



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 12:12 PM UTC

PDB ID : 5TGA / pdb_00005tga
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

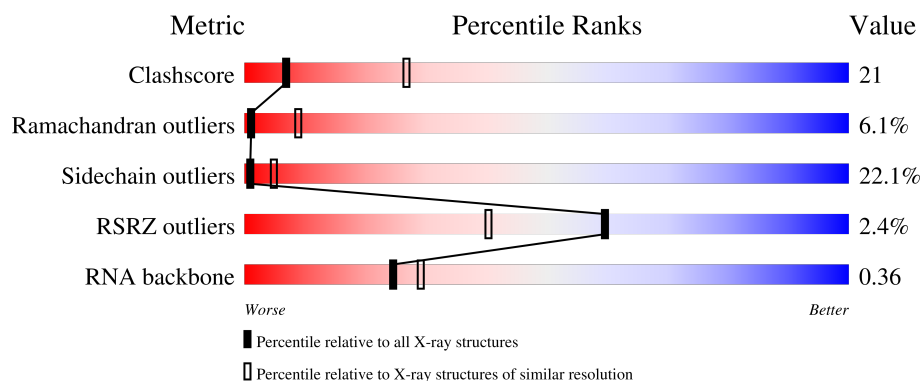
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

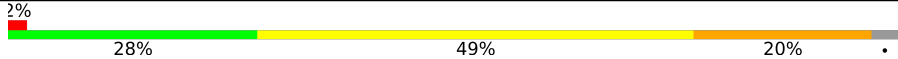
The reported resolution of this entry is 3.30 Å.

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))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	2	1829	
2	S0	206	
2	s0	206	
3	S1	216	
3	s1	216	

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Mol	Chain	Length	Quality of chain
4	S2	217	
4	s2	217	
5	S3	223	
5	s3	223	
6	S4	260	
6	s4	260	
7	S5	206	
7	s5	206	
8	S6	226	
8	s6	226	
9	S7	186	
9	s7	186	
10	S8	199	
10	s8	199	
11	S9	185	
11	s9	185	
12	C0	96	
13	C1	155	
13	c1	155	
14	C2	124	
14	c2	124	
15	C3	150	
15	c3	150	
16	C4	128	
16	c4	128	

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Mol	Chain	Length	Quality of chain
17	C5	135	
17	c5	135	
18	C6	142	
18	c6	142	
19	C7	125	
19	c7	125	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	110	
22	d0	110	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	70	
27	d5	70	
28	D6	97	
28	d6	97	
29	D7	81	

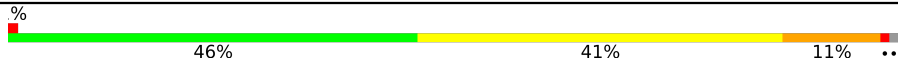
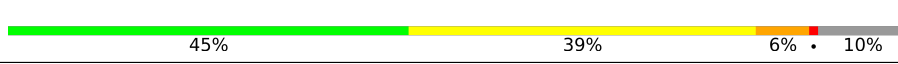
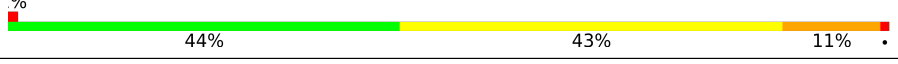
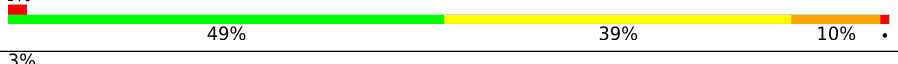
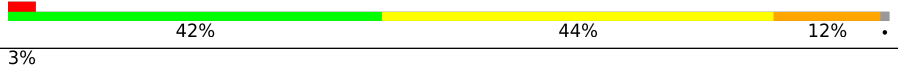
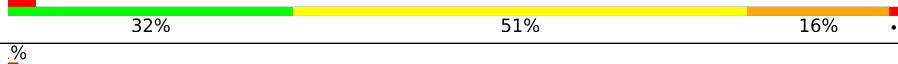
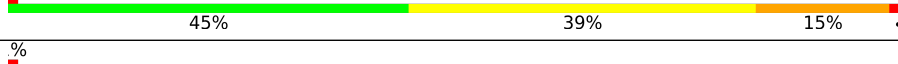
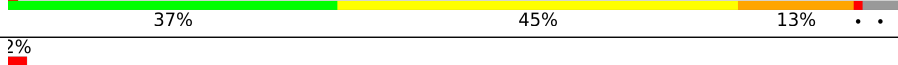
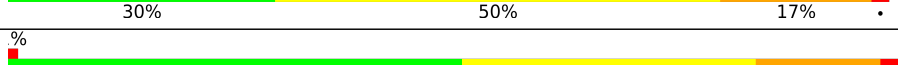
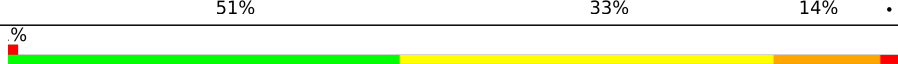
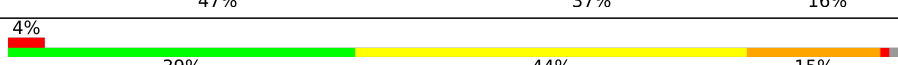
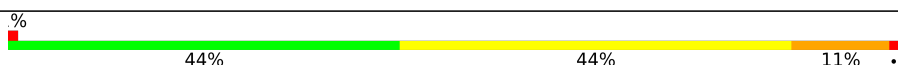
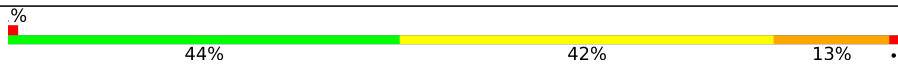
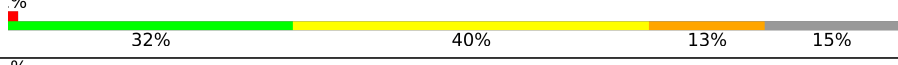
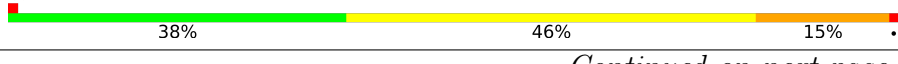
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Mol	Chain	Length	Quality of chain
29	d7	81	
30	D8	63	
30	d8	63	
31	D9	53	
31	d9	53	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	159	
36	1	3394	
36	5	3394	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	252	
39	l2	252	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	

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Mol	Chain	Length	Quality of chain
42	l5	296	
43	L6	175	
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	

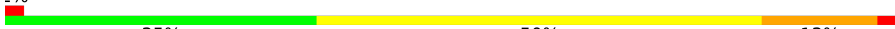
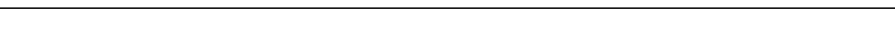
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Mol	Chain	Length	Quality of chain
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	100	
58	n2	100	
59	N3	136	
59	n3	136	
60	N4	135	
60	n4	135	
61	N5	121	
61	n5	121	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	100	
66	o0	100	
67	O1	109	

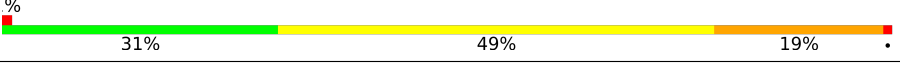
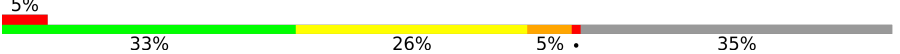
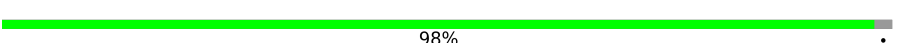
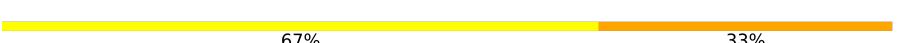
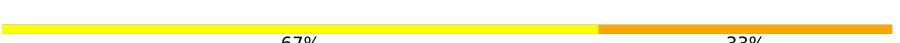
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Mol	Chain	Length	Quality of chain
67	o1	109	
68	O2	127	
68	o2	127	
69	O3	106	
69	o3	106	
70	O4	112	
70	o4	112	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	

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Mol	Chain	Length	Quality of chain
80	6	1800	
81	c0	96	
82	sM	104	
83	m2	150	
84	p0	219	
85	p1	47	
85	p2	47	
86	A	3	
86	B	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	8AN	A	3403	-	-	X	-
86	8AN	B	3403	-	-	X	-
87	OHX	1	3433	-	-	X	-
87	OHX	1	3496	-	-	X	-
87	OHX	1	3665	-	-	-	X
87	OHX	1	3670	-	-	-	X
87	OHX	1	3671	-	-	-	X
87	OHX	1	3691	-	-	X	-
87	OHX	1	3724	-	-	-	X
87	OHX	1	3729	-	-	-	X
87	OHX	1	3733	-	-	X	X
87	OHX	1	3738	-	-	-	X
87	OHX	1	3747	-	-	X	-
87	OHX	1	3752	-	-	-	X
87	OHX	1	3765	-	-	-	X
87	OHX	1	3768	-	-	-	X
87	OHX	1	3772	-	-	X	-
87	OHX	1	3779	-	-	-	X
87	OHX	1	3781	-	-	-	X
87	OHX	1	3793	-	-	X	-
87	OHX	1	3799	-	-	-	X
87	OHX	1	3802	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	1	3804	-	-	-	X
87	OHX	1	3805	-	-	X	-
87	OHX	1	3806	-	-	X	-
87	OHX	2	1909	-	-	X	-
87	OHX	2	1962	-	-	X	-
87	OHX	2	1964	-	-	X	-
87	OHX	2	1969	-	-	X	-
87	OHX	2	2035	-	-	X	-
87	OHX	2	2080	-	-	-	X
87	OHX	4	214	-	-	-	X
87	OHX	5	3449	-	-	X	-
87	OHX	5	3593	-	-	X	-
87	OHX	5	3632	-	-	-	X
87	OHX	5	3638	-	-	-	X
87	OHX	5	3654	-	-	-	X
87	OHX	5	3670	-	-	-	X
87	OHX	5	3684	-	-	X	X
87	OHX	5	3691	-	-	-	X
87	OHX	5	3708	-	-	-	X
87	OHX	5	3716	-	-	-	X
87	OHX	5	3726	-	-	-	X
87	OHX	5	3735	-	-	-	X
87	OHX	5	3737	-	-	-	X
87	OHX	5	3741	-	-	-	X
87	OHX	5	3744	-	-	-	X
87	OHX	5	3751	-	-	-	X
87	OHX	5	3752	-	-	-	X
87	OHX	5	3758	-	-	-	X
87	OHX	5	3759	-	-	-	X
87	OHX	5	3763	-	-	-	X
87	OHX	5	3764	-	-	-	X
87	OHX	5	3778	-	-	-	X
87	OHX	5	3781	-	-	-	X
87	OHX	5	3788	-	-	-	X
87	OHX	5	3793	-	-	-	X
87	OHX	5	3802	-	-	-	X
87	OHX	5	3804	-	-	X	-
87	OHX	5	3807	-	-	-	X
87	OHX	5	3808	-	-	-	X
87	OHX	5	3814	-	-	-	X
87	OHX	6	1920	-	-	X	-
87	OHX	6	2028	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	OHX	6	2042	-	-	-	X
87	OHX	6	2054	-	-	-	X
87	OHX	6	2060	-	-	-	X
87	OHX	6	2064	-	-	-	X
87	OHX	6	2068	-	-	-	X
87	OHX	6	2075	-	-	-	X
87	OHX	6	2087	-	-	-	X
87	OHX	6	2089	-	-	-	X
87	OHX	6	2095	-	-	-	X
87	OHX	6	2097	-	-	-	X
87	OHX	6	2098	-	-	X	-
87	OHX	7	211	-	-	-	X
87	OHX	8	215	-	-	-	X
87	OHX	M0	303	-	-	X	X
87	OHX	M0	304	-	-	X	-
87	OHX	O7	102	-	-	X	-
87	OHX	c5	202	-	-	X	-
87	OHX	m0	302	-	-	-	X
87	OHX	n3	202	-	-	-	X
87	OHX	o9	101	-	-	-	X
88	MG	1	3852	-	-	-	X
88	MG	1	3921	-	-	-	X
88	MG	1	4099	-	-	-	X
88	MG	2	2093	-	-	-	X
88	MG	2	2096	-	-	-	X
88	MG	2	2101	-	-	-	X
88	MG	2	2114	-	-	-	X
88	MG	2	2128	-	-	-	X
88	MG	2	2140	-	-	-	X
88	MG	2	2156	-	-	-	X
88	MG	2	2162	-	-	-	X
88	MG	2	2173	-	-	-	X
88	MG	2	2225	-	-	-	X
88	MG	3	229	-	-	-	X
88	MG	5	4067	-	-	-	X
88	MG	5	4182	-	-	-	X
88	MG	5	4512	-	-	-	X
88	MG	6	2143	-	-	-	X
88	MG	6	2305	-	-	-	X
88	MG	E1	502	-	-	-	X
88	MG	M5	305	-	-	-	X
89	ZN	Q2	501	-	-	X	-

2 Entry composition

There are 90 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 Small ribosomal subunit protein eS1A.

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 Small ribosomal subunit protein uS5.

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 Small ribosomal subunit protein uS3.

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 Small ribosomal subunit protein eS4A.

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 Rps5p.

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 Small ribosomal subunit protein eS6A.

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 Small ribosomal subunit protein eS7A.

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 Small ribosomal subunit protein eS8A.

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 Small ribosomal subunit protein uS4A.

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 Small ribosomal subunit protein eS10A.

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 Small ribosomal subunit protein uS17A.

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 Small ribosomal subunit protein eS12.

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 Small ribosomal subunit protein uS11B.

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 Small ribosomal subunit protein uS19.

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 Small ribosomal subunit protein uS9A.

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-A.

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

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

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

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

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS10.

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 Small ribosomal subunit protein eS25A.

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 Small ribosomal subunit protein eS30A.

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 Small ribosomal subunit protein eS31.

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 Small ribosomal subunit protein RACK1.

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,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 Large ribosomal subunit protein eL6A.

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 Large ribosomal subunit protein uL30A.

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 Large ribosomal subunit protein eL13A.

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 Large ribosomal subunit protein eL14A.

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 Large ribosomal subunit protein eL24A.

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 Large ribosomal subunit protein uL24A.

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 Large ribosomal subunit protein eL30.

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 60S ribosomal protein L40-A.

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 Large ribosomal subunit protein eL41B.

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 Small ribosomal subunit protein eS10A,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,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 Large ribosomal subunit protein uL10.

