	-	-		
86	OHX	5	3541	86	0,6,6	-	-	-		
86	OHX	5	3795	-	0,6,6	-	-	-		
86	OHX	1	3596	86	0,6,6	-	-	-		
86	OHX	1	3544	-	0,6,6	-	-	-		
86	OHX	5	3568	-	0,6,6	-	-	-		
86	OHX	6	2091	86	0,6,6	-	-	-		
86	OHX	5	3422	-	0,6,6	-	-	-		
86	OHX	6	2074	80	0,6,6	-	-	-		
86	OHX	1	3539	86	0,6,6	-	-	-		
86	OHX	1	3522	-	0,6,6	-	-	-		
86	OHX	1	3757	86,36	0,6,6	-	-	-		
86	OHX	1	3411	86	0,6,6	-	-	-		
86	OHX	5	3811	86	0,6,6	-	-	-		
86	OHX	1	3426	-	0,6,6	-	-	-		
86	OHX	1	3785	86	0,6,6	-	-	-		
86	OHX	1	3427	-	0,6,6	-	-	-		
86	OHX	2	1996	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3484	-	0,6,6	-	-	-		
86	OHX	5	3465	86	0,6,6	-	-	-		
86	OHX	6	2052	80	0,6,6	-	-	-		
86	OHX	2	1978	-	0,6,6	-	-	-		
86	OHX	5	3659	86,36	0,6,6	-	-	-		
86	OHX	8	208	-	0,6,6	-	-	-		
86	OHX	5	3424	36	0,6,6	-	-	-		
86	OHX	6	1966	-	0,6,6	-	-	-		
86	OHX	6	2075	86,80	0,6,6	-	-	-		
86	OHX	5	3619	-	0,6,6	-	-	-		
86	OHX	1	3451	-	0,6,6	-	-	-		
86	OHX	6	2008	-	0,6,6	-	-	-		
86	OHX	1	3687	36	0,6,6	-	-	-		
86	OHX	5	3661	86,36	0,6,6	-	-	-		
86	OHX	2	2029	1	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	5	3473	-	0,6,6	-	-	-		
86	OHX	2	1950	-	0,6,6	-	-	-		
86	OHX	5	3461	-	0,6,6	-	-	-		
86	OHX	2	1952	1	0,6,6	-	-	-		
86	OHX	5	3669	-	0,6,6	-	-	-		
86	OHX	5	3570	36	0,6,6	-	-	-		
86	OHX	6	2069	86	0,6,6	-	-	-		
86	OHX	1	3770	-	0,6,6	-	-	-		
86	OHX	5	3504	-	0,6,6	-	-	-		
86	OHX	6	2038	-	0,6,6	-	-	-		
86	OHX	1	3694	-	0,6,6	-	-	-		
86	OHX	3	211	86	0,6,6	-	-	-		
86	OHX	q1	101	86	0,6,6	-	-	-		
86	OHX	5	3542	36	0,6,6	-	-	-		
86	OHX	2	2077	86,1	0,6,6	-	-	-		
86	OHX	1	3640	-	0,6,6	-	-	-		
86	OHX	1	3595	86	0,6,6	-	-	-		
86	OHX	1	3453	-	0,6,6	-	-	-		
86	OHX	1	3744	86	0,6,6	-	-	-		
86	OHX	5	3440	-	0,6,6	-	-	-		
86	OHX	2	2073	86	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	5	3564	86	0,6,6	-	-	-		
86	OHX	M7	201	-	0,6,6	-	-	-		
86	OHX	1	3480	86	0,6,6	-	-	-		
86	OHX	1	3703	36	0,6,6	-	-	-		
86	OHX	6	1992	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3438	36	0,6,6	-	-	-		
86	OHX	5	3672	-	0,6,6	-	-	-		
86	OHX	1	3805	86	0,6,6	-	-	-		
86	OHX	5	3766	-	0,6,6	-	-	-		
86	OHX	2	1915	86,1	0,6,6	-	-	-		
86	OHX	1	3708	-	0,6,6	-	-	-		
86	OHX	1	3585	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
90	8AN	1	3403	89	19,24,25	1.05	1 (5%)	13,35,38	1.70	4 (30%)
86	OHX	5	3638	-	0,6,6	-	-	-		
86	OHX	5	3441	-	0,6,6	-	-	-		
86	OHX	5	3457	86	0,6,6	-	-	-		
86	OHX	1	3542	-	0,6,6	-	-	-		
86	OHX	1	3807	-	0,6,6	-	-	-		
86	OHX	5	3536	86	0,6,6	-	-	-		
86	OHX	1	3797	86,36	0,6,6	-	-	-		
86	OHX	12	301	86	0,6,6	-	-	-		
86	OHX	5	3487	-	0,6,6	-	-	-		
86	OHX	6	1995	-	0,6,6	-	-	-		
86	OHX	1	3704	-	0,6,6	-	-	-		
86	OHX	2	1983	-	0,6,6	-	-	-		
86	OHX	2	1954	86	0,6,6	-	-	-		
86	OHX	5	3581	36	0,6,6	-	-	-		
86	OHX	1	3711	86	0,6,6	-	-	-		
86	OHX	6	2054	86,80	0,6,6	-	-	-		
86	OHX	1	3697	-	0,6,6	-	-	-		
86	OHX	5	3469	-	0,6,6	-	-	-		
86	OHX	5	3643	-	0,6,6	-	-	-		
86	OHX	1	3718	86	0,6,6	-	-	-		
86	OHX	8	211	38	0,6,6	-	-	-		
86	OHX	2	2020	-	0,6,6	-	-	-		
86	OHX	5	3631	-	0,6,6	-	-	-		
86	OHX	1	3457	-	0,6,6	-	-	-		
86	OHX	1	3555	-	0,6,6	-	-	-		
86	OHX	5	3515	-	0,6,6	-	-	-		
86	OHX	6	1907	80	0,6,6	-	-	-		
86	OHX	5	3755	36	0,6,6	-	-	-		
86	OHX	5	3777	-	0,6,6	-	-	-		
86	OHX	1	3771	-	0,6,6	-	-	-		
86	OHX	5	3717	-	0,6,6	-	-	-		
86	OHX	5	3492	36	0,6,6	-	-	-		
86	OHX	1	3419	-	0,6,6	-	-	-		
86	OHX	5	3563	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3603	36	0,6,6	-	-	-		
86	OHX	6	1939	86	0,6,6	-	-	-		
86	OHX	2	1921	86	0,6,6	-	-	-		
86	OHX	5	3771	86	0,6,6	-	-	-		
86	OHX	C8	202	86,36	0,6,6	-	-	-		
86	OHX	1	3736	-	0,6,6	-	-	-		
86	OHX	1	3802	-	0,6,6	-	-	-		
86	OHX	6	2018	86	0,6,6	-	-	-		
86	OHX	1	3523	-	0,6,6	-	-	-		
86	OHX	5	3596	86	0,6,6	-	-	-		
86	OHX	5	3814	86	0,6,6	-	-	-		
86	OHX	1	3429	-	0,6,6	-	-	-		
86	OHX	8	210	-	0,6,6	-	-	-		
86	OHX	2	1992	-	0,6,6	-	-	-		
86	OHX	5	3609	86	0,6,6	-	-	-		
86	OHX	2	1962	-	0,6,6	-	-	-		
86	OHX	7	201	37	0,6,6	-	-	-		
86	OHX	8	206	-	0,6,6	-	-	-		
86	OHX	6	2012	80	0,6,6	-	-	-		
86	OHX	2	2048	86	0,6,6	-	-	-		
86	OHX	6	2030	-	0,6,6	-	-	-		
86	OHX	6	2032	86,80	0,6,6	-	-	-		
89	C	5	3402	90	18,21,22	0.57	0	26,30,33	0.78	1 (3%)
86	OHX	6	1990	80	0,6,6	-	-	-		
86	OHX	6	2024	80	0,6,6	-	-	-		
86	OHX	o7	503	86	0,6,6	-	-	-		
86	OHX	M9	203	-	0,6,6	-	-	-		
86	OHX	2	1938	-	0,6,6	-	-	-		
86	OHX	5	3449	86	0,6,6	-	-	-		
86	OHX	5	3420	36	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	5	3405	36	0,6,6	-	-	-		
86	OHX	1	3495	86	0,6,6	-	-	-		
86	OHX	5	3470	-	0,6,6	-	-	-		
86	OHX	6	2049	80	0,6,6	-	-	-		
86	OHX	M0	301	86	0,6,6	-	-	-		
86	OHX	5	3576	-	0,6,6	-	-	-		
86	OHX	6	1965	86	0,6,6	-	-	-		
86	OHX	1	3745	-	0,6,6	-	-	-		
86	OHX	5	3779	86	0,6,6	-	-	-		
86	OHX	1	3636	-	0,6,6	-	-	-		
86	OHX	2	2084	86	0,6,6	-	-	-		
86	OHX	6	1915	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	1940	86	0,6,6	-	-	-		
86	OHX	5	3757	86	0,6,6	-	-	-		
86	OHX	6	2006	-	0,6,6	-	-	-		
86	OHX	5	3433	36	0,6,6	-	-	-		
86	OHX	5	3548	-	0,6,6	-	-	-		
86	OHX	5	3613	-	0,6,6	-	-	-		
86	OHX	1	3728	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	1	3528	-	0,6,6	-	-	-		
86	OHX	1	3604	-	0,6,6	-	-	-		
89	C	1	3401	-	18,21,22	0.65	0	26,30,33	1.43	5 (19%)
86	OHX	5	3543	86	0,6,6	-	-	-		
86	OHX	1	3525	-	0,6,6	-	-	-		
86	OHX	5	3467	-	0,6,6	-	-	-		
86	OHX	1	3428	-	0,6,6	-	-	-		
86	OHX	4	218	86	0,6,6	-	-	-		
86	OHX	1	3633	-	0,6,6	-	-	-		
91	PRO	1	3404	-	5,7,8	0.51	0	7,8,10	1.39	1 (14%)
86	OHX	1	3413	-	0,6,6	-	-	-		
86	OHX	6	1918	86	0,6,6	-	-	-		
86	OHX	1	3787	-	0,6,6	-	-	-		
86	OHX	5	3503	36	0,6,6	-	-	-		
86	OHX	5	3628	-	0,6,6	-	-	-		
86	OHX	5	3679	-	0,6,6	-	-	-		
86	OHX	6	2064	80	0,6,6	-	-	-		
86	OHX	5	3577	36	0,6,6	-	-	-		
86	OHX	1	3813	86	0,6,6	-	-	-		
86	OHX	2	2050	1	0,6,6	-	-	-		
86	OHX	5	3500	-	0,6,6	-	-	-		
86	OHX	1	3551	-	0,6,6	-	-	-		
86	OHX	5	3635	36	0,6,6	-	-	-		
86	OHX	2	1935	-	0,6,6	-	-	-		
86	OHX	1	3447	-	0,6,6	-	-	-		
86	OHX	1	3473	-	0,6,6	-	-	-		
86	OHX	1	3497	-	0,6,6	-	-	-		
86	OHX	2	2069	86	0,6,6	-	-	-		
86	OHX	5	3697	-	0,6,6	-	-	-		
86	OHX	1	3768	86,36	0,6,6	-	-	-		
86	OHX	5	3793	-	0,6,6	-	-	-		
86	OHX	1	3812	86	0,6,6	-	-	-		
86	OHX	5	3598	86,36	0,6,6	-	-	-		
86	OHX	1	3545	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3531	36	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	5	3442	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	2	1928	-	0,6,6	-	-	-		
86	OHX	1	3607	-	0,6,6	-	-	-		
86	OHX	1	3481	-	0,6,6	-	-	-		
86	OHX	5	3590	86	0,6,6	-	-	-		
86	OHX	5	3800	-	0,6,6	-	-	-		
86	OHX	5	3610	-	0,6,6	-	-	-		
86	OHX	1	3788	86	0,6,6	-	-	-		
86	OHX	6	1931	86,80	0,6,6	-	-	-		
86	OHX	8	202	38	0,6,6	-	-	-		
86	OHX	2	1943	86	0,6,6	-	-	-		
86	OHX	c5	202	17	0,6,6	-	-	-		
86	OHX	1	3635	-	0,6,6	-	-	-		
86	OHX	2	2002	-	0,6,6	-	-	-		
86	OHX	1	3662	-	0,6,6	-	-	-		
86	OHX	1	3524	-	0,6,6	-	-	-		
86	OHX	5	3606	36	0,6,6	-	-	-		
86	OHX	5	3434	86	0,6,6	-	-	-		
86	OHX	5	3736	86	0,6,6	-	-	-		
86	OHX	5	3767	86,36	0,6,6	-	-	-		
86	OHX	2	1970	86	0,6,6	-	-	-		
86	OHX	5	3751	-	0,6,6	-	-	-		
86	OHX	5	3569	86	0,6,6	-	-	-		
86	OHX	2	1942	1	0,6,6	-	-	-		
86	OHX	6	1946	-	0,6,6	-	-	-		
86	OHX	5	3670	36	0,6,6	-	-	-		
86	OHX	6	2090	86	0,6,6	-	-	-		
86	OHX	1	3639	86	0,6,6	-	-	-		
86	OHX	s1	301	-	0,6,6	-	-	-		
86	OHX	1	3801	86	0,6,6	-	-	-		
86	OHX	8	203	86	0,6,6	-	-	-		
86	OHX	5	3808	86	0,6,6	-	-	-		
86	OHX	1	3620	-	0,6,6	-	-	-		
86	OHX	5	3491	-	0,6,6	-	-	-		
86	OHX	5	3680	-	0,6,6	-	-	-		
86	OHX	2	1971	-	0,6,6	-	-	-		
86	OHX	6	1961	-	0,6,6	-	-	-		
86	OHX	5	3539	86	0,6,6	-	-	-		
86	OHX	1	3454	-	0,6,6	-	-	-		
86	OHX	6	1997	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	1963	80	0,6,6	-	-	-		
86	OHX	1	3750	86	0,6,6	-	-	-		
86	OHX	1	3760	-	0,6,6	-	-	-		
86	OHX	5	3769	86	0,6,6	-	-	-		
86	OHX	6	1948	86,80	0,6,6	-	-	-		
86	OHX	1	3790	-	0,6,6	-	-	-		
86	OHX	1	3746	86	0,6,6	-	-	-		
86	OHX	1	3754	-	0,6,6	-	-	-		
86	OHX	1	3562	86	0,6,6	-	-	-		
86	OHX	m0	301	86	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	2	1941	-	0,6,6	-	-	-		
86	OHX	3	203	-	0,6,6	-	-	-		
86	OHX	1	3632	-	0,6,6	-	-	-		
86	OHX	6	1906	-	0,6,6	-	-	-		
86	OHX	5	3450	-	0,6,6	-	-	-		
86	OHX	5	3622	-	0,6,6	-	-	-		
86	OHX	1	3498	-	0,6,6	-	-	-		
86	OHX	6	1937	-	0,6,6	-	-	-		
86	OHX	1	3688	86	0,6,6	-	-	-		
86	OHX	1	3534	-	0,6,6	-	-	-		
86	OHX	6	1924	-	0,6,6	-	-	-		
86	OHX	5	3719	36	0,6,6	-	-	-		
86	OHX	1	3612	86	0,6,6	-	-	-		
86	OHX	2	1910	1	0,6,6	-	-	-		
86	OHX	6	2043	86	0,6,6	-	-	-		
86	OHX	1	3443	-	0,6,6	-	-	-		
86	OHX	1	3455	86	0,6,6	-	-	-		
86	OHX	1	3655	-	0,6,6	-	-	-		
86	OHX	6	1920	86	0,6,6	-	-	-		
86	OHX	2	1907	86	0,6,6	-	-	-		
86	OHX	1	3712	-	0,6,6	-	-	-		
86	OHX	2	1932	-	0,6,6	-	-	-		
86	OHX	7	210	-	0,6,6	-	-	-		
86	OHX	5	3525	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	1	3456	86	0,6,6	-	-	-		
86	OHX	6	2071	86	0,6,6	-	-	-		
86	OHX	1	3735	-	0,6,6	-	-	-		
91	PRO	5	3404	-	5,7,8	0.51	0	7,8,10	1.39	1 (14%)
86	OHX	3	205	86	0,6,6	-	-	-		
86	OHX	2	1963	-	0,6,6	-	-	-		
86	OHX	5	3554	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	1919	1	0,6,6	-	-	-		
86	OHX	5	3694	-	0,6,6	-	-	-		
86	OHX	5	3733	86	0,6,6	-	-	-		
86	OHX	2	1961	86	0,6,6	-	-	-		
86	OHX	6	1926	-	0,6,6	-	-	-		
86	OHX	6	2013	-	0,6,6	-	-	-		
86	OHX	1	3583	-	0,6,6	-	-	-		
86	OHX	1	3656	86	0,6,6	-	-	-		
86	OHX	6	2045	80	0,6,6	-	-	-		
86	OHX	5	3648	-	0,6,6	-	-	-		
86	OHX	6	1930	80	0,6,6	-	-	-		
86	OHX	5	3496	-	0,6,6	-	-	-		
86	OHX	1	3609	-	0,6,6	-	-	-		
86	OHX	1	3570	-	0,6,6	-	-	-		
86	OHX	5	3707	-	0,6,6	-	-	-		
86	OHX	1	3680	-	0,6,6	-	-	-		
86	OHX	1	3513	86	0,6,6	-	-	-		
86	OHX	1	3430	-	0,6,6	-	-	-		
86	OHX	5	3627	-	0,6,6	-	-	-		
86	OHX	5	3772	86,36	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	1	3721	86	0,6,6	-	-	-		
86	OHX	2	2014	-	0,6,6	-	-	-		
86	OHX	1	3670	-	0,6,6	-	-	-		
86	OHX	M9	202	86	0,6,6	-	-	-		
86	OHX	2	2064	86	0,6,6	-	-	-		
86	OHX	5	3724	-	0,6,6	-	-	-		
86	OHX	6	2023	-	0,6,6	-	-	-		
86	OHX	5	3715	86,36	0,6,6	-	-	-		
86	OHX	5	3729	86	0,6,6	-	-	-		
86	OHX	5	3683	86,36	0,6,6	-	-	-		
86	OHX	6	2096	86,80	0,6,6	-	-	-		
86	OHX	2	1945	86	0,6,6	-	-	-		
86	OHX	5	3807	86,36	0,6,6	-	-	-		
86	OHX	5	3501	86	0,6,6	-	-	-		
86	OHX	5	3580	-	0,6,6	-	-	-		
86	OHX	1	3566	-	0,6,6	-	-	-		
86	OHX	5	3410	36	0,6,6	-	-	-		
86	OHX	1	3494	86	0,6,6	-	-	-		
86	OHX	1	3709	86,36	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	6	1964	80	0,6,6	-	-	-		
86	OHX	1	3696	86	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2019	-	0,6,6	-	-	-		
86	OHX	5	3691	86	0,6,6	-	-	-		
86	OHX	1	3795	-	0,6,6	-	-	-		
86	OHX	5	3668	-	0,6,6	-	-	-		
86	OHX	8	205	-	0,6,6	-	-	-		
86	OHX	6	2089	80	0,6,6	-	-	-		
86	OHX	5	3723	-	0,6,6	-	-	-		
86	OHX	1	3472	36	0,6,6	-	-	-		
86	OHX	1	3422	86,36	0,6,6	-	-	-		
86	OHX	5	3660	36	0,6,6	-	-	-		
86	OHX	5	3726	36	0,6,6	-	-	-		
86	OHX	6	1914	86,80	0,6,6	-	-	-		
86	OHX	4	204	-	0,6,6	-	-	-		
86	OHX	2	1957	-	0,6,6	-	-	-		
86	OHX	1	3543	-	0,6,6	-	-	-		
86	OHX	5	3784	-	0,6,6	-	-	-		
86	OHX	6	1927	80	0,6,6	-	-	-		
86	OHX	7	207	-	0,6,6	-	-	-		
86	OHX	5	3586	86	0,6,6	-	-	-		
86	OHX	5	3700	86,36	0,6,6	-	-	-		
86	OHX	5	3780	-	0,6,6	-	-	-		
86	OHX	1	3509	-	0,6,6	-	-	-		
86	OHX	3	206	-	0,6,6	-	-	-		
86	OHX	5	3744	-	0,6,6	-	-	-		
86	OHX	6	2076	80	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	1	3414	-	0,6,6	-	-	-		
86	OHX	1	3642	-	0,6,6	-	-	-		
86	OHX	1	3659	-	0,6,6	-	-	-		
86	OHX	1	3672	-	0,6,6	-	-	-		
86	OHX	13	402	-	0,6,6	-	-	-		
86	OHX	5	3752	-	0,6,6	-	-	-		
86	OHX	2	2017	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	6	1950	80	0,6,6	-	-	-		
86	OHX	1	3460	-	0,6,6	-	-	-		
86	OHX	1	3803	-	0,6,6	-	-	-		
86	OHX	2	1981	-	0,6,6	-	-	-		
86	OHX	6	1902	-	0,6,6	-	-	-		
86	OHX	2	2087	86	0,6,6	-	-	-		
86	OHX	1	3705	86	0,6,6	-	-	-		
86	OHX	1	3488	86	0,6,6	-	-	-		
86	OHX	5	3479	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3471	-	0,6,6	-	-	-		
86	OHX	M0	304	86	0,6,6	-	-	-		
86	OHX	5	3520	-	0,6,6	-	-	-		
86	OHX	5	3761	86	0,6,6	-	-	-		
86	OHX	1	3496	-	0,6,6	-	-	-		
86	OHX	2	1931	-	0,6,6	-	-	-		
86	OHX	5	3488	36	0,6,6	-	-	-		
86	OHX	1	3800	86	0,6,6	-	-	-		
86	OHX	8	221	86	0,6,6	-	-	-		
86	OHX	1	3775	86	0,6,6	-	-	-		
86	OHX	1	3610	-	0,6,6	-	-	-		
86	OHX	1	3608	-	0,6,6	-	-	-		
86	OHX	5	3650	36	0,6,6	-	-	-		
86	OHX	1	3572	-	0,6,6	-	-	-		
86	OHX	5	3647	36	0,6,6	-	-	-		
86	OHX	1	3645	-	0,6,6	-	-	-		
86	OHX	1	3547	86	0,6,6	-	-	-		
86	OHX	5	3499	-	0,6,6	-	-	-		
86	OHX	5	3775	-	0,6,6	-	-	-		
86	OHX	5	3416	-	0,6,6	-	-	-		
86	OHX	2	1964	-	0,6,6	-	-	-		
86	OHX	4	216	86	0,6,6	-	-	-		
86	OHX	6	1986	-	0,6,6	-	-	-		
86	OHX	5	3510	-	0,6,6	-	-	-		
86	OHX	1	3767	86	0,6,6	-	-	-		
86	OHX	5	3734	86	0,6,6	-	-	-		
86	OHX	5	3484	-	0,6,6	-	-	-		
86	OHX	5	3685	-	0,6,6	-	-	-		
86	OHX	6	1936	80	0,6,6	-	-	-		
86	OHX	1	3436	-	0,6,6	-	-	-		
86	OHX	8	218	38	0,6,6	-	-	-		
86	OHX	1	3407	-	0,6,6	-	-	-		
86	OHX	5	3664	86	0,6,6	-	-	-		
86	OHX	6	2015	86	0,6,6	-	-	-		
86	OHX	5	3591	-	0,6,6	-	-	-		
86	OHX	1	3761	-	0,6,6	-	-	-		
86	OHX	5	3630	-	0,6,6	-	-	-		
86	OHX	5	3740	-	0,6,6	-	-	-		
86	OHX	5	3419	-	0,6,6	-	-	-		
86	OHX	1	3441	86	0,6,6	-	-	-		
86	OHX	2	1926	-	0,6,6	-	-	-		
86	OHX	2	1987	-	0,6,6	-	-	-		
86	OHX	6	1985	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3538	-	0,6,6	-	-	-		
86	OHX	2	2076	86,1	0,6,6	-	-	-		
86	OHX	5	3671	-	0,6,6	-	-	-		
86	OHX	2	1916	1	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	5	3533	86,36	0,6,6	-	-	-		
86	OHX	5	3604	-	0,6,6	-	-	-		
86	OHX	m5	501	-	0,6,6	-	-	-		
86	OHX	6	1910	-	0,6,6	-	-	-		
86	OHX	8	212	86	0,6,6	-	-	-		
86	OHX	1	3782	-	0,6,6	-	-	-		
86	OHX	5	3557	36	0,6,6	-	-	-		
86	OHX	1	3512	-	0,6,6	-	-	-		
86	OHX	6	2004	-	0,6,6	-	-	-		
86	OHX	6	1969	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	5	3714	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	1	3591	-	0,6,6	-	-	-		
86	OHX	3	202	-	0,6,6	-	-	-		
86	OHX	6	1911	80	0,6,6	-	-	-		
86	OHX	1	3643	-	0,6,6	-	-	-		
86	OHX	5	3686	-	0,6,6	-	-	-		
86	OHX	1	3739	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	1	3741	86	0,6,6	-	-	-		
86	OHX	2	1974	-	0,6,6	-	-	-		
86	OHX	5	3810	86	0,6,6	-	-	-		
86	OHX	5	3720	36	0,6,6	-	-	-		
86	OHX	1	3514	-	0,6,6	-	-	-		
86	OHX	2	1933	86	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	2	1946	-	0,6,6	-	-	-		
86	OHX	1	3689	86	0,6,6	-	-	-		
86	OHX	4	210	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	3812	-	0,6,6	-	-	-		
86	OHX	m7	201	-	0,6,6	-	-	-		
86	OHX	2	1960	-	0,6,6	-	-	-		
86	OHX	1	3518	86	0,6,6	-	-	-		
86	OHX	5	3768	36	0,6,6	-	-	-		
86	OHX	5	3561	86	0,6,6	-	-	-		
86	OHX	5	3743	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	1	3725	36	0,6,6	-	-	-		
86	OHX	2	2089	86	0,6,6	-	-	-		
86	OHX	5	3607	36	0,6,6	-	-	-		
86	OHX	1	3666	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	5	3502	86,36	0,6,6	-	-	-		
86	OHX	1	3799	86	0,6,6	-	-	-		
86	OHX	2	1985	-	0,6,6	-	-	-		
86	OHX	6	1973	86	0,6,6	-	-	-		
86	OHX	5	3644	36	0,6,6	-	-	-		
86	OHX	1	3619	36	0,6,6	-	-	-		
86	OHX	1	3742	-	0,6,6	-	-	-		
86	OHX	5	3727	86	0,6,6	-	-	-		
86	OHX	1	3720	-	0,6,6	-	-	-		
86	OHX	6	2022	86,80	0,6,6	-	-	-		
86	OHX	5	3528	-	0,6,6	-	-	-		
86	OHX	1	3605	86	0,6,6	-	-	-		
86	OHX	5	3555	-	0,6,6	-	-	-		
86	OHX	1	3669	86	0,6,6	-	-	-		
86	OHX	o9	101	-	0,6,6	-	-	-		
86	OHX	2	2027	86	0,6,6	-	-	-		
86	OHX	6	1996	-	0,6,6	-	-	-		
86	OHX	5	3718	-	0,6,6	-	-	-		
86	OHX	2	1937	-	0,6,6	-	-	-		
86	OHX	1	3675	86,36	0,6,6	-	-	-		
86	OHX	6	2082	86	0,6,6	-	-	-		
86	OHX	5	3776	-	0,6,6	-	-	-		
86	OHX	6	1987	-	0,6,6	-	-	-		
86	OHX	1	3526	-	0,6,6	-	-	-		
86	OHX	2	2004	-	0,6,6	-	-	-		
86	OHX	1	3683	-	0,6,6	-	-	-		
86	OHX	2	2011	-	0,6,6	-	-	-		
86	OHX	5	3595	-	0,6,6	-	-	-		
86	OHX	6	2010	86,80	0,6,6	-	-	-		
86	OHX	5	3748	-	0,6,6	-	-	-		
86	OHX	1	3467	-	0,6,6	-	-	-		
86	OHX	1	3531	-	0,6,6	-	-	-		
86	OHX	1	3674	-	0,6,6	-	-	-		
86	OHX	5	3641	-	0,6,6	-	-	-		
86	OHX	3	212	-	0,6,6	-	-	-		
86	OHX	5	3588	-	0,6,6	-	-	-		
86	OHX	6	1967	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3677	-	0,6,6	-	-	-		
86	OHX	5	3754	-	0,6,6	-	-	-		
86	OHX	1	3552	-	0,6,6	-	-	-		
86	OHX	1	3556	-	0,6,6	-	-	-		
86	OHX	d9	102	86	0,6,6	-	-	-		
86	OHX	5	3448	86	0,6,6	-	-	-		
86	OHX	6	1928	80	0,6,6	-	-	-		
86	OHX	1	3535	86	0,6,6	-	-	-		
86	OHX	6	2002	86,80	0,6,6	-	-	-		
86	OHX	1	3647	86	0,6,6	-	-	-		
86	OHX	5	3597	-	0,6,6	-	-	-		
86	OHX	1	3663	86	0,6,6	-	-	-		
86	OHX	5	3802	86	0,6,6	-	-	-		
86	OHX	6	1929	-	0,6,6	-	-	-		
86	OHX	5	3498	-	0,6,6	-	-	-		
86	OHX	6	2059	86	0,6,6	-	-	-		
86	OHX	5	3788	86	0,6,6	-	-	-		
86	OHX	n3	202	-	0,6,6	-	-	-		
86	OHX	1	3792	86	0,6,6	-	-	-		
86	OHX	1	3412	-	0,6,6	-	-	-		
86	OHX	5	3682	-	0,6,6	-	-	-		
86	OHX	2	1982	-	0,6,6	-	-	-		
86	OHX	2	2016	-	0,6,6	-	-	-		
86	OHX	5	3443	-	0,6,6	-	-	-		
86	OHX	o3	201	-	0,6,6	-	-	-		
86	OHX	6	2057	86,80	0,6,6	-	-	-		
86	OHX	5	3599	86	0,6,6	-	-	-		
86	OHX	1	3503	-	0,6,6	-	-	-		
86	OHX	5	3412	-	0,6,6	-	-	-		
86	OHX	5	3782	36	0,6,6	-	-	-		
86	OHX	1	3489	86	0,6,6	-	-	-		
86	OHX	5	3474	36	0,6,6	-	-	-		
86	OHX	1	3440	-	0,6,6	-	-	-		
86	OHX	1	3500	-	0,6,6	-	-	-		
86	OHX	5	3485	-	0,6,6	-	-	-		
86	OHX	2	1955	-	0,6,6	-	-	-		
86	OHX	5	3806	86,36	0,6,6	-	-	-		
86	OHX	5	3575	-	0,6,6	-	-	-		
86	OHX	2	2010	-	0,6,6	-	-	-		
86	OHX	3	204	-	0,6,6	-	-	-		
86	OHX	1	3445	-	0,6,6	-	-	-		
86	OHX	5	3464	86	0,6,6	-	-	-		
86	OHX	2	2039	86	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3511	86	0,6,6	-	-	-		
86	OHX	1	3789	86	0,6,6	-	-	-		
86	OHX	6	2034	86,80	0,6,6	-	-	-		
86	OHX	4	202	-	0,6,6	-	-	-		
86	OHX	2	1972	1	0,6,6	-	-	-		
86	OHX	1	3476	86	0,6,6	-	-	-		
86	OHX	5	3781	-	0,6,6	-	-	-		
86	OHX	5	3454	86,36	0,6,6	-	-	-		
86	OHX	6	2035	-	0,6,6	-	-	-		
86	OHX	5	3741	-	0,6,6	-	-	-		
86	OHX	1	3576	-	0,6,6	-	-	-		
86	OHX	5	3493	36	0,6,6	-	-	-		
86	OHX	14	402	-	0,6,6	-	-	-		
86	OHX	5	3409	36	0,6,6	-	-	-		
86	OHX	1	3446	-	0,6,6	-	-	-		
86	OHX	1	3717	86	0,6,6	-	-	-		
86	OHX	6	1984	80	0,6,6	-	-	-		
86	OHX	1	3657	-	0,6,6	-	-	-		
86	OHX	5	3578	-	0,6,6	-	-	-		
86	OHX	1	3631	-	0,6,6	-	-	-		
86	OHX	1	3730	-	0,6,6	-	-	-		
86	OHX	2	2080	86	0,6,6	-	-	-		
86	OHX	1	3529	-	0,6,6	-	-	-		
86	OHX	1	3527	-	0,6,6	-	-	-		
86	OHX	1	3673	-	0,6,6	-	-	-		
86	OHX	1	3540	36	0,6,6	-	-	-		
86	OHX	5	3749	86	0,6,6	-	-	-		
86	OHX	1	3571	86	0,6,6	-	-	-		
86	OHX	1	3493	86	0,6,6	-	-	-		
86	OHX	5	3411	36	0,6,6	-	-	-		
86	OHX	2	1908	-	0,6,6	-	-	-		
86	OHX	5	3421	36	0,6,6	-	-	-		
86	OHX	1	3434	-	0,6,6	-	-	-		
86	OHX	5	3618	-	0,6,6	-	-	-		
86	OHX	1	3431	86	0,6,6	-	-	-		
86	OHX	2	1949	-	0,6,6	-	-	-		
86	OHX	1	3706	-	0,6,6	-	-	-		
86	OHX	5	3594	36	0,6,6	-	-	-		
86	OHX	5	3508	36	0,6,6	-	-	-		
86	OHX	5	3567	-	0,6,6	-	-	-		
86	OHX	6	1932	-	0,6,6	-	-	-		
86	OHX	1	3568	-	0,6,6	-	-	-		
86	OHX	1	3764	86	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3516	-	0,6,6	-	-	-		
86	OHX	5	3615	86,89,36	0,6,6	-	-	-		
86	OHX	1	3622	-	0,6,6	-	-	-		
86	OHX	2	1902	-	0,6,6	-	-	-		
86	OHX	2	1998	86	0,6,6	-	-	-		
86	OHX	5	3427	-	0,6,6	-	-	-		
86	OHX	1	3671	-	0,6,6	-	-	-		
86	OHX	2	1903	-	0,6,6	-	-	-		
86	OHX	6	2061	86	0,6,6	-	-	-		
86	OHX	1	3482	-	0,6,6	-	-	-		
86	OHX	2	1979	86	0,6,6	-	-	-		
86	OHX	2	1913	-	0,6,6	-	-	-		
86	OHX	6	1974	80	0,6,6	-	-	-		
86	OHX	6	2021	-	0,6,6	-	-	-		
86	OHX	15	303	-	0,6,6	-	-	-		
86	OHX	1	3425	-	0,6,6	-	-	-		
86	OHX	5	3583	86	0,6,6	-	-	-		
86	OHX	5	3626	-	0,6,6	-	-	-		
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	6	2016	80	0,6,6	-	-	-		
86	OHX	5	3656	-	0,6,6	-	-	-		
86	OHX	6	1999	-	0,6,6	-	-	-		
86	OHX	1	3468	-	0,6,6	-	-	-		
86	OHX	5	3451	86	0,6,6	-	-	-		
86	OHX	1	3618	-	0,6,6	-	-	-		
86	OHX	6	2040	-	0,6,6	-	-	-		
86	OHX	5	3687	-	0,6,6	-	-	-		
86	OHX	1	3627	-	0,6,6	-	-	-		
86	OHX	1	3634	-	0,6,6	-	-	-		
86	OHX	1	3638	-	0,6,6	-	-	-		
86	OHX	1	3804	86	0,6,6	-	-	-		
86	OHX	1	3406	-	0,6,6	-	-	-		
86	OHX	7	206	-	0,6,6	-	-	-		
86	OHX	4	207	-	0,6,6	-	-	-		
86	OHX	2	1905	-	0,6,6	-	-	-		
86	OHX	6	2044	-	0,6,6	-	-	-		
86	OHX	5	3693	36	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	1	3423	-	0,6,6	-	-	-		
86	OHX	5	3634	86	0,6,6	-	-	-		
86	OHX	M0	303	86	0,6,6	-	-	-		
86	OHX	5	3667	-	0,6,6	-	-	-		
86	OHX	6	2053	80	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2036	80	0,6,6	-	-	-		
86	OHX	6	1956	-	0,6,6	-	-	-		
86	OHX	l3	401	-	0,6,6	-	-	-		
86	OHX	3	210	-	0,6,6	-	-	-		
86	OHX	1	3504	86	0,6,6	-	-	-		
86	OHX	1	3637	-	0,6,6	-	-	-		
86	OHX	5	3742	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	5	3471	86	0,6,6	-	-	-		
86	OHX	1	3625	86	0,6,6	-	-	-		
86	OHX	6	1959	86	0,6,6	-	-	-		
86	OHX	5	3639	-	0,6,6	-	-	-		
86	OHX	5	3750	36	0,6,6	-	-	-		
86	OHX	2	1988	86	0,6,6	-	-	-		
86	OHX	1	3698	-	0,6,6	-	-	-		
86	OHX	5	3805	86	0,6,6	-	-	-		
86	OHX	1	3654	-	0,6,6	-	-	-		
86	OHX	5	3658	36	0,6,6	-	-	-		
86	OHX	S2	301	86	0,6,6	-	-	-		
86	OHX	1	3651	36	0,6,6	-	-	-		
86	OHX	1	3733	-	0,6,6	-	-	-		
86	OHX	1	3546	86	0,6,6	-	-	-		
86	OHX	6	1981	-	0,6,6	-	-	-		
86	OHX	5	3632	86	0,6,6	-	-	-		
86	OHX	1	3648	-	0,6,6	-	-	-		
86	OHX	5	3703	36	0,6,6	-	-	-		
86	OHX	6	1972	-	0,6,6	-	-	-		
86	OHX	1	3410	36	0,6,6	-	-	-		
86	OHX	5	3546	-	0,6,6	-	-	-		
86	OHX	1	3766	-	0,6,6	-	-	-		
86	OHX	6	1998	80	0,6,6	-	-	-		
86	OHX	5	3711	-	0,6,6	-	-	-		
86	OHX	4	217	-	0,6,6	-	-	-		
86	OHX	6	1925	80	0,6,6	-	-	-		
86	OHX	1	3737	36	0,6,6	-	-	-		
86	OHX	1	3772	-	0,6,6	-	-	-		
86	OHX	5	3629	36	0,6,6	-	-	-		
86	OHX	2	2008	86	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	7	213	-	0,6,6	-	-	-		
86	OHX	5	3436	-	0,6,6	-	-	-		
86	OHX	5	3524	86	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	1947	-	0,6,6	-	-	-		
86	OHX	1	3508	86	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	5	3816	86	0,6,6	-	-	-		
86	OHX	5	3517	86	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	M9	201	-	0,6,6	-	-	-		
86	OHX	1	3450	86	0,6,6	-	-	-		
86	OHX	1	3729	-	0,6,6	-	-	-		
86	OHX	1	3506	86	0,6,6	-	-	-		
86	OHX	5	3737	36	0,6,6	-	-	-		
86	OHX	1	3601	86	0,6,6	-	-	-		
86	OHX	5	3553	-	0,6,6	-	-	-		
86	OHX	5	3460	86,36	0,6,6	-	-	-		
86	OHX	5	3803	86	0,6,6	-	-	-		
86	OHX	5	3705	-	0,6,6	-	-	-		
86	OHX	m0	304	86	0,6,6	-	-	-		
86	OHX	c1	201	86	0,6,6	-	-	-		
86	OHX	1	3664	-	0,6,6	-	-	-		
86	OHX	5	3456	-	0,6,6	-	-	-		
86	OHX	5	3678	-	0,6,6	-	-	-		
86	OHX	2	1929	-	0,6,6	-	-	-		
86	OHX	1	3691	86,36	0,6,6	-	-	-		
86	OHX	1	3668	-	0,6,6	-	-	-		
86	OHX	1	3458	-	0,6,6	-	-	-		
86	OHX	2	1997	-	0,6,6	-	-	-		
86	OHX	5	3513	36	0,6,6	-	-	-		
86	OHX	6	2003	80	0,6,6	-	-	-		
86	OHX	1	3483	-	0,6,6	-	-	-		
86	OHX	2	2074	86	0,6,6	-	-	-		
86	OHX	O7	102	73	0,6,6	-	-	-		
86	OHX	5	3614	-	0,6,6	-	-	-		
86	OHX	2	2059	86	0,6,6	-	-	-		
86	OHX	2	2026	86	0,6,6	-	-	-		
86	OHX	5	3739	36	0,6,6	-	-	-		
86	OHX	7	205	-	0,6,6	-	-	-		
86	OHX	6	2098	86	0,6,6	-	-	-		
86	OHX	2	1977	86	0,6,6	-	-	-		
86	OHX	1	3586	-	0,6,6	-	-	-		
86	OHX	6	2033	-	0,6,6	-	-	-		
86	OHX	6	2092	86	0,6,6	-	-	-		
86	OHX	5	3514	86,36	0,6,6	-	-	-		
86	OHX	5	3547	36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3468	86	0,6,6	-	-	-		
86	OHX	6	1943	-	0,6,6	-	-	-		
86	OHX	2	1909	86	0,6,6	-	-	-		
86	OHX	6	1978	80	0,6,6	-	-	-		
86	OHX	1	3699	86	0,6,6	-	-	-		
86	OHX	4	213	-	0,6,6	-	-	-		
86	OHX	5	3646	-	0,6,6	-	-	-		
86	OHX	6	1903	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	5	3425	-	0,6,6	-	-	-		
86	OHX	1	3752	-	0,6,6	-	-	-		
86	OHX	1	3814	86,36	0,6,6	-	-	-		
86	OHX	5	3582	86	0,6,6	-	-	-		
86	OHX	6	2042	86,80	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	6	2093	86,80	0,6,6	-	-	-		
86	OHX	6	1947	-	0,6,6	-	-	-		
86	OHX	5	3655	86,36	0,6,6	-	-	-		
86	OHX	5	3545	-	0,6,6	-	-	-		
86	OHX	4	214	38	0,6,6	-	-	-		
86	OHX	2	1968	-	0,6,6	-	-	-		
86	OHX	5	3426	-	0,6,6	-	-	-		
86	OHX	3	207	86	0,6,6	-	-	-		
86	OHX	1	3758	36	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	2	1917	-	0,6,6	-	-	-		
86	OHX	5	3585	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	6	1923	80	0,6,6	-	-	-		
86	OHX	5	3653	-	0,6,6	-	-	-		
86	OHX	2	1953	-	0,6,6	-	-	-		
86	OHX	5	3636	86	0,6,6	-	-	-		
86	OHX	S8	301	-	0,6,6	-	-	-		
86	OHX	5	3558	36	0,6,6	-	-	-		
86	OHX	5	3651	86	0,6,6	-	-	-		
86	OHX	5	3530	-	0,6,6	-	-	-		
86	OHX	5	3414	-	0,6,6	-	-	-		
86	OHX	1	3521	-	0,6,6	-	-	-		
86	OHX	1	3439	-	0,6,6	-	-	-		
86	OHX	4	211	-	0,6,6	-	-	-		
86	OHX	5	3584	-	0,6,6	-	-	-		
86	OHX	5	3552	-	0,6,6	-	-	-		
86	OHX	5	3728	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3430	36	0,6,6	-	-	-		
86	OHX	1	3630	-	0,6,6	-	-	-		
86	OHX	6	1991	80	0,6,6	-	-	-		
86	OHX	2	1958	-	0,6,6	-	-	-		
86	OHX	1	3740	-	0,6,6	-	-	-		
89	C	5	3401	86	18,21,22	0.65	0	26,30,33	1.43	5 (19%)
86	OHX	2	2018	86	0,6,6	-	-	-		
86	OHX	8	201	-	0,6,6	-	-	-		
86	OHX	2	1966	-	0,6,6	-	-	-		
86	OHX	5	3439	-	0,6,6	-	-	-		
86	OHX	5	3413	36	0,6,6	-	-	-		
86	OHX	2	1922	86	0,6,6	-	-	-		
86	OHX	1	3464	86	0,6,6	-	-	-		
86	OHX	5	3423	36	0,6,6	-	-	-		
86	OHX	5	3608	36	0,6,6	-	-	-		
86	OHX	2	2012	-	0,6,6	-	-	-		
86	OHX	6	1951	-	0,6,6	-	-	-		
86	OHX	5	3444	36	0,6,6	-	-	-		
86	OHX	2	1990	86,1	0,6,6	-	-	-		
86	OHX	6	1957	80	0,6,6	-	-	-		
86	OHX	6	1952	86,80	0,6,6	-	-	-		
86	OHX	5	3453	-	0,6,6	-	-	-		
86	OHX	6	1909	86,80	0,6,6	-	-	-		
86	OHX	1	3731	86	0,6,6	-	-	-		
86	OHX	1	3693	-	0,6,6	-	-	-		
86	OHX	8	207	38,86	0,6,6	-	-	-		
86	OHX	1	3602	86	0,6,6	-	-	-		
86	OHX	1	3710	-	0,6,6	-	-	-		
86	OHX	5	3579	36	0,6,6	-	-	-		
86	OHX	1	3452	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	1	3588	86	0,6,6	-	-	-		
86	OHX	1	3753	86	0,6,6	-	-	-		
86	OHX	5	3511	36	0,6,6	-	-	-		
86	OHX	1	3791	86	0,6,6	-	-	-		
86	OHX	5	3677	-	0,6,6	-	-	-		
86	OHX	2	2068	86	0,6,6	-	-	-		
86	OHX	2	2006	-	0,6,6	-	-	-		
86	OHX	1	3743	86	0,6,6	-	-	-		
86	OHX	5	3801	86	0,6,6	-	-	-		
86	OHX	5	3556	-	0,6,6	-	-	-		
86	OHX	5	3676	36	0,6,6	-	-	-		
86	OHX	2	1994	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3614	-	0,6,6	-	-	-		
86	OHX	1	3732	-	0,6,6	-	-	-		
86	OHX	1	3726	-	0,6,6	-	-	-		
86	OHX	5	3657	86	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	3529	-	0,6,6	-	-	-		
86	OHX	1	3606	86	0,6,6	-	-	-		
86	OHX	6	1934	-	0,6,6	-	-	-		
86	OHX	O1	201	86	0,6,6	-	-	-		
86	OHX	5	3571	36	0,6,6	-	-	-		
86	OHX	1	3538	36	0,6,6	-	-	-		
86	OHX	1	3727	-	0,6,6	-	-	-		
86	OHX	1	3751	86,36	0,6,6	-	-	-		
86	OHX	1	3681	86	0,6,6	-	-	-		
86	OHX	2	2015	86,1	0,6,6	-	-	-		
86	OHX	5	3665	-	0,6,6	-	-	-		
86	OHX	6	2029	-	0,6,6	-	-	-		
86	OHX	n3	201	-	0,6,6	-	-	-		
86	OHX	2	2030	86	0,6,6	-	-	-		
86	OHX	5	3706	-	0,6,6	-	-	-		
86	OHX	1	3459	-	0,6,6	-	-	-		
86	OHX	D9	102	86	0,6,6	-	-	-		
86	OHX	6	2084	86	0,6,6	-	-	-		
86	OHX	2	2054	86	0,6,6	-	-	-		
86	OHX	1	3505	86	0,6,6	-	-	-		
86	OHX	5	3692	-	0,6,6	-	-	-		
86	OHX	1	3676	-	0,6,6	-	-	-		
86	OHX	5	3489	36	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	6	1922	-	0,6,6	-	-	-		
86	OHX	6	1953	-	0,6,6	-	-	-		
86	OHX	2	2031	86	0,6,6	-	-	-		

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
89	C	1	3402	90	-	0/7/25/26	0/2/2/2
89	C	1	3401	-	-	0/7/25/26	0/2/2/2
90	8AN	1	3403	89	-	0/3/25/26	0/3/3/3
91	PRO	1	3404	-	-	0/0/9/11	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	C	5	3402	90	-	0/7/25/26	0/2/2/2
91	PRO	5	3404	-	-	0/0/9/11	0/1/1/1
89	C	5	3401	86	-	0/7/25/26	0/2/2/2
90	8AN	5	3403	89	-	0/3/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	5	3403	8AN	C3'-N3'	-35.17	0.93	1.47
90	5	3403	8AN	O2'-C2'	5.86	1.56	1.43
90	1	3403	8AN	C5-C4	2.50	1.47	1.40
90	5	3403	8AN	C5-C4	-2.25	1.35	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	1	3401	C	C5-C4-N4	3.61	126.26	120.57
89	5	3401	C	C5-C4-N4	3.60	126.24	120.57
89	1	3401	C	O2-C2-N3	-3.22	117.09	122.33
89	5	3401	C	O2-C2-N3	-3.22	117.10	122.33
90	5	3403	8AN	N3-C2-N1	-3.18	123.70	128.68

There are no chirality outliers.

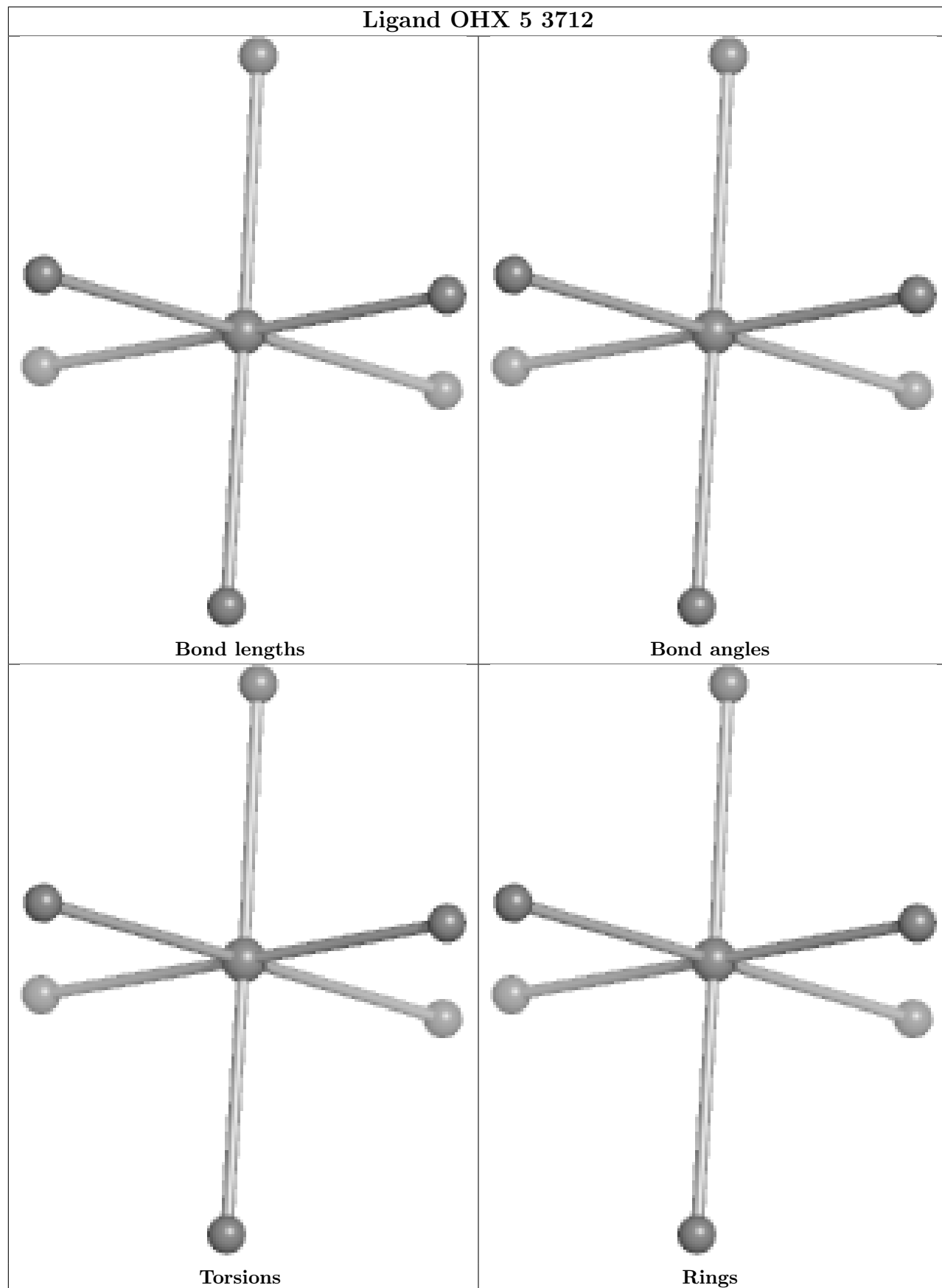
There are no torsion outliers.

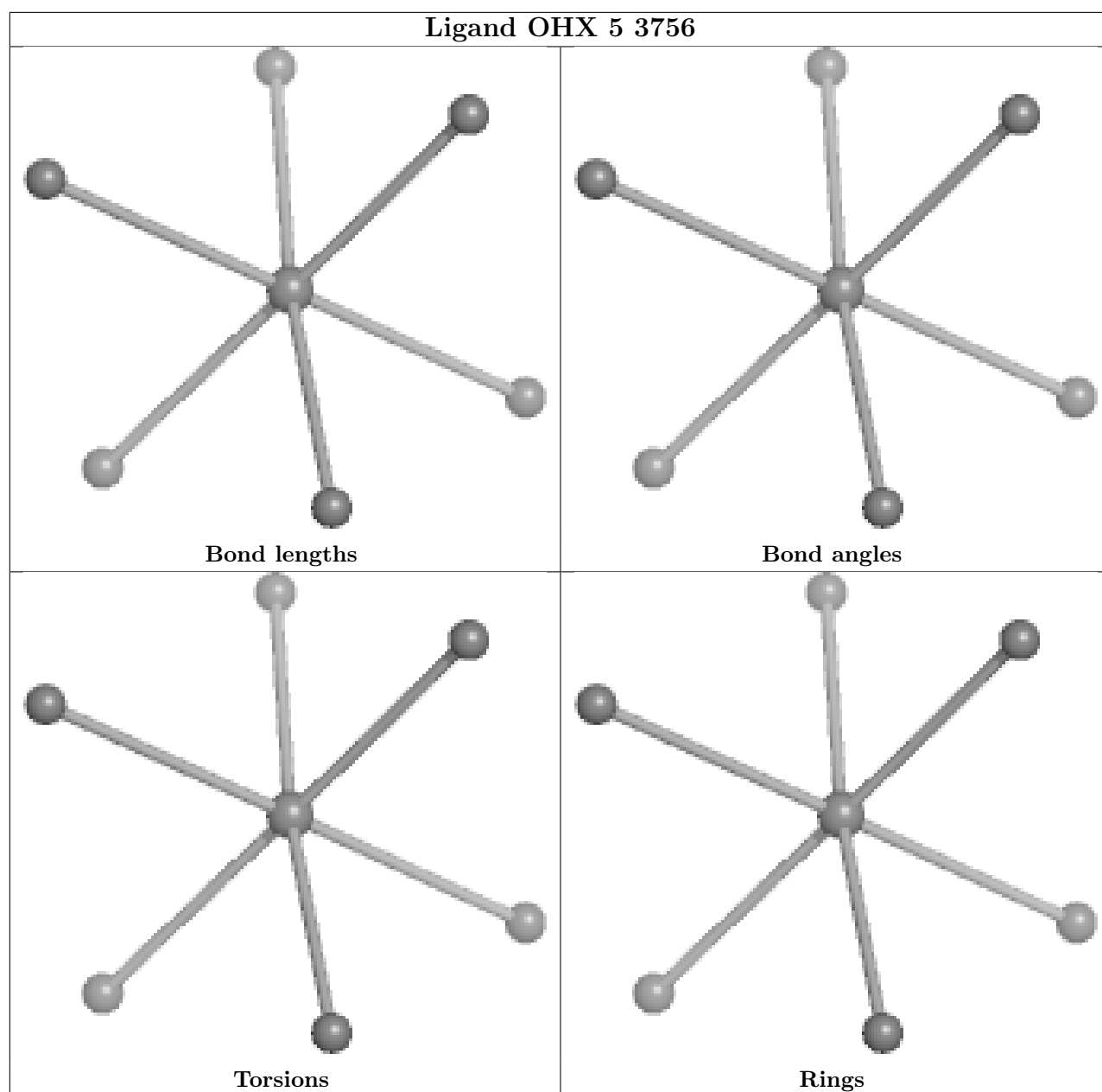
There are no ring outliers.

No monomer is involved in short contacts.

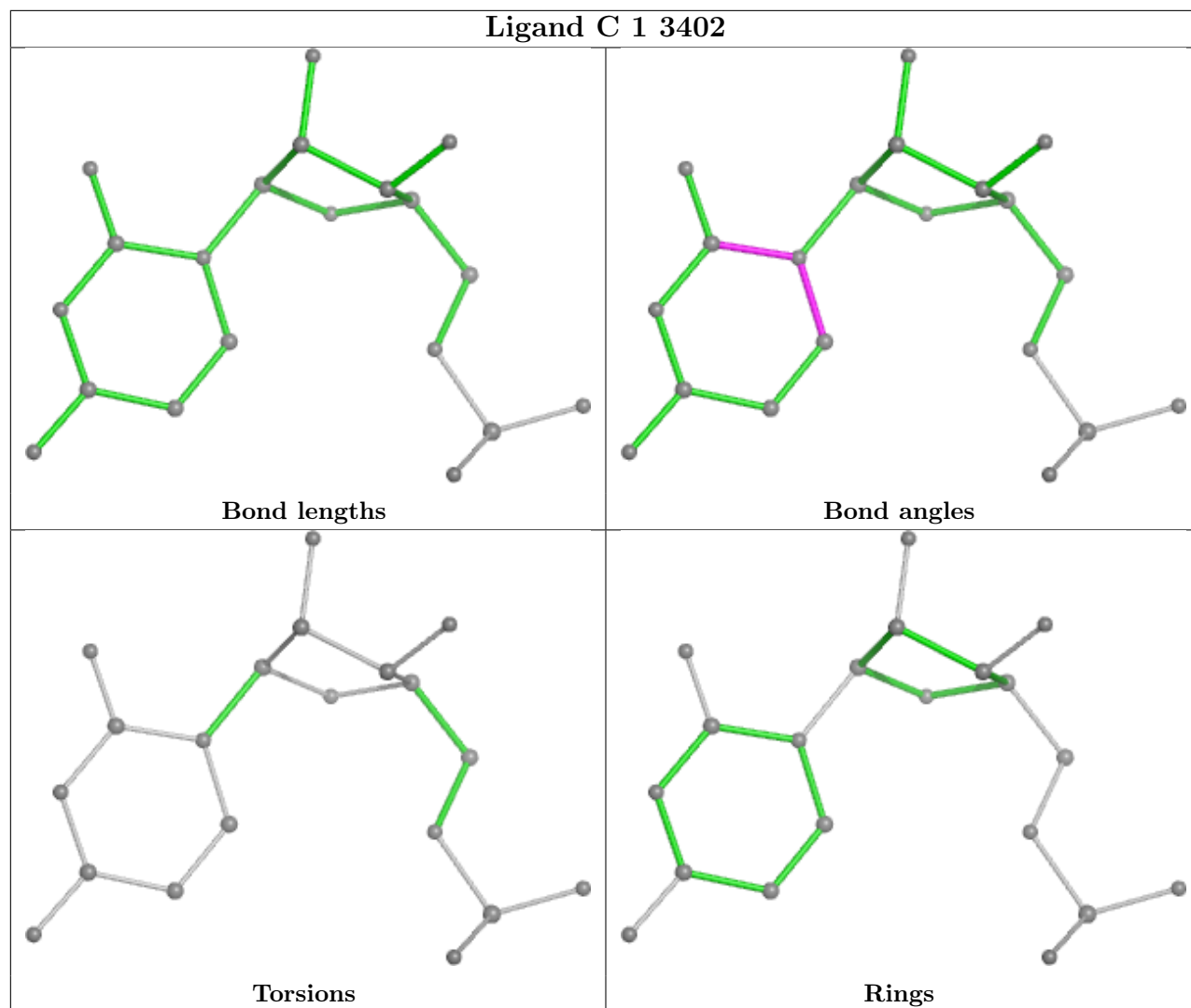
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand OHX 5 3712