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

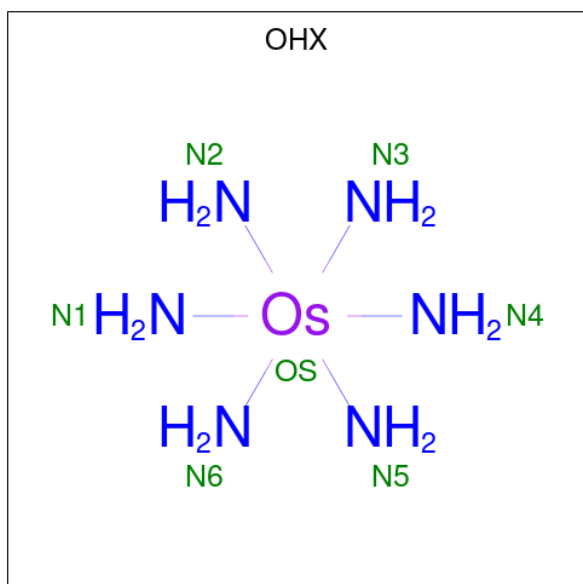
- Molecule 85 is a protein called 60S Ribosomal Protein P1/2.

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 a RNA chain called Peptidyl-tRNA analog ACCA-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
86	A	3	Total	C	N	O	P	0	0	0
			62	28	12	19	3			
86	B	3	Total	C	N	O	P	0	0	0
			62	28	12	19	3			

- Molecule 87 is osmium (III) hexammine (CCD ID: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
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87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	2	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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87	2	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
87	2	1	Total	N	Os	0	0
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87	S2	1	Total	N	Os	0	0
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87	S8	1	Total	N	Os	0	0
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87	C3	1	Total	N	Os	0	0
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87	C5	1	Total	N	Os	0	0
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87	C8	1	Total	N	Os	0	0
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87	C8	1	Total	N	Os	0	0
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87	D9	1	Total	N	Os	0	0
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87	SR	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	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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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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87	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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87	L3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	M5	1	Total	N	Os	0	0
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87	M7	1	Total	N	Os	0	0
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87	M8	1	Total	N	Os	0	0
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87	M9	1	Total	N	Os	0	0
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87	N9	1	Total	N	Os	0	0
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87	O1	1	Total	N	Os	0	0
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87	O3	1	Total	N	Os	0	0
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87	O7	1	Total	N	Os	0	0
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87	Q2	1	Total	N	Os	0	0
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87	6	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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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	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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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	s1	1	Total 7	N 6	Os 1	0	0
87	s1	1	Total 7	N 6	Os 1	0	0
87	s4	1	Total 7	N 6	Os 1	0	0
87	s8	1	Total 7	N 6	Os 1	0	0
87	c1	1	Total 7	N 6	Os 1	0	0
87	c3	1	Total 7	N 6	Os 1	0	0
87	c5	1	Total 7	N 6	Os 1	0	0
87	c5	1	Total 7	N 6	Os 1	0	0
87	c8	1	Total 7	N 6	Os 1	0	0
87	d9	1	Total 7	N 6	Os 1	0	0
87	sR	1	Total 7	N 6	Os 1	0	0
87	5	1	Total 7	N 6	Os 1	2	0
87	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	1	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	5	1	Total	N	Os	0	0
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87	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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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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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	1	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	12	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	13	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		
87	14	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	15	1	Total	N	Os	0	0
			7	6	1		
87	19	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m0	1	Total	N	Os	0	0
			7	6	1		
87	m1	1	Total	N	Os	0	0
			7	6	1		
87	m4	1	Total	N	Os	0	0
			7	6	1		
87	m5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	m5	1	Total	N	Os	0	0
			7	6	1		
87	m7	1	Total	N	Os	0	0
			7	6	1		
87	m9	1	Total	N	Os	0	0
			7	6	1		
87	n1	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n3	1	Total	N	Os	0	0
			7	6	1		
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o9	1	Total	N	Os	0	0
			7	6	1		
87	q1	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	2	170	Total	Mg	0	0
			170	170		
88	S1	1	Total	Mg	0	0
			1	1		
88	S2	1	Total	Mg	0	0
			1	1		
88	S4	2	Total	Mg	0	0
			2	2		
88	S6	1	Total	Mg	0	0
			1	1		
88	S8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	C1	2	Total 2	Mg 2	0	0
88	C5	1	Total 1	Mg 1	0	0
88	C8	1	Total 1	Mg 1	0	0
88	D0	1	Total 1	Mg 1	0	0
88	D4	1	Total 1	Mg 1	0	0
88	D6	1	Total 1	Mg 1	0	0
88	D9	3	Total 3	Mg 3	0	0
88	E1	1	Total 1	Mg 1	0	0
88	SM	1	Total 1	Mg 1	0	0
88	1	698	Total 698	Mg 698	0	0
88	3	18	Total 18	Mg 18	0	0
88	4	28	Total 28	Mg 28	0	0
88	L2	3	Total 3	Mg 3	0	0
88	L3	5	Total 5	Mg 5	0	0
88	L4	7	Total 7	Mg 7	0	0
88	L7	3	Total 3	Mg 3	0	0
88	L8	1	Total 1	Mg 1	0	0
88	M0	5	Total 5	Mg 5	0	0
88	M1	2	Total 2	Mg 2	0	0
88	M3	3	Total 3	Mg 3	0	0
88	M4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	M5	4	Total 4	Mg 4	0	0
88	M6	4	Total 4	Mg 4	0	0
88	M7	10	Total 10	Mg 10	0	0
88	M8	3	Total 3	Mg 3	0	0
88	M9	2	Total 2	Mg 2	0	0
88	N0	2	Total 2	Mg 2	0	0
88	N1	1	Total 1	Mg 1	0	0
88	N3	3	Total 3	Mg 3	0	0
88	N6	2	Total 2	Mg 2	0	0
88	N8	7	Total 7	Mg 7	0	0
88	N9	1	Total 1	Mg 1	0	0
88	O1	5	Total 5	Mg 5	0	0
88	O2	4	Total 4	Mg 4	0	0
88	O3	2	Total 2	Mg 2	0	0
88	O4	1	Total 1	Mg 1	0	0
88	O5	2	Total 2	Mg 2	0	0
88	O7	6	Total 6	Mg 6	0	0
88	Q0	2	Total 2	Mg 2	0	0
88	Q2	3	Total 3	Mg 3	0	0
88	6	235	Total 235	Mg 235	0	0
88	s1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	s4	1	Total 1	Mg 1	0	0
88	s6	2	Total 2	Mg 2	0	0
88	s8	4	Total 4	Mg 4	0	0
88	c6	2	Total 2	Mg 2	0	0
88	c7	1	Total 1	Mg 1	0	0
88	c8	4	Total 4	Mg 4	0	0
88	c9	3	Total 3	Mg 3	0	0
88	d2	1	Total 1	Mg 1	0	0
88	d3	2	Total 2	Mg 2	0	0
88	d4	2	Total 2	Mg 2	0	0
88	d5	1	Total 1	Mg 1	0	0
88	d9	2	Total 2	Mg 2	0	0
88	sM	2	Total 2	Mg 2	0	0
88	5	759	Total 759	Mg 759	0	0
88	7	28	Total 28	Mg 28	0	0
88	8	19	Total 19	Mg 19	0	0
88	12	6	Total 6	Mg 6	0	0
88	13	13	Total 13	Mg 13	0	0
88	14	1	Total 1	Mg 1	0	0
88	15	6	Total 6	Mg 6	0	0
88	17	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	l8	1	Total 1	Mg 1	0	0
88	l9	3	Total 3	Mg 3	0	0
88	m0	1	Total 1	Mg 1	0	0
88	m3	1	Total 1	Mg 1	0	0
88	m4	1	Total 1	Mg 1	0	0
88	m5	3	Total 3	Mg 3	0	0
88	m6	4	Total 4	Mg 4	0	0
88	m7	8	Total 8	Mg 8	0	0
88	m8	4	Total 4	Mg 4	0	0
88	m9	1	Total 1	Mg 1	0	0
88	n0	5	Total 5	Mg 5	0	0
88	n1	3	Total 3	Mg 3	0	0
88	n3	3	Total 3	Mg 3	0	0
88	n6	1	Total 1	Mg 1	0	0
88	n8	7	Total 7	Mg 7	0	0
88	n9	2	Total 2	Mg 2	0	0
88	o2	3	Total 3	Mg 3	0	0
88	o3	4	Total 4	Mg 4	0	0
88	o4	1	Total 1	Mg 1	0	0
88	o6	1	Total 1	Mg 1	0	0
88	o7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total 1	Mg 1	0	0
88	q1	2	Total 2	Mg 2	0	0
88	q2	1	Total 1	Mg 1	0	0
88	q3	1	Total 1	Mg 1	0	0
88	p0	1	Total 1	Mg 1	0	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

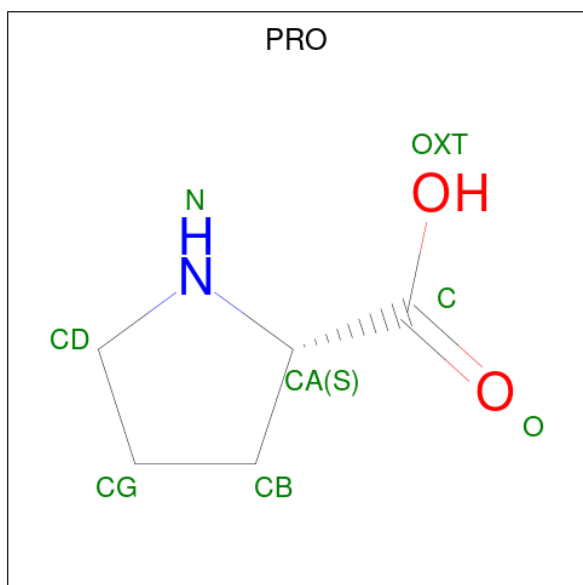
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	D6	1	Total 1	Zn 1	0	0
89	D7	1	Total 1	Zn 1	0	0
89	D9	1	Total 1	Zn 1	0	0
89	E1	1	Total 1	Zn 1	0	0
89	O7	1	Total 1	Zn 1	0	0
89	Q0	1	Total 1	Zn 1	0	0
89	Q2	1	Total 1	Zn 1	0	0
89	Q3	1	Total 1	Zn 1	0	0
89	d6	1	Total 1	Zn 1	0	0
89	d7	1	Total 1	Zn 1	0	0
89	d9	1	Total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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	q2	1	Total	Zn	0	0
			1	1		
89	q3	1	Total	Zn	0	0
			1	1		

- Molecule 90 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).

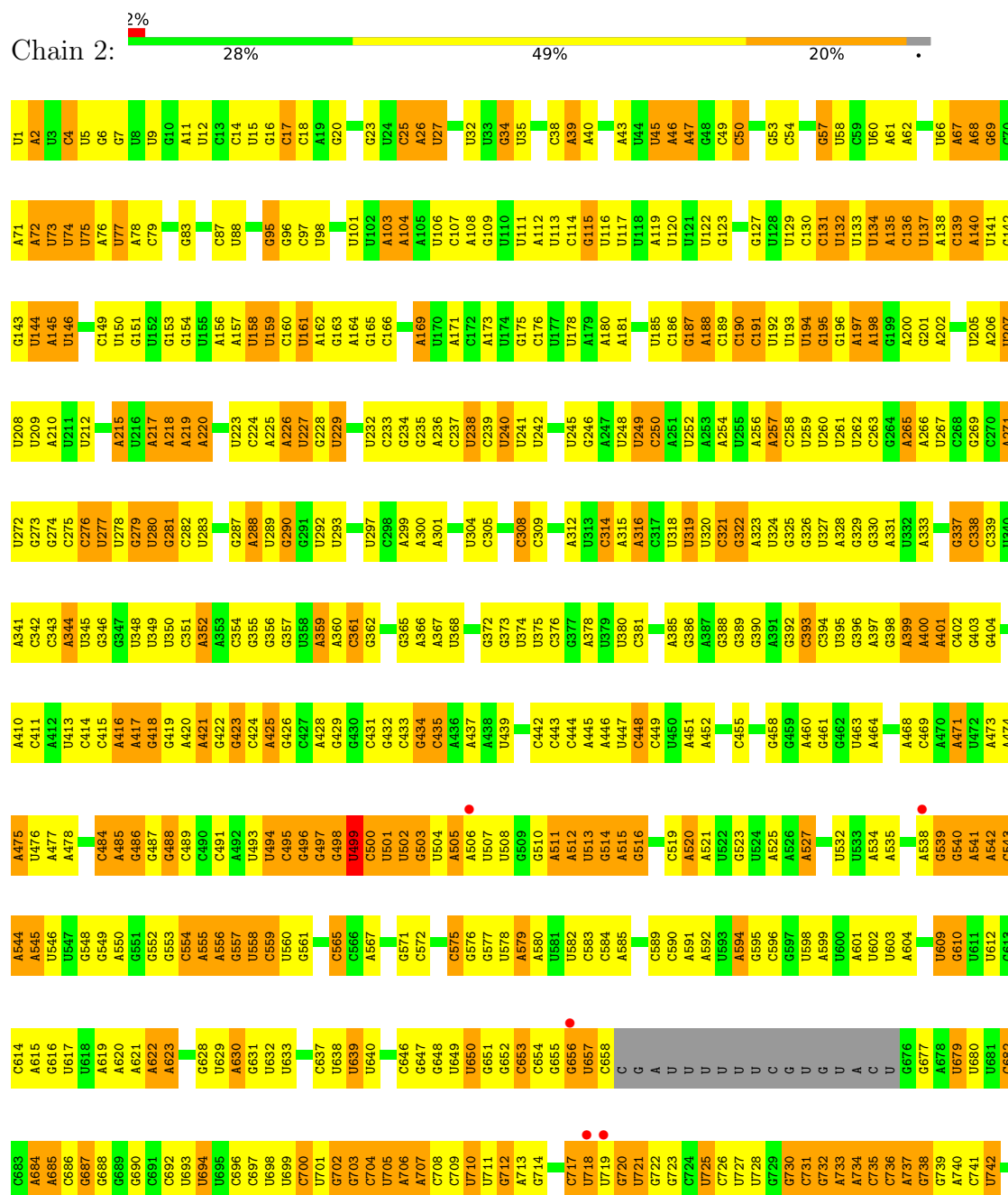


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
90	A	1	Total	C	N	O	0	0
			7	5	1	1		
90	B	1	Total	C	N	O	0	0
			7	5	1	1		

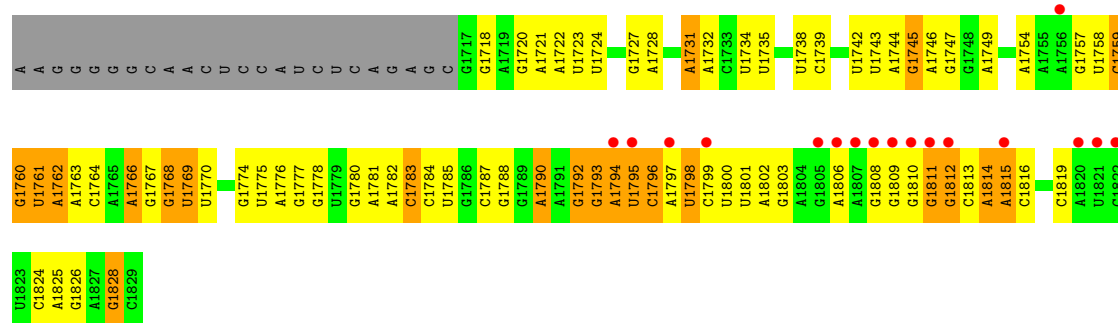
3 Residue-property plots

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.