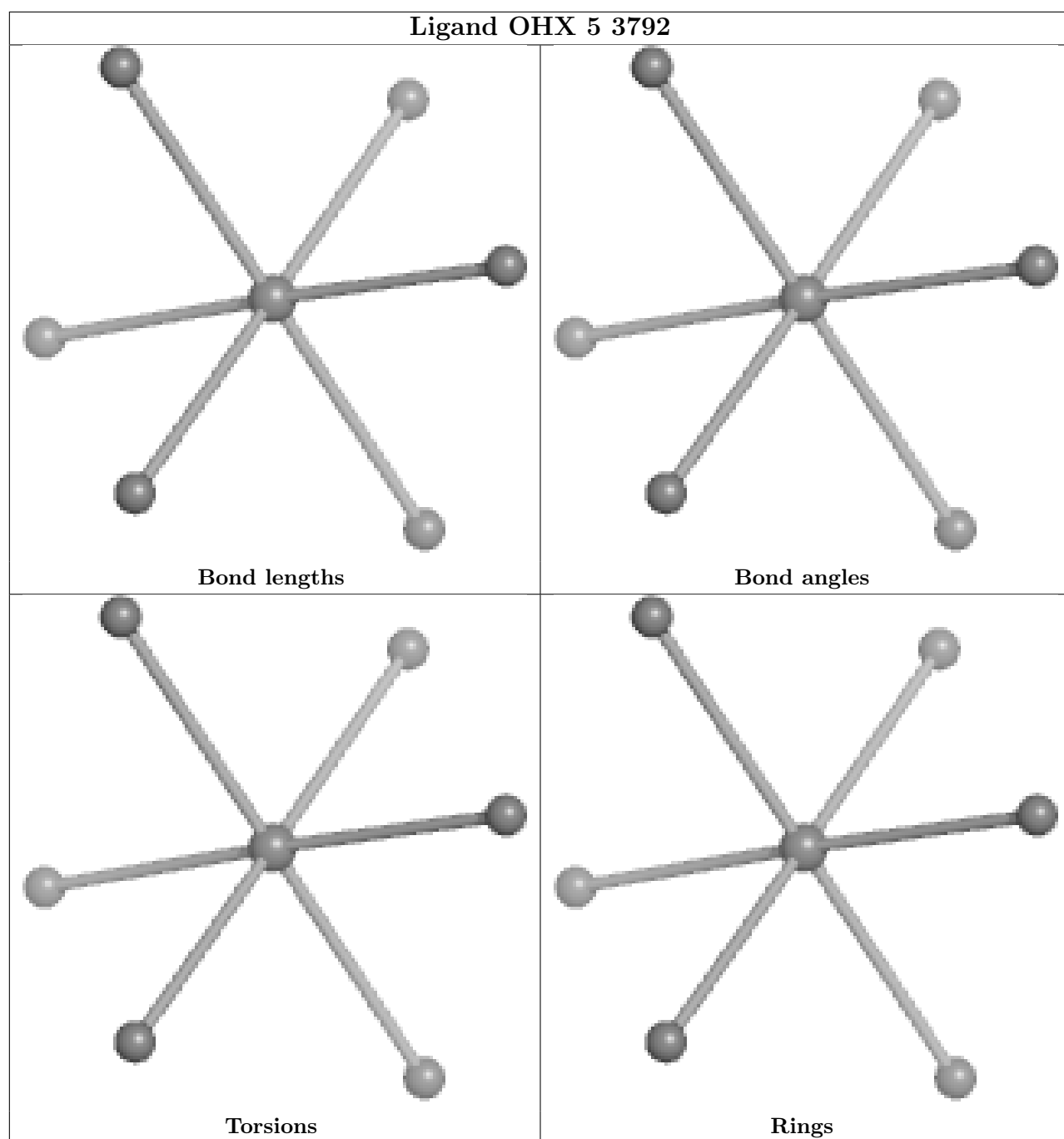


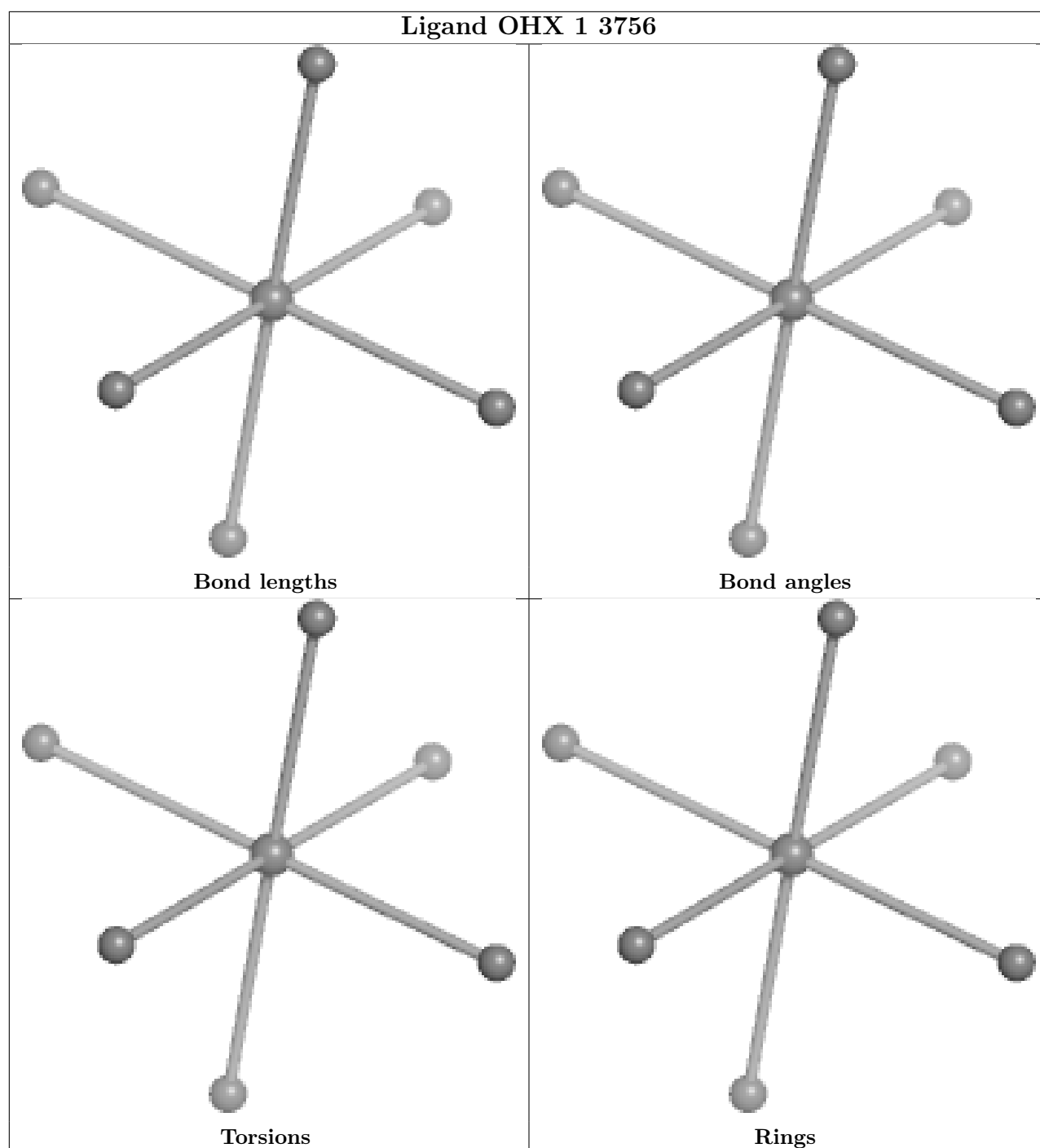


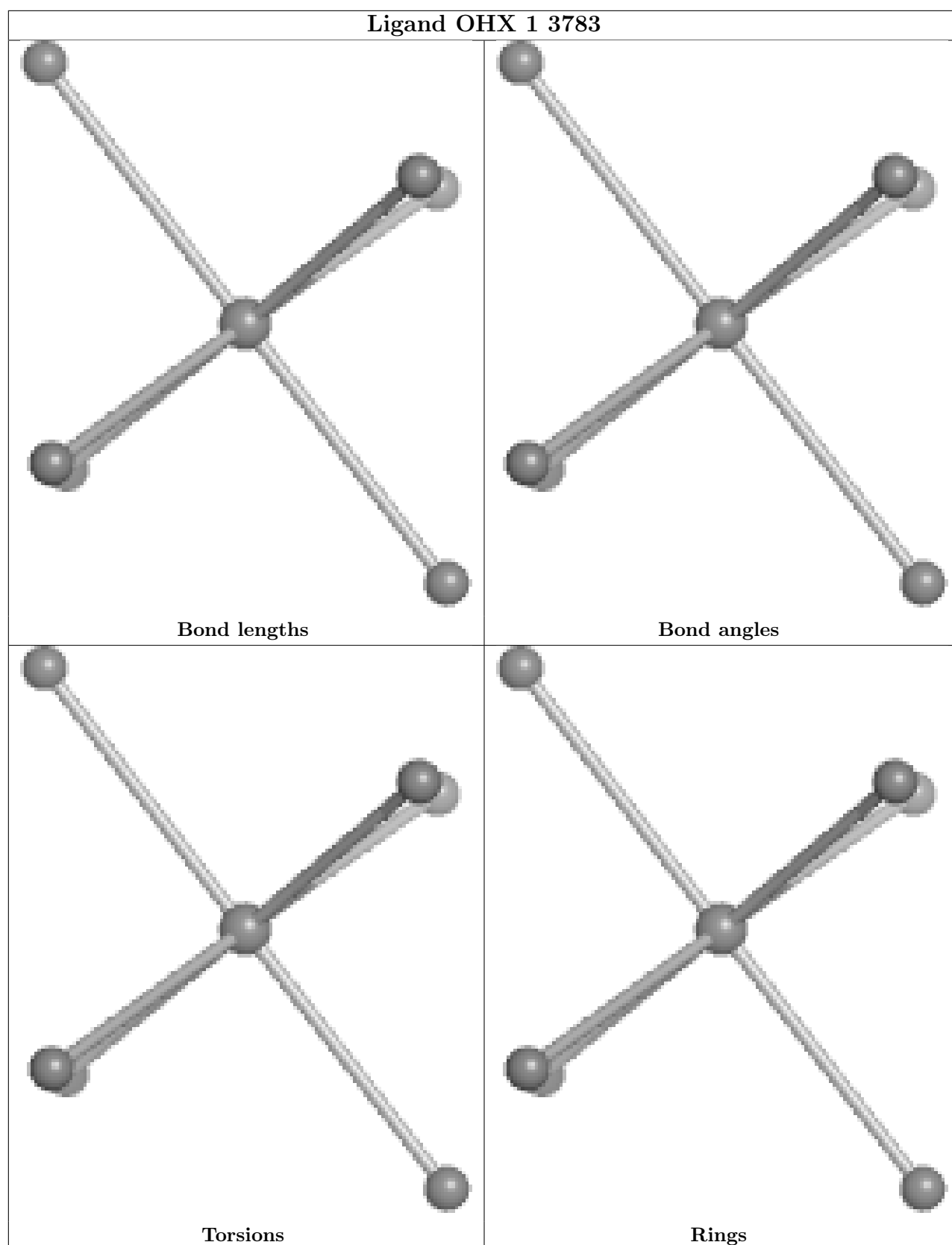
## Ligand C 1 3402

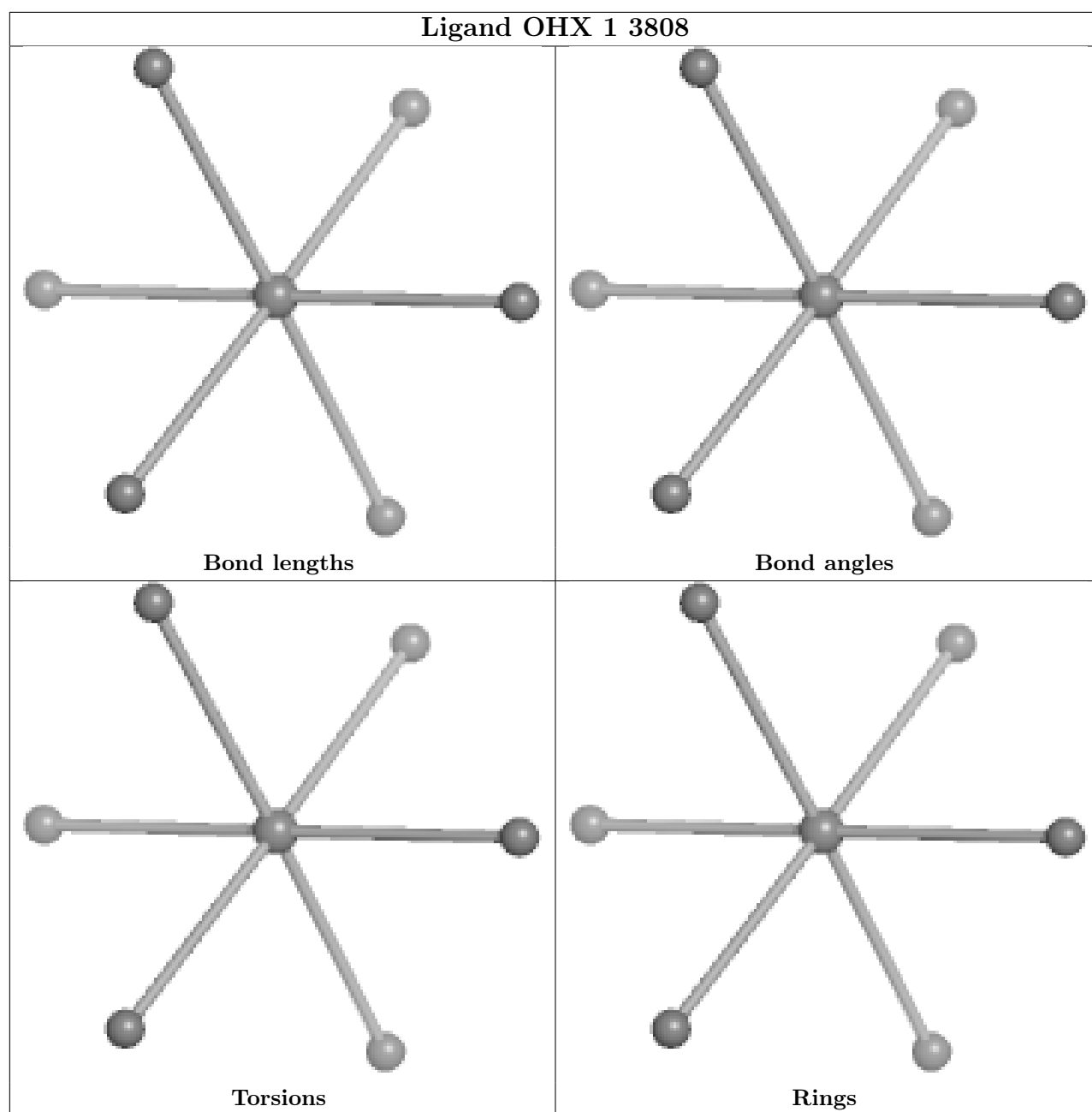


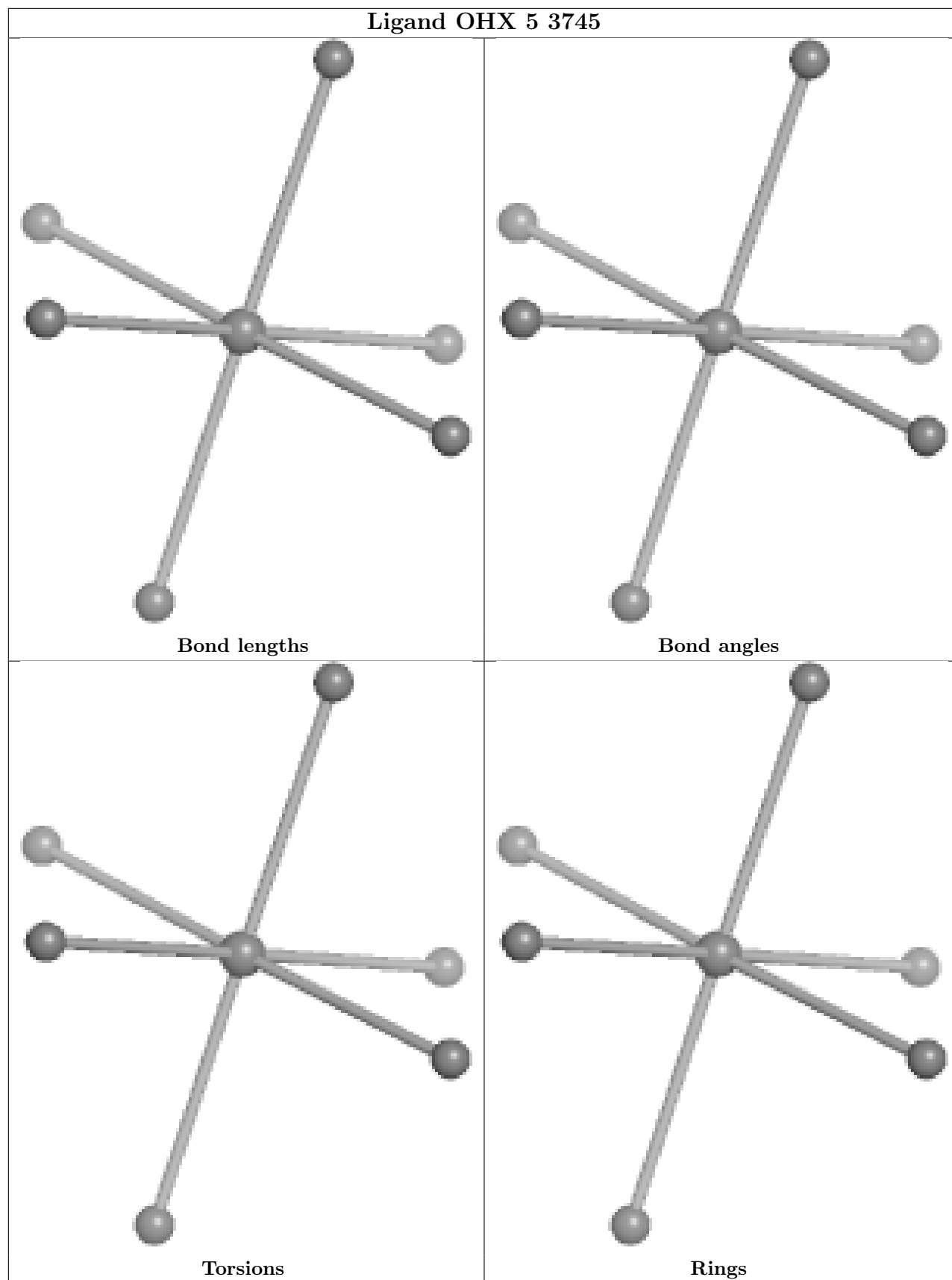


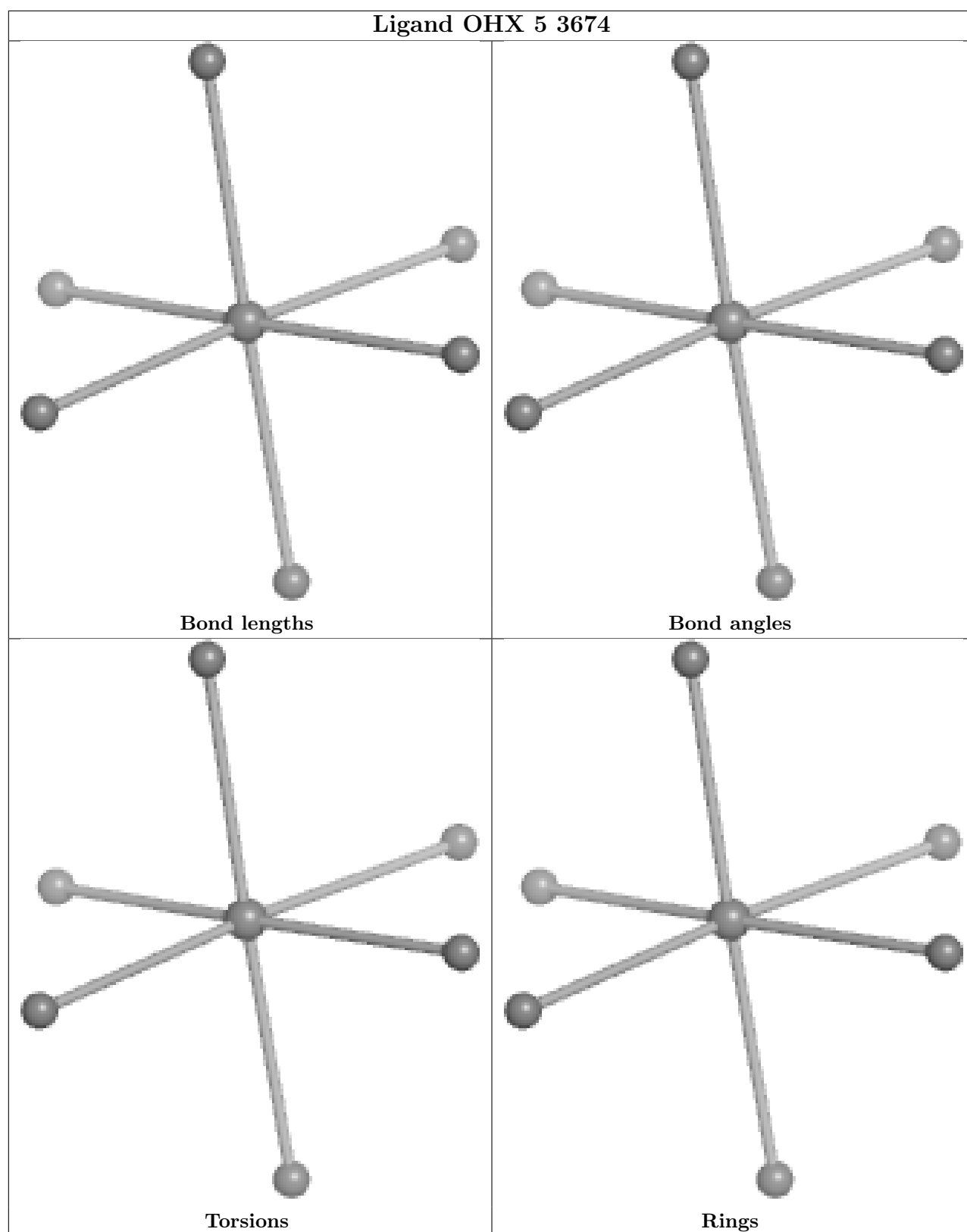




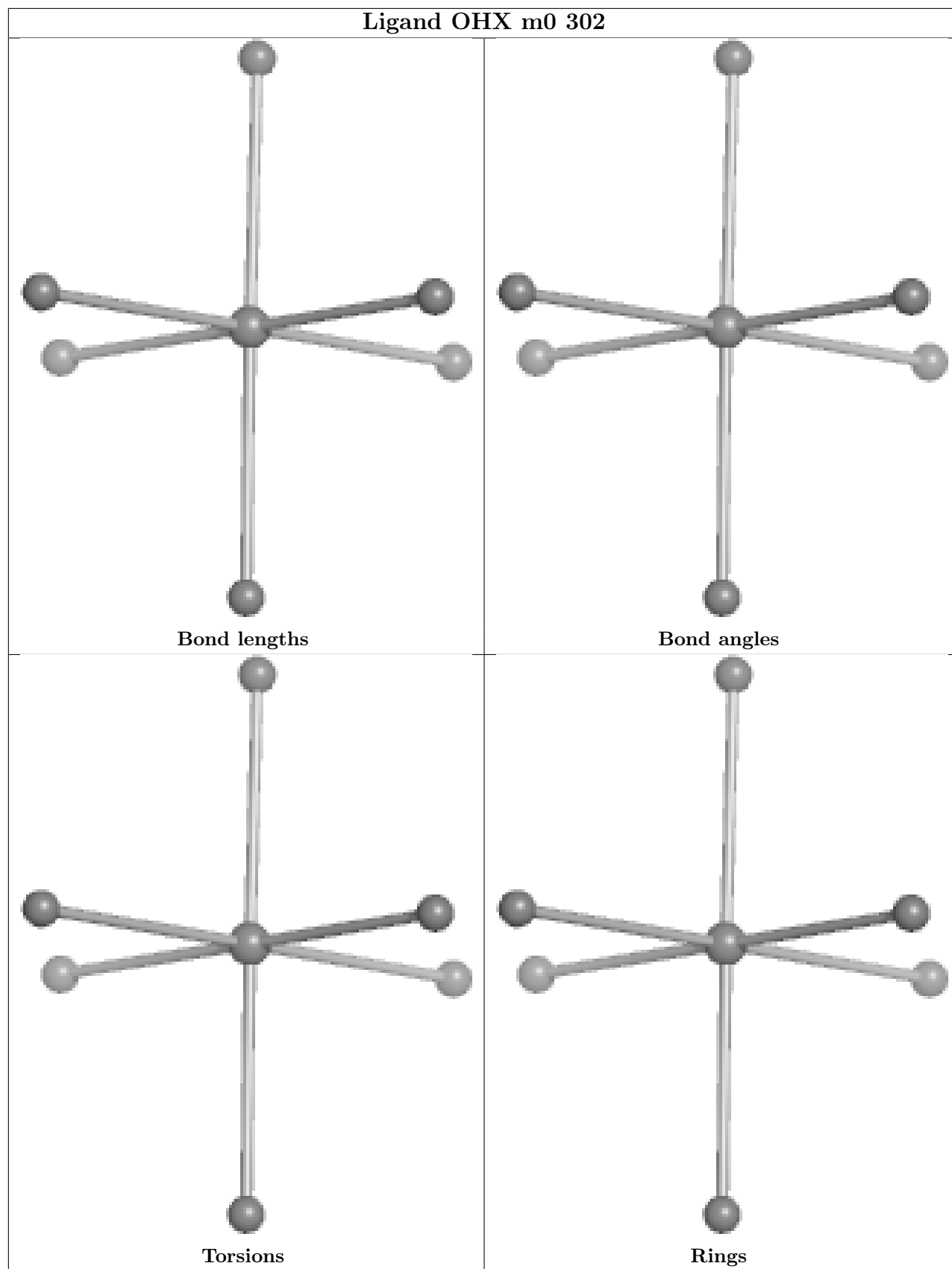


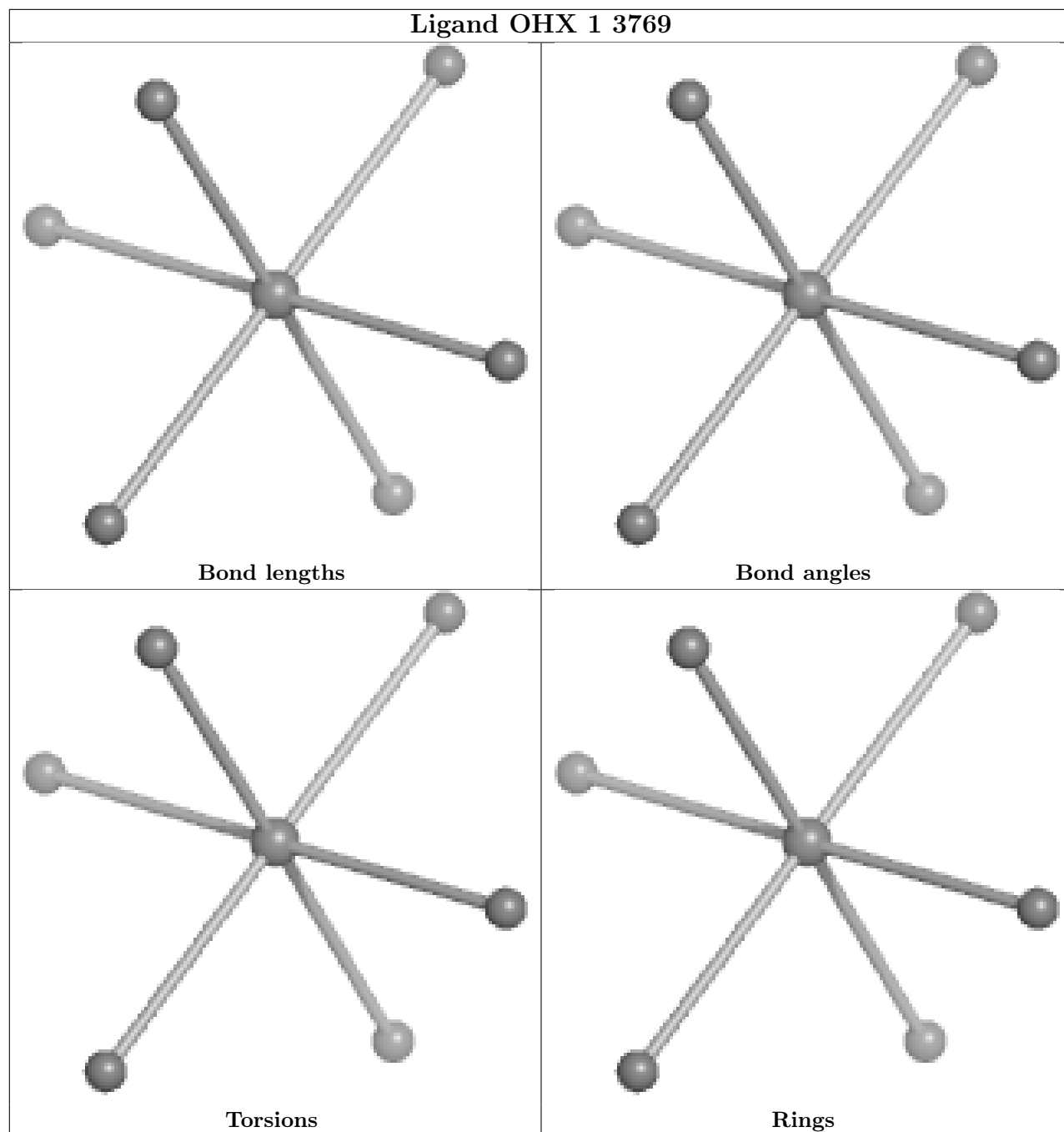




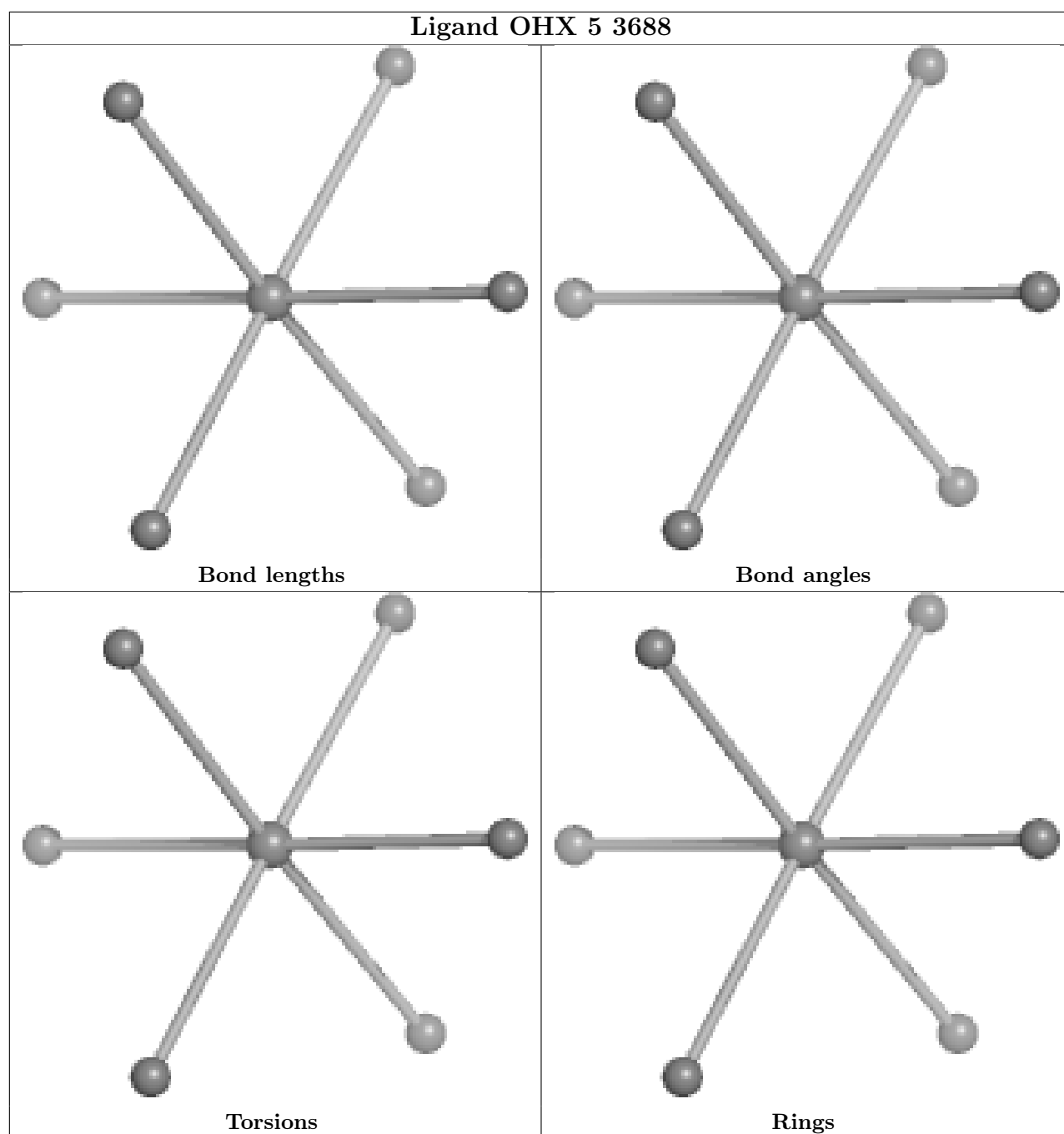


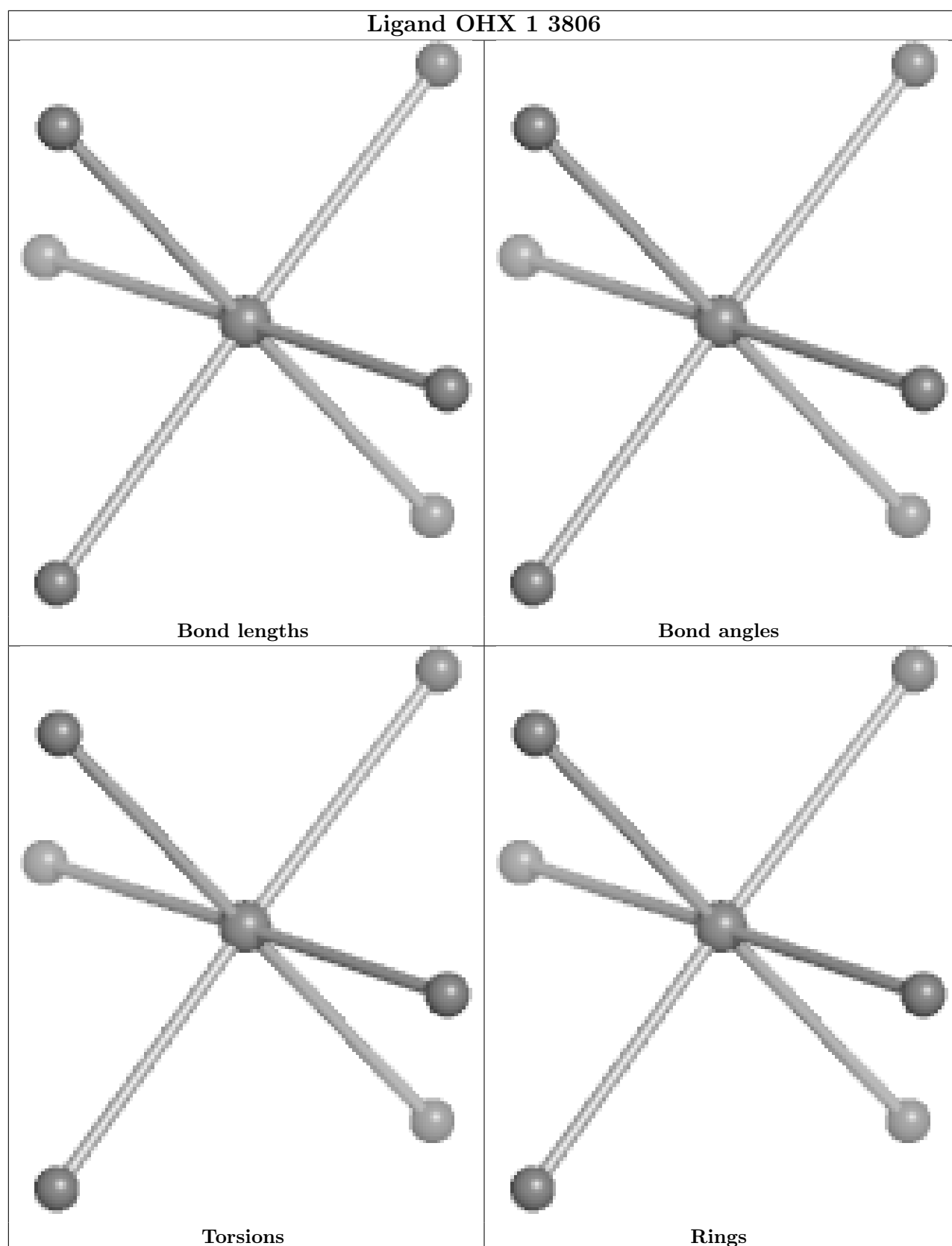
## Ligand OHX m0 302

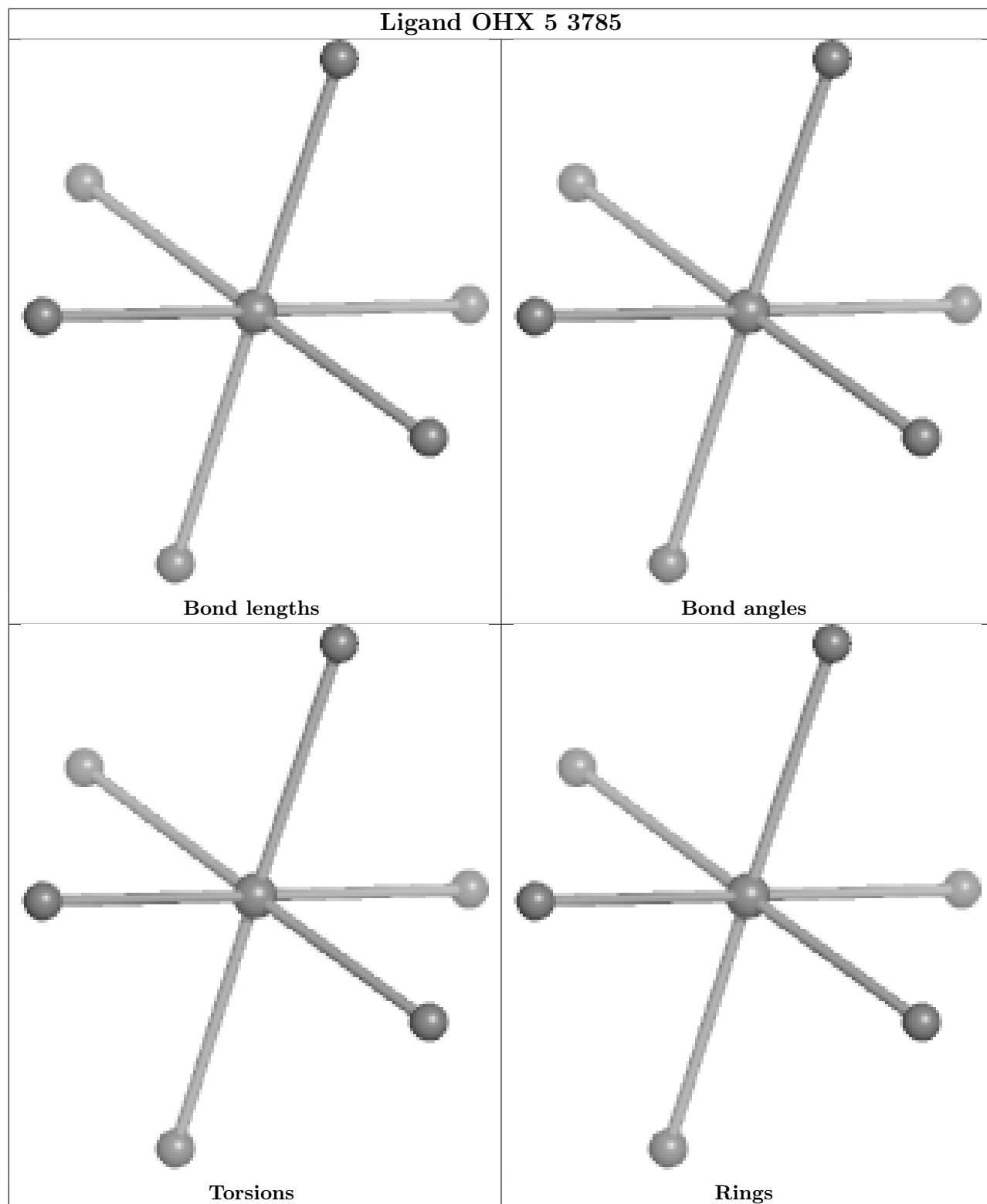


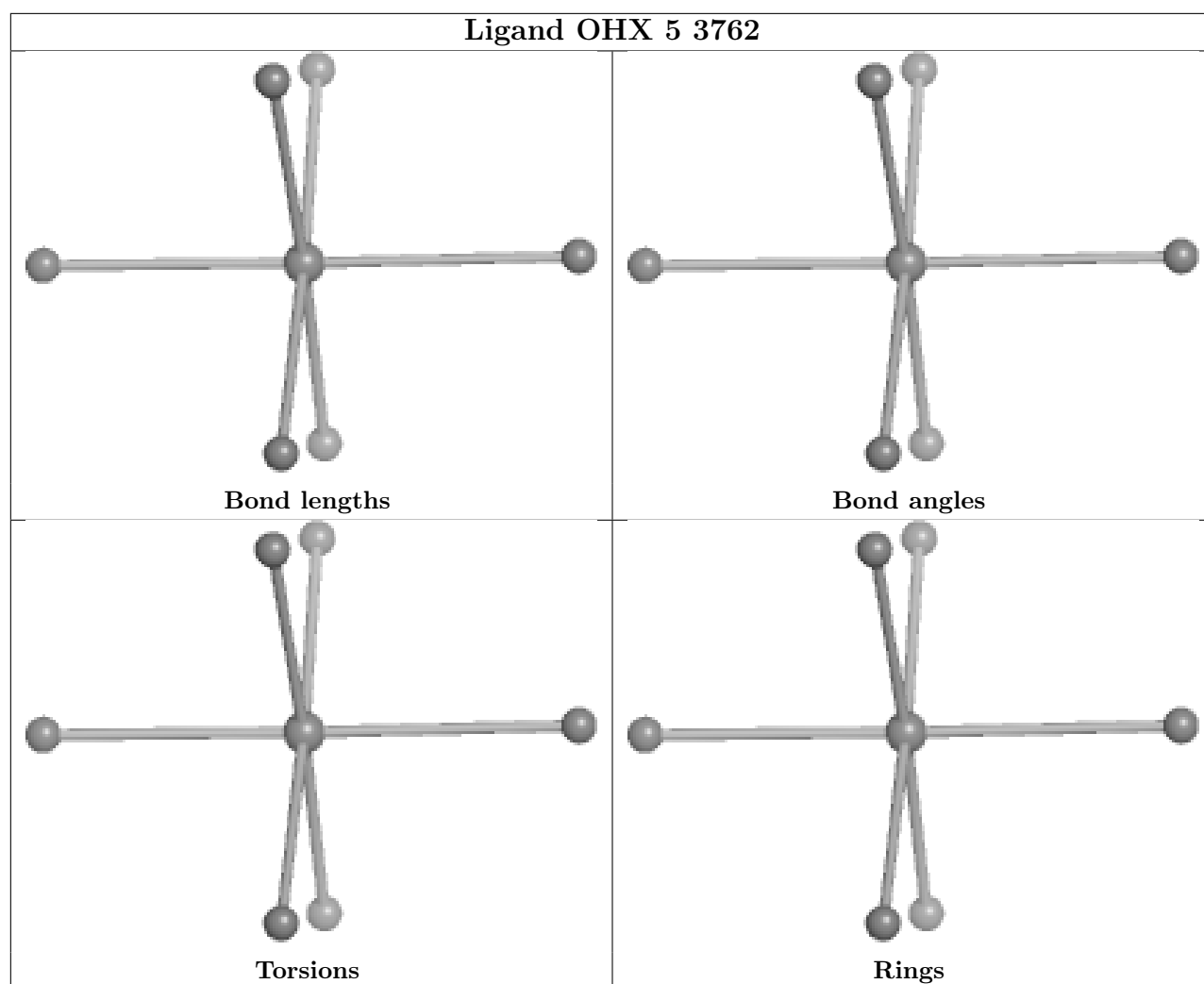


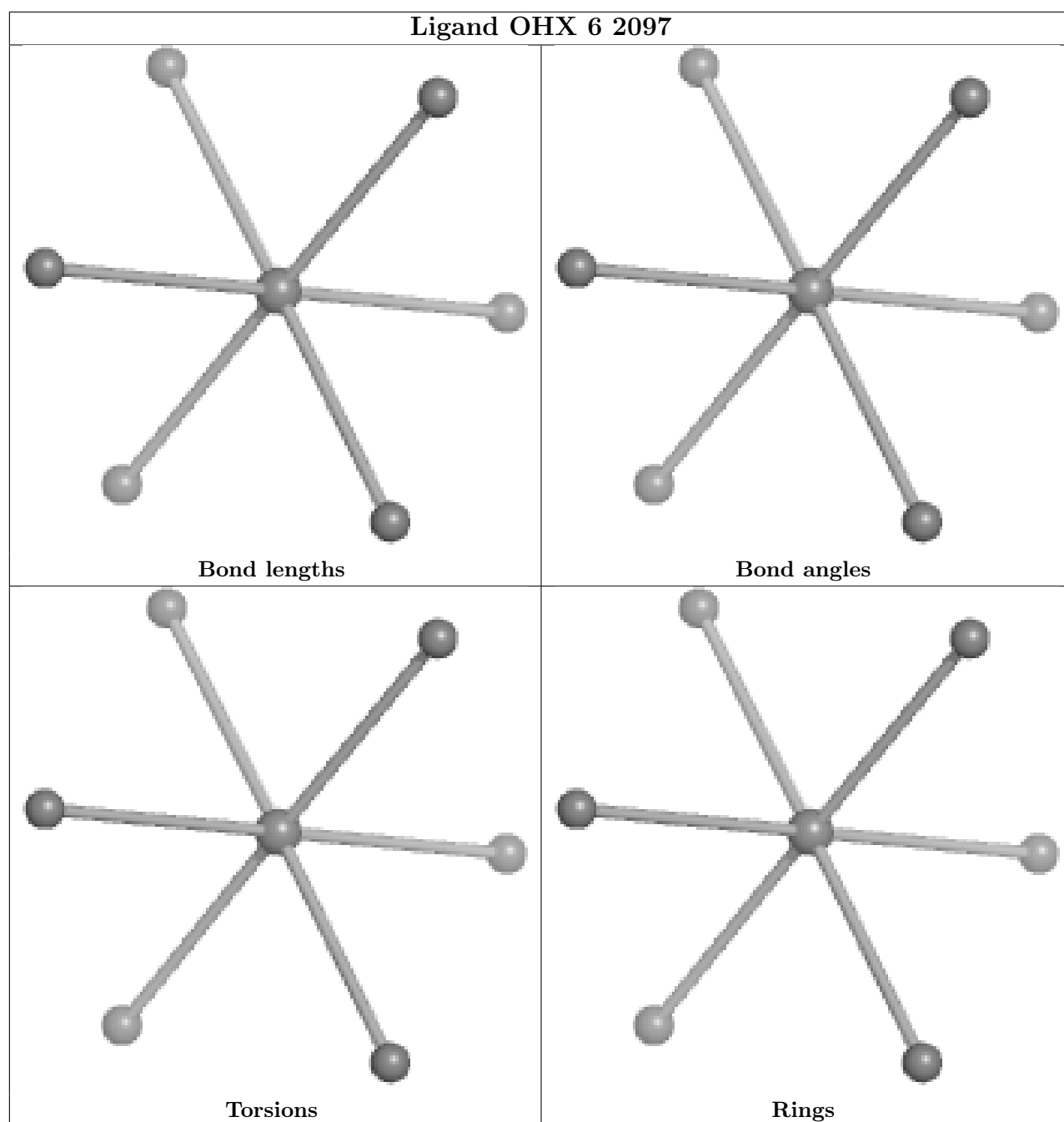


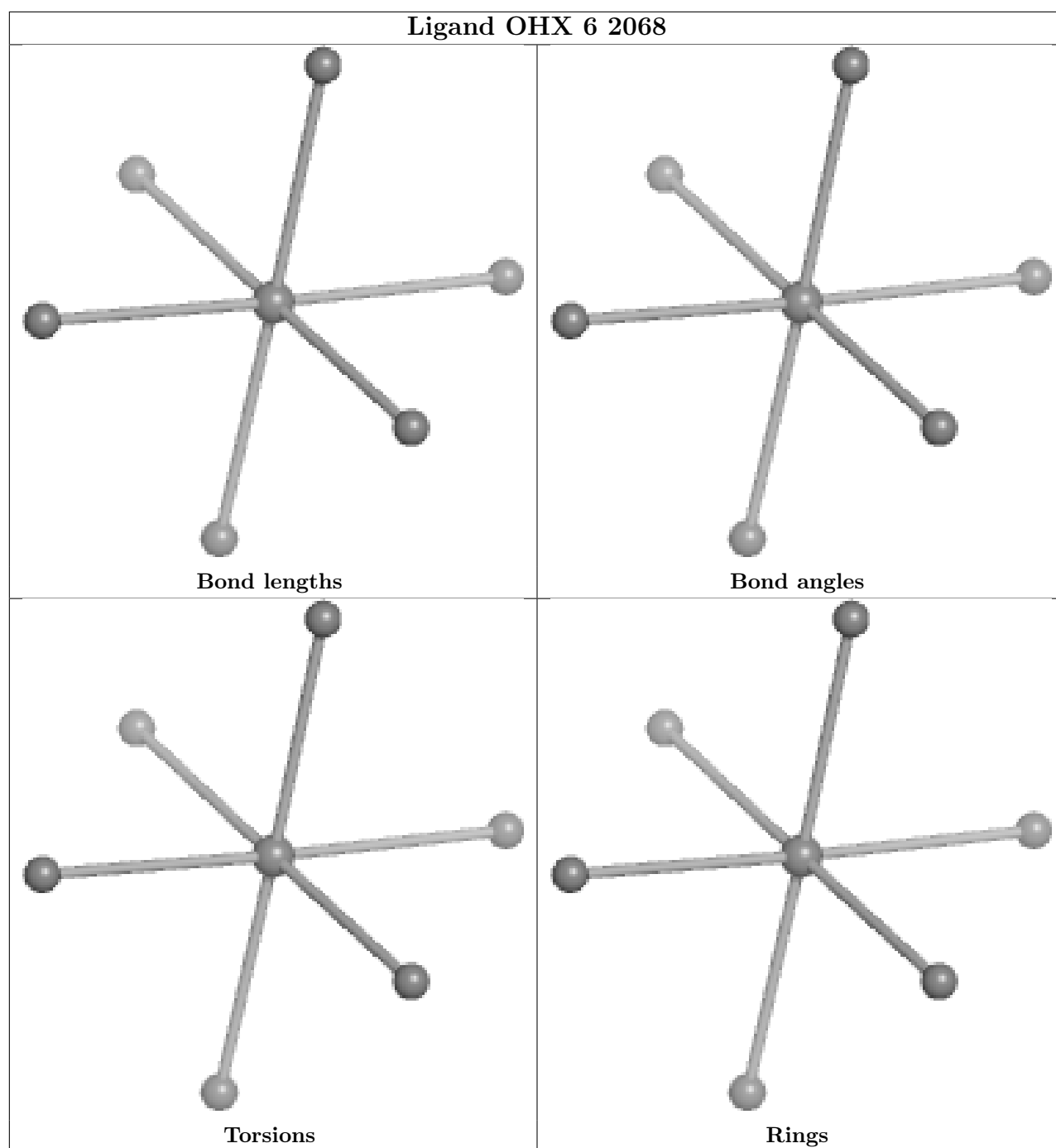


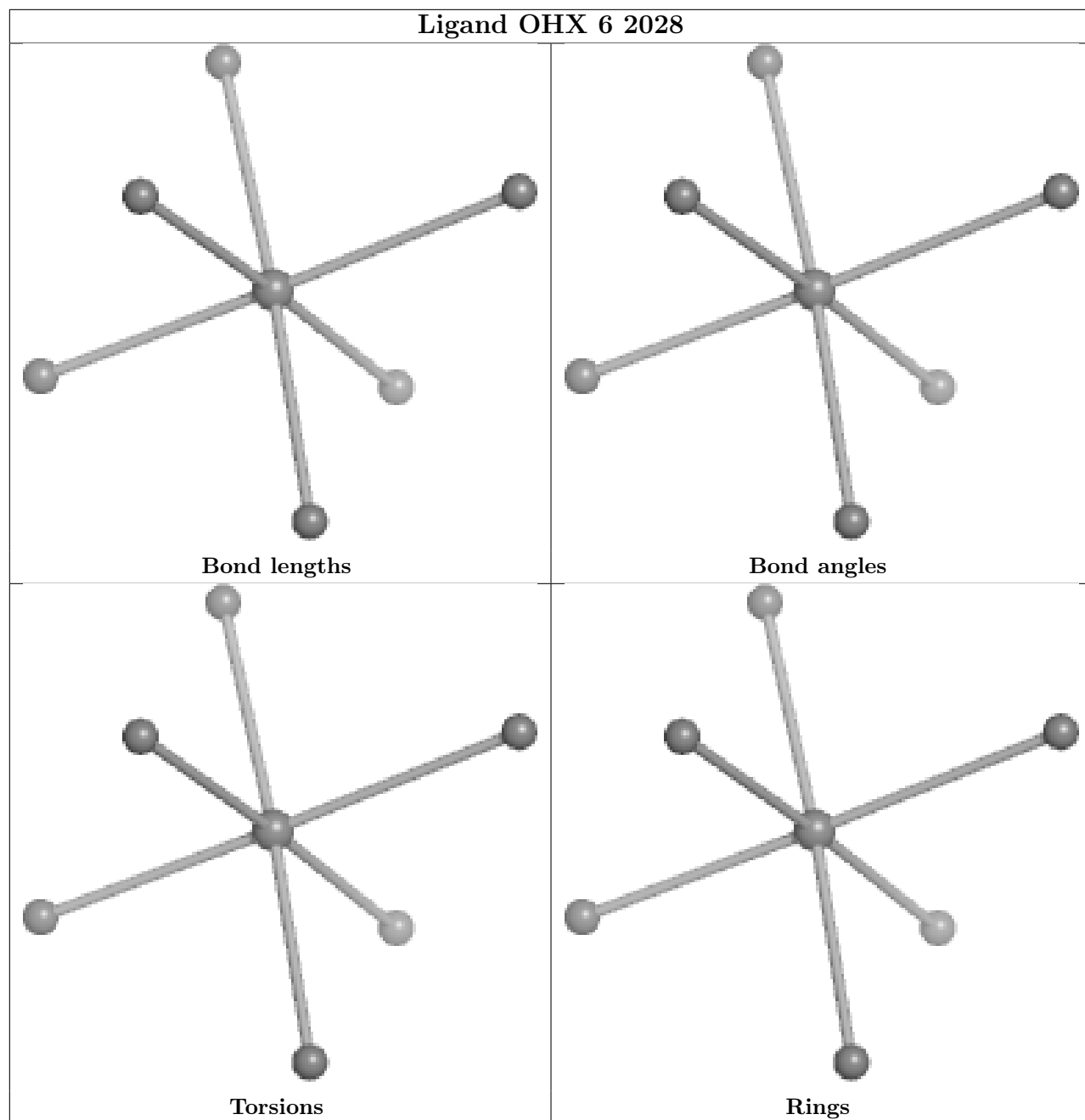


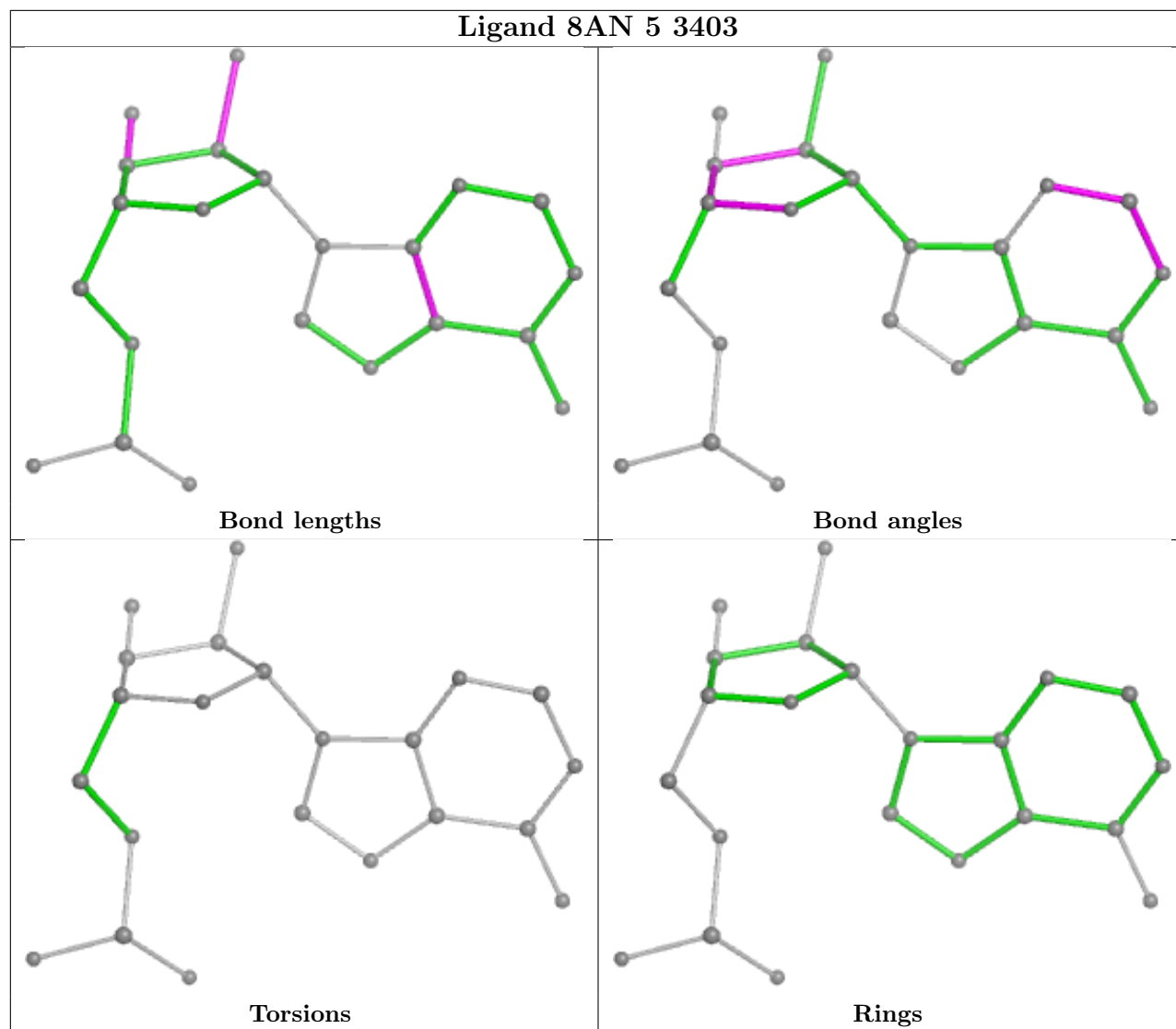




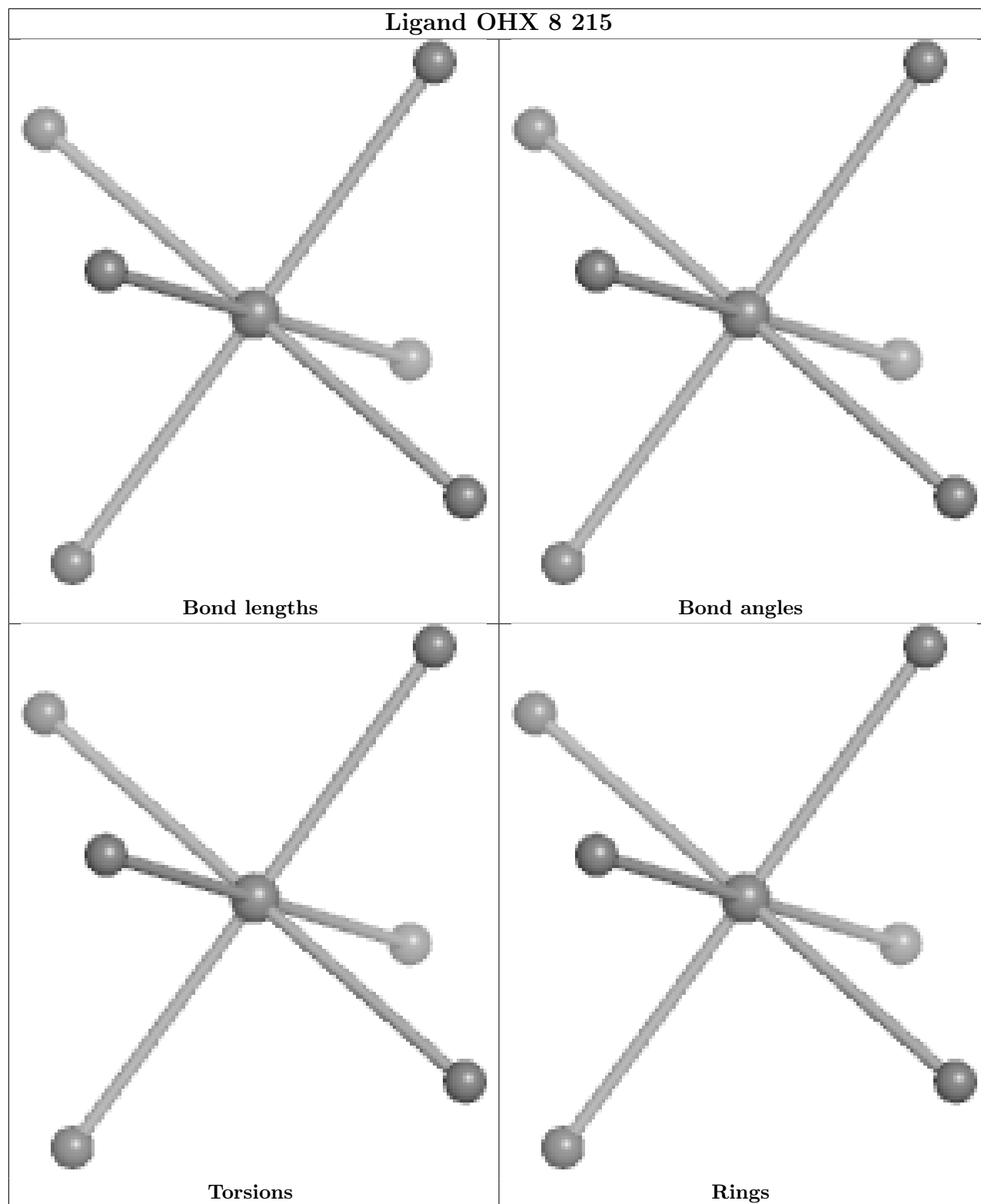




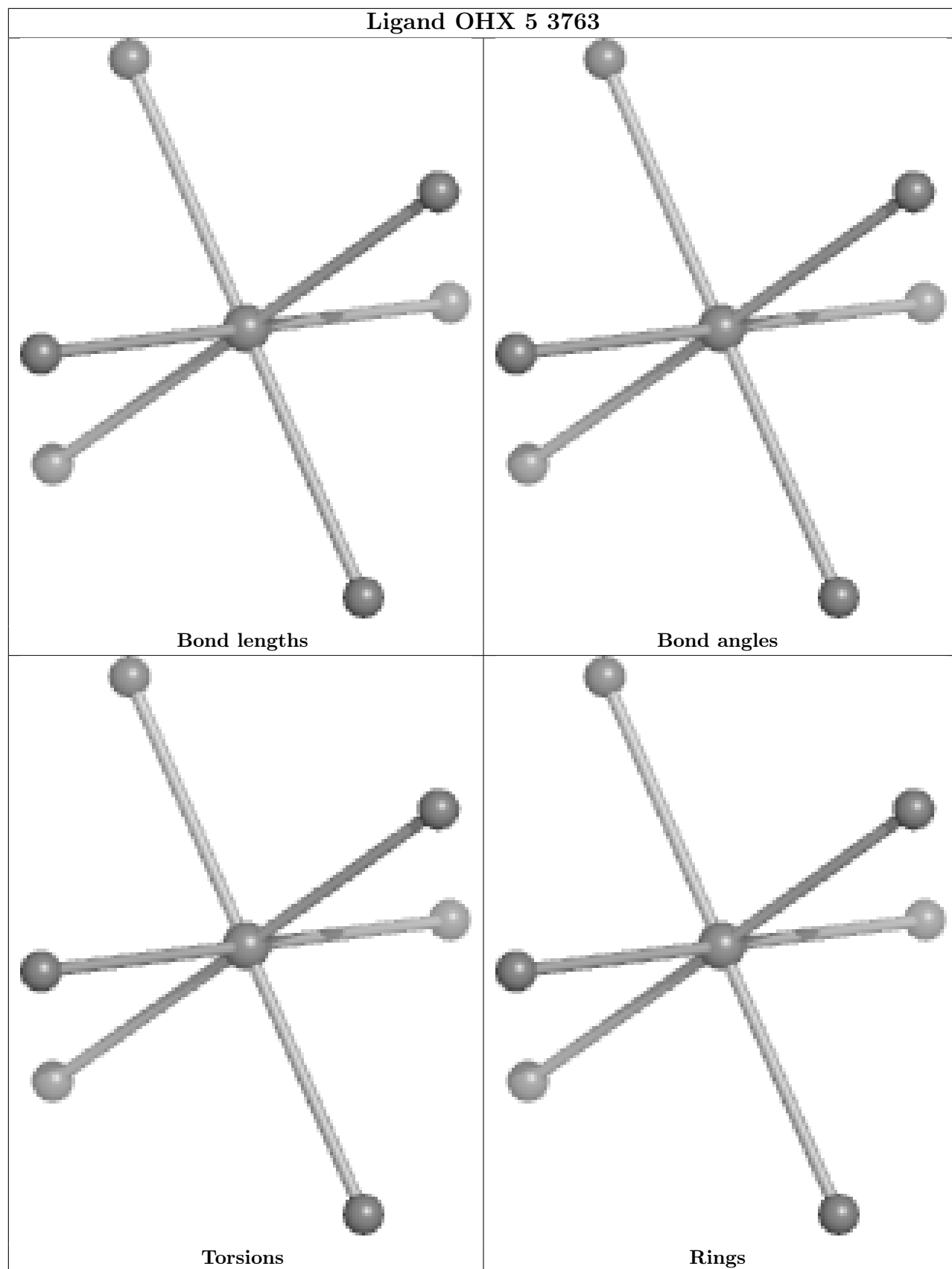


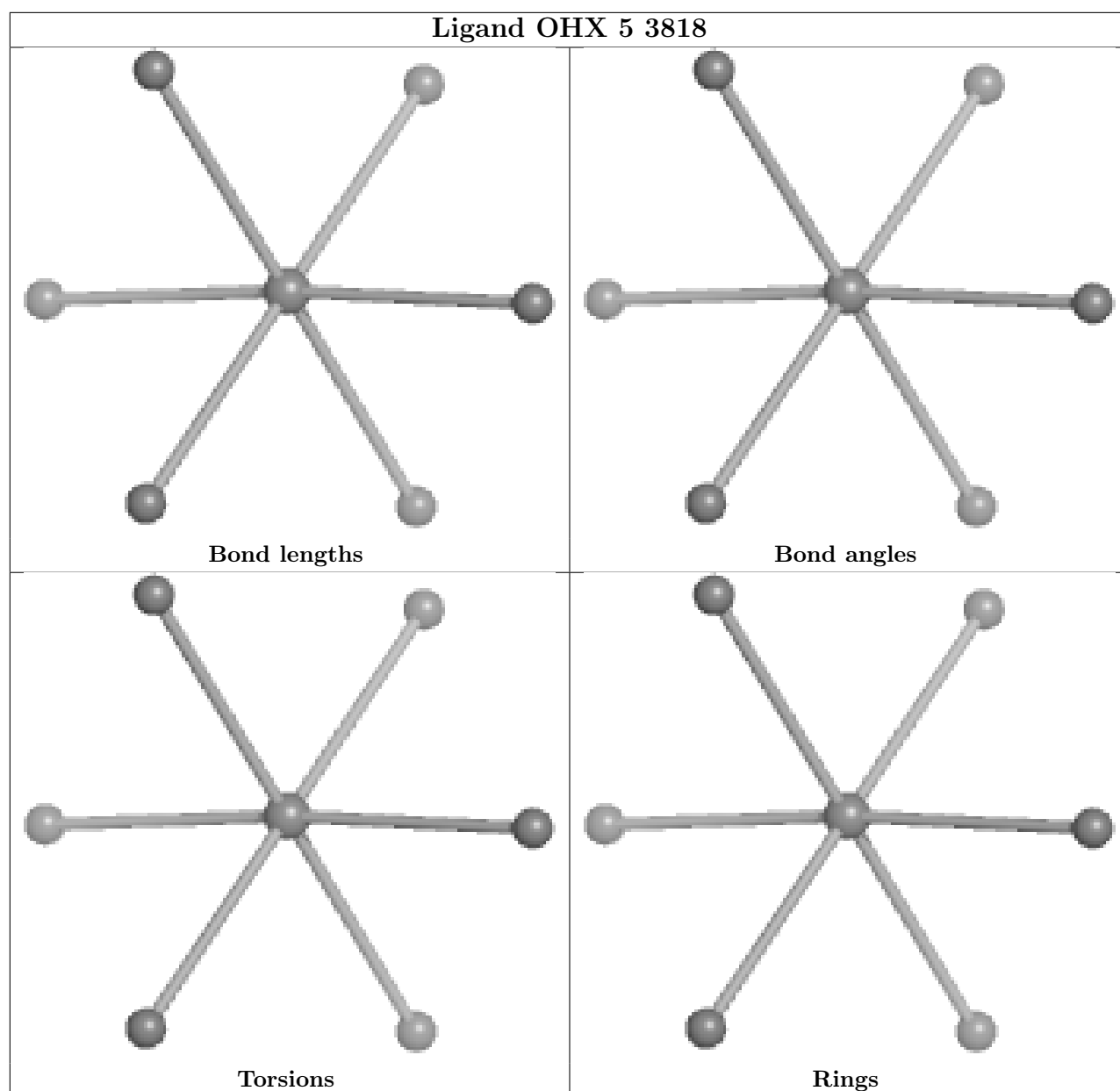


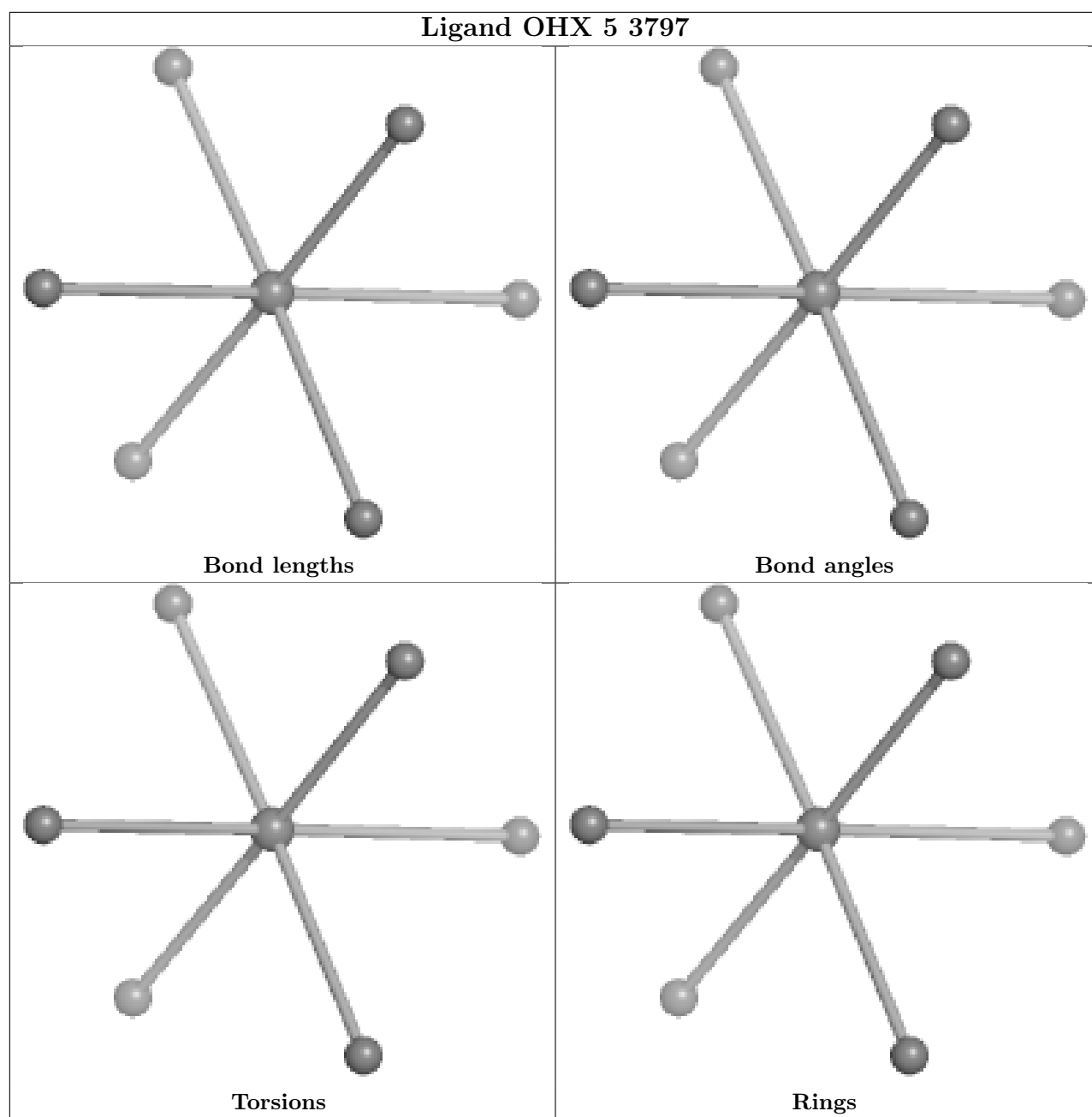


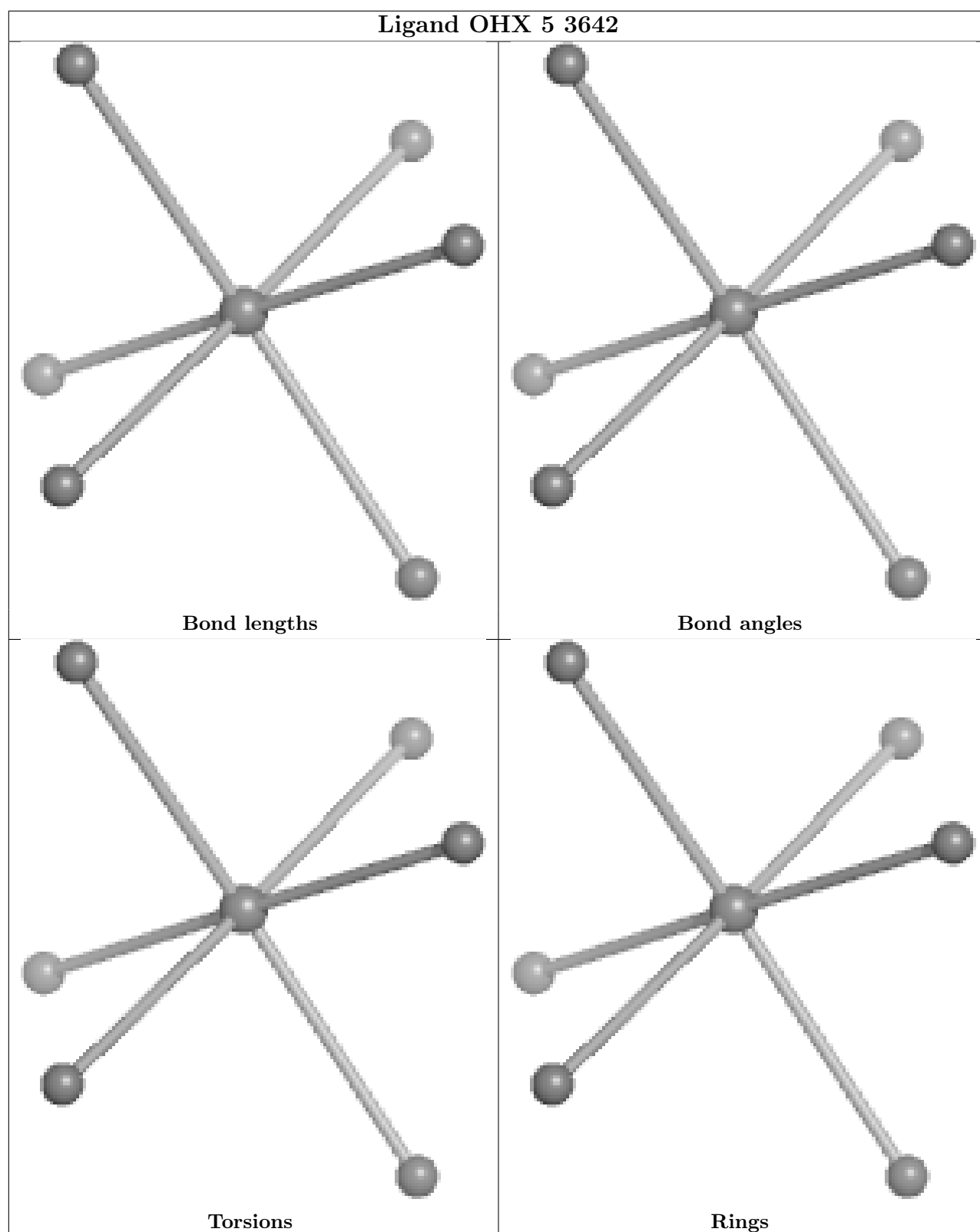


## Ligand OHX 5 3763

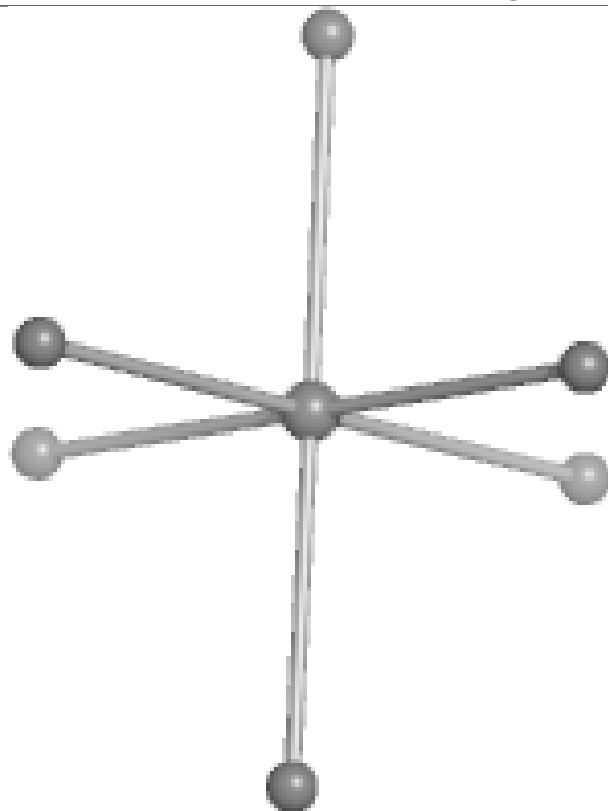




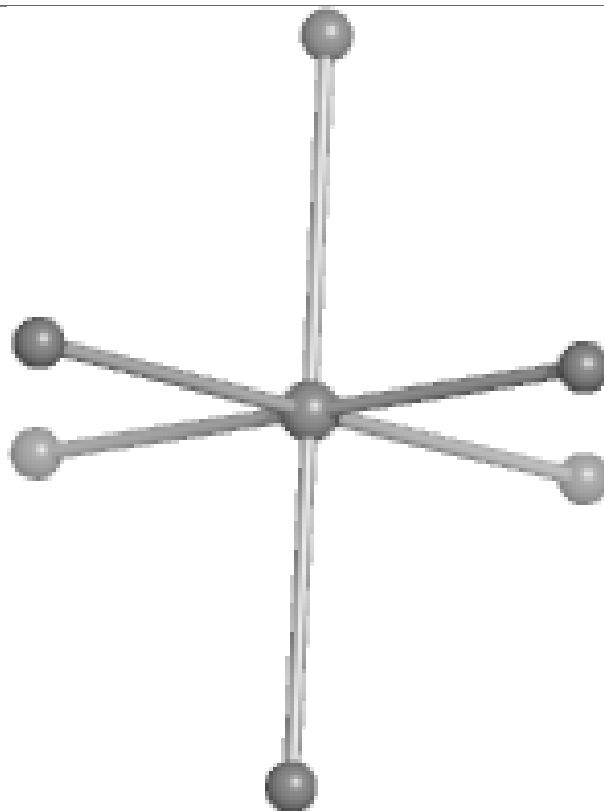




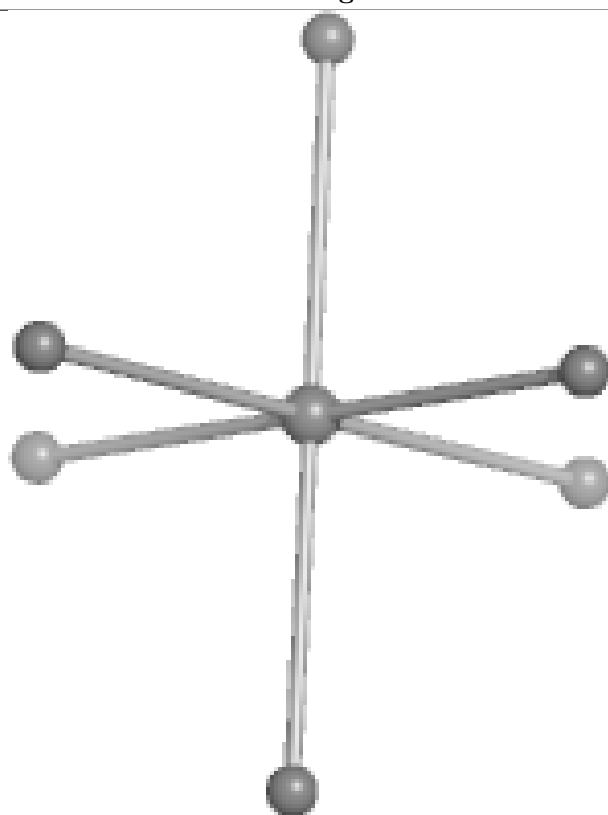
## Ligand OHX 5 3695



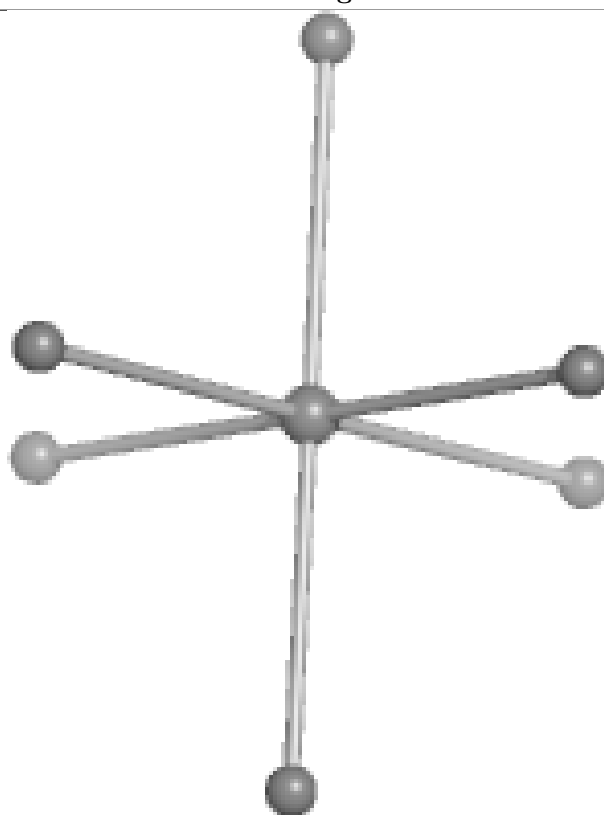
Bond lengths



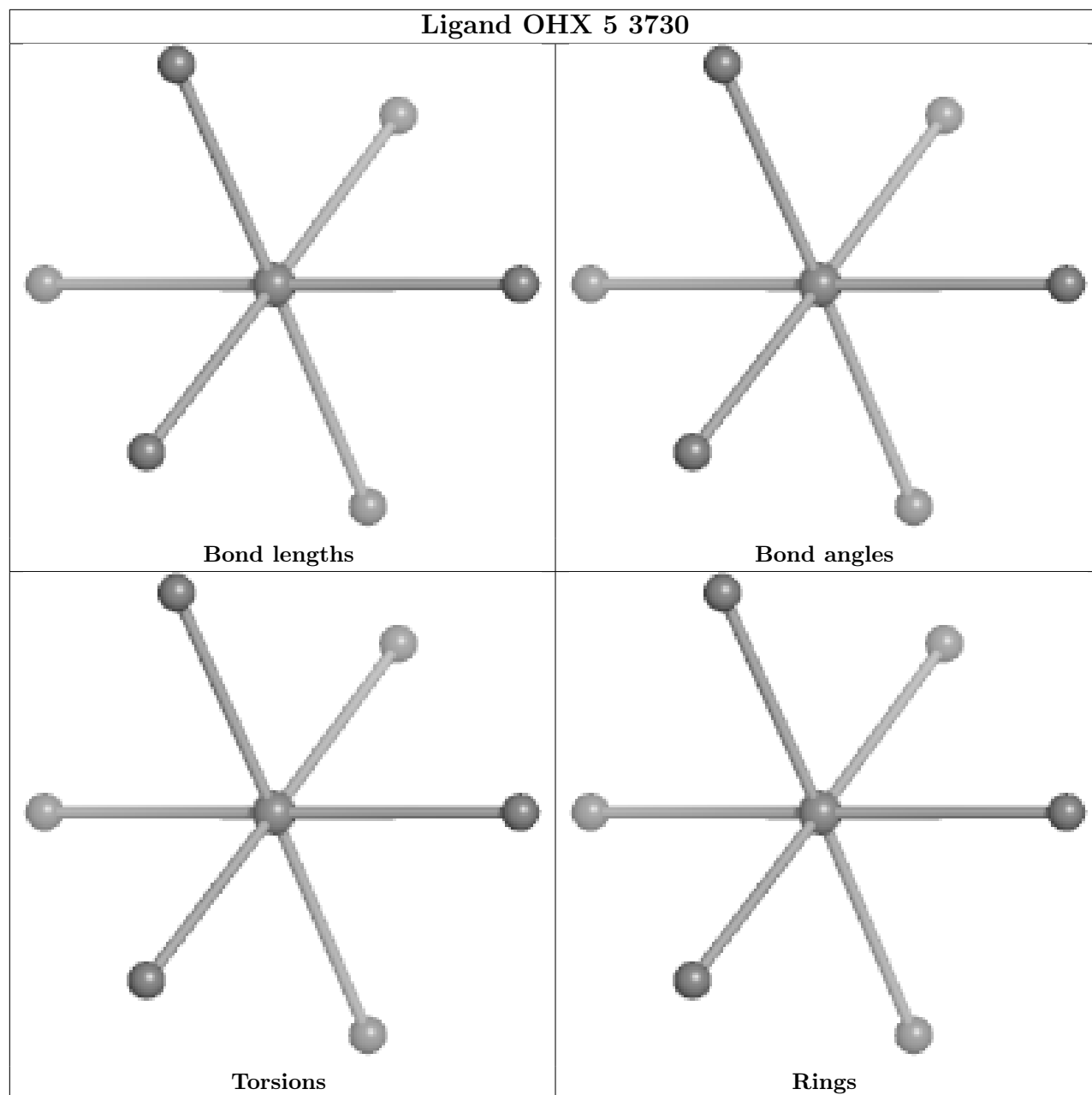
Bond angles

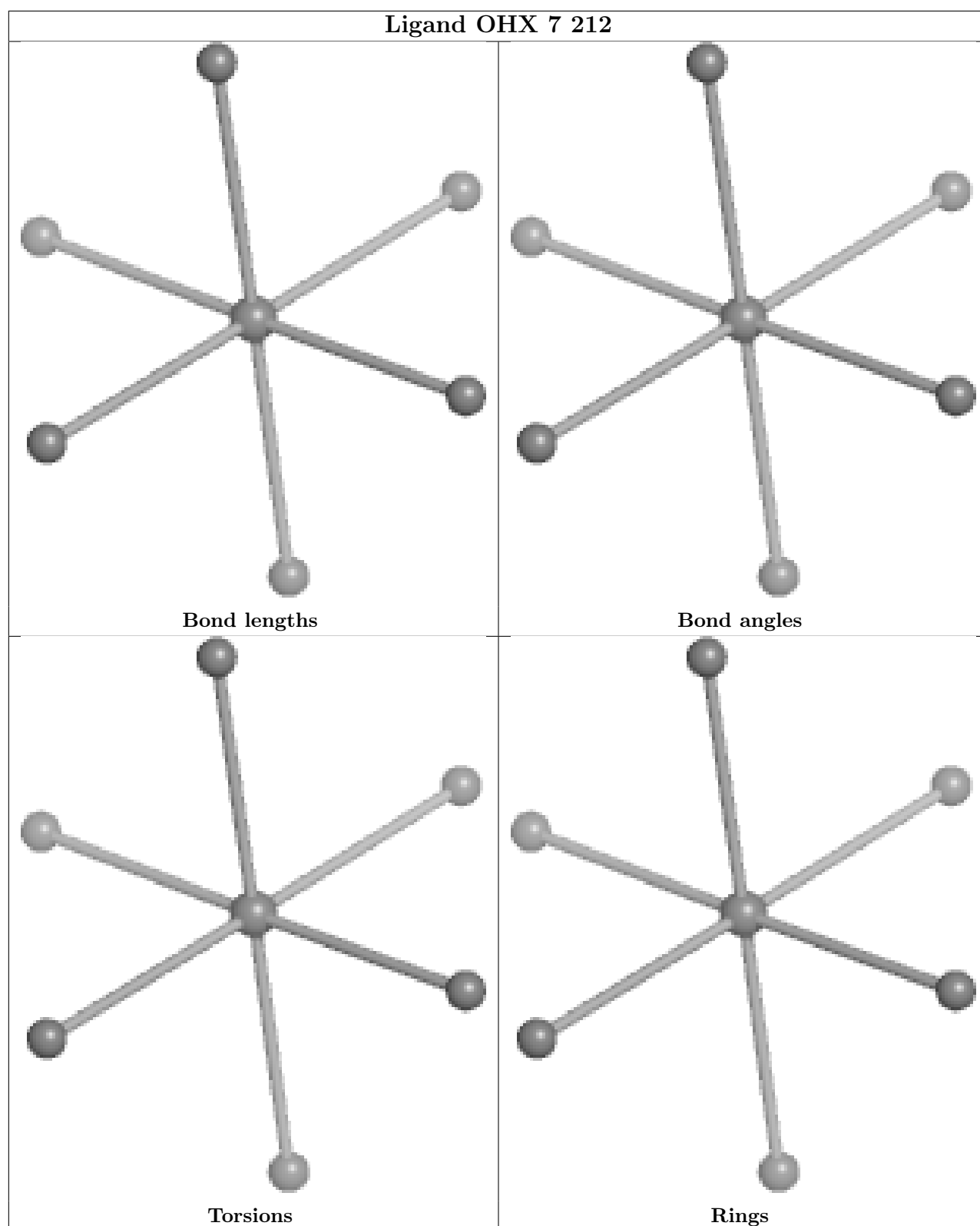


Torsions



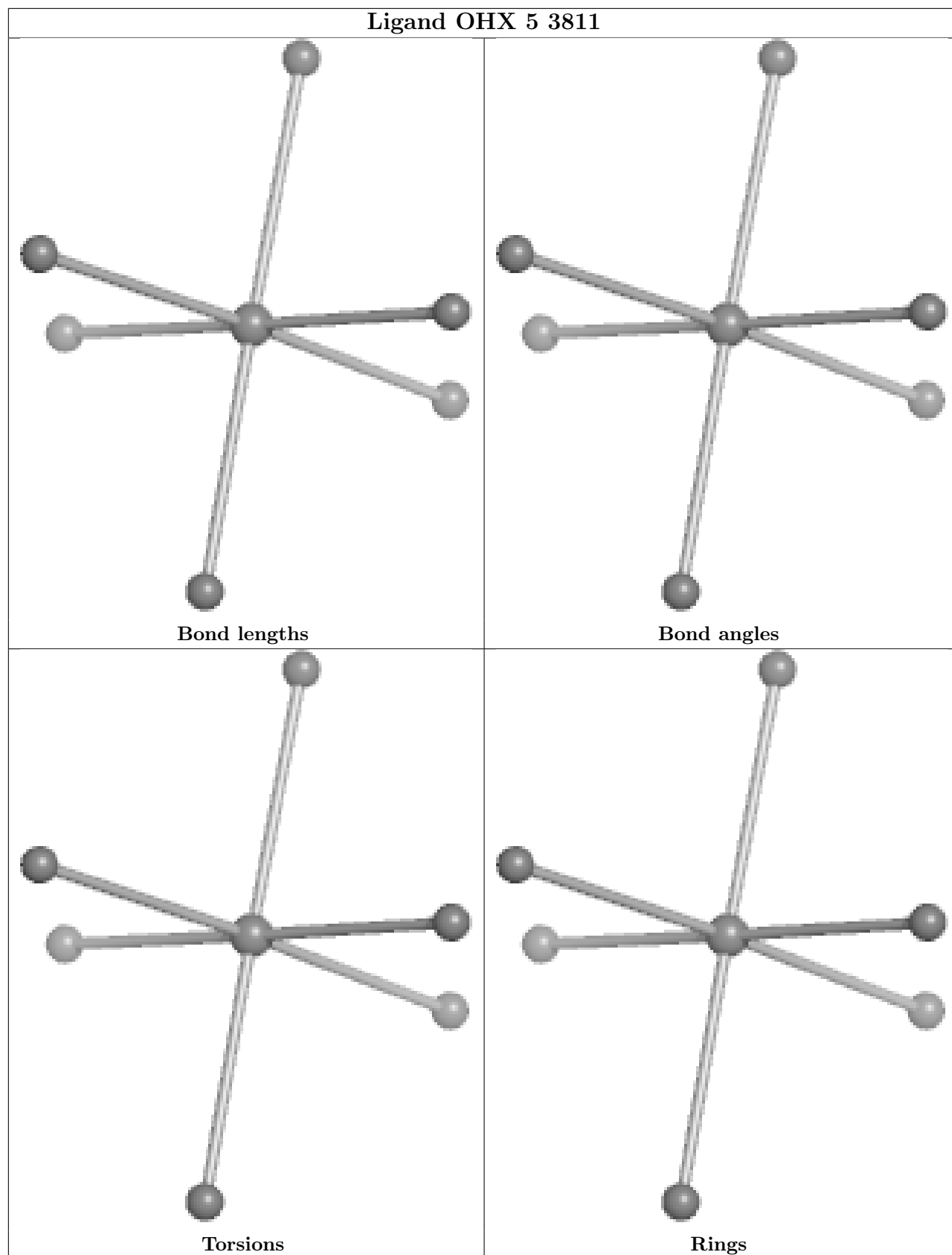
Rings

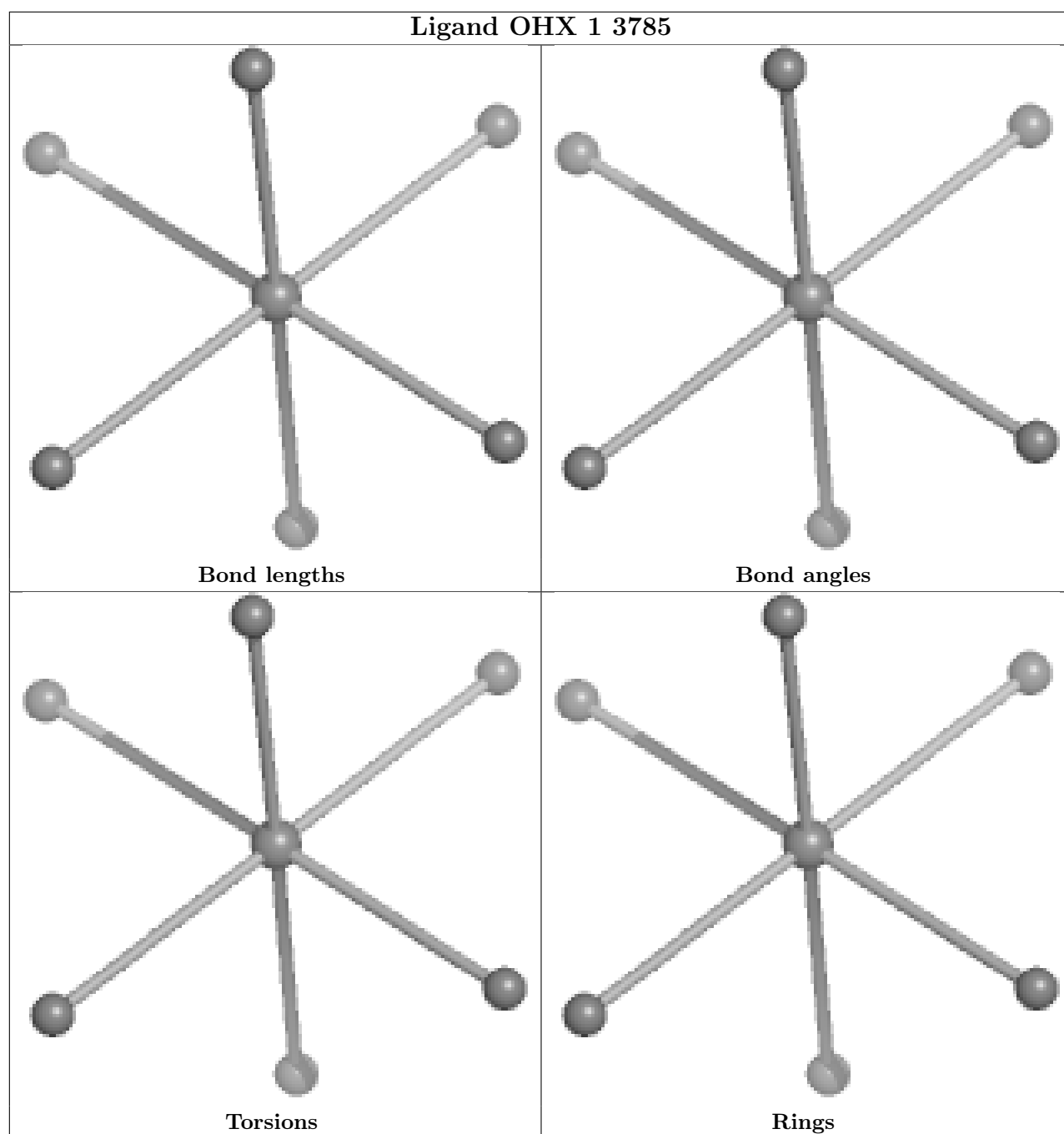


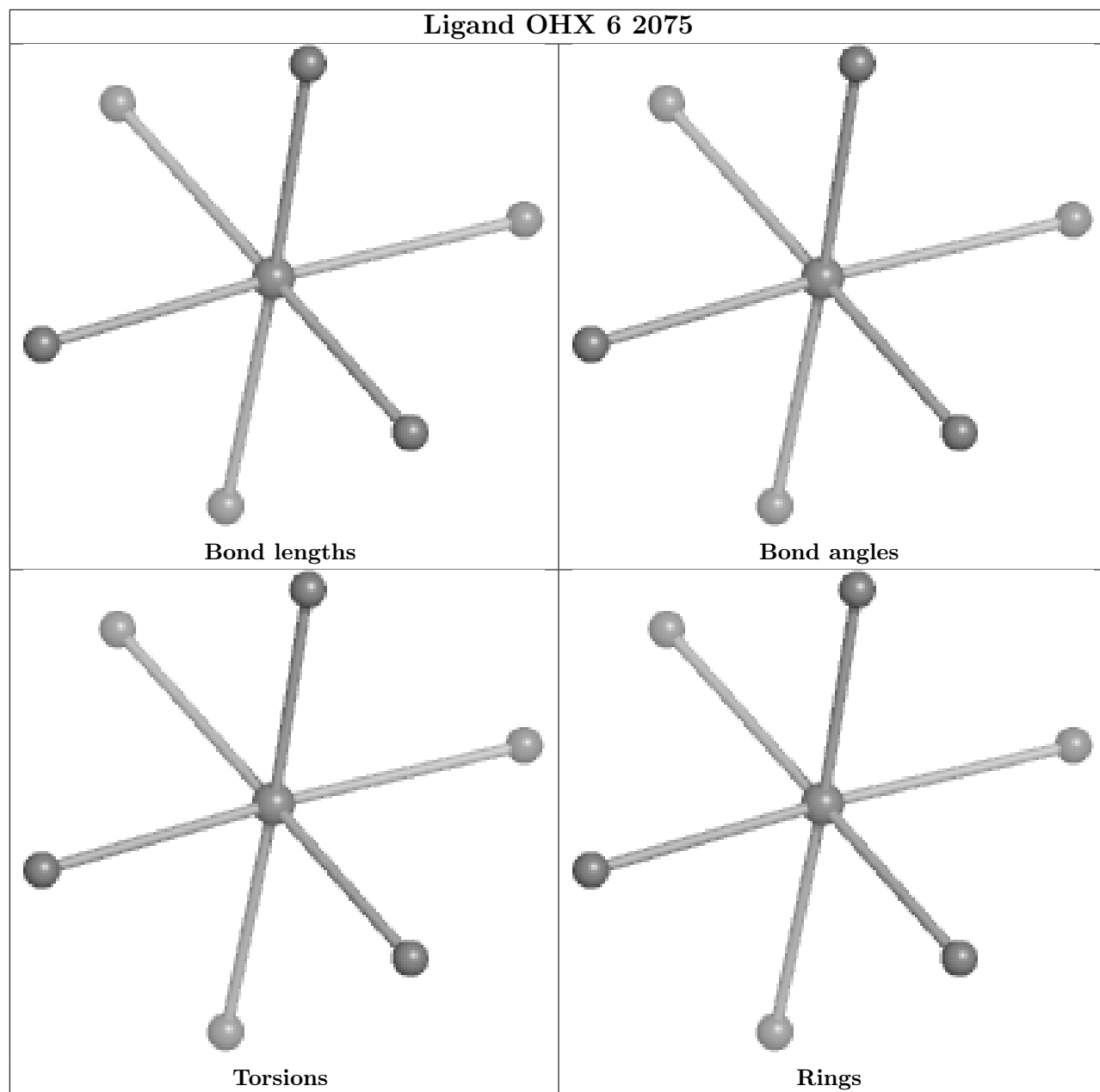


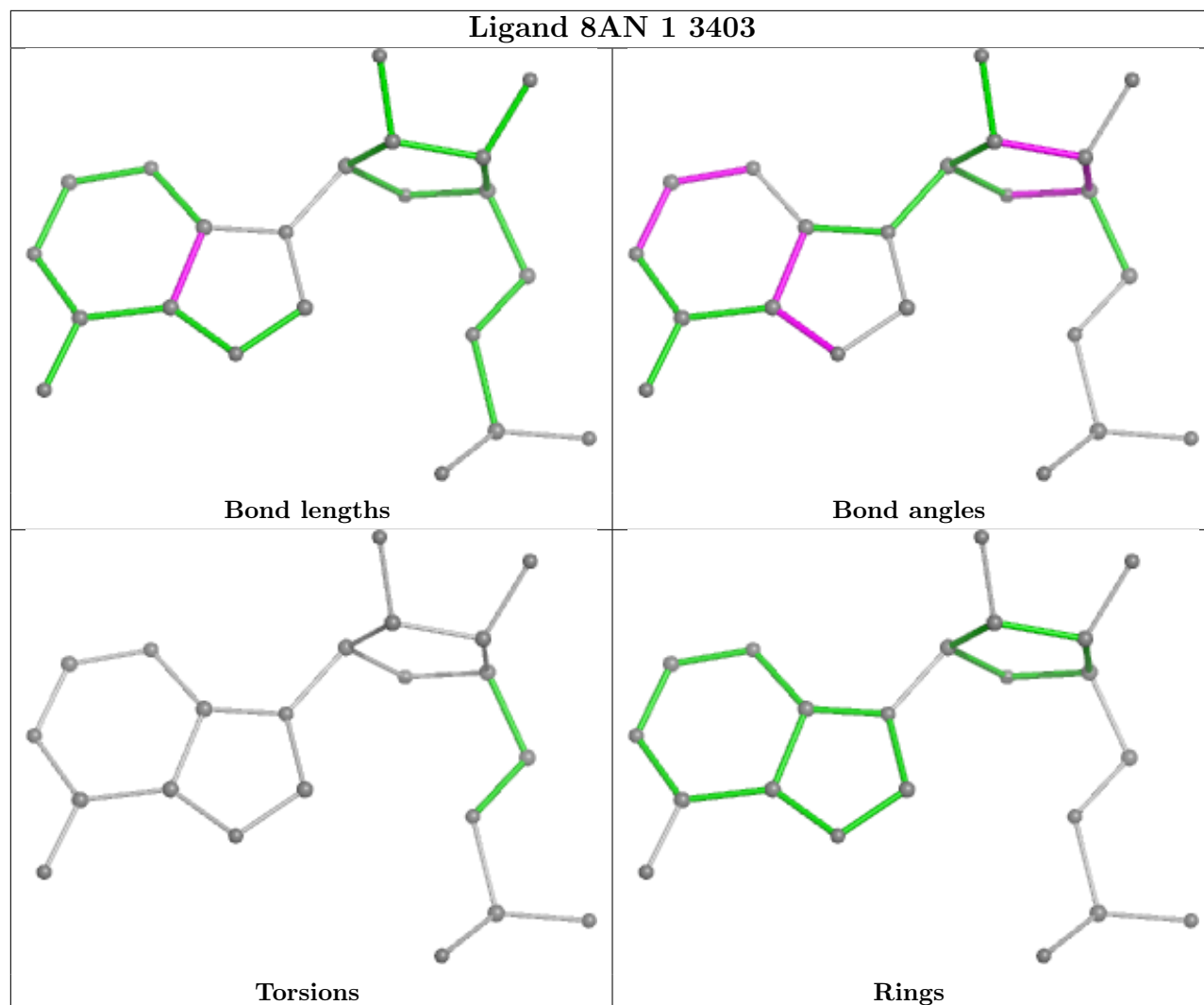


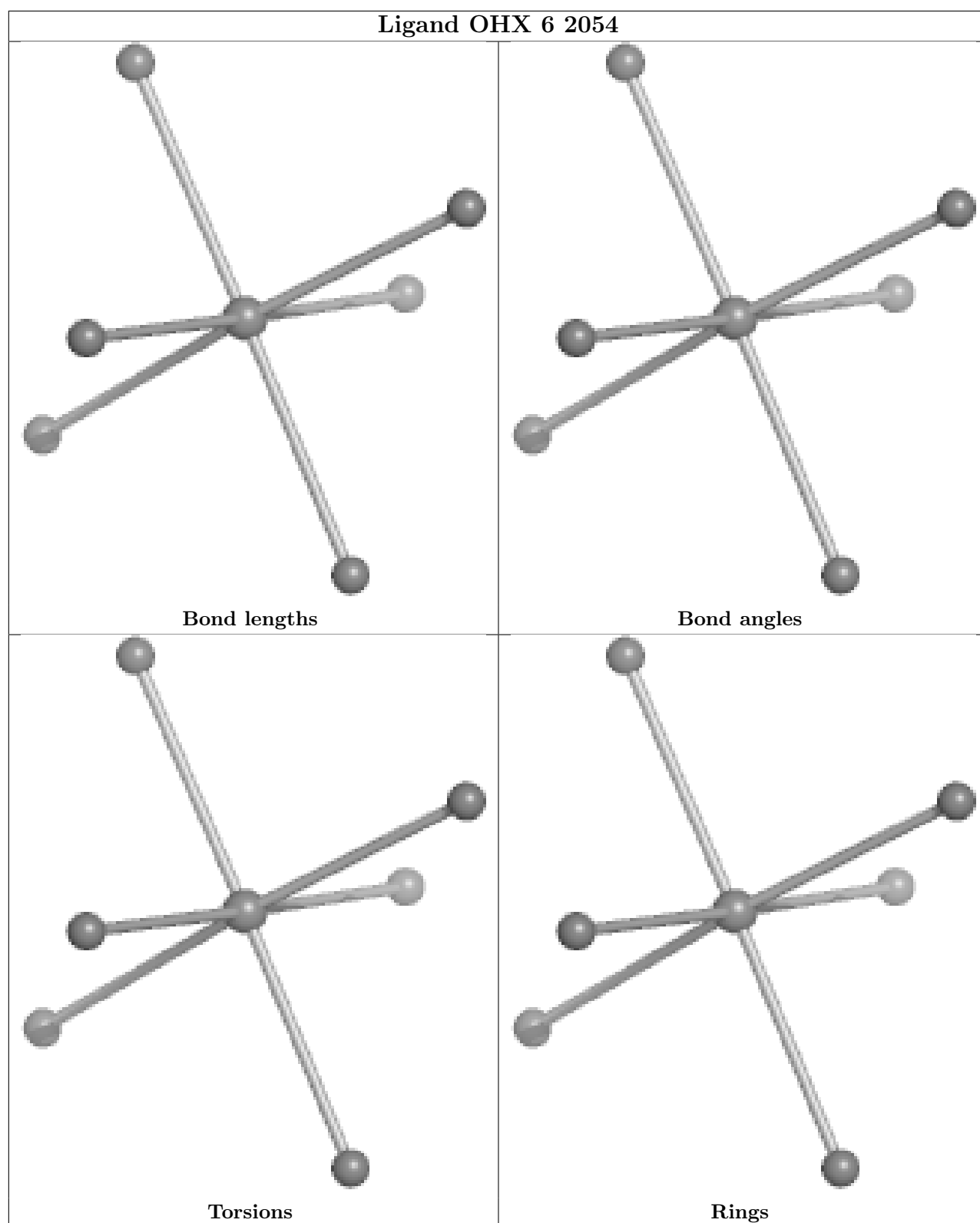
## Ligand OHX 5 3811

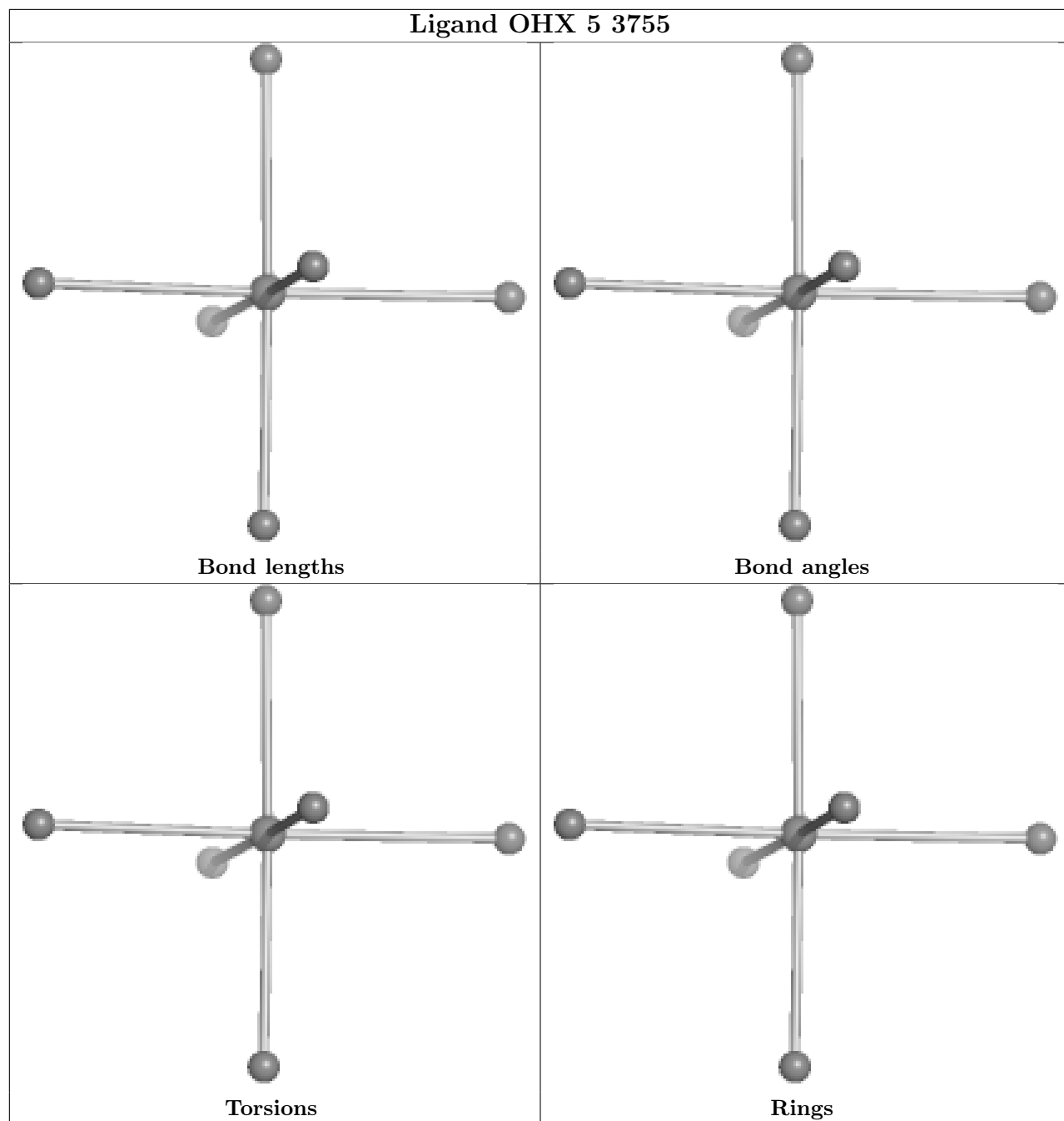




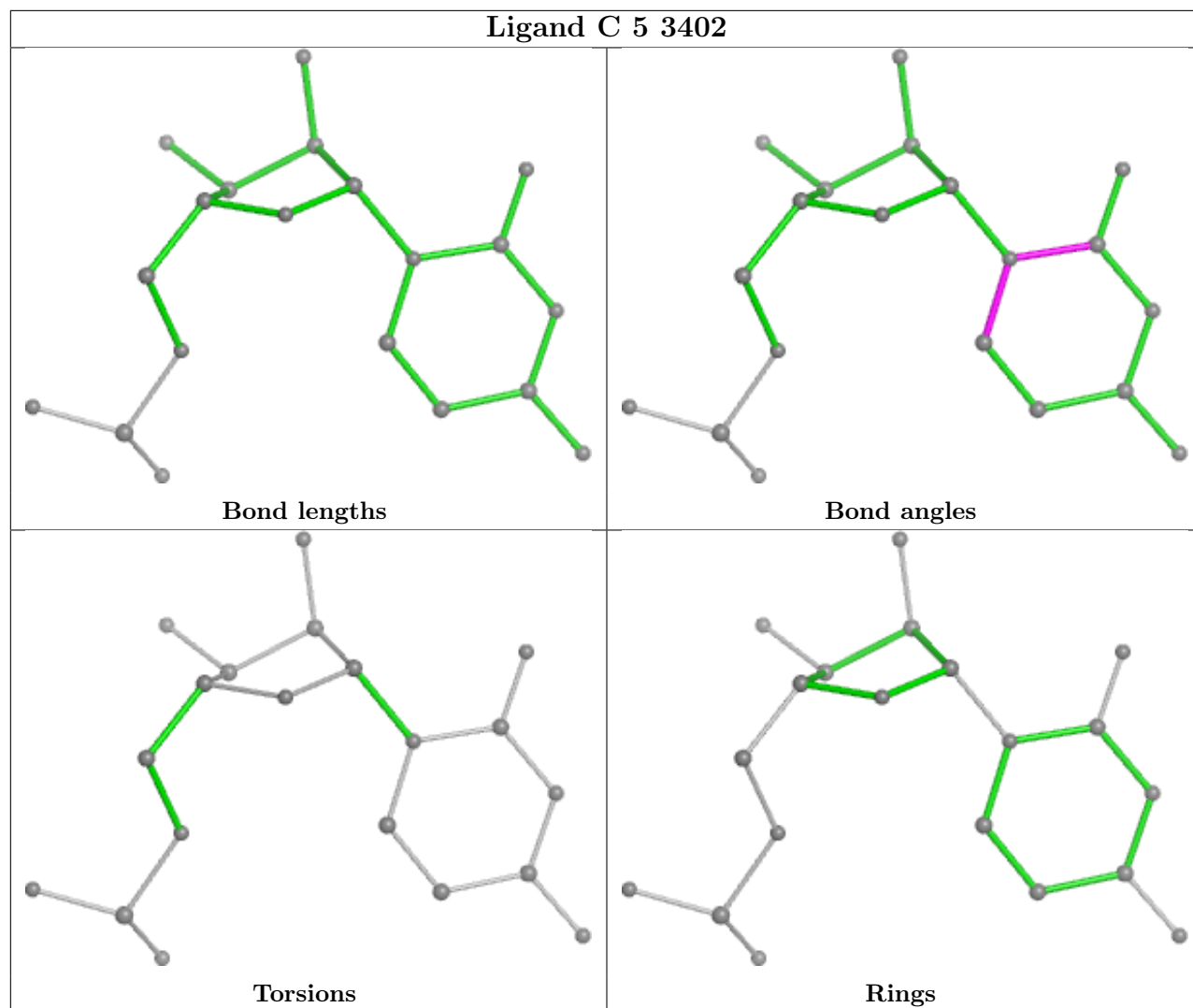


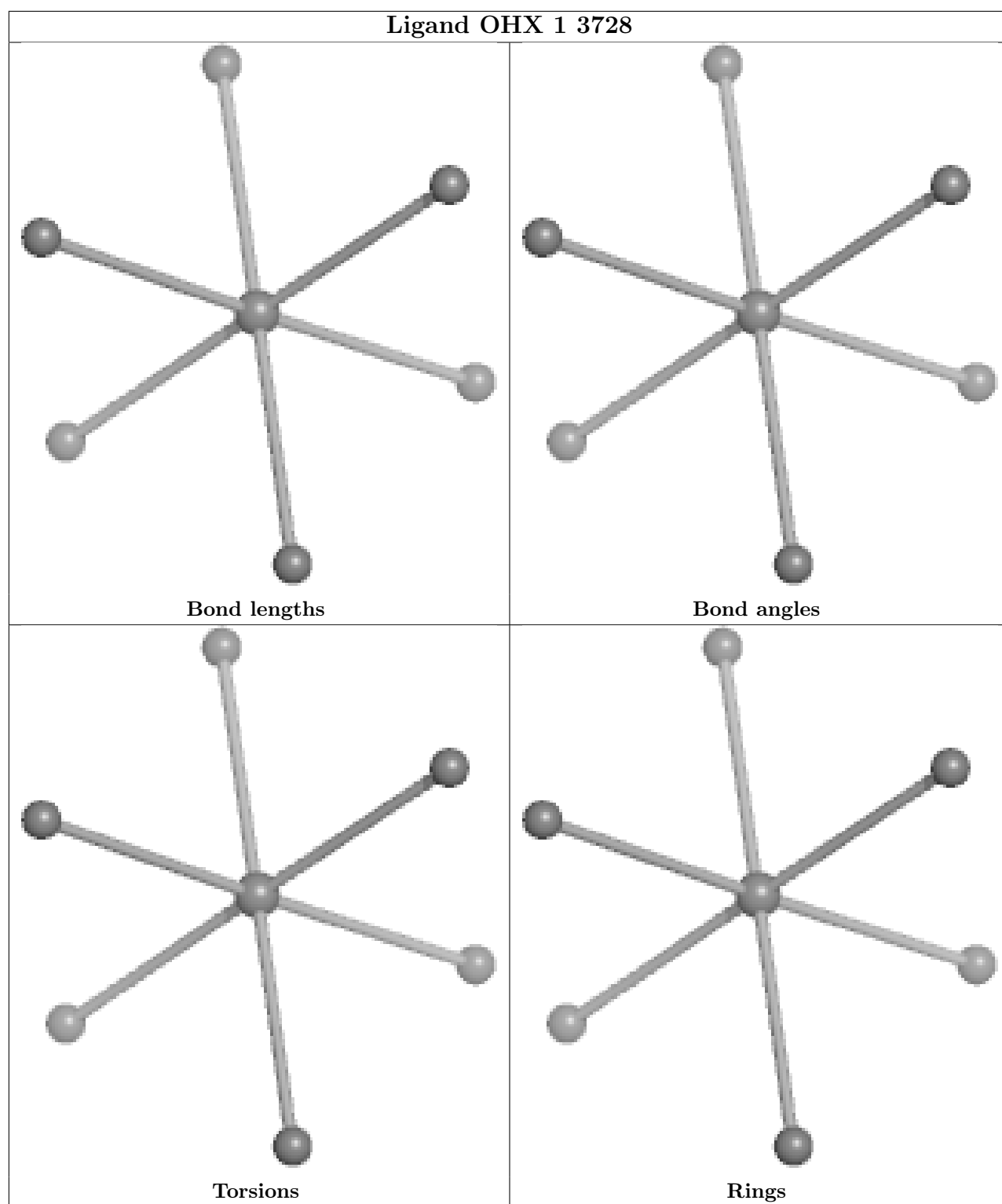






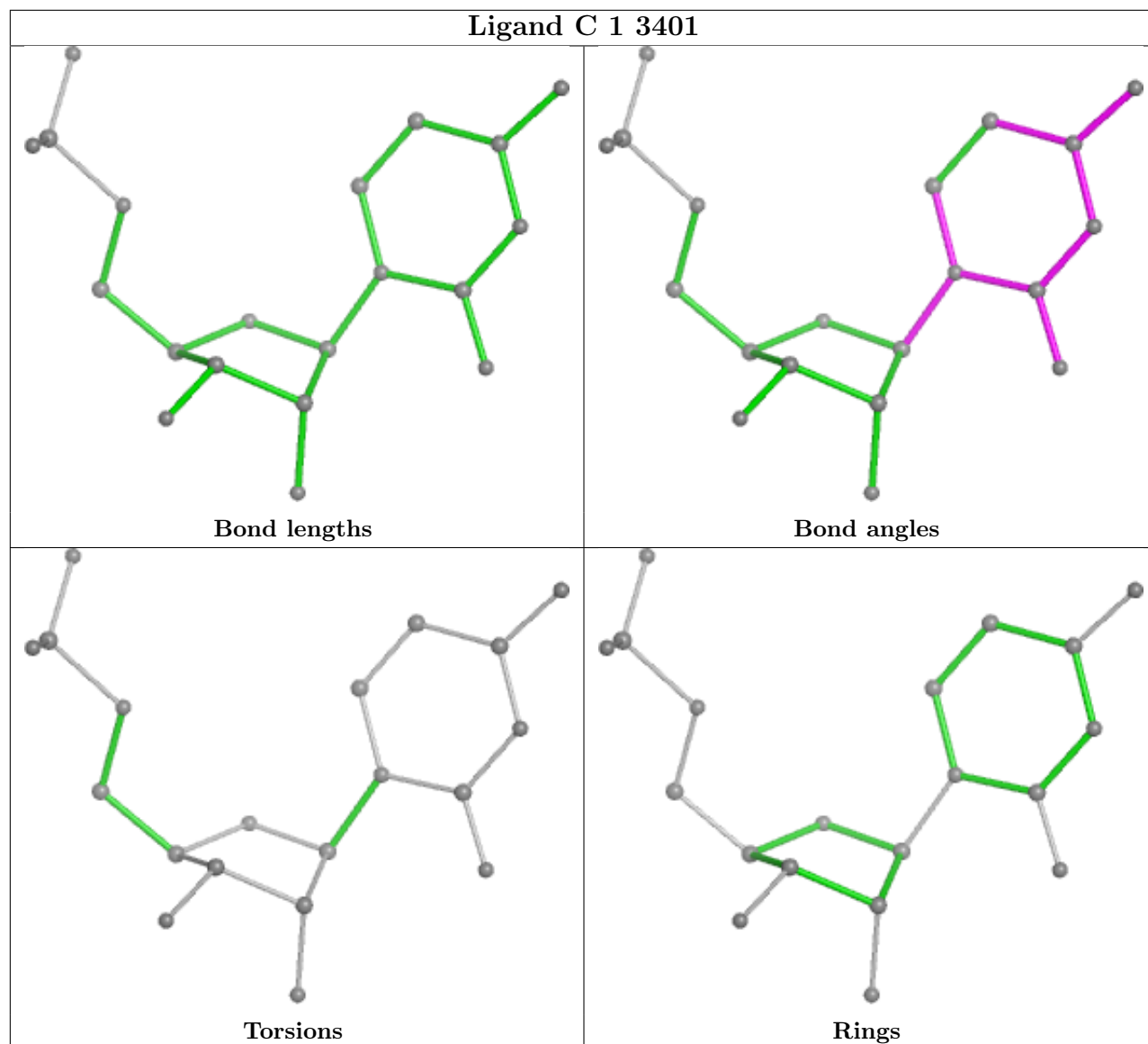
## Ligand C 5 3402

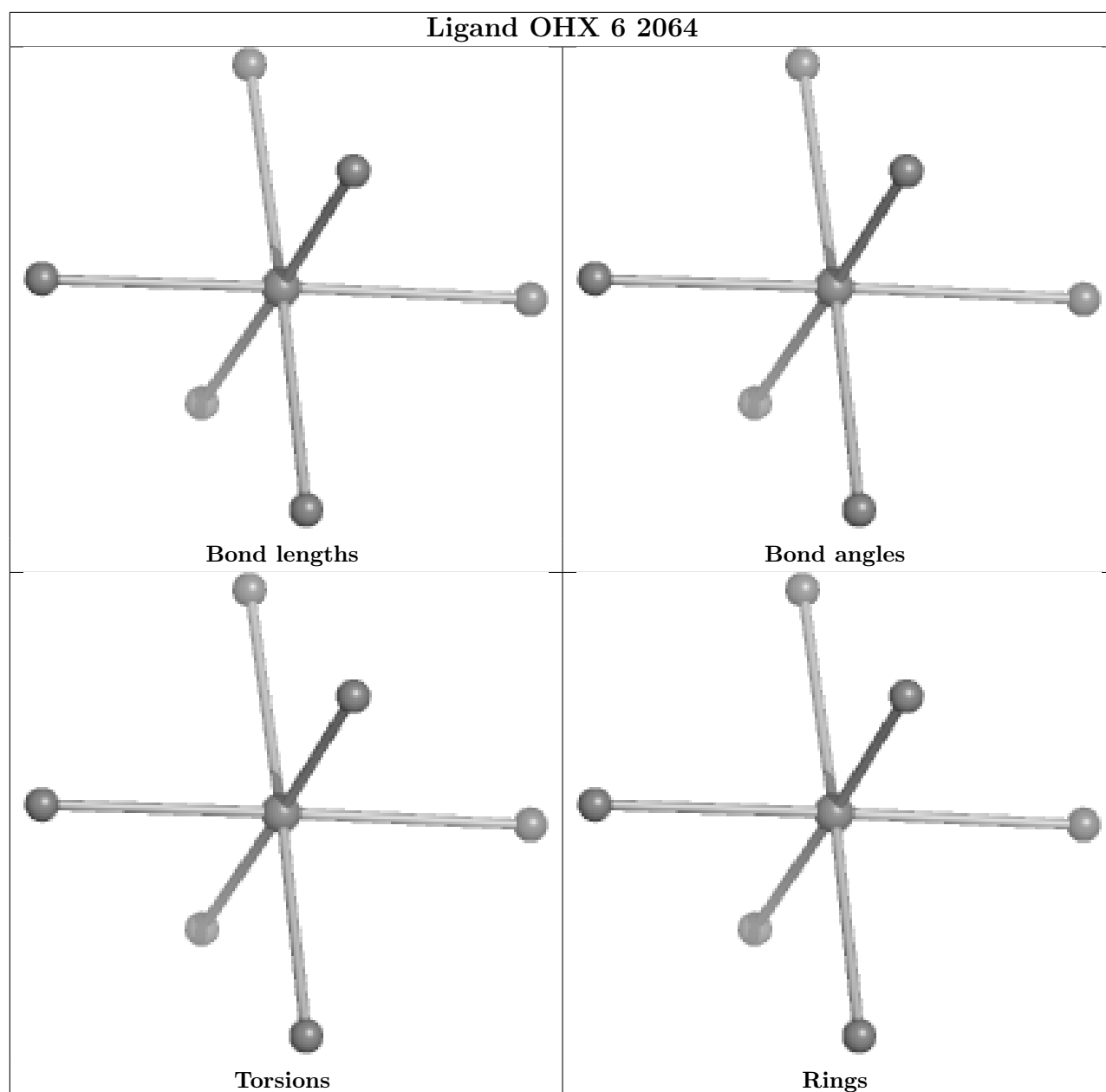


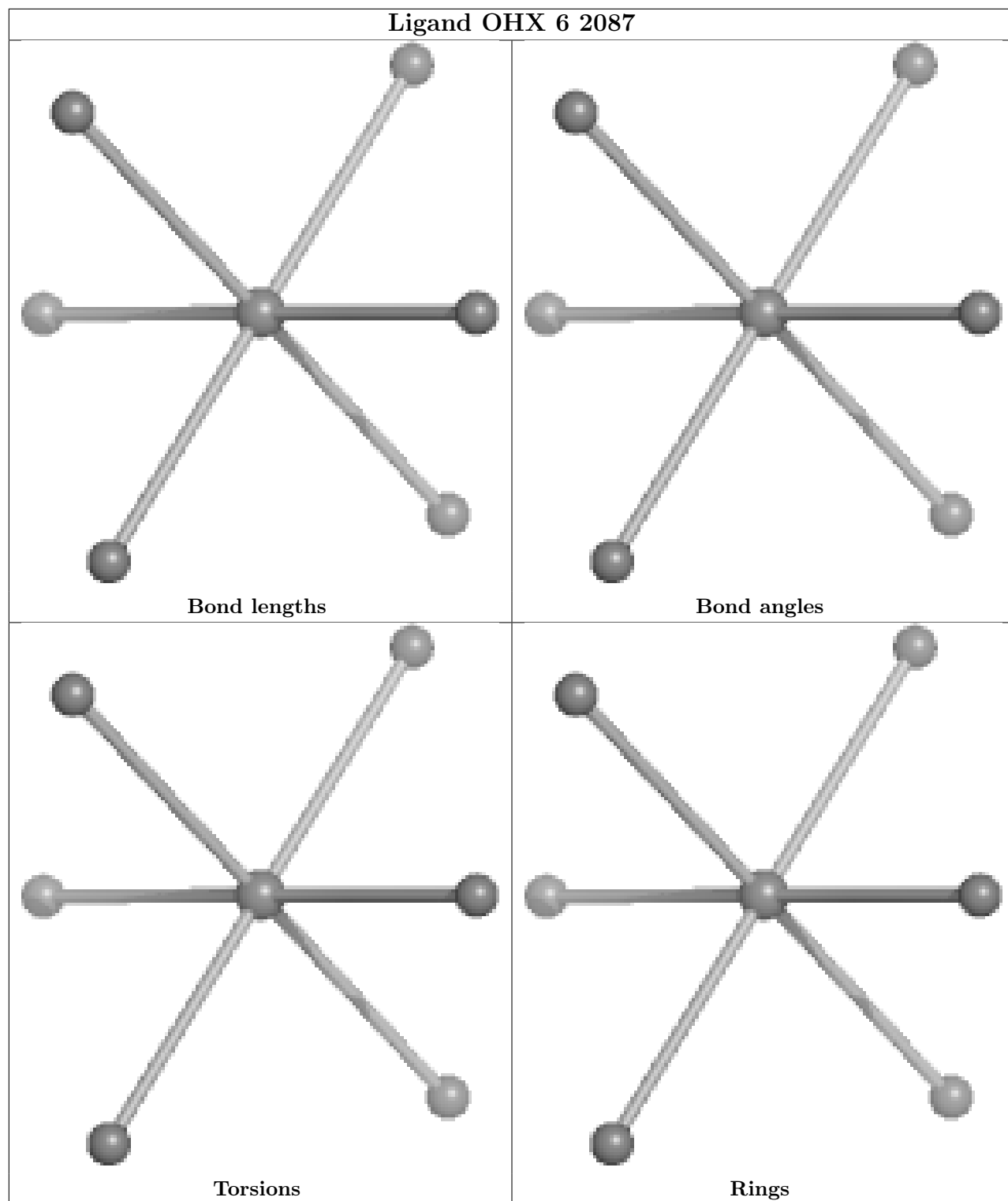


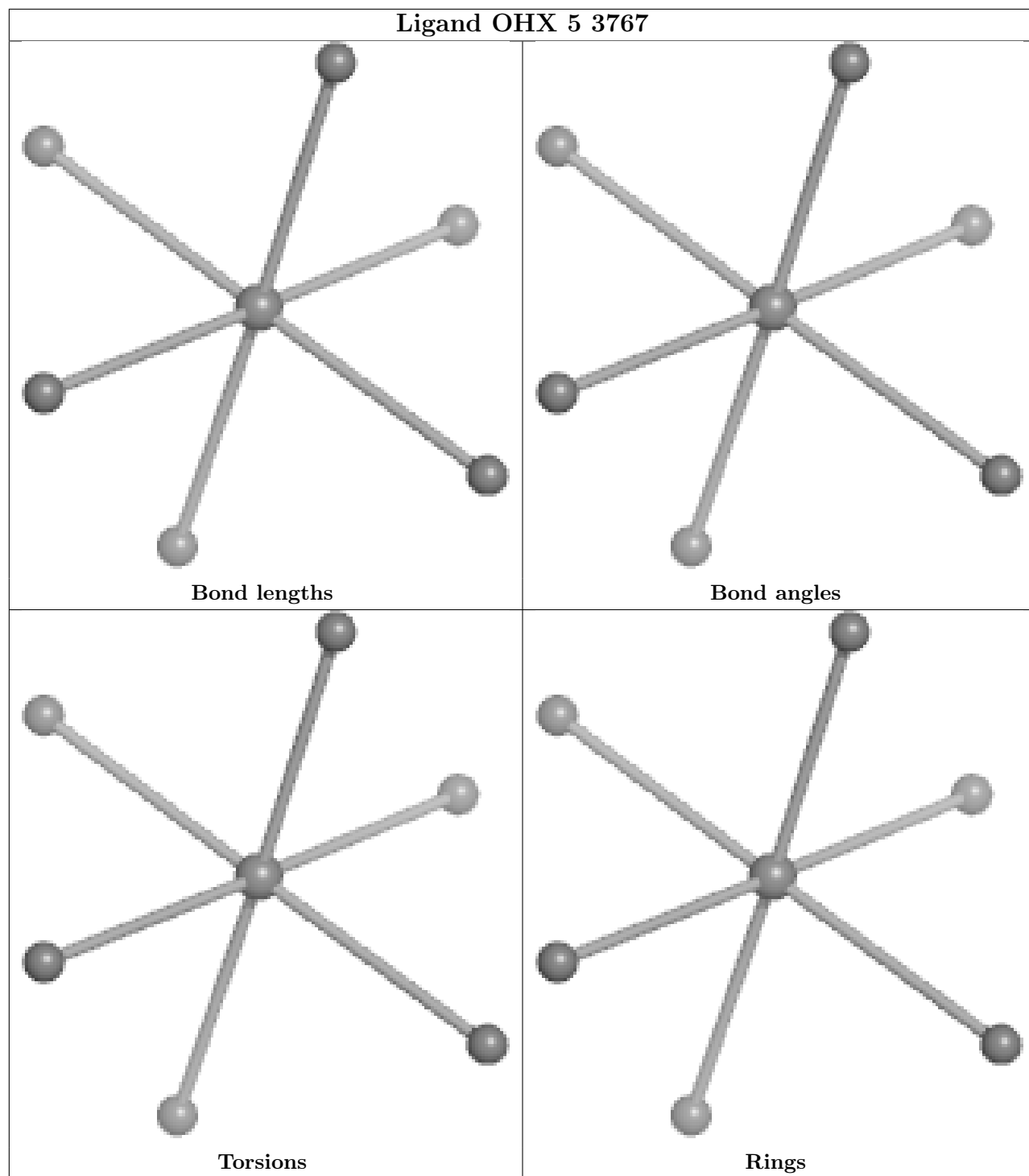


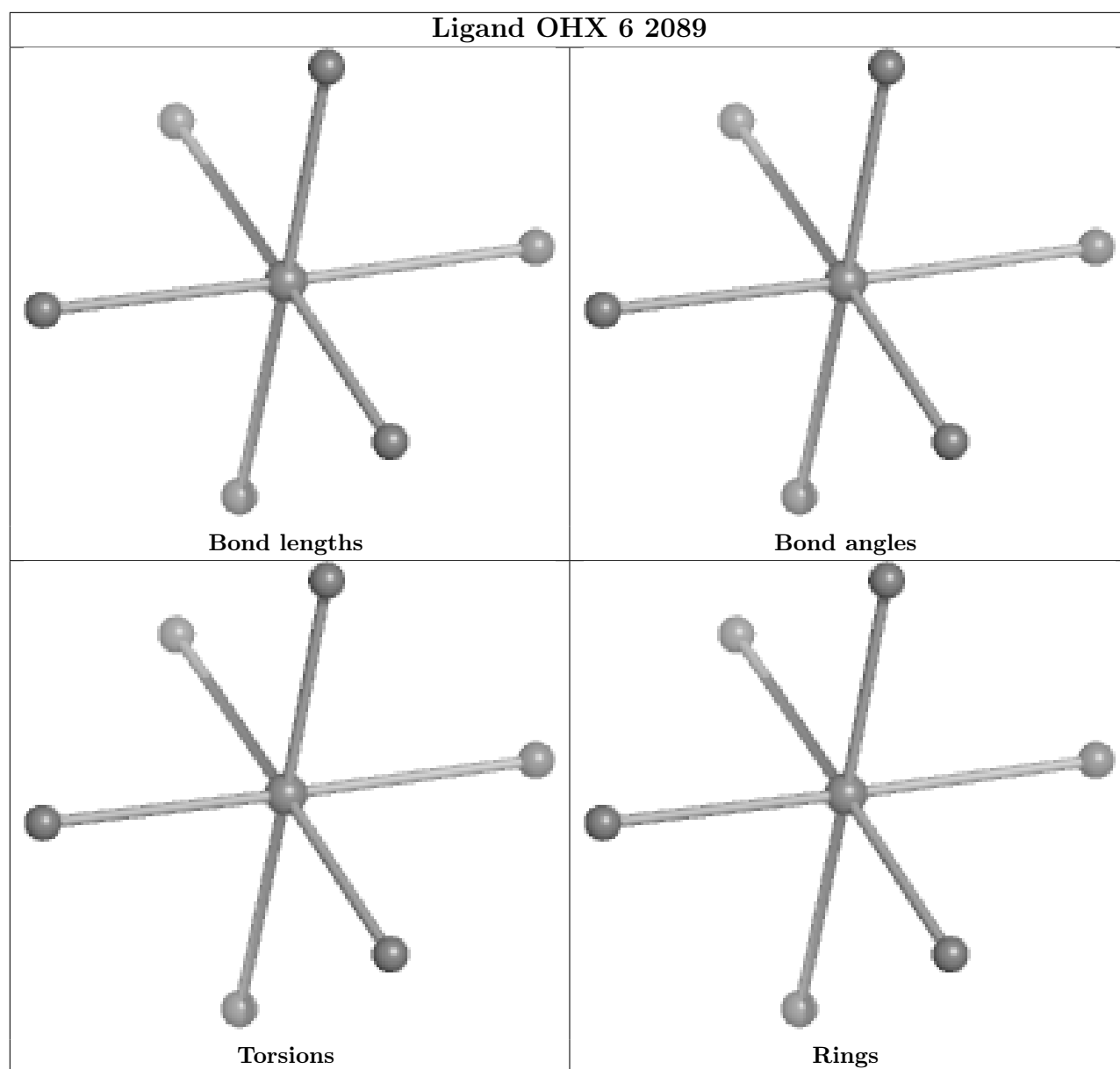
## Ligand C 1 3401



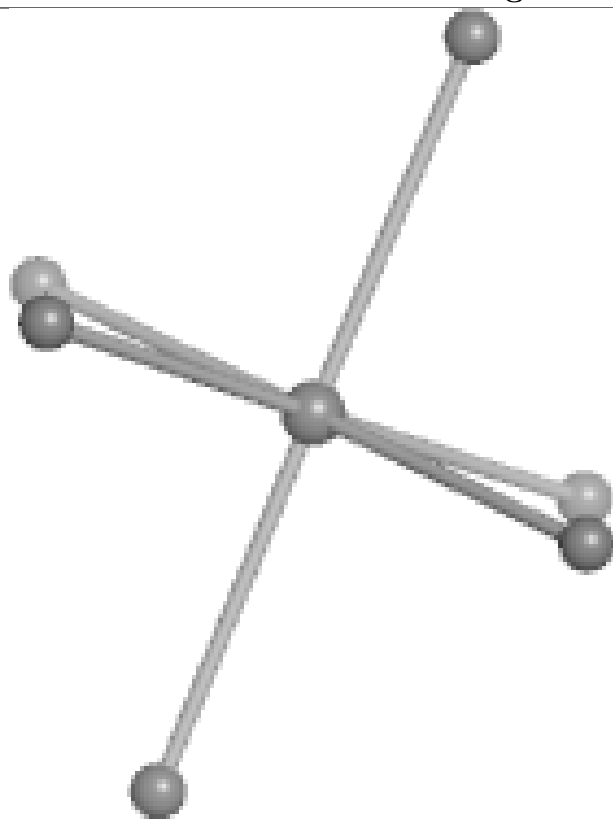




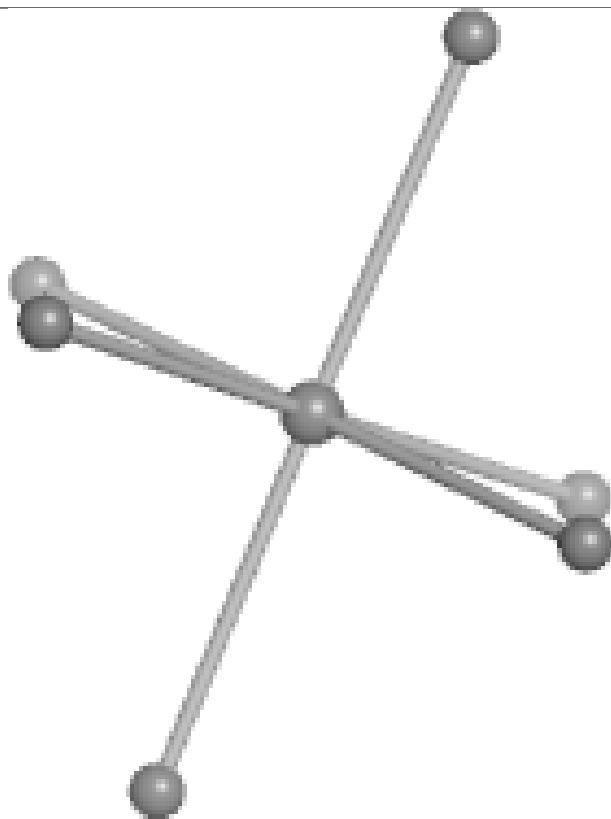




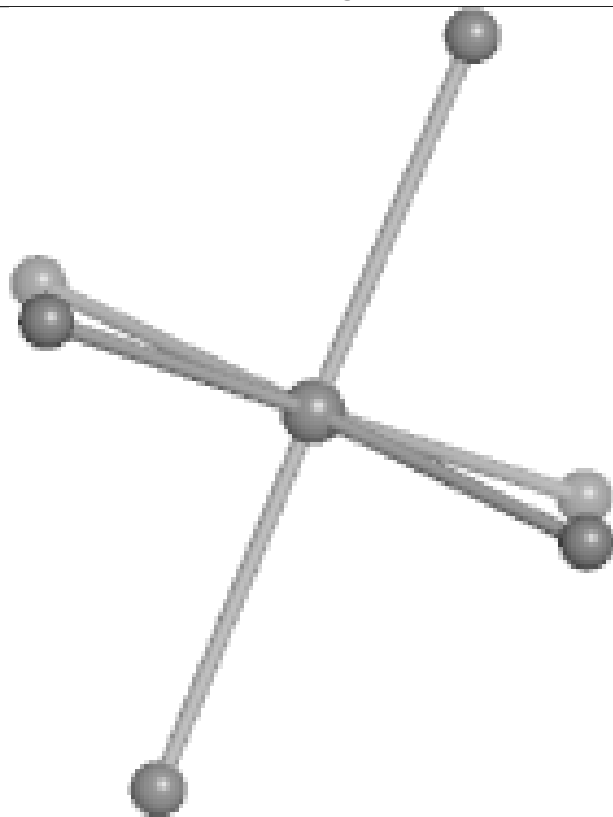
## Ligand OHX 1 3803



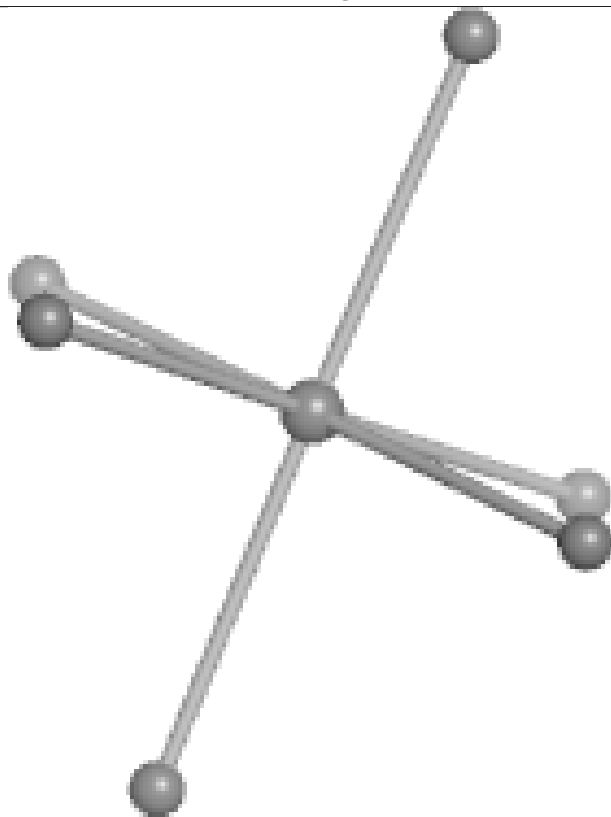
Bond lengths



Bond angles

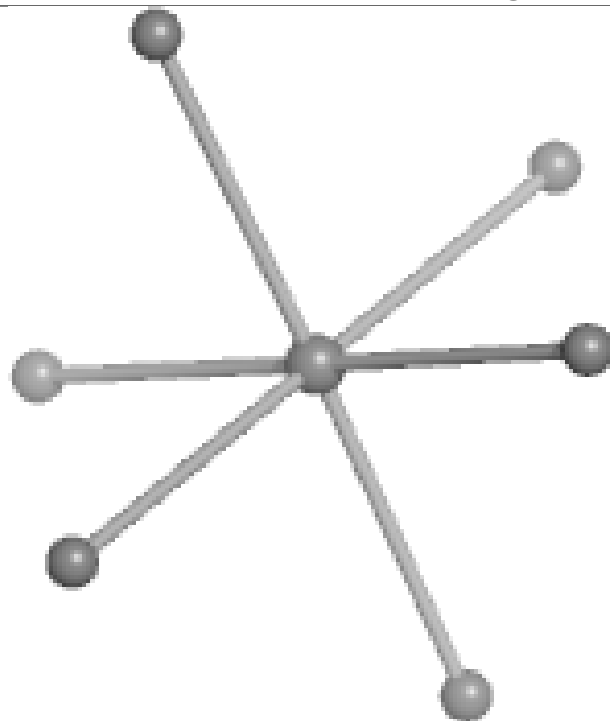


Torsions

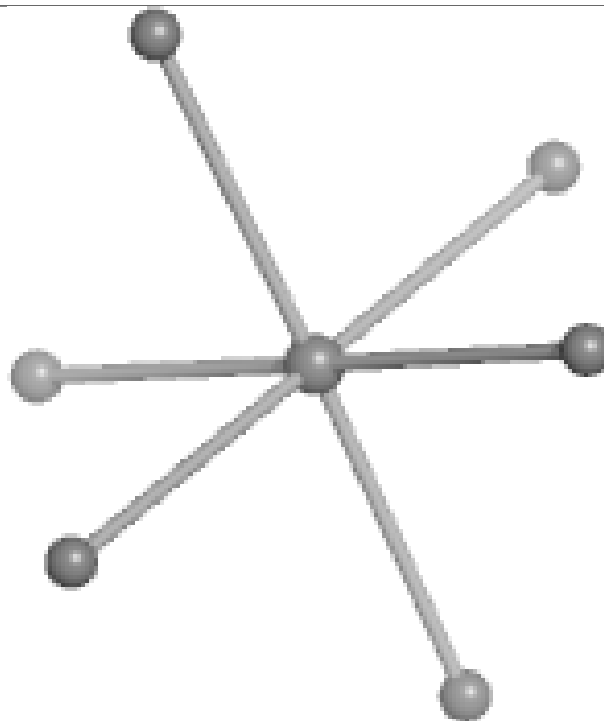


Rings

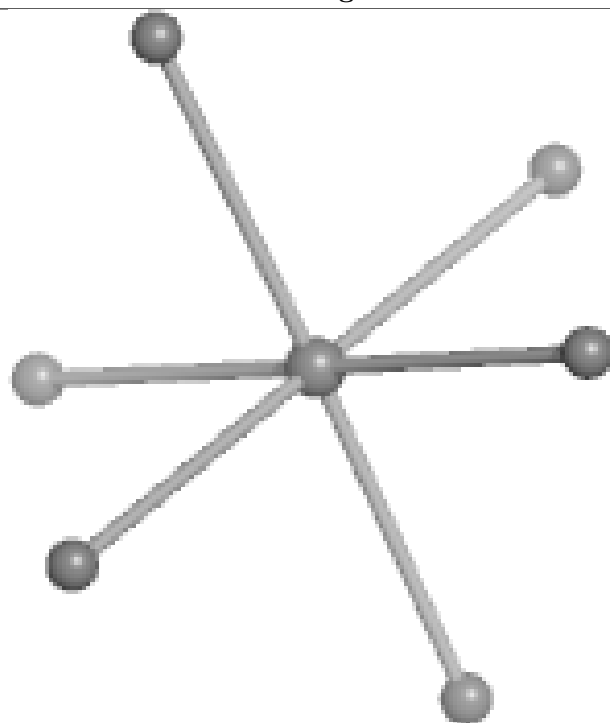
## Ligand OHX 1 3739



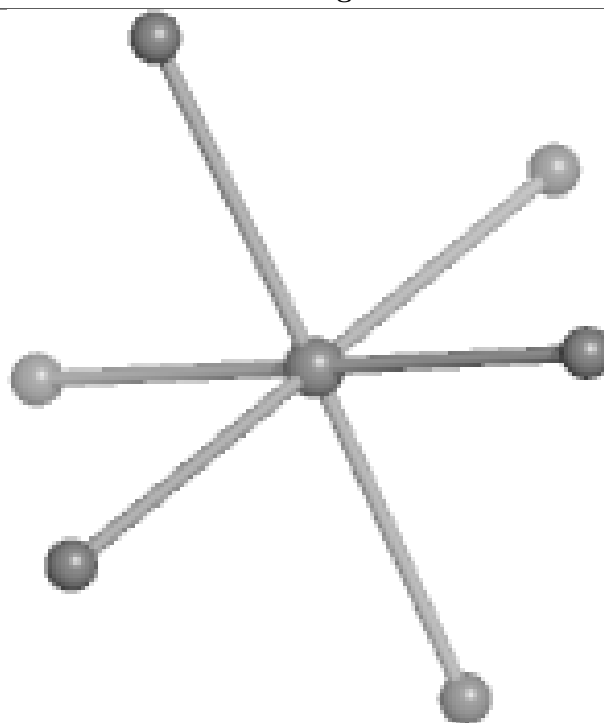
Bond lengths



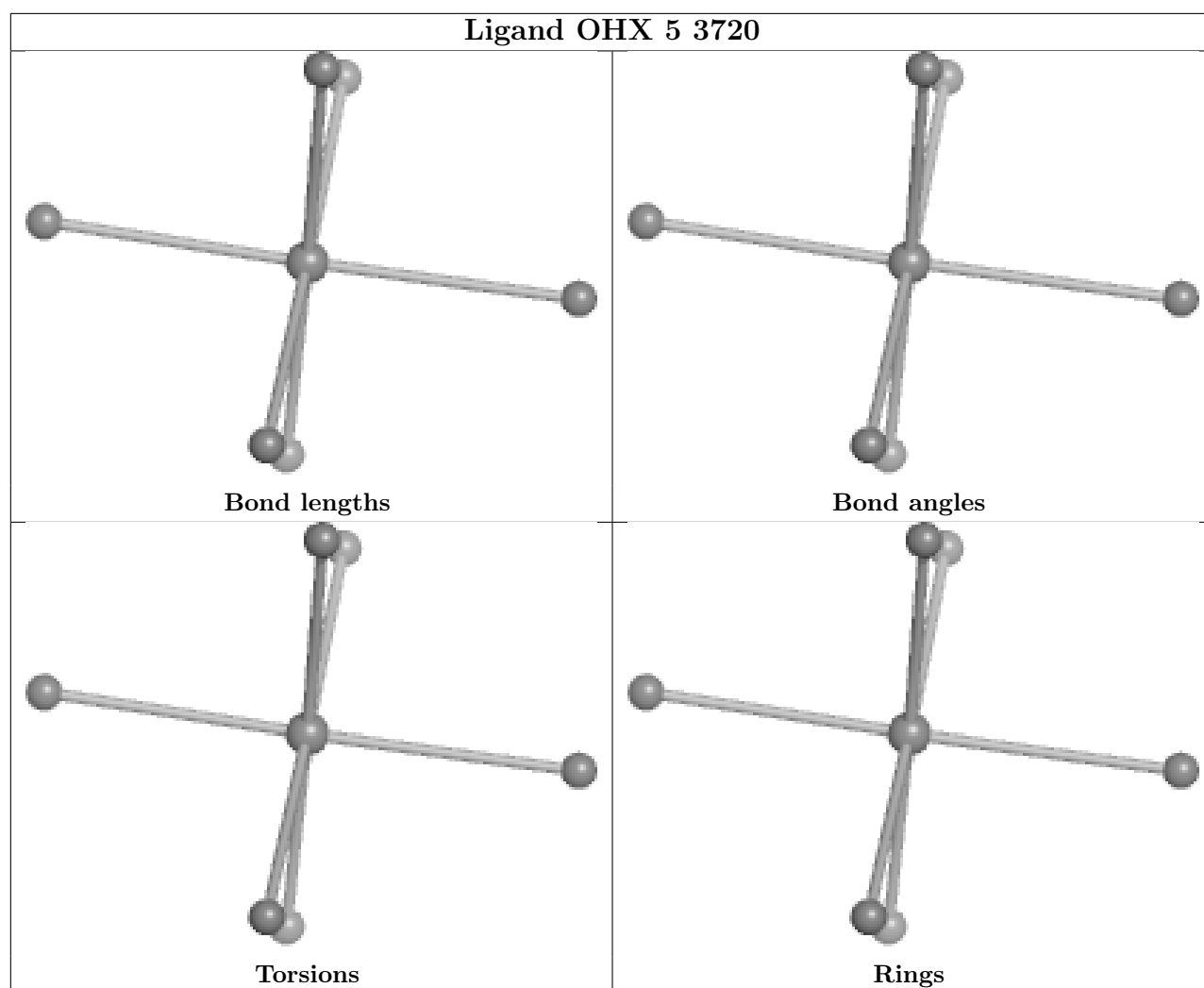
Bond angles



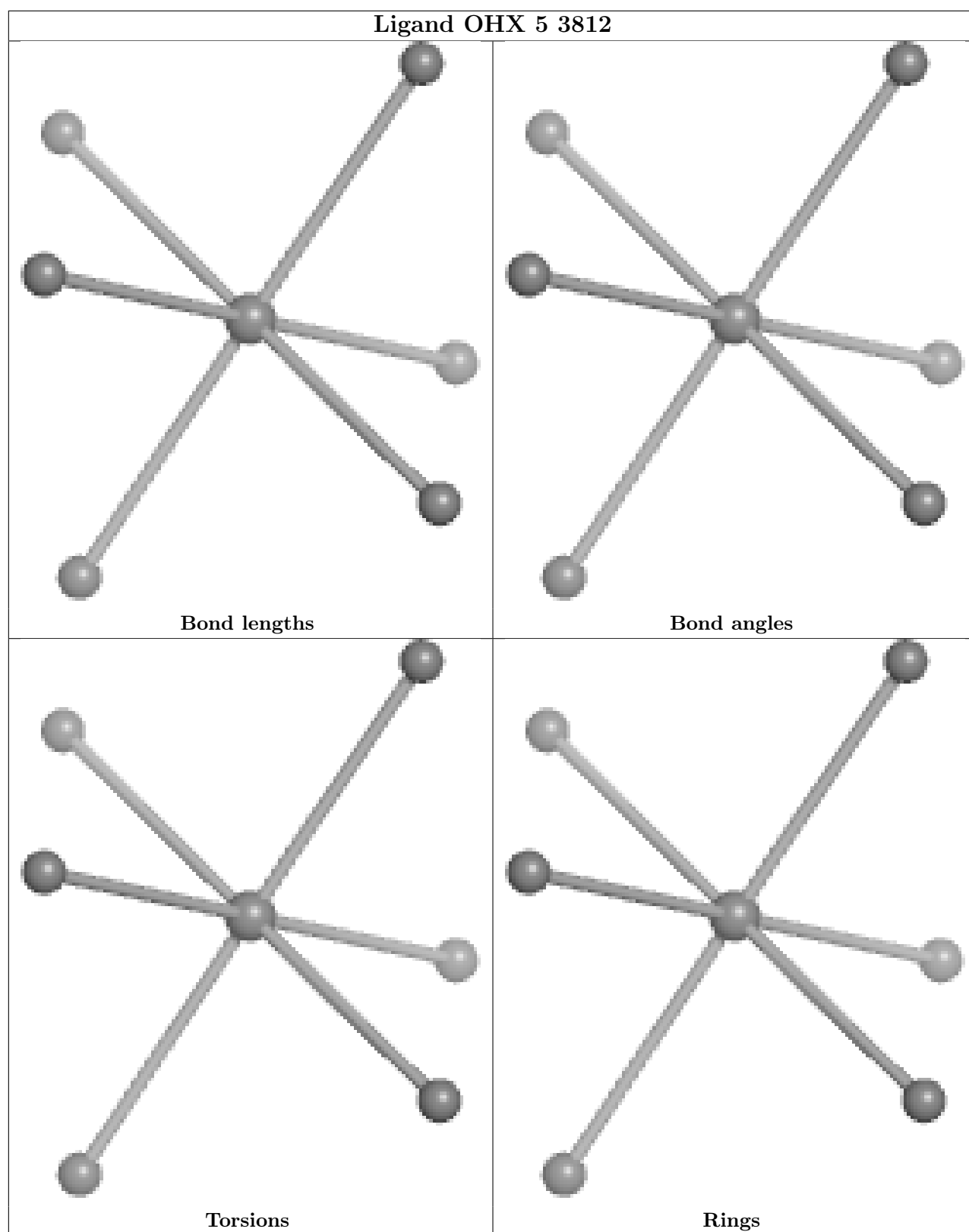
Torsions

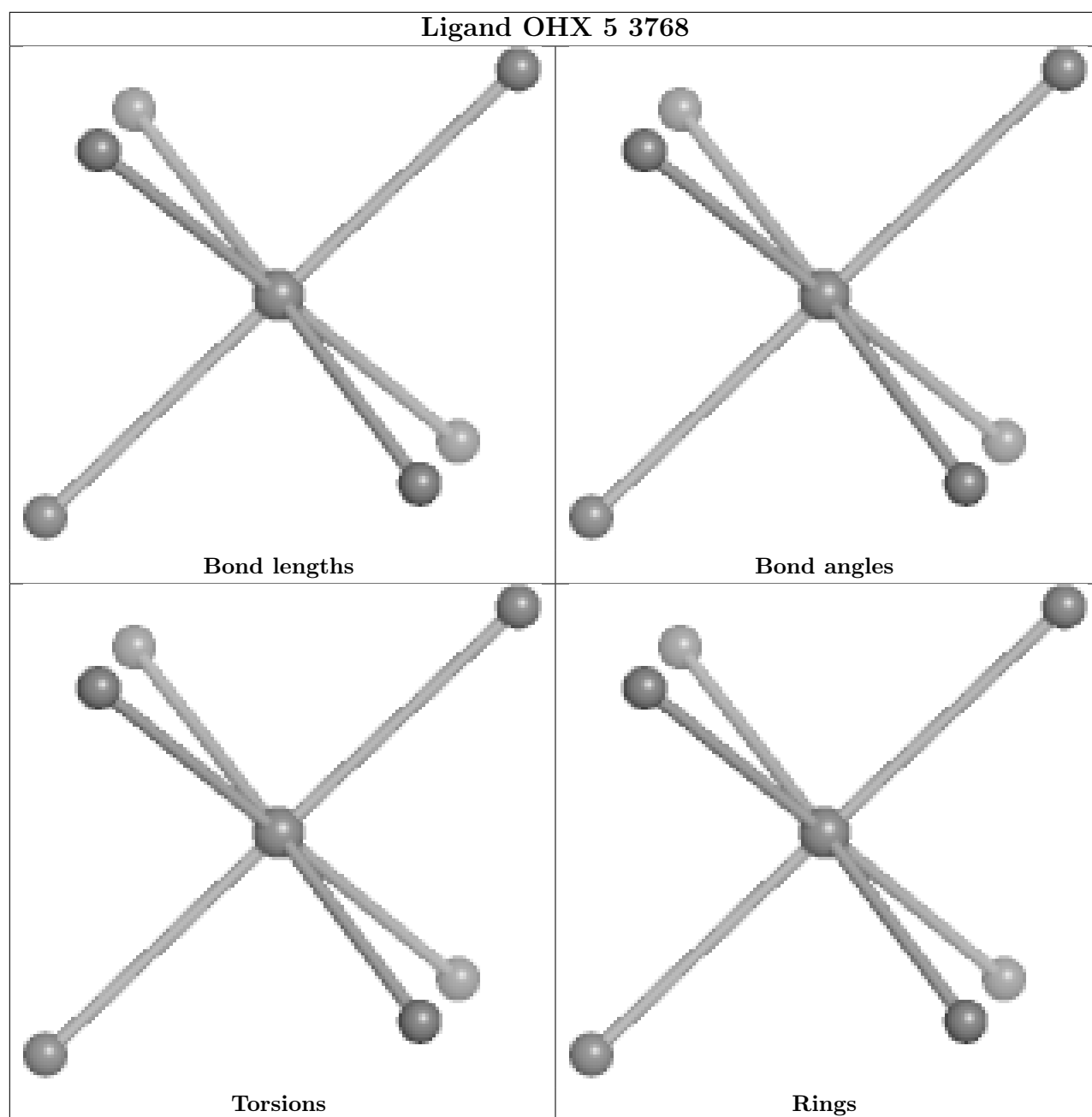


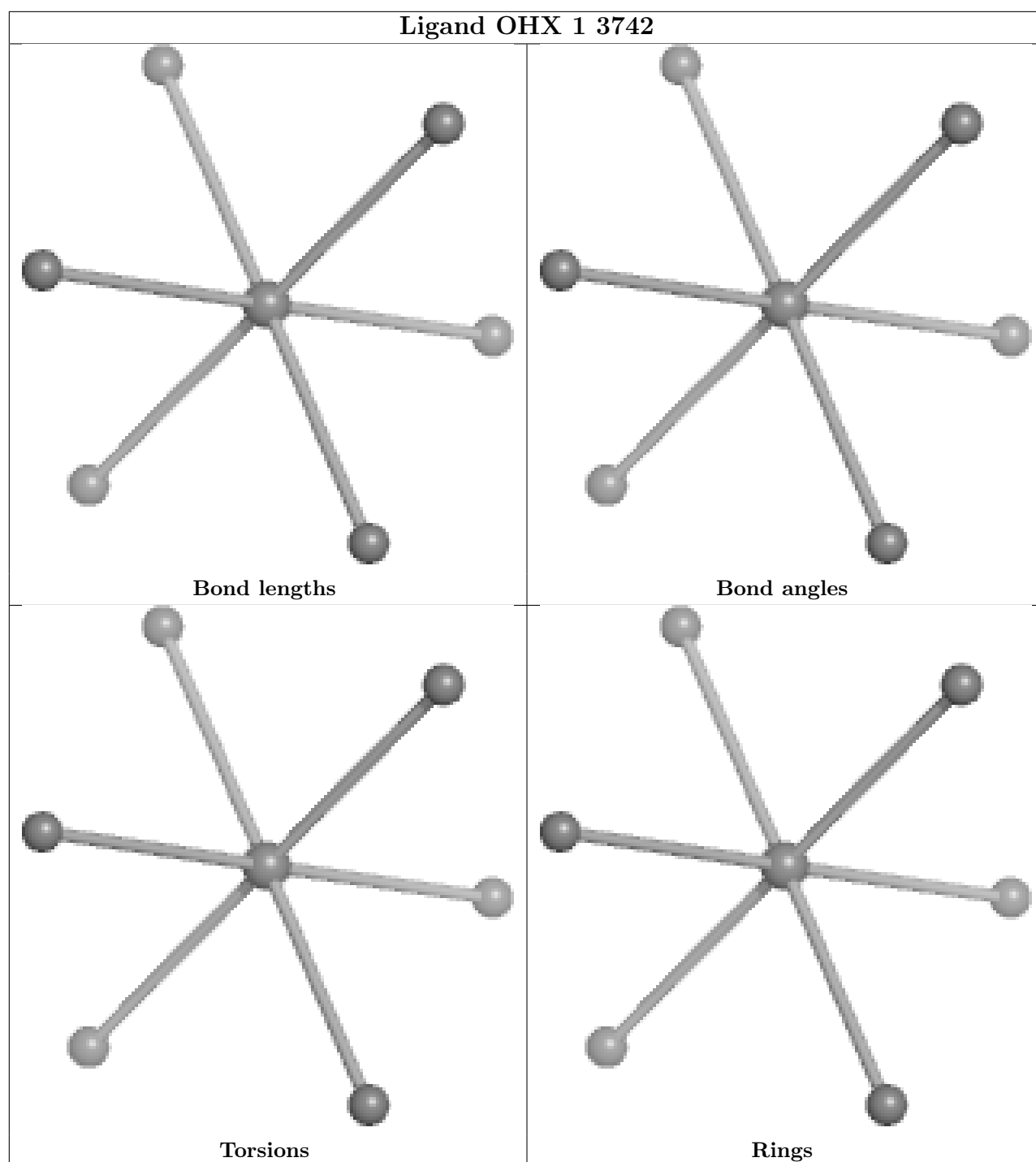
Rings

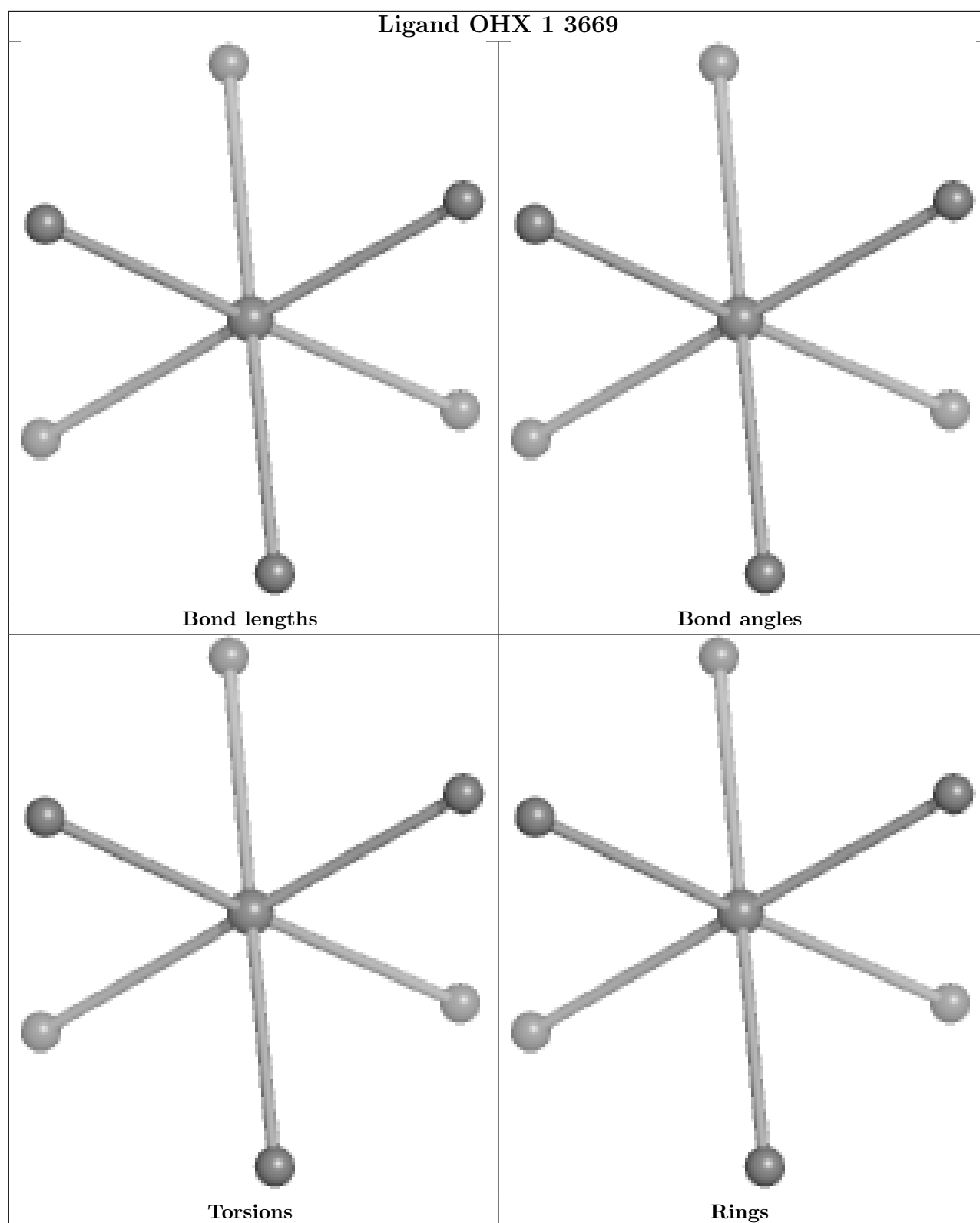


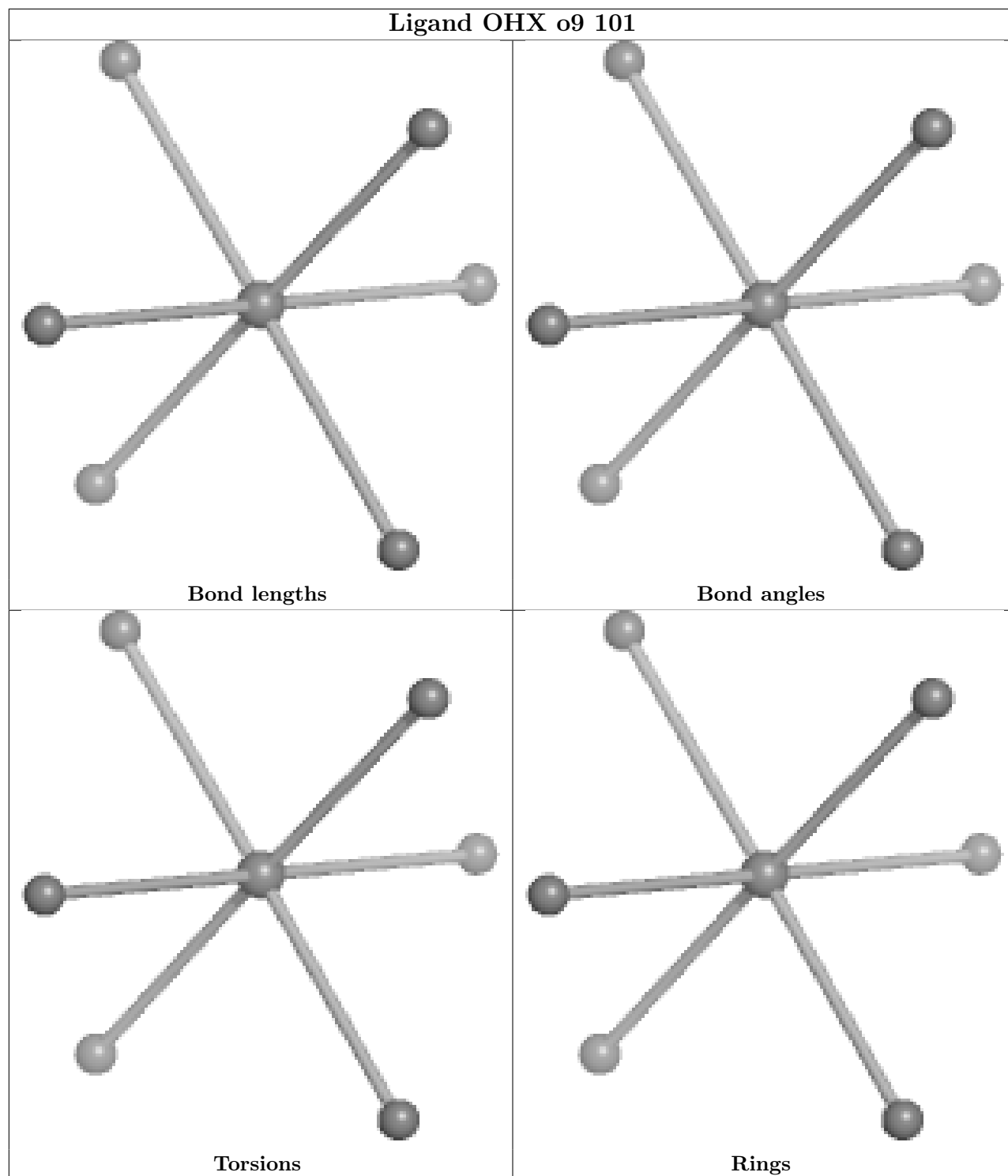


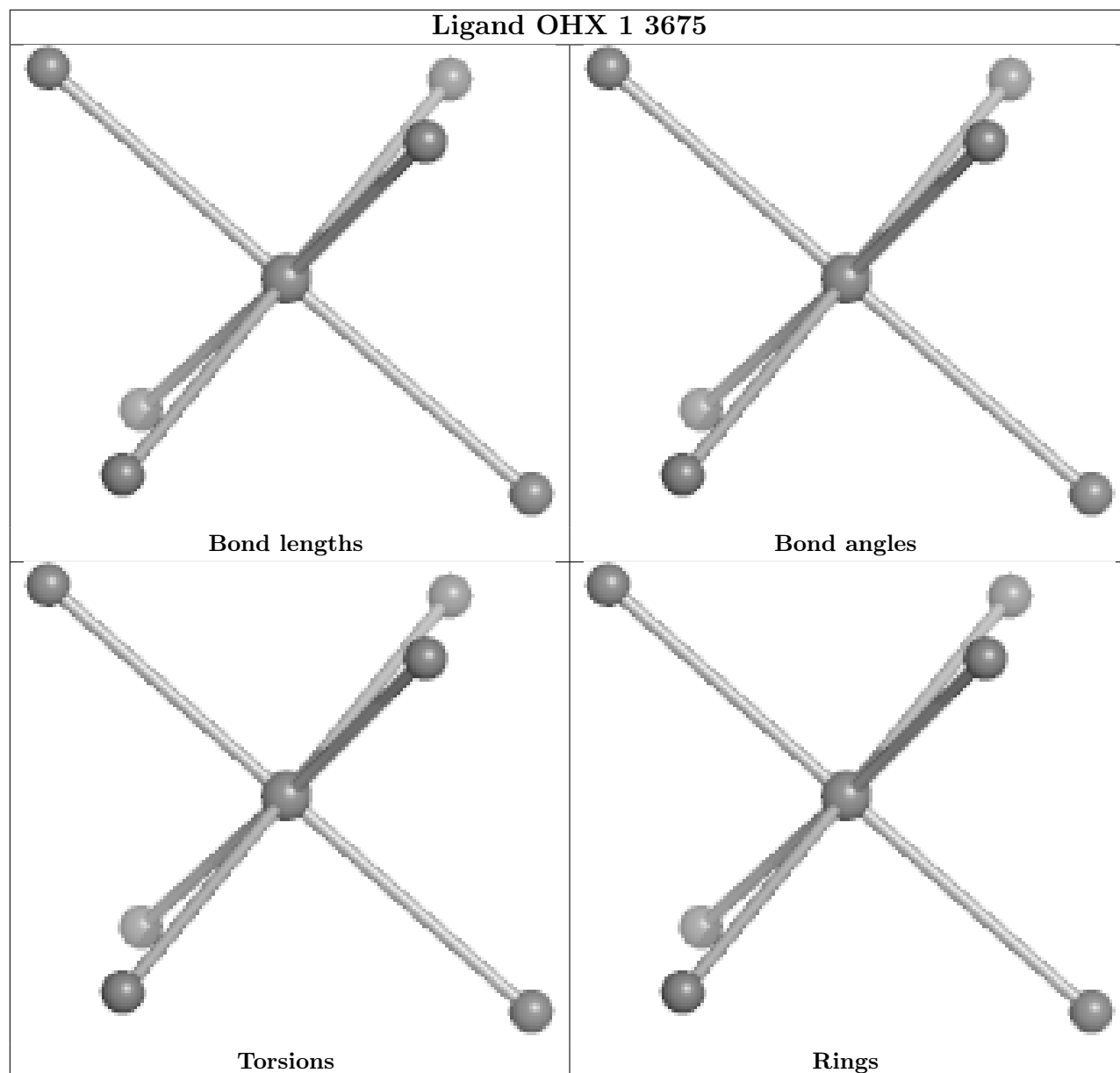




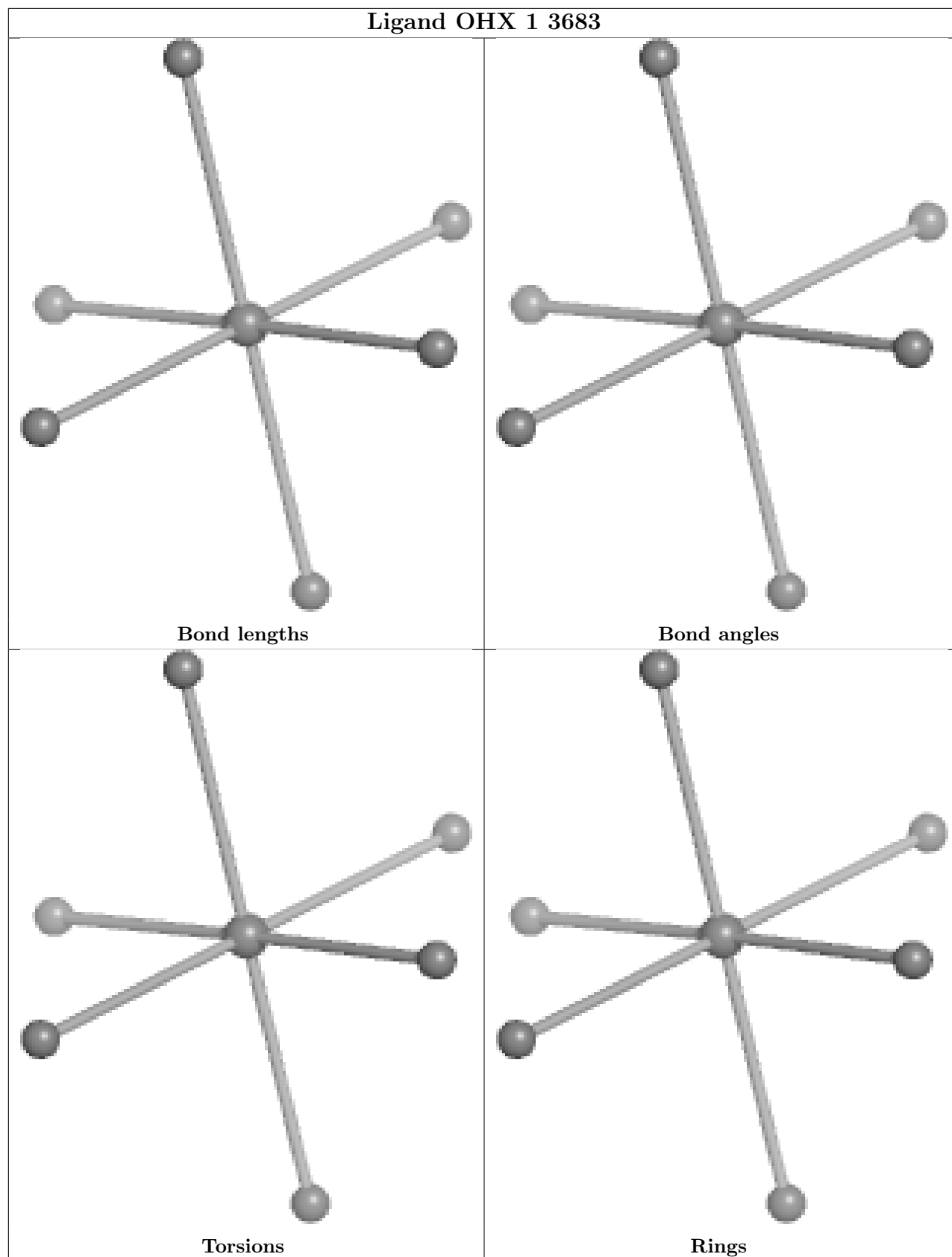




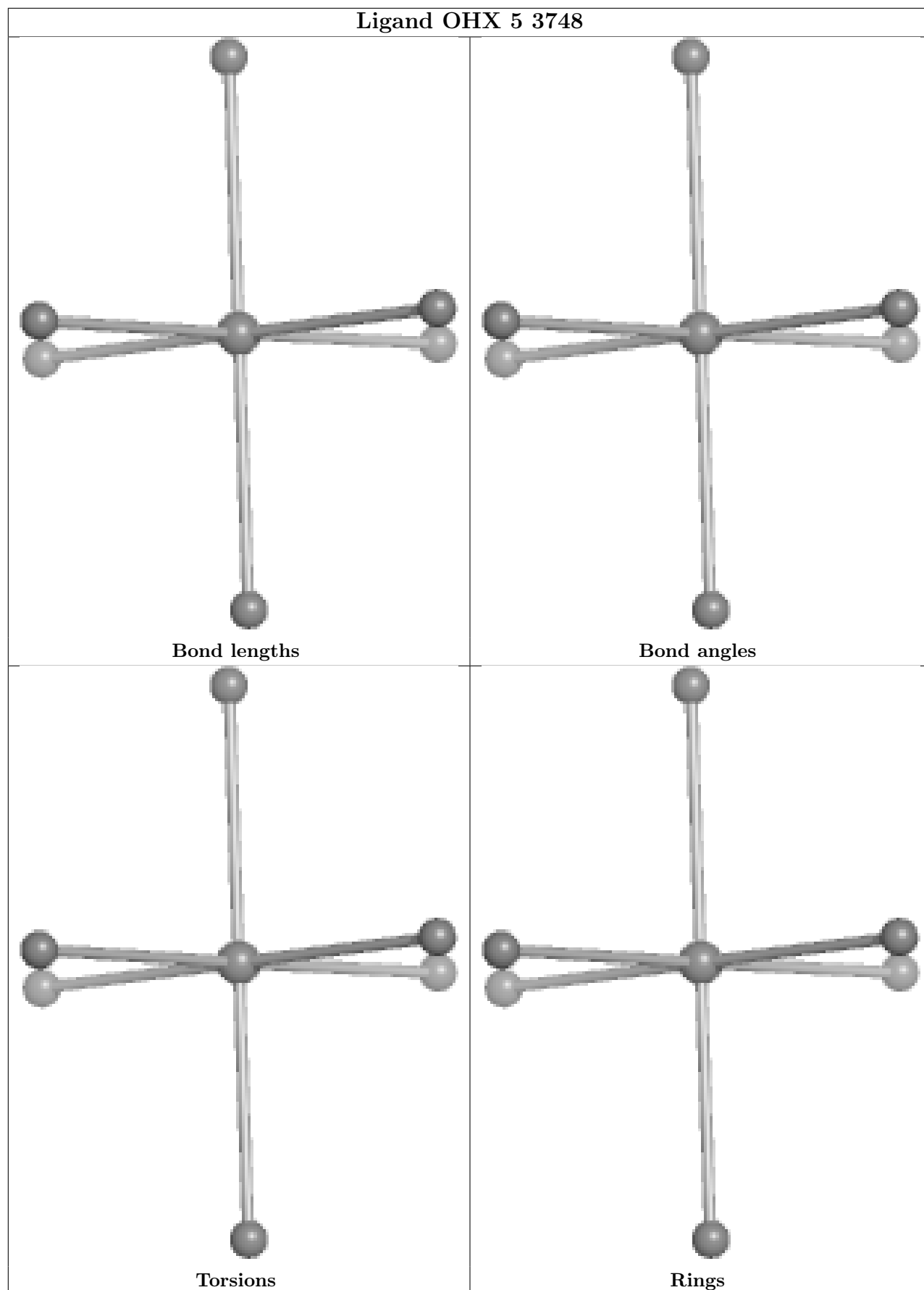




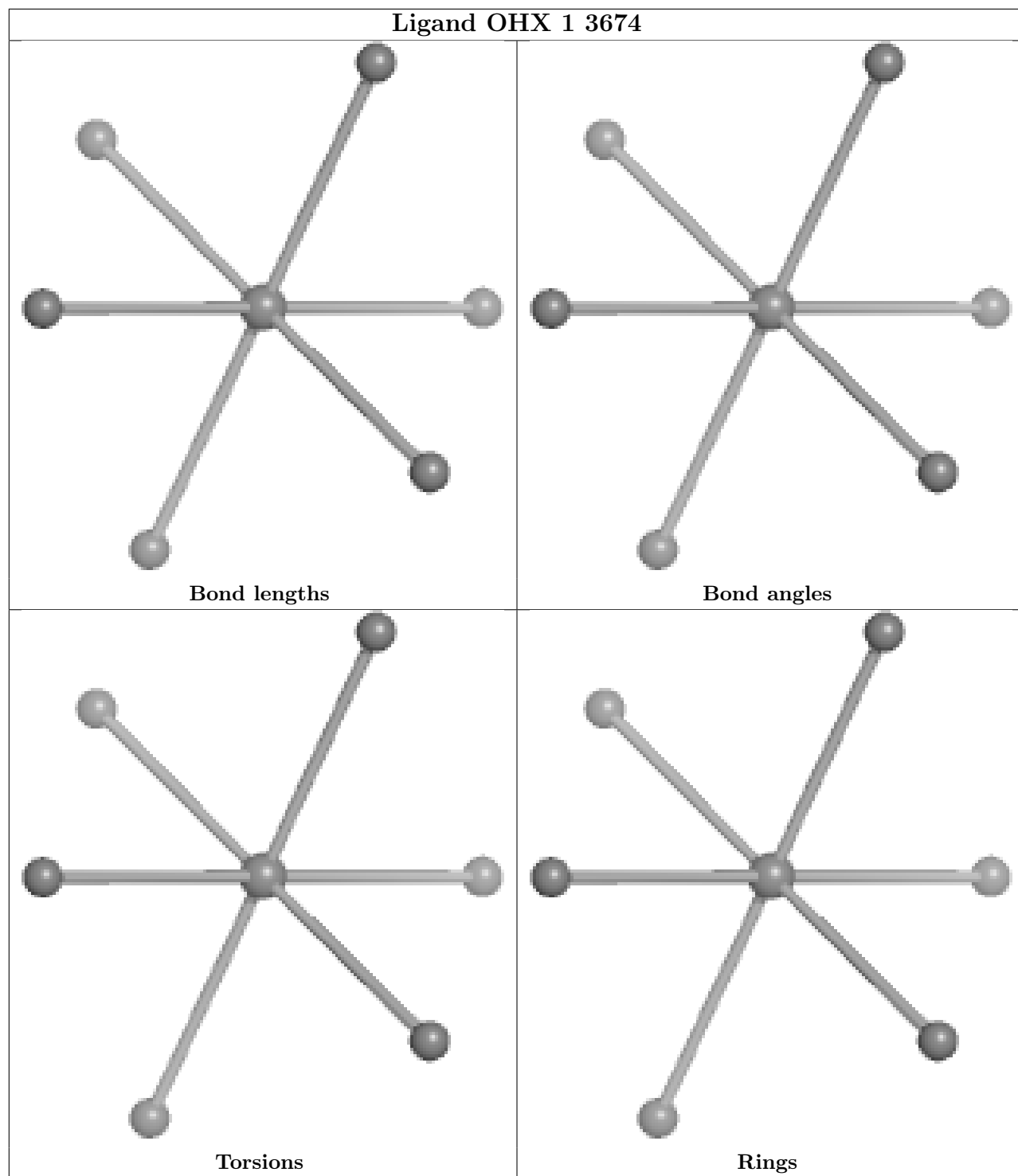
## Ligand OHX 1 3683

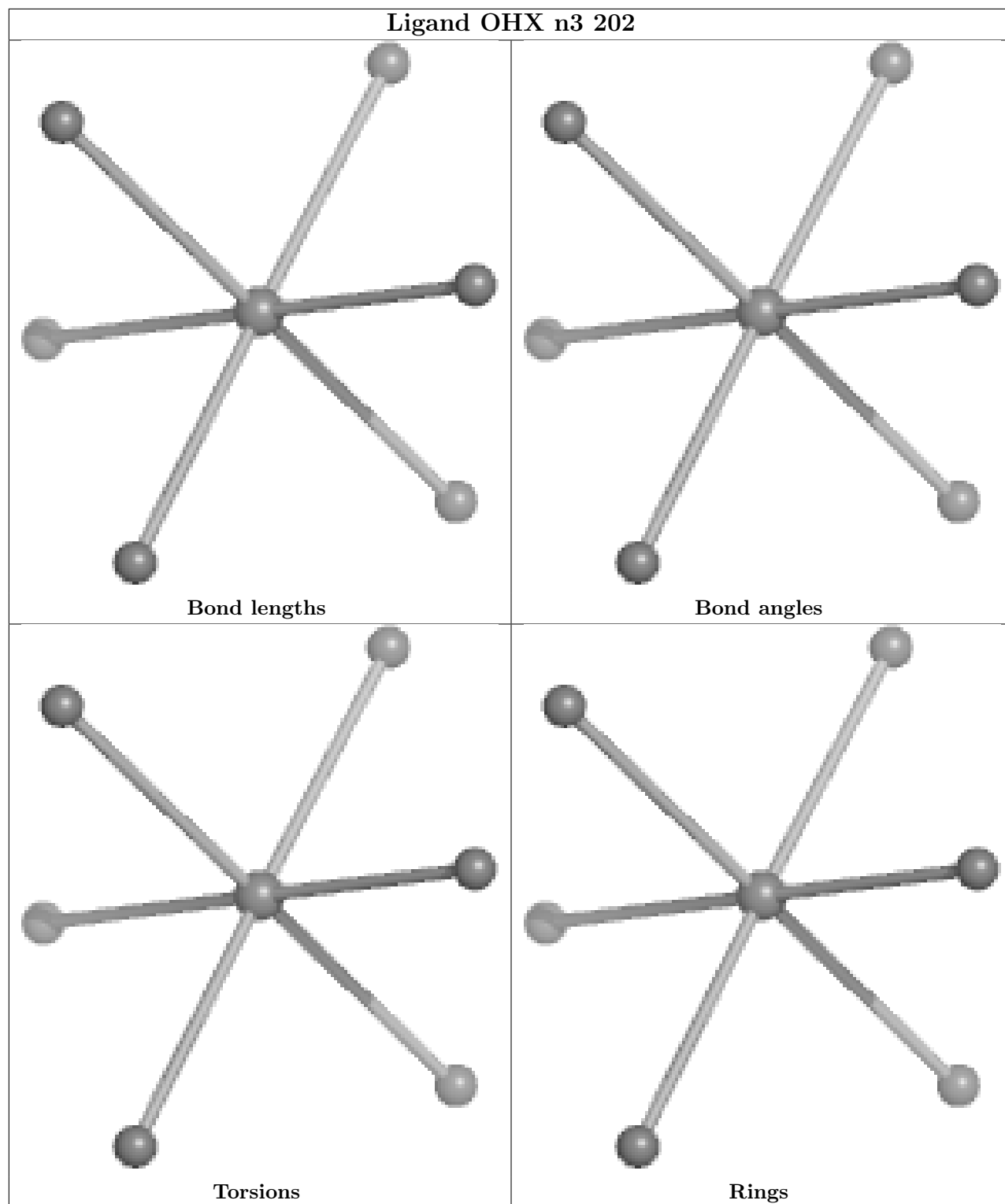


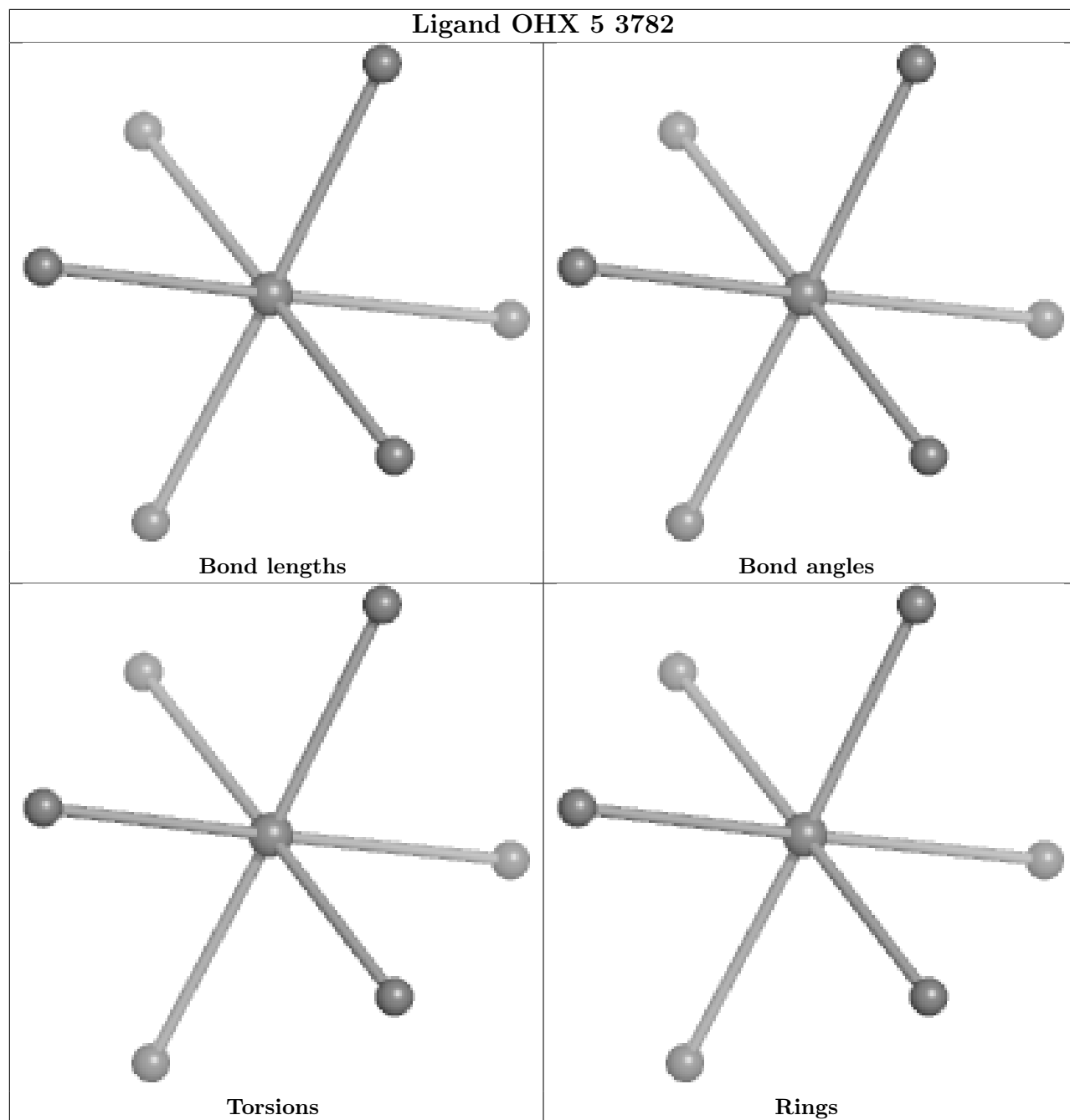
## Ligand OHX 5 3748

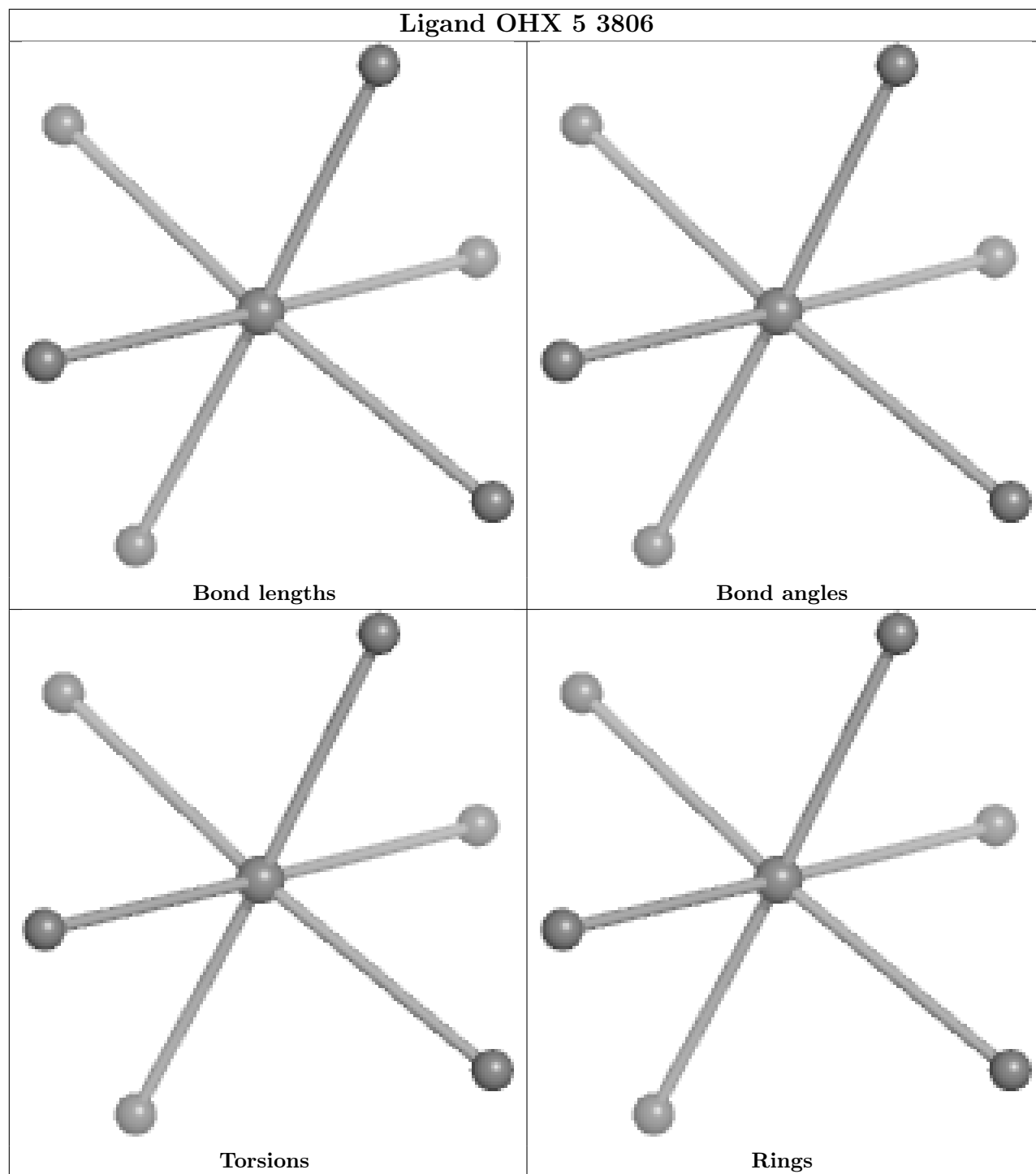




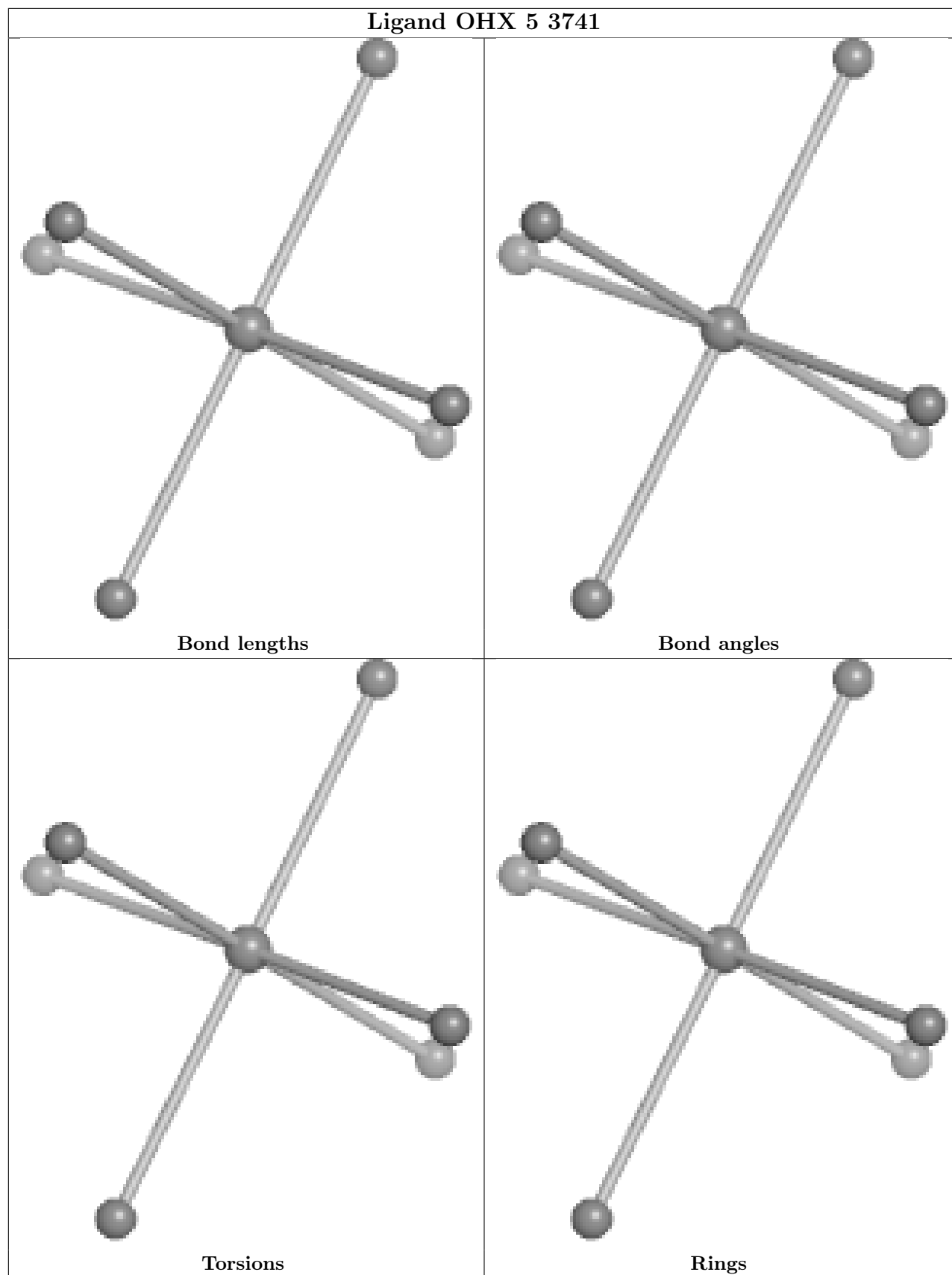




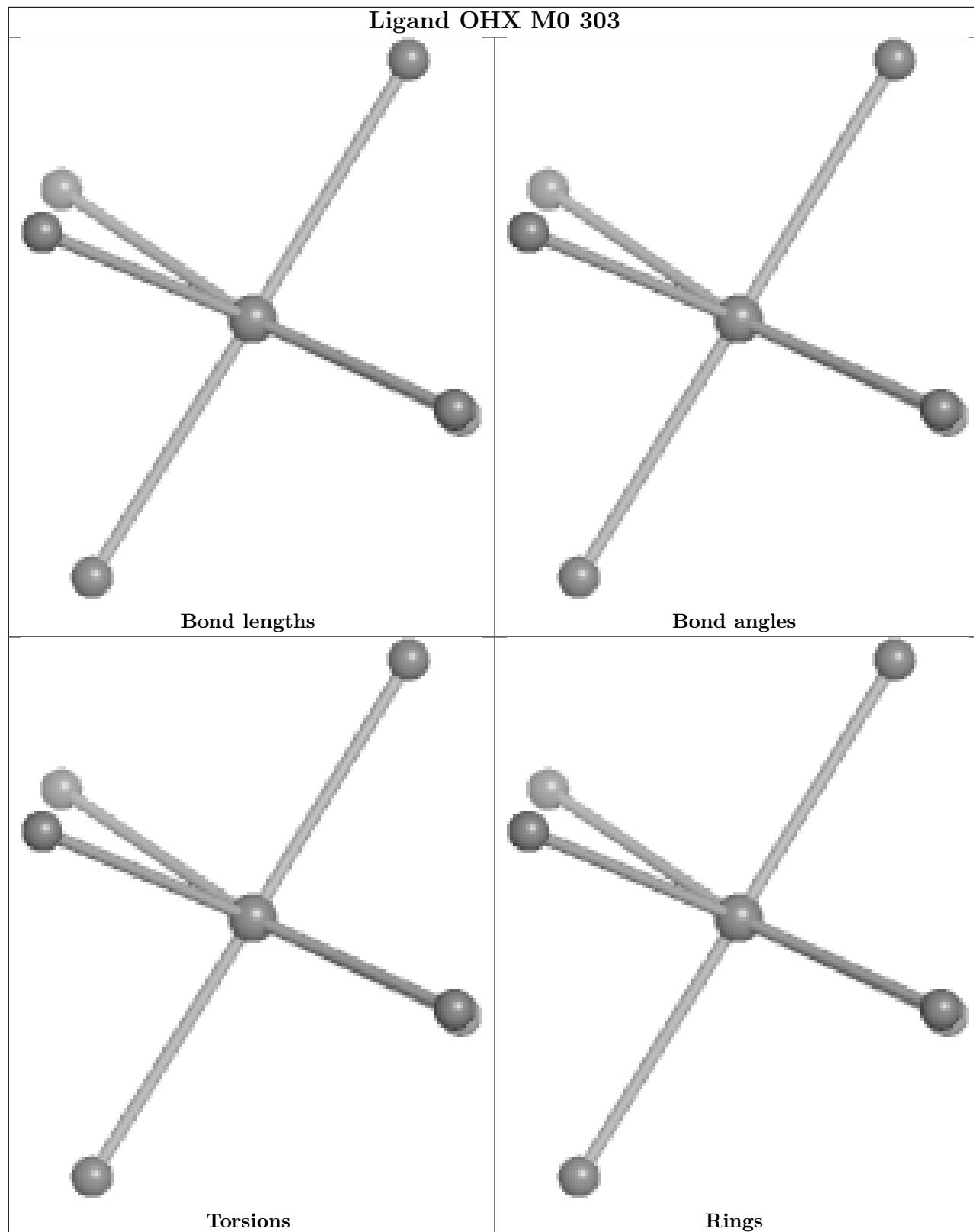


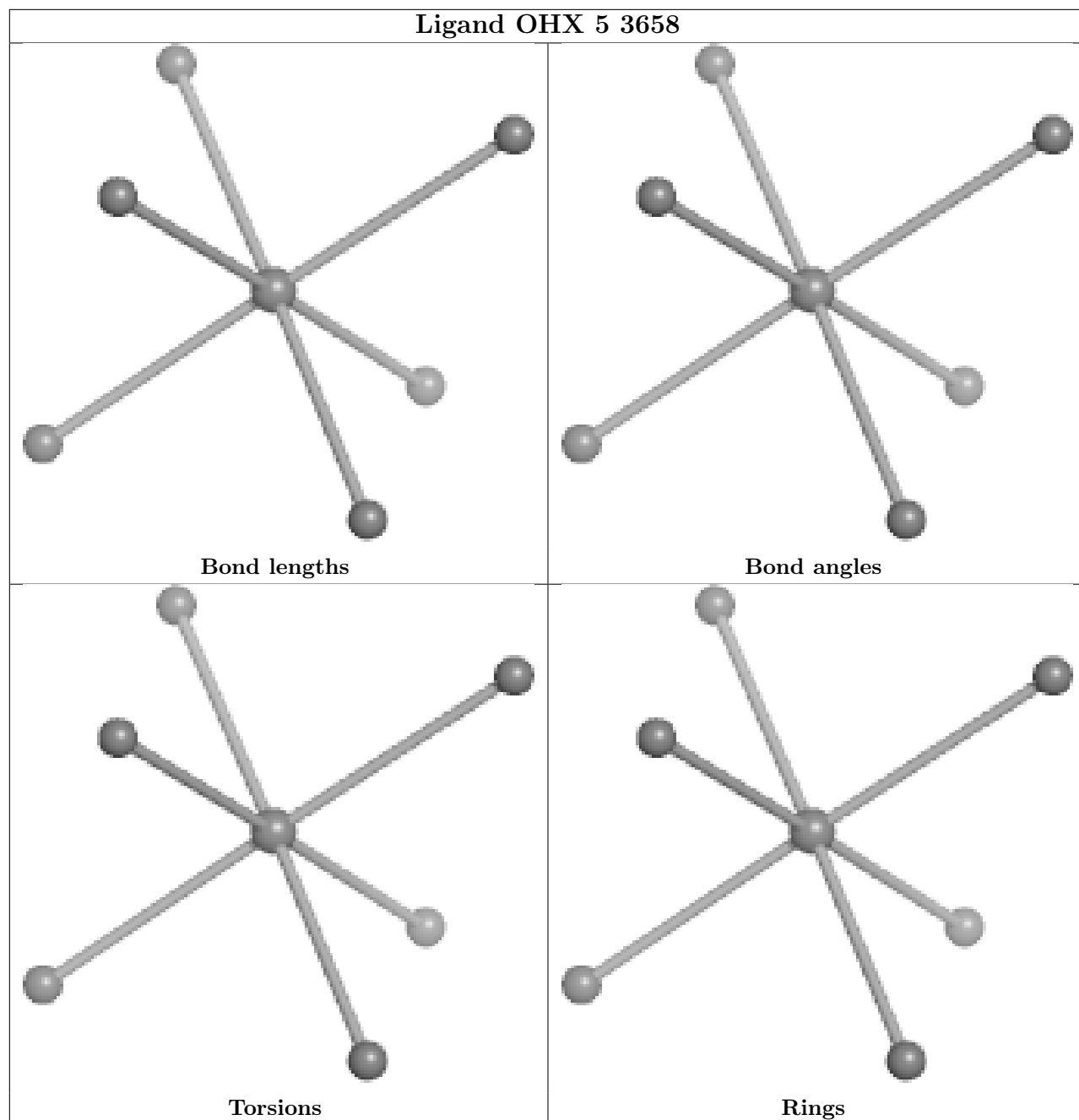


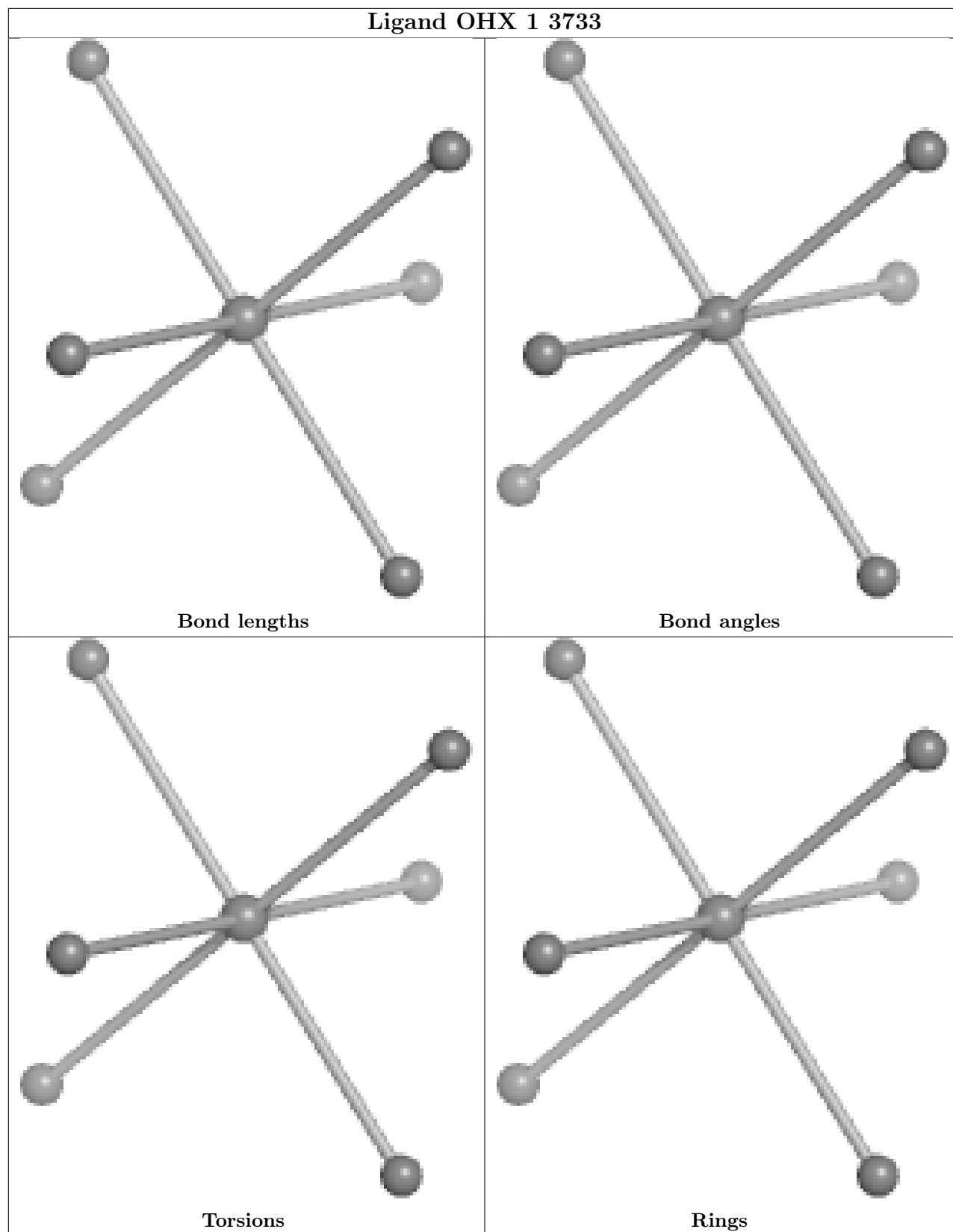
## Ligand OHX 5 3741



## Ligand OHX M0 303

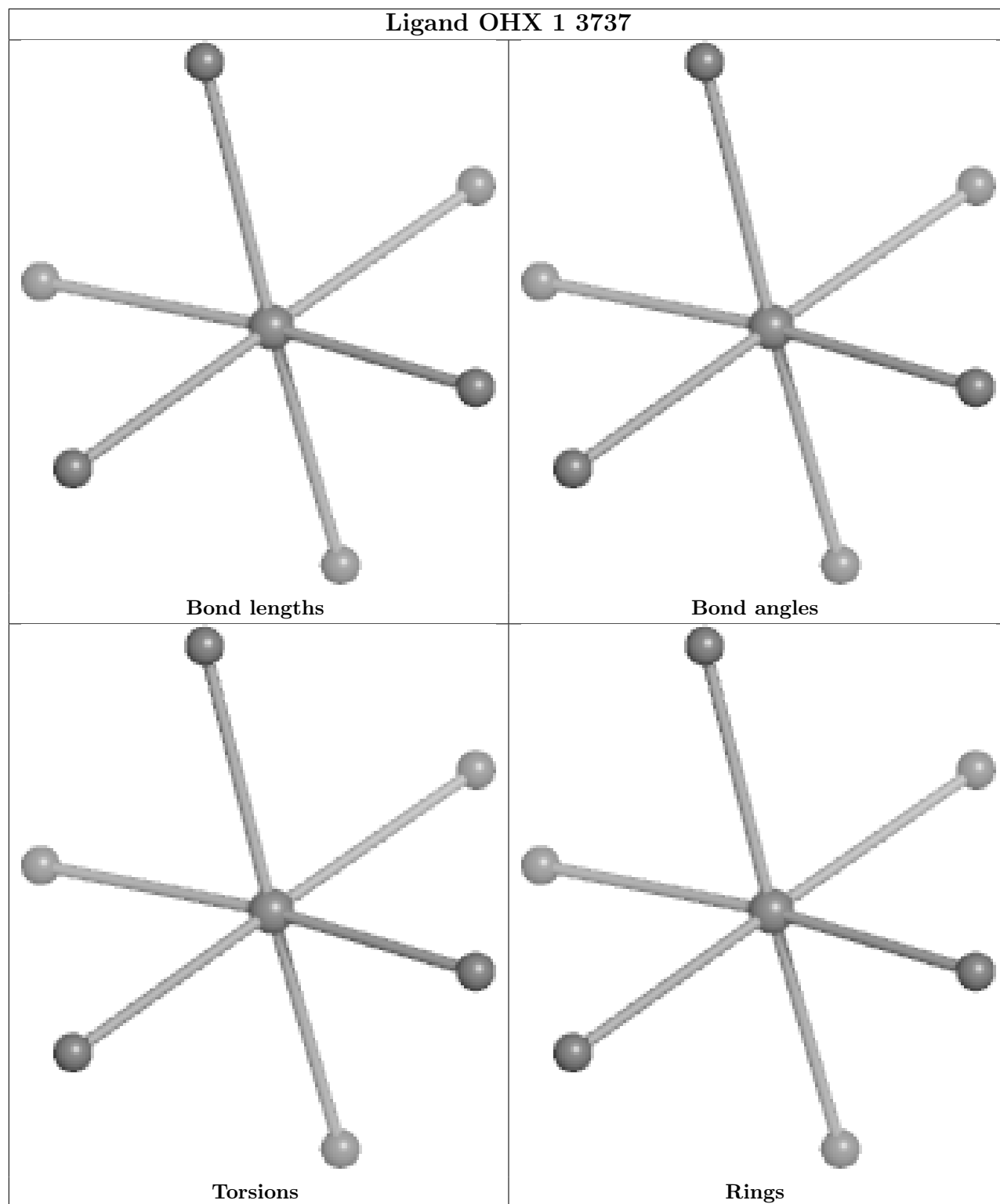




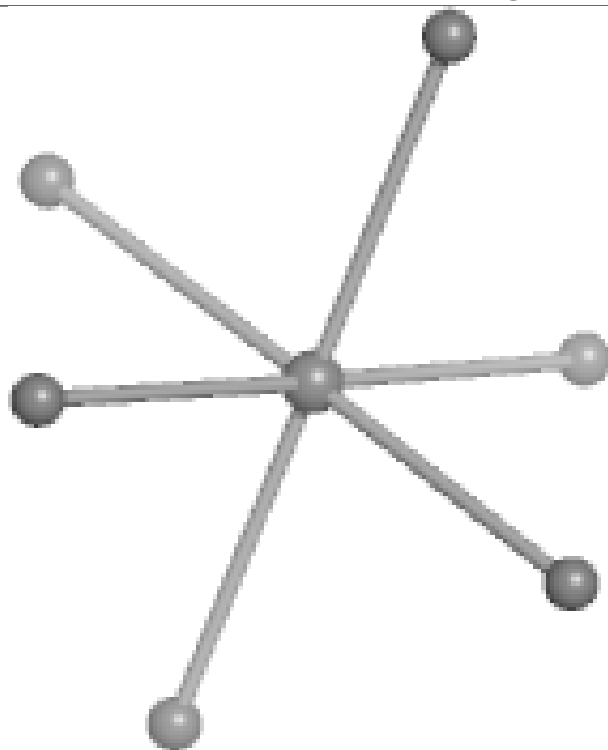




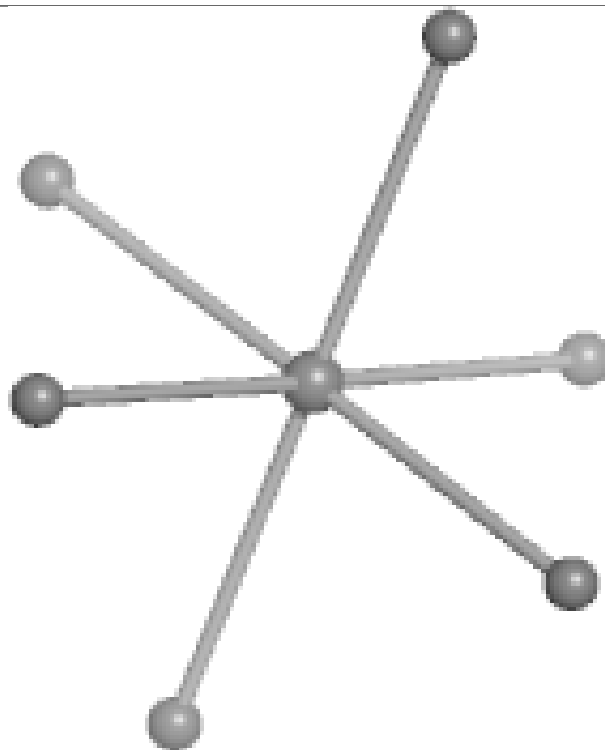
## Ligand OHX 1 3737



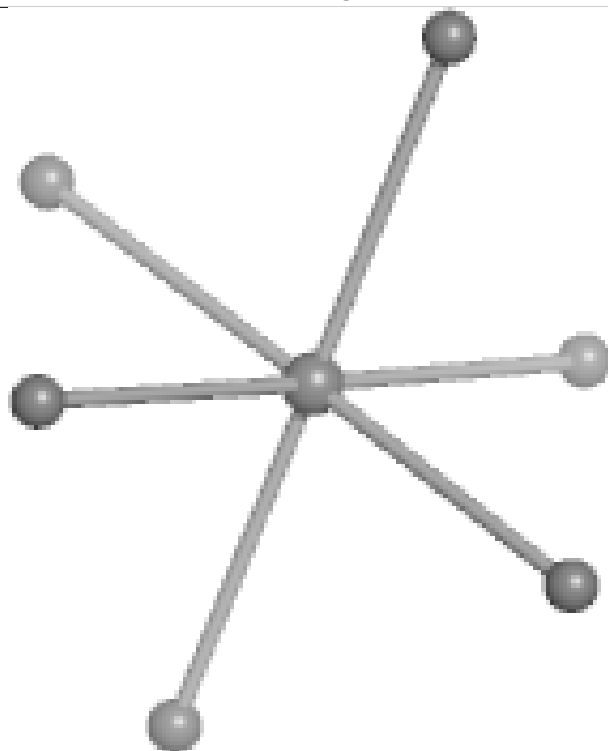
## Ligand OHX 1 3772



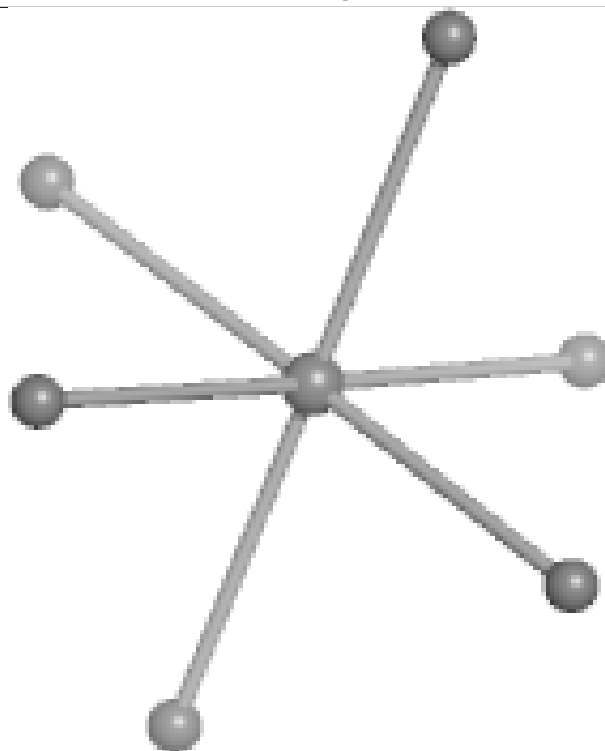
Bond lengths



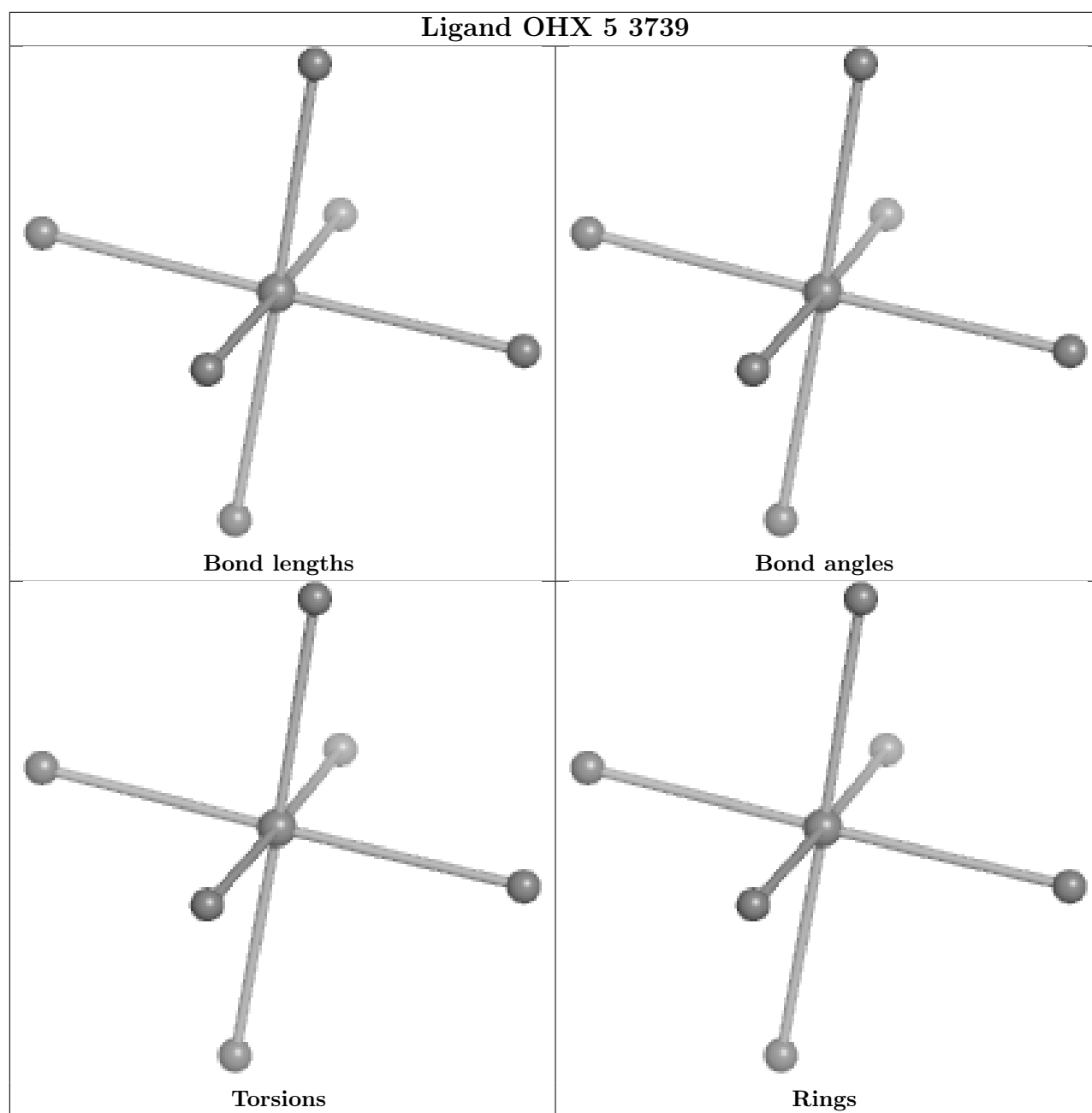
Bond angles

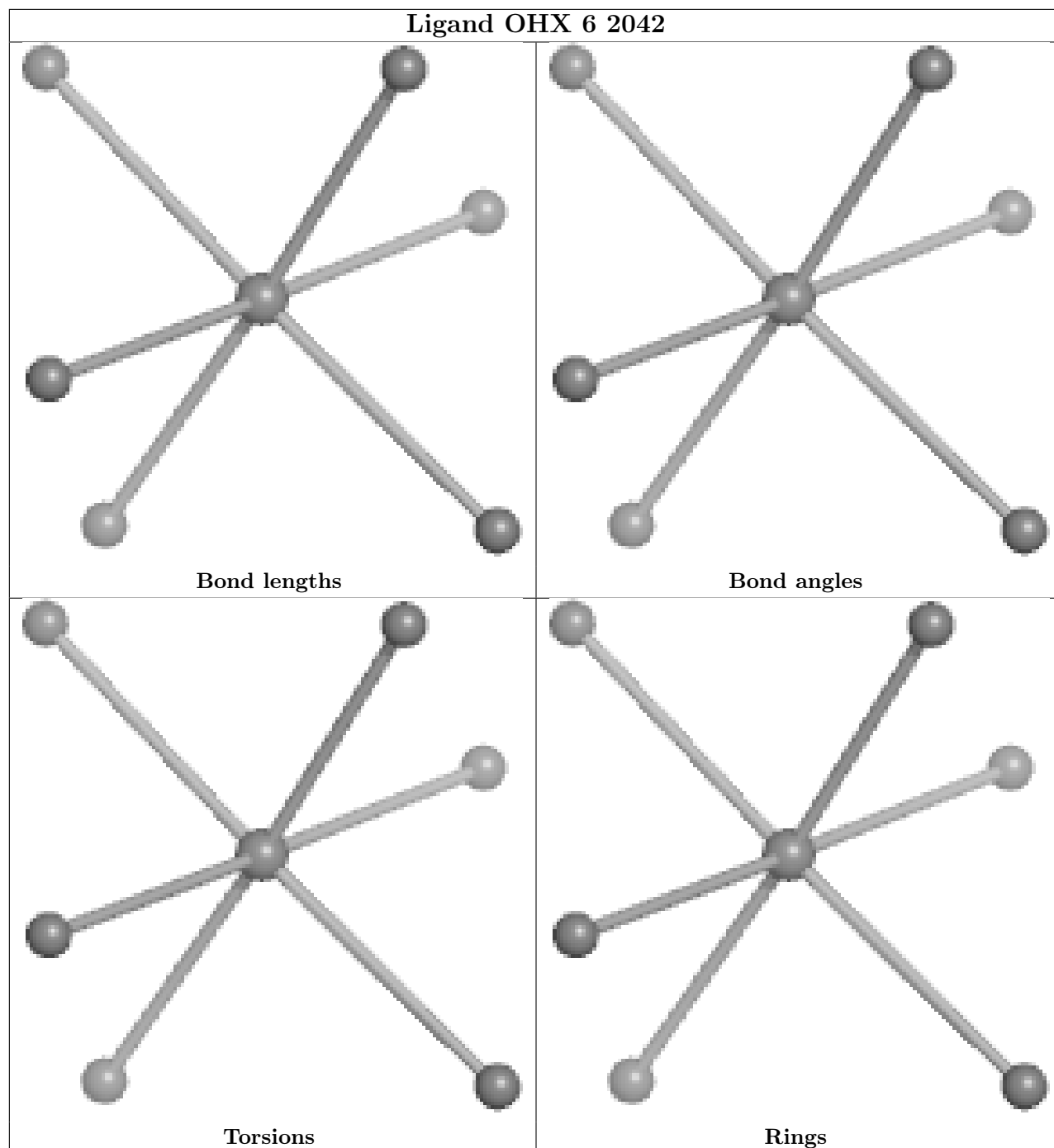


Torsions

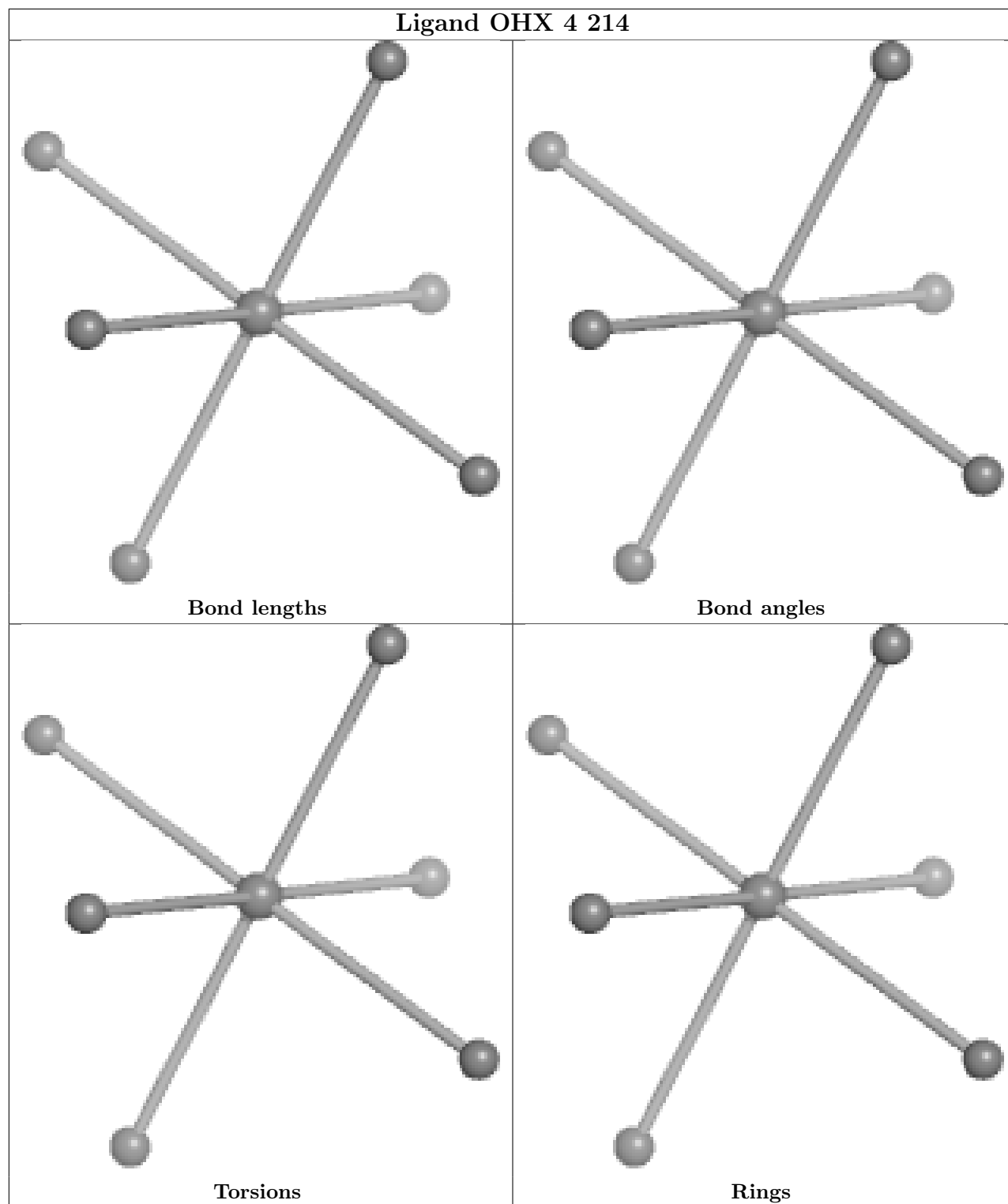


Rings

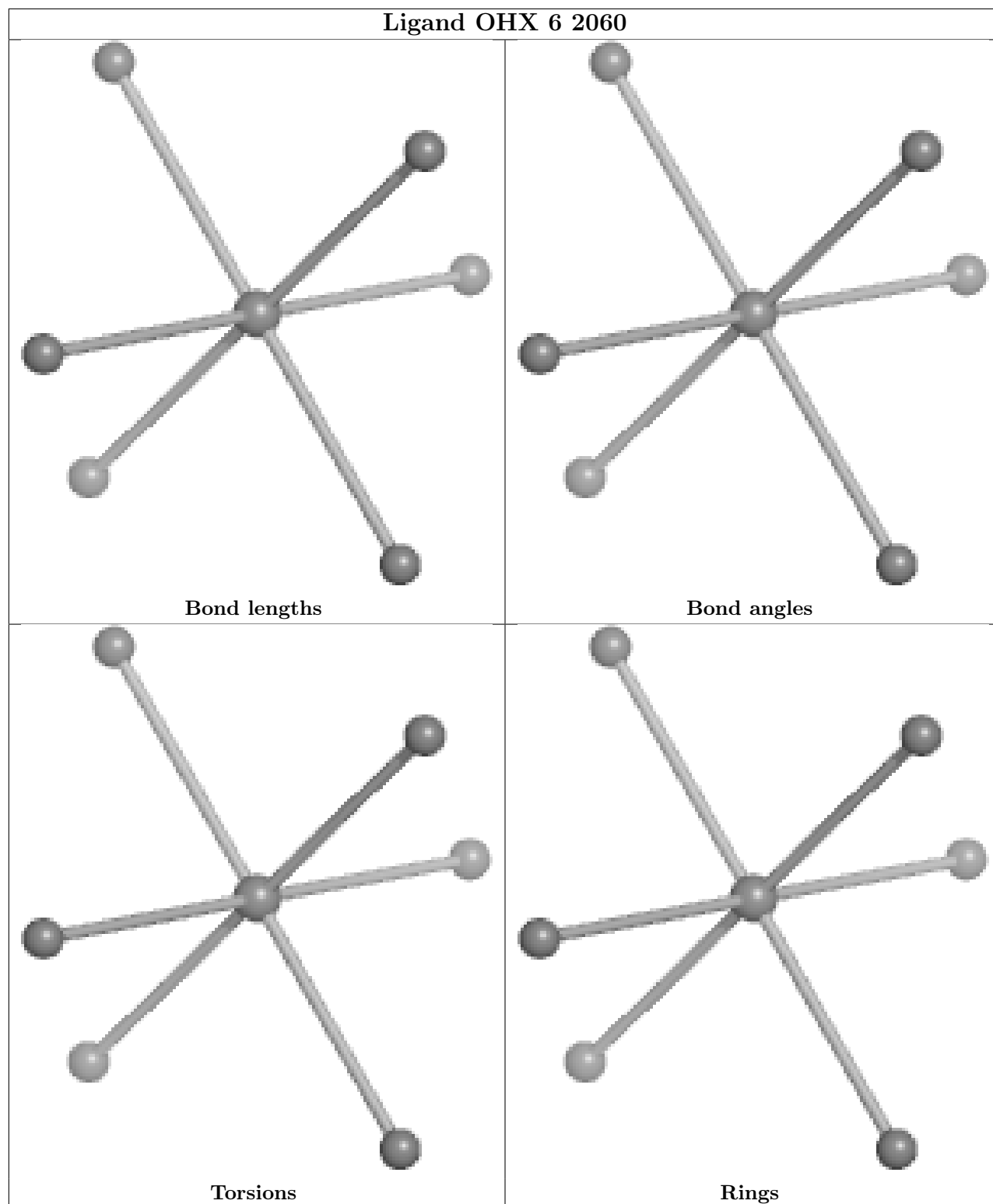




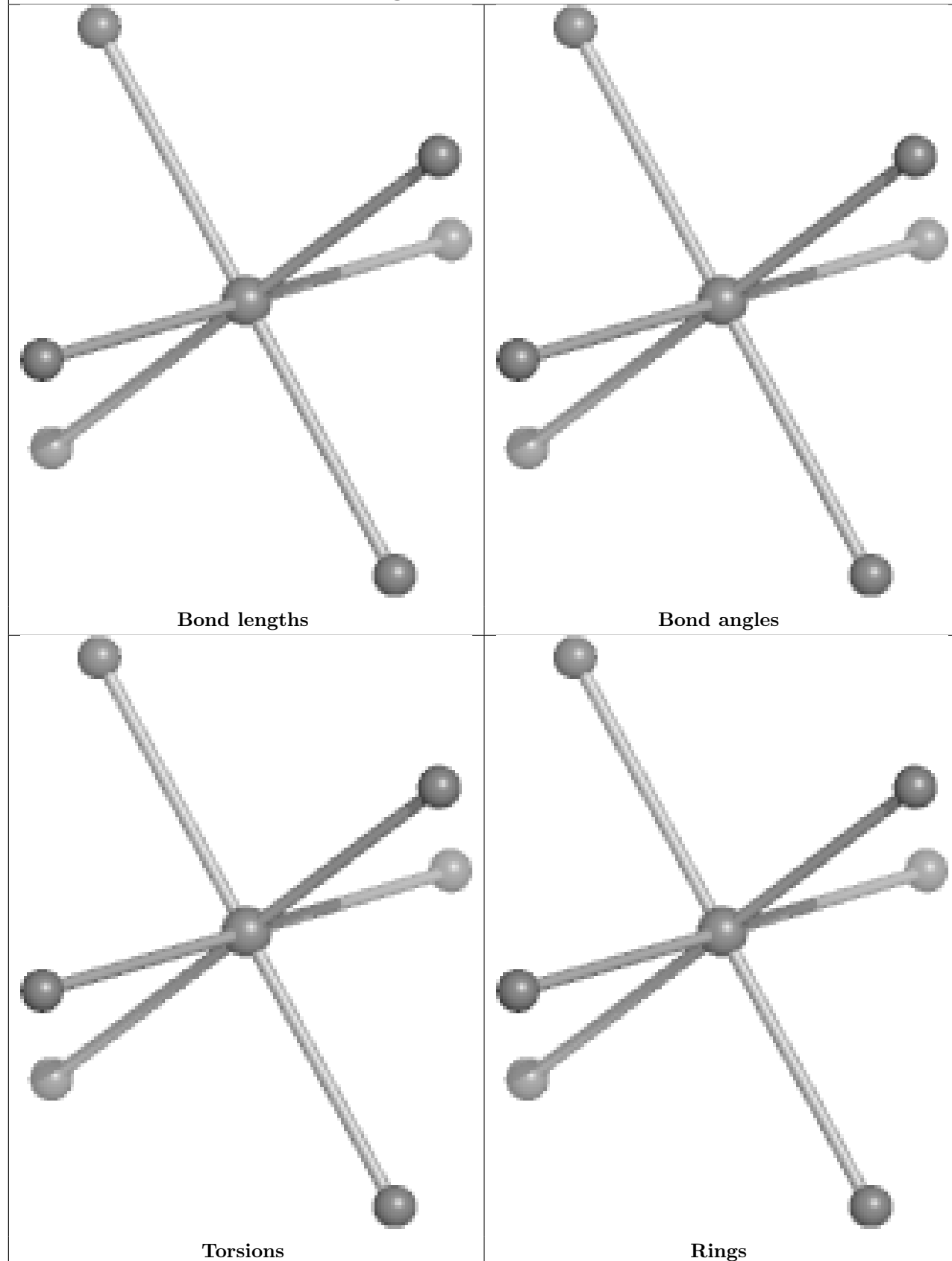
## Ligand OHX 4 214



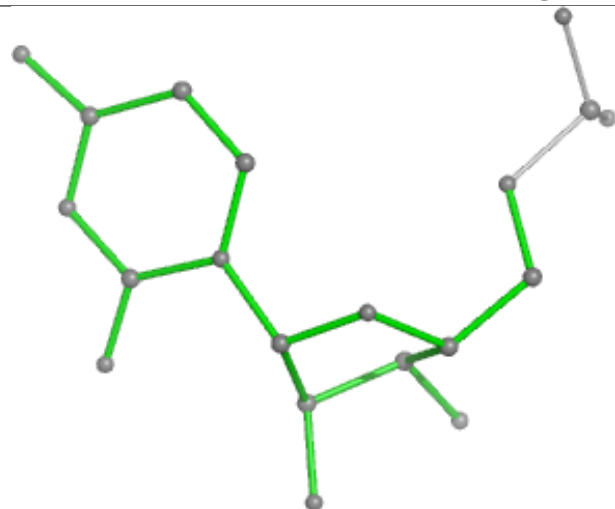
## Ligand OHX 6 2060



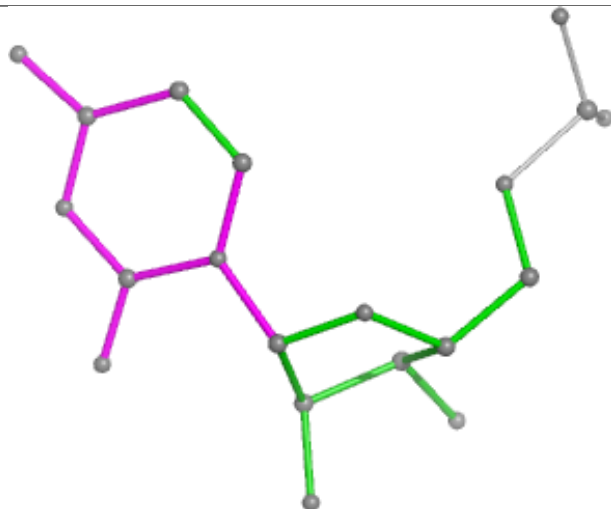
## Ligand OHX 5 3636



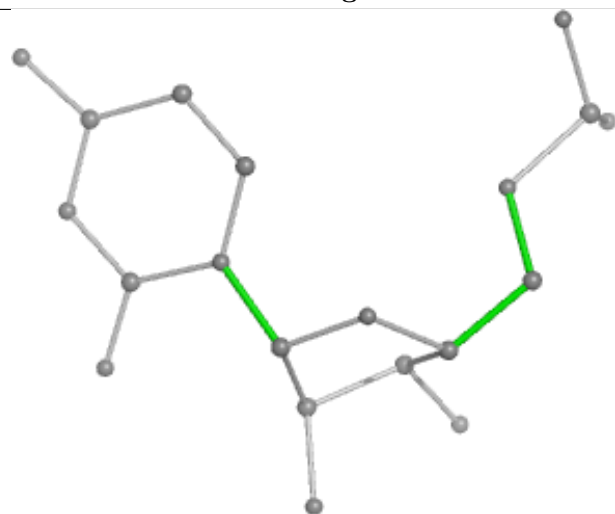
## Ligand C 5 3401



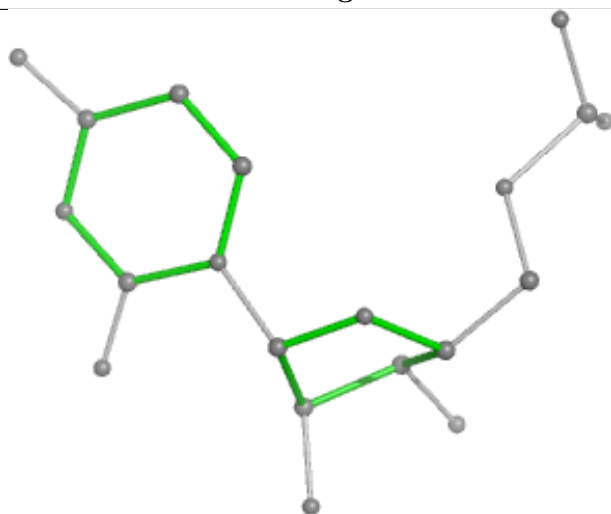
Bond lengths



Bond angles

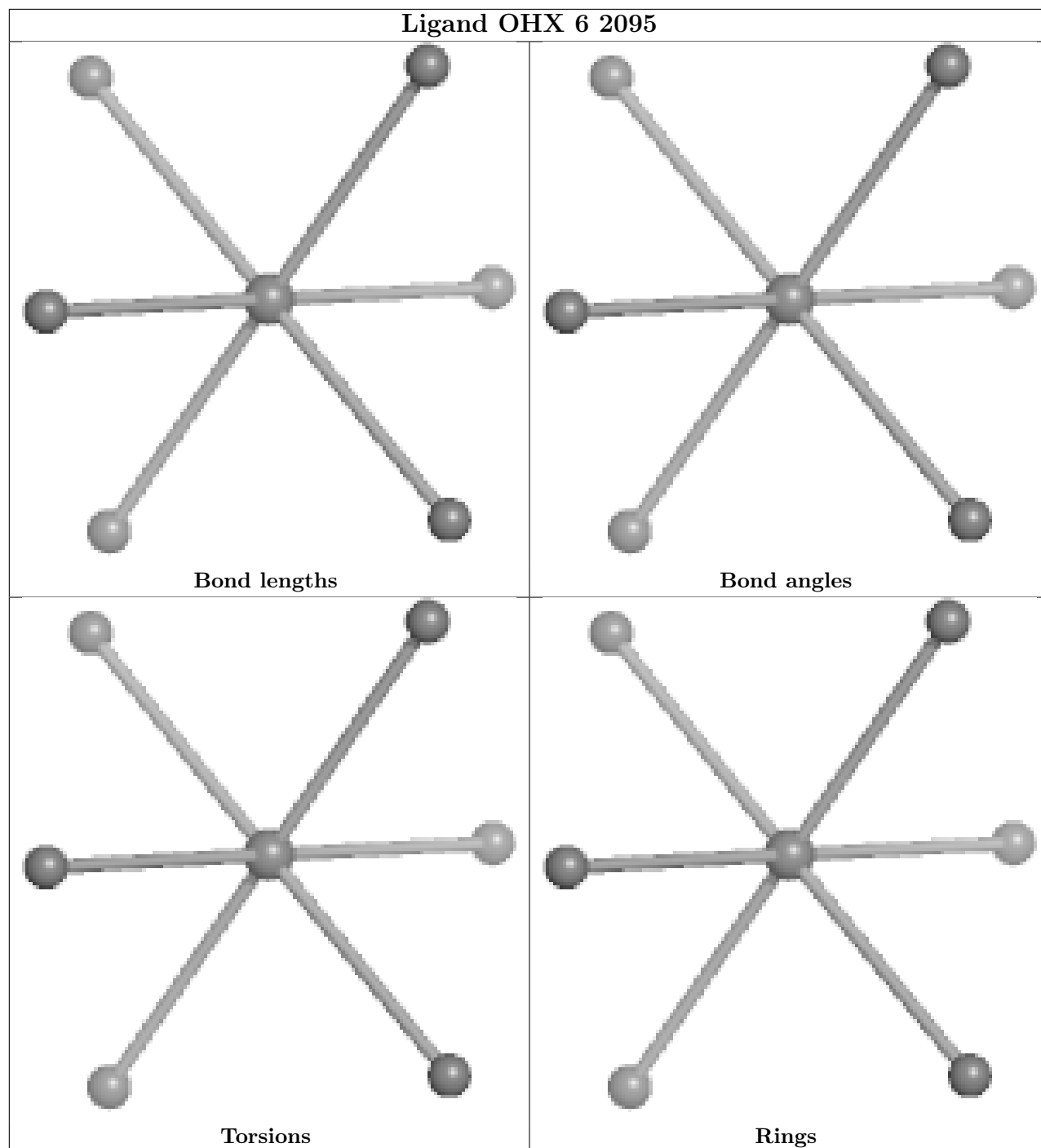


Torsions



Rings





## 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
82	sM	2
83	m2	2
1	2	1
35	SM	1
81	c0	1
2	S0	1
47	m0	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1798:U	O3'	1799:C	P	144.70
1	sM	85:SER	C	119:UNK	N	44.14
1	sM	139:UNK	C	155:UNK	N	37.81
1	SM	141:ALA	C	151:UNK	N	26.32
1	c0	84:GLU	C	87:UNK	N	7.55

## 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	1781/1829 (97%)	-0.05	28 (1%) 70 57	38, 90, 174, 223	1 (0%)
2	S0	206/206 (100%)	0.48	9 (4%) 39 30	91, 107, 116, 121	0
2	s0	206/206 (100%)	0.27	5 (2%) 59 44	68, 84, 96, 105	0