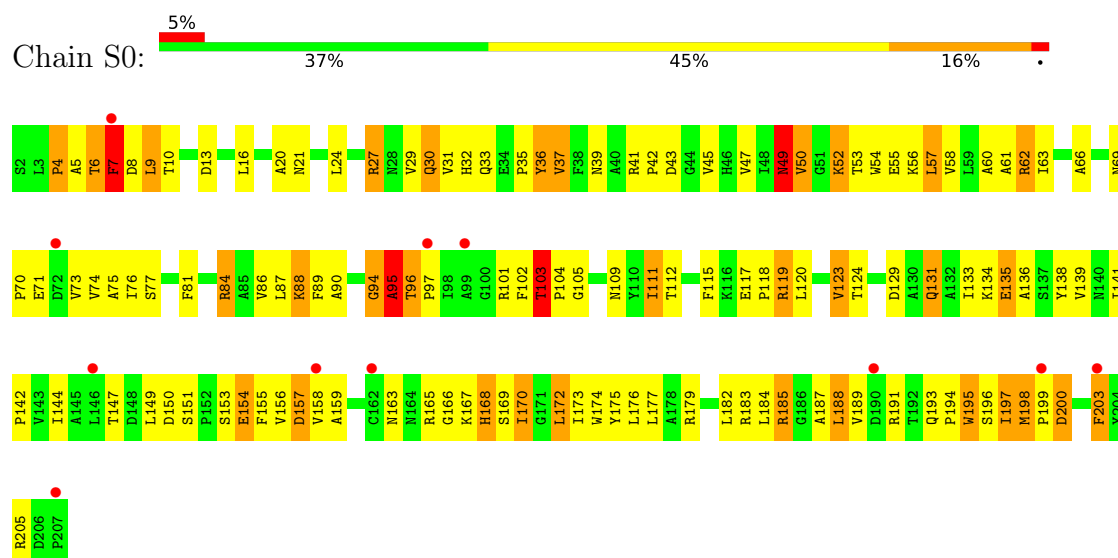
- Molecule 1: 18S ribosomal RNA



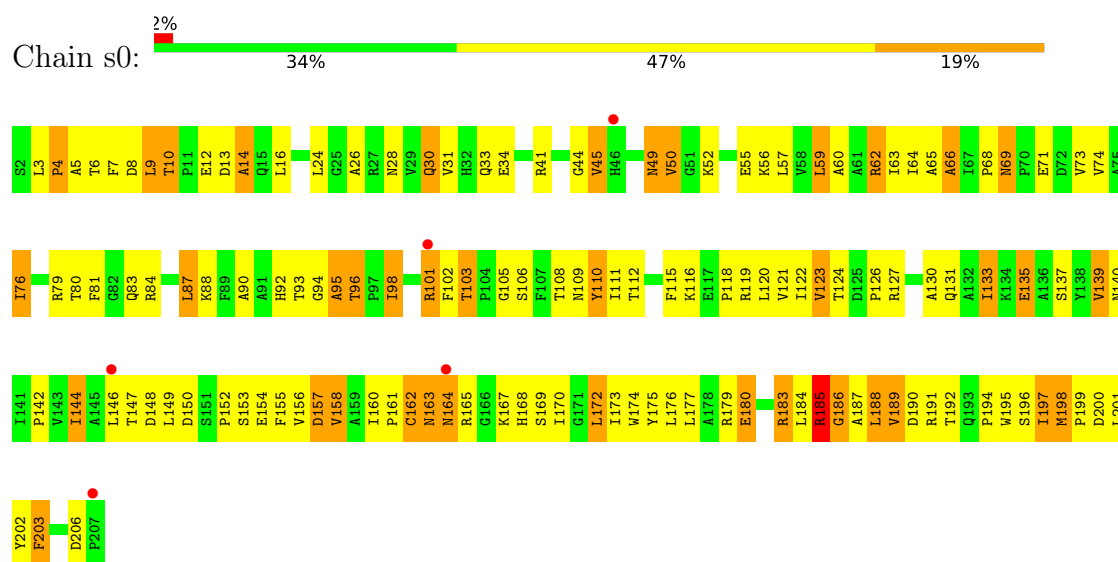
C1624	C1625	U1626	G1629	U1630	A1631	A1635	C1636	C1637	G1638	C1639	C1640	C1641	C1642	U1643	C1644	G1645	C1646	G1649	U1650	C1653	U1654	A1655	U1656	U1657	G1658	A1659	A1660	U1661	G1662	G1663	A1667	G1670	A1671	G1672	G1673	C1674	C1675	U1676	C1677	G1680	A1681	U1682	C1683	U1684	C1685	C	U	U	A	G																					
G1562	C1563	U1564	C1565	U1566	U1567	U1568	A1569	U1569	C1570	U1508	C1571	A1572	C1573	U1574	C1575	U1576	U1577	U1578	U1579	C1583	U1584	U1585	U1586	A1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	C1596	U1597	U1598	C1599	A1600	G1536	G1601	C1602	U1538	G1539	G1540	G1541	G1542	A1543	U1544	U1545	G1546	A1547	U1550	U1551	U1552	G1553	U1554	A1555	U1556	A1557	U1558	A1559	C1623										
G1429	U1430	C1431	U1432	G1433	U1434	G1435	A1436	U1444	G1445	A1446	C1447	G1448	U1449	U1450	C1451	U1452	G1453	G1454	U1455	G1456	C1457	G1458	C1459	A1460	C1461	U1462	U1468	A1469	C1470	A1471	C1472	U1473	G1474	A1475	C1476	G1477	U1478	A1479	G1480	C1481	C1482	A1483	G1484	C1485	G1486	A1487	U1488	U1489	C1490	U1491	A1492	A1493	C1494	C1495	U1496	U1497	G1498														
G1358	C1359	A1360	U1361	U1362	U1363	G1364	C1365	U1366	G1367	U1368	U1369	A1370	A1371	U1372	C1373	C1374	C1375	C1376	U1377	U1378	G1379	U1380	U1381	A1382	G1383	U1384	G1385	U1386	G1387	A1388	C1389	U1390	U1398	C1399	A1400	A1401	G1402	C1403	U1407	G1408	G1409	A1410	A1411	G1412	G1413	U1414	U1415	G1416	A1417	G1418	U1419	A1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439
A1237	G1238	U1239	U1288	U1289	G1290	U1291	G1292	U1293	G1294	U1298	G1299	A1300	U1301	U1302	U1303	G1308	C1309	U1310	U1311	U1312	A1313	U1314	U1315	G1316	C1317	G1318	A1319	C1320	U1321	A1322	U1323	U1324	A1325	A1331	C1332	C1333	U1334	U1335	A1336	A1337	C1338	C1339	U1340	A1341	A1344	A1345	A1346	G1349	U1350	C1351	G1352	U1353	G1354	C1355	U1356	A1357															
A1151	A1152	G1153	A1087	U1088	U1089	C1090	A1091	A1092	A1093	G1094	U1095	U1096	U1097	U1098	U1099	G1100	G1101	G1102	U1103	U1104	C1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	U1113	U1114	U1115	A1116	U1117	G1118	G1119	U1120	A1125	G1126	G1130	A1131	A1132	A1133	C1134	U1135	U1136	A1137	A1138	A1139	G1140	G1141	A1142	U1143	U1144	U1145	G1146	A1147	G1148	G1150													
U1017	U1018	A1019	A1018	A1020	C1021	C1022	A1023	U1024	A1025	A1026	A1027	C1028	U1029	A1030	U1031	C1032	C1033	A1039	G1040	A1041	G1042	G1043	G1044	A1045	G1046	G1051	U1052	G1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	A1061	A1062	U1063	G1064	A1065	A1066	U1067	C1068	A1069	C1070	U1071	G1074	C1077	U1078	U1079	U1080	G1081	C1082	G1083	U1084	G1085															
U945	A951	A952	C953	G954	A955	U959	U959	U960	U960	U964	U965	A966	U967	U968	C969	G972	A973	A974	C975	G976	A977	A978	A979	U981	U982	A983	G984	G985	A986	U987	A988	U989	C990	G991	A992	A993	G994	A995	U996	G997	A998	G1002	A1003	U1004	A1005	C1006	U1009	U1010	G1011	A1012	A1013	U1014	U1015	C1016																	
G877	C880	A881	U882	C883	A884	C885	U886	U887	U888	U889	C890	U894	G895	U896	C969	G972	A973	A974	C975	G976	A977	A978	A979	U981	U982	A983	G984	G985	A986	U987	A988	U989	C990	G991	A992	A993	G994	A995	U996	G997	A998	G1002	A1003	U1004	A1005	C1006	U1009	U1010	G1011	A1012	A1013	U1014	U1015	C1016																	
U813	A814	G815	A816	U817	C818	G819	U820	U821	U822	U823	U824	U825	U826	C827	U828	U829	U830	U831	U832	U833	G834	G837	G838	U839	U840	U841	U842	U843	U844	G845	U846	A847	C848	U851	C852	G853	U854	A855	A856	U857	G858	A859	U860	U861	A862	A863	U864	A865	G866	U867	G868	A869	U870	G871	G872	G876															
U748	U749	U750	G751	U752	A753	A754	A755	U756	A757	U758	U759	G761	A762	G763	U764	G765	U766	U767	U768	A769	G772	G773	A774	G775	G776	C777	U778	C778	U779	A780	U781	C782	C783	C784	U785	C786	A789	U792	A793	U794	U795	A796	U800	G801	A802	A803	A804	G805	A806	A807	U808	U809	G810	A811	A812																