3	S1	214/216 (99%)	0.58	14 (6%) 26 21	104, 134, 158, 165	0
3	s1	216/216 (100%)	0.02	4 (1%) 66 51	72, 84, 102, 115	0
4	S2	217/217 (100%)	0.44	6 (2%) 55 40	75, 86, 98, 108	0
4	s2	217/217 (100%)	0.09	6 (2%) 55 40	55, 68, 78, 87	0
5	S3	223/223 (100%)	0.36	3 (1%) 74 61	82, 93, 112, 124	0
5	s3	223/223 (100%)	0.33	5 (2%) 62 47	74, 99, 116, 124	0
6	S4	260/260 (100%)	0.32	2 (0%) 82 72	69, 91, 98, 119	0
6	s4	260/260 (100%)	-0.02	0 100 100	47, 69, 82, 106	0
7	S5	206/206 (100%)	0.69	16 (7%) 20 18	96, 112, 124, 132	0
7	s5	206/206 (100%)	0.39	9 (4%) 39 30	79, 97, 113, 121	0
8	S6	226/226 (100%)	0.74	19 (8%) 18 17	72, 106, 120, 125	0
8	s6	218/226 (96%)	0.22	10 (4%) 38 29	49, 77, 94, 110	0
9	S7	184/186 (98%)	0.51	7 (3%) 44 33	90, 114, 139, 144	0
9	s7	186/186 (100%)	0.26	7 (3%) 44 33	65, 96, 124, 132	0
10	S8	188/199 (94%)	0.20	2 (1%) 77 66	63, 79, 113, 125	0
10	s8	188/199 (94%)	0.26	6 (3%) 50 37	46, 66, 107, 124	0
11	S9	185/185 (100%)	0.34	1 (0%) 87 80	81, 95, 126, 141	0
11	s9	185/185 (100%)	0.17	4 (2%) 62 47	57, 74, 104, 122	0
12	C0	96/96 (100%)	0.54	6 (6%) 27 22	84, 105, 126, 135	0
13	C1	155/155 (100%)	0.40	11 (7%) 23 20	64, 76, 112, 121	0
13	c1	146/155 (94%)	0.32	8 (5%) 32 25	48, 61, 89, 110	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	C2	124/124 (100%)	0.59	8 (6%) 26 21	133, 139, 151, 157	0
14	c2	124/124 (100%)	0.91	16 (12%) 9 9	167, 183, 195, 200	0
15	C3	150/150 (100%)	0.34	4 (2%) 56 41	75, 88, 104, 108	0
15	c3	150/150 (100%)	0.01	2 (1%) 74 61	57, 70, 86, 88	0
16	C4	127/128 (99%)	0.67	7 (5%) 32 25	75, 129, 142, 144	0
16	c4	128/128 (100%)	0.16	3 (2%) 61 46	54, 86, 94, 104	0
17	C5	124/135 (91%)	0.32	3 (2%) 59 44	79, 94, 110, 126	0
17	c5	135/135 (100%)	0.33	6 (4%) 39 30	67, 97, 112, 115	0
18	C6	141/142 (99%)	0.63	6 (4%) 40 30	82, 102, 107, 110	0
18	c6	142/142 (100%)	0.53	10 (7%) 24 20	73, 91, 104, 121	0
19	C7	120/125 (96%)	0.40	2 (1%) 69 55	91, 105, 124, 126	0
19	c7	117/125 (93%)	0.33	3 (2%) 57 42	78, 91, 105, 112	0
20	C8	145/145 (100%)	0.32	2 (1%) 73 60	77, 97, 120, 127	0
20	c8	145/145 (100%)	0.27	7 (4%) 36 28	73, 89, 109, 114	0
21	C9	143/143 (100%)	0.52	5 (3%) 47 35	85, 99, 111, 120	0
21	c9	143/143 (100%)	0.15	4 (2%) 55 40	76, 85, 99, 107	0
22	D0	107/110 (97%)	0.76	10 (9%) 16 15	77, 105, 124, 127	0
22	d0	110/110 (100%)	0.51	4 (3%) 46 34	74, 102, 127, 134	0
23	D1	87/87 (100%)	0.27	2 (2%) 61 46	87, 95, 109, 115	0
23	d1	87/87 (100%)	-0.00	0 100 100	65, 73, 93, 100	0
24	D2	129/129 (100%)	0.38	3 (2%) 61 46	73, 84, 90, 100	0
24	d2	129/129 (100%)	-0.19	0 100 100	53, 61, 68, 76	0
25	D3	144/144 (100%)	0.27	9 (6%) 27 22	64, 71, 83, 97	0
25	d3	144/144 (100%)	0.14	4 (2%) 55 40	45, 52, 62, 77	0
26	D4	134/134 (100%)	0.27	1 (0%) 84 75	81, 102, 113, 118	0
26	d4	134/134 (100%)	0.12	2 (1%) 71 58	56, 76, 87, 91	0
27	D5	70/70 (100%)	0.31	1 (1%) 73 60	108, 118, 124, 125	0
27	d5	69/70 (98%)	0.24	1 (1%) 73 60	89, 104, 111, 113	0
28	D6	97/97 (100%)	1.03	16 (16%) 5 5	79, 94, 142, 143	0
28	d6	97/97 (100%)	0.30	2 (2%) 63 48	58, 72, 97, 100	0
29	D7	81/81 (100%)	0.55	1 (1%) 76 64	90, 106, 133, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	d7	81/81 (100%)	0.21	2 (2%) 58 43	66, 83, 117, 120	0
30	D8	63/63 (100%)	0.93	9 (14%) 7 7	106, 122, 129, 131	0
30	d8	63/63 (100%)	0.44	1 (1%) 70 57	96, 110, 117, 119	0
31	D9	53/53 (100%)	0.24	1 (1%) 66 51	75, 80, 100, 104	0
31	d9	53/53 (100%)	0.14	0 100 100	71, 83, 117, 130	0
32	E0	60/62 (96%)	0.45	2 (3%) 49 36	70, 100, 125, 128	0
32	e0	62/62 (100%)	0.11	3 (4%) 36 28	55, 79, 104, 105	0
33	E1	71/76 (93%)	0.47	4 (5%) 31 25	96, 129, 140, 142	0
33	e1	76/76 (100%)	0.92	10 (13%) 8 8	100, 155, 176, 178	0
34	SR	318/318 (100%)	0.39	10 (3%) 51 38	100, 111, 126, 148	0
34	sR	318/318 (100%)	0.62	20 (6%) 27 22	96, 110, 122, 137	0
35	SM	133/159 (83%)	0.68	13 (9%) 14 14	54, 86, 117, 122	0
36	1	3149/3394 (92%)	-0.42	19 (0%) 85 78	30, 54, 125, 221	0
36	5	3150/3394 (92%)	-0.50	18 (0%) 85 78	31, 50, 117, 193	0
37	3	121/121 (100%)	-0.46	0 100 100	40, 70, 86, 94	0
37	7	121/121 (100%)	-0.71	1 (0%) 82 72	35, 53, 64, 71	0
38	4	158/158 (100%)	-0.53	1 (0%) 85 78	40, 60, 96, 129	0
38	8	158/158 (100%)	-0.45	1 (0%) 85 78	42, 64, 97, 126	0
39	L2	252/252 (100%)	0.04	4 (1%) 70 57	40, 57, 74, 83	0
39	l2	252/252 (100%)	-0.06	3 (1%) 76 64	38, 56, 74, 87	0
40	L3	386/386 (100%)	-0.07	4 (1%) 79 68	38, 57, 69, 83	0
40	l3	386/386 (100%)	-0.21	10 (2%) 57 42	30, 42, 56, 76	0
41	L4	361/361 (100%)	-0.25	2 (0%) 85 78	34, 48, 63, 70	0
41	l4	361/361 (100%)	-0.24	1 (0%) 90 85	37, 52, 70, 76	0
42	L5	296/296 (100%)	0.13	3 (1%) 79 68	51, 76, 94, 108	0
42	l5	294/296 (99%)	-0.21	2 (0%) 84 75	42, 54, 75, 94	0
43	L6	156/175 (89%)	-0.22	0 100 100	44, 53, 66, 77	0
43	l6	157/175 (89%)	-0.30	0 100 100	44, 54, 71, 83	0