• Molecule 2: 40S ribosomal protein S0-A

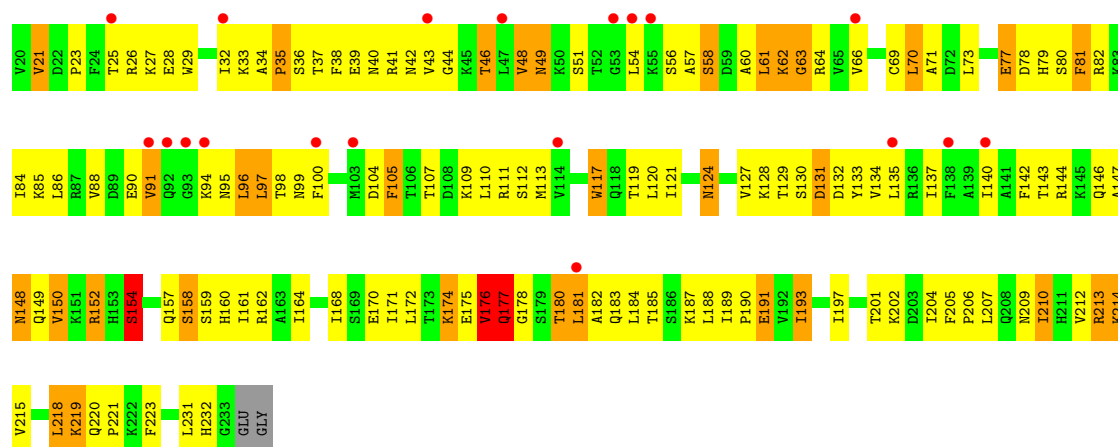


• Molecule 2: 40S ribosomal protein S0-A

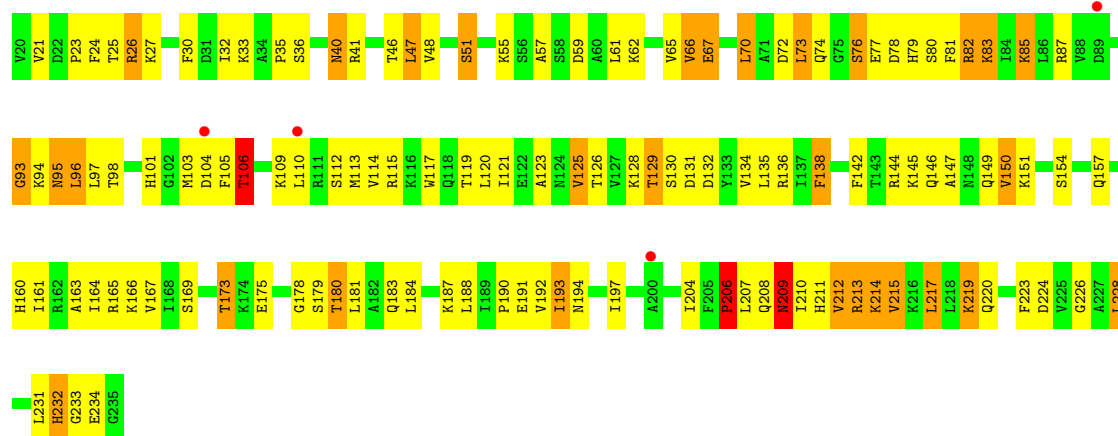


• Molecule 3: Small ribosomal subunit protein eS1A

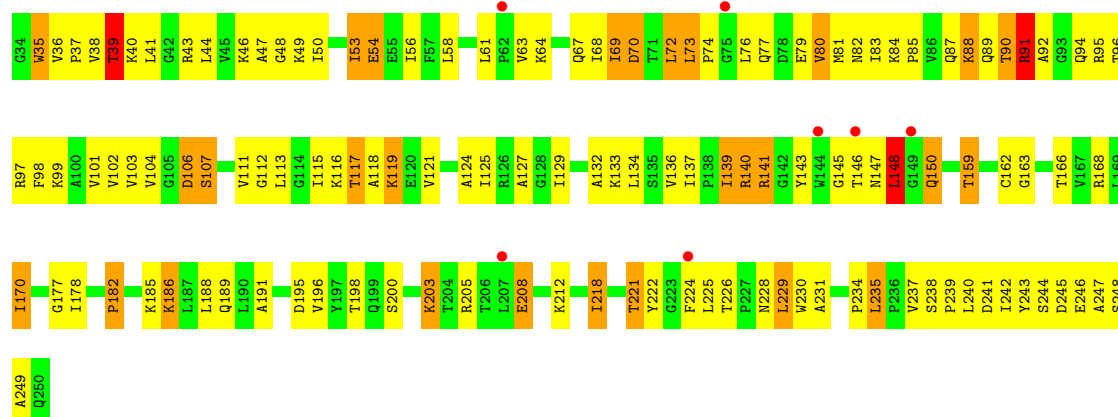




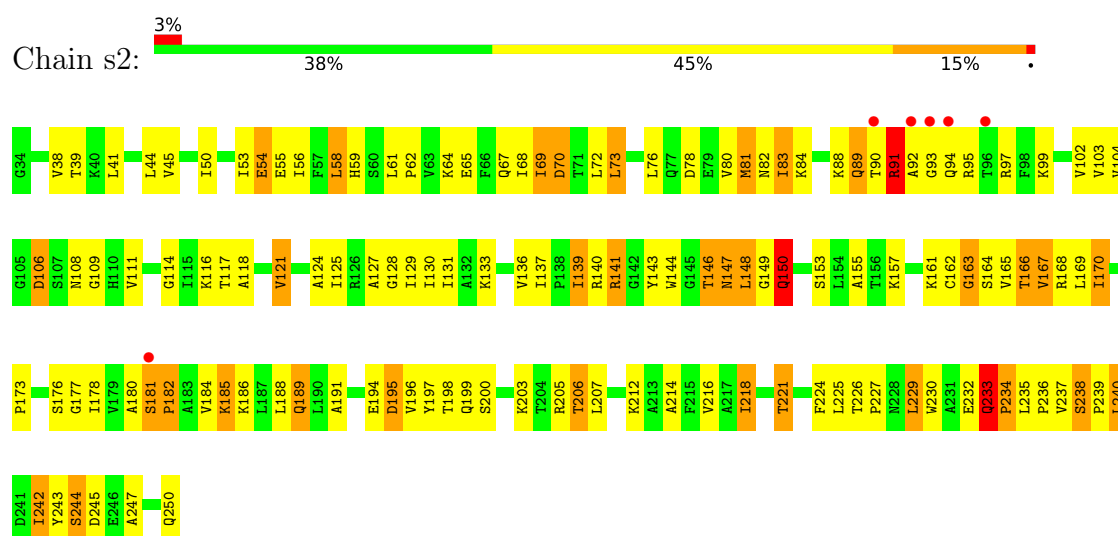
• Molecule 3: Small ribosomal subunit protein eS1A



• Molecule 4: Small ribosomal subunit protein uS5



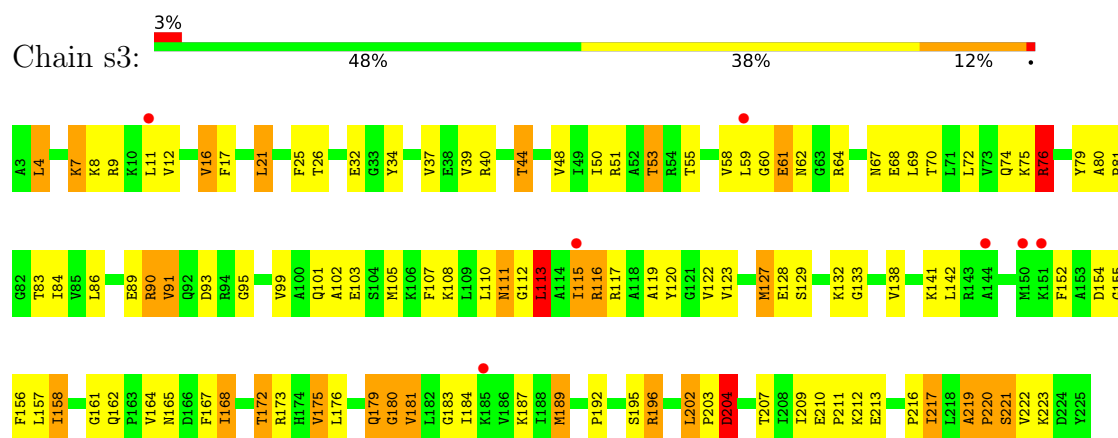
• Molecule 4: Small ribosomal subunit protein uS5



• Molecule 5: Small ribosomal subunit protein uS3

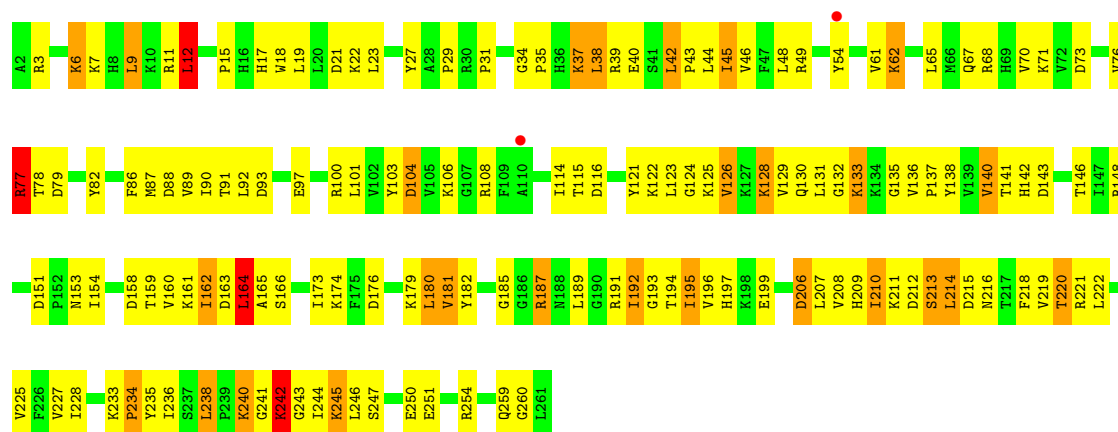


• Molecule 5: Small ribosomal subunit protein uS3



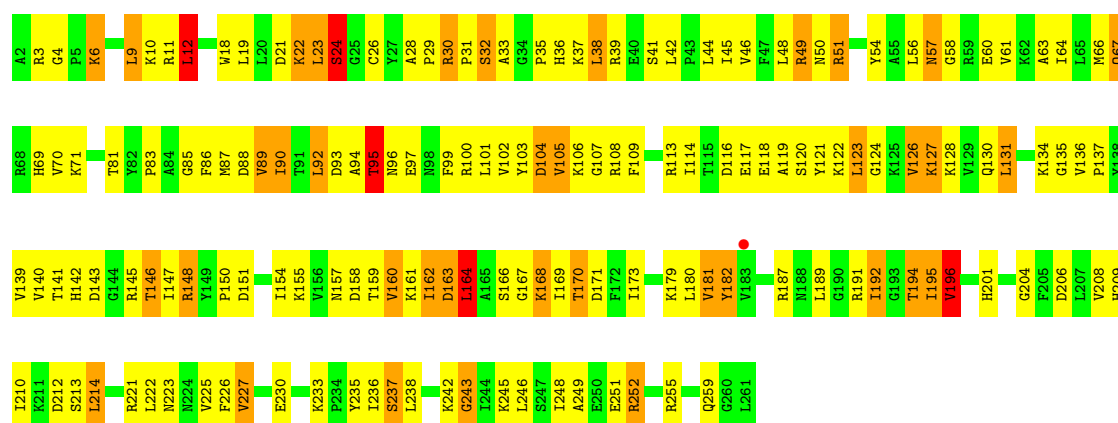
• Molecule 6: Small ribosomal subunit protein eS4A





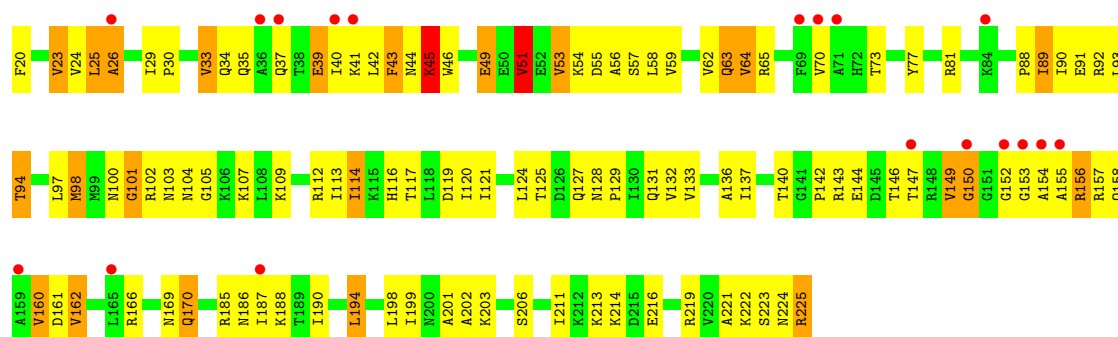
• Molecule 6: Small ribosomal subunit protein eS4A

Chain s4: 38% 46% 14% .



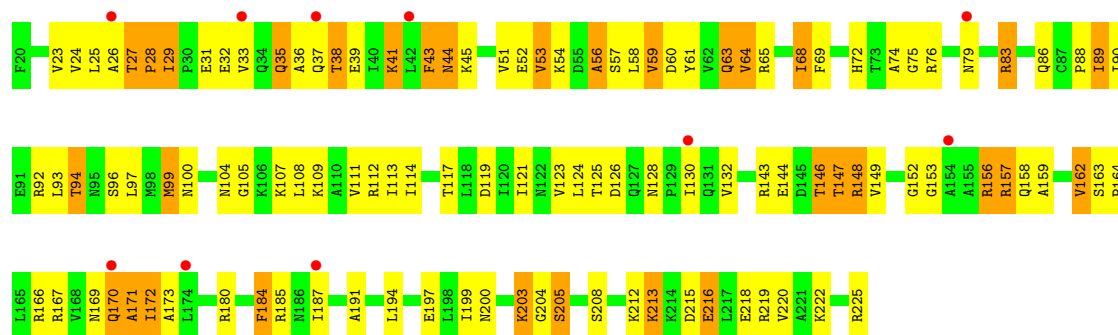
• Molecule 7: Rps5p

Chain S5: 9% 45% 43% 11% .

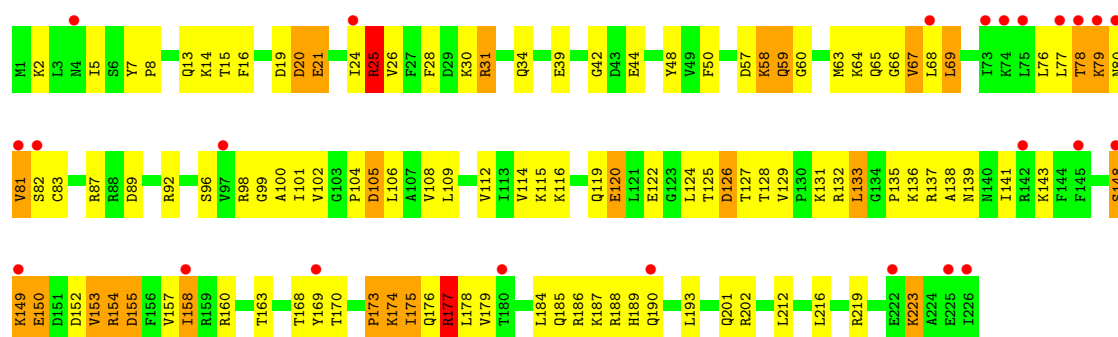


• Molecule 7: Rps5p

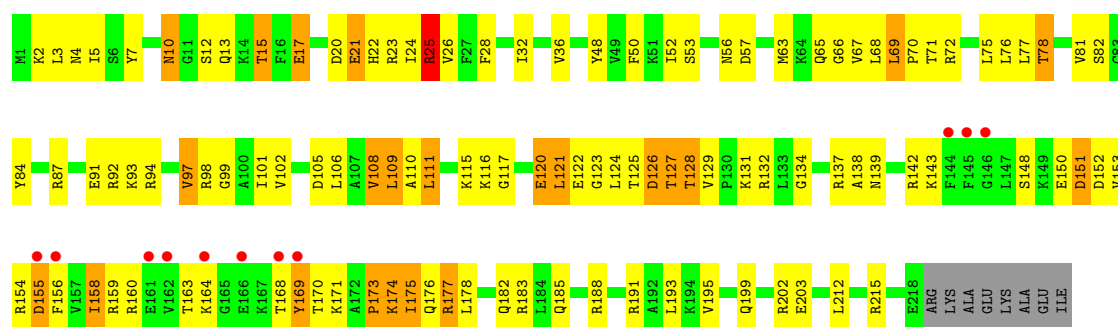
Chain s5: 5% 45% 40% 16%



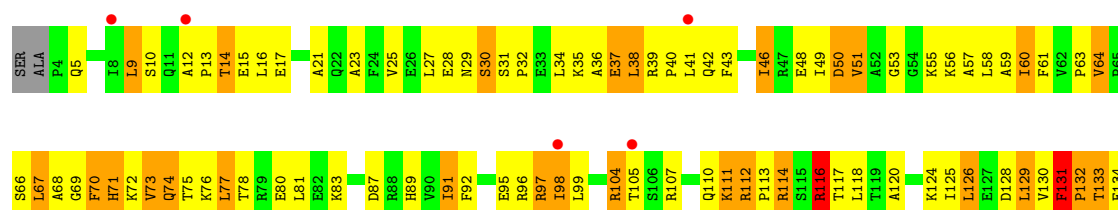
• Molecule 8: Small ribosomal subunit protein eS6A



• Molecule 8: Small ribosomal subunit protein eS6A

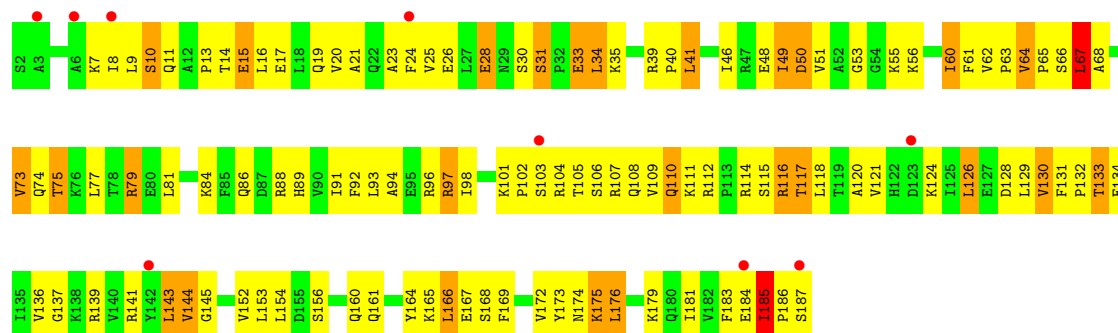


• Molecule 9: Small ribosomal subunit protein eS7A

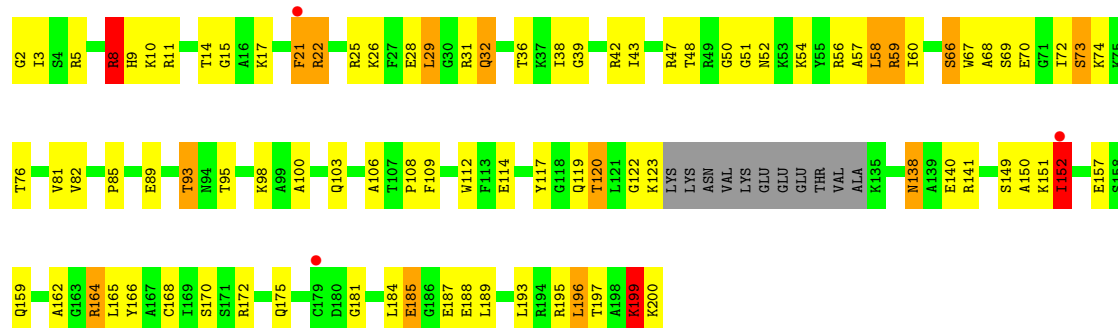




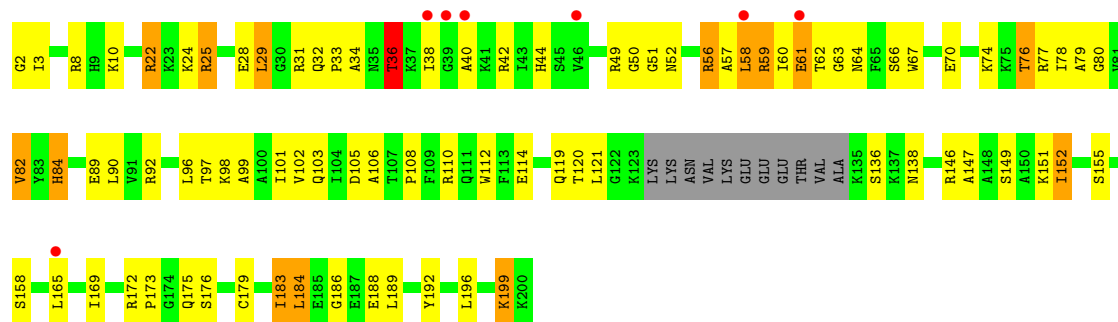
• Molecule 9: Small ribosomal subunit protein eS7A



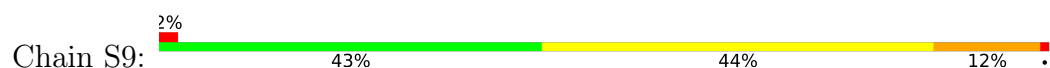
• Molecule 10: Small ribosomal subunit protein eS8A

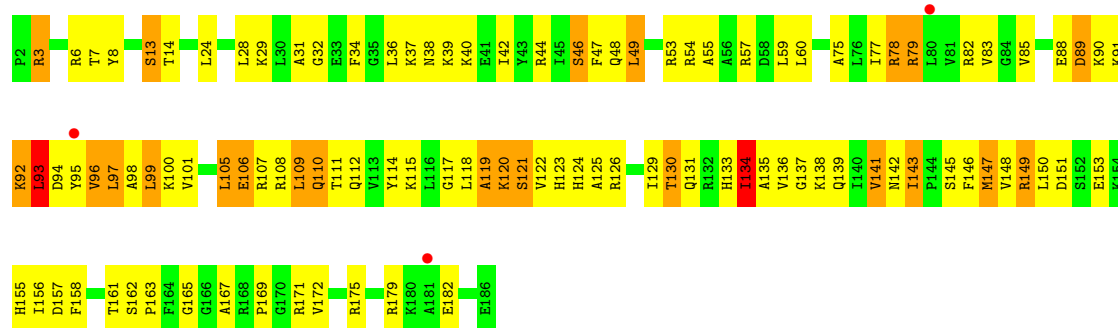


• Molecule 10: Small ribosomal subunit protein eS8A

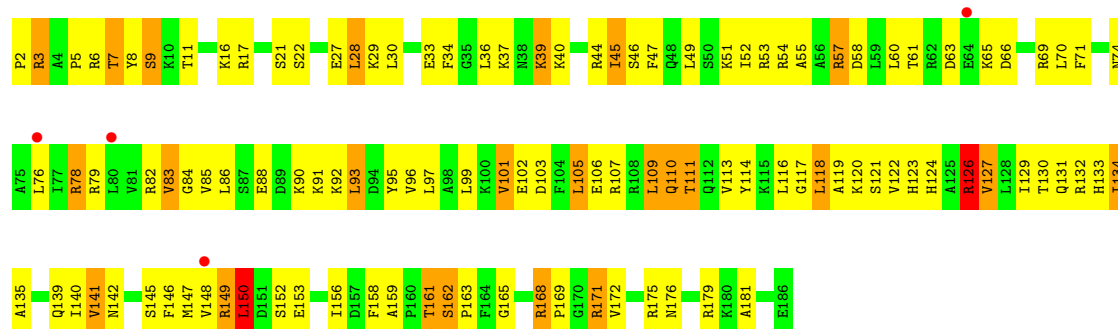


• Molecule 11: Small ribosomal subunit protein uS4A

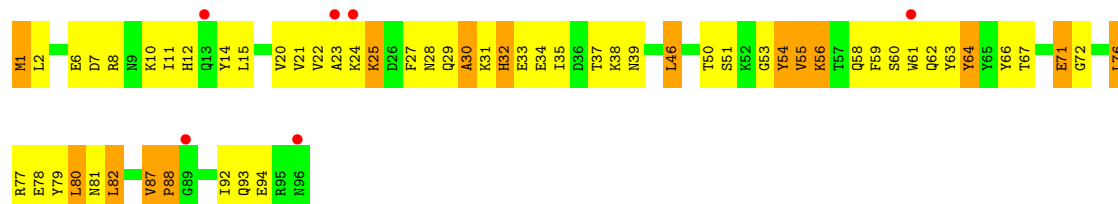




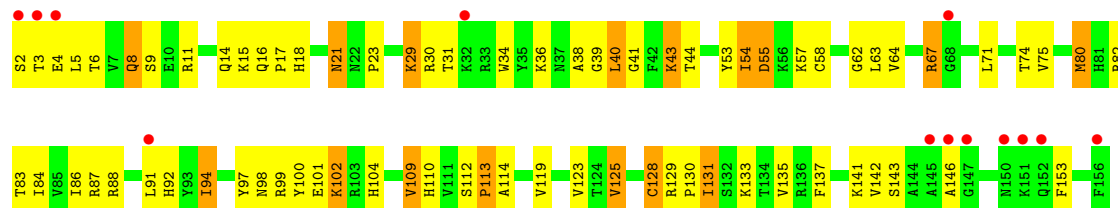
• Molecule 11: Small ribosomal subunit protein uS4A



• Molecule 12: Small ribosomal subunit protein eS10A

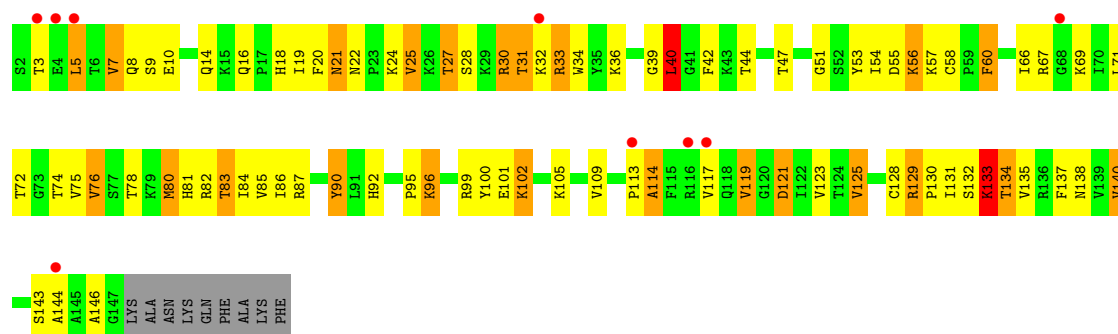


• Molecule 13: Small ribosomal subunit protein uS17A

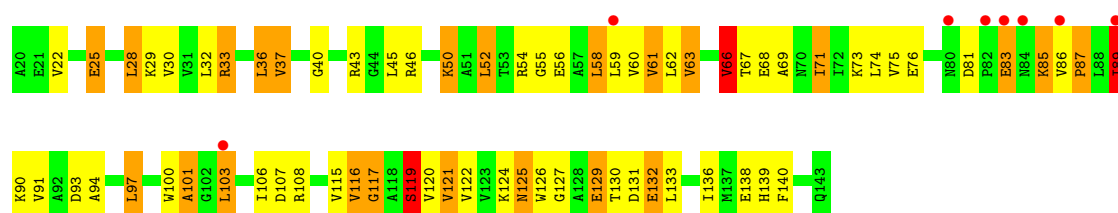


• Molecule 13: Small ribosomal subunit protein uS17A

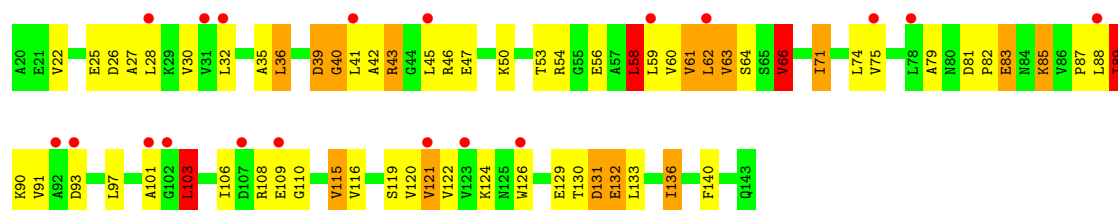




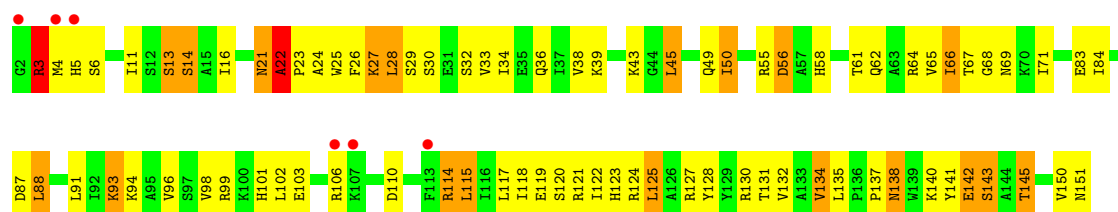
- Molecule 14: Small ribosomal subunit protein eS12



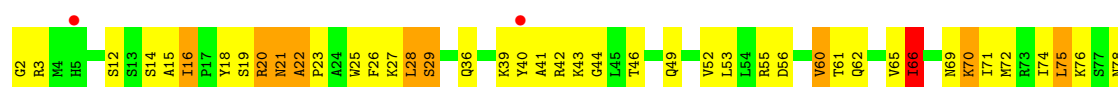
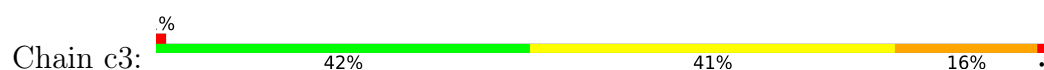
- Molecule 14: Small ribosomal subunit protein eS12



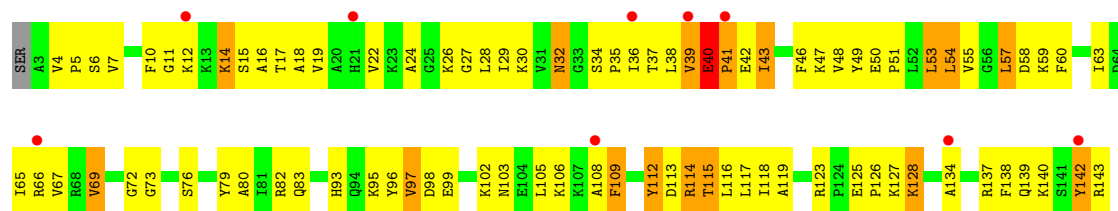
- Molecule 15: 40S ribosomal protein S13



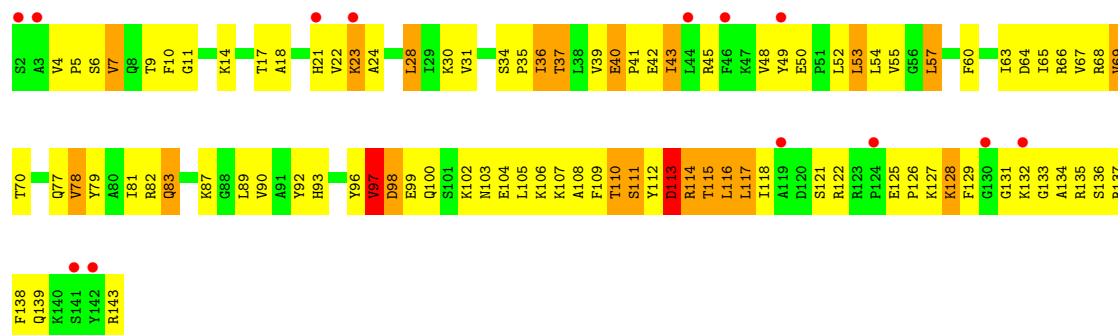
- Molecule 15: 40S ribosomal protein S13



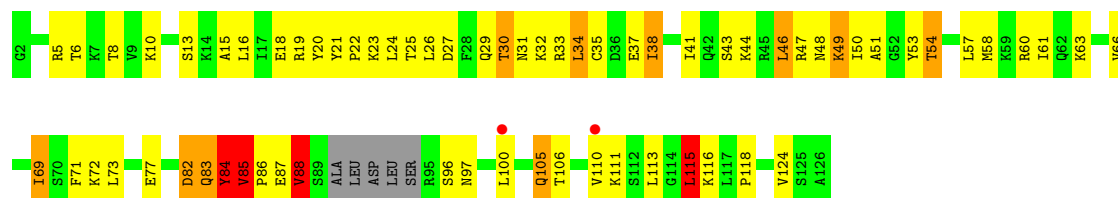
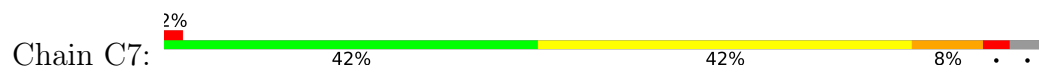