44	L7	222/223 (99%)	-0.31	1 (0%) 87 80	35, 45, 70, 99	0
44	l7	223/223 (100%)	-0.26	0 100 100	35, 43, 74, 102	0
45	L8	233/233 (100%)	0.27	3 (1%) 74 61	65, 83, 108, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	l8	231/233 (99%)	0.26	6 (2%) 57 42	72, 87, 109, 112	0
46	L9	191/191 (100%)	0.02	3 (1%) 70 57	57, 65, 74, 85	0
46	l9	191/191 (100%)	-0.34	0 100 100	39, 48, 63, 72	0
47	M0	211/220 (95%)	-0.03	2 (0%) 81 70	41, 54, 88, 102	0
47	m0	213/220 (96%)	-0.05	4 (1%) 66 51	36, 50, 74, 87	0
48	M1	169/169 (100%)	0.06	2 (1%) 76 64	62, 77, 87, 93	0
48	m1	169/169 (100%)	-0.22	0 100 100	45, 61, 68, 72	0
49	M3	193/194 (99%)	-0.16	2 (1%) 79 68	35, 58, 94, 119	0
49	m3	194/194 (100%)	-0.01	1 (0%) 87 80	38, 67, 100, 109	0
50	M4	136/137 (99%)	-0.15	4 (2%) 54 40	50, 59, 70, 74	0
50	m4	137/137 (100%)	-0.29	2 (1%) 71 58	44, 50, 66, 72	0
51	M5	203/203 (100%)	0.00	2 (0%) 79 68	38, 55, 66, 68	0
51	m5	203/203 (100%)	0.10	3 (1%) 71 58	42, 61, 73, 76	0
52	M6	197/197 (100%)	-0.10	2 (1%) 79 68	38, 45, 63, 65	0
52	m6	197/197 (100%)	-0.19	2 (1%) 79 68	31, 37, 63, 68	0
53	M7	183/183 (100%)	0.02	7 (3%) 44 33	41, 47, 96, 121	0
53	m7	155/183 (84%)	-0.32	0 100 100	37, 42, 52, 70	0
54	M8	185/185 (100%)	-0.21	2 (1%) 77 66	37, 48, 61, 75	0
54	m8	185/185 (100%)	-0.18	0 100 100	37, 52, 62, 69	0
55	M9	188/188 (100%)	0.26	9 (4%) 36 28	61, 73, 137, 144	0
55	m9	188/188 (100%)	0.00	2 (1%) 77 66	49, 63, 121, 132	0
56	N0	172/172 (100%)	0.06	3 (1%) 69 55	46, 54, 65, 73	0
56	n0	172/172 (100%)	-0.37	0 100 100	38, 45, 55, 63	0
57	N1	159/159 (100%)	-0.08	5 (3%) 51 38	37, 51, 92, 98	0
57	n1	159/159 (100%)	-0.10	0 100 100	36, 44, 78, 83	0
58	N2	100/100 (100%)	0.33	2 (2%) 64 50	92, 102, 107, 115	0
58	n2	98/100 (98%)	0.13	1 (1%) 79 68	74, 85, 91, 93	0
59	N3	136/136 (100%)	-0.08	0 100 100	44, 54, 64, 69	0
59	n3	136/136 (100%)	-0.22	1 (0%) 84 75	31, 38, 47, 50	0
60	N4	98/135 (72%)	0.68	11 (11%) 11 11	55, 67, 134, 136	0
60	n4	135/135 (100%)	0.40	7 (5%) 34 27	39, 83, 109, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
61	N5	121/121 (100%)	0.04	2 (1%) 69 55	57, 69, 85, 106	0
61	n5	120/121 (99%)	0.04	0 100 100	56, 69, 87, 93	0
62	N6	126/126 (100%)	-0.08	1 (0%) 82 72	44, 61, 70, 79	0
62	n6	126/126 (100%)	-0.09	0 100 100	50, 66, 80, 83	0
63	N7	135/135 (100%)	0.22	1 (0%) 84 75	83, 96, 107, 111	0
63	n7	135/135 (100%)	0.24	0 100 100	82, 96, 113, 117	0
64	N8	148/148 (100%)	-0.26	1 (0%) 84 75	31, 49, 67, 75	0
64	n8	148/148 (100%)	-0.13	1 (0%) 84 75	33, 54, 68, 71	0
65	N9	58/58 (100%)	-0.06	1 (1%) 69 55	34, 54, 89, 101	0
65	n9	58/58 (100%)	0.07	2 (3%) 48 35	35, 52, 73, 77	0
66	O0	97/100 (97%)	0.13	3 (3%) 51 38	80, 88, 103, 106	0
66	o0	100/100 (100%)	0.10	1 (1%) 79 68	72, 83, 100, 103	0
67	O1	109/109 (100%)	0.20	2 (1%) 67 53	55, 65, 88, 92	0
67	o1	109/109 (100%)	-0.17	0 100 100	43, 53, 80, 96	0
68	O2	127/127 (100%)	-0.24	1 (0%) 82 72	33, 44, 55, 67	0
68	o2	127/127 (100%)	-0.24	0 100 100	34, 49, 59, 64	0
69	O3	106/106 (100%)	-0.18	0 100 100	37, 45, 66, 74	0
69	o3	106/106 (100%)	-0.25	0 100 100	36, 42, 64, 74	0
70	O4	112/112 (100%)	0.44	5 (4%) 39 29	54, 74, 103, 109	0
70	o4	112/112 (100%)	0.45	6 (5%) 32 26	51, 73, 105, 111	0
71	O5	119/119 (100%)	0.10	2 (1%) 69 55	55, 70, 77, 80	0
71	o5	119/119 (100%)	0.11	1 (0%) 82 72	63, 71, 86, 95	0
72	O6	99/99 (100%)	-0.09	2 (2%) 64 50	55, 67, 92, 100	0
72	o6	99/99 (100%)	-0.10	1 (1%) 79 68	61, 72, 86, 99	0
73	O7	87/87 (100%)	-0.09	1 (1%) 77 66	41, 46, 67, 75	0
73	o7	87/87 (100%)	-0.07	1 (1%) 77 66	37, 49, 77, 91	0
74	O8	77/77 (100%)	0.21	1 (1%) 74 61	82, 92, 103, 106	0
74	o8	77/77 (100%)	0.11	0 100 100	81, 89, 97, 99	0
75	O9	50/50 (100%)	0.06	0 100 100	47, 55, 57, 57	0
75	o9	50/50 (100%)	0.04	0 100 100	48, 55, 60, 62	0
76	Q0	52/52 (100%)	-0.13	0 100 100	49, 53, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
76	q0	52/52 (100%)	-0.55	0 100 100	36, 40, 49, 54	0
77	Q1	25/25 (100%)	0.33	0 100 100	57, 62, 66, 66	0
77	q1	25/25 (100%)	-0.21	0 100 100	45, 47, 48, 50	0
78	Q2	105/105 (100%)	-0.25	0 100 100	41, 51, 72, 93	0
78	q2	105/105 (100%)	-0.32	0 100 100	42, 50, 64, 85	0
79	Q3	91/91 (100%)	0.03	3 (3%) 49 36	46, 59, 74, 81	0
79	q3	91/91 (100%)	-0.03	1 (1%) 77 66	42, 55, 67, 73	0
80	6	1795/1800 (99%)	-0.29	22 (1%) 76 64	29, 75, 157, 226	1 (0%)
81	c0	84/96 (87%)	0.72	7 (8%) 19 17	94, 126, 139, 141	0
82	sM	63/104 (60%)	0.41	5 (7%) 20 18	47, 97, 105, 110	0
83	m2	0/150	-	-	-	-
84	p0	143/219 (65%)	0.43	5 (3%) 47 35	88, 109, 177, 181	0
85	p1	0/47	-	-	-	-
85	p2	0/47	-	-	-	-
All	All	33015/34167 (96%)	-0.02	644 (1%) 64 50	29, 69, 125, 226	2 (0%)

The worst 5 of 644 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	86	SER	8.1
13	c1	3	THR	8.0
8	s6	162	VAL	6.4
7	s5	37	GLN	5.8
53	M7	161	ALA	5.7

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

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
87	MG	6	2332	1/1	-0.16	0.23	213,213,213,213	0
87	MG	1	4348	1/1	-0.09	0.25	191,191,191,191	0
87	MG	2	2173	1/1	0.03	0.41	116,116,116,116	0
87	MG	1	4293	1/1	0.04	0.25	127,127,127,127	0
87	MG	2	2198	1/1	0.07	0.35	120,120,120,120	0
87	MG	2	2247	1/1	0.10	0.23	115,115,115,115	0
87	MG	6	2281	1/1	0.15	0.34	124,124,124,124	0
87	MG	2	2230	1/1	0.16	0.27	124,124,124,124	0
87	MG	5	4392	1/1	0.17	0.25	134,134,134,134	0
87	MG	5	4186	1/1	0.20	0.43	123,123,123,123	0
86	OHX	8	219	7/7	0.22	0.36	92,92,92,92	7
87	MG	2	2148	1/1	0.25	0.27	130,130,130,130	0
87	MG	1	4306	1/1	0.26	0.16	126,126,126,126	0
87	MG	2	2147	1/1	0.29	0.27	100,100,100,100	0
86	OHX	5	3806	7/7	0.31	0.47	76,76,76,76	7
87	MG	1	4465	1/1	0.33	0.33	109,109,109,109	0
87	MG	2	2204	1/1	0.35	0.31	106,106,106,106	0
86	OHX	m1	201	7/7	0.36	0.36	73,73,73,73	7
86	OHX	5	3720	7/7	0.37	0.43	73,73,73,73	7
86	OHX	5	3739	7/7	0.37	0.41	72,72,72,72	7
87	MG	2	2224	1/1	0.38	0.39	99,99,99,99	0
86	OHX	6	2068	7/7	0.39	0.44	83,83,83,83	7
86	OHX	M0	303	7/7	0.39	0.40	96,96,96,96	7
87	MG	1	4153	1/1	0.40	0.33	101,101,101,101	0
87	MG	2	2162	1/1	0.41	0.60	85,85,85,85	0
87	MG	1	4367	1/1	0.44	0.39	92,92,92,92	0
87	MG	2	2157	1/1	0.44	0.34	103,103,103,103	0
87	MG	2	2156	1/1	0.46	0.44	86,86,86,86	0
87	MG	5	4138	1/1	0.46	0.25	100,100,100,100	0
87	MG	6	2305	1/1	0.47	0.43	98,98,98,98	0
87	MG	p0	301	1/1	0.47	0.33	93,93,93,93	0
87	MG	1	4486	1/1	0.48	0.17	53,53,53,53	0
87	MG	E1	502	1/1	0.48	0.48	125,125,125,125	0
87	MG	6	2333	1/1	0.49	0.23	59,59,59,59	1
87	MG	5	4569	1/1	0.49	0.15	117,117,117,117	0
87	MG	d5	201	1/1	0.49	0.26	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2072	7/7	0.50	0.33	104,104,104,104	7
87	MG	1	4318	1/1	0.50	0.27	115,115,115,115	0
87	MG	6	2169	1/1	0.51	0.30	85,85,85,85	0
87	MG	6	2262	1/1	0.51	0.39	114,114,114,114	0
86	OHX	6	2064	7/7	0.51	0.51	68,68,68,68	7
86	OHX	6	2089	7/7	0.52	0.48	74,74,74,74	7
87	MG	2	2212	1/1	0.52	0.32	86,86,86,86	0
86	OHX	2	2079	7/7	0.53	0.27	103,103,103,103	7
87	MG	2	2137	1/1	0.53	0.27	126,126,126,126	0
87	MG	2	2252	1/1	0.53	0.15	126,126,126,126	0
86	OHX	6	2093	7/7	0.53	0.32	83,83,83,83	7
87	MG	1	4054	1/1	0.53	0.24	105,105,105,105	0
87	MG	M1	201	1/1	0.54	0.13	73,73,73,73	0
87	MG	5	4317	1/1	0.54	0.20	102,102,102,102	0
87	MG	2	2211	1/1	0.54	0.31	106,106,106,106	0
87	MG	5	3911	1/1	0.54	0.25	53,53,53,53	1
86	OHX	5	3762	7/7	0.54	0.46	53,53,53,53	7
86	OHX	5	3767	7/7	0.55	0.66	39,39,39,39	7
87	MG	1	4209	1/1	0.55	0.23	67,67,67,67	1
87	MG	2	2150	1/1	0.56	0.18	74,74,74,74	0
87	MG	O4	201	1/1	0.56	0.35	77,77,77,77	0
87	MG	1	4214	1/1	0.56	0.16	36,36,36,36	0
86	OHX	5	3769	7/7	0.56	0.35	78,78,78,78	7
87	MG	5	3889	1/1	0.57	0.18	111,111,111,111	0
86	OHX	5	3658	7/7	0.57	0.49	51,51,51,51	7
87	MG	2	2101	1/1	0.57	0.38	73,73,73,73	0
86	OHX	5	3785	7/7	0.57	0.65	53,53,53,53	7
87	MG	1	4087	1/1	0.58	0.34	101,101,101,101	0
87	MG	1	4331	1/1	0.58	0.23	86,86,86,86	0
87	MG	6	2164	1/1	0.58	0.35	87,87,87,87	0
87	MG	2	2169	1/1	0.59	0.18	101,101,101,101	0
87	MG	6	2191	1/1	0.59	0.29	86,86,86,86	0
87	MG	1	3859	1/1	0.59	0.31	89,89,89,89	0
86	OHX	2	2060	7/7	0.59	0.27	98,98,98,98	7
87	MG	6	2154	1/1	0.60	0.28	76,76,76,76	0
87	MG	2	2090	1/1	0.60	0.28	83,83,83,83	0
86	OHX	5	3800	7/7	0.60	0.33	87,87,87,87	7
87	MG	5	4359	1/1	0.60	0.31	73,73,73,73	0
87	MG	2	2191	1/1	0.60	0.37	99,99,99,99	0
87	MG	5	4485	1/1	0.60	0.31	95,95,95,95	0
87	MG	2	2214	1/1	0.60	0.19	78,78,78,78	0
86	OHX	6	2087	7/7	0.60	0.50	71,71,71,71	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3741	7/7	0.61	0.62	53,53,53,53	7
87	MG	1	4490	1/1	0.61	0.32	100,100,100,100	0
86	OHX	5	3730	7/7	0.61	0.63	42,42,42,42	7
87	MG	6	2302	1/1	0.61	0.29	106,106,106,106	0
87	MG	D9	103	1/1	0.61	0.24	94,94,94,94	0
87	MG	6	2108	1/1	0.61	0.27	98,98,98,98	0
87	MG	2	2119	1/1	0.61	0.34	92,92,92,92	0
87	MG	1	3819	1/1	0.61	0.35	106,106,106,106	0
86	OHX	2	2029	7/7	0.61	0.35	95,95,95,95	7
88	ZN	d7	101	1/1	0.61	0.16	135,135,135,135	0
86	OHX	1	3775	7/7	0.62	0.33	84,84,84,84	7
87	MG	2	2250	1/1	0.62	0.16	79,79,79,79	0
87	MG	d9	104	1/1	0.62	0.25	109,109,109,109	0
87	MG	5	3886	1/1	0.62	0.27	97,97,97,97	0
86	OHX	2	2030	7/7	0.62	0.21	112,112,112,112	7
87	MG	1	4013	1/1	0.63	0.39	47,47,47,47	0
87	MG	2	2142	1/1	0.63	0.40	61,61,61,61	0
86	OHX	6	2095	7/7	0.63	0.48	73,73,73,73	7
86	OHX	5	3776	7/7	0.63	0.36	80,80,80,80	7
87	MG	2	2149	1/1	0.63	0.30	92,92,92,92	0
86	OHX	5	3782	7/7	0.63	0.52	45,45,45,45	7
86	OHX	5	3756	7/7	0.64	0.76	42,42,42,42	7
87	MG	1	4481	1/1	0.64	0.12	82,82,82,82	0
87	MG	5	4345	1/1	0.64	0.10	95,95,95,95	0
86	OHX	6	2054	7/7	0.64	0.41	65,65,65,65	7
87	MG	2	2216	1/1	0.64	0.28	69,69,69,69	0
86	OHX	1	3660	7/7	0.64	0.16	127,127,127,127	7
87	MG	2	2164	1/1	0.64	0.26	122,122,122,122	0
86	OHX	1	3737	7/7	0.64	0.50	42,42,42,42	7
87	MG	6	2153	1/1	0.64	0.34	44,44,44,44	0
87	MG	6	2203	1/1	0.65	0.21	68,68,68,68	0
87	MG	5	4135	1/1	0.65	0.32	69,69,69,69	0
87	MG	c9	203	1/1	0.65	0.34	87,87,87,87	0
86	OHX	5	3755	7/7	0.65	0.43	49,49,49,49	7
86	OHX	6	2010	7/7	0.66	0.37	84,84,84,84	7
87	MG	2	2255	1/1	0.66	0.23	88,88,88,88	0
86	OHX	6	2036	7/7	0.66	0.39	48,48,48,48	7
86	OHX	2	2019	7/7	0.66	0.30	105,105,105,105	7
87	MG	2	2217	1/1	0.66	0.28	103,103,103,103	0
87	MG	1	4181	1/1	0.66	0.29	75,75,75,75	0
87	MG	5	4203	1/1	0.66	0.19	36,36,36,36	1
87	MG	5	4298	1/1	0.66	0.16	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	2	2242	1/1	0.67	0.24	85,85,85,85	0
87	MG	1	4506	1/1	0.67	0.21	94,94,94,94	0
87	MG	2	2176	1/1	0.67	0.14	84,84,84,84	0
87	MG	2	2190	1/1	0.67	0.14	78,78,78,78	0
87	MG	2	2105	1/1	0.67	0.38	72,72,72,72	0
88	ZN	D7	101	1/1	0.67	0.19	147,147,147,147	0
86	OHX	1	3796	7/7	0.67	0.34	71,71,71,71	7
87	MG	3	226	1/1	0.68	0.15	65,65,65,65	0
86	OHX	3	212	7/7	0.68	0.24	79,79,79,79	7
86	OHX	1	3684	7/7	0.68	0.34	81,81,81,81	7
87	MG	1	4345	1/1	0.68	0.21	44,44,44,44	1
87	MG	1	4142	1/1	0.68	0.18	45,45,45,45	1
86	OHX	6	2074	7/7	0.68	0.24	108,108,108,108	7
87	MG	2	2154	1/1	0.68	0.28	68,68,68,68	0
86	OHX	6	2081	7/7	0.68	0.34	91,91,91,91	7
86	OHX	O1	201	7/7	0.68	0.33	77,77,77,77	7
87	MG	6	2202	1/1	0.68	0.26	81,81,81,81	0
87	MG	2	2143	1/1	0.68	0.23	91,91,91,91	0
87	MG	5	4129	1/1	0.68	0.34	82,82,82,82	0
86	OHX	5	3783	7/7	0.68	0.35	56,56,56,56	7
86	OHX	1	3802	7/7	0.69	0.37	63,63,63,63	7
87	MG	6	2166	1/1	0.69	0.26	88,88,88,88	0
87	MG	5	3905	1/1	0.69	0.20	71,71,71,71	0
86	OHX	5	3813	7/7	0.69	0.12	173,173,173,173	7
86	OHX	1	3735	7/7	0.69	0.39	71,71,71,71	7
87	MG	1	3900	1/1	0.69	0.25	104,104,104,104	0
86	OHX	5	3798	7/7	0.69	0.39	73,73,73,73	7
86	OHX	1	3703	7/7	0.69	0.28	101,101,101,101	7
87	MG	6	2274	1/1	0.69	0.32	42,42,42,42	1
87	MG	5	4242	1/1	0.69	0.27	44,44,44,44	0
86	OHX	6	2075	7/7	0.70	0.43	54,54,54,54	7
86	OHX	6	2066	7/7	0.70	0.38	70,70,70,70	7
87	MG	4	236	1/1	0.70	0.24	98,98,98,98	0
87	MG	4	240	1/1	0.70	0.16	57,57,57,57	0
87	MG	1	4197	1/1	0.70	0.25	56,56,56,56	0
87	MG	5	3854	1/1	0.70	0.31	72,72,72,72	0
87	MG	1	3916	1/1	0.70	0.25	86,86,86,86	0
86	OHX	6	2096	7/7	0.70	0.32	78,78,78,78	7
87	MG	6	2278	1/1	0.70	0.13	83,83,83,83	0
87	MG	5	4456	1/1	0.70	0.26	100,100,100,100	0
86	OHX	o9	101	7/7	0.70	0.62	52,52,52,52	7
87	MG	5	4071	1/1	0.70	0.44	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4104	1/1	0.70	0.19	45,45,45,45	1
86	OHX	1	3697	7/7	0.70	0.12	169,169,169,169	7
86	OHX	2	2053	7/7	0.70	0.33	80,80,80,80	7
87	MG	Q2	503	1/1	0.71	0.34	62,62,62,62	0
87	MG	2	2098	1/1	0.71	0.28	80,80,80,80	0
87	MG	2	2163	1/1	0.71	0.30	70,70,70,70	0
87	MG	1	4372	1/1	0.71	0.18	76,76,76,76	0
86	OHX	5	3799	7/7	0.71	0.32	72,72,72,72	7
86	OHX	2	2075	7/7	0.71	0.35	87,87,87,87	7
86	OHX	m4	201	7/7	0.71	0.21	101,101,101,101	7
87	MG	6	2184	1/1	0.71	0.17	69,69,69,69	0
86	OHX	6	2028	7/7	0.71	0.46	58,58,58,58	7
87	MG	2	2182	1/1	0.71	0.37	87,87,87,87	0
87	MG	2	2139	1/1	0.71	0.38	70,70,70,70	0
87	MG	2	2140	1/1	0.71	0.48	81,81,81,81	0
87	MG	1	4328	1/1	0.71	0.20	70,70,70,70	0
87	MG	5	4572	1/1	0.71	0.36	69,69,69,69	0
87	MG	8	230	1/1	0.71	0.18	72,72,72,72	0
87	MG	2	2193	1/1	0.71	0.31	71,71,71,71	0
87	MG	5	4121	1/1	0.71	0.21	52,52,52,52	0
86	OHX	5	3768	7/7	0.71	0.43	47,47,47,47	7
86	OHX	1	3683	7/7	0.72	0.41	61,61,61,61	7
86	OHX	5	3808	7/7	0.72	0.29	83,83,83,83	7
87	MG	2	2165	1/1	0.72	0.12	98,98,98,98	0
87	MG	1	4485	1/1	0.72	0.17	63,63,63,63	0
86	OHX	6	2042	7/7	0.72	0.47	54,54,54,54	7
86	OHX	8	218	7/7	0.72	0.40	48,48,48,48	7
86	OHX	5	3792	7/7	0.72	0.53	51,51,51,51	7
87	MG	2	2181	1/1	0.72	0.28	80,80,80,80	0
86	OHX	5	3712	7/7	0.72	0.67	36,36,36,36	7
87	MG	4	237	1/1	0.72	0.18	67,67,67,67	0
87	MG	2	2186	1/1	0.72	0.29	65,65,65,65	0
87	MG	1	4033	1/1	0.72	0.38	73,73,73,73	0
86	OHX	6	2077	7/7	0.72	0.26	85,85,85,85	7
87	MG	6	2295	1/1	0.72	0.27	58,58,58,58	1
86	OHX	n3	202	7/7	0.72	0.43	44,44,44,44	7
86	OHX	1	3772	7/7	0.72	0.42	61,61,61,61	7
89	C	1	3401	20/21	0.72	0.15	54,111,113,113	0
86	OHX	1	3806	7/7	0.73	0.40	54,54,54,54	7
87	MG	2	2124	1/1	0.73	0.29	77,77,77,77	0
86	OHX	1	3756	7/7	0.73	0.43	59,59,59,59	7
86	OHX	5	3681	7/7	0.73	0.40	80,80,80,80	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	2	2225	1/1	0.73	0.44	58,58,58,58	1
87	MG	2	2161	1/1	0.73	0.28	63,63,63,63	0
87	MG	5	4265	1/1	0.73	0.21	61,61,61,61	0
87	MG	6	2117	1/1	0.73	0.34	61,61,61,61	0
87	MG	6	2124	1/1	0.73	0.41	71,71,71,71	0
86	OHX	5	3748	7/7	0.73	0.46	54,54,54,54	7
87	MG	2	2192	1/1	0.73	0.34	64,64,64,64	0
86	OHX	5	3688	7/7	0.73	0.53	37,37,37,37	7
86	OHX	1	3761	7/7	0.73	0.22	117,117,117,117	7
87	MG	1	4178	1/1	0.73	0.14	93,93,93,93	0
86	OHX	1	3754	7/7	0.73	0.17	99,99,99,99	7
87	MG	2	2257	1/1	0.73	0.13	121,121,121,121	0
87	MG	S4	302	1/1	0.73	0.20	87,87,87,87	0
86	OHX	5	3763	7/7	0.73	0.45	56,56,56,56	7
87	MG	2	2116	1/1	0.73	0.27	89,89,89,89	0
87	MG	5	4107	1/1	0.73	0.31	59,59,59,59	0
87	MG	6	2273	1/1	0.73	0.20	80,80,80,80	0
86	OHX	6	2051	7/7	0.74	0.30	82,82,82,82	7
87	MG	6	2301	1/1	0.74	0.20	57,57,57,57	0
87	MG	2	2134	1/1	0.74	0.23	76,76,76,76	0
86	OHX	N8	201	7/7	0.74	0.24	94,94,94,94	7
87	MG	6	2323	1/1	0.74	0.31	70,70,70,70	0
87	MG	6	2326	1/1	0.74	0.15	79,79,79,79	0
86	OHX	6	2060	7/7	0.74	0.42	58,58,58,58	7
86	OHX	6	2063	7/7	0.74	0.36	77,77,77,77	7
87	MG	1	3824	1/1	0.74	0.28	55,55,55,55	0
87	MG	5	4332	1/1	0.74	0.11	106,106,106,106	0
86	OHX	2	2034	7/7	0.74	0.29	86,86,86,86	7
87	MG	1	4492	1/1	0.74	0.25	65,65,65,65	0
87	MG	5	4376	1/1	0.74	0.21	72,72,72,72	0
87	MG	1	4258	1/1	0.74	0.20	77,77,77,77	0
87	MG	5	4423	1/1	0.74	0.18	59,59,59,59	0
86	OHX	1	3695	7/7	0.74	0.39	56,56,56,56	7
86	OHX	1	3811	7/7	0.74	0.25	89,89,89,89	7
87	MG	5	4528	1/1	0.74	0.21	83,83,83,83	1
86	OHX	8	217	7/7	0.74	0.30	82,82,82,82	7
86	OHX	1	3671	7/7	0.74	0.35	85,85,85,85	7
87	MG	2	2254	1/1	0.74	0.12	97,97,97,97	0
87	MG	5	4099	1/1	0.74	0.26	61,61,61,61	0
87	MG	M5	305	1/1	0.74	0.42	69,69,69,69	0
86	OHX	2	2081	7/7	0.74	0.15	120,120,120,120	7
87	MG	1	4103	1/1	0.74	0.42	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2234	1/1	0.75	0.19	79,79,79,79	0
86	OHX	C3	201	7/7	0.75	0.29	99,99,99,99	7
87	MG	2	2244	1/1	0.75	0.20	78,78,78,78	0
86	OHX	5	3674	7/7	0.75	0.43	39,39,39,39	7
87	MG	6	2139	1/1	0.75	0.38	63,63,63,63	0
87	MG	6	2143	1/1	0.75	0.44	86,86,86,86	0
87	MG	1	3856	1/1	0.75	0.40	63,63,63,63	0
86	OHX	2	2084	7/7	0.75	0.13	183,183,183,183	7
86	OHX	1	3704	7/7	0.75	0.40	55,55,55,55	7
86	OHX	6	2094	7/7	0.75	0.22	102,102,102,102	7
86	OHX	1	3729	7/7	0.75	0.39	57,57,57,57	7
87	MG	6	2178	1/1	0.75	0.23	54,54,54,54	0
87	MG	2	2125	1/1	0.75	0.27	85,85,85,85	0
87	MG	5	4162	1/1	0.75	0.31	49,49,49,49	0
87	MG	l2	305	1/1	0.75	0.11	71,71,71,71	0
87	MG	N6	201	1/1	0.75	0.23	63,63,63,63	0
86	OHX	5	3812	7/7	0.75	0.61	54,54,54,54	7
86	OHX	1	3731	7/7	0.75	0.20	100,100,100,100	7
87	MG	6	2207	1/1	0.75	0.20	93,93,93,93	0
87	MG	2	2178	1/1	0.76	0.25	79,79,79,79	0
86	OHX	2	2058	7/7	0.76	0.10	193,193,193,193	7
87	MG	6	2156	1/1	0.76	0.58	66,66,66,66	0
87	MG	2	2117	1/1	0.76	0.21	74,74,74,74	0
86	OHX	5	3758	7/7	0.76	0.38	42,42,42,42	7
87	MG	5	4255	1/1	0.76	0.17	37,37,37,37	0
86	OHX	5	3759	7/7	0.76	0.18	110,110,110,110	7
86	OHX	1	3803	7/7	0.76	0.51	48,48,48,48	7
87	MG	c8	205	1/1	0.76	0.22	93,93,93,93	0
86	OHX	1	3769	7/7	0.76	0.60	49,49,49,49	7
87	MG	L8	301	1/1	0.76	0.13	82,82,82,82	0
86	OHX	1	3742	7/7	0.76	0.55	41,41,41,41	7
87	MG	sM	201	1/1	0.76	0.20	48,48,48,48	0
87	MG	1	4047	1/1	0.76	0.18	83,83,83,83	0
86	OHX	2	2066	7/7	0.76	0.39	80,80,80,80	7
87	MG	6	2222	1/1	0.76	0.20	81,81,81,81	0
87	MG	1	4067	1/1	0.76	0.34	71,71,71,71	0
87	MG	2	2203	1/1	0.76	0.12	85,85,85,85	0
87	MG	5	3913	1/1	0.76	0.17	55,55,55,55	0
87	MG	6	2272	1/1	0.76	0.29	98,98,98,98	0
87	MG	5	4576	1/1	0.76	0.13	53,53,53,53	0
86	OHX	5	3745	7/7	0.76	0.64	37,37,37,37	7
87	MG	2	2093	1/1	0.76	0.40	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	l5	305	1/1	0.76	0.15	62,62,62,62	0
86	OHX	1	3675	7/7	0.76	0.57	49,49,49,49	7
86	OHX	6	2049	7/7	0.76	0.33	70,70,70,70	7
87	MG	6	2283	1/1	0.76	0.17	69,69,69,69	1
86	OHX	7	212	7/7	0.76	0.45	61,61,61,61	7
90	8AN	1	3403	22/23	0.76	0.20	48,103,107,107	0
86	OHX	2	2063	7/7	0.77	0.34	81,81,81,81	7
87	MG	2	2251	1/1	0.77	0.15	59,59,59,59	1
86	OHX	1	3795	7/7	0.77	0.29	79,79,79,79	7
87	MG	6	2304	1/1	0.77	0.33	52,52,52,52	1
87	MG	1	4093	1/1	0.77	0.39	43,43,43,43	0
86	OHX	5	3703	7/7	0.77	0.21	86,86,86,86	7
86	OHX	19	201	7/7	0.77	0.33	62,62,62,62	7
87	MG	1	4149	1/1	0.77	0.18	82,82,82,82	0
86	OHX	6	2052	7/7	0.77	0.13	127,127,127,127	7
87	MG	5	4325	1/1	0.77	0.14	74,74,74,74	0
87	MG	s4	302	1/1	0.77	0.28	55,55,55,55	0
87	MG	1	4176	1/1	0.77	0.14	72,72,72,72	0
86	OHX	6	2012	7/7	0.77	0.28	64,64,64,64	7
86	OHX	2	2086	7/7	0.77	0.19	105,105,105,105	7
87	MG	5	4389	1/1	0.77	0.18	63,63,63,63	0
86	OHX	1	3745	7/7	0.77	0.33	72,72,72,72	7
86	OHX	5	3815	7/7	0.77	0.39	66,66,66,66	7
86	OHX	5	3818	7/7	0.77	0.43	63,63,63,63	7
87	MG	6	2212	1/1	0.77	0.10	84,84,84,84	0
87	MG	6	2216	1/1	0.77	0.19	86,86,86,86	0
87	MG	2	2094	1/1	0.77	0.32	62,62,62,62	0
86	OHX	2	2078	7/7	0.77	0.25	102,102,102,102	7
87	MG	6	2258	1/1	0.77	0.26	84,84,84,84	0
87	MG	5	4067	1/1	0.77	0.14	54,54,54,54	0
87	MG	M9	204	1/1	0.77	0.11	70,70,70,70	0
87	MG	l2	306	1/1	0.77	0.37	53,53,53,53	1
87	MG	l5	304	1/1	0.77	0.20	61,61,61,61	0
87	MG	2	2099	1/1	0.77	0.32	63,63,63,63	0
86	OHX	7	213	7/7	0.77	0.25	56,56,56,56	7
87	MG	1	3925	1/1	0.77	0.42	49,49,49,49	0
87	MG	2	2104	1/1	0.77	0.30	70,70,70,70	0
86	OHX	8	215	7/7	0.77	0.44	48,48,48,48	7
87	MG	2	2249	1/1	0.77	0.38	97,97,97,97	0
87	MG	2	2185	1/1	0.78	0.39	74,74,74,74	0
87	MG	5	4137	1/1	0.78	0.33	63,63,63,63	0
86	OHX	5	3696	7/7	0.78	0.31	49,49,49,49	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4155	1/1	0.78	0.25	80,80,80,80	0
87	MG	2	2188	1/1	0.78	0.10	84,84,84,84	0
87	MG	5	4164	1/1	0.78	0.13	83,83,83,83	0
87	MG	1	4360	1/1	0.78	0.35	55,55,55,55	1
86	OHX	6	2085	7/7	0.78	0.13	128,128,128,128	7
86	OHX	6	2062	7/7	0.78	0.30	74,74,74,74	7
86	OHX	5	3719	7/7	0.78	0.26	64,64,64,64	7
87	MG	1	4467	1/1	0.78	0.25	58,58,58,58	0
87	MG	2	2111	1/1	0.78	0.35	63,63,63,63	0
87	MG	5	4308	1/1	0.78	0.22	58,58,58,58	0
87	MG	1	4126	1/1	0.78	0.11	66,66,66,66	0
87	MG	6	2175	1/1	0.78	0.21	56,56,56,56	0
87	MG	c6	201	1/1	0.78	0.24	97,97,97,97	0
86	OHX	4	214	7/7	0.78	0.51	46,46,46,46	7
87	MG	c9	201	1/1	0.78	0.15	78,78,78,78	0
86	OHX	1	3770	7/7	0.78	0.17	141,141,141,141	7
86	OHX	1	3706	7/7	0.78	0.34	60,60,60,60	7
86	OHX	1	3728	7/7	0.78	0.52	37,37,37,37	7
86	OHX	6	1993	7/7	0.78	0.26	78,78,78,78	7
87	MG	3	229	1/1	0.78	0.48	52,52,52,52	1
86	OHX	5	3648	7/7	0.78	0.28	69,69,69,69	7
87	MG	5	4494	1/1	0.78	0.19	69,69,69,69	0
87	MG	1	4184	1/1	0.78	0.18	63,63,63,63	0
86	OHX	1	3674	7/7	0.78	0.43	64,64,64,64	7
86	OHX	6	2076	7/7	0.78	0.27	74,74,74,74	7
87	MG	6	2256	1/1	0.78	0.27	73,73,73,73	0
87	MG	5	3921	1/1	0.78	0.12	51,51,51,51	0
87	MG	5	3982	1/1	0.78	0.34	57,57,57,57	0
87	MG	5	4058	1/1	0.78	0.19	37,37,37,37	0
86	OHX	5	3676	7/7	0.78	0.37	42,42,42,42	7
86	OHX	1	3669	7/7	0.78	0.56	54,54,54,54	7
87	MG	1	4282	1/1	0.78	0.14	47,47,47,47	1
86	OHX	5	3686	7/7	0.78	0.36	56,56,56,56	7
87	MG	2	2232	1/1	0.78	0.15	90,90,90,90	0
87	MG	1	3939	1/1	0.78	0.38	37,37,37,37	0
86	OHX	6	2023	7/7	0.78	0.26	80,80,80,80	7
86	OHX	1	3740	7/7	0.79	0.27	70,70,70,70	7
87	MG	5	4252	1/1	0.79	0.23	58,58,58,58	0
86	OHX	M9	203	7/7	0.79	0.18	78,78,78,78	7
87	MG	2	2102	1/1	0.79	0.29	84,84,84,84	0
86	OHX	6	2097	7/7	0.79	0.40	70,70,70,70	7
86	OHX	5	3573	7/7	0.79	0.40	64,64,64,64	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3642	7/7	0.79	0.50	39,39,39,39	7
86	OHX	1	3730	7/7	0.79	0.36	59,59,59,59	7
87	MG	5	3860	1/1	0.79	0.25	39,39,39,39	0
87	MG	6	2255	1/1	0.79	0.33	54,54,54,54	0
87	MG	5	4349	1/1	0.79	0.11	41,41,41,41	1
86	OHX	5	3655	7/7	0.79	0.31	47,47,47,47	7
86	OHX	5	3797	7/7	0.79	0.51	42,42,42,42	7
87	MG	1	4349	1/1	0.79	0.10	69,69,69,69	0
87	MG	6	2268	1/1	0.79	0.39	84,84,84,84	0
86	OHX	2	1989	7/7	0.79	0.24	104,104,104,104	7
87	MG	2	2209	1/1	0.79	0.24	71,71,71,71	0
86	OHX	2	2041	7/7	0.79	0.34	83,83,83,83	7
87	MG	6	2129	1/1	0.79	0.29	59,59,59,59	0
87	MG	5	4513	1/1	0.79	0.12	97,97,97,97	0
87	MG	1	4435	1/1	0.79	0.24	41,41,41,41	1
87	MG	5	4541	1/1	0.79	0.10	56,56,56,56	0
86	OHX	6	2056	7/7	0.79	0.14	97,97,97,97	7
86	OHX	2	2049	7/7	0.79	0.29	84,84,84,84	7
87	MG	1	4468	1/1	0.79	0.11	70,70,70,70	1
86	OHX	1	3808	7/7	0.79	0.41	60,60,60,60	7
87	MG	8	233	1/1	0.79	0.19	88,88,88,88	0
86	OHX	1	3783	7/7	0.79	0.48	48,48,48,48	7
87	MG	1	3842	1/1	0.79	0.32	45,45,45,45	0
87	MG	2	2218	1/1	0.79	0.15	82,82,82,82	0
87	MG	6	2325	1/1	0.79	0.19	59,59,59,59	0
87	MG	6	2171	1/1	0.79	0.17	79,79,79,79	0
86	OHX	1	3787	7/7	0.79	0.36	69,69,69,69	7
87	MG	1	4198	1/1	0.79	0.39	47,47,47,47	0
86	OHX	1	3789	7/7	0.79	0.39	56,56,56,56	7
87	MG	2	2146	1/1	0.79	0.27	86,86,86,86	0
86	OHX	1	3764	7/7	0.80	0.49	49,49,49,49	7
86	OHX	1	3721	7/7	0.80	0.25	96,96,96,96	7
86	OHX	1	3722	7/7	0.80	0.34	69,69,69,69	7
86	OHX	1	3771	7/7	0.80	0.45	52,52,52,52	7
86	OHX	1	3812	7/7	0.80	0.26	88,88,88,88	7
87	MG	4	221	1/1	0.80	0.36	65,65,65,65	0
86	OHX	c3	201	7/7	0.80	0.28	79,79,79,79	7
87	MG	1	4131	1/1	0.80	0.25	63,63,63,63	0
86	OHX	1	3814	7/7	0.80	0.14	149,149,149,149	7
86	OHX	m0	302	7/7	0.80	0.53	45,45,45,45	7
87	MG	6	2287	1/1	0.80	0.26	62,62,62,62	0
87	MG	2	2155	1/1	0.80	0.32	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2300	1/1	0.80	0.17	82,82,82,82	0
86	OHX	5	3636	7/7	0.80	0.49	44,44,44,44	7
86	OHX	1	3738	7/7	0.80	0.29	68,68,68,68	7
87	MG	5	4274	1/1	0.80	0.12	46,46,46,46	0
86	OHX	1	3739	7/7	0.80	0.45	52,52,52,52	7
86	OHX	4	216	7/7	0.80	0.29	73,73,73,73	7
87	MG	5	4310	1/1	0.80	0.08	50,50,50,50	0
87	MG	6	2306	1/1	0.80	0.17	79,79,79,79	0
87	MG	6	2320	1/1	0.80	0.13	62,62,62,62	0
86	OHX	1	3725	7/7	0.80	0.29	68,68,68,68	7
86	OHX	6	2065	7/7	0.80	0.14	129,129,129,129	7
86	OHX	1	3785	7/7	0.80	0.68	47,47,47,47	7
87	MG	2	2096	1/1	0.80	0.41	61,61,61,61	0
86	OHX	2	2045	7/7	0.80	0.30	73,73,73,73	7
87	MG	1	4262	1/1	0.80	0.15	74,74,74,74	0
86	OHX	5	3784	7/7	0.80	0.57	55,55,55,55	7
87	MG	S4	301	1/1	0.80	0.30	76,76,76,76	0
86	OHX	2	2080	7/7	0.80	0.60	66,66,66,66	7
86	OHX	5	3786	7/7	0.80	0.44	42,42,42,42	7
86	OHX	1	3790	7/7	0.80	0.24	69,69,69,69	7
86	OHX	5	3695	7/7	0.80	0.60	55,55,55,55	7
86	OHX	1	3793	7/7	0.80	0.54	46,46,46,46	7
86	OHX	1	3707	7/7	0.80	0.21	106,106,106,106	7
86	OHX	5	3704	7/7	0.80	0.29	67,67,67,67	7
86	OHX	1	3713	7/7	0.80	0.41	58,58,58,58	7
86	OHX	6	2024	7/7	0.80	0.24	86,86,86,86	7
86	OHX	5	3811	7/7	0.80	0.43	44,44,44,44	7
87	MG	2	2128	1/1	0.80	0.46	60,60,60,60	0
87	MG	1	3938	1/1	0.80	0.40	36,36,36,36	0
86	OHX	6	2086	7/7	0.80	0.15	147,147,147,147	7
87	MG	5	3981	1/1	0.80	0.32	50,50,50,50	0
86	OHX	5	3726	7/7	0.80	0.32	62,62,62,62	7
87	MG	6	2214	1/1	0.80	0.09	79,79,79,79	0
87	MG	1	4476	1/1	0.80	0.16	81,81,81,81	0
86	OHX	1	3798	7/7	0.80	0.25	93,93,93,93	7
87	MG	1	4046	1/1	0.80	0.19	59,59,59,59	0
86	OHX	1	3733	7/7	0.80	0.70	46,46,46,46	7
86	OHX	1	3774	7/7	0.81	0.35	53,53,53,53	7
86	OHX	5	3746	7/7	0.81	0.12	149,149,149,149	7
87	MG	1	4404	1/1	0.81	0.24	57,57,57,57	0
87	MG	1	4434	1/1	0.81	0.29	38,38,38,38	1
86	OHX	5	3770	7/7	0.81	0.26	96,96,96,96	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2155	1/1	0.81	0.22	72,72,72,72	0
87	MG	1	3821	1/1	0.81	0.22	55,55,55,55	0
86	OHX	5	3705	7/7	0.81	0.43	46,46,46,46	7
87	MG	1	3838	1/1	0.81	0.22	59,59,59,59	0
87	MG	1	4469	1/1	0.81	0.12	55,55,55,55	0
87	MG	1	4173	1/1	0.81	0.40	52,52,52,52	0
86	OHX	6	2073	7/7	0.81	0.31	64,64,64,64	7
86	OHX	m5	502	7/7	0.81	0.41	78,78,78,78	7
87	MG	5	4289	1/1	0.81	0.41	57,57,57,57	1
86	OHX	1	3755	7/7	0.81	0.30	79,79,79,79	7
87	MG	1	3879	1/1	0.81	0.24	61,61,61,61	0
87	MG	c8	204	1/1	0.81	0.21	81,81,81,81	0
87	MG	1	3899	1/1	0.81	0.17	40,40,40,40	0
87	MG	2	2189	1/1	0.81	0.28	94,94,94,94	0
87	MG	3	214	1/1	0.81	0.21	46,46,46,46	0
87	MG	6	2210	1/1	0.81	0.33	79,79,79,79	0
87	MG	5	4346	1/1	0.81	0.36	68,68,68,68	1
87	MG	1	4207	1/1	0.81	0.16	58,58,58,58	0
87	MG	1	3903	1/1	0.81	0.28	51,51,51,51	0
86	OHX	1	3663	7/7	0.81	0.47	48,48,48,48	7
87	MG	1	4244	1/1	0.81	0.14	72,72,72,72	0
87	MG	6	2229	1/1	0.81	0.24	45,45,45,45	0
87	MG	5	4394	1/1	0.81	0.34	62,62,62,62	0
87	MG	1	3923	1/1	0.81	0.31	75,75,75,75	0
87	MG	5	3895	1/1	0.81	0.23	59,59,59,59	0
87	MG	6	2251	1/1	0.81	0.31	74,74,74,74	0
86	OHX	3	209	7/7	0.81	0.32	82,82,82,82	7
87	MG	2	2159	1/1	0.81	0.24	75,75,75,75	0
86	OHX	5	3760	7/7	0.81	0.21	89,89,89,89	7
87	MG	5	3946	1/1	0.81	0.34	33,33,33,33	0
87	MG	5	3965	1/1	0.81	0.17	55,55,55,55	0
87	MG	6	2260	1/1	0.81	0.21	55,55,55,55	0
86	OHX	5	3789	7/7	0.81	0.18	90,90,90,90	7
87	MG	2	2095	1/1	0.81	0.26	63,63,63,63	0
86	OHX	5	3790	7/7	0.81	0.59	40,40,40,40	7
86	OHX	2	2077	7/7	0.81	0.17	139,139,139,139	7
87	MG	5	4088	1/1	0.81	0.22	42,42,42,42	1
87	MG	5	4098	1/1	0.81	0.24	50,50,50,50	0
87	MG	O7	108	1/1	0.81	0.34	69,69,69,69	0
87	MG	l5	306	1/1	0.81	0.11	54,54,54,54	0
86	OHX	6	2079	7/7	0.81	0.31	60,60,60,60	7
87	MG	S1	301	1/1	0.81	0.16	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2083	7/7	0.81	0.18	106,106,106,106	7
87	MG	2	2175	1/1	0.81	0.30	87,87,87,87	0
87	MG	5	4134	1/1	0.81	0.10	37,37,37,37	0
87	MG	2	2145	1/1	0.82	0.42	97,97,97,97	0
86	OHX	5	3644	7/7	0.82	0.35	47,47,47,47	7
86	OHX	6	2044	7/7	0.82	0.24	78,78,78,78	7
86	OHX	1	3766	7/7	0.82	0.54	59,59,59,59	7
86	OHX	6	2078	7/7	0.82	0.23	93,93,93,93	7
86	OHX	2	2039	7/7	0.82	0.23	103,103,103,103	7
87	MG	1	3857	1/1	0.82	0.18	51,51,51,51	0
86	OHX	6	2080	7/7	0.82	0.18	126,126,126,126	7
87	MG	1	4229	1/1	0.82	0.22	64,64,64,64	0
87	MG	1	3872	1/1	0.82	0.31	54,54,54,54	0
86	OHX	6	1989	7/7	0.82	0.29	84,84,84,84	7
87	MG	1	3889	1/1	0.82	0.28	37,37,37,37	0
87	MG	1	3894	1/1	0.82	0.29	53,53,53,53	0
87	MG	6	2123	1/1	0.82	0.27	67,67,67,67	0
86	OHX	1	3748	7/7	0.82	0.28	89,89,89,89	7
86	OHX	6	2003	7/7	0.82	0.33	61,61,61,61	7
87	MG	6	2138	1/1	0.82	0.13	73,73,73,73	0
86	OHX	5	3692	7/7	0.82	0.52	38,38,38,38	7
86	OHX	6	2059	7/7	0.82	0.20	104,104,104,104	7
86	OHX	6	2007	7/7	0.82	0.28	62,62,62,62	7
87	MG	2	2229	1/1	0.82	0.19	84,84,84,84	0
86	OHX	6	2092	7/7	0.82	0.20	104,104,104,104	7
87	MG	s6	302	1/1	0.82	0.31	75,75,75,75	0
87	MG	5	4327	1/1	0.82	0.38	82,82,82,82	0
87	MG	2	2114	1/1	0.82	0.55	79,79,79,79	0
87	MG	1	4359	1/1	0.82	0.16	51,51,51,51	1
86	OHX	1	3749	7/7	0.82	0.37	62,62,62,62	7
87	MG	1	4024	1/1	0.82	0.27	37,37,37,37	0
87	MG	1	4032	1/1	0.82	0.29	49,49,49,49	0
86	OHX	2	2046	7/7	0.82	0.15	114,114,114,114	7
86	OHX	6	2018	7/7	0.82	0.42	54,54,54,54	7
86	OHX	1	3665	7/7	0.82	0.38	59,59,59,59	7
86	OHX	8	220	7/7	0.82	0.27	77,77,77,77	7
87	MG	2	2126	1/1	0.82	0.40	69,69,69,69	0
87	MG	1	4076	1/1	0.82	0.28	76,76,76,76	0
86	OHX	2	2055	7/7	0.82	0.34	72,72,72,72	7
87	MG	2	2253	1/1	0.82	0.26	76,76,76,76	0
87	MG	1	4477	1/1	0.82	0.14	47,47,47,47	0
87	MG	5	4516	1/1	0.82	0.41	62,62,62,62	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3908	1/1	0.82	0.31	76,76,76,76	0
87	MG	5	3910	1/1	0.82	0.35	88,88,88,88	0
86	OHX	1	3782	7/7	0.82	0.36	55,55,55,55	7
87	MG	2	2135	1/1	0.82	0.18	72,72,72,72	0
87	MG	2	2136	1/1	0.82	0.27	71,71,71,71	0
86	OHX	5	3727	7/7	0.82	0.46	53,53,53,53	7
87	MG	6	2233	1/1	0.82	0.36	83,83,83,83	0
87	MG	5	3976	1/1	0.82	0.25	41,41,41,41	0
87	MG	1	4148	1/1	0.82	0.12	69,69,69,69	0
87	MG	6	2240	1/1	0.82	0.18	74,74,74,74	0
87	MG	6	2242	1/1	0.82	0.37	55,55,55,55	1
86	OHX	6	2034	7/7	0.82	0.10	134,134,134,134	7
87	MG	n0	201	1/1	0.82	0.38	49,49,49,49	1
86	OHX	S8	301	7/7	0.82	0.19	108,108,108,108	7
87	MG	3	220	1/1	0.82	0.23	55,55,55,55	0
87	MG	1	4172	1/1	0.82	0.27	53,53,53,53	0
86	OHX	m9	201	7/7	0.82	0.22	70,70,70,70	7
86	OHX	2	2065	7/7	0.82	0.20	110,110,110,110	7
90	8AN	5	3403	22/23	0.82	0.18	42,97,101,102	0
87	MG	4	241	1/1	0.83	0.23	53,53,53,53	0
87	MG	4	245	1/1	0.83	0.14	95,95,95,95	0
87	MG	5	4110	1/1	0.83	0.27	50,50,50,50	0
87	MG	1	3921	1/1	0.83	0.34	37,37,37,37	0
87	MG	2	2245	1/1	0.83	0.17	71,71,71,71	0
87	MG	1	4259	1/1	0.83	0.23	61,61,61,61	0
87	MG	M7	211	1/1	0.83	0.18	75,75,75,75	0
86	OHX	5	3672	7/7	0.83	0.29	71,71,71,71	7
87	MG	N3	202	1/1	0.83	0.16	67,67,67,67	0
87	MG	5	4140	1/1	0.83	0.23	82,82,82,82	0
87	MG	5	4154	1/1	0.83	0.18	44,44,44,44	0
86	OHX	2	2069	7/7	0.83	0.28	78,78,78,78	7
86	OHX	1	3752	7/7	0.83	0.10	180,180,180,180	7
87	MG	1	3959	1/1	0.83	0.23	55,55,55,55	0
87	MG	5	4178	1/1	0.83	0.19	38,38,38,38	1
87	MG	5	4185	1/1	0.83	0.14	50,50,50,50	0
86	OHX	5	3750	7/7	0.83	0.12	131,131,131,131	7
87	MG	6	2102	1/1	0.83	0.15	81,81,81,81	0
87	MG	5	4211	1/1	0.83	0.20	46,46,46,46	0
86	OHX	5	3751	7/7	0.83	0.34	61,61,61,61	7
86	OHX	4	215	7/7	0.83	0.27	74,74,74,74	7
86	OHX	2	2027	7/7	0.83	0.18	111,111,111,111	7
87	MG	5	4261	1/1	0.83	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3810	7/7	0.83	0.31	63,63,63,63	7
86	OHX	2	2052	7/7	0.83	0.10	189,189,189,189	7
87	MG	1	4356	1/1	0.83	0.11	88,88,88,88	0
86	OHX	1	3604	7/7	0.83	0.33	62,62,62,62	7
86	OHX	6	2070	7/7	0.83	0.28	71,71,71,71	7
86	OHX	1	3777	7/7	0.83	0.30	68,68,68,68	7
87	MG	5	4311	1/1	0.83	0.17	37,37,37,37	1
86	OHX	1	3778	7/7	0.83	0.36	56,56,56,56	7
87	MG	5	4322	1/1	0.83	0.09	62,62,62,62	0
86	OHX	1	3781	7/7	0.83	0.23	63,63,63,63	7
86	OHX	1	3759	7/7	0.83	0.34	45,45,45,45	7
87	MG	6	2161	1/1	0.83	0.29	59,59,59,59	0
86	OHX	5	3614	7/7	0.83	0.38	60,60,60,60	7
87	MG	1	4448	1/1	0.83	0.47	37,37,37,37	1
87	MG	2	2158	1/1	0.83	0.29	68,68,68,68	0
86	OHX	5	3715	7/7	0.83	0.31	69,69,69,69	7
87	MG	1	4147	1/1	0.83	0.24	48,48,48,48	0
87	MG	6	2176	1/1	0.83	0.15	73,73,73,73	0
87	MG	1	3839	1/1	0.83	0.28	46,46,46,46	0
86	OHX	5	3633	7/7	0.83	0.34	43,43,43,43	7
87	MG	5	4413	1/1	0.83	0.08	72,72,72,72	0
87	MG	5	4418	1/1	0.83	0.23	64,64,64,64	0
86	OHX	1	3606	7/7	0.83	0.27	68,68,68,68	7
87	MG	6	2192	1/1	0.83	0.34	75,75,75,75	0
87	MG	2	2122	1/1	0.83	0.41	68,68,68,68	0
87	MG	2	2219	1/1	0.83	0.23	62,62,62,62	0
87	MG	6	2205	1/1	0.83	0.21	84,84,84,84	0
87	MG	1	3868	1/1	0.83	0.23	70,70,70,70	0
87	MG	1	3870	1/1	0.83	0.25	34,34,34,34	0
86	OHX	6	2053	7/7	0.83	0.22	85,85,85,85	7
87	MG	1	4503	1/1	0.83	0.15	47,47,47,47	0
86	OHX	2	2047	7/7	0.83	0.20	106,106,106,106	7
87	MG	5	3935	1/1	0.83	0.24	54,54,54,54	0
87	MG	6	2217	1/1	0.83	0.11	66,66,66,66	0
87	MG	5	3947	1/1	0.83	0.25	43,43,43,43	0
87	MG	2	2228	1/1	0.83	0.26	56,56,56,56	0
87	MG	5	3971	1/1	0.83	0.31	27,27,27,27	0
87	MG	2	2168	1/1	0.83	0.45	68,68,68,68	0
86	OHX	1	3710	7/7	0.83	0.40	55,55,55,55	7
86	OHX	2	2067	7/7	0.83	0.27	92,92,92,92	7
87	MG	3	230	1/1	0.83	0.22	58,58,58,58	0
87	MG	5	4064	1/1	0.83	0.10	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3740	7/7	0.83	0.33	62,62,62,62	7
87	MG	4	227	1/1	0.83	0.20	58,58,58,58	0
87	MG	1	4224	1/1	0.83	0.19	74,74,74,74	0
87	MG	1	4226	1/1	0.83	0.21	72,72,72,72	0
86	OHX	6	2015	7/7	0.83	0.39	65,65,65,65	7
86	OHX	2	2018	7/7	0.84	0.22	102,102,102,102	7
86	OHX	6	2048	7/7	0.84	0.44	51,51,51,51	7
86	OHX	5	3744	7/7	0.84	0.34	56,56,56,56	7
86	OHX	2	2061	7/7	0.84	0.26	78,78,78,78	7
87	MG	2	2100	1/1	0.84	0.35	66,66,66,66	0
86	OHX	1	3813	7/7	0.84	0.57	60,60,60,60	7
86	OHX	2	2070	7/7	0.84	0.37	78,78,78,78	7
86	OHX	6	2008	7/7	0.84	0.25	82,82,82,82	7
86	OHX	1	3681	7/7	0.84	0.34	56,56,56,56	7
87	MG	2	2109	1/1	0.84	0.38	73,73,73,73	0
86	OHX	1	3656	7/7	0.84	0.32	69,69,69,69	7
87	MG	O7	104	1/1	0.84	0.24	81,81,81,81	0
87	MG	5	4167	1/1	0.84	0.37	39,39,39,39	0
87	MG	1	4296	1/1	0.84	0.24	72,72,72,72	0
86	OHX	5	3684	7/7	0.84	0.40	43,43,43,43	7
87	MG	1	3964	1/1	0.84	0.23	51,51,51,51	0
87	MG	5	4191	1/1	0.84	0.22	44,44,44,44	1
87	MG	1	3970	1/1	0.84	0.31	66,66,66,66	0
87	MG	1	3972	1/1	0.84	0.26	41,41,41,41	0
87	MG	5	4225	1/1	0.84	0.32	71,71,71,71	0
87	MG	1	4000	1/1	0.84	0.18	39,39,39,39	0
87	MG	6	2312	1/1	0.84	0.18	75,75,75,75	0
87	MG	1	4006	1/1	0.84	0.23	39,39,39,39	0
87	MG	6	2128	1/1	0.84	0.23	68,68,68,68	0
86	OHX	5	3817	7/7	0.84	0.22	85,85,85,85	7
87	MG	6	2131	1/1	0.84	0.36	53,53,53,53	0
87	MG	6	2137	1/1	0.84	0.13	83,83,83,83	0
86	OHX	6	2013	7/7	0.84	0.27	82,82,82,82	7
87	MG	5	4304	1/1	0.84	0.25	70,70,70,70	0
87	MG	2	2170	1/1	0.84	0.17	78,78,78,78	0
86	OHX	1	3718	7/7	0.84	0.30	73,73,73,73	7
87	MG	1	4365	1/1	0.84	0.32	38,38,38,38	1
87	MG	2	2120	1/1	0.84	0.16	70,70,70,70	0
86	OHX	2	2020	7/7	0.84	0.22	84,84,84,84	7
87	MG	1	4399	1/1	0.84	0.12	54,54,54,54	0
87	MG	1	4050	1/1	0.84	0.18	35,35,35,35	0
87	MG	1	4428	1/1	0.84	0.38	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4340	1/1	0.84	0.32	34,34,34,34	0
86	OHX	6	2022	7/7	0.84	0.14	139,139,139,139	7
87	MG	2	2179	1/1	0.84	0.27	85,85,85,85	0
87	MG	5	3846	1/1	0.84	0.19	43,43,43,43	0
87	MG	1	4068	1/1	0.84	0.18	62,62,62,62	0
86	OHX	2	2064	7/7	0.84	0.10	130,130,130,130	7
87	MG	5	3876	1/1	0.84	0.23	33,33,33,33	0
86	OHX	5	3702	7/7	0.84	0.18	86,86,86,86	7
86	OHX	M0	302	7/7	0.84	0.38	48,48,48,48	7
87	MG	2	2130	1/1	0.84	0.26	75,75,75,75	0
86	OHX	2	2042	7/7	0.84	0.15	113,113,113,113	7
87	MG	1	4130	1/1	0.84	0.33	58,58,58,58	0
87	MG	5	4428	1/1	0.84	0.11	69,69,69,69	0
87	MG	6	2198	1/1	0.84	0.12	90,90,90,90	0
87	MG	5	4474	1/1	0.84	0.09	62,62,62,62	0
87	MG	6	2199	1/1	0.84	0.39	83,83,83,83	0
86	OHX	8	221	7/7	0.84	0.25	74,74,74,74	7
86	OHX	6	2029	7/7	0.84	0.30	82,82,82,82	7
87	MG	6	2204	1/1	0.84	0.13	47,47,47,47	0
86	OHX	1	3763	7/7	0.84	0.30	64,64,64,64	7
86	OHX	5	3714	7/7	0.84	0.28	82,82,82,82	7
87	MG	5	4555	1/1	0.84	0.09	53,53,53,53	0
87	MG	5	4556	1/1	0.84	0.18	43,43,43,43	0
87	MG	5	3958	1/1	0.84	0.62	61,61,61,61	0
86	OHX	2	2044	7/7	0.84	0.14	134,134,134,134	7
87	MG	1	4494	1/1	0.84	0.26	58,58,58,58	0
87	MG	1	4151	1/1	0.84	0.20	50,50,50,50	0
87	MG	2	2194	1/1	0.84	0.27	72,72,72,72	0
87	MG	2	2196	1/1	0.84	0.18	82,82,82,82	0
87	MG	5	3999	1/1	0.84	0.47	32,32,32,32	0
87	MG	5	4055	1/1	0.84	0.13	33,33,33,33	0
87	MG	3	219	1/1	0.84	0.37	63,63,63,63	0
86	OHX	5	3615	7/7	0.84	0.27	51,51,51,51	7
87	MG	m6	203	1/1	0.84	0.15	41,41,41,41	1
86	OHX	5	3624	7/7	0.84	0.24	51,51,51,51	7
86	OHX	5	3629	7/7	0.84	0.26	67,67,67,67	7
87	MG	2	2205	1/1	0.84	0.24	76,76,76,76	0
86	OHX	6	2037	7/7	0.84	0.25	75,75,75,75	7
86	OHX	5	3728	7/7	0.84	0.36	57,57,57,57	7
89	C	5	3401	20/21	0.84	0.12	48,105,107,107	0
86	OHX	6	2041	7/7	0.84	0.29	62,62,62,62	7
86	OHX	1	3765	7/7	0.84	0.23	93,93,93,93	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4124	1/1	0.85	0.10	46,46,46,46	0
86	OHX	2	2005	7/7	0.85	0.24	86,86,86,86	7
87	MG	1	4127	1/1	0.85	0.18	49,49,49,49	0
87	MG	5	4173	1/1	0.85	0.26	82,82,82,82	0
86	OHX	5	3635	7/7	0.85	0.19	81,81,81,81	7
86	OHX	1	3727	7/7	0.85	0.11	141,141,141,141	7
87	MG	1	4133	1/1	0.85	0.12	83,83,83,83	0
86	OHX	6	2055	7/7	0.85	0.37	59,59,59,59	7
86	OHX	8	213	7/7	0.85	0.18	77,77,77,77	7
87	MG	1	3881	1/1	0.85	0.21	47,47,47,47	0
87	MG	5	4217	1/1	0.85	0.35	66,66,66,66	0
86	OHX	2	2089	7/7	0.85	0.17	121,121,121,121	7
87	MG	5	4226	1/1	0.85	0.12	36,36,36,36	0
87	MG	2	2167	1/1	0.85	0.18	84,84,84,84	0
87	MG	6	2170	1/1	0.85	0.08	49,49,49,49	0
86	OHX	5	3647	7/7	0.85	0.33	35,35,35,35	7
87	MG	6	2172	1/1	0.85	0.22	76,76,76,76	0
87	MG	6	2174	1/1	0.85	0.26	58,58,58,58	0
87	MG	d4	201	1/1	0.85	0.26	68,68,68,68	0
86	OHX	5	3773	7/7	0.85	0.10	145,145,145,145	7
86	OHX	1	3807	7/7	0.85	0.14	112,112,112,112	7
86	OHX	5	3780	7/7	0.85	0.16	110,110,110,110	7
87	MG	5	3825	1/1	0.85	0.20	48,48,48,48	0
87	MG	5	3834	1/1	0.85	0.21	46,46,46,46	0
87	MG	1	3917	1/1	0.85	0.20	49,49,49,49	0
86	OHX	5	3781	7/7	0.85	0.33	53,53,53,53	7
86	OHX	1	3614	7/7	0.85	0.39	53,53,53,53	7
86	OHX	6	1984	7/7	0.85	0.20	82,82,82,82	7
87	MG	1	3937	1/1	0.85	0.26	33,33,33,33	0
87	MG	2	2132	1/1	0.85	0.23	70,70,70,70	0
87	MG	5	4335	1/1	0.85	0.13	35,35,35,35	0
86	OHX	5	3664	7/7	0.85	0.29	63,63,63,63	7
87	MG	5	4342	1/1	0.85	0.24	34,34,34,34	0
87	MG	1	4211	1/1	0.85	0.19	58,58,58,58	0
86	OHX	1	3747	7/7	0.85	0.45	46,46,46,46	7
86	OHX	2	2016	7/7	0.85	0.22	101,101,101,101	7
87	MG	6	2208	1/1	0.85	0.10	67,67,67,67	0
87	MG	5	4368	1/1	0.85	0.18	53,53,53,53	1
86	OHX	1	3716	7/7	0.85	0.39	61,61,61,61	7
86	OHX	5	3742	7/7	0.85	0.35	49,49,49,49	7
87	MG	1	4233	1/1	0.85	0.15	63,63,63,63	0
87	MG	1	3974	1/1	0.85	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	4	238	1/1	0.85	0.13	59,59,59,59	0
87	MG	5	3948	1/1	0.85	0.30	24,24,24,24	0
87	MG	1	3985	1/1	0.85	0.42	28,28,28,28	0
87	MG	5	4424	1/1	0.85	0.13	63,63,63,63	0
87	MG	5	3963	1/1	0.85	0.22	43,43,43,43	0
87	MG	5	4434	1/1	0.85	0.14	93,93,93,93	0
87	MG	1	3994	1/1	0.85	0.47	56,56,56,56	0
86	OHX	1	3701	7/7	0.85	0.23	68,68,68,68	7
86	OHX	5	3793	7/7	0.85	0.37	58,58,58,58	7
86	OHX	2	2071	7/7	0.85	0.20	94,94,94,94	7
87	MG	5	4499	1/1	0.85	0.24	55,55,55,55	0
87	MG	1	4295	1/1	0.85	0.49	41,41,41,41	1
87	MG	6	2248	1/1	0.85	0.41	53,53,53,53	0
87	MG	5	4006	1/1	0.85	0.32	37,37,37,37	0
87	MG	5	4015	1/1	0.85	0.41	38,38,38,38	0
87	MG	5	4039	1/1	0.85	0.22	57,57,57,57	0
87	MG	2	2144	1/1	0.85	0.17	66,66,66,66	0
87	MG	1	4297	1/1	0.85	0.16	46,46,46,46	0
86	OHX	6	2043	7/7	0.85	0.23	86,86,86,86	7
86	OHX	1	3560	7/7	0.85	0.26	72,72,72,72	7
87	MG	8	229	1/1	0.85	0.11	52,52,52,52	0
87	MG	O3	203	1/1	0.85	0.26	47,47,47,47	1
87	MG	1	4043	1/1	0.85	0.15	66,66,66,66	0
86	OHX	5	3749	7/7	0.85	0.52	39,39,39,39	7
87	MG	2	2097	1/1	0.85	0.21	82,82,82,82	0
87	MG	1	4347	1/1	0.85	0.10	41,41,41,41	1
86	OHX	5	3690	7/7	0.85	0.25	90,90,90,90	7
87	MG	6	2105	1/1	0.85	0.29	49,49,49,49	0
86	OHX	6	2045	7/7	0.85	0.25	61,61,61,61	7
87	MG	6	2109	1/1	0.85	0.23	47,47,47,47	0
87	MG	n6	201	1/1	0.85	0.18	54,54,54,54	0
87	MG	1	4066	1/1	0.85	0.26	55,55,55,55	0
87	MG	1	3834	1/1	0.85	0.39	71,71,71,71	0
86	OHX	5	3612	7/7	0.85	0.29	39,39,39,39	7
86	OHX	1	3773	7/7	0.85	0.22	71,71,71,71	7
89	C	1	3402	20/21	0.85	0.12	50,107,109,109	0
86	OHX	1	3723	7/7	0.85	0.35	57,57,57,57	7
86	OHX	6	2014	7/7	0.85	0.31	74,74,74,74	7
86	OHX	1	3758	7/7	0.85	0.34	55,55,55,55	7
91	PRO	1	3404	7/8	0.85	0.25	75,75,75,75	0
86	OHX	1	3666	7/7	0.86	0.26	62,62,62,62	7
87	MG	6	2249	1/1	0.86	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2062	7/7	0.86	0.22	85,85,85,85	7
87	MG	5	4131	1/1	0.86	0.16	35,35,35,35	1
87	MG	1	3908	1/1	0.86	0.28	43,43,43,43	0
86	OHX	5	3809	7/7	0.86	0.23	86,86,86,86	7
86	OHX	1	3670	7/7	0.86	0.27	50,50,50,50	7
87	MG	2	2160	1/1	0.86	0.07	67,67,67,67	0
86	OHX	3	210	7/7	0.86	0.37	53,53,53,53	7
87	MG	5	4144	1/1	0.86	0.17	44,44,44,44	0
86	OHX	3	211	7/7	0.86	0.24	81,81,81,81	7
87	MG	1	3933	1/1	0.86	0.29	49,49,49,49	0
86	OHX	5	3585	7/7	0.86	0.42	44,44,44,44	7
87	MG	2	2110	1/1	0.86	0.22	66,66,66,66	0
87	MG	2	2239	1/1	0.86	0.19	86,86,86,86	0
87	MG	1	3941	1/1	0.86	0.29	36,36,36,36	0
87	MG	1	4228	1/1	0.86	0.19	62,62,62,62	0
86	OHX	5	3699	7/7	0.86	0.35	39,39,39,39	7
87	MG	1	4232	1/1	0.86	0.32	61,61,61,61	0
87	MG	5	4187	1/1	0.86	0.25	53,53,53,53	0
86	OHX	5	3605	7/7	0.86	0.36	44,44,44,44	7
87	MG	5	4196	1/1	0.86	0.13	52,52,52,52	0
87	MG	1	3968	1/1	0.86	0.36	43,43,43,43	0
86	OHX	1	3627	7/7	0.86	0.41	45,45,45,45	7
86	OHX	7	210	7/7	0.86	0.24	63,63,63,63	7
87	MG	2	2248	1/1	0.86	0.20	78,78,78,78	0
87	MG	1	4271	1/1	0.86	0.15	48,48,48,48	0
87	MG	5	4230	1/1	0.86	0.15	55,55,55,55	0
87	MG	1	3975	1/1	0.86	0.31	41,41,41,41	0
87	MG	1	3976	1/1	0.86	0.34	44,44,44,44	0
86	OHX	1	3762	7/7	0.86	0.17	63,63,63,63	7
87	MG	6	2106	1/1	0.86	0.23	68,68,68,68	0
87	MG	2	2171	1/1	0.86	0.18	90,90,90,90	0
86	OHX	1	3788	7/7	0.86	0.20	105,105,105,105	7
87	MG	1	4304	1/1	0.86	0.18	44,44,44,44	1
87	MG	6	2121	1/1	0.86	0.30	61,61,61,61	0
86	OHX	5	3709	7/7	0.86	0.59	41,41,41,41	7
86	OHX	1	3673	7/7	0.86	0.33	47,47,47,47	7
87	MG	c6	202	1/1	0.86	0.29	87,87,87,87	0
87	MG	6	2125	1/1	0.86	0.38	40,40,40,40	0
87	MG	1	4322	1/1	0.86	0.10	65,65,65,65	0
87	MG	1	4014	1/1	0.86	0.29	49,49,49,49	0
87	MG	c9	202	1/1	0.86	0.23	80,80,80,80	0
87	MG	1	4023	1/1	0.86	0.27	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2132	1/1	0.86	0.27	69,69,69,69	0
87	MG	2	2177	1/1	0.86	0.28	69,69,69,69	0
87	MG	5	4336	1/1	0.86	0.25	69,69,69,69	0
86	OHX	8	216	7/7	0.86	0.22	67,67,67,67	7
86	OHX	4	218	7/7	0.86	0.34	51,51,51,51	7
86	OHX	1	3646	7/7	0.86	0.35	54,54,54,54	7
87	MG	1	4350	1/1	0.86	0.18	40,40,40,40	1
87	MG	5	3838	1/1	0.86	0.28	40,40,40,40	0
87	MG	5	4351	1/1	0.86	0.20	59,59,59,59	0
87	MG	5	4355	1/1	0.86	0.12	53,53,53,53	0
86	OHX	5	3778	7/7	0.86	0.15	109,109,109,109	7
87	MG	5	3848	1/1	0.86	0.20	33,33,33,33	0
86	OHX	1	3792	7/7	0.86	0.12	147,147,147,147	7
86	OHX	2	2010	7/7	0.86	0.16	101,101,101,101	7
87	MG	5	3871	1/1	0.86	0.28	36,36,36,36	0
87	MG	1	4052	1/1	0.86	0.29	49,49,49,49	0
87	MG	5	4408	1/1	0.86	0.14	57,57,57,57	0
86	OHX	1	3680	7/7	0.86	0.30	60,60,60,60	7
87	MG	5	4414	1/1	0.86	0.22	38,38,38,38	1
86	OHX	2	1981	7/7	0.86	0.24	106,106,106,106	7
87	MG	1	4373	1/1	0.86	0.21	69,69,69,69	0
86	OHX	m0	304	7/7	0.86	0.47	43,43,43,43	7
87	MG	2	2138	1/1	0.86	0.13	76,76,76,76	0
87	MG	1	4425	1/1	0.86	0.27	46,46,46,46	1
87	MG	5	4455	1/1	0.86	0.24	37,37,37,37	1
86	OHX	1	3682	7/7	0.86	0.19	75,75,75,75	7
87	MG	5	4464	1/1	0.86	0.17	66,66,66,66	0
86	OHX	1	3662	7/7	0.86	0.28	60,60,60,60	7
87	MG	5	4481	1/1	0.86	0.12	44,44,44,44	1
86	OHX	6	1990	7/7	0.86	0.24	65,65,65,65	7
87	MG	5	3926	1/1	0.86	0.27	65,65,65,65	0
87	MG	1	4439	1/1	0.86	0.15	200,200,200,200	0
87	MG	5	3940	1/1	0.86	0.31	34,34,34,34	0
87	MG	5	3945	1/1	0.86	0.20	41,41,41,41	0
87	MG	1	4096	1/1	0.86	0.29	76,76,76,76	0
87	MG	5	4529	1/1	0.86	0.37	37,37,37,37	1
87	MG	6	2185	1/1	0.86	0.24	44,44,44,44	0
87	MG	5	4543	1/1	0.86	0.27	41,41,41,41	1
87	MG	1	4453	1/1	0.86	0.18	82,82,82,82	0
86	OHX	5	3787	7/7	0.86	0.15	111,111,111,111	7
87	MG	5	4563	1/1	0.86	0.24	85,85,85,85	0
87	MG	1	4107	1/1	0.86	0.22	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4108	1/1	0.86	0.12	56,56,56,56	0
87	MG	2	2197	1/1	0.86	0.32	76,76,76,76	0
87	MG	7	225	1/1	0.86	0.21	39,39,39,39	0
87	MG	7	235	1/1	0.86	0.27	60,60,60,60	0
86	OHX	2	2087	7/7	0.86	0.33	71,71,71,71	7
86	OHX	6	1998	7/7	0.86	0.23	64,64,64,64	7
87	MG	1	4128	1/1	0.86	0.21	55,55,55,55	0