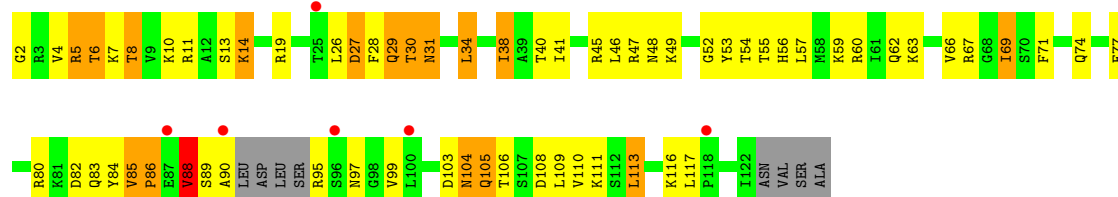
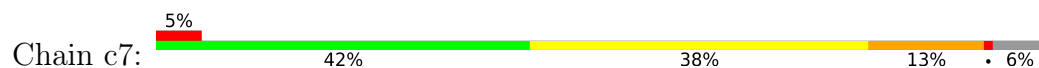
• Molecule 18: Small ribosomal subunit protein uS9A



• Molecule 19: 40S ribosomal protein S17-A

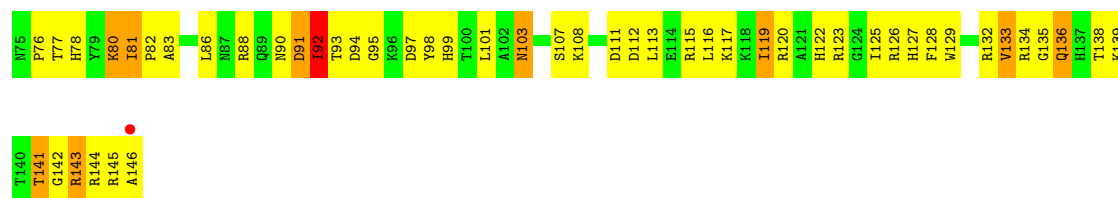


• Molecule 19: 40S ribosomal protein S17-A

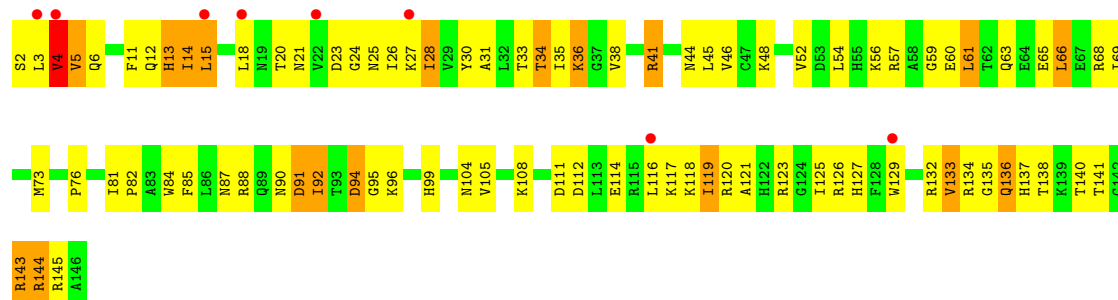
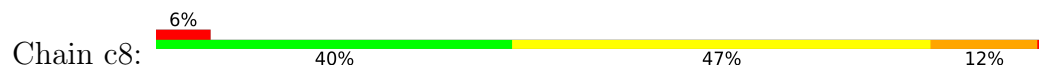


• Molecule 20: 40S ribosomal protein S18-A

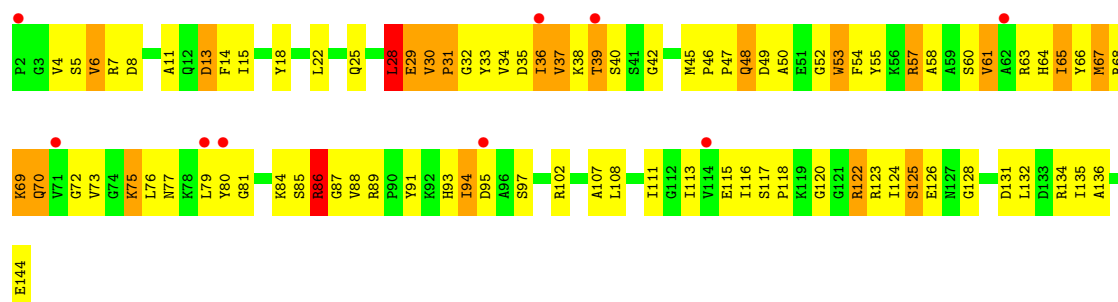




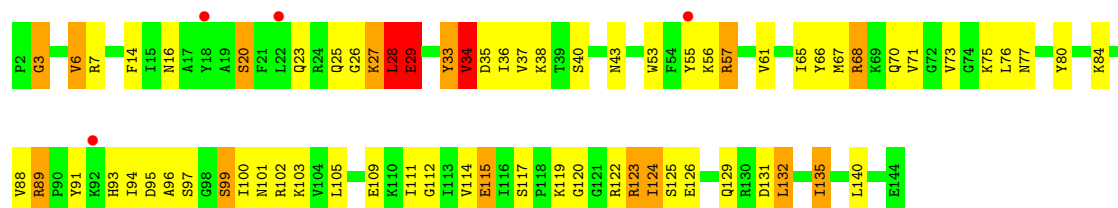
- Molecule 20: 40S ribosomal protein S18-A



- Molecule 21: 40S ribosomal protein S19-A

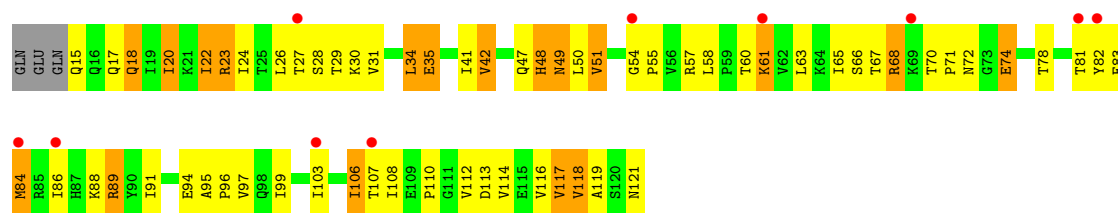


- Molecule 21: 40S ribosomal protein S19-A

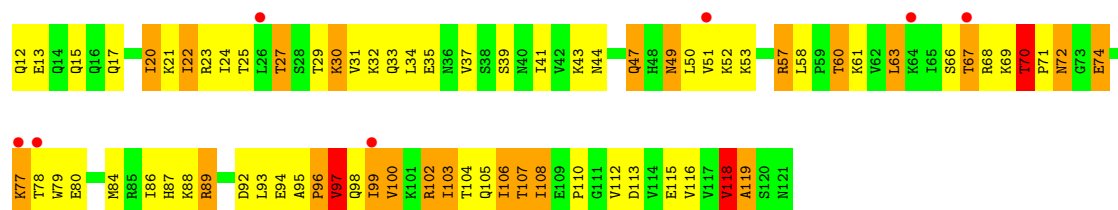


- Molecule 22: Small ribosomal subunit protein uS10

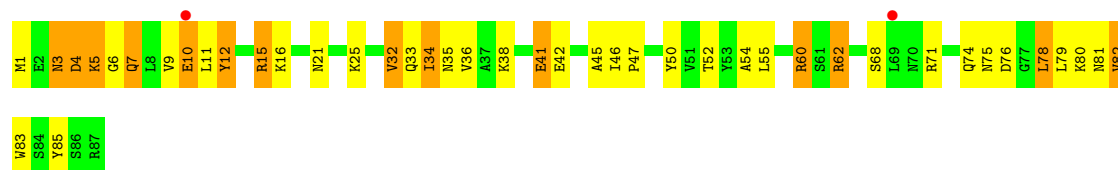




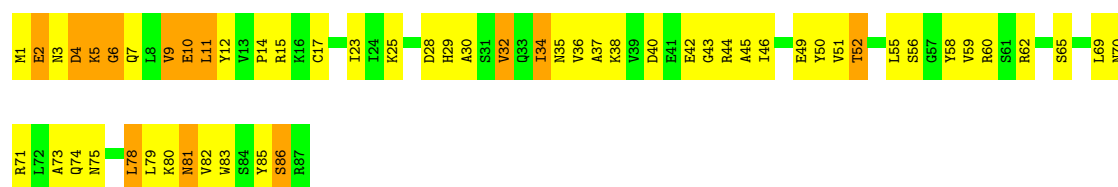
- Molecule 22: Small ribosomal subunit protein uS10



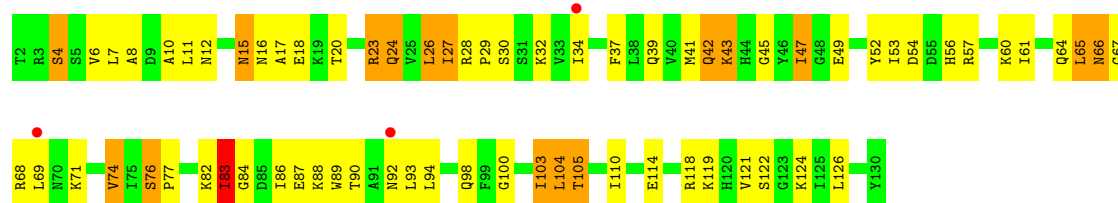
- Molecule 23: 40S ribosomal protein S21-A



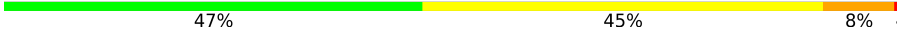
- Molecule 23: 40S ribosomal protein S21-A

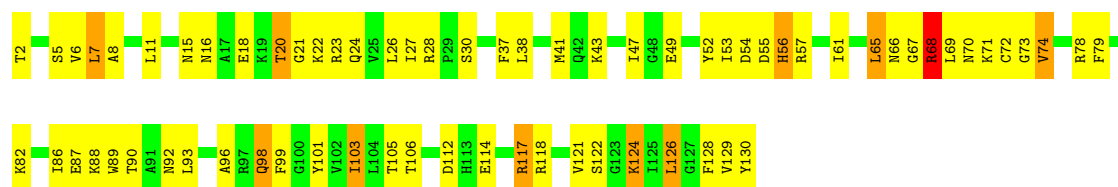


- Molecule 24: 40S ribosomal protein S22-A

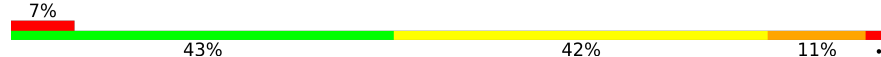


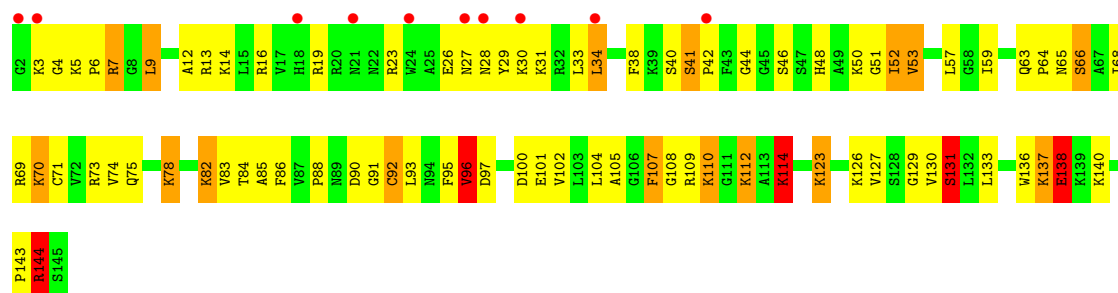
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:  47% 45% 8% .



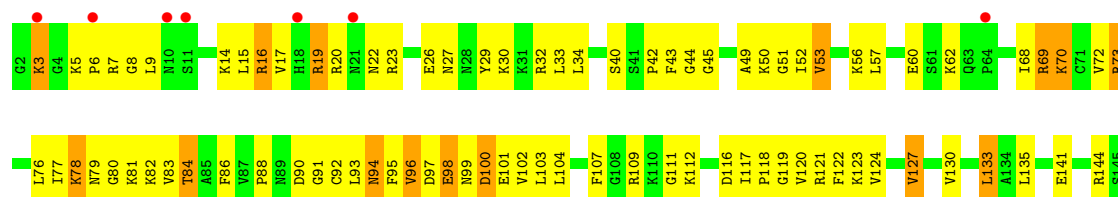
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:  7% 43% 42% 11% .



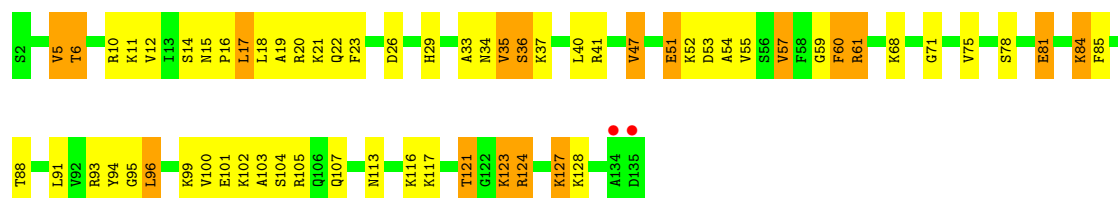
• Molecule 25: 40S ribosomal protein S23-A

Chain d3:  5% 41% 49% 10% .



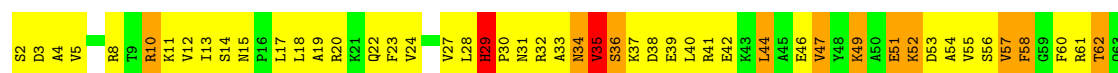
• Molecule 26: 40S ribosomal protein S24-A

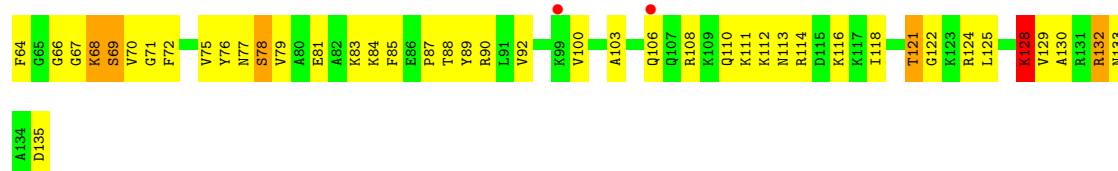
Chain D4:  % 53% 34% 13% .



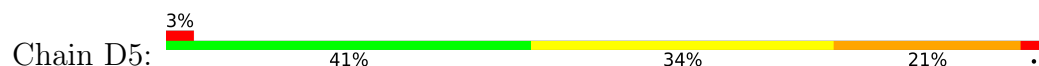
• Molecule 26: 40S ribosomal protein S24-A

Chain d4:  % 31% 54% 12% .