87	MG	8	237	1/1	0.86	0.10	71,71,71,71	0
87	MG	1	4483	1/1	0.86	0.24	59,59,59,59	0
87	MG	1	3864	1/1	0.86	0.41	55,55,55,55	0
86	OHX	5	3671	7/7	0.86	0.32	56,56,56,56	7
87	MG	5	4025	1/1	0.86	0.50	32,32,32,32	0
86	OHX	1	3685	7/7	0.86	0.18	95,95,95,95	7
86	OHX	5	3795	7/7	0.86	0.33	54,54,54,54	7
87	MG	2	2210	1/1	0.86	0.26	69,69,69,69	0
87	MG	1	4501	1/1	0.86	0.14	66,66,66,66	0
86	OHX	1	3724	7/7	0.86	0.17	100,100,100,100	7
86	OHX	1	3688	7/7	0.86	0.33	54,54,54,54	7
87	MG	5	4074	1/1	0.86	0.26	86,86,86,86	0
87	MG	6	2232	1/1	0.86	0.14	53,53,53,53	0
87	MG	5	4095	1/1	0.86	0.24	60,60,60,60	0
86	OHX	1	3692	7/7	0.86	0.27	65,65,65,65	7
87	MG	1	3896	1/1	0.86	0.34	66,66,66,66	0
86	OHX	2	2056	7/7	0.86	0.09	155,155,155,155	7
87	MG	3	223	1/1	0.86	0.11	62,62,62,62	0
86	OHX	5	3724	7/7	0.87	0.28	58,58,58,58	7
87	MG	5	4176	1/1	0.87	0.20	45,45,45,45	0
87	MG	1	4400	1/1	0.87	0.27	59,59,59,59	0
87	MG	5	4182	1/1	0.87	0.35	66,66,66,66	0
86	OHX	1	3760	7/7	0.87	0.36	52,52,52,52	7
87	MG	1	4408	1/1	0.87	0.10	56,56,56,56	1
86	OHX	2	1960	7/7	0.87	0.19	97,97,97,97	7
87	MG	1	4426	1/1	0.87	0.19	63,63,63,63	0
86	OHX	1	3661	7/7	0.87	0.44	45,45,45,45	7
87	MG	6	2142	1/1	0.87	0.19	73,73,73,73	0
87	MG	5	4209	1/1	0.87	0.15	50,50,50,50	0
87	MG	2	2223	1/1	0.87	0.27	69,69,69,69	0
87	MG	5	4214	1/1	0.87	0.12	52,52,52,52	0
86	OHX	5	3729	7/7	0.87	0.33	58,58,58,58	7
86	OHX	6	2050	7/7	0.87	0.11	132,132,132,132	7
86	OHX	4	217	7/7	0.87	0.31	70,70,70,70	7
87	MG	1	3922	1/1	0.87	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4455	1/1	0.87	0.21	43,43,43,43	0
87	MG	5	4243	1/1	0.87	0.19	58,58,58,58	0
87	MG	6	2163	1/1	0.87	0.34	40,40,40,40	0
87	MG	1	4460	1/1	0.87	0.17	75,75,75,75	0
87	MG	1	4462	1/1	0.87	0.23	53,53,53,53	0
86	OHX	6	2082	7/7	0.87	0.34	54,54,54,54	7
86	OHX	5	3651	7/7	0.87	0.29	63,63,63,63	7
86	OHX	5	3654	7/7	0.87	0.37	55,55,55,55	7
87	MG	5	4290	1/1	0.87	0.11	72,72,72,72	0
86	OHX	2	2043	7/7	0.87	0.14	119,119,119,119	7
86	OHX	L3	403	7/7	0.87	0.16	85,85,85,85	7
87	MG	2	2166	1/1	0.87	0.24	55,55,55,55	0
86	OHX	1	3702	7/7	0.87	0.39	42,42,42,42	7
87	MG	1	3946	1/1	0.87	0.41	39,39,39,39	0
87	MG	5	3870	1/1	0.87	0.20	34,34,34,34	0
87	MG	5	4319	1/1	0.87	0.17	59,59,59,59	0
87	MG	6	2179	1/1	0.87	0.17	67,67,67,67	0
87	MG	6	2180	1/1	0.87	0.17	52,52,52,52	0
87	MG	1	4484	1/1	0.87	0.20	49,49,49,49	1
87	MG	5	3887	1/1	0.87	0.16	34,34,34,34	0
87	MG	5	4334	1/1	0.87	0.17	37,37,37,37	0
87	MG	1	3950	1/1	0.87	0.25	31,31,31,31	0
87	MG	1	3951	1/1	0.87	0.39	35,35,35,35	0
86	OHX	6	2017	7/7	0.87	0.29	50,50,50,50	7
86	OHX	1	3612	7/7	0.87	0.40	46,46,46,46	7
87	MG	1	4493	1/1	0.87	0.16	46,46,46,46	0
87	MG	6	2200	1/1	0.87	0.22	74,74,74,74	0
87	MG	2	2115	1/1	0.87	0.45	71,71,71,71	0
86	OHX	6	2057	7/7	0.87	0.27	78,78,78,78	7
86	OHX	M7	201	7/7	0.87	0.57	42,42,42,42	7
87	MG	5	3931	1/1	0.87	0.19	42,42,42,42	0
87	MG	5	4365	1/1	0.87	0.30	45,45,45,45	0
86	OHX	5	3753	7/7	0.87	0.29	49,49,49,49	7
87	MG	5	3938	1/1	0.87	0.42	28,28,28,28	0
87	MG	5	4386	1/1	0.87	0.17	37,37,37,37	1
86	OHX	1	3664	7/7	0.87	0.29	65,65,65,65	7
86	OHX	5	3683	7/7	0.87	0.31	60,60,60,60	7
87	MG	1	3981	1/1	0.87	0.21	51,51,51,51	0
87	MG	2	2123	1/1	0.87	0.16	68,68,68,68	0
86	OHX	7	211	7/7	0.87	0.32	52,52,52,52	7
86	OHX	2	1994	7/7	0.87	0.17	111,111,111,111	7
86	OHX	2	2051	7/7	0.87	0.23	86,86,86,86	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2220	1/1	0.87	0.14	47,47,47,47	0
87	MG	5	3970	1/1	0.87	0.29	38,38,38,38	0
86	OHX	s1	302	7/7	0.87	0.17	93,93,93,93	7
87	MG	5	3973	1/1	0.87	0.32	34,34,34,34	0
87	MG	5	4444	1/1	0.87	0.09	39,39,39,39	0
86	OHX	1	3639	7/7	0.87	0.23	85,85,85,85	7
87	MG	5	3977	1/1	0.87	0.37	55,55,55,55	0
87	MG	6	2230	1/1	0.87	0.29	59,59,59,59	0
87	MG	1	4016	1/1	0.87	0.24	38,38,38,38	0
87	MG	5	4476	1/1	0.87	0.11	46,46,46,46	0
87	MG	5	3992	1/1	0.87	0.33	33,33,33,33	0
86	OHX	sR	401	7/7	0.87	0.14	122,122,122,122	7
86	OHX	5	3764	7/7	0.87	0.23	71,71,71,71	7
86	OHX	5	3536	7/7	0.87	0.34	53,53,53,53	7
87	MG	5	4022	1/1	0.87	0.31	31,31,31,31	0
86	OHX	6	2031	7/7	0.87	0.21	81,81,81,81	7
87	MG	5	4518	1/1	0.87	0.18	41,41,41,41	0
87	MG	5	4527	1/1	0.87	0.21	55,55,55,55	0
87	MG	5	4026	1/1	0.87	0.33	37,37,37,37	0
86	OHX	2	2024	7/7	0.87	0.18	91,91,91,91	7
86	OHX	5	3700	7/7	0.87	0.30	43,43,43,43	7
86	OHX	5	3601	7/7	0.87	0.23	89,89,89,89	7
87	MG	5	4547	1/1	0.87	0.33	46,46,46,46	0
87	MG	5	4549	1/1	0.87	0.22	77,77,77,77	0
86	OHX	1	3686	7/7	0.87	0.19	117,117,117,117	7
87	MG	1	4311	1/1	0.87	0.17	57,57,57,57	1
86	OHX	5	3607	7/7	0.87	0.18	112,112,112,112	7
86	OHX	1	3571	7/7	0.87	0.25	64,64,64,64	7
87	MG	5	4086	1/1	0.87	0.18	48,48,48,48	0
87	MG	1	4327	1/1	0.87	0.27	51,51,51,51	0
87	MG	7	222	1/1	0.87	0.14	61,61,61,61	0
87	MG	O1	204	1/1	0.87	0.33	63,63,63,63	0
86	OHX	6	2072	7/7	0.87	0.27	66,66,66,66	7
87	MG	1	4330	1/1	0.87	0.10	59,59,59,59	0
87	MG	5	4100	1/1	0.87	0.20	32,32,32,32	0
87	MG	8	232	1/1	0.87	0.27	64,64,64,64	0
86	OHX	1	3672	7/7	0.87	0.36	46,46,46,46	7
87	MG	6	2275	1/1	0.87	0.25	67,67,67,67	1
87	MG	8	239	1/1	0.87	0.31	71,71,71,71	0
86	OHX	6	2001	7/7	0.87	0.29	68,68,68,68	7
87	MG	5	4119	1/1	0.87	0.31	61,61,61,61	0
87	MG	6	2279	1/1	0.87	0.17	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4069	1/1	0.87	0.18	56,56,56,56	0
87	MG	1	4074	1/1	0.87	0.21	50,50,50,50	0
86	OHX	5	3625	7/7	0.87	0.26	52,52,52,52	7
87	MG	m7	205	1/1	0.87	0.07	50,50,50,50	0
86	OHX	4	212	7/7	0.87	0.35	42,42,42,42	7
87	MG	1	3876	1/1	0.87	0.20	30,30,30,30	0
87	MG	n8	201	1/1	0.87	0.23	33,33,33,33	0
86	OHX	6	2005	7/7	0.87	0.23	80,80,80,80	7
87	MG	1	4099	1/1	0.87	0.22	59,59,59,59	0
87	MG	6	2119	1/1	0.87	0.34	59,59,59,59	0
86	OHX	5	3722	7/7	0.87	0.22	76,76,76,76	7
87	MG	2	2151	1/1	0.87	0.27	58,58,58,58	0
87	MG	2	2215	1/1	0.87	0.30	78,78,78,78	0
87	MG	6	2317	1/1	0.87	0.22	59,59,59,59	0
87	MG	1	4121	1/1	0.87	0.17	37,37,37,37	0
87	MG	5	4171	1/1	0.87	0.07	115,115,115,115	0
91	PRO	5	3404	7/8	0.87	0.27	71,71,71,71	0
87	MG	4	232	1/1	0.88	0.15	42,42,42,42	0
86	OHX	5	3580	7/7	0.88	0.34	63,63,63,63	7
86	OHX	5	3685	7/7	0.88	0.15	88,88,88,88	7
86	OHX	6	2035	7/7	0.88	0.19	82,82,82,82	7
86	OHX	1	3708	7/7	0.88	0.17	103,103,103,103	7
87	MG	1	3979	1/1	0.88	0.38	45,45,45,45	0
86	OHX	5	3689	7/7	0.88	0.14	116,116,116,116	7
86	OHX	6	2000	7/7	0.88	0.36	63,63,63,63	7
87	MG	M0	305	1/1	0.88	0.23	62,62,62,62	0
87	MG	1	3992	1/1	0.88	0.30	27,27,27,27	0
87	MG	M5	302	1/1	0.88	0.26	42,42,42,42	1
86	OHX	6	2038	7/7	0.88	0.17	88,88,88,88	7
86	OHX	2	1968	7/7	0.88	0.25	77,77,77,77	7
86	OHX	1	3637	7/7	0.88	0.26	76,76,76,76	7
87	MG	S8	302	1/1	0.88	0.09	69,69,69,69	1
87	MG	1	4294	1/1	0.88	0.21	58,58,58,58	0
87	MG	6	2321	1/1	0.88	0.09	72,72,72,72	0
87	MG	2	2183	1/1	0.88	0.29	66,66,66,66	0
86	OHX	5	3697	7/7	0.88	0.50	44,44,44,44	7
87	MG	1	3815	1/1	0.88	0.33	44,44,44,44	0
86	OHX	1	3693	7/7	0.88	0.17	81,81,81,81	7
87	MG	1	4025	1/1	0.88	0.18	39,39,39,39	0
86	OHX	1	3677	7/7	0.88	0.25	74,74,74,74	7
87	MG	s6	301	1/1	0.88	0.17	71,71,71,71	0
86	OHX	1	3757	7/7	0.88	0.59	49,49,49,49	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2046	7/7	0.88	0.19	100,100,100,100	7
87	MG	2	2133	1/1	0.88	0.26	76,76,76,76	0
87	MG	c8	202	1/1	0.88	0.34	81,81,81,81	0
86	OHX	1	3736	7/7	0.88	0.15	113,113,113,113	7
87	MG	5	4293	1/1	0.88	0.14	43,43,43,43	0
87	MG	1	3841	1/1	0.88	0.17	55,55,55,55	0
87	MG	6	2112	1/1	0.88	0.25	42,42,42,42	0
87	MG	6	2113	1/1	0.88	0.13	75,75,75,75	0
87	MG	6	2116	1/1	0.88	0.22	61,61,61,61	0
86	OHX	1	3804	7/7	0.88	0.31	67,67,67,67	7
87	MG	1	3851	1/1	0.88	0.19	53,53,53,53	0
87	MG	1	4055	1/1	0.88	0.20	51,51,51,51	0
86	OHX	L5	301	7/7	0.88	0.22	78,78,78,78	7
87	MG	5	3819	1/1	0.88	0.43	36,36,36,36	0
86	OHX	1	3719	7/7	0.88	0.23	86,86,86,86	7
87	MG	5	4331	1/1	0.88	0.16	62,62,62,62	0
87	MG	5	3829	1/1	0.88	0.23	39,39,39,39	0
86	OHX	l3	402	7/7	0.88	0.21	73,73,73,73	7
86	OHX	l4	401	7/7	0.88	0.22	69,69,69,69	7
87	MG	2	2202	1/1	0.88	0.15	69,69,69,69	0
86	OHX	5	3777	7/7	0.88	0.43	38,38,38,38	7
87	MG	5	3850	1/1	0.88	0.21	65,65,65,65	0
87	MG	5	3851	1/1	0.88	0.12	36,36,36,36	0
87	MG	1	4361	1/1	0.88	0.26	67,67,67,67	0
87	MG	1	4082	1/1	0.88	0.61	52,52,52,52	1
87	MG	1	4083	1/1	0.88	0.20	29,29,29,29	0
87	MG	5	4354	1/1	0.88	0.17	61,61,61,61	0
86	OHX	5	3713	7/7	0.88	0.28	70,70,70,70	7
87	MG	1	4088	1/1	0.88	0.19	52,52,52,52	0
87	MG	1	4395	1/1	0.88	0.28	34,34,34,34	1
87	MG	6	2150	1/1	0.88	0.46	59,59,59,59	0
87	MG	5	4369	1/1	0.88	0.20	52,52,52,52	1
86	OHX	5	3779	7/7	0.88	0.17	122,122,122,122	7
86	OHX	2	2038	7/7	0.88	0.27	85,85,85,85	7
86	OHX	M0	304	7/7	0.88	0.21	96,96,96,96	7
87	MG	1	4405	1/1	0.88	0.12	44,44,44,44	0
87	MG	6	2158	1/1	0.88	0.34	40,40,40,40	0
87	MG	1	4406	1/1	0.88	0.12	46,46,46,46	1
87	MG	1	3886	1/1	0.88	0.18	39,39,39,39	0
87	MG	1	4423	1/1	0.88	0.70	40,40,40,40	1
86	OHX	2	2002	7/7	0.88	0.25	86,86,86,86	7
86	OHX	m7	201	7/7	0.88	0.28	49,49,49,49	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3649	7/7	0.88	0.32	41,41,41,41	7
87	MG	1	4432	1/1	0.88	0.13	47,47,47,47	1
86	OHX	1	3654	7/7	0.88	0.26	65,65,65,65	7
87	MG	1	4125	1/1	0.88	0.17	35,35,35,35	0
86	OHX	o7	503	7/7	0.88	0.40	53,53,53,53	7
87	MG	1	4440	1/1	0.88	0.15	43,43,43,43	0
87	MG	5	4457	1/1	0.88	0.13	54,54,54,54	0
86	OHX	5	3723	7/7	0.88	0.26	62,62,62,62	7
87	MG	5	4468	1/1	0.88	0.24	43,43,43,43	0
87	MG	5	4473	1/1	0.88	0.11	49,49,49,49	0
86	OHX	1	3784	7/7	0.88	0.28	66,66,66,66	7
87	MG	1	3911	1/1	0.88	0.23	40,40,40,40	0
87	MG	1	4457	1/1	0.88	0.17	43,43,43,43	0
87	MG	5	3969	1/1	0.88	0.27	41,41,41,41	0
86	OHX	1	3505	7/7	0.88	0.34	50,50,50,50	7
87	MG	6	2187	1/1	0.88	0.09	77,77,77,77	0
87	MG	2	2222	1/1	0.88	0.11	80,80,80,80	0
87	MG	1	4464	1/1	0.88	0.33	60,60,60,60	0
87	MG	1	4139	1/1	0.88	0.35	44,44,44,44	0
87	MG	5	3980	1/1	0.88	0.29	58,58,58,58	0
87	MG	1	4140	1/1	0.88	0.18	39,39,39,39	0
86	OHX	6	2027	7/7	0.88	0.26	83,83,83,83	7
87	MG	1	4146	1/1	0.88	0.14	50,50,50,50	0
87	MG	1	4472	1/1	0.88	0.29	61,61,61,61	0
87	MG	5	4002	1/1	0.88	0.26	37,37,37,37	0
86	OHX	5	3663	7/7	0.88	0.31	57,57,57,57	7
86	OHX	5	3791	7/7	0.88	0.32	68,68,68,68	7
87	MG	6	2206	1/1	0.88	0.25	67,67,67,67	0
87	MG	5	4559	1/1	0.88	0.25	73,73,73,73	1
87	MG	1	4479	1/1	0.88	0.20	41,41,41,41	1
86	OHX	1	3744	7/7	0.88	0.37	60,60,60,60	7
86	OHX	2	2040	7/7	0.88	0.23	88,88,88,88	7
86	OHX	5	3735	7/7	0.88	0.24	62,62,62,62	7
87	MG	7	220	1/1	0.88	0.19	58,58,58,58	0
87	MG	1	4156	1/1	0.88	0.09	60,60,60,60	0
87	MG	1	4159	1/1	0.88	0.23	45,45,45,45	0
87	MG	1	4169	1/1	0.88	0.33	72,72,72,72	0
87	MG	6	2219	1/1	0.88	0.34	60,60,60,60	0
87	MG	5	4072	1/1	0.88	0.18	55,55,55,55	0
87	MG	8	231	1/1	0.88	0.18	50,50,50,50	0
87	MG	1	4491	1/1	0.88	0.13	36,36,36,36	0
87	MG	5	4076	1/1	0.88	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	2	2231	1/1	0.88	0.23	82,82,82,82	0
87	MG	6	2223	1/1	0.88	0.14	52,52,52,52	0
87	MG	8	240	1/1	0.88	0.14	72,72,72,72	0
86	OHX	6	2030	7/7	0.88	0.11	105,105,105,105	7
86	OHX	5	3673	7/7	0.88	0.33	44,44,44,44	7
87	MG	1	4497	1/1	0.88	0.12	51,51,51,51	0
87	MG	1	3942	1/1	0.88	0.34	32,32,32,32	0
86	OHX	1	3619	7/7	0.88	0.24	70,70,70,70	7
87	MG	1	3949	1/1	0.88	0.23	31,31,31,31	0
87	MG	1	4509	1/1	0.88	0.15	90,90,90,90	0
87	MG	m7	206	1/1	0.88	0.18	35,35,35,35	0
87	MG	6	2243	1/1	0.88	0.32	68,68,68,68	0
87	MG	1	4195	1/1	0.88	0.42	52,52,52,52	0
86	OHX	5	3675	7/7	0.88	0.32	49,49,49,49	7
87	MG	n8	205	1/1	0.88	0.22	39,39,39,39	0
86	OHX	6	2033	7/7	0.88	0.24	67,67,67,67	7
87	MG	1	4206	1/1	0.88	0.11	48,48,48,48	0
87	MG	3	225	1/1	0.88	0.31	68,68,68,68	0
87	MG	1	3952	1/1	0.88	0.25	48,48,48,48	0
87	MG	3	227	1/1	0.88	0.16	78,78,78,78	0
86	OHX	5	3678	7/7	0.88	0.27	51,51,51,51	7
86	OHX	1	3624	7/7	0.88	0.20	63,63,63,63	7
86	OHX	6	2067	7/7	0.88	0.35	70,70,70,70	7
87	MG	4	224	1/1	0.88	0.18	37,37,37,37	0
87	MG	2	2112	1/1	0.88	0.21	69,69,69,69	0
87	MG	1	4105	1/1	0.89	0.18	47,47,47,47	0
87	MG	3	228	1/1	0.89	0.17	78,78,78,78	0
87	MG	5	4268	1/1	0.89	0.17	46,46,46,46	0
86	OHX	5	3752	7/7	0.89	0.30	49,49,49,49	7
86	OHX	1	3559	7/7	0.89	0.20	90,90,90,90	7
87	MG	4	220	1/1	0.89	0.14	64,64,64,64	0
87	MG	1	4340	1/1	0.89	0.14	49,49,49,49	1
87	MG	5	3896	1/1	0.89	0.10	50,50,50,50	0
87	MG	5	3904	1/1	0.89	0.25	44,44,44,44	0
86	OHX	5	3801	7/7	0.89	0.27	66,66,66,66	7
86	OHX	5	3657	7/7	0.89	0.36	41,41,41,41	7
87	MG	4	228	1/1	0.89	0.10	58,58,58,58	0
87	MG	5	4313	1/1	0.89	0.21	57,57,57,57	0
86	OHX	2	2022	7/7	0.89	0.27	66,66,66,66	7
87	MG	4	234	1/1	0.89	0.21	67,67,67,67	0
87	MG	5	3916	1/1	0.89	0.23	57,57,57,57	0
87	MG	5	3918	1/1	0.89	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3710	7/7	0.89	0.31	79,79,79,79	7
87	MG	D6	102	1/1	0.89	0.15	77,77,77,77	0
87	MG	1	4352	1/1	0.89	0.14	52,52,52,52	0
86	OHX	5	3711	7/7	0.89	0.22	83,83,83,83	7
86	OHX	M9	202	7/7	0.89	0.23	78,78,78,78	7
87	MG	6	2218	1/1	0.89	0.06	81,81,81,81	0
87	MG	4	243	1/1	0.89	0.10	57,57,57,57	1
87	MG	SM	201	1/1	0.89	0.24	55,55,55,55	0
87	MG	2	2201	1/1	0.89	0.12	61,61,61,61	0
87	MG	1	3967	1/1	0.89	0.29	40,40,40,40	0
87	MG	M0	306	1/1	0.89	0.10	53,53,53,53	0
86	OHX	1	3567	7/7	0.89	0.39	48,48,48,48	7
87	MG	5	3964	1/1	0.89	0.26	33,33,33,33	0
86	OHX	1	3631	7/7	0.89	0.34	51,51,51,51	7
86	OHX	1	3633	7/7	0.89	0.19	79,79,79,79	7
87	MG	1	3827	1/1	0.89	0.19	67,67,67,67	0
87	MG	1	4398	1/1	0.89	0.10	72,72,72,72	0
87	MG	2	2103	1/1	0.89	0.12	65,65,65,65	0
87	MG	5	3975	1/1	0.89	0.23	74,74,74,74	0
87	MG	1	3835	1/1	0.89	0.20	41,41,41,41	0
87	MG	6	2247	1/1	0.89	0.14	50,50,50,50	0
87	MG	N8	202	1/1	0.89	0.18	37,37,37,37	0
87	MG	1	4150	1/1	0.89	0.21	73,73,73,73	0
87	MG	5	4400	1/1	0.89	0.15	43,43,43,43	1
87	MG	O2	204	1/1	0.89	0.21	33,33,33,33	0
87	MG	2	2208	1/1	0.89	0.14	72,72,72,72	0
86	OHX	5	3610	7/7	0.89	0.32	60,60,60,60	7
87	MG	O5	201	1/1	0.89	0.09	58,58,58,58	0
87	MG	5	4004	1/1	0.89	0.28	42,42,42,42	0
86	OHX	6	2040	7/7	0.89	0.34	58,58,58,58	7
87	MG	1	4413	1/1	0.89	0.11	52,52,52,52	1
87	MG	6	2267	1/1	0.89	0.15	54,54,54,54	0
87	MG	5	4442	1/1	0.89	0.70	34,34,34,34	1
87	MG	1	4422	1/1	0.89	0.29	60,60,60,60	0
87	MG	6	2271	1/1	0.89	0.15	42,42,42,42	0
87	MG	5	4034	1/1	0.89	0.09	45,45,45,45	0
87	MG	5	4037	1/1	0.89	0.25	35,35,35,35	0
87	MG	6	2099	1/1	0.89	0.44	43,43,43,43	0
86	OHX	6	1968	7/7	0.89	0.28	74,74,74,74	7
87	MG	6	2104	1/1	0.89	0.27	52,52,52,52	0
87	MG	1	4424	1/1	0.89	0.09	54,54,54,54	0
87	MG	1	3993	1/1	0.89	0.23	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	3845	1/1	0.89	0.19	44,44,44,44	0
87	MG	1	3849	1/1	0.89	0.19	44,44,44,44	0
86	OHX	1	3705	7/7	0.89	0.25	64,64,64,64	7
87	MG	1	4008	1/1	0.89	0.27	52,52,52,52	0
87	MG	5	4507	1/1	0.89	0.22	46,46,46,46	1
87	MG	1	4009	1/1	0.89	0.35	48,48,48,48	0
86	OHX	5	3620	7/7	0.89	0.36	42,42,42,42	7
87	MG	5	4093	1/1	0.89	0.14	34,34,34,34	0
86	OHX	5	3774	7/7	0.89	0.21	66,66,66,66	7
87	MG	5	4097	1/1	0.89	0.15	40,40,40,40	0
87	MG	1	4196	1/1	0.89	0.20	55,55,55,55	0
87	MG	5	4535	1/1	0.89	0.23	56,56,56,56	0
87	MG	5	4539	1/1	0.89	0.17	56,56,56,56	0
87	MG	1	4015	1/1	0.89	0.37	53,53,53,53	0
86	OHX	1	3570	7/7	0.89	0.34	41,41,41,41	7
86	OHX	2	2088	7/7	0.89	0.13	94,94,94,94	7
86	OHX	2	2007	7/7	0.89	0.20	101,101,101,101	7
87	MG	6	2313	1/1	0.89	0.13	71,71,71,71	0
86	OHX	6	1997	7/7	0.89	0.19	94,94,94,94	7
86	OHX	6	2025	7/7	0.89	0.11	113,113,113,113	7
86	OHX	6	2071	7/7	0.89	0.36	55,55,55,55	7
87	MG	1	4222	1/1	0.89	0.10	45,45,45,45	0
87	MG	2	2121	1/1	0.89	0.15	73,73,73,73	0
86	OHX	5	3736	7/7	0.89	0.17	93,93,93,93	7
87	MG	1	4227	1/1	0.89	0.14	45,45,45,45	0
86	OHX	5	3738	7/7	0.89	0.26	53,53,53,53	7
87	MG	6	2144	1/1	0.89	0.17	55,55,55,55	0
87	MG	6	2146	1/1	0.89	0.34	37,37,37,37	0
87	MG	8	224	1/1	0.89	0.28	52,52,52,52	0
87	MG	5	4153	1/1	0.89	0.26	41,41,41,41	0
86	OHX	5	3638	7/7	0.89	0.24	73,73,73,73	7
87	MG	2	2172	1/1	0.89	0.22	65,65,65,65	0
86	OHX	2	1961	7/7	0.89	0.16	112,112,112,112	7
87	MG	2	2174	1/1	0.89	0.27	68,68,68,68	0
87	MG	8	236	1/1	0.89	0.24	57,57,57,57	0
87	MG	1	4249	1/1	0.89	0.12	54,54,54,54	0
87	MG	6	2157	1/1	0.89	0.35	46,46,46,46	0
87	MG	1	4058	1/1	0.89	0.09	44,44,44,44	0
86	OHX	2	2085	7/7	0.89	0.25	93,93,93,93	7
87	MG	1	3901	1/1	0.89	0.22	66,66,66,66	0
86	OHX	5	3694	7/7	0.89	0.31	55,55,55,55	7
86	OHX	m0	303	7/7	0.89	0.20	86,86,86,86	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4289	1/1	0.89	0.20	57,57,57,57	0
87	MG	18	301	1/1	0.89	0.29	70,70,70,70	0
87	MG	1	4071	1/1	0.89	0.35	40,40,40,40	0
86	OHX	5	3646	7/7	0.89	0.26	52,52,52,52	7
87	MG	5	3823	1/1	0.89	0.28	33,33,33,33	0
87	MG	1	3912	1/1	0.89	0.07	52,52,52,52	0
87	MG	n1	204	1/1	0.89	0.23	56,56,56,56	0
86	OHX	s8	301	7/7	0.89	0.18	104,104,104,104	7
86	OHX	2	2000	7/7	0.89	0.19	110,110,110,110	7
87	MG	1	4300	1/1	0.89	0.17	46,46,46,46	0
87	MG	o6	201	1/1	0.89	0.14	69,69,69,69	1
87	MG	3	213	1/1	0.89	0.18	78,78,78,78	0
86	OHX	5	3747	7/7	0.89	0.21	66,66,66,66	7
86	OHX	1	3616	7/7	0.89	0.31	60,60,60,60	7
86	OHX	5	3650	7/7	0.89	0.25	46,46,46,46	7
87	MG	5	4236	1/1	0.89	0.16	42,42,42,42	0
86	OHX	5	3796	7/7	0.89	0.27	63,63,63,63	7
89	C	5	3402	20/21	0.89	0.12	43,100,102,102	0
86	OHX	1	3696	7/7	0.89	0.23	63,63,63,63	7
87	MG	5	4249	1/1	0.89	0.15	60,60,60,60	0
87	MG	5	3869	1/1	0.89	0.20	62,62,62,62	0
86	OHX	5	3542	7/7	0.89	0.22	84,84,84,84	7
87	MG	1	3947	1/1	0.90	0.20	37,37,37,37	0
87	MG	1	4101	1/1	0.90	0.10	57,57,57,57	0
87	MG	5	3833	1/1	0.90	0.29	59,59,59,59	0
86	OHX	5	3682	7/7	0.90	0.22	75,75,75,75	7
86	OHX	5	3725	7/7	0.90	0.23	75,75,75,75	7
87	MG	5	3841	1/1	0.90	0.31	43,43,43,43	0
87	MG	5	4223	1/1	0.90	0.09	53,53,53,53	0
87	MG	5	3843	1/1	0.90	0.21	62,62,62,62	0
87	MG	3	215	1/1	0.90	0.35	51,51,51,51	0
87	MG	5	4227	1/1	0.90	0.11	48,48,48,48	0
87	MG	5	4228	1/1	0.90	0.12	44,44,44,44	0
87	MG	3	216	1/1	0.90	0.31	55,55,55,55	0
87	MG	5	3849	1/1	0.90	0.19	34,34,34,34	0
86	OHX	1	3732	7/7	0.90	0.28	55,55,55,55	7
87	MG	6	2177	1/1	0.90	0.10	80,80,80,80	0
87	MG	5	3852	1/1	0.90	0.24	40,40,40,40	0
87	MG	1	4302	1/1	0.90	0.25	48,48,48,48	0
87	MG	3	221	1/1	0.90	0.12	70,70,70,70	0
86	OHX	1	3714	7/7	0.90	0.31	45,45,45,45	7
87	MG	6	2181	1/1	0.90	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4109	1/1	0.90	0.08	46,46,46,46	0
87	MG	1	4308	1/1	0.90	0.34	55,55,55,55	0
87	MG	5	4282	1/1	0.90	0.13	39,39,39,39	0
87	MG	1	4114	1/1	0.90	0.07	67,67,67,67	0
87	MG	1	4115	1/1	0.90	0.23	49,49,49,49	0
86	OHX	C5	201	7/7	0.90	0.14	112,112,112,112	7
87	MG	5	3893	1/1	0.90	0.17	47,47,47,47	0
87	MG	6	2194	1/1	0.90	0.19	52,52,52,52	0
87	MG	1	4123	1/1	0.90	0.29	56,56,56,56	0
87	MG	5	4309	1/1	0.90	0.11	74,74,74,74	0
87	MG	5	3898	1/1	0.90	0.30	39,39,39,39	0
87	MG	5	3902	1/1	0.90	0.23	71,71,71,71	0
87	MG	2	2213	1/1	0.90	0.12	55,55,55,55	0
87	MG	1	3965	1/1	0.90	0.30	31,31,31,31	0
86	OHX	5	3775	7/7	0.90	0.30	59,59,59,59	7
87	MG	4	226	1/1	0.90	0.07	61,61,61,61	0
87	MG	1	4335	1/1	0.90	0.34	45,45,45,45	1
87	MG	1	4339	1/1	0.90	0.14	73,73,73,73	1
87	MG	5	4329	1/1	0.90	0.18	47,47,47,47	0
87	MG	5	3914	1/1	0.90	0.32	33,33,33,33	0
86	OHX	8	208	7/7	0.90	0.26	63,63,63,63	7
86	OHX	1	3780	7/7	0.90	0.37	45,45,45,45	7
86	OHX	2	2009	7/7	0.90	0.27	70,70,70,70	7
86	OHX	1	3574	7/7	0.90	0.30	56,56,56,56	7
87	MG	5	3929	1/1	0.90	0.23	39,39,39,39	0
87	MG	5	3930	1/1	0.90	0.19	34,34,34,34	0
87	MG	1	3848	1/1	0.90	0.22	46,46,46,46	0
87	MG	5	3934	1/1	0.90	0.30	35,35,35,35	0
87	MG	5	4348	1/1	0.90	0.27	46,46,46,46	1
87	MG	2	2118	1/1	0.90	0.26	46,46,46,46	0
87	MG	1	4351	1/1	0.90	0.17	43,43,43,43	0
86	OHX	1	3720	7/7	0.90	0.13	104,104,104,104	7
87	MG	5	3941	1/1	0.90	0.35	30,30,30,30	0
87	MG	1	4141	1/1	0.90	0.12	51,51,51,51	0
87	MG	L3	407	1/1	0.90	0.35	51,51,51,51	1
87	MG	L4	407	1/1	0.90	0.11	55,55,55,55	1
86	OHX	1	3593	7/7	0.90	0.30	56,56,56,56	7
87	MG	5	3952	1/1	0.90	0.29	34,34,34,34	0
87	MG	5	3956	1/1	0.90	0.30	47,47,47,47	0
86	OHX	c5	202	7/7	0.90	0.14	98,98,98,98	7
86	OHX	1	3630	7/7	0.90	0.30	57,57,57,57	7
87	MG	1	4364	1/1	0.90	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2231	1/1	0.90	0.18	86,86,86,86	0
87	MG	5	3966	1/1	0.90	0.24	39,39,39,39	0
87	MG	M4	201	1/1	0.90	0.09	53,53,53,53	0
87	MG	1	3863	1/1	0.90	0.20	38,38,38,38	0
87	MG	5	4416	1/1	0.90	0.14	38,38,38,38	0
87	MG	2	2227	1/1	0.90	0.10	63,63,63,63	0
87	MG	6	2238	1/1	0.90	0.10	66,66,66,66	0
87	MG	M7	202	1/1	0.90	0.42	52,52,52,52	0
87	MG	6	2241	1/1	0.90	0.16	70,70,70,70	0
86	OHX	1	3545	7/7	0.90	0.21	91,91,91,91	7
86	OHX	5	3539	7/7	0.90	0.31	54,54,54,54	7
87	MG	N1	201	1/1	0.90	0.21	42,42,42,42	1
87	MG	1	4378	1/1	0.90	0.27	41,41,41,41	1
87	MG	5	3983	1/1	0.90	0.23	35,35,35,35	0
87	MG	1	4152	1/1	0.90	0.19	75,75,75,75	0
87	MG	5	3995	1/1	0.90	0.35	34,34,34,34	0
86	OHX	3	208	7/7	0.90	0.20	85,85,85,85	7
86	OHX	15	301	7/7	0.90	0.18	90,90,90,90	7
86	OHX	5	3549	7/7	0.90	0.34	55,55,55,55	7
86	OHX	1	3605	7/7	0.90	0.15	107,107,107,107	7
87	MG	5	4012	1/1	0.90	0.27	33,33,33,33	0
87	MG	5	4482	1/1	0.90	0.20	45,45,45,45	1
87	MG	1	4171	1/1	0.90	0.15	46,46,46,46	0
87	MG	5	4492	1/1	0.90	0.16	41,41,41,41	1
87	MG	6	2261	1/1	0.90	0.11	60,60,60,60	0
87	MG	1	3884	1/1	0.90	0.12	50,50,50,50	0
86	OHX	6	1981	7/7	0.90	0.30	45,45,45,45	7
87	MG	5	4027	1/1	0.90	0.24	41,41,41,41	0
86	OHX	2	1992	7/7	0.90	0.25	75,75,75,75	7
87	MG	Q0	203	1/1	0.90	0.33	52,52,52,52	0
87	MG	5	4524	1/1	0.90	0.07	47,47,47,47	0
86	OHX	6	1985	7/7	0.90	0.23	90,90,90,90	7
87	MG	5	4042	1/1	0.90	0.27	35,35,35,35	0
87	MG	5	4043	1/1	0.90	0.22	37,37,37,37	0
87	MG	5	4052	1/1	0.90	0.20	39,39,39,39	0
86	OHX	5	3662	7/7	0.90	0.34	45,45,45,45	7
86	OHX	1	3726	7/7	0.90	0.34	54,54,54,54	7
87	MG	5	4060	1/1	0.90	0.15	45,45,45,45	0
87	MG	5	4062	1/1	0.90	0.22	39,39,39,39	0
87	MG	1	4188	1/1	0.90	0.25	47,47,47,47	0
87	MG	5	4553	1/1	0.90	0.86	50,50,50,50	1
87	MG	5	4554	1/1	0.90	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2082	7/7	0.90	0.10	137,137,137,137	7
87	MG	1	4035	1/1	0.90	0.14	44,44,44,44	0
86	OHX	5	3608	7/7	0.90	0.31	44,44,44,44	7
87	MG	1	4044	1/1	0.90	0.29	69,69,69,69	0
87	MG	5	4564	1/1	0.90	0.24	34,34,34,34	1
87	MG	6	2110	1/1	0.90	0.18	82,82,82,82	0
87	MG	5	4079	1/1	0.90	0.15	44,44,44,44	0
87	MG	1	4199	1/1	0.90	0.23	46,46,46,46	0
87	MG	7	214	1/1	0.90	0.19	46,46,46,46	0
87	MG	1	4200	1/1	0.90	0.14	51,51,51,51	0
86	OHX	5	3754	7/7	0.90	0.08	161,161,161,161	7
86	OHX	1	3640	7/7	0.90	0.19	83,83,83,83	7
86	OHX	4	213	7/7	0.90	0.25	64,64,64,64	7
87	MG	7	237	1/1	0.90	0.26	53,53,53,53	1
87	MG	7	240	1/1	0.90	0.11	53,53,53,53	1
86	OHX	5	3757	7/7	0.90	0.20	75,75,75,75	7
87	MG	8	225	1/1	0.90	0.20	55,55,55,55	0
87	MG	1	4053	1/1	0.90	0.18	44,44,44,44	0
87	MG	1	4216	1/1	0.90	0.41	52,52,52,52	1
86	OHX	2	2021	7/7	0.90	0.23	72,72,72,72	7
87	MG	2	2256	1/1	0.90	0.10	66,66,66,66	0
86	OHX	5	3718	7/7	0.90	0.10	136,136,136,136	7
86	OHX	1	3648	7/7	0.90	0.29	65,65,65,65	7
86	OHX	5	3761	7/7	0.90	0.31	69,69,69,69	7
87	MG	6	2133	1/1	0.90	0.07	39,39,39,39	0
87	MG	1	3924	1/1	0.90	0.20	36,36,36,36	0
87	MG	l2	303	1/1	0.90	0.24	55,55,55,55	1
87	MG	1	4231	1/1	0.90	0.08	44,44,44,44	0
86	OHX	1	3615	7/7	0.90	0.22	68,68,68,68	7
87	MG	l3	403	1/1	0.90	0.34	26,26,26,26	0
87	MG	l3	414	1/1	0.90	0.12	32,32,32,32	1
87	MG	6	2141	1/1	0.90	0.16	40,40,40,40	0
87	MG	1	4070	1/1	0.90	0.14	70,70,70,70	0
87	MG	1	4241	1/1	0.90	0.23	57,57,57,57	0
87	MG	l7	304	1/1	0.90	0.19	49,49,49,49	1
87	MG	s8	305	1/1	0.90	0.14	56,56,56,56	0
87	MG	m0	305	1/1	0.90	0.29	32,32,32,32	0
87	MG	5	4151	1/1	0.90	0.19	52,52,52,52	0
87	MG	1	3932	1/1	0.90	0.24	28,28,28,28	0
86	OHX	5	3721	7/7	0.90	0.24	50,50,50,50	7
87	MG	1	4252	1/1	0.90	0.14	58,58,58,58	0
87	MG	5	4160	1/1	0.90	0.07	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2152	1/1	0.90	0.23	50,50,50,50	0
87	MG	C5	202	1/1	0.90	0.17	76,76,76,76	0
87	MG	n8	204	1/1	0.90	0.13	55,55,55,55	1
87	MG	5	4165	1/1	0.90	0.06	54,54,54,54	0
87	MG	o2	202	1/1	0.90	0.09	49,49,49,49	0
87	MG	o3	202	1/1	0.90	0.11	53,53,53,53	0
86	OHX	5	3622	7/7	0.90	0.24	74,74,74,74	7
87	MG	q2	503	1/1	0.90	0.13	42,42,42,42	1
86	OHX	5	3766	7/7	0.90	0.24	66,66,66,66	7
87	MG	1	4264	1/1	0.90	0.36	53,53,53,53	0
87	MG	1	3940	1/1	0.90	0.23	38,38,38,38	0
87	MG	1	4280	1/1	0.90	0.13	76,76,76,76	0
87	MG	5	4179	1/1	0.90	0.27	44,44,44,44	0
86	OHX	5	3814	7/7	0.90	0.17	70,70,70,70	7
87	MG	1	4285	1/1	0.90	0.17	52,52,52,52	0
86	OHX	1	3800	7/7	0.90	0.45	41,41,41,41	7
87	MG	5	3821	1/1	0.90	0.26	54,54,54,54	0
86	OHX	5	3816	7/7	0.90	0.31	43,43,43,43	7
87	MG	5	4195	1/1	0.90	0.45	35,35,35,35	1
87	MG	6	2167	1/1	0.91	0.20	55,55,55,55	0
87	MG	1	4042	1/1	0.91	0.15	50,50,50,50	0
86	OHX	5	3587	7/7	0.91	0.26	53,53,53,53	7
87	MG	1	3874	1/1	0.91	0.27	31,31,31,31	0
87	MG	5	3878	1/1	0.91	0.28	54,54,54,54	0
87	MG	5	3880	1/1	0.91	0.27	34,34,34,34	0
87	MG	5	4256	1/1	0.91	0.17	44,44,44,44	0
86	OHX	2	2003	7/7	0.91	0.14	103,103,103,103	7
87	MG	5	4263	1/1	0.91	0.24	32,32,32,32	1
86	OHX	1	3799	7/7	0.91	0.26	54,54,54,54	7
87	MG	1	3880	1/1	0.91	0.18	49,49,49,49	0
86	OHX	2	2011	7/7	0.91	0.22	69,69,69,69	7
86	OHX	6	2069	7/7	0.91	0.18	78,78,78,78	7
86	OHX	1	3801	7/7	0.91	0.25	57,57,57,57	7
87	MG	1	4236	1/1	0.91	0.14	52,52,52,52	0
87	MG	5	4292	1/1	0.91	0.19	37,37,37,37	0
86	OHX	l5	302	7/7	0.91	0.18	88,88,88,88	7
87	MG	1	4056	1/1	0.91	0.12	44,44,44,44	0
86	OHX	l5	303	7/7	0.91	0.20	69,69,69,69	7
87	MG	1	4063	1/1	0.91	0.30	53,53,53,53	0
87	MG	1	4255	1/1	0.91	0.21	48,48,48,48	0
87	MG	1	4508	1/1	0.91	0.33	37,37,37,37	1
87	MG	1	4256	1/1	0.91	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3767	7/7	0.91	0.34	45,45,45,45	7
87	MG	6	2196	1/1	0.91	0.15	45,45,45,45	1
87	MG	6	2197	1/1	0.91	0.28	60,60,60,60	0
86	OHX	5	3701	7/7	0.91	0.10	120,120,120,120	7
87	MG	5	3923	1/1	0.91	0.13	35,35,35,35	0
86	OHX	5	3772	7/7	0.91	0.15	115,115,115,115	7
87	MG	5	4328	1/1	0.91	0.15	53,53,53,53	0
86	OHX	1	3768	7/7	0.91	0.44	50,50,50,50	7
87	MG	6	2201	1/1	0.91	0.10	83,83,83,83	0
87	MG	3	218	1/1	0.91	0.31	35,35,35,35	0
87	MG	2	2152	1/1	0.91	0.12	88,88,88,88	0
87	MG	1	4276	1/1	0.91	0.29	37,37,37,37	0
86	OHX	1	3676	7/7	0.91	0.22	71,71,71,71	7
86	OHX	O3	201	7/7	0.91	0.31	49,49,49,49	7
86	OHX	6	1961	7/7	0.91	0.24	65,65,65,65	7
87	MG	1	4288	1/1	0.91	0.19	52,52,52,52	0
87	MG	1	4077	1/1	0.91	0.16	54,54,54,54	0
87	MG	5	4347	1/1	0.91	0.14	60,60,60,60	0
87	MG	1	4081	1/1	0.91	0.22	46,46,46,46	0
87	MG	1	3914	1/1	0.91	0.28	34,34,34,34	0
86	OHX	6	1966	7/7	0.91	0.28	56,56,56,56	7
86	OHX	1	3805	7/7	0.91	0.23	73,73,73,73	7
87	MG	2	2234	1/1	0.91	0.14	76,76,76,76	0
87	MG	4	222	1/1	0.91	0.37	46,46,46,46	0
86	OHX	5	3626	7/7	0.91	0.21	69,69,69,69	7
87	MG	5	4367	1/1	0.91	0.16	44,44,44,44	0
87	MG	6	2221	1/1	0.91	0.09	53,53,53,53	1
86	OHX	6	1971	7/7	0.91	0.22	85,85,85,85	7
86	OHX	5	3631	7/7	0.91	0.17	89,89,89,89	7
87	MG	5	4381	1/1	0.91	0.30	79,79,79,79	0
87	MG	1	4305	1/1	0.91	0.16	59,59,59,59	0
86	OHX	2	2012	7/7	0.91	0.14	102,102,102,102	7
87	MG	1	3927	1/1	0.91	0.33	40,40,40,40	0
87	MG	1	3931	1/1	0.91	0.23	41,41,41,41	0
87	MG	5	4395	1/1	0.91	0.12	41,41,41,41	0
87	MG	1	4312	1/1	0.91	0.19	41,41,41,41	0
87	MG	5	4404	1/1	0.91	0.22	38,38,38,38	1
86	OHX	6	1982	7/7	0.91	0.16	98,98,98,98	7
86	OHX	2	2015	7/7	0.91	0.17	87,87,87,87	7
86	OHX	5	3637	7/7	0.91	0.15	109,109,109,109	7
87	MG	5	4415	1/1	0.91	0.13	33,33,33,33	1
87	MG	1	4113	1/1	0.91	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3582	7/7	0.91	0.21	67,67,67,67	7
86	OHX	2	1988	7/7	0.91	0.22	80,80,80,80	7
86	OHX	2	2057	7/7	0.91	0.29	67,67,67,67	7
87	MG	5	3996	1/1	0.91	0.30	31,31,31,31	0
87	MG	1	4122	1/1	0.91	0.11	45,45,45,45	0
86	OHX	2	2074	7/7	0.91	0.22	92,92,92,92	7
87	MG	1	4342	1/1	0.91	0.17	58,58,58,58	0
86	OHX	2	2006	7/7	0.91	0.27	72,72,72,72	7
86	OHX	2	2032	7/7	0.91	0.19	82,82,82,82	7
86	OHX	6	2047	7/7	0.91	0.23	67,67,67,67	7
87	MG	5	4020	1/1	0.91	0.25	30,30,30,30	0
87	MG	5	4467	1/1	0.91	0.10	37,37,37,37	0
86	OHX	6	1999	7/7	0.91	0.18	85,85,85,85	7
87	MG	5	4023	1/1	0.91	0.25	32,32,32,32	0
86	OHX	2	2001	7/7	0.91	0.18	82,82,82,82	7
86	OHX	1	3690	7/7	0.91	0.29	66,66,66,66	7
87	MG	5	4479	1/1	0.91	0.24	56,56,56,56	1
87	MG	6	2266	1/1	0.91	0.11	71,71,71,71	0
87	MG	5	4030	1/1	0.91	0.42	34,34,34,34	0
87	MG	2	2108	1/1	0.91	0.46	59,59,59,59	0
87	MG	1	4354	1/1	0.91	0.09	62,62,62,62	0
87	MG	6	2269	1/1	0.91	0.15	89,89,89,89	0
87	MG	5	4040	1/1	0.91	0.21	35,35,35,35	0
87	MG	5	4504	1/1	0.91	0.18	39,39,39,39	1
87	MG	1	4355	1/1	0.91	0.25	67,67,67,67	0
86	OHX	1	3753	7/7	0.91	0.26	51,51,51,51	7
87	MG	1	4358	1/1	0.91	0.17	51,51,51,51	0
87	MG	O1	203	1/1	0.91	0.26	57,57,57,57	0
87	MG	1	4136	1/1	0.91	0.19	58,58,58,58	0
86	OHX	5	3656	7/7	0.91	0.33	58,58,58,58	7
86	OHX	2	2036	7/7	0.91	0.11	123,123,123,123	7
87	MG	1	4363	1/1	0.91	0.20	45,45,45,45	1
86	OHX	s4	301	7/7	0.91	0.22	79,79,79,79	7
87	MG	5	4536	1/1	0.91	0.39	42,42,42,42	1
87	MG	6	2284	1/1	0.91	0.29	59,59,59,59	0
87	MG	O5	202	1/1	0.91	0.23	54,54,54,54	1
86	OHX	5	3660	7/7	0.91	0.71	42,42,42,42	7
87	MG	1	4144	1/1	0.91	0.11	41,41,41,41	0
87	MG	5	4078	1/1	0.91	0.09	41,41,41,41	0
87	MG	1	4369	1/1	0.91	0.09	43,43,43,43	0
87	MG	1	4370	1/1	0.91	0.08	41,41,41,41	1
87	MG	1	3969	1/1	0.91	0.29	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4090	1/1	0.91	0.08	52,52,52,52	0
86	OHX	5	3661	7/7	0.91	0.24	50,50,50,50	7
86	OHX	1	3521	7/7	0.91	0.29	59,59,59,59	7
87	MG	6	2307	1/1	0.91	0.16	68,68,68,68	0
86	OHX	1	3694	7/7	0.91	0.18	85,85,85,85	7
86	OHX	1	3617	7/7	0.91	0.39	36,36,36,36	7
86	OHX	5	3669	7/7	0.91	0.32	37,37,37,37	7
87	MG	5	4577	1/1	0.91	0.19	44,44,44,44	0
87	MG	5	4101	1/1	0.91	0.07	49,49,49,49	0
87	MG	7	216	1/1	0.91	0.31	53,53,53,53	0
87	MG	6	2319	1/1	0.91	0.23	57,57,57,57	0
86	OHX	2	2048	7/7	0.91	0.22	83,83,83,83	7
87	MG	1	3980	1/1	0.91	0.22	54,54,54,54	0
87	MG	7	227	1/1	0.91	0.22	50,50,50,50	1
87	MG	1	4154	1/1	0.91	0.20	81,81,81,81	0
87	MG	7	236	1/1	0.91	0.11	44,44,44,44	0
87	MG	1	4155	1/1	0.91	0.12	54,54,54,54	0
87	MG	6	2114	1/1	0.91	0.23	49,49,49,49	0
87	MG	8	223	1/1	0.91	0.14	60,60,60,60	0
87	MG	6	2115	1/1	0.91	0.25	75,75,75,75	0
87	MG	1	3830	1/1	0.91	0.24	40,40,40,40	0
87	MG	1	3983	1/1	0.91	0.25	40,40,40,40	0
87	MG	1	4161	1/1	0.91	0.18	47,47,47,47	0
86	OHX	5	3509	7/7	0.91	0.24	66,66,66,66	7
87	MG	s8	303	1/1	0.91	0.24	46,46,46,46	0
87	MG	5	4142	1/1	0.91	0.08	40,40,40,40	0
86	OHX	5	3523	7/7	0.91	0.15	120,120,120,120	7
86	OHX	1	3547	7/7	0.91	0.32	56,56,56,56	7
86	OHX	1	3699	7/7	0.91	0.38	44,44,44,44	7
86	OHX	1	3625	7/7	0.91	0.33	61,61,61,61	7
86	OHX	5	3548	7/7	0.91	0.26	48,48,48,48	7
87	MG	5	4156	1/1	0.91	0.17	41,41,41,41	0
87	MG	6	2130	1/1	0.91	0.10	55,55,55,55	0
87	MG	1	4007	1/1	0.91	0.25	46,46,46,46	0
87	MG	1	4182	1/1	0.91	0.10	55,55,55,55	0
87	MG	l3	415	1/1	0.91	0.13	36,36,36,36	1
87	MG	1	4438	1/1	0.91	0.16	64,64,64,64	0
87	MG	6	2135	1/1	0.91	0.34	50,50,50,50	0
86	OHX	6	2016	7/7	0.91	0.14	91,91,91,91	7
87	MG	2	2200	1/1	0.91	0.22	65,65,65,65	0
87	MG	1	4443	1/1	0.91	0.21	41,41,41,41	1
87	MG	1	4444	1/1	0.91	0.23	41,41,41,41	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	m4	202	1/1	0.91	0.12	53,53,53,53	1
87	MG	1	4012	1/1	0.91	0.29	35,35,35,35	0
87	MG	2	2129	1/1	0.91	0.17	66,66,66,66	0
86	OHX	5	3561	7/7	0.91	0.31	51,51,51,51	7
87	MG	m8	1503	1/1	0.91	0.13	52,52,52,52	0
87	MG	1	3853	1/1	0.91	0.31	41,41,41,41	0
87	MG	n0	203	1/1	0.91	0.21	41,41,41,41	0
87	MG	6	2147	1/1	0.91	0.33	58,58,58,58	0
87	MG	n3	203	1/1	0.91	0.27	29,29,29,29	0
87	MG	5	4188	1/1	0.91	0.13	45,45,45,45	0
87	MG	1	4459	1/1	0.91	0.35	46,46,46,46	1
86	OHX	5	3564	7/7	0.91	0.26	89,89,89,89	7
86	OHX	5	3569	7/7	0.91	0.21	78,78,78,78	7
87	MG	5	4198	1/1	0.91	0.30	43,43,43,43	0
87	MG	o2	203	1/1	0.91	0.43	34,34,34,34	1
87	MG	1	4203	1/1	0.91	0.80	42,42,42,42	1
86	OHX	1	3553	7/7	0.91	0.24	60,60,60,60	7
86	OHX	5	3575	7/7	0.91	0.23	66,66,66,66	7
87	MG	5	4212	1/1	0.91	0.10	41,41,41,41	0
87	MG	5	4213	1/1	0.91	0.10	59,59,59,59	0
87	MG	1	4208	1/1	0.91	0.15	47,47,47,47	1
87	MG	1	4027	1/1	0.91	0.20	43,43,43,43	0
86	OHX	2	1980	7/7	0.91	0.21	93,93,93,93	7
87	MG	1	4473	1/1	0.91	0.21	51,51,51,51	0
86	OHX	5	3583	7/7	0.91	0.13	148,148,148,148	7
86	OHX	2	2050	7/7	0.91	0.16	96,96,96,96	7
87	MG	5	3866	1/1	0.91	0.05	34,34,34,34	0
87	MG	5	4229	1/1	0.91	0.17	43,43,43,43	0
87	MG	5	3868	1/1	0.91	0.21	36,36,36,36	0
87	MG	M7	203	1/1	0.92	0.39	36,36,36,36	0
87	MG	5	4280	1/1	0.92	0.08	39,39,39,39	0
87	MG	6	2228	1/1	0.92	0.13	59,59,59,59	1
87	MG	5	3933	1/1	0.92	0.20	46,46,46,46	0
86	OHX	L4	401	7/7	0.92	0.22	59,59,59,59	7
86	OHX	1	3555	7/7	0.92	0.21	89,89,89,89	7
86	OHX	5	3617	7/7	0.92	0.20	74,74,74,74	7
87	MG	5	4295	1/1	0.92	0.32	43,43,43,43	0
87	MG	5	3939	1/1	0.92	0.26	39,39,39,39	0
87	MG	N3	201	1/1	0.92	0.33	39,39,39,39	0
87	MG	1	4064	1/1	0.92	0.19	56,56,56,56	0
87	MG	5	3944	1/1	0.92	0.32	32,32,32,32	0
87	MG	N3	203	1/1	0.92	0.20	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2235	1/1	0.92	0.16	76,76,76,76	0
86	OHX	M0	301	7/7	0.92	0.31	49,49,49,49	7
87	MG	5	4315	1/1	0.92	0.59	31,31,31,31	1
87	MG	1	4414	1/1	0.92	0.16	50,50,50,50	1
87	MG	N8	203	1/1	0.92	0.20	33,33,33,33	0
86	OHX	5	3621	7/7	0.92	0.24	43,43,43,43	7
86	OHX	5	3680	7/7	0.92	0.30	38,38,38,38	7
87	MG	5	4326	1/1	0.92	0.16	53,53,53,53	0
87	MG	O2	202	1/1	0.92	0.29	32,32,32,32	0
87	MG	1	3936	1/1	0.92	0.39	31,31,31,31	0
87	MG	1	4223	1/1	0.92	0.28	37,37,37,37	1
86	OHX	1	3636	7/7	0.92	0.20	75,75,75,75	7
87	MG	1	3820	1/1	0.92	0.16	44,44,44,44	0
86	OHX	c1	201	7/7	0.92	0.21	79,79,79,79	7
87	MG	1	3822	1/1	0.92	0.28	34,34,34,34	0
86	OHX	2	1984	7/7	0.92	0.09	177,177,177,177	7
87	MG	Q0	202	1/1	0.92	0.15	54,54,54,54	0
87	MG	1	4230	1/1	0.92	0.27	41,41,41,41	1
87	MG	6	2263	1/1	0.92	0.17	40,40,40,40	0
87	MG	5	3978	1/1	0.92	0.32	40,40,40,40	0
87	MG	5	3979	1/1	0.92	0.27	48,48,48,48	0
86	OHX	c5	201	7/7	0.92	0.11	118,118,118,118	7
86	OHX	5	3628	7/7	0.92	0.23	66,66,66,66	7
87	MG	5	4350	1/1	0.92	0.15	44,44,44,44	1
87	MG	6	2100	1/1	0.92	0.07	60,60,60,60	0
87	MG	5	4352	1/1	0.92	0.13	54,54,54,54	1
87	MG	6	2101	1/1	0.92	0.31	39,39,39,39	0
87	MG	5	3985	1/1	0.92	0.41	50,50,50,50	0
87	MG	5	4356	1/1	0.92	0.15	45,45,45,45	0
87	MG	5	3991	1/1	0.92	0.24	34,34,34,34	0
87	MG	5	4360	1/1	0.92	0.20	50,50,50,50	0
87	MG	1	3831	1/1	0.92	0.21	44,44,44,44	0
87	MG	5	3993	1/1	0.92	0.34	29,29,29,29	0
87	MG	1	3948	1/1	0.92	0.20	34,34,34,34	0
87	MG	1	3833	1/1	0.92	0.22	84,84,84,84	0
87	MG	1	4091	1/1	0.92	0.11	39,39,39,39	0
86	OHX	5	3743	7/7	0.92	0.16	105,105,105,105	7
87	MG	5	4382	1/1	0.92	0.15	47,47,47,47	0
87	MG	5	4385	1/1	0.92	0.27	34,34,34,34	1
87	MG	6	2277	1/1	0.92	0.09	48,48,48,48	0
87	MG	5	4005	1/1	0.92	0.23	30,30,30,30	0
87	MG	1	4094	1/1	0.92	0.24	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4010	1/1	0.92	0.40	46,46,46,46	0
87	MG	1	4458	1/1	0.92	0.13	47,47,47,47	0
87	MG	5	4399	1/1	0.92	0.12	46,46,46,46	1
87	MG	5	4014	1/1	0.92	0.17	30,30,30,30	0
86	OHX	1	3511	7/7	0.92	0.24	66,66,66,66	7
86	OHX	6	2006	7/7	0.92	0.27	54,54,54,54	7
87	MG	1	4100	1/1	0.92	0.21	44,44,44,44	1
87	MG	1	3955	1/1	0.92	0.21	36,36,36,36	0
87	MG	6	2288	1/1	0.92	0.12	65,65,65,65	0
87	MG	6	2293	1/1	0.92	0.22	46,46,46,46	1
86	OHX	1	3608	7/7	0.92	0.22	51,51,51,51	7
87	MG	5	4421	1/1	0.92	0.16	46,46,46,46	0
87	MG	6	2296	1/1	0.92	0.16	54,54,54,54	1
87	MG	5	4033	1/1	0.92	0.17	43,43,43,43	0
87	MG	1	4104	1/1	0.92	0.28	52,52,52,52	0
87	MG	6	2118	1/1	0.92	0.23	38,38,38,38	0
87	MG	1	3960	1/1	0.92	0.27	43,43,43,43	0
87	MG	6	2120	1/1	0.92	0.29	43,43,43,43	0
87	MG	5	4454	1/1	0.92	0.21	47,47,47,47	0
87	MG	1	4274	1/1	0.92	0.14	43,43,43,43	1
87	MG	1	4471	1/1	0.92	0.38	33,33,33,33	1
87	MG	5	4048	1/1	0.92	0.14	34,34,34,34	0
87	MG	5	4050	1/1	0.92	0.11	42,42,42,42	0
87	MG	1	3961	1/1	0.92	0.37	37,37,37,37	0
86	OHX	5	3634	7/7	0.92	0.26	42,42,42,42	7
87	MG	5	4056	1/1	0.92	0.21	40,40,40,40	0
86	OHX	M8	201	7/7	0.92	0.28	53,53,53,53	7
87	MG	1	4284	1/1	0.92	0.13	50,50,50,50	0
87	MG	5	4061	1/1	0.92	0.17	51,51,51,51	0
87	MG	1	4110	1/1	0.92	0.30	51,51,51,51	0
87	MG	1	3844	1/1	0.92	0.22	39,39,39,39	0
86	OHX	1	3561	7/7	0.92	0.17	76,76,76,76	7
87	MG	1	3847	1/1	0.92	0.19	49,49,49,49	0
87	MG	6	2134	1/1	0.92	0.22	42,42,42,42	0
87	MG	1	4118	1/1	0.92	0.23	42,42,42,42	0
86	OHX	1	3786	7/7	0.92	0.27	73,73,73,73	7
86	OHX	5	3804	7/7	0.92	0.20	52,52,52,52	7
87	MG	5	4510	1/1	0.92	0.19	33,33,33,33	0
86	OHX	1	3565	7/7	0.92	0.20	84,84,84,84	7
87	MG	5	4085	1/1	0.92	0.07	57,57,57,57	0
87	MG	1	4298	1/1	0.92	0.14	53,53,53,53	0
87	MG	5	4087	1/1	0.92	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3641	7/7	0.92	0.31	52,52,52,52	7
86	OHX	5	3698	7/7	0.92	0.18	66,66,66,66	7
87	MG	s8	304	1/1	0.92	0.13	56,56,56,56	0
87	MG	1	4495	1/1	0.92	0.30	71,71,71,71	0
87	MG	1	3977	1/1	0.92	0.26	41,41,41,41	0
87	MG	1	4498	1/1	0.92	0.14	41,41,41,41	0
87	MG	1	4499	1/1	0.92	0.15	60,60,60,60	0
87	MG	1	3978	1/1	0.92	0.37	28,28,28,28	0
86	OHX	1	3649	7/7	0.92	0.23	52,52,52,52	7
86	OHX	2	2008	7/7	0.92	0.24	83,83,83,83	7
87	MG	1	4309	1/1	0.92	0.51	44,44,44,44	1
86	OHX	1	3535	7/7	0.92	0.33	47,47,47,47	7
87	MG	d2	201	1/1	0.92	0.22	46,46,46,46	0
87	MG	d3	201	1/1	0.92	0.19	47,47,47,47	0
87	MG	1	4511	1/1	0.92	0.11	52,52,52,52	0
87	MG	1	4512	1/1	0.92	0.07	41,41,41,41	0
86	OHX	1	3791	7/7	0.92	0.27	68,68,68,68	7
87	MG	5	4565	1/1	0.92	0.13	37,37,37,37	0
86	OHX	5	3565	7/7	0.92	0.21	72,72,72,72	7
87	MG	1	4138	1/1	0.92	0.11	46,46,46,46	0
87	MG	1	3987	1/1	0.92	0.19	40,40,40,40	0
86	OHX	1	3543	7/7	0.92	0.19	64,64,64,64	7
87	MG	5	4141	1/1	0.92	0.14	54,54,54,54	0
87	MG	7	215	1/1	0.92	0.30	27,27,27,27	0
87	MG	5	3824	1/1	0.92	0.16	39,39,39,39	0
87	MG	7	218	1/1	0.92	0.25	30,30,30,30	0
86	OHX	6	2019	7/7	0.92	0.25	55,55,55,55	7
86	OHX	5	3707	7/7	0.92	0.22	46,46,46,46	7
87	MG	5	3832	1/1	0.92	0.25	35,35,35,35	0
86	OHX	2	2025	7/7	0.92	0.17	94,94,94,94	7
87	MG	7	229	1/1	0.92	0.09	38,38,38,38	0
87	MG	7	232	1/1	0.92	0.09	50,50,50,50	0
87	MG	3	222	1/1	0.92	0.23	45,45,45,45	0
87	MG	6	2173	1/1	0.92	0.17	56,56,56,56	0
87	MG	5	4158	1/1	0.92	0.06	45,45,45,45	0
87	MG	7	239	1/1	0.92	0.15	50,50,50,50	1
87	MG	1	4003	1/1	0.92	0.30	44,44,44,44	0
87	MG	3	224	1/1	0.92	0.12	47,47,47,47	0
87	MG	1	4005	1/1	0.92	0.19	29,29,29,29	0
87	MG	2	2113	1/1	0.92	0.35	68,68,68,68	0
86	OHX	7	209	7/7	0.92	0.28	40,40,40,40	7
86	OHX	5	3577	7/7	0.92	0.23	53,53,53,53	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4172	1/1	0.92	0.21	40,40,40,40	0
87	MG	1	3883	1/1	0.92	0.26	48,48,48,48	0
87	MG	5	4175	1/1	0.92	0.12	86,86,86,86	0
86	OHX	2	1998	7/7	0.92	0.18	94,94,94,94	7
86	OHX	1	3585	7/7	0.92	0.29	54,54,54,54	7
86	OHX	2	2028	7/7	0.92	0.11	134,134,134,134	7
87	MG	1	3893	1/1	0.92	0.29	51,51,51,51	0
86	OHX	6	2088	7/7	0.92	0.23	71,71,71,71	7
87	MG	1	3895	1/1	0.92	0.19	44,44,44,44	0
87	MG	6	2193	1/1	0.92	0.12	57,57,57,57	0
86	OHX	5	3594	7/7	0.92	0.29	42,42,42,42	7
87	MG	l3	407	1/1	0.92	0.29	38,38,38,38	1
87	MG	5	4190	1/1	0.92	0.18	44,44,44,44	1
87	MG	6	2195	1/1	0.92	0.24	46,46,46,46	0
87	MG	5	3877	1/1	0.92	0.27	38,38,38,38	0
87	MG	1	3897	1/1	0.92	0.21	43,43,43,43	0
87	MG	4	230	1/1	0.92	0.14	47,47,47,47	0
87	MG	l7	303	1/1	0.92	0.17	34,34,34,34	1
86	OHX	5	3716	7/7	0.92	0.25	60,60,60,60	7
87	MG	l7	307	1/1	0.92	0.14	38,38,38,38	1
87	MG	5	4205	1/1	0.92	0.13	60,60,60,60	0