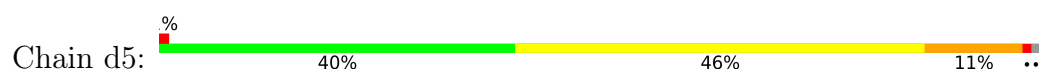




- Molecule 27: Small ribosomal subunit protein eS25A



- Molecule 27: Small ribosomal subunit protein eS25A



- Molecule 28: 40S ribosomal protein S26-B



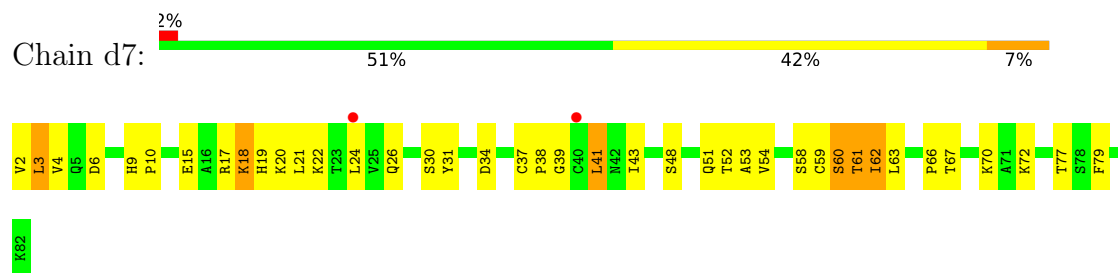
- Molecule 28: 40S ribosomal protein S26-B



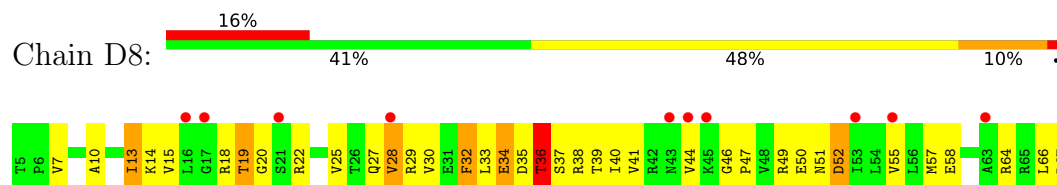
- Molecule 29: 40S ribosomal protein S27-A



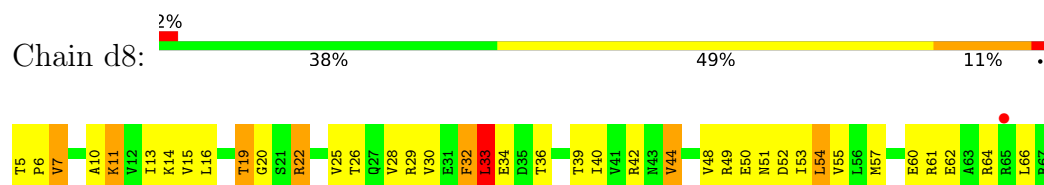
- Molecule 29: 40S ribosomal protein S27-A



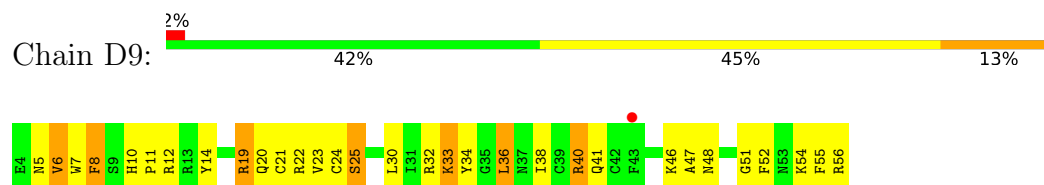
- Molecule 30: 40S ribosomal protein S28-A



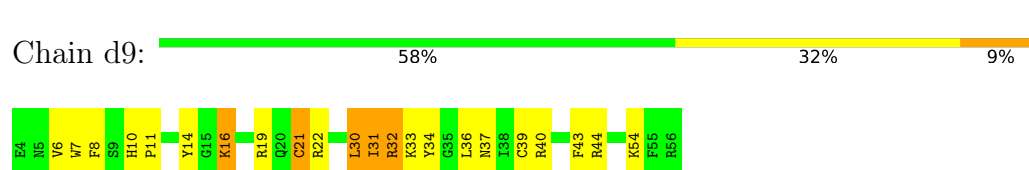
- Molecule 30: 40S ribosomal protein S28-A



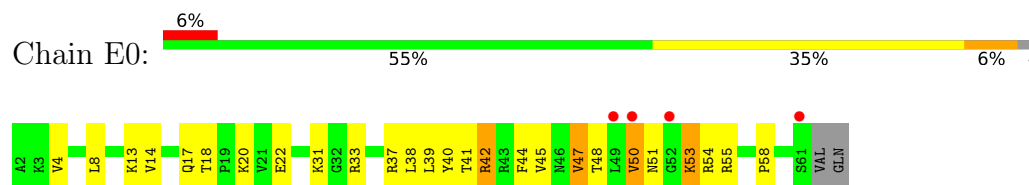
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 31: 40S ribosomal protein S29-A

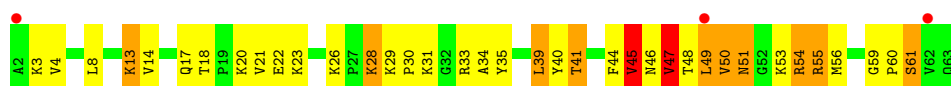


- Molecule 32: Small ribosomal subunit protein eS30A

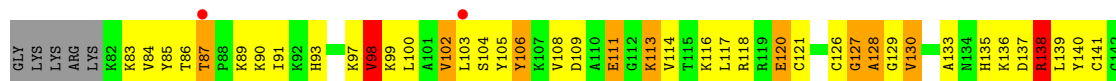


- Molecule 32: Small ribosomal subunit protein eS30A

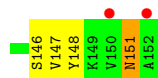
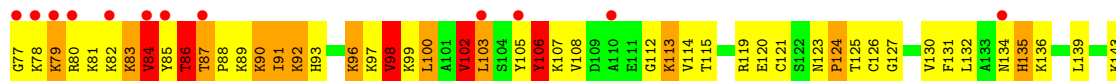




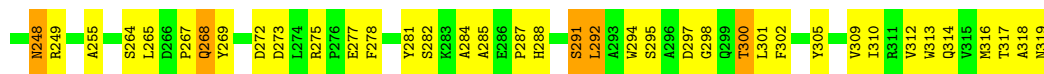
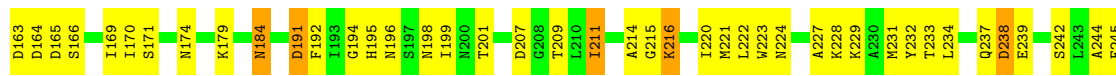
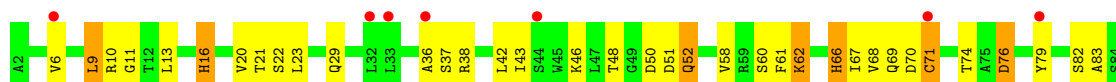
- Molecule 33: Small ribosomal subunit protein eS31



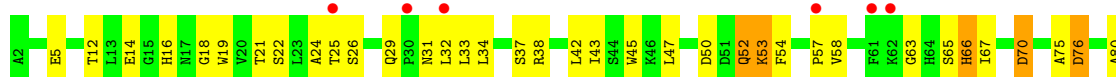
- Molecule 33: Small ribosomal subunit protein eS31

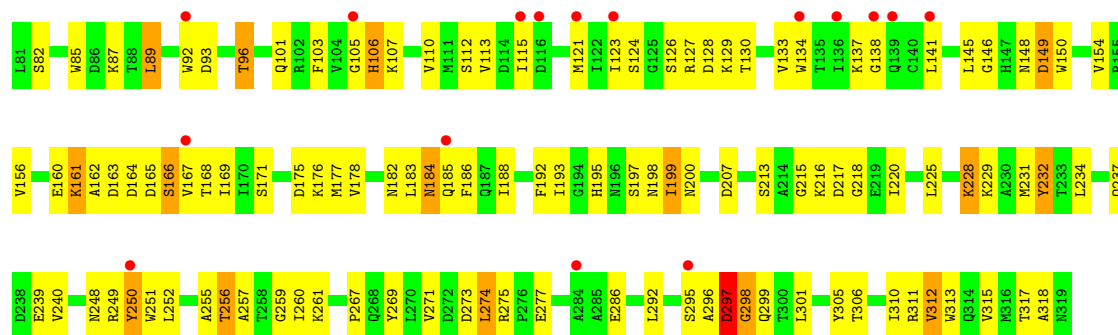


- Molecule 34: Small ribosomal subunit protein RACK1

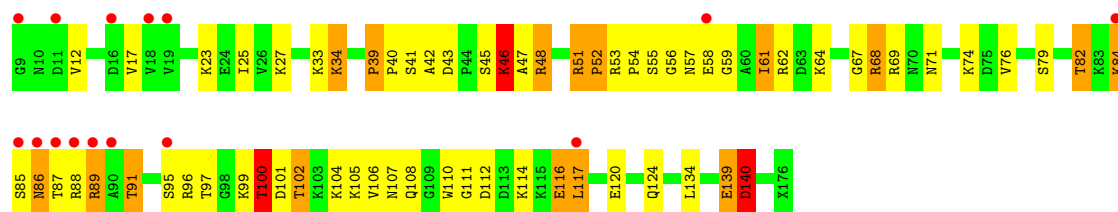


- Molecule 34: Small ribosomal subunit protein RACK1

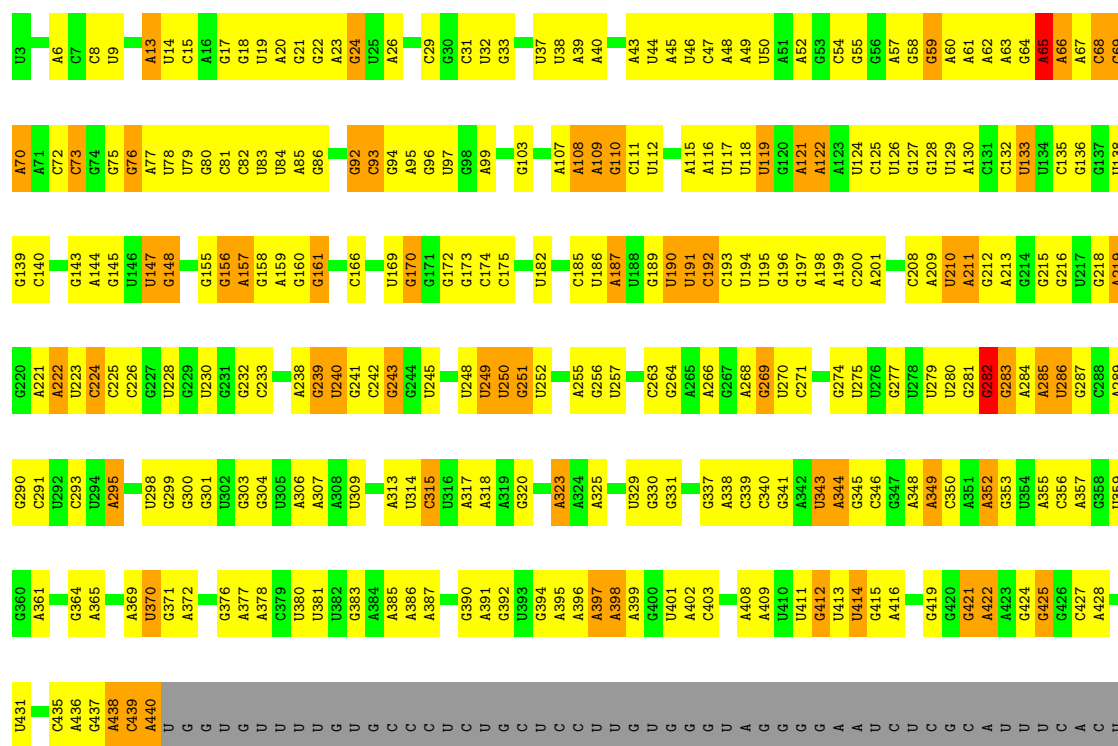




- Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1, Ribosome-bound protein Stm1