87	MG	4	233	1/1	0.92	0.15	43,43,43,43	1
87	MG	m3	201	1/1	0.92	0.46	55,55,55,55	1
86	OHX	5	3771	7/7	0.92	0.28	60,60,60,60	7
87	MG	4	235	1/1	0.92	0.13	90,90,90,90	1
87	MG	5	3894	1/1	0.92	0.12	40,40,40,40	1
86	OHX	1	3596	7/7	0.92	0.22	70,70,70,70	7
87	MG	1	4034	1/1	0.92	0.15	54,54,54,54	0
86	OHX	5	3604	7/7	0.92	0.24	70,70,70,70	7
87	MG	1	4041	1/1	0.92	0.19	33,33,33,33	0
87	MG	5	3903	1/1	0.92	0.13	61,61,61,61	0
86	OHX	1	3709	7/7	0.92	0.26	59,59,59,59	7
86	OHX	1	3602	7/7	0.92	0.09	152,152,152,152	7
87	MG	5	3906	1/1	0.92	0.20	48,48,48,48	0
87	MG	2	2127	1/1	0.92	0.26	60,60,60,60	0
87	MG	5	4233	1/1	0.92	0.30	58,58,58,58	1
87	MG	n8	206	1/1	0.92	0.14	37,37,37,37	1
87	MG	n9	102	1/1	0.92	0.12	37,37,37,37	0
87	MG	5	4235	1/1	0.92	0.24	38,38,38,38	0
86	OHX	5	3665	7/7	0.92	0.37	47,47,47,47	7
86	OHX	5	3666	7/7	0.92	0.27	65,65,65,65	7
86	OHX	1	3711	7/7	0.92	0.22	67,67,67,67	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4244	1/1	0.92	0.22	58,58,58,58	0
87	MG	5	4247	1/1	0.92	0.22	37,37,37,37	0
87	MG	1	4388	1/1	0.92	0.28	35,35,35,35	1
87	MG	1	4394	1/1	0.92	0.17	41,41,41,41	1
87	MG	5	4253	1/1	0.92	0.09	44,44,44,44	0
87	MG	1	3918	1/1	0.92	0.16	57,57,57,57	0
87	MG	5	3920	1/1	0.92	0.14	41,41,41,41	0
86	OHX	14	402	7/7	0.92	0.25	55,55,55,55	7
86	OHX	1	3779	7/7	0.92	0.28	50,50,50,50	7
86	OHX	6	2032	7/7	0.92	0.22	61,61,61,61	7
87	MG	1	4403	1/1	0.92	0.21	65,65,65,65	0
87	MG	5	4273	1/1	0.92	0.14	34,34,34,34	1
87	MG	6	2226	1/1	0.93	0.11	107,107,107,107	0
87	MG	5	4258	1/1	0.93	0.11	57,57,57,57	0
87	MG	5	3936	1/1	0.93	0.24	28,28,28,28	0
87	MG	5	4262	1/1	0.93	0.12	39,39,39,39	0
87	MG	6	2227	1/1	0.93	0.12	52,52,52,52	0
86	OHX	2	1999	7/7	0.93	0.17	94,94,94,94	7
86	OHX	1	3607	7/7	0.93	0.27	55,55,55,55	7
87	MG	5	4271	1/1	0.93	0.21	40,40,40,40	1
86	OHX	2	1950	7/7	0.93	0.19	97,97,97,97	7
87	MG	1	4164	1/1	0.93	0.23	62,62,62,62	0
87	MG	5	4279	1/1	0.93	0.31	36,36,36,36	1
87	MG	M1	202	1/1	0.93	0.21	72,72,72,72	0
87	MG	2	2221	1/1	0.93	0.12	61,61,61,61	0
86	OHX	1	3810	7/7	0.93	0.18	62,62,62,62	7
87	MG	1	4017	1/1	0.93	0.20	35,35,35,35	0
87	MG	5	3949	1/1	0.93	0.24	28,28,28,28	0
87	MG	6	2237	1/1	0.93	0.19	55,55,55,55	0
87	MG	5	3954	1/1	0.93	0.24	40,40,40,40	0
87	MG	M6	201	1/1	0.93	0.26	40,40,40,40	1
87	MG	5	4299	1/1	0.93	0.13	47,47,47,47	0
87	MG	1	4374	1/1	0.93	0.16	44,44,44,44	0
87	MG	5	3959	1/1	0.93	0.28	35,35,35,35	0
87	MG	5	3960	1/1	0.93	0.26	37,37,37,37	0
87	MG	5	3962	1/1	0.93	0.25	44,44,44,44	0
86	OHX	6	1979	7/7	0.93	0.16	79,79,79,79	7
87	MG	1	4379	1/1	0.93	0.12	33,33,33,33	0
87	MG	1	4380	1/1	0.93	0.13	30,30,30,30	0
87	MG	5	4316	1/1	0.93	0.11	74,74,74,74	0
87	MG	6	2244	1/1	0.93	0.17	53,53,53,53	0
87	MG	1	4382	1/1	0.93	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4386	1/1	0.93	0.12	53,53,53,53	0
87	MG	5	4323	1/1	0.93	0.19	36,36,36,36	1
86	OHX	6	2091	7/7	0.93	0.13	96,96,96,96	7
87	MG	5	3972	1/1	0.93	0.27	31,31,31,31	0
86	OHX	6	1980	7/7	0.93	0.23	61,61,61,61	7
87	MG	1	4179	1/1	0.93	0.18	53,53,53,53	1
87	MG	1	4180	1/1	0.93	0.07	58,58,58,58	0
87	MG	6	2257	1/1	0.93	0.15	72,72,72,72	0
87	MG	1	3887	1/1	0.93	0.28	31,31,31,31	0
87	MG	N8	204	1/1	0.93	0.10	48,48,48,48	0
87	MG	N9	102	1/1	0.93	0.12	38,38,38,38	0
86	OHX	2	1986	7/7	0.93	0.21	80,80,80,80	7
86	OHX	1	3613	7/7	0.93	0.24	62,62,62,62	7
87	MG	O1	205	1/1	0.93	0.17	65,65,65,65	0
87	MG	5	3984	1/1	0.93	0.17	50,50,50,50	0
86	OHX	2	1971	7/7	0.93	0.25	80,80,80,80	7
87	MG	5	3986	1/1	0.93	0.25	35,35,35,35	0
87	MG	5	3988	1/1	0.93	0.15	28,28,28,28	0
87	MG	5	3990	1/1	0.93	0.18	57,57,57,57	0
87	MG	O2	203	1/1	0.93	0.15	44,44,44,44	1
86	OHX	1	3563	7/7	0.93	0.29	50,50,50,50	7
86	OHX	6	1988	7/7	0.93	0.25	57,57,57,57	7
86	OHX	3	202	7/7	0.93	0.28	48,48,48,48	7
86	OHX	3	206	7/7	0.93	0.21	81,81,81,81	7
86	OHX	5	3639	7/7	0.93	0.10	138,138,138,138	7
87	MG	5	4000	1/1	0.93	0.23	34,34,34,34	0
87	MG	1	4418	1/1	0.93	0.18	60,60,60,60	1
87	MG	5	4361	1/1	0.93	0.20	37,37,37,37	1
87	MG	5	4003	1/1	0.93	0.28	27,27,27,27	0
87	MG	5	4366	1/1	0.93	0.25	41,41,41,41	0
87	MG	O7	105	1/1	0.93	0.12	51,51,51,51	0
87	MG	1	4421	1/1	0.93	0.33	41,41,41,41	1
87	MG	2	2240	1/1	0.93	0.27	66,66,66,66	0
87	MG	5	4373	1/1	0.93	0.28	38,38,38,38	1
86	OHX	SR	401	7/7	0.93	0.10	130,130,130,130	7
86	OHX	6	1994	7/7	0.93	0.16	76,76,76,76	7
87	MG	5	4013	1/1	0.93	0.28	39,39,39,39	0
86	OHX	5	3643	7/7	0.93	0.30	53,53,53,53	7
87	MG	2	2246	1/1	0.93	0.19	77,77,77,77	0
87	MG	5	4018	1/1	0.93	0.12	34,34,34,34	0
87	MG	5	4391	1/1	0.93	0.12	52,52,52,52	0
86	OHX	6	1996	7/7	0.93	0.15	90,90,90,90	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2289	1/1	0.93	0.20	57,57,57,57	0
87	MG	1	4429	1/1	0.93	0.16	49,49,49,49	1
87	MG	5	4396	1/1	0.93	0.16	52,52,52,52	1
86	OHX	2	1979	7/7	0.93	0.18	75,75,75,75	7
87	MG	2	2091	1/1	0.93	0.24	44,44,44,44	0
86	OHX	5	3717	7/7	0.93	0.24	56,56,56,56	7
87	MG	5	4028	1/1	0.93	0.30	38,38,38,38	0
87	MG	5	4412	1/1	0.93	0.22	39,39,39,39	0
87	MG	6	2107	1/1	0.93	0.19	47,47,47,47	0
87	MG	5	4032	1/1	0.93	0.08	49,49,49,49	0
87	MG	1	4218	1/1	0.93	0.14	50,50,50,50	0
86	OHX	2	2004	7/7	0.93	0.15	89,89,89,89	7
86	OHX	1	3621	7/7	0.93	0.19	73,73,73,73	7
87	MG	1	4065	1/1	0.93	0.19	50,50,50,50	0
86	OHX	2	1935	7/7	0.93	0.13	98,98,98,98	7
86	OHX	4	208	7/7	0.93	0.15	85,85,85,85	7
87	MG	5	4426	1/1	0.93	0.09	62,62,62,62	0
87	MG	5	4427	1/1	0.93	0.20	39,39,39,39	1
86	OHX	4	210	7/7	0.93	0.17	101,101,101,101	7
87	MG	5	4429	1/1	0.93	0.27	37,37,37,37	1
87	MG	1	3926	1/1	0.93	0.25	34,34,34,34	0
87	MG	5	4049	1/1	0.93	0.13	48,48,48,48	0
86	OHX	5	3652	7/7	0.93	0.19	65,65,65,65	7
86	OHX	5	3653	7/7	0.93	0.20	64,64,64,64	7
87	MG	5	4053	1/1	0.93	0.35	44,44,44,44	0
87	MG	1	4073	1/1	0.93	0.12	37,37,37,37	0
86	OHX	6	2004	7/7	0.93	0.26	54,54,54,54	7
87	MG	1	4461	1/1	0.93	0.17	54,54,54,54	1
86	OHX	4	211	7/7	0.93	0.13	99,99,99,99	7
87	MG	6	2331	1/1	0.93	0.10	76,76,76,76	0
87	MG	5	4472	1/1	0.93	0.07	42,42,42,42	0
87	MG	1	4237	1/1	0.93	0.38	54,54,54,54	0
87	MG	1	4240	1/1	0.93	0.15	46,46,46,46	0
86	OHX	1	3530	7/7	0.93	0.17	67,67,67,67	7
87	MG	5	4068	1/1	0.93	0.29	42,42,42,42	0
87	MG	5	4069	1/1	0.93	0.13	50,50,50,50	0
87	MG	S6	301	1/1	0.93	0.08	103,103,103,103	0
87	MG	5	4484	1/1	0.93	0.11	39,39,39,39	1
86	OHX	1	3626	7/7	0.93	0.17	84,84,84,84	7
87	MG	5	4489	1/1	0.93	0.08	57,57,57,57	0
87	MG	1	4251	1/1	0.93	0.59	45,45,45,45	1
87	MG	5	4075	1/1	0.93	0.23	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2061	7/7	0.93	0.14	102,102,102,102	7
87	MG	1	4086	1/1	0.93	0.08	57,57,57,57	0
87	MG	1	4474	1/1	0.93	0.23	55,55,55,55	0
87	MG	5	4082	1/1	0.93	0.17	62,62,62,62	0
87	MG	5	4083	1/1	0.93	0.23	36,36,36,36	1
87	MG	5	4084	1/1	0.93	0.17	41,41,41,41	0
87	MG	C8	203	1/1	0.93	0.12	96,96,96,96	0
87	MG	D0	201	1/1	0.93	0.34	71,71,71,71	0
87	MG	c8	203	1/1	0.93	0.05	86,86,86,86	0
87	MG	1	4089	1/1	0.93	0.08	44,44,44,44	0
87	MG	1	4480	1/1	0.93	0.13	48,48,48,48	0
87	MG	D4	201	1/1	0.93	0.22	83,83,83,83	0
87	MG	2	2107	1/1	0.93	0.28	60,60,60,60	0
87	MG	5	4096	1/1	0.93	0.11	34,34,34,34	0
86	OHX	1	3750	7/7	0.93	0.27	46,46,46,46	7
87	MG	1	4095	1/1	0.93	0.09	41,41,41,41	0
86	OHX	6	2009	7/7	0.93	0.27	56,56,56,56	7
87	MG	1	4488	1/1	0.93	0.10	55,55,55,55	0
87	MG	6	2149	1/1	0.93	0.35	65,65,65,65	0
87	MG	1	4277	1/1	0.93	0.12	37,37,37,37	0
87	MG	5	4105	1/1	0.93	0.16	38,38,38,38	0
87	MG	1	4098	1/1	0.93	0.18	46,46,46,46	0
87	MG	1	4281	1/1	0.93	0.11	40,40,40,40	0
87	MG	5	4562	1/1	0.93	0.12	68,68,68,68	0
87	MG	5	4112	1/1	0.93	0.11	28,28,28,28	0
86	OHX	1	3579	7/7	0.93	0.29	53,53,53,53	7
86	OHX	5	3737	7/7	0.93	0.21	73,73,73,73	7
87	MG	5	4125	1/1	0.93	0.19	38,38,38,38	0
86	OHX	5	3571	7/7	0.93	0.22	62,62,62,62	7
87	MG	5	4573	1/1	0.93	0.12	30,30,30,30	0
87	MG	1	4287	1/1	0.93	0.51	40,40,40,40	1
87	MG	5	3828	1/1	0.93	0.25	54,54,54,54	0
87	MG	1	4102	1/1	0.93	0.31	44,44,44,44	0
87	MG	5	4136	1/1	0.93	0.31	48,48,48,48	0
87	MG	5	3831	1/1	0.93	0.28	43,43,43,43	0
87	MG	7	217	1/1	0.93	0.38	43,43,43,43	0
86	OHX	2	2031	7/7	0.93	0.17	90,90,90,90	7
87	MG	1	4500	1/1	0.93	0.15	49,49,49,49	0
87	MG	7	221	1/1	0.93	0.10	41,41,41,41	0
87	MG	1	3954	1/1	0.93	0.22	47,47,47,47	0
87	MG	5	3835	1/1	0.93	0.19	37,37,37,37	0
87	MG	7	226	1/1	0.93	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	3837	1/1	0.93	0.29	33,33,33,33	0
87	MG	5	4146	1/1	0.93	0.07	43,43,43,43	0
86	OHX	1	3584	7/7	0.93	0.14	106,106,106,106	7
87	MG	7	234	1/1	0.93	0.08	45,45,45,45	0
87	MG	1	3957	1/1	0.93	0.16	34,34,34,34	0
87	MG	1	4507	1/1	0.93	0.32	36,36,36,36	1
86	OHX	1	3678	7/7	0.93	0.24	44,44,44,44	7
86	OHX	5	3579	7/7	0.93	0.17	55,55,55,55	7
87	MG	5	4157	1/1	0.93	0.31	51,51,51,51	0
86	OHX	1	3679	7/7	0.93	0.30	42,42,42,42	7
86	OHX	1	3539	7/7	0.93	0.12	147,147,147,147	7
86	OHX	1	3635	7/7	0.93	0.29	45,45,45,45	7
87	MG	8	226	1/1	0.93	0.11	63,63,63,63	0
87	MG	5	4163	1/1	0.93	0.16	59,59,59,59	0
87	MG	1	3832	1/1	0.93	0.16	39,39,39,39	0
86	OHX	2	1993	7/7	0.93	0.20	80,80,80,80	7
87	MG	5	3857	1/1	0.93	0.11	47,47,47,47	0
87	MG	5	4169	1/1	0.93	0.08	43,43,43,43	0
87	MG	1	4119	1/1	0.93	0.19	52,52,52,52	0
86	OHX	5	3590	7/7	0.93	0.17	83,83,83,83	7
87	MG	8	238	1/1	0.93	0.16	45,45,45,45	0
87	MG	2	2195	1/1	0.93	0.34	65,65,65,65	0
87	MG	1	3837	1/1	0.93	0.29	41,41,41,41	0
86	OHX	1	3595	7/7	0.93	0.17	95,95,95,95	7
86	OHX	5	3596	7/7	0.93	0.23	43,43,43,43	7
87	MG	1	3840	1/1	0.93	0.20	43,43,43,43	0
87	MG	5	4181	1/1	0.93	0.14	55,55,55,55	0
87	MG	13	405	1/1	0.93	0.10	35,35,35,35	0
87	MG	1	4324	1/1	0.93	0.15	54,54,54,54	0
87	MG	13	409	1/1	0.93	0.09	41,41,41,41	1
87	MG	5	4183	1/1	0.93	0.12	54,54,54,54	0
87	MG	6	2188	1/1	0.93	0.15	52,52,52,52	0
87	MG	5	3879	1/1	0.93	0.24	33,33,33,33	0
86	OHX	5	3679	7/7	0.93	0.29	47,47,47,47	7
86	OHX	2	2059	7/7	0.93	0.28	66,66,66,66	7
86	OHX	5	3602	7/7	0.93	0.22	86,86,86,86	7
86	OHX	1	3598	7/7	0.93	0.19	100,100,100,100	7
87	MG	17	306	1/1	0.93	0.22	37,37,37,37	1
87	MG	1	4332	1/1	0.93	0.25	37,37,37,37	1
87	MG	1	4132	1/1	0.93	0.15	51,51,51,51	0
87	MG	19	204	1/1	0.93	0.16	41,41,41,41	1
87	MG	4	219	1/1	0.93	0.35	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4199	1/1	0.93	0.14	41,41,41,41	0
87	MG	1	4337	1/1	0.93	0.18	42,42,42,42	0
87	MG	1	3846	1/1	0.93	0.16	35,35,35,35	0
87	MG	m7	202	1/1	0.93	0.33	36,36,36,36	0
87	MG	5	4207	1/1	0.93	0.39	62,62,62,62	0
87	MG	5	3900	1/1	0.93	0.30	41,41,41,41	0
86	OHX	1	3641	7/7	0.93	0.19	89,89,89,89	7
86	OHX	8	206	7/7	0.93	0.16	94,94,94,94	7
87	MG	1	3986	1/1	0.93	0.14	54,54,54,54	0
87	MG	1	4346	1/1	0.93	0.14	48,48,48,48	1
86	OHX	1	3687	7/7	0.93	0.19	61,61,61,61	7
87	MG	5	4219	1/1	0.93	0.11	39,39,39,39	0
87	MG	5	4221	1/1	0.93	0.20	54,54,54,54	0
87	MG	5	4222	1/1	0.93	0.10	49,49,49,49	0
87	MG	1	3988	1/1	0.93	0.08	42,42,42,42	0
87	MG	2	2206	1/1	0.93	0.09	58,58,58,58	0
86	OHX	8	210	7/7	0.93	0.29	49,49,49,49	7
87	MG	o2	201	1/1	0.93	0.14	35,35,35,35	1
86	OHX	1	3644	7/7	0.93	0.18	91,91,91,91	7
87	MG	1	3997	1/1	0.93	0.35	43,43,43,43	0
87	MG	6	2211	1/1	0.93	0.07	50,50,50,50	0
87	MG	1	4353	1/1	0.93	0.11	59,59,59,59	0
87	MG	5	3919	1/1	0.93	0.17	44,44,44,44	0
87	MG	1	3999	1/1	0.93	0.27	32,32,32,32	0
86	OHX	8	214	7/7	0.93	0.18	100,100,100,100	7
86	OHX	2	1947	7/7	0.93	0.10	130,130,130,130	7
87	MG	5	3925	1/1	0.93	0.17	43,43,43,43	1
86	OHX	1	3603	7/7	0.93	0.10	128,128,128,128	7
87	MG	5	4245	1/1	0.93	0.07	65,65,65,65	0
86	OHX	1	3552	7/7	0.93	0.26	60,60,60,60	7
86	OHX	2	1983	7/7	0.93	0.16	70,70,70,70	7
87	MG	L2	303	1/1	0.93	0.07	53,53,53,53	0
86	OHX	6	1945	7/7	0.93	0.24	58,58,58,58	7
86	OHX	6	2083	7/7	0.93	0.20	82,82,82,82	7
87	MG	1	4362	1/1	0.94	0.20	42,42,42,42	0
87	MG	5	4267	1/1	0.94	0.11	38,38,38,38	0
87	MG	5	3950	1/1	0.94	0.41	36,36,36,36	0
87	MG	1	4021	1/1	0.94	0.32	37,37,37,37	0
87	MG	L4	408	1/1	0.94	0.22	34,34,34,34	1
87	MG	5	3955	1/1	0.94	0.32	32,32,32,32	0
87	MG	5	4277	1/1	0.94	0.14	35,35,35,35	1
87	MG	L7	302	1/1	0.94	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	L7	303	1/1	0.94	0.10	42,42,42,42	0
86	OHX	1	3546	7/7	0.94	0.20	52,52,52,52	7
86	OHX	5	3541	7/7	0.94	0.26	55,55,55,55	7
86	OHX	2	1976	7/7	0.94	0.21	92,92,92,92	7
87	MG	M0	307	1/1	0.94	0.18	45,45,45,45	0
87	MG	1	4368	1/1	0.94	0.09	38,38,38,38	0
87	MG	1	4175	1/1	0.94	0.27	46,46,46,46	0
86	OHX	1	3551	7/7	0.94	0.18	65,65,65,65	7
87	MG	1	4177	1/1	0.94	0.13	49,49,49,49	1
87	MG	1	4028	1/1	0.94	0.17	48,48,48,48	0
87	MG	1	4030	1/1	0.94	0.20	46,46,46,46	0
87	MG	M6	204	1/1	0.94	0.18	39,39,39,39	1
87	MG	1	4031	1/1	0.94	0.31	44,44,44,44	0
87	MG	5	3974	1/1	0.94	0.25	36,36,36,36	0
86	OHX	2	2068	7/7	0.94	0.22	66,66,66,66	7
87	MG	M7	209	1/1	0.94	0.10	42,42,42,42	0
86	OHX	5	3554	7/7	0.94	0.18	57,57,57,57	7
86	OHX	5	3557	7/7	0.94	0.19	49,49,49,49	7
87	MG	5	4318	1/1	0.94	0.28	64,64,64,64	0
87	MG	N0	202	1/1	0.94	0.21	51,51,51,51	1
87	MG	5	4320	1/1	0.94	0.22	35,35,35,35	1
87	MG	6	2259	1/1	0.94	0.05	48,48,48,48	0
87	MG	1	4186	1/1	0.94	0.10	43,43,43,43	0
87	MG	5	4324	1/1	0.94	0.16	42,42,42,42	1
87	MG	1	3902	1/1	0.94	0.19	43,43,43,43	0
87	MG	1	4393	1/1	0.94	0.19	49,49,49,49	0
87	MG	1	4190	1/1	0.94	0.10	65,65,65,65	0
87	MG	1	4037	1/1	0.94	0.31	45,45,45,45	0
87	MG	1	4397	1/1	0.94	0.17	38,38,38,38	1
87	MG	1	4038	1/1	0.94	0.21	45,45,45,45	0
87	MG	1	4039	1/1	0.94	0.15	32,32,32,32	0
87	MG	N8	206	1/1	0.94	0.26	39,39,39,39	0
87	MG	N8	208	1/1	0.94	0.18	45,45,45,45	1
86	OHX	1	3628	7/7	0.94	0.14	74,74,74,74	7
87	MG	5	4339	1/1	0.94	0.23	43,43,43,43	0
86	OHX	6	1944	7/7	0.94	0.16	60,60,60,60	7
86	OHX	2	1962	7/7	0.94	0.15	97,97,97,97	7
87	MG	5	3997	1/1	0.94	0.20	31,31,31,31	0
86	OHX	5	3566	7/7	0.94	0.20	96,96,96,96	7
87	MG	1	4204	1/1	0.94	0.12	60,60,60,60	0
87	MG	5	4001	1/1	0.94	0.24	36,36,36,36	0
87	MG	1	4407	1/1	0.94	0.39	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2021	7/7	0.94	0.19	53,53,53,53	7
87	MG	1	4412	1/1	0.94	0.24	32,32,32,32	1
87	MG	1	3915	1/1	0.94	0.18	48,48,48,48	0
87	MG	6	2285	1/1	0.94	0.21	68,68,68,68	1
87	MG	5	4009	1/1	0.94	0.22	38,38,38,38	0
87	MG	6	2286	1/1	0.94	0.18	65,65,65,65	0
86	OHX	5	3794	7/7	0.94	0.20	57,57,57,57	7
87	MG	1	4416	1/1	0.94	0.20	60,60,60,60	0
86	OHX	6	1959	7/7	0.94	0.24	57,57,57,57	7
87	MG	5	4363	1/1	0.94	0.08	42,42,42,42	0
87	MG	6	2292	1/1	0.94	0.67	50,50,50,50	1
86	OHX	1	3599	7/7	0.94	0.21	42,42,42,42	7
87	MG	O7	106	1/1	0.94	0.12	59,59,59,59	0
87	MG	1	3919	1/1	0.94	0.20	42,42,42,42	0
87	MG	6	2297	1/1	0.94	0.19	70,70,70,70	1
87	MG	6	2299	1/1	0.94	0.26	59,59,59,59	0
87	MG	5	4374	1/1	0.94	0.11	45,45,45,45	1
87	MG	5	4375	1/1	0.94	0.18	61,61,61,61	0
86	OHX	6	1963	7/7	0.94	0.19	72,72,72,72	7
87	MG	5	4378	1/1	0.94	0.17	55,55,55,55	0
86	OHX	1	3743	7/7	0.94	0.17	76,76,76,76	7
86	OHX	5	3732	7/7	0.94	0.20	49,49,49,49	7
87	MG	Q2	504	1/1	0.94	0.12	50,50,50,50	0
87	MG	5	4031	1/1	0.94	0.55	30,30,30,30	0
87	MG	5	4387	1/1	0.94	0.12	45,45,45,45	0
86	OHX	5	3733	7/7	0.94	0.19	57,57,57,57	7
86	OHX	5	3734	7/7	0.94	0.20	70,70,70,70	7
86	OHX	5	3802	7/7	0.94	0.22	55,55,55,55	7
87	MG	5	4393	1/1	0.94	0.16	34,34,34,34	0
86	OHX	6	2026	7/7	0.94	0.10	151,151,151,151	7
87	MG	6	2103	1/1	0.94	0.16	66,66,66,66	0
87	MG	6	2315	1/1	0.94	0.10	54,54,54,54	0
87	MG	5	4397	1/1	0.94	0.37	38,38,38,38	1
87	MG	5	4041	1/1	0.94	0.16	51,51,51,51	0
87	MG	6	2316	1/1	0.94	0.17	60,60,60,60	1
87	MG	5	4402	1/1	0.94	0.16	42,42,42,42	1
86	OHX	1	3601	7/7	0.94	0.26	49,49,49,49	7
86	OHX	6	1969	7/7	0.94	0.18	68,68,68,68	7
87	MG	D9	104	1/1	0.94	0.11	85,85,85,85	0
87	MG	1	3935	1/1	0.94	0.36	32,32,32,32	0
87	MG	6	2322	1/1	0.94	0.14	62,62,62,62	0
86	OHX	1	3451	7/7	0.94	0.22	77,77,77,77	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4054	1/1	0.94	0.23	50,50,50,50	0
87	MG	6	2324	1/1	0.94	0.21	47,47,47,47	1
87	MG	5	4420	1/1	0.94	0.19	40,40,40,40	1
86	OHX	3	207	7/7	0.94	0.14	85,85,85,85	7
87	MG	1	4235	1/1	0.94	0.14	49,49,49,49	1
87	MG	1	4447	1/1	0.94	0.15	44,44,44,44	0
86	OHX	2	1963	7/7	0.94	0.18	83,83,83,83	7
87	MG	1	4075	1/1	0.94	0.15	43,43,43,43	0
87	MG	5	4063	1/1	0.94	0.10	37,37,37,37	0
87	MG	1	4239	1/1	0.94	0.08	45,45,45,45	0
87	MG	5	4430	1/1	0.94	0.12	45,45,45,45	0
87	MG	5	4433	1/1	0.94	0.20	45,45,45,45	1
87	MG	5	4065	1/1	0.94	0.14	39,39,39,39	0
86	OHX	5	3591	7/7	0.94	0.21	52,52,52,52	7
86	OHX	5	3593	7/7	0.94	0.28	44,44,44,44	7
87	MG	5	4446	1/1	0.94	0.15	45,45,45,45	0
87	MG	5	4449	1/1	0.94	0.17	48,48,48,48	0
87	MG	1	4080	1/1	0.94	0.26	51,51,51,51	0
87	MG	5	4070	1/1	0.94	0.12	49,49,49,49	0
87	MG	1	4248	1/1	0.94	0.26	55,55,55,55	0
86	OHX	2	1949	7/7	0.94	0.12	108,108,108,108	7
87	MG	5	4459	1/1	0.94	0.12	36,36,36,36	1
87	MG	5	4462	1/1	0.94	0.11	54,54,54,54	0
87	MG	1	4250	1/1	0.94	0.10	53,53,53,53	1
87	MG	6	2122	1/1	0.94	0.16	49,49,49,49	0
86	OHX	2	1955	7/7	0.94	0.17	91,91,91,91	7
87	MG	5	4471	1/1	0.94	0.13	55,55,55,55	0
87	MG	5	4077	1/1	0.94	0.07	34,34,34,34	0
87	MG	1	3944	1/1	0.94	0.21	35,35,35,35	0
86	OHX	1	3523	7/7	0.94	0.18	95,95,95,95	7
87	MG	5	4080	1/1	0.94	0.13	37,37,37,37	0
87	MG	5	4478	1/1	0.94	0.24	33,33,33,33	0
87	MG	1	3825	1/1	0.94	0.25	38,38,38,38	0
86	OHX	1	3751	7/7	0.94	0.09	146,146,146,146	7
87	MG	1	4470	1/1	0.94	0.36	35,35,35,35	1
87	MG	1	3828	1/1	0.94	0.16	40,40,40,40	0
87	MG	1	4260	1/1	0.94	0.09	40,40,40,40	0
86	OHX	1	3715	7/7	0.94	0.20	77,77,77,77	7
86	OHX	7	208	7/7	0.94	0.25	54,54,54,54	7
87	MG	1	4475	1/1	0.94	0.14	62,62,62,62	0
87	MG	5	4091	1/1	0.94	0.26	53,53,53,53	0
87	MG	5	4503	1/1	0.94	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	d9	103	1/1	0.94	0.15	83,83,83,83	1
87	MG	1	4268	1/1	0.94	0.19	32,32,32,32	0
87	MG	1	4269	1/1	0.94	0.13	68,68,68,68	0
87	MG	5	4512	1/1	0.94	0.08	53,53,53,53	1
87	MG	1	4478	1/1	0.94	0.26	47,47,47,47	1
87	MG	5	3820	1/1	0.94	0.19	32,32,32,32	0
87	MG	1	4270	1/1	0.94	0.10	77,77,77,77	0
87	MG	5	4519	1/1	0.94	0.12	42,42,42,42	1
87	MG	5	4521	1/1	0.94	0.27	59,59,59,59	0
87	MG	5	4523	1/1	0.94	0.16	43,43,43,43	1
87	MG	5	3822	1/1	0.94	0.10	48,48,48,48	0
87	MG	5	4526	1/1	0.94	0.18	51,51,51,51	1
86	OHX	4	209	7/7	0.94	0.26	45,45,45,45	7
87	MG	5	4102	1/1	0.94	0.21	44,44,44,44	0
86	OHX	1	3529	7/7	0.94	0.24	66,66,66,66	7
86	OHX	6	1992	7/7	0.94	0.16	71,71,71,71	7
87	MG	5	3827	1/1	0.94	0.32	46,46,46,46	0
87	MG	1	3956	1/1	0.94	0.31	40,40,40,40	0
87	MG	5	4111	1/1	0.94	0.17	36,36,36,36	0
87	MG	1	4278	1/1	0.94	0.31	46,46,46,46	1
87	MG	5	4545	1/1	0.94	0.33	34,34,34,34	1
87	MG	5	4114	1/1	0.94	0.27	43,43,43,43	0
87	MG	5	4117	1/1	0.94	0.16	46,46,46,46	0
87	MG	5	4118	1/1	0.94	0.13	32,32,32,32	1
87	MG	6	2148	1/1	0.94	0.39	45,45,45,45	0
87	MG	1	4279	1/1	0.94	0.08	58,58,58,58	0
87	MG	5	4124	1/1	0.94	0.21	57,57,57,57	0
86	OHX	5	3609	7/7	0.94	0.18	96,96,96,96	7
87	MG	5	4560	1/1	0.94	0.12	40,40,40,40	0
86	OHX	1	3642	7/7	0.94	0.21	52,52,52,52	7
87	MG	5	4130	1/1	0.94	0.11	35,35,35,35	1
86	OHX	5	3611	7/7	0.94	0.25	52,52,52,52	7
87	MG	5	4133	1/1	0.94	0.12	57,57,57,57	0
86	OHX	1	3643	7/7	0.94	0.21	52,52,52,52	7
87	MG	1	3962	1/1	0.94	0.12	46,46,46,46	0
87	MG	5	3840	1/1	0.94	0.27	60,60,60,60	0
87	MG	1	3963	1/1	0.94	0.27	31,31,31,31	0
86	OHX	5	3613	7/7	0.94	0.20	70,70,70,70	7
86	OHX	8	211	7/7	0.94	0.15	105,105,105,105	7
87	MG	6	2159	1/1	0.94	0.40	45,45,45,45	0
86	OHX	1	3566	7/7	0.94	0.15	92,92,92,92	7
86	OHX	2	1996	7/7	0.94	0.15	93,93,93,93	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3531	7/7	0.94	0.23	49,49,49,49	7
87	MG	5	4149	1/1	0.94	0.14	50,50,50,50	0
87	MG	6	2165	1/1	0.94	0.11	45,45,45,45	0
87	MG	5	3853	1/1	0.94	0.31	43,43,43,43	0
87	MG	7	223	1/1	0.94	0.15	52,52,52,52	0
87	MG	1	4111	1/1	0.94	0.21	40,40,40,40	1
87	MG	5	3855	1/1	0.94	0.19	36,36,36,36	0
87	MG	5	3856	1/1	0.94	0.17	35,35,35,35	0
87	MG	1	4502	1/1	0.94	0.10	46,46,46,46	0
87	MG	6	2168	1/1	0.94	0.15	59,59,59,59	0
87	MG	5	3865	1/1	0.94	0.24	44,44,44,44	0
86	OHX	1	3532	7/7	0.94	0.25	59,59,59,59	7
87	MG	1	4505	1/1	0.94	0.10	51,51,51,51	0
87	MG	1	3971	1/1	0.94	0.14	43,43,43,43	0
87	MG	7	238	1/1	0.94	0.12	51,51,51,51	1
86	OHX	1	3652	7/7	0.94	0.27	58,58,58,58	7
86	OHX	2	1973	7/7	0.94	0.15	103,103,103,103	7
87	MG	5	3874	1/1	0.94	0.17	43,43,43,43	0
86	OHX	6	2002	7/7	0.94	0.21	52,52,52,52	7
87	MG	1	3850	1/1	0.94	0.17	37,37,37,37	0
86	OHX	1	3797	7/7	0.94	0.15	85,85,85,85	7
87	MG	1	3852	1/1	0.94	0.33	30,30,30,30	0
86	OHX	2	1985	7/7	0.94	0.19	59,59,59,59	7
87	MG	5	3884	1/1	0.94	0.17	40,40,40,40	0
87	MG	5	3885	1/1	0.94	0.29	58,58,58,58	0
87	MG	1	3855	1/1	0.94	0.17	32,32,32,32	0
86	OHX	5	3765	7/7	0.94	0.18	42,42,42,42	7
87	MG	1	4314	1/1	0.94	0.48	40,40,40,40	1
87	MG	5	3891	1/1	0.94	0.23	39,39,39,39	0
87	MG	5	3892	1/1	0.94	0.24	46,46,46,46	0
87	MG	6	2182	1/1	0.94	0.13	51,51,51,51	0
86	OHX	1	3657	7/7	0.94	0.24	40,40,40,40	7
87	MG	12	304	1/1	0.94	0.27	44,44,44,44	1
87	MG	1	4321	1/1	0.94	0.64	44,44,44,44	1
87	MG	6	2186	1/1	0.94	0.19	53,53,53,53	0
86	OHX	1	3659	7/7	0.94	0.28	48,48,48,48	7
87	MG	5	3899	1/1	0.94	0.21	32,32,32,32	0
86	OHX	2	1974	7/7	0.94	0.09	137,137,137,137	7
87	MG	5	3901	1/1	0.94	0.11	67,67,67,67	0
87	MG	13	412	1/1	0.94	0.13	34,34,34,34	0
87	MG	5	4202	1/1	0.94	0.14	32,32,32,32	1
87	MG	6	2190	1/1	0.94	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4204	1/1	0.94	0.26	60,60,60,60	0
87	MG	1	4325	1/1	0.94	0.28	52,52,52,52	0
87	MG	5	4206	1/1	0.94	0.10	40,40,40,40	0
86	OHX	5	3632	7/7	0.94	0.19	63,63,63,63	7
87	MG	5	4208	1/1	0.94	0.30	32,32,32,32	0
87	MG	1	3866	1/1	0.94	0.24	49,49,49,49	0
87	MG	1	3989	1/1	0.94	0.35	37,37,37,37	0
87	MG	1	3990	1/1	0.94	0.19	31,31,31,31	0
86	OHX	1	3583	7/7	0.94	0.23	54,54,54,54	7
87	MG	1	3869	1/1	0.94	0.34	62,62,62,62	0
86	OHX	1	3620	7/7	0.94	0.25	60,60,60,60	7
87	MG	1	3871	1/1	0.94	0.22	46,46,46,46	0
87	MG	m6	202	1/1	0.94	0.18	36,36,36,36	1
87	MG	5	4220	1/1	0.94	0.17	49,49,49,49	1
87	MG	1	3998	1/1	0.94	0.24	27,27,27,27	0
86	OHX	2	2033	7/7	0.94	0.10	113,113,113,113	7
87	MG	1	4343	1/1	0.94	0.18	62,62,62,62	0
87	MG	1	4145	1/1	0.94	0.17	47,47,47,47	0
87	MG	4	225	1/1	0.94	0.39	55,55,55,55	0
87	MG	5	3922	1/1	0.94	0.18	33,33,33,33	0
86	OHX	6	2058	7/7	0.94	0.10	148,148,148,148	7
87	MG	1	3875	1/1	0.94	0.23	35,35,35,35	0
87	MG	n3	204	1/1	0.94	0.17	42,42,42,42	0
86	OHX	5	3708	7/7	0.94	0.26	43,43,43,43	7
87	MG	5	4231	1/1	0.94	0.17	35,35,35,35	1
87	MG	5	3927	1/1	0.94	0.19	38,38,38,38	0
87	MG	1	3877	1/1	0.94	0.24	39,39,39,39	0
86	OHX	6	2011	7/7	0.94	0.24	57,57,57,57	7
87	MG	5	4239	1/1	0.94	0.34	34,34,34,34	1
87	MG	5	4240	1/1	0.94	0.25	37,37,37,37	1
86	OHX	5	3525	7/7	0.94	0.29	42,42,42,42	7
87	MG	2	2235	1/1	0.94	0.14	102,102,102,102	1
87	MG	2	2237	1/1	0.94	0.14	80,80,80,80	0
87	MG	o3	204	1/1	0.94	0.17	37,37,37,37	1
86	OHX	5	3526	7/7	0.94	0.26	46,46,46,46	7
86	OHX	5	3531	7/7	0.94	0.18	57,57,57,57	7
87	MG	5	4248	1/1	0.94	0.25	39,39,39,39	1
87	MG	2	2241	1/1	0.94	0.25	60,60,60,60	0
87	MG	1	4357	1/1	0.94	0.07	49,49,49,49	0
86	OHX	5	3535	7/7	0.94	0.24	42,42,42,42	7
87	MG	4	242	1/1	0.94	0.20	45,45,45,45	0
86	OHX	1	3622	7/7	0.94	0.20	56,56,56,56	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	4	244	1/1	0.94	0.61	41,41,41,41	1
87	MG	1	4163	1/1	0.94	0.28	52,52,52,52	0
87	MG	1	4018	1/1	0.94	0.33	30,30,30,30	0
87	MG	L3	404	1/1	0.94	0.17	42,42,42,42	1
87	MG	5	4264	1/1	0.94	0.24	63,63,63,63	0
87	MG	5	4300	1/1	0.95	0.09	32,32,32,32	0
87	MG	L3	405	1/1	0.95	0.14	42,42,42,42	0
86	OHX	1	3618	7/7	0.95	0.14	78,78,78,78	7
87	MG	1	4338	1/1	0.95	0.30	37,37,37,37	1
86	OHX	5	3562	7/7	0.95	0.20	51,51,51,51	7
86	OHX	5	3563	7/7	0.95	0.15	93,93,93,93	7
86	OHX	S2	301	7/7	0.95	0.17	81,81,81,81	7
86	OHX	2	2023	7/7	0.95	0.15	71,71,71,71	7
87	MG	2	2258	1/1	0.95	0.14	74,74,74,74	1
87	MG	2	2259	1/1	0.95	0.16	74,74,74,74	1
86	OHX	6	1976	7/7	0.95	0.11	95,95,95,95	7
87	MG	S2	302	1/1	0.95	0.11	75,75,75,75	0
87	MG	1	3958	1/1	0.95	0.35	32,32,32,32	0
86	OHX	5	3687	7/7	0.95	0.24	46,46,46,46	7
86	OHX	5	3568	7/7	0.95	0.26	53,53,53,53	7
87	MG	M5	304	1/1	0.95	0.15	40,40,40,40	1
86	OHX	2	1982	7/7	0.95	0.12	100,100,100,100	7
87	MG	1	4134	1/1	0.95	0.04	49,49,49,49	1
87	MG	6	2276	1/1	0.95	0.25	40,40,40,40	0
86	OHX	2	1943	7/7	0.95	0.16	95,95,95,95	7
86	OHX	2	2026	7/7	0.95	0.18	93,93,93,93	7
87	MG	2	2141	1/1	0.95	0.25	67,67,67,67	0
87	MG	M7	205	1/1	0.95	0.22	42,42,42,42	0
87	MG	5	4333	1/1	0.95	0.10	43,43,43,43	0
87	MG	M7	207	1/1	0.95	0.19	43,43,43,43	0
86	OHX	5	3574	7/7	0.95	0.19	53,53,53,53	7
86	OHX	2	1946	7/7	0.95	0.12	110,110,110,110	7
86	OHX	6	1983	7/7	0.95	0.16	95,95,95,95	7
87	MG	M9	205	1/1	0.95	0.18	68,68,68,68	1
87	MG	5	4011	1/1	0.95	0.20	33,33,33,33	0
87	MG	1	4143	1/1	0.95	0.13	54,54,54,54	0
86	OHX	1	3473	7/7	0.95	0.18	60,60,60,60	7
86	OHX	1	3490	7/7	0.95	0.26	54,54,54,54	7
87	MG	D9	105	1/1	0.95	0.08	76,76,76,76	0
86	OHX	5	3582	7/7	0.95	0.19	67,67,67,67	7
87	MG	5	4019	1/1	0.95	0.55	30,30,30,30	0
86	OHX	5	3807	7/7	0.95	0.11	147,147,147,147	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4021	1/1	0.95	0.41	36,36,36,36	0
87	MG	N6	202	1/1	0.95	0.08	58,58,58,58	1
87	MG	6	2298	1/1	0.95	0.12	86,86,86,86	0
86	OHX	1	3746	7/7	0.95	0.13	71,71,71,71	7
86	OHX	1	3568	7/7	0.95	0.14	79,79,79,79	7
86	OHX	1	3502	7/7	0.95	0.20	63,63,63,63	7
87	MG	N8	205	1/1	0.95	0.17	31,31,31,31	1
87	MG	5	4029	1/1	0.95	0.24	26,26,26,26	0
87	MG	6	2303	1/1	0.95	0.09	78,78,78,78	0
86	OHX	2	1932	7/7	0.95	0.12	92,92,92,92	7
87	MG	N8	207	1/1	0.95	0.39	39,39,39,39	1
86	OHX	1	3691	7/7	0.95	0.19	67,67,67,67	7
86	OHX	5	3592	7/7	0.95	0.18	63,63,63,63	7
87	MG	5	4371	1/1	0.95	0.11	38,38,38,38	1
87	MG	5	4035	1/1	0.95	0.11	46,46,46,46	0
87	MG	6	2309	1/1	0.95	0.25	65,65,65,65	0
87	MG	6	2310	1/1	0.95	0.44	48,48,48,48	1
87	MG	6	2311	1/1	0.95	0.07	60,60,60,60	1
86	OHX	1	3809	7/7	0.95	0.15	83,83,83,83	7
87	MG	5	4379	1/1	0.95	0.12	37,37,37,37	1
87	MG	5	4380	1/1	0.95	0.10	45,45,45,45	0
87	MG	1	4376	1/1	0.95	0.25	34,34,34,34	1
87	MG	6	2314	1/1	0.95	0.19	48,48,48,48	0
87	MG	5	4045	1/1	0.95	0.16	40,40,40,40	0
87	MG	5	4047	1/1	0.95	0.10	40,40,40,40	1
87	MG	1	3982	1/1	0.95	0.29	31,31,31,31	0
87	MG	1	3826	1/1	0.95	0.19	43,43,43,43	0
86	OHX	1	3572	7/7	0.95	0.13	95,95,95,95	7
87	MG	1	4162	1/1	0.95	0.07	42,42,42,42	0
87	MG	O3	202	1/1	0.95	0.24	38,38,38,38	1
87	MG	1	4384	1/1	0.95	0.10	64,64,64,64	0
86	OHX	1	3634	7/7	0.95	0.07	121,121,121,121	7
87	MG	1	3829	1/1	0.95	0.12	58,58,58,58	0
87	MG	1	4390	1/1	0.95	0.20	36,36,36,36	1
87	MG	1	4166	1/1	0.95	0.14	36,36,36,36	0
86	OHX	5	3597	7/7	0.95	0.22	46,46,46,46	7
87	MG	5	4401	1/1	0.95	0.24	48,48,48,48	0
87	MG	6	2329	1/1	0.95	0.09	48,48,48,48	0
87	MG	6	2330	1/1	0.95	0.28	55,55,55,55	1
87	MG	5	4406	1/1	0.95	0.16	37,37,37,37	0
87	MG	1	4170	1/1	0.95	0.18	45,45,45,45	0
87	MG	5	4409	1/1	0.95	0.31	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3599	7/7	0.95	0.18	56,56,56,56	7
87	MG	5	4066	1/1	0.95	0.13	53,53,53,53	0
86	OHX	7	205	7/7	0.95	0.21	68,68,68,68	7
87	MG	s1	303	1/1	0.95	0.10	77,77,77,77	0
86	OHX	7	207	7/7	0.95	0.17	78,78,78,78	7
87	MG	5	4417	1/1	0.95	0.14	56,56,56,56	0
87	MG	1	4174	1/1	0.95	0.35	35,35,35,35	0
86	OHX	5	3600	7/7	0.95	0.20	57,57,57,57	7
87	MG	Q2	505	1/1	0.95	0.09	45,45,45,45	1
87	MG	5	4073	1/1	0.95	0.07	36,36,36,36	0
86	OHX	1	3573	7/7	0.95	0.26	58,58,58,58	7
86	OHX	1	3510	7/7	0.95	0.15	93,93,93,93	7
86	OHX	5	3603	7/7	0.95	0.18	43,43,43,43	7
86	OHX	1	3575	7/7	0.95	0.22	47,47,47,47	7
86	OHX	1	3577	7/7	0.95	0.14	114,114,114,114	7
87	MG	1	4409	1/1	0.95	0.14	46,46,46,46	0
87	MG	1	4002	1/1	0.95	0.35	36,36,36,36	0
87	MG	5	4081	1/1	0.95	0.17	48,48,48,48	0
87	MG	5	4437	1/1	0.95	0.24	37,37,37,37	1
86	OHX	8	204	7/7	0.95	0.17	66,66,66,66	7
87	MG	5	4443	1/1	0.95	0.12	32,32,32,32	0
87	MG	1	4183	1/1	0.95	0.27	37,37,37,37	0
87	MG	1	4004	1/1	0.95	0.10	44,44,44,44	0
87	MG	1	4417	1/1	0.95	0.17	44,44,44,44	1
86	OHX	3	203	7/7	0.95	0.24	56,56,56,56	7
87	MG	1	3843	1/1	0.95	0.29	43,43,43,43	0
86	OHX	3	204	7/7	0.95	0.17	85,85,85,85	7
87	MG	d4	202	1/1	0.95	0.12	55,55,55,55	0
86	OHX	8	209	7/7	0.95	0.18	88,88,88,88	7
86	OHX	2	2073	7/7	0.95	0.18	89,89,89,89	7
87	MG	5	4094	1/1	0.95	0.18	52,52,52,52	0
86	OHX	1	3700	7/7	0.95	0.32	47,47,47,47	7
86	OHX	1	3517	7/7	0.95	0.23	61,61,61,61	7
87	MG	sM	202	1/1	0.95	0.09	44,44,44,44	0
86	OHX	2	1965	7/7	0.95	0.14	91,91,91,91	7
86	OHX	2	1967	7/7	0.95	0.18	92,92,92,92	7
86	OHX	1	3525	7/7	0.95	0.27	44,44,44,44	7
87	MG	5	4475	1/1	0.95	0.08	39,39,39,39	0
86	OHX	1	3645	7/7	0.95	0.21	58,58,58,58	7
86	OHX	5	3616	7/7	0.95	0.24	46,46,46,46	7
87	MG	5	4103	1/1	0.95	0.31	35,35,35,35	0
87	MG	5	4480	1/1	0.95	0.16	50,50,50,50	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4020	1/1	0.95	0.33	32,32,32,32	0
87	MG	1	3854	1/1	0.95	0.12	48,48,48,48	0
87	MG	5	4106	1/1	0.95	0.17	35,35,35,35	0
87	MG	1	4022	1/1	0.95	0.36	22,22,22,22	0
86	OHX	4	207	7/7	0.95	0.20	61,61,61,61	7
86	OHX	5	3618	7/7	0.95	0.23	52,52,52,52	7
87	MG	1	4445	1/1	0.95	0.17	41,41,41,41	0
87	MG	1	4215	1/1	0.95	0.31	37,37,37,37	0
87	MG	5	4500	1/1	0.95	0.19	54,54,54,54	0
87	MG	5	4501	1/1	0.95	0.13	33,33,33,33	1
87	MG	5	4115	1/1	0.95	0.14	35,35,35,35	0
87	MG	2	2184	1/1	0.95	0.12	59,59,59,59	0
87	MG	5	4505	1/1	0.95	0.24	49,49,49,49	0
87	MG	1	4217	1/1	0.95	0.23	39,39,39,39	1
86	OHX	5	3619	7/7	0.95	0.27	38,38,38,38	7
87	MG	1	4456	1/1	0.95	0.18	56,56,56,56	1
87	MG	1	4220	1/1	0.95	0.19	39,39,39,39	0
87	MG	1	4221	1/1	0.95	0.21	43,43,43,43	0
87	MG	5	4127	1/1	0.95	0.10	44,44,44,44	1
87	MG	1	3861	1/1	0.95	0.20	40,40,40,40	0
87	MG	5	3842	1/1	0.95	0.12	45,45,45,45	0
86	OHX	12	301	7/7	0.95	0.20	63,63,63,63	7
87	MG	5	4132	1/1	0.95	0.17	33,33,33,33	1
86	OHX	1	3587	7/7	0.95	0.18	77,77,77,77	7
87	MG	1	4225	1/1	0.95	0.19	37,37,37,37	1
86	OHX	1	3588	7/7	0.95	0.18	47,47,47,47	7
86	OHX	1	3589	7/7	0.95	0.19	50,50,50,50	7
86	OHX	2	1933	7/7	0.95	0.22	71,71,71,71	7
86	OHX	1	3653	7/7	0.95	0.17	59,59,59,59	7
86	OHX	2	1991	7/7	0.95	0.10	104,104,104,104	7
86	OHX	1	3712	7/7	0.95	0.19	62,62,62,62	7
87	MG	5	4542	1/1	0.95	0.26	45,45,45,45	0
87	MG	1	3873	1/1	0.95	0.25	39,39,39,39	0
87	MG	5	4544	1/1	0.95	0.19	37,37,37,37	0
86	OHX	6	2090	7/7	0.95	0.15	68,68,68,68	7
87	MG	1	4234	1/1	0.95	0.08	51,51,51,51	0
87	MG	5	4147	1/1	0.95	0.16	36,36,36,36	0
86	OHX	5	3630	7/7	0.95	0.14	75,75,75,75	7
87	MG	5	4150	1/1	0.95	0.12	41,41,41,41	1
87	MG	5	3863	1/1	0.95	0.24	35,35,35,35	0
86	OHX	2	1969	7/7	0.95	0.16	62,62,62,62	7
86	OHX	6	2020	7/7	0.95	0.15	49,49,49,49	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	2	2199	1/1	0.95	0.17	81,81,81,81	0
86	OHX	2	1931	7/7	0.95	0.12	116,116,116,116	7
87	MG	1	4048	1/1	0.95	0.23	44,44,44,44	0
87	MG	1	4242	1/1	0.95	0.18	37,37,37,37	0
87	MG	1	4243	1/1	0.95	0.20	45,45,45,45	0
87	MG	5	4161	1/1	0.95	0.17	38,38,38,38	0
87	MG	5	3875	1/1	0.95	0.22	31,31,31,31	0
87	MG	1	4482	1/1	0.95	0.24	46,46,46,46	0
87	MG	5	4574	1/1	0.95	0.10	49,49,49,49	0
86	OHX	1	3658	7/7	0.95	0.20	49,49,49,49	7
86	OHX	1	3533	7/7	0.95	0.09	129,129,129,129	7
86	OHX	1	3600	7/7	0.95	0.18	68,68,68,68	7
87	MG	1	3885	1/1	0.95	0.17	41,41,41,41	0
87	MG	5	3881	1/1	0.95	0.16	41,41,41,41	0
87	MG	5	3882	1/1	0.95	0.12	37,37,37,37	0
87	MG	5	3883	1/1	0.95	0.27	41,41,41,41	0
87	MG	1	4487	1/1	0.95	0.17	62,62,62,62	0
86	OHX	1	3776	7/7	0.95	0.17	59,59,59,59	7
87	MG	1	4489	1/1	0.95	0.27	56,56,56,56	1
86	OHX	o3	201	7/7	0.95	0.25	51,51,51,51	7
87	MG	7	224	1/1	0.95	0.07	55,55,55,55	0
87	MG	1	4253	1/1	0.95	0.23	66,66,66,66	0
87	MG	1	3888	1/1	0.95	0.22	66,66,66,66	0
87	MG	1	4060	1/1	0.95	0.07	44,44,44,44	0
87	MG	1	4061	1/1	0.95	0.14	32,32,32,32	0
87	MG	7	231	1/1	0.95	0.09	43,43,43,43	0
87	MG	1	4062	1/1	0.95	0.07	33,33,33,33	1
87	MG	1	4496	1/1	0.95	0.10	56,56,56,56	1
86	OHX	1	3534	7/7	0.95	0.18	65,65,65,65	7
87	MG	5	3897	1/1	0.95	0.24	52,52,52,52	0
87	MG	1	4261	1/1	0.95	0.17	41,41,41,41	1
87	MG	5	4194	1/1	0.95	0.11	39,39,39,39	0
86	OHX	2	2013	7/7	0.95	0.08	158,158,158,158	7
87	MG	1	4263	1/1	0.95	0.05	45,45,45,45	1
86	OHX	1	3537	7/7	0.95	0.10	112,112,112,112	7
86	OHX	2	2037	7/7	0.95	0.17	60,60,60,60	7
87	MG	5	4200	1/1	0.95	0.26	43,43,43,43	1
86	OHX	2	1972	7/7	0.95	0.20	81,81,81,81	7
87	MG	8	227	1/1	0.95	0.19	61,61,61,61	0
86	OHX	2	1951	7/7	0.95	0.19	87,87,87,87	7
87	MG	1	3898	1/1	0.95	0.23	48,48,48,48	0
86	OHX	1	3667	7/7	0.95	0.18	49,49,49,49	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	1952	7/7	0.95	0.09	131,131,131,131	7
87	MG	5	3909	1/1	0.95	0.15	49,49,49,49	0
87	MG	8	234	1/1	0.95	0.19	41,41,41,41	1
86	OHX	5	3493	7/7	0.95	0.16	67,67,67,67	7
87	MG	1	4510	1/1	0.95	0.07	50,50,50,50	0
86	OHX	5	3506	7/7	0.95	0.24	41,41,41,41	7
86	OHX	2	1954	7/7	0.95	0.17	88,88,88,88	7
87	MG	5	3915	1/1	0.95	0.11	39,39,39,39	0
86	OHX	5	3511	7/7	0.95	0.20	61,61,61,61	7
86	OHX	5	3512	7/7	0.95	0.23	69,69,69,69	7
86	OHX	5	3515	7/7	0.95	0.25	40,40,40,40	7
87	MG	1	3913	1/1	0.95	0.21	49,49,49,49	0
87	MG	3	217	1/1	0.95	0.31	36,36,36,36	0
86	OHX	5	3521	7/7	0.95	0.16	56,56,56,56	7
87	MG	1	4286	1/1	0.95	0.20	40,40,40,40	0
86	OHX	1	3611	7/7	0.95	0.25	42,42,42,42	7
86	OHX	1	3548	7/7	0.95	0.22	59,59,59,59	7
87	MG	2	2106	1/1	0.95	0.12	60,60,60,60	0
87	MG	5	3928	1/1	0.95	0.26	38,38,38,38	0
87	MG	1	4290	1/1	0.95	0.22	40,40,40,40	1
87	MG	2	2226	1/1	0.95	0.12	76,76,76,76	0
87	MG	6	2209	1/1	0.95	0.10	46,46,46,46	0
87	MG	15	307	1/1	0.95	0.06	46,46,46,46	1
87	MG	17	301	1/1	0.95	0.23	36,36,36,36	1
86	OHX	1	3549	7/7	0.95	0.23	54,54,54,54	7
86	OHX	2	1938	7/7	0.95	0.19	70,70,70,70	7
87	MG	1	4092	1/1	0.95	0.28	42,42,42,42	0
86	OHX	5	3532	7/7	0.95	0.21	38,38,38,38	7
86	OHX	2	1957	7/7	0.95	0.16	79,79,79,79	7
86	OHX	6	1950	7/7	0.95	0.11	100,100,100,100	7
87	MG	1	4301	1/1	0.95	0.11	52,52,52,52	0
86	OHX	5	3538	7/7	0.95	0.20	42,42,42,42	7
87	MG	5	3942	1/1	0.95	0.20	40,40,40,40	0
87	MG	m5	504	1/1	0.95	0.08	45,45,45,45	0
87	MG	m5	505	1/1	0.95	0.12	58,58,58,58	0
87	MG	5	4246	1/1	0.95	0.15	45,45,45,45	0
86	OHX	6	1953	7/7	0.95	0.09	137,137,137,137	7
86	OHX	6	1954	7/7	0.95	0.10	149,149,149,149	7
87	MG	1	3928	1/1	0.95	0.22	43,43,43,43	0
87	MG	1	4307	1/1	0.95	0.11	58,58,58,58	1
86	OHX	2	1940	7/7	0.95	0.15	85,85,85,85	7
87	MG	m8	1504	1/1	0.95	0.29	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3668	7/7	0.95	0.25	39,39,39,39	7
86	OHX	5	3543	7/7	0.95	0.22	60,60,60,60	7
87	MG	n0	204	1/1	0.95	0.27	45,45,45,45	0
87	MG	n0	205	1/1	0.95	0.18	41,41,41,41	1
87	MG	4	229	1/1	0.95	0.29	66,66,66,66	0
87	MG	5	4259	1/1	0.95	0.09	54,54,54,54	0
87	MG	5	3953	1/1	0.95	0.39	45,45,45,45	0
86	OHX	5	3670	7/7	0.95	0.21	51,51,51,51	7
87	MG	4	231	1/1	0.95	0.20	56,56,56,56	0
87	MG	n8	202	1/1	0.95	0.14	51,51,51,51	0
86	OHX	5	3544	7/7	0.95	0.15	99,99,99,99	7
87	MG	1	4106	1/1	0.95	0.12	45,45,45,45	0
87	MG	5	4266	1/1	0.95	0.20	42,42,42,42	1
87	MG	n8	207	1/1	0.95	0.12	39,39,39,39	1
86	OHX	1	3734	7/7	0.95	0.20	52,52,52,52	7
87	MG	n9	103	1/1	0.95	0.18	40,40,40,40	1
86	OHX	6	1962	7/7	0.95	0.21	62,62,62,62	7
87	MG	1	4323	1/1	0.95	0.28	42,42,42,42	1
87	MG	5	4272	1/1	0.95	0.21	48,48,48,48	0
86	OHX	5	3551	7/7	0.95	0.16	66,66,66,66	7
87	MG	6	2239	1/1	0.95	0.16	56,56,56,56	1
87	MG	5	4275	1/1	0.95	0.46	36,36,36,36	1
87	MG	q1	102	1/1	0.95	0.19	43,43,43,43	0
86	OHX	5	3552	7/7	0.95	0.18	47,47,47,47	7
87	MG	1	4326	1/1	0.95	0.14	42,42,42,42	0
86	OHX	1	3554	7/7	0.95	0.15	78,78,78,78	7
87	MG	5	4281	1/1	0.95	0.41	44,44,44,44	1
86	OHX	5	3677	7/7	0.95	0.18	48,48,48,48	7
86	OHX	5	3556	7/7	0.95	0.14	107,107,107,107	7
87	MG	6	2246	1/1	0.95	0.10	50,50,50,50	1
86	OHX	1	3794	7/7	0.95	0.17	68,68,68,68	7
87	MG	1	4116	1/1	0.95	0.20	36,36,36,36	0
87	MG	L2	301	1/1	0.95	0.13	39,39,39,39	0
86	OHX	5	3559	7/7	0.95	0.22	53,53,53,53	7
87	MG	1	4336	1/1	0.95	0.13	43,43,43,43	0
86	OHX	2	1970	7/7	0.96	0.16	89,89,89,89	7
87	MG	1	4213	1/1	0.96	0.32	35,35,35,35	0
87	MG	5	4383	1/1	0.96	0.12	53,53,53,53	0
86	OHX	1	3580	7/7	0.96	0.14	89,89,89,89	7
87	MG	2	2233	1/1	0.96	0.20	72,72,72,72	0
87	MG	1	3904	1/1	0.96	0.34	42,42,42,42	0
87	MG	5	4108	1/1	0.96	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4390	1/1	0.96	0.10	39,39,39,39	1
87	MG	5	4109	1/1	0.96	0.09	40,40,40,40	0
87	MG	5	3888	1/1	0.96	0.08	37,37,37,37	0
87	MG	1	3906	1/1	0.96	0.20	42,42,42,42	1
87	MG	6	2224	1/1	0.96	0.11	47,47,47,47	0
87	MG	5	4113	1/1	0.96	0.06	39,39,39,39	0
87	MG	6	2225	1/1	0.96	0.34	55,55,55,55	0
87	MG	1	4401	1/1	0.96	0.22	36,36,36,36	1
87	MG	1	3907	1/1	0.96	0.15	59,59,59,59	0
87	MG	M6	203	1/1	0.96	0.33	40,40,40,40	1
86	OHX	2	2014	7/7	0.96	0.12	80,80,80,80	7
87	MG	5	4120	1/1	0.96	0.27	39,39,39,39	0
86	OHX	2	1944	7/7	0.96	0.18	72,72,72,72	7
87	MG	5	4405	1/1	0.96	0.09	70,70,70,70	1
87	MG	1	4057	1/1	0.96	0.16	38,38,38,38	0
86	OHX	2	1927	7/7	0.96	0.14	94,94,94,94	7
87	MG	M7	206	1/1	0.96	0.15	43,43,43,43	0
87	MG	5	4411	1/1	0.96	0.10	55,55,55,55	0
87	MG	5	4128	1/1	0.96	0.13	40,40,40,40	0
86	OHX	2	2017	7/7	0.96	0.10	108,108,108,108	7
86	OHX	1	3586	7/7	0.96	0.16	50,50,50,50	7
87	MG	1	4411	1/1	0.96	0.21	42,42,42,42	1
87	MG	M8	203	1/1	0.96	0.16	41,41,41,41	0
87	MG	M8	204	1/1	0.96	0.20	46,46,46,46	1
86	OHX	5	3567	7/7	0.96	0.22	39,39,39,39	7
87	MG	5	4419	1/1	0.96	0.15	39,39,39,39	1
87	MG	5	3907	1/1	0.96	0.26	28,28,28,28	0
86	OHX	L3	401	7/7	0.96	0.16	56,56,56,56	7
87	MG	2	2243	1/1	0.96	0.10	61,61,61,61	0
86	OHX	2	2035	7/7	0.96	0.13	95,95,95,95	7
87	MG	5	4139	1/1	0.96	0.10	38,38,38,38	0
86	OHX	5	3788	7/7	0.96	0.18	58,58,58,58	7
87	MG	5	3912	1/1	0.96	0.18	40,40,40,40	0
87	MG	1	3920	1/1	0.96	0.18	52,52,52,52	0
87	MG	1	4419	1/1	0.96	0.12	34,34,34,34	1
87	MG	5	4145	1/1	0.96	0.18	49,49,49,49	0
86	OHX	5	3570	7/7	0.96	0.09	98,98,98,98	7
86	OHX	2	2054	7/7	0.96	0.14	87,87,87,87	7
87	MG	5	4438	1/1	0.96	0.25	40,40,40,40	0
86	OHX	1	3689	7/7	0.96	0.17	55,55,55,55	7
87	MG	6	2253	1/1	0.96	0.14	47,47,47,47	0
86	OHX	D9	102	7/7	0.96	0.12	83,83,83,83	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3741	7/7	0.96	0.20	56,56,56,56	7
86	OHX	5	3576	7/7	0.96	0.18	56,56,56,56	7
87	MG	1	4238	1/1	0.96	0.13	46,46,46,46	0
87	MG	5	3924	1/1	0.96	0.15	42,42,42,42	0
86	OHX	1	3592	7/7	0.96	0.20	52,52,52,52	7
86	OHX	1	3541	7/7	0.96	0.17	54,54,54,54	7
87	MG	5	4458	1/1	0.96	0.23	38,38,38,38	1
87	MG	5	4159	1/1	0.96	0.17	37,37,37,37	0
87	MG	1	3929	1/1	0.96	0.34	40,40,40,40	0
87	MG	1	4079	1/1	0.96	0.08	43,43,43,43	0
86	OHX	M5	301	7/7	0.96	0.17	75,75,75,75	7
86	OHX	1	3594	7/7	0.96	0.15	74,74,74,74	7
87	MG	1	4245	1/1	0.96	0.17	47,47,47,47	1
87	MG	1	4441	1/1	0.96	0.06	43,43,43,43	1
87	MG	5	4166	1/1	0.96	0.21	44,44,44,44	0
87	MG	1	4246	1/1	0.96	0.14	41,41,41,41	1
87	MG	6	2270	1/1	0.96	0.17	61,61,61,61	0
86	OHX	5	3691	7/7	0.96	0.21	54,54,54,54	7
87	MG	5	3937	1/1	0.96	0.35	33,33,33,33	0
87	MG	1	3934	1/1	0.96	0.16	40,40,40,40	0
87	MG	1	4446	1/1	0.96	0.10	45,45,45,45	1
87	MG	1	4084	1/1	0.96	0.10	49,49,49,49	0
87	MG	5	4177	1/1	0.96	0.22	42,42,42,42	0
87	MG	1	4085	1/1	0.96	0.14	46,46,46,46	0
87	MG	1	4449	1/1	0.96	0.10	49,49,49,49	1
87	MG	5	4487	1/1	0.96	0.09	37,37,37,37	0
87	MG	5	4488	1/1	0.96	0.12	46,46,46,46	0
87	MG	5	4180	1/1	0.96	0.16	51,51,51,51	0
86	OHX	2	1953	7/7	0.96	0.12	64,64,64,64	7
87	MG	1	4454	1/1	0.96	0.15	50,50,50,50	0
87	MG	5	4498	1/1	0.96	0.17	45,45,45,45	1
86	OHX	2	1987	7/7	0.96	0.17	75,75,75,75	7
87	MG	5	4184	1/1	0.96	0.13	40,40,40,40	1
86	OHX	5	3586	7/7	0.96	0.15	83,83,83,83	7
87	MG	6	2282	1/1	0.96	0.25	55,55,55,55	0
86	OHX	5	3803	7/7	0.96	0.21	69,69,69,69	7
86	OHX	2	2076	7/7	0.96	0.10	122,122,122,122	7
86	OHX	5	3805	7/7	0.96	0.15	88,88,88,88	7
87	MG	5	4509	1/1	0.96	0.08	33,33,33,33	0
86	OHX	5	3588	7/7	0.96	0.19	43,43,43,43	7
87	MG	5	4193	1/1	0.96	0.12	39,39,39,39	1
86	OHX	1	3647	7/7	0.96	0.17	64,64,64,64	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3481	7/7	0.96	0.13	88,88,88,88	7
87	MG	C1	202	1/1	0.96	0.13	72,72,72,72	1
87	MG	5	4197	1/1	0.96	0.17	36,36,36,36	0
87	MG	5	4520	1/1	0.96	0.11	43,43,43,43	0
87	MG	5	3957	1/1	0.96	0.23	30,30,30,30	0
87	MG	6	2290	1/1	0.96	0.11	52,52,52,52	0
87	MG	6	2291	1/1	0.96	0.07	65,65,65,65	0
87	MG	5	4525	1/1	0.96	0.08	41,41,41,41	0
86	OHX	1	3486	7/7	0.96	0.19	65,65,65,65	7
86	OHX	O7	102	7/7	0.96	0.18	73,73,73,73	7
86	OHX	Q2	502	7/7	0.96	0.20	45,45,45,45	7
86	OHX	6	1921	7/7	0.96	0.20	51,51,51,51	7
86	OHX	6	1925	7/7	0.96	0.11	87,87,87,87	7
86	OHX	5	3598	7/7	0.96	0.14	73,73,73,73	7
87	MG	5	4537	1/1	0.96	0.16	38,38,38,38	0
87	MG	5	3968	1/1	0.96	0.23	27,27,27,27	0
86	OHX	6	1931	7/7	0.96	0.18	71,71,71,71	7
87	MG	2	2153	1/1	0.96	0.11	72,72,72,72	0
86	OHX	6	1939	7/7	0.96	0.16	103,103,103,103	7
86	OHX	6	1940	7/7	0.96	0.15	64,64,64,64	7
86	OHX	1	3488	7/7	0.96	0.19	49,49,49,49	7
87	MG	1	3817	1/1	0.96	0.28	40,40,40,40	0
87	MG	5	4218	1/1	0.96	0.18	41,41,41,41	0
87	MG	1	3818	1/1	0.96	0.20	58,58,58,58	0
86	OHX	2	1941	7/7	0.96	0.11	92,92,92,92	7
86	OHX	7	206	7/7	0.96	0.16	67,67,67,67	7
86	OHX	6	2098	7/7	0.96	0.10	113,113,113,113	7
87	MG	5	4558	1/1	0.96	0.10	50,50,50,50	1
86	OHX	6	1949	7/7	0.96	0.16	73,73,73,73	7
86	OHX	5	3606	7/7	0.96	0.13	74,74,74,74	7
87	MG	1	3966	1/1	0.96	0.16	41,41,41,41	0
86	OHX	1	3491	7/7	0.96	0.10	118,118,118,118	7
87	MG	1	4291	1/1	0.96	0.16	41,41,41,41	0
86	OHX	1	3655	7/7	0.96	0.17	64,64,64,64	7
87	MG	5	4566	1/1	0.96	0.11	40,40,40,40	0
87	MG	5	4568	1/1	0.96	0.14	38,38,38,38	1
86	OHX	2	1964	7/7	0.96	0.14	101,101,101,101	7
87	MG	5	4570	1/1	0.96	0.27	50,50,50,50	0
87	MG	6	2126	1/1	0.96	0.32	43,43,43,43	0
87	MG	5	4232	1/1	0.96	0.14	35,35,35,35	1
87	MG	5	3987	1/1	0.96	0.26	45,45,45,45	0
87	MG	6	2127	1/1	0.96	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	1955	7/7	0.96	0.09	145,145,145,145	7
87	MG	5	4238	1/1	0.96	0.08	33,33,33,33	1
86	OHX	6	1958	7/7	0.96	0.17	77,77,77,77	7
86	OHX	8	205	7/7	0.96	0.19	64,64,64,64	7
86	OHX	1	3503	7/7	0.96	0.17	57,57,57,57	7
86	OHX	d9	102	7/7	0.96	0.11	97,97,97,97	7
86	OHX	6	1960	7/7	0.96	0.18	72,72,72,72	7
86	OHX	5	3444	7/7	0.96	0.15	70,70,70,70	7
86	OHX	5	3465	7/7	0.96	0.22	40,40,40,40	7
87	MG	6	2136	1/1	0.96	0.18	54,54,54,54	0
86	OHX	5	3478	7/7	0.96	0.24	45,45,45,45	7
86	OHX	5	3479	7/7	0.96	0.15	79,79,79,79	7
87	MG	5	4251	1/1	0.96	0.07	51,51,51,51	0
86	OHX	5	3483	7/7	0.96	0.23	49,49,49,49	7
87	MG	6	2140	1/1	0.96	0.28	44,44,44,44	0
87	MG	7	230	1/1	0.96	0.39	37,37,37,37	1
87	MG	5	4254	1/1	0.96	0.07	38,38,38,38	1
86	OHX	5	3484	7/7	0.96	0.17	57,57,57,57	7
87	MG	1	4137	1/1	0.96	0.10	38,38,38,38	0
87	MG	5	4008	1/1	0.96	0.27	48,48,48,48	0
86	OHX	5	3487	7/7	0.96	0.20	48,48,48,48	7
87	MG	5	4260	1/1	0.96	0.13	59,59,59,59	0
87	MG	s8	302	1/1	0.96	0.20	45,45,45,45	0
86	OHX	5	3488	7/7	0.96	0.17	48,48,48,48	7
87	MG	6	2145	1/1	0.96	0.20	33,33,33,33	0
86	OHX	5	3491	7/7	0.96	0.24	51,51,51,51	7
86	OHX	1	3504	7/7	0.96	0.14	90,90,90,90	7
86	OHX	5	3494	7/7	0.96	0.16	89,89,89,89	7
87	MG	5	4017	1/1	0.96	0.33	33,33,33,33	0
87	MG	c7	201	1/1	0.96	0.14	81,81,81,81	1
87	MG	8	228	1/1	0.96	0.28	46,46,46,46	1
86	OHX	5	3627	7/7	0.96	0.15	81,81,81,81	7
86	OHX	5	3496	7/7	0.96	0.19	48,48,48,48	7
86	OHX	5	3500	7/7	0.96	0.14	75,75,75,75	7
86	OHX	6	2039	7/7	0.96	0.16	46,46,46,46	7
86	OHX	5	3507	7/7	0.96	0.21	62,62,62,62	7
87	MG	1	3995	1/1	0.96	0.18	36,36,36,36	0
87	MG	1	3996	1/1	0.96	0.26	32,32,32,32	0
86	OHX	1	3558	7/7	0.96	0.16	62,62,62,62	7
86	OHX	2	1990	7/7	0.96	0.10	111,111,111,111	7
86	OHX	1	3609	7/7	0.96	0.21	49,49,49,49	7
87	MG	5	4287	1/1	0.96	0.16	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	6	2160	1/1	0.96	0.35	59,59,59,59	0
87	MG	1	4334	1/1	0.96	0.09	56,56,56,56	0
86	OHX	1	3610	7/7	0.96	0.09	110,110,110,110	7
87	MG	1	4001	1/1	0.96	0.34	28,28,28,28	0
86	OHX	5	3517	7/7	0.96	0.18	56,56,56,56	7
86	OHX	5	3519	7/7	0.96	0.08	132,132,132,132	7
87	MG	l3	406	1/1	0.96	0.15	31,31,31,31	1
87	MG	1	4158	1/1	0.96	0.35	42,42,42,42	1
86	OHX	5	3520	7/7	0.96	0.22	42,42,42,42	7
87	MG	l3	411	1/1	0.96	0.14	33,33,33,33	1
87	MG	5	4301	1/1	0.96	0.05	37,37,37,37	0
87	MG	1	4160	1/1	0.96	0.12	46,46,46,46	0
87	MG	5	4305	1/1	0.96	0.14	34,34,34,34	1
86	OHX	1	3509	7/7	0.96	0.24	42,42,42,42	7
86	OHX	m5	501	7/7	0.96	0.16	81,81,81,81	7
86	OHX	5	3522	7/7	0.96	0.17	56,56,56,56	7
86	OHX	2	1977	7/7	0.96	0.09	138,138,138,138	7
87	MG	l5	308	1/1	0.96	0.18	49,49,49,49	1
87	MG	5	3826	1/1	0.96	0.06	35,35,35,35	0
87	MG	l7	302	1/1	0.96	0.15	35,35,35,35	1
86	OHX	6	1974	7/7	0.96	0.16	67,67,67,67	7
87	MG	1	4010	1/1	0.96	0.36	41,41,41,41	0
87	MG	l7	305	1/1	0.96	0.11	40,40,40,40	0
86	OHX	1	3562	7/7	0.96	0.18	71,71,71,71	7
87	MG	5	3830	1/1	0.96	0.26	31,31,31,31	0
86	OHX	5	3645	7/7	0.96	0.19	68,68,68,68	7
86	OHX	5	3527	7/7	0.96	0.18	49,49,49,49	7
87	MG	4	223	1/1	0.96	0.32	32,32,32,32	0
86	OHX	5	3529	7/7	0.96	0.18	51,51,51,51	7
86	OHX	2	1942	7/7	0.96	0.14	74,74,74,74	7
87	MG	m5	503	1/1	0.96	0.13	48,48,48,48	0
86	OHX	1	3513	7/7	0.96	0.21	49,49,49,49	7
87	MG	6	2183	1/1	0.96	0.16	54,54,54,54	1
87	MG	m6	201	1/1	0.96	0.13	38,38,38,38	1
87	MG	5	3839	1/1	0.96	0.20	55,55,55,55	0
87	MG	2	2092	1/1	0.96	0.28	40,40,40,40	0
87	MG	1	4019	1/1	0.96	0.59	27,27,27,27	0
87	MG	5	4330	1/1	0.96	0.08	79,79,79,79	0
86	OHX	5	3533	7/7	0.96	0.16	47,47,47,47	7
87	MG	m8	1501	1/1	0.96	0.32	42,42,42,42	1
86	OHX	1	3717	7/7	0.96	0.16	50,50,50,50	7
87	MG	5	3844	1/1	0.96	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	m9	202	1/1	0.96	0.16	54,54,54,54	1
87	MG	5	3845	1/1	0.96	0.25	46,46,46,46	0
86	OHX	1	3668	7/7	0.96	0.17	50,50,50,50	7
86	OHX	1	3516	7/7	0.96	0.17	65,65,65,65	7
86	OHX	2	1923	7/7	0.96	0.14	80,80,80,80	7
86	OHX	1	3520	7/7	0.96	0.18	52,52,52,52	7
86	OHX	6	1987	7/7	0.96	0.16	70,70,70,70	7
87	MG	1	4185	1/1	0.96	0.16	40,40,40,40	1
86	OHX	1	3569	7/7	0.96	0.13	79,79,79,79	7
86	OHX	2	1958	7/7	0.96	0.18	75,75,75,75	7
86	OHX	5	3659	7/7	0.96	0.14	58,58,58,58	7
87	MG	1	4191	1/1	0.96	0.14	90,90,90,90	0
87	MG	1	4371	1/1	0.96	0.07	43,43,43,43	1
87	MG	5	3859	1/1	0.96	0.27	32,32,32,32	0
87	MG	1	4192	1/1	0.96	0.16	38,38,38,38	0
87	MG	5	3861	1/1	0.96	0.16	36,36,36,36	0
86	OHX	5	3547	7/7	0.96	0.09	136,136,136,136	7
87	MG	5	3864	1/1	0.96	0.13	35,35,35,35	0
87	MG	5	4358	1/1	0.96	0.10	54,54,54,54	0
86	OHX	2	1995	7/7	0.96	0.16	86,86,86,86	7
86	OHX	2	1959	7/7	0.96	0.08	127,127,127,127	7
87	MG	o3	203	1/1	0.96	0.10	40,40,40,40	1
87	MG	L2	302	1/1	0.96	0.20	46,46,46,46	0
87	MG	o4	201	1/1	0.96	0.17	70,70,70,70	1
87	MG	1	3891	1/1	0.96	0.15	45,45,45,45	0
87	MG	5	4089	1/1	0.96	0.18	37,37,37,37	0
86	OHX	1	3526	7/7	0.96	0.21	47,47,47,47	7
86	OHX	1	3527	7/7	0.96	0.15	81,81,81,81	7
87	MG	5	3873	1/1	0.96	0.28	45,45,45,45	0
88	ZN	Q2	501	1/1	0.96	0.14	73,73,73,73	0
86	OHX	5	3553	7/7	0.96	0.14	84,84,84,84	7
88	ZN	e1	501	1/1	0.96	0.06	163,163,163,163	0
86	OHX	6	1995	7/7	0.96	0.10	113,113,113,113	7
87	MG	1	4385	1/1	0.96	0.10	32,32,32,32	1
86	OHX	5	3667	7/7	0.96	0.18	41,41,41,41	7
86	OHX	5	3555	7/7	0.96	0.18	60,60,60,60	7
86	OHX	1	3528	7/7	0.96	0.15	68,68,68,68	7
87	MG	6	2215	1/1	0.96	0.31	52,52,52,52	0
87	MG	1	4391	1/1	0.96	0.10	37,37,37,37	1
86	OHX	2	1997	7/7	0.96	0.13	88,88,88,88	7
86	OHX	1	3515	7/7	0.97	0.13	98,98,98,98	7
86	OHX	C8	202	7/7	0.97	0.09	94,94,94,94	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	1975	7/7	0.97	0.08	112,112,112,112	7
87	MG	5	3872	1/1	0.97	0.10	32,32,32,32	0
86	OHX	L3	402	7/7	0.97	0.16	67,67,67,67	7
86	OHX	5	3572	7/7	0.97	0.15	66,66,66,66	7
86	OHX	5	3693	7/7	0.97	0.16	45,45,45,45	7
87	MG	1	3984	1/1	0.97	0.30	37,37,37,37	0
86	OHX	1	3518	7/7	0.97	0.19	41,41,41,41	7
86	OHX	1	3519	7/7	0.97	0.15	50,50,50,50	7
87	MG	1	4341	1/1	0.97	0.18	38,38,38,38	1
86	OHX	2	1912	7/7	0.97	0.10	109,109,109,109	0
86	OHX	1	3436	7/7	0.97	0.18	46,46,46,46	7
86	OHX	7	203	7/7	0.97	0.21	54,54,54,54	7
86	OHX	1	3522	7/7	0.97	0.20	40,40,40,40	7
87	MG	1	3991	1/1	0.97	0.19	36,36,36,36	0
86	OHX	5	3578	7/7	0.97	0.16	55,55,55,55	7
87	MG	5	4407	1/1	0.97	0.06	48,48,48,48	0
86	OHX	1	3445	7/7	0.97	0.16	51,51,51,51	7
86	OHX	1	3524	7/7	0.97	0.16	55,55,55,55	7
86	OHX	5	3581	7/7	0.97	0.16	46,46,46,46	7
86	OHX	1	3629	7/7	0.97	0.07	186,186,186,186	7
87	MG	5	3890	1/1	0.97	0.28	46,46,46,46	0
86	OHX	1	3576	7/7	0.97	0.14	53,53,53,53	7
86	OHX	2	1945	7/7	0.97	0.10	110,110,110,110	7
87	MG	6	2213	1/1	0.97	0.12	68,68,68,68	1
86	OHX	5	3706	7/7	0.97	0.14	74,74,74,74	7
87	MG	1	4165	1/1	0.97	0.22	54,54,54,54	0
86	OHX	8	203	7/7	0.97	0.16	86,86,86,86	7
87	MG	1	4167	1/1	0.97	0.15	42,42,42,42	1
86	OHX	M9	201	7/7	0.97	0.14	68,68,68,68	7
87	MG	5	4422	1/1	0.97	0.07	35,35,35,35	0
87	MG	4	246	1/1	0.97	0.22	51,51,51,51	0
86	OHX	1	3452	7/7	0.97	0.15	70,70,70,70	7
86	OHX	1	3456	7/7	0.97	0.13	85,85,85,85	7
86	OHX	5	3589	7/7	0.97	0.20	46,46,46,46	7
87	MG	5	4143	1/1	0.97	0.10	34,34,34,34	1
87	MG	2	2180	1/1	0.97	0.20	68,68,68,68	0
86	OHX	1	3457	7/7	0.97	0.17	50,50,50,50	7
87	MG	5	4431	1/1	0.97	0.24	44,44,44,44	1
87	MG	5	4432	1/1	0.97	0.09	36,36,36,36	1
86	OHX	1	3458	7/7	0.97	0.13	79,79,79,79	7
87	MG	L4	403	1/1	0.97	0.22	34,34,34,34	0
87	MG	5	4435	1/1	0.97	0.22	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4436	1/1	0.97	0.08	39,39,39,39	0
87	MG	L4	405	1/1	0.97	0.17	38,38,38,38	1
86	OHX	1	3464	7/7	0.97	0.22	50,50,50,50	7
87	MG	5	4439	1/1	0.97	0.09	40,40,40,40	0
86	OHX	8	212	7/7	0.97	0.12	85,85,85,85	7
87	MG	5	4152	1/1	0.97	0.12	40,40,40,40	0
87	MG	L7	301	1/1	0.97	0.06	39,39,39,39	0
87	MG	5	4445	1/1	0.97	0.19	32,32,32,32	1
87	MG	1	3860	1/1	0.97	0.22	49,49,49,49	0
87	MG	5	4448	1/1	0.97	0.12	42,42,42,42	1
86	OHX	1	3638	7/7	0.97	0.09	82,82,82,82	7
87	MG	5	4450	1/1	0.97	0.08	44,44,44,44	0
87	MG	5	4451	1/1	0.97	0.08	39,39,39,39	1
87	MG	5	4452	1/1	0.97	0.14	38,38,38,38	1
87	MG	1	3862	1/1	0.97	0.16	41,41,41,41	0
86	OHX	O7	103	7/7	0.97	0.16	60,60,60,60	7
86	OHX	5	3595	7/7	0.97	0.22	46,46,46,46	7
87	MG	1	3865	1/1	0.97	0.09	42,42,42,42	0
87	MG	M0	308	1/1	0.97	0.18	44,44,44,44	1
86	OHX	1	3470	7/7	0.97	0.14	88,88,88,88	7
87	MG	5	4460	1/1	0.97	0.14	62,62,62,62	0
87	MG	1	3867	1/1	0.97	0.21	42,42,42,42	0
87	MG	M3	201	1/1	0.97	0.12	45,45,45,45	0
87	MG	5	4466	1/1	0.97	0.07	39,39,39,39	0
87	MG	M3	203	1/1	0.97	0.10	46,46,46,46	1
86	OHX	6	1914	7/7	0.97	0.14	52,52,52,52	7
87	MG	5	4470	1/1	0.97	0.24	36,36,36,36	1
87	MG	1	4187	1/1	0.97	0.15	47,47,47,47	1
87	MG	6	2245	1/1	0.97	0.11	60,60,60,60	0
87	MG	5	4168	1/1	0.97	0.13	45,45,45,45	0
87	MG	M5	303	1/1	0.97	0.10	41,41,41,41	1
86	OHX	6	1918	7/7	0.97	0.19	56,56,56,56	7
86	OHX	c8	201	7/7	0.97	0.10	95,95,95,95	7
86	OHX	2	1978	7/7	0.97	0.07	121,121,121,121	7
87	MG	5	4174	1/1	0.97	0.07	41,41,41,41	0
87	MG	6	2250	1/1	0.97	0.27	47,47,47,47	0
86	OHX	1	3474	7/7	0.97	0.16	90,90,90,90	7
87	MG	6	2252	1/1	0.97	0.22	47,47,47,47	0
87	MG	5	4483	1/1	0.97	0.26	34,34,34,34	1
87	MG	1	4193	1/1	0.97	0.09	40,40,40,40	1
87	MG	6	2254	1/1	0.97	0.09	53,53,53,53	0
87	MG	5	4486	1/1	0.97	0.20	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3434	7/7	0.97	0.24	38,38,38,38	7
86	OHX	l3	401	7/7	0.97	0.20	52,52,52,52	7
87	MG	1	4392	1/1	0.97	0.13	37,37,37,37	1
87	MG	5	4491	1/1	0.97	0.31	35,35,35,35	1
86	OHX	5	3438	7/7	0.97	0.15	48,48,48,48	7
87	MG	5	4493	1/1	0.97	0.06	38,38,38,38	0
86	OHX	6	1929	7/7	0.97	0.20	53,53,53,53	7
87	MG	5	4496	1/1	0.97	0.07	57,57,57,57	0
87	MG	M7	208	1/1	0.97	0.11	40,40,40,40	0
87	MG	1	4029	1/1	0.97	0.08	62,62,62,62	0
87	MG	5	3943	1/1	0.97	0.16	48,48,48,48	0
86	OHX	5	3445	7/7	0.97	0.16	63,63,63,63	7
87	MG	M8	202	1/1	0.97	0.38	39,39,39,39	1
87	MG	6	2265	1/1	0.97	0.09	48,48,48,48	0
86	OHX	5	3457	7/7	0.97	0.17	67,67,67,67	7
87	MG	5	4506	1/1	0.97	0.32	38,38,38,38	1
86	OHX	5	3461	7/7	0.97	0.16	72,72,72,72	7
87	MG	1	4205	1/1	0.97	0.12	52,52,52,52	1
86	OHX	5	3462	7/7	0.97	0.13	56,56,56,56	7
87	MG	5	3951	1/1	0.97	0.36	39,39,39,39	0
87	MG	1	4402	1/1	0.97	0.10	48,48,48,48	0
87	MG	5	4515	1/1	0.97	0.09	34,34,34,34	0
87	MG	1	3882	1/1	0.97	0.10	49,49,49,49	0
87	MG	5	4517	1/1	0.97	0.08	54,54,54,54	0
86	OHX	5	3463	7/7	0.97	0.16	58,58,58,58	7
87	MG	5	4201	1/1	0.97	0.09	43,43,43,43	0
87	MG	1	4036	1/1	0.97	0.15	41,41,41,41	0
86	OHX	m0	301	7/7	0.97	0.13	86,86,86,86	7
86	OHX	6	1930	7/7	0.97	0.15	59,59,59,59	7
86	OHX	5	3473	7/7	0.97	0.15	61,61,61,61	7
87	MG	1	4040	1/1	0.97	0.35	47,47,47,47	0
87	MG	1	4410	1/1	0.97	0.10	56,56,56,56	0
86	OHX	5	3475	7/7	0.97	0.13	81,81,81,81	7
87	MG	6	2280	1/1	0.97	0.09	46,46,46,46	0
86	OHX	5	3477	7/7	0.97	0.13	44,44,44,44	7
87	MG	5	4530	1/1	0.97	0.07	43,43,43,43	0
87	MG	5	4532	1/1	0.97	0.14	43,43,43,43	0
87	MG	5	4534	1/1	0.97	0.12	54,54,54,54	0
86	OHX	1	3479	7/7	0.97	0.19	55,55,55,55	7
87	MG	1	4219	1/1	0.97	0.09	54,54,54,54	0
87	MG	5	3967	1/1	0.97	0.30	28,28,28,28	0
87	MG	5	4215	1/1	0.97	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4415	1/1	0.97	0.05	60,60,60,60	1
87	MG	1	3890	1/1	0.97	0.15	49,49,49,49	0
87	MG	O1	202	1/1	0.97	0.20	60,60,60,60	1
86	OHX	6	1933	7/7	0.97	0.11	82,82,82,82	7
86	OHX	6	1937	7/7	0.97	0.10	88,88,88,88	7
87	MG	5	4546	1/1	0.97	0.16	34,34,34,34	1
86	OHX	6	1938	7/7	0.97	0.13	69,69,69,69	7
86	OHX	5	3485	7/7	0.97	0.17	46,46,46,46	7
86	OHX	1	3480	7/7	0.97	0.20	75,75,75,75	7
86	OHX	1	3591	7/7	0.97	0.10	90,90,90,90	7
86	OHX	o7	502	7/7	0.97	0.18	64,64,64,64	7
87	MG	6	2294	1/1	0.97	0.08	43,43,43,43	0
86	OHX	5	3489	7/7	0.97	0.13	51,51,51,51	7
86	OHX	6	1942	7/7	0.97	0.12	70,70,70,70	7
86	OHX	q1	101	7/7	0.97	0.18	46,46,46,46	7
87	MG	5	4561	1/1	0.97	0.06	41,41,41,41	0
86	OHX	5	3623	7/7	0.97	0.18	46,46,46,46	7
87	MG	1	4430	1/1	0.97	0.23	49,49,49,49	0
86	OHX	5	3492	7/7	0.97	0.16	42,42,42,42	7
87	MG	1	4433	1/1	0.97	0.14	43,43,43,43	0
87	MG	O7	107	1/1	0.97	0.28	42,42,42,42	1
86	OHX	6	1943	7/7	0.97	0.10	108,108,108,108	7
87	MG	O7	109	1/1	0.97	0.24	46,46,46,46	1
87	MG	5	3989	1/1	0.97	0.26	32,32,32,32	0
86	OHX	1	3698	7/7	0.97	0.16	51,51,51,51	7
87	MG	1	4436	1/1	0.97	0.08	41,41,41,41	0
87	MG	1	4437	1/1	0.97	0.16	39,39,39,39	1
87	MG	6	2308	1/1	0.97	0.14	51,51,51,51	1
86	OHX	2	1913	7/7	0.97	0.14	87,87,87,87	7
86	OHX	6	1946	7/7	0.97	0.13	71,71,71,71	7
87	MG	1	3909	1/1	0.97	0.08	43,43,43,43	0
87	MG	5	4250	1/1	0.97	0.22	58,58,58,58	0
87	MG	5	3998	1/1	0.97	0.38	41,41,41,41	0
86	OHX	5	3501	7/7	0.97	0.16	57,57,57,57	7
87	MG	1	4442	1/1	0.97	0.20	51,51,51,51	0
86	OHX	5	3505	7/7	0.97	0.15	59,59,59,59	7
86	OHX	6	1947	7/7	0.97	0.17	59,59,59,59	7
86	OHX	6	1948	7/7	0.97	0.12	86,86,86,86	7
87	MG	5	4257	1/1	0.97	0.13	29,29,29,29	0
86	OHX	5	3508	7/7	0.97	0.17	38,38,38,38	7
86	OHX	1	3485	7/7	0.97	0.15	87,87,87,87	7
86	OHX	2	1916	7/7	0.97	0.11	89,89,89,89	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	7	228	1/1	0.97	0.14	41,41,41,41	1
86	OHX	6	1952	7/7	0.97	0.13	84,84,84,84	7
87	MG	1	4451	1/1	0.97	0.21	58,58,58,58	1
87	MG	1	4452	1/1	0.97	0.19	44,44,44,44	0
87	MG	6	2111	1/1	0.97	0.33	49,49,49,49	0
87	MG	7	233	1/1	0.97	0.13	52,52,52,52	0
87	MG	2	2236	1/1	0.97	0.08	64,64,64,64	0
86	OHX	5	3513	7/7	0.97	0.09	107,107,107,107	7
87	MG	6	2327	1/1	0.97	0.12	78,78,78,78	0
87	MG	6	2328	1/1	0.97	0.12	54,54,54,54	1
87	MG	5	4269	1/1	0.97	0.18	39,39,39,39	1
87	MG	5	4270	1/1	0.97	0.22	45,45,45,45	0
87	MG	2	2238	1/1	0.97	0.05	89,89,89,89	0
87	MG	7	241	1/1	0.97	0.13	47,47,47,47	1
87	MG	8	222	1/1	0.97	0.18	41,41,41,41	0
87	MG	1	4078	1/1	0.97	0.16	31,31,31,31	0
86	OHX	5	3514	7/7	0.97	0.19	39,39,39,39	7
86	OHX	1	3542	7/7	0.97	0.20	49,49,49,49	7
86	OHX	1	3487	7/7	0.97	0.13	74,74,74,74	7
86	OHX	1	3650	7/7	0.97	0.13	96,96,96,96	7
86	OHX	6	1956	7/7	0.97	0.12	90,90,90,90	7
87	MG	5	4024	1/1	0.97	0.34	37,37,37,37	0
86	OHX	6	1957	7/7	0.97	0.14	63,63,63,63	7
87	MG	1	4463	1/1	0.97	0.08	51,51,51,51	0
87	MG	5	4284	1/1	0.97	0.18	44,44,44,44	1
87	MG	5	4285	1/1	0.97	0.15	38,38,38,38	1
87	MG	5	4286	1/1	0.97	0.13	34,34,34,34	1
87	MG	8	235	1/1	0.97	0.14	61,61,61,61	1
86	OHX	1	3651	7/7	0.97	0.07	199,199,199,199	7
86	OHX	1	3597	7/7	0.97	0.17	37,37,37,37	7
87	MG	1	4466	1/1	0.97	0.12	43,43,43,43	0
87	MG	1	3930	1/1	0.97	0.13	41,41,41,41	0
86	OHX	3	201	7/7	0.97	0.13	71,71,71,71	7
87	MG	12	302	1/1	0.97	0.17	36,36,36,36	0
87	MG	5	4294	1/1	0.97	0.10	39,39,39,39	0
86	OHX	1	3544	7/7	0.97	0.15	52,52,52,52	7
87	MG	5	4296	1/1	0.97	0.07	48,48,48,48	1
86	OHX	2	1948	7/7	0.97	0.17	67,67,67,67	7
87	MG	12	307	1/1	0.97	0.52	46,46,46,46	1
87	MG	1	4266	1/1	0.97	0.11	33,33,33,33	0
87	MG	13	404	1/1	0.97	0.05	33,33,33,33	0
87	MG	1	4267	1/1	0.97	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4036	1/1	0.97	0.08	34,34,34,34	0
87	MG	5	4302	1/1	0.97	0.12	40,40,40,40	0
86	OHX	5	3528	7/7	0.97	0.14	62,62,62,62	7
87	MG	l3	410	1/1	0.97	0.13	31,31,31,31	1
86	OHX	2	1934	7/7	0.97	0.11	103,103,103,103	7
87	MG	5	4307	1/1	0.97	0.09	41,41,41,41	1
86	OHX	6	1964	7/7	0.97	0.14	49,49,49,49	7
86	OHX	6	1965	7/7	0.97	0.14	83,83,83,83	7
87	MG	1	4272	1/1	0.97	0.29	46,46,46,46	1
87	MG	1	4273	1/1	0.97	0.17	45,45,45,45	1
87	MG	5	4312	1/1	0.97	0.08	29,29,29,29	0
87	MG	5	4044	1/1	0.97	0.16	35,35,35,35	0
86	OHX	3	205	7/7	0.97	0.13	80,80,80,80	7
87	MG	d3	202	1/1	0.97	0.14	49,49,49,49	1
87	MG	1	4275	1/1	0.97	0.04	46,46,46,46	0
87	MG	1	4097	1/1	0.97	0.09	42,42,42,42	0
86	OHX	5	3534	7/7	0.97	0.16	42,42,42,42	7
87	MG	5	4051	1/1	0.97	0.16	33,33,33,33	0
87	MG	5	4321	1/1	0.97	0.44	66,66,66,66	1
86	OHX	6	1967	7/7	0.97	0.14	47,47,47,47	7
86	OHX	2	1922	7/7	0.97	0.11	75,75,75,75	7
87	MG	l9	202	1/1	0.97	0.16	38,38,38,38	0
86	OHX	5	3537	7/7	0.97	0.10	114,114,114,114	7
87	MG	1	3943	1/1	0.97	0.19	38,38,38,38	0
86	OHX	1	3492	7/7	0.97	0.09	113,113,113,113	7
87	MG	5	4057	1/1	0.97	0.07	45,45,45,45	0
87	MG	1	3945	1/1	0.97	0.16	43,43,43,43	0
87	MG	5	4059	1/1	0.97	0.20	39,39,39,39	0
86	OHX	6	1970	7/7	0.97	0.12	88,88,88,88	7
86	OHX	5	3540	7/7	0.97	0.19	54,54,54,54	7
86	OHX	1	3495	7/7	0.97	0.19	44,44,44,44	7
87	MG	6	2151	1/1	0.97	0.34	47,47,47,47	0
86	OHX	6	1972	7/7	0.97	0.16	59,59,59,59	7
87	MG	m7	203	1/1	0.97	0.22	33,33,33,33	0
87	MG	m7	204	1/1	0.97	0.15	40,40,40,40	1
86	OHX	6	1973	7/7	0.97	0.15	86,86,86,86	7
86	OHX	1	3550	7/7	0.97	0.15	55,55,55,55	7
87	MG	5	4338	1/1	0.97	0.15	39,39,39,39	1
87	MG	m8	1502	1/1	0.97	0.07	47,47,47,47	0
86	OHX	5	3545	7/7	0.97	0.16	46,46,46,46	7
87	MG	1	4292	1/1	0.97	0.09	39,39,39,39	0
87	MG	5	4341	1/1	0.97	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4112	1/1	0.97	0.12	48,48,48,48	0
87	MG	5	4344	1/1	0.97	0.09	35,35,35,35	1
87	MG	1	3953	1/1	0.97	0.28	38,38,38,38	0
86	OHX	5	3546	7/7	0.97	0.15	52,52,52,52	7
87	MG	n1	202	1/1	0.97	0.07	40,40,40,40	1
86	OHX	6	1975	7/7	0.97	0.15	61,61,61,61	7
86	OHX	1	3496	7/7	0.97	0.21	45,45,45,45	7
87	MG	6	2162	1/1	0.97	0.29	53,53,53,53	0
87	MG	1	4117	1/1	0.97	0.11	59,59,59,59	0
86	OHX	6	1977	7/7	0.97	0.13	86,86,86,86	7
86	OHX	1	3499	7/7	0.97	0.14	54,54,54,54	7
87	MG	n8	203	1/1	0.97	0.05	41,41,41,41	0
86	OHX	1	3501	7/7	0.97	0.13	83,83,83,83	7
87	MG	1	4303	1/1	0.97	0.16	41,41,41,41	1
86	OHX	4	203	7/7	0.97	0.15	61,61,61,61	7
86	OHX	4	206	7/7	0.97	0.14	88,88,88,88	7
86	OHX	2	1936	7/7	0.97	0.17	72,72,72,72	7
86	OHX	2	1908	7/7	0.97	0.09	104,104,104,104	0
86	OHX	1	3557	7/7	0.97	0.15	87,87,87,87	7
87	MG	5	4362	1/1	0.97	0.06	49,49,49,49	1
87	MG	1	3816	1/1	0.97	0.34	49,49,49,49	0
87	MG	5	4364	1/1	0.97	0.07	35,35,35,35	1
86	OHX	5	3558	7/7	0.97	0.13	45,45,45,45	7
87	MG	1	4129	1/1	0.97	0.06	36,36,36,36	0
87	MG	1	4313	1/1	0.97	0.17	41,41,41,41	1
86	OHX	2	1939	7/7	0.97	0.10	98,98,98,98	7
86	OHX	5	3560	7/7	0.97	0.13	50,50,50,50	7
87	MG	1	4319	1/1	0.97	0.09	59,59,59,59	0
87	MG	5	4372	1/1	0.97	0.16	38,38,38,38	1
86	OHX	2	1924	7/7	0.97	0.13	89,89,89,89	7
86	OHX	2	1909	7/7	0.97	0.11	94,94,94,94	7
86	OHX	2	1956	7/7	0.97	0.12	91,91,91,91	7
87	MG	1	3823	1/1	0.97	0.18	31,31,31,31	0
87	MG	1	3973	1/1	0.97	0.17	29,29,29,29	0
86	OHX	6	1991	7/7	0.97	0.12	83,83,83,83	7
87	MG	5	3862	1/1	0.97	0.28	35,35,35,35	0
86	OHX	2	1928	7/7	0.97	0.13	75,75,75,75	7
86	OHX	2	1930	7/7	0.97	0.14	77,77,77,77	7
87	MG	1	4329	1/1	0.97	0.31	60,60,60,60	0
87	MG	6	2189	1/1	0.97	0.22	47,47,47,47	0
86	OHX	1	3514	7/7	0.97	0.16	50,50,50,50	7
86	OHX	1	3420	7/7	0.98	0.11	59,59,59,59	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4495	1/1	0.98	0.29	53,53,53,53	0
87	MG	1	4333	1/1	0.98	0.06	49,49,49,49	0
87	MG	5	4497	1/1	0.98	0.13	41,41,41,41	1
87	MG	5	4276	1/1	0.98	0.09	33,33,33,33	1
87	MG	1	4045	1/1	0.98	0.15	35,35,35,35	0
87	MG	5	4278	1/1	0.98	0.12	35,35,35,35	1
86	OHX	1	3540	7/7	0.98	0.06	128,128,128,128	7
87	MG	5	4502	1/1	0.98	0.13	42,42,42,42	1
86	OHX	1	3421	7/7	0.98	0.15	48,48,48,48	7
86	OHX	5	3480	7/7	0.98	0.13	63,63,63,63	7
87	MG	1	4049	1/1	0.98	0.10	42,42,42,42	0
86	OHX	5	3481	7/7	0.98	0.11	69,69,69,69	7
87	MG	1	4051	1/1	0.98	0.16	41,41,41,41	0
87	MG	5	4508	1/1	0.98	0.10	40,40,40,40	1
86	OHX	5	3482	7/7	0.98	0.16	54,54,54,54	7
86	OHX	1	3422	7/7	0.98	0.14	56,56,56,56	7
87	MG	5	4511	1/1	0.98	0.08	52,52,52,52	1
87	MG	5	4092	1/1	0.98	0.20	36,36,36,36	1
87	MG	1	4504	1/1	0.98	0.11	60,60,60,60	0
86	OHX	1	3489	7/7	0.98	0.10	89,89,89,89	7
87	MG	1	4344	1/1	0.98	0.11	40,40,40,40	0
87	MG	5	3917	1/1	0.98	0.12	39,39,39,39	0
86	OHX	1	3435	7/7	0.98	0.13	45,45,45,45	7
86	OHX	5	3486	7/7	0.98	0.13	64,64,64,64	7
87	MG	1	4194	1/1	0.98	0.07	47,47,47,47	1
86	OHX	2	1906	7/7	0.98	0.10	82,82,82,82	7
87	MG	5	4522	1/1	0.98	0.06	35,35,35,35	1
87	MG	C1	201	1/1	0.98	0.15	69,69,69,69	0
87	MG	1	4059	1/1	0.98	0.21	38,38,38,38	0
86	OHX	1	3439	7/7	0.98	0.10	69,69,69,69	7
87	MG	5	4303	1/1	0.98	0.06	43,43,43,43	1
86	OHX	7	201	7/7	0.98	0.13	70,70,70,70	7
86	OHX	7	202	7/7	0.98	0.11	60,60,60,60	7
87	MG	5	4306	1/1	0.98	0.16	35,35,35,35	1
87	MG	1	4201	1/1	0.98	0.08	38,38,38,38	0
87	MG	1	4202	1/1	0.98	0.06	59,59,59,59	1
87	MG	5	4533	1/1	0.98	0.19	36,36,36,36	1
86	OHX	1	3493	7/7	0.98	0.14	56,56,56,56	7
86	OHX	7	204	7/7	0.98	0.14	43,43,43,43	7
86	OHX	5	3490	7/7	0.98	0.14	50,50,50,50	7
87	MG	5	3932	1/1	0.98	0.07	39,39,39,39	0
87	MG	5	4538	1/1	0.98	0.26	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3443	7/7	0.98	0.16	61,61,61,61	7
87	MG	5	4540	1/1	0.98	0.19	39,39,39,39	1
86	OHX	2	1917	7/7	0.98	0.13	85,85,85,85	7
86	OHX	1	3497	7/7	0.98	0.15	50,50,50,50	7
86	OHX	1	3498	7/7	0.98	0.12	62,62,62,62	7
87	MG	5	4116	1/1	0.98	0.20	36,36,36,36	1
86	OHX	1	3446	7/7	0.98	0.12	65,65,65,65	7
87	MG	1	4212	1/1	0.98	0.14	41,41,41,41	1
86	OHX	5	3497	7/7	0.98	0.14	62,62,62,62	7
87	MG	5	4548	1/1	0.98	0.16	42,42,42,42	1
87	MG	1	4072	1/1	0.98	0.30	40,40,40,40	0
87	MG	5	4550	1/1	0.98	0.07	49,49,49,49	1
87	MG	5	4551	1/1	0.98	0.15	41,41,41,41	1
87	MG	5	4552	1/1	0.98	0.05	39,39,39,39	0
86	OHX	5	3498	7/7	0.98	0.11	66,66,66,66	7
87	MG	5	4122	1/1	0.98	0.26	48,48,48,48	1
87	MG	5	4123	1/1	0.98	0.08	42,42,42,42	0
86	OHX	5	3499	7/7	0.98	0.16	46,46,46,46	7
87	MG	5	4557	1/1	0.98	0.09	50,50,50,50	0
86	OHX	1	3500	7/7	0.98	0.15	41,41,41,41	7
87	MG	5	4126	1/1	0.98	0.14	55,55,55,55	0
86	OHX	6	1978	7/7	0.98	0.11	52,52,52,52	7
86	OHX	5	3502	7/7	0.98	0.13	46,46,46,46	7
86	OHX	5	3503	7/7	0.98	0.13	104,104,104,104	7
86	OHX	8	207	7/7	0.98	0.13	74,74,74,74	7
87	MG	1	4375	1/1	0.98	0.08	43,43,43,43	1
86	OHX	1	3448	7/7	0.98	0.12	59,59,59,59	7
87	MG	1	4377	1/1	0.98	0.18	35,35,35,35	1
86	OHX	1	3449	7/7	0.98	0.10	88,88,88,88	7
86	OHX	1	3556	7/7	0.98	0.13	70,70,70,70	7
86	OHX	2	1918	7/7	0.98	0.14	80,80,80,80	7
87	MG	5	4571	1/1	0.98	0.09	34,34,34,34	1
87	MG	1	4381	1/1	0.98	0.10	60,60,60,60	0
86	OHX	2	1921	7/7	0.98	0.10	88,88,88,88	7
87	MG	1	4383	1/1	0.98	0.09	33,33,33,33	1
87	MG	5	4575	1/1	0.98	0.24	48,48,48,48	1
87	MG	5	4343	1/1	0.98	0.09	53,53,53,53	1
86	OHX	5	3510	7/7	0.98	0.17	48,48,48,48	7
86	OHX	1	3454	7/7	0.98	0.14	61,61,61,61	7
86	OHX	1	3506	7/7	0.98	0.22	38,38,38,38	7
87	MG	1	4387	1/1	0.98	0.07	51,51,51,51	1
87	MG	5	3961	1/1	0.98	0.37	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3731	7/7	0.98	0.19	48,48,48,48	7
87	MG	7	219	1/1	0.98	0.13	39,39,39,39	0
86	OHX	6	1986	7/7	0.98	0.12	73,73,73,73	7
87	MG	4	239	1/1	0.98	0.08	40,40,40,40	1
87	MG	1	4090	1/1	0.98	0.14	50,50,50,50	0
86	OHX	1	3507	7/7	0.98	0.15	60,60,60,60	7
86	OHX	1	3508	7/7	0.98	0.11	71,71,71,71	7
86	OHX	5	3516	7/7	0.98	0.12	60,60,60,60	7
87	MG	1	3836	1/1	0.98	0.11	38,38,38,38	1
86	OHX	1	3455	7/7	0.98	0.13	70,70,70,70	7
86	OHX	5	3518	7/7	0.98	0.11	60,60,60,60	7
86	OHX	2	1911	7/7	0.98	0.08	109,109,109,109	0
86	OHX	1	3623	7/7	0.98	0.11	51,51,51,51	7
86	OHX	2	1907	7/7	0.98	0.08	93,93,93,93	7
86	OHX	1	3512	7/7	0.98	0.13	74,74,74,74	7
86	OHX	6	1905	7/7	0.98	0.10	74,74,74,74	0
87	MG	L3	406	1/1	0.98	0.16	39,39,39,39	1
86	OHX	5	3524	7/7	0.98	0.12	88,88,88,88	7
87	MG	L3	408	1/1	0.98	0.20	53,53,53,53	1
87	MG	2	2187	1/1	0.98	0.12	87,87,87,87	0
87	MG	L4	404	1/1	0.98	0.12	42,42,42,42	1
86	OHX	6	1907	7/7	0.98	0.08	76,76,76,76	0
87	MG	1	4247	1/1	0.98	0.15	44,44,44,44	1
86	OHX	6	1911	7/7	0.98	0.09	59,59,59,59	7
86	OHX	6	1913	7/7	0.98	0.08	85,85,85,85	7
87	MG	5	4170	1/1	0.98	0.13	36,36,36,36	1
87	MG	5	4377	1/1	0.98	0.08	36,36,36,36	1
86	OHX	2	1903	7/7	0.98	0.10	90,90,90,90	0
86	OHX	6	1915	7/7	0.98	0.16	63,63,63,63	7
86	OHX	5	3530	7/7	0.98	0.11	94,94,94,94	7
86	OHX	5	3640	7/7	0.98	0.10	73,73,73,73	7
87	MG	1	4254	1/1	0.98	0.11	51,51,51,51	0
86	OHX	1	3460	7/7	0.98	0.18	60,60,60,60	7
86	OHX	6	1919	7/7	0.98	0.12	68,68,68,68	7
87	MG	M0	309	1/1	0.98	0.07	46,46,46,46	1
87	MG	5	3994	1/1	0.98	0.21	21,21,21,21	0
86	OHX	6	1920	7/7	0.98	0.07	114,114,114,114	7
86	OHX	1	3461	7/7	0.98	0.12	96,96,96,96	7
86	OHX	6	1923	7/7	0.98	0.12	71,71,71,71	7
87	MG	1	4420	1/1	0.98	0.10	56,56,56,56	0
87	MG	1	3858	1/1	0.98	0.10	51,51,51,51	0
86	OHX	1	3462	7/7	0.98	0.12	59,59,59,59	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2084	7/7	0.98	0.11	79,79,79,79	7
86	OHX	6	1926	7/7	0.98	0.14	55,55,55,55	7
87	MG	1	4265	1/1	0.98	0.14	56,56,56,56	0
87	MG	5	4398	1/1	0.98	0.20	38,38,38,38	1
87	MG	5	4189	1/1	0.98	0.15	35,35,35,35	1
87	MG	1	4120	1/1	0.98	0.40	51,51,51,51	0
87	MG	M6	202	1/1	0.98	0.18	41,41,41,41	1
86	OHX	6	1927	7/7	0.98	0.08	109,109,109,109	7
87	MG	5	4403	1/1	0.98	0.10	40,40,40,40	1
87	MG	5	4007	1/1	0.98	0.24	28,28,28,28	0
86	OHX	6	1928	7/7	0.98	0.08	118,118,118,118	7
86	OHX	2	1937	7/7	0.98	0.10	94,94,94,94	7
87	MG	l3	408	1/1	0.98	0.08	31,31,31,31	0
86	OHX	q2	502	7/7	0.98	0.14	51,51,51,51	7
87	MG	5	3836	1/1	0.98	0.10	34,34,34,34	0
87	MG	M7	204	1/1	0.98	0.25	40,40,40,40	0
87	MG	5	4410	1/1	0.98	0.09	47,47,47,47	1
87	MG	l3	413	1/1	0.98	0.11	32,32,32,32	1
87	MG	2	2207	1/1	0.98	0.15	61,61,61,61	0
86	OHX	1	3465	7/7	0.98	0.14	62,62,62,62	7
87	MG	l4	403	1/1	0.98	0.06	39,39,39,39	0
86	OHX	1	3632	7/7	0.98	0.14	43,43,43,43	7
87	MG	5	4016	1/1	0.98	0.32	29,29,29,29	0
86	OHX	1	3466	7/7	0.98	0.12	45,45,45,45	7
86	OHX	6	1934	7/7	0.98	0.15	57,57,57,57	7
86	OHX	6	1935	7/7	0.98	0.11	56,56,56,56	7
87	MG	l5	309	1/1	0.98	0.07	54,54,54,54	1
86	OHX	6	1936	7/7	0.98	0.13	57,57,57,57	7
86	OHX	1	3467	7/7	0.98	0.10	113,113,113,113	7
86	OHX	1	3468	7/7	0.98	0.13	65,65,65,65	7
87	MG	5	4210	1/1	0.98	0.11	35,35,35,35	1
87	MG	5	3847	1/1	0.98	0.32	38,38,38,38	0
86	OHX	5	3550	7/7	0.98	0.21	47,47,47,47	7
86	OHX	1	3469	7/7	0.98	0.15	75,75,75,75	7
86	OHX	1	3578	7/7	0.98	0.17	40,40,40,40	7
87	MG	1	4283	1/1	0.98	0.08	38,38,38,38	1
87	MG	l9	203	1/1	0.98	0.06	46,46,46,46	1
87	MG	5	4216	1/1	0.98	0.10	44,44,44,44	0
86	OHX	2	1926	7/7	0.98	0.10	81,81,81,81	7
87	MG	2	2220	1/1	0.98	0.07	70,70,70,70	1
86	OHX	1	3471	7/7	0.98	0.17	43,43,43,43	7
86	OHX	1	3581	7/7	0.98	0.13	54,54,54,54	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	1914	7/7	0.98	0.13	69,69,69,69	7
86	OHX	C8	201	7/7	0.98	0.09	94,94,94,94	7
87	MG	5	3858	1/1	0.98	0.17	58,58,58,58	0
87	MG	5	4224	1/1	0.98	0.18	38,38,38,38	0
86	OHX	1	3475	7/7	0.98	0.14	49,49,49,49	7
87	MG	m6	204	1/1	0.98	0.05	40,40,40,40	0
87	MG	1	4011	1/1	0.98	0.30	31,31,31,31	0
86	OHX	1	3476	7/7	0.98	0.12	70,70,70,70	7
87	MG	5	4440	1/1	0.98	0.12	33,33,33,33	0
87	MG	5	4038	1/1	0.98	0.18	29,29,29,29	0
86	OHX	1	3477	7/7	0.98	0.14	62,62,62,62	7
87	MG	m7	207	1/1	0.98	0.08	41,41,41,41	1
87	MG	m7	208	1/1	0.98	0.12	40,40,40,40	1
87	MG	m7	209	1/1	0.98	0.16	42,42,42,42	1
87	MG	6	2236	1/1	0.98	0.11	54,54,54,54	0
86	OHX	2	1915	7/7	0.98	0.09	122,122,122,122	7
86	OHX	6	1951	7/7	0.98	0.06	133,133,133,133	7
86	OHX	5	3431	7/7	0.98	0.10	61,61,61,61	7
87	MG	5	3867	1/1	0.98	0.14	41,41,41,41	0
86	OHX	5	3433	7/7	0.98	0.10	47,47,47,47	7
87	MG	n0	202	1/1	0.98	0.17	38,38,38,38	1
87	MG	5	4237	1/1	0.98	0.09	36,36,36,36	1
87	MG	5	4046	1/1	0.98	0.38	51,51,51,51	0
87	MG	5	4453	1/1	0.98	0.11	33,33,33,33	1
87	MG	1	3892	1/1	0.98	0.18	41,41,41,41	0
87	MG	1	4299	1/1	0.98	0.10	44,44,44,44	1
86	OHX	2	1929	7/7	0.98	0.13	66,66,66,66	7
87	MG	O2	201	1/1	0.98	0.19	30,30,30,30	0
86	OHX	2	1966	7/7	0.98	0.11	61,61,61,61	7
86	OHX	1	3590	7/7	0.98	0.11	91,91,91,91	7
86	OHX	1	3482	7/7	0.98	0.14	59,59,59,59	7
87	MG	1	4157	1/1	0.98	0.08	42,42,42,42	0
87	MG	5	4463	1/1	0.98	0.25	36,36,36,36	1
86	OHX	5	3447	7/7	0.98	0.14	60,60,60,60	7
87	MG	5	4465	1/1	0.98	0.06	44,44,44,44	0
86	OHX	5	3448	7/7	0.98	0.16	46,46,46,46	7
86	OHX	5	3449	7/7	0.98	0.11	72,72,72,72	7
87	MG	1	4026	1/1	0.98	0.07	40,40,40,40	0
86	OHX	5	3451	7/7	0.98	0.15	43,43,43,43	7
86	OHX	5	3452	7/7	0.98	0.13	70,70,70,70	7
86	OHX	5	3453	7/7	0.98	0.12	79,79,79,79	7
86	OHX	5	3455	7/7	0.98	0.15	54,54,54,54	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3456	7/7	0.98	0.09	115,115,115,115	0
87	MG	1	4315	1/1	0.98	0.08	35,35,35,35	1
87	MG	o3	205	1/1	0.98	0.22	35,35,35,35	1
87	MG	1	4316	1/1	0.98	0.15	51,51,51,51	0
87	MG	5	4477	1/1	0.98	0.08	38,38,38,38	1
87	MG	o7	504	1/1	0.98	0.11	37,37,37,37	1
87	MG	1	3905	1/1	0.98	0.06	48,48,48,48	0
87	MG	q1	103	1/1	0.98	0.14	46,46,46,46	1
87	MG	1	4168	1/1	0.98	0.07	35,35,35,35	1
87	MG	q3	502	1/1	0.98	0.23	43,43,43,43	1
87	MG	1	4320	1/1	0.98	0.17	36,36,36,36	1
86	OHX	4	204	7/7	0.98	0.13	57,57,57,57	7
88	ZN	E1	501	1/1	0.98	0.04	132,132,132,132	0
87	MG	6	2264	1/1	0.98	0.10	46,46,46,46	1
86	OHX	5	3458	7/7	0.98	0.18	42,42,42,42	7
86	OHX	4	205	7/7	0.98	0.11	75,75,75,75	7
88	ZN	q2	501	1/1	0.98	0.12	69,69,69,69	0
86	OHX	1	3483	7/7	0.98	0.15	55,55,55,55	7
86	OHX	1	3484	7/7	0.98	0.15	62,62,62,62	7
86	OHX	1	3536	7/7	0.98	0.13	54,54,54,54	7
87	MG	2	2131	1/1	0.98	0.09	73,73,73,73	0
86	OHX	1	3419	7/7	0.98	0.10	66,66,66,66	7
86	OHX	5	3474	7/7	0.98	0.12	78,78,78,78	7
86	OHX	1	3538	7/7	0.98	0.13	62,62,62,62	7
86	OHX	5	3476	7/7	0.98	0.15	46,46,46,46	7
86	OHX	5	3471	7/7	0.99	0.09	76,76,76,76	7
86	OHX	5	3472	7/7	0.99	0.12	53,53,53,53	7
86	OHX	1	3415	7/7	0.99	0.11	53,53,53,53	7
87	MG	5	4425	1/1	0.99	0.06	48,48,48,48	1
87	MG	1	4210	1/1	0.99	0.08	47,47,47,47	0
86	OHX	1	3417	7/7	0.99	0.08	56,56,56,56	7
86	OHX	1	3418	7/7	0.99	0.12	49,49,49,49	7
86	OHX	2	1910	7/7	0.99	0.08	94,94,94,94	7
86	OHX	2	1902	7/7	0.99	0.08	86,86,86,86	0
87	MG	5	4283	1/1	0.99	0.10	41,41,41,41	0
87	MG	M3	202	1/1	0.99	0.08	49,49,49,49	1
87	MG	5	4148	1/1	0.99	0.06	32,32,32,32	1
86	OHX	1	3459	7/7	0.99	0.10	81,81,81,81	7
86	OHX	5	3584	7/7	0.99	0.13	52,52,52,52	7
87	MG	5	4288	1/1	0.99	0.09	39,39,39,39	1
86	OHX	2	1901	7/7	0.99	0.10	81,81,81,81	0
86	OHX	2	1925	7/7	0.99	0.06	112,112,112,112	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4291	1/1	0.99	0.15	35,35,35,35	1
86	OHX	1	3423	7/7	0.99	0.10	62,62,62,62	7
87	MG	1	3878	1/1	0.99	0.20	46,46,46,46	0
86	OHX	1	3463	7/7	0.99	0.10	74,74,74,74	7
86	OHX	1	3424	7/7	0.99	0.11	49,49,49,49	7
86	OHX	N9	101	7/7	0.99	0.11	58,58,58,58	7
87	MG	5	4297	1/1	0.99	0.19	33,33,33,33	1
87	MG	5	4447	1/1	0.99	0.09	34,34,34,34	1
86	OHX	1	3425	7/7	0.99	0.09	71,71,71,71	7
86	OHX	1	3426	7/7	0.99	0.08	71,71,71,71	7
86	OHX	1	3427	7/7	0.99	0.13	65,65,65,65	7
86	OHX	1	3428	7/7	0.99	0.08	79,79,79,79	0
86	OHX	1	3429	7/7	0.99	0.12	62,62,62,62	7
86	OHX	6	1902	7/7	0.99	0.08	77,77,77,77	2
86	OHX	6	1903	7/7	0.99	0.10	63,63,63,63	3
86	OHX	6	1904	7/7	0.99	0.08	71,71,71,71	7
86	OHX	1	3430	7/7	0.99	0.12	55,55,55,55	7
87	MG	M7	210	1/1	0.99	0.05	45,45,45,45	1
86	OHX	6	1906	7/7	0.99	0.11	55,55,55,55	7
86	OHX	5	3495	7/7	0.99	0.13	47,47,47,47	7
86	OHX	1	3431	7/7	0.99	0.08	86,86,86,86	7
87	MG	5	4461	1/1	0.99	0.08	45,45,45,45	1
86	OHX	6	1908	7/7	0.99	0.09	71,71,71,71	7
87	MG	6	2318	1/1	0.99	0.07	54,54,54,54	0
86	OHX	6	1909	7/7	0.99	0.10	79,79,79,79	7
87	MG	5	4314	1/1	0.99	0.04	33,33,33,33	0
86	OHX	6	1910	7/7	0.99	0.07	60,60,60,60	7
87	MG	N0	201	1/1	0.99	0.11	49,49,49,49	1
86	OHX	1	3472	7/7	0.99	0.08	54,54,54,54	7
87	MG	5	4469	1/1	0.99	0.08	38,38,38,38	0
86	OHX	6	1912	7/7	0.99	0.09	72,72,72,72	7
86	OHX	1	3432	7/7	0.99	0.09	64,64,64,64	7
86	OHX	1	3433	7/7	0.99	0.09	53,53,53,53	7
86	OHX	5	3504	7/7	0.99	0.10	75,75,75,75	7
86	OHX	1	3434	7/7	0.99	0.08	68,68,68,68	7
86	OHX	s1	301	7/7	0.99	0.06	80,80,80,80	0
86	OHX	6	1916	7/7	0.99	0.10	65,65,65,65	7
87	MG	1	4366	1/1	0.99	0.08	42,42,42,42	1
86	OHX	6	1917	7/7	0.99	0.08	55,55,55,55	7
86	OHX	2	1904	7/7	0.99	0.10	89,89,89,89	7
86	OHX	4	201	7/7	0.99	0.14	52,52,52,52	2
86	OHX	4	202	7/7	0.99	0.09	55,55,55,55	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	1	4135	1/1	0.99	0.10	41,41,41,41	0
86	OHX	2	1919	7/7	0.99	0.06	78,78,78,78	7
87	MG	1	3910	1/1	0.99	0.45	44,44,44,44	0
87	MG	5	4192	1/1	0.99	0.04	36,36,36,36	0
86	OHX	6	1922	7/7	0.99	0.07	58,58,58,58	7
86	OHX	8	201	7/7	0.99	0.07	55,55,55,55	7
86	OHX	8	202	7/7	0.99	0.12	49,49,49,49	2
87	MG	5	4337	1/1	0.99	0.06	47,47,47,47	0
87	MG	5	4490	1/1	0.99	0.12	46,46,46,46	0
87	MG	O1	206	1/1	0.99	0.15	59,59,59,59	1
87	MG	1	4257	1/1	0.99	0.11	44,44,44,44	1
86	OHX	1	3564	7/7	0.99	0.11	54,54,54,54	7
86	OHX	6	1924	7/7	0.99	0.10	54,54,54,54	7
86	OHX	1	3478	7/7	0.99	0.09	58,58,58,58	7
86	OHX	5	3408	7/7	0.99	0.09	42,42,42,42	2
86	OHX	5	3409	7/7	0.99	0.10	57,57,57,57	1
86	OHX	5	3411	7/7	0.99	0.10	50,50,50,50	7
86	OHX	5	3412	7/7	0.99	0.10	64,64,64,64	7
86	OHX	5	3413	7/7	0.99	0.08	51,51,51,51	7
86	OHX	5	3414	7/7	0.99	0.10	43,43,43,43	7
86	OHX	5	3415	7/7	0.99	0.09	74,74,74,74	1
86	OHX	5	3416	7/7	0.99	0.10	46,46,46,46	7
87	MG	1	4389	1/1	0.99	0.06	59,59,59,59	1
86	OHX	5	3417	7/7	0.99	0.09	63,63,63,63	0
87	MG	5	4353	1/1	0.99	0.10	39,39,39,39	1
86	OHX	5	3418	7/7	0.99	0.11	58,58,58,58	7
86	OHX	5	3419	7/7	0.99	0.10	55,55,55,55	7
86	OHX	5	3420	7/7	0.99	0.08	56,56,56,56	7
87	MG	5	4357	1/1	0.99	0.07	36,36,36,36	1
86	OHX	5	3422	7/7	0.99	0.10	55,55,55,55	7
86	OHX	5	3423	7/7	0.99	0.06	56,56,56,56	7
87	MG	1	4396	1/1	0.99	0.09	45,45,45,45	1
87	MG	5	4514	1/1	0.99	0.21	30,30,30,30	1
86	OHX	5	3424	7/7	0.99	0.08	70,70,70,70	0
86	OHX	5	3425	7/7	0.99	0.09	49,49,49,49	7
86	OHX	5	3427	7/7	0.99	0.07	66,66,66,66	7
86	OHX	5	3428	7/7	0.99	0.09	64,64,64,64	0
86	OHX	5	3429	7/7	0.99	0.10	49,49,49,49	7
86	OHX	5	3430	7/7	0.99	0.10	40,40,40,40	7
86	OHX	1	3437	7/7	0.99	0.10	61,61,61,61	7
86	OHX	5	3432	7/7	0.99	0.09	59,59,59,59	7
86	OHX	1	3438	7/7	0.99	0.12	59,59,59,59	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
87	MG	5	4370	1/1	0.99	0.29	47,47,47,47	1
86	OHX	2	1920	7/7	0.99	0.12	84,84,84,84	7
86	OHX	5	3436	7/7	0.99	0.12	54,54,54,54	7
86	OHX	5	3437	7/7	0.99	0.07	100,100,100,100	0
86	OHX	1	3440	7/7	0.99	0.10	75,75,75,75	7
86	OHX	5	3439	7/7	0.99	0.12	57,57,57,57	7
86	OHX	5	3440	7/7	0.99	0.14	51,51,51,51	7
87	MG	5	4531	1/1	0.99	0.10	39,39,39,39	0
86	OHX	5	3441	7/7	0.99	0.09	54,54,54,54	7
86	OHX	5	3442	7/7	0.99	0.11	56,56,56,56	7
87	MG	5	4234	1/1	0.99	0.10	44,44,44,44	0
86	OHX	5	3443	7/7	0.99	0.07	82,82,82,82	7
87	MG	n1	203	1/1	0.99	0.06	37,37,37,37	1
86	OHX	1	3441	7/7	0.99	0.12	52,52,52,52	7
86	OHX	1	3442	7/7	0.99	0.10	55,55,55,55	7
86	OHX	5	3446	7/7	0.99	0.11	56,56,56,56	7
87	MG	n3	205	1/1	0.99	0.12	34,34,34,34	1
87	MG	5	4384	1/1	0.99	0.06	34,34,34,34	1
86	OHX	n1	201	7/7	0.99	0.10	48,48,48,48	7
86	OHX	n3	201	7/7	0.99	0.11	55,55,55,55	7
87	MG	5	4241	1/1	0.99	0.10	38,38,38,38	1
87	MG	5	4388	1/1	0.99	0.04	40,40,40,40	0
86	OHX	6	1932	7/7	0.99	0.09	47,47,47,47	7
86	OHX	n9	101	7/7	0.99	0.11	59,59,59,59	7
86	OHX	2	1905	7/7	0.99	0.11	71,71,71,71	7
86	OHX	1	3444	7/7	0.99	0.11	61,61,61,61	7
86	OHX	5	3450	7/7	0.99	0.12	41,41,41,41	7
86	OHX	1	3405	7/7	0.99	0.08	48,48,48,48	0
86	OHX	1	3406	7/7	0.99	0.09	58,58,58,58	2
87	MG	1	4427	1/1	0.99	0.06	55,55,55,55	1
86	OHX	1	3447	7/7	0.99	0.12	69,69,69,69	7
87	MG	1	4189	1/1	0.99	0.06	46,46,46,46	0
86	OHX	5	3454	7/7	0.99	0.10	77,77,77,77	7
87	MG	1	4431	1/1	0.99	0.15	42,42,42,42	1
86	OHX	1	3408	7/7	0.99	0.07	59,59,59,59	2
86	OHX	1	3409	7/7	0.99	0.09	58,58,58,58	1
87	MG	1	4310	1/1	0.99	0.04	45,45,45,45	1
87	MG	q0	202	1/1	0.99	0.13	42,42,42,42	0
86	OHX	1	3450	7/7	0.99	0.09	46,46,46,46	7
86	OHX	6	1941	7/7	0.99	0.09	79,79,79,79	7
86	OHX	5	3459	7/7	0.99	0.10	80,80,80,80	7
86	OHX	5	3460	7/7	0.99	0.12	68,68,68,68	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3411	7/7	0.99	0.09	64,64,64,64	0
88	ZN	D6	101	1/1	0.99	0.04	88,88,88,88	0
86	OHX	1	3494	7/7	0.99	0.11	66,66,66,66	7
87	MG	1	4317	1/1	0.99	0.13	38,38,38,38	1
87	MG	L4	402	1/1	0.99	0.13	43,43,43,43	0
88	ZN	d6	500	1/1	0.99	0.04	67,67,67,67	0
87	MG	5	4567	1/1	0.99	0.07	48,48,48,48	1
86	OHX	1	3413	7/7	0.99	0.07	55,55,55,55	1
86	OHX	5	3464	7/7	0.99	0.11	45,45,45,45	7
86	OHX	1	3453	7/7	0.99	0.09	74,74,74,74	7
87	MG	L4	406	1/1	0.99	0.10	38,38,38,38	1
86	OHX	5	3466	7/7	0.99	0.08	63,63,63,63	7
86	OHX	5	3467	7/7	0.99	0.11	66,66,66,66	7
86	OHX	5	3468	7/7	0.99	0.12	63,63,63,63	7
86	OHX	5	3469	7/7	0.99	0.13	49,49,49,49	7
86	OHX	5	3470	7/7	0.99	0.06	90,90,90,90	7
87	MG	1	4450	1/1	0.99	0.08	54,54,54,54	0
88	ZN	D9	101	1/1	1.00	0.02	79,79,79,79	0
86	OHX	5	3407	7/7	1.00	0.09	44,44,44,44	2
88	ZN	O7	101	1/1	1.00	0.02	47,47,47,47	0
88	ZN	Q0	201	1/1	1.00	0.03	53,53,53,53	0
86	OHX	1	3416	7/7	1.00	0.09	69,69,69,69	0
88	ZN	Q3	501	1/1	1.00	0.01	73,73,73,73	0
86	OHX	6	1901	7/7	1.00	0.09	62,62,62,62	0
86	OHX	5	3410	7/7	1.00	0.08	58,58,58,58	2
88	ZN	d9	101	1/1	1.00	0.03	81,81,81,81	0
86	OHX	5	3421	7/7	1.00	0.07	45,45,45,45	7
88	ZN	o7	501	1/1	1.00	0.01	53,53,53,53	0
88	ZN	q0	201	1/1	1.00	0.01	40,40,40,40	0
86	OHX	1	3412	7/7	1.00	0.07	47,47,47,47	7
88	ZN	q3	501	1/1	1.00	0.03	64,64,64,64	0
86	OHX	5	3435	7/7	1.00	0.08	50,50,50,50	7
86	OHX	1	3410	7/7	1.00	0.07	53,53,53,53	3
86	OHX	1	3414	7/7	1.00	0.04	67,67,67,67	0
86	OHX	1	3407	7/7	1.00	0.09	48,48,48,48	2
86	OHX	5	3426	7/7	1.00	0.07	59,59,59,59	7
87	MG	5	4441	1/1	1.00	0.04	33,33,33,33	0
86	OHX	5	3405	7/7	1.00	0.07	48,48,48,48	3
86	OHX	5	3406	7/7	1.00	0.07	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.