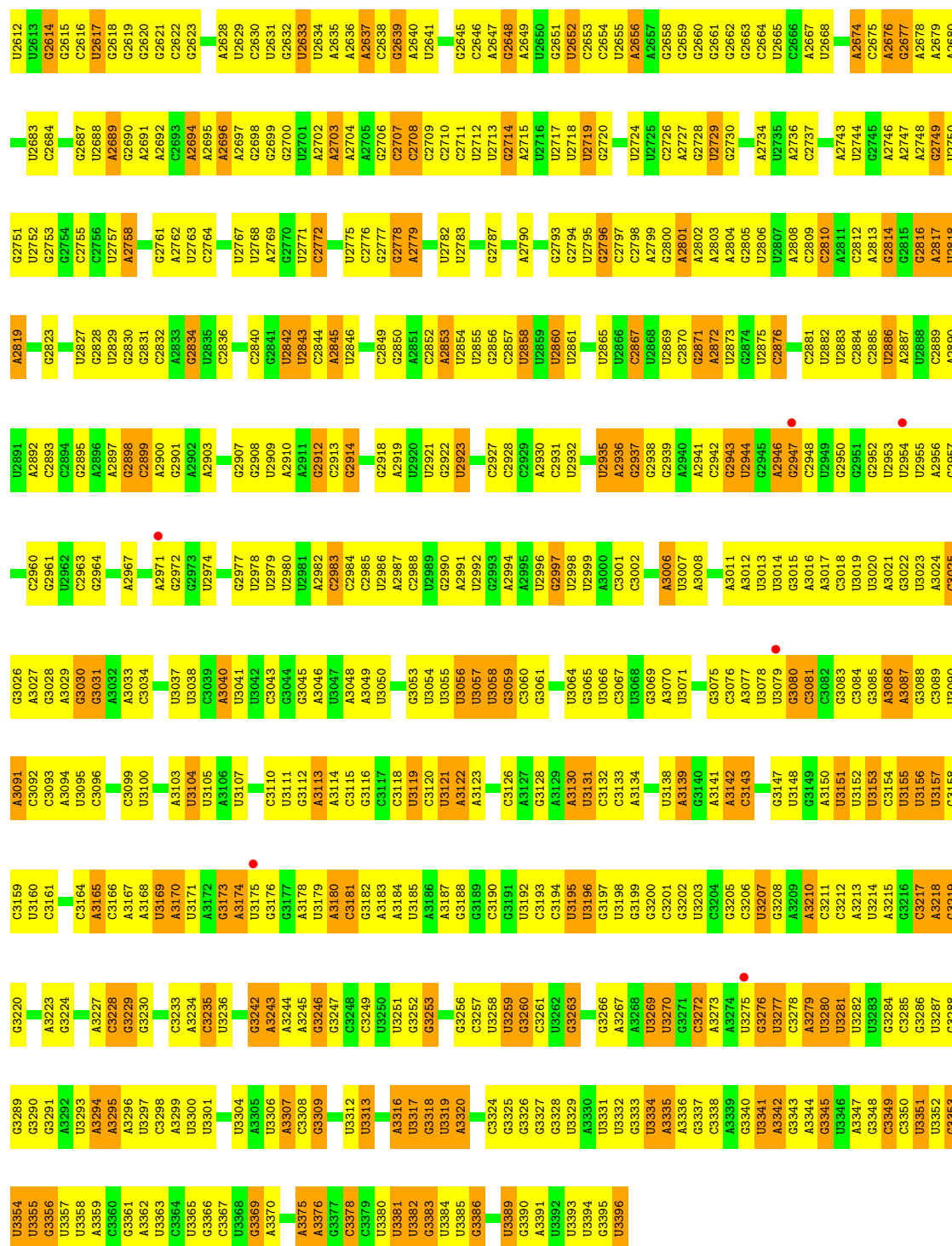


- Molecule 36: 25S ribosomal RNA



U1501	A1428	U1356	C1283	C1219	C1141	U1071	A997	C948	A847	U778	A705	G566	G
C1502	G1429	G1357	C1284	U1220	G1142	G1072	A998	U919	A848	G779	A706	G567	G494
C1505	U1430	C1358	G1285	G1221	A1143	U1073	G999	A920	C849	A780	A709	G568	G496
G1506	G1431	C1359	A1286	G1222	U1144	A1075	C1000	A921	G854	G781	A709	A569	C496
G1507	C1432	C1360	A1287	A1225	G1145	A1076	A1001	U922	G855	U782	G712	A572	C497
C1508	A1433	G1361	C1282	G1226	G1148	A1079	A1002	C923	U855	A783	U713	C573	A498
A1509	G1434	A1362	U1293	C1227	G1149	A1080	A1003	G924	G856	G784	U714	U574	G499
G1510	A1435	C1363	A1294	G1230	G1150	U1081	A1004	A925	G857	G785	G715	C500	C500
U1511	U1436	G1364	C1295	G1231	U1151	U1082	A1005	C926	A786	G786	A716	U502	A501
U1512	U1437	A1365	C1296	A1231	G1152	U1083	A1006	C927	G860	G787	C717	C503	C503
G1517	U1438	A1366	C1297	G1232	U1153	G1083	A1009	U930	C861	G788	G718	U507	U507
U1518	U1439	C1367	C1298	G1233	A1154	C1086	A1010	C931	U862	G789	U719	U508	U508
G1521	G1443	U1368	C1299	G1234	G1155	G1087	G1010	U932	G864	A791	A720	G582	U509
U1522	U1444	A1369	G1300	U1235	A1159	G1090	G1013	A936	G867	U796	G721	G583	G513
U1523	U1445	G1375	A1301	G1236	U1160	G1091	U1014	A937	C868	U797	G722	U587	G514
A1524	A1446	C1381	A1302	G1237	C1160	A1091	U1015	C938	G869	G798	G725	G588	G518
G1525	U1447	G1382	A1303	C1238	G1161	G1092	C1016	U939	U871	A801	G726	A589	A519
U1526	U1448	C1383	A1304	C1239	U1162	U1093	C1017	U943	U872	C802	G727	G590	G518
G1527	A1449	G1384	U1305	A1240	A1163	U1094	G1018	C944	U873	C803	G728	G591	A519
G1528	G1450	A1385	G1306	U1241	G1164	U1095	G1019	C945	U874	C804	G729	A592	A521
A1529	G1451	C1386	A1307	G1242	G1165	U1096	G1020	U946	U875	C805	C730	C593	A521
U1533	A1453	A1387	A1308	G1243	G1166	U1097	G1021	G950	G876	A806	G731	U594	A527
A1534	U1454	U1388	U1309	A1244	A1170	A1098	G1024	A951	G878	A807	G732	G595	U528
A1537	U1455	G1389	G1310	A1245	G1171	G1101	A1025	A952	U879	A808	G733	C596	U529
G1538	U1456	A1390	C1312	G1246	G1172	A1102	U1028	A953	A883	C809	G734	G597	G530
A1539	A1457	G1391	G1313	U1247	A1179	A1103	G1029	G954	A884	A810	A735	G600	G531
U1540	G1458	C1392	A1314	G1248	U1180	G1104	U1030	U955	U885	U811	A736	U601	A532
G1541	U1459	A1393	C1316	G1249	U1181	U1105	A1031	C957	G887	A812	G742	A602	A533
G1542	A1460	C1394	A1317	A1251	A1182	C1107	C1032	U956	U888	U821	G743	A603	U534
U1543	G1461	G1395	U1318	U1252	G1186	U1108	U1033	C958	C890	A816	A744	G604	G535
G1544	U1462	C1396	G1319	U1253	A1187	U1109	U1034	U959	G891	A817	A745	U605	U540
A1545	A1463	U1397	C1320	C1254	A1190	U1110	G1035	U960	U892	C818	U748	U606	U541
U1546	G1464	C1398	G1321	C1255	U1191	U1111	A1036	U961	U893	U819	C749	A607	G542
G1547	U1465	A1399	U1322	G1256	U1192	G1112	C1037	G963	G894	A820	G750	A608	C543
U1548	A1466	G1400	G1323	U1257	A1193	U1113	C1038	G964	A895	U822	A751	G609	C544
C1550	U1467	C1401	U1329	U1258	A1194	G1114	U1041	A965	A896	G823	G754	G610	U545
U1553	G1468	G1402	A1330	G1261	A1195	G1115	C1045	U966	U897	C824	A755	G611	C546
U1554	U1469	C1403	U1331	A1262	C1196	G1116	A1046	A967	U898	U825	G756	G612	G547
U1555	G1470	G1404	A1332	G1263	A1197	C1117	A1047	U968	U899	G826	U759	U681	G548
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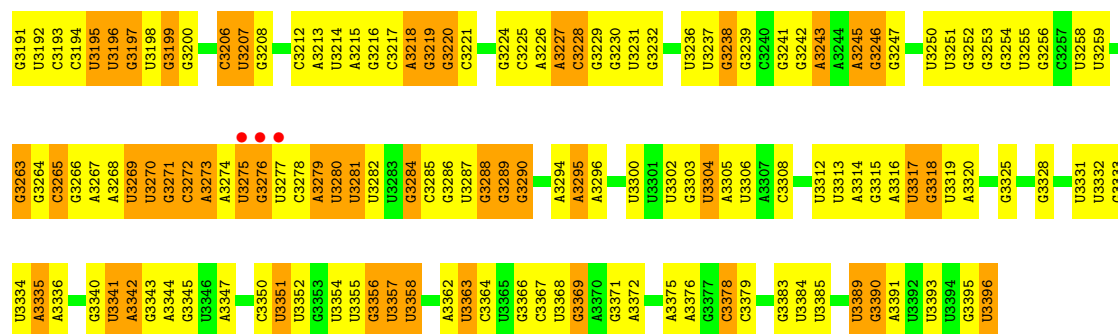




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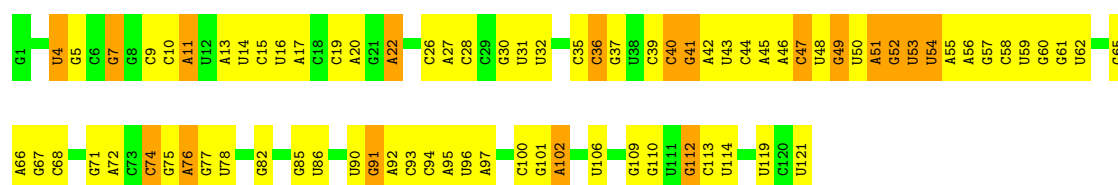
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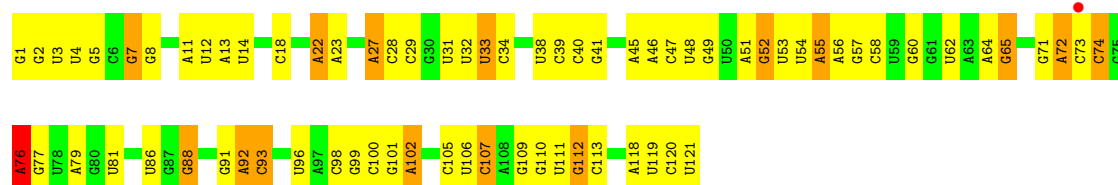
• Molecule 37: 5S ribosomal RNA

Chain 3: 34% 51% 15%



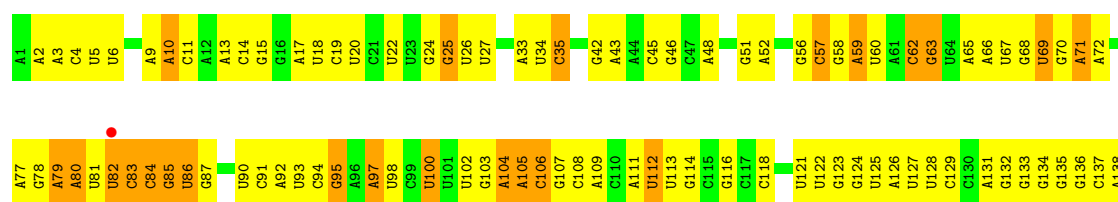
• Molecule 37: 5S ribosomal RNA

Chain 7: 40% 47% 12%



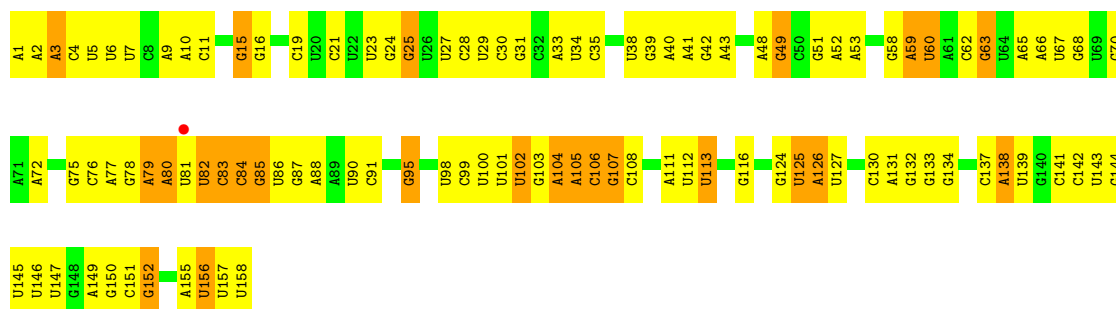
• Molecule 38: 5.8S ribosomal RNA

Chain 4: 32% 54% 15%

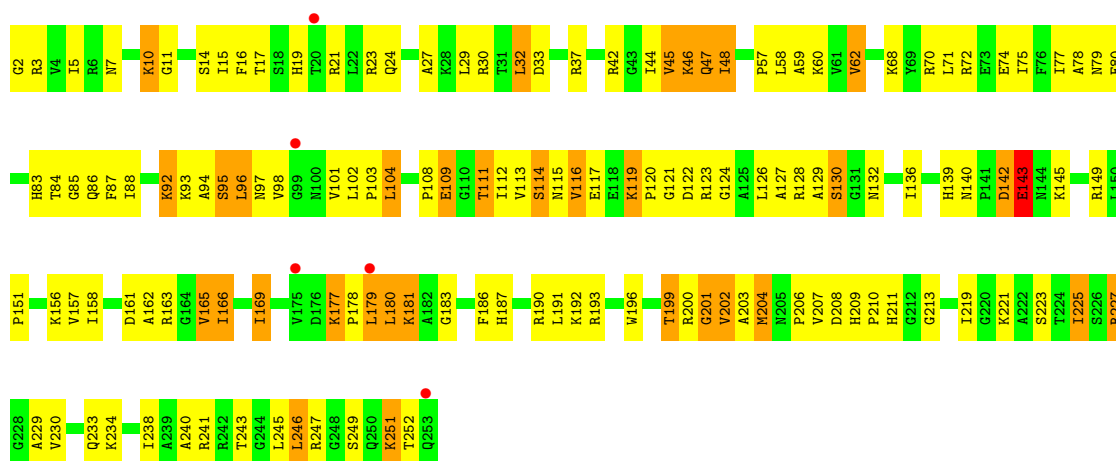


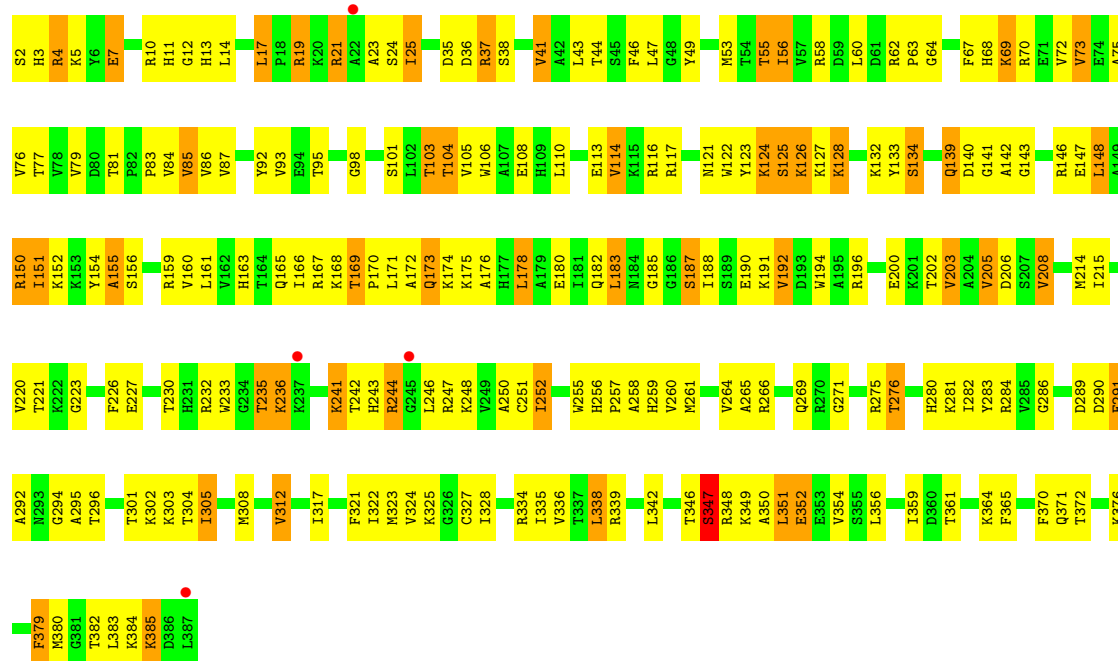
• Molecule 38: 5.8S ribosomal RNA

Chain 8: 33% 51% 16%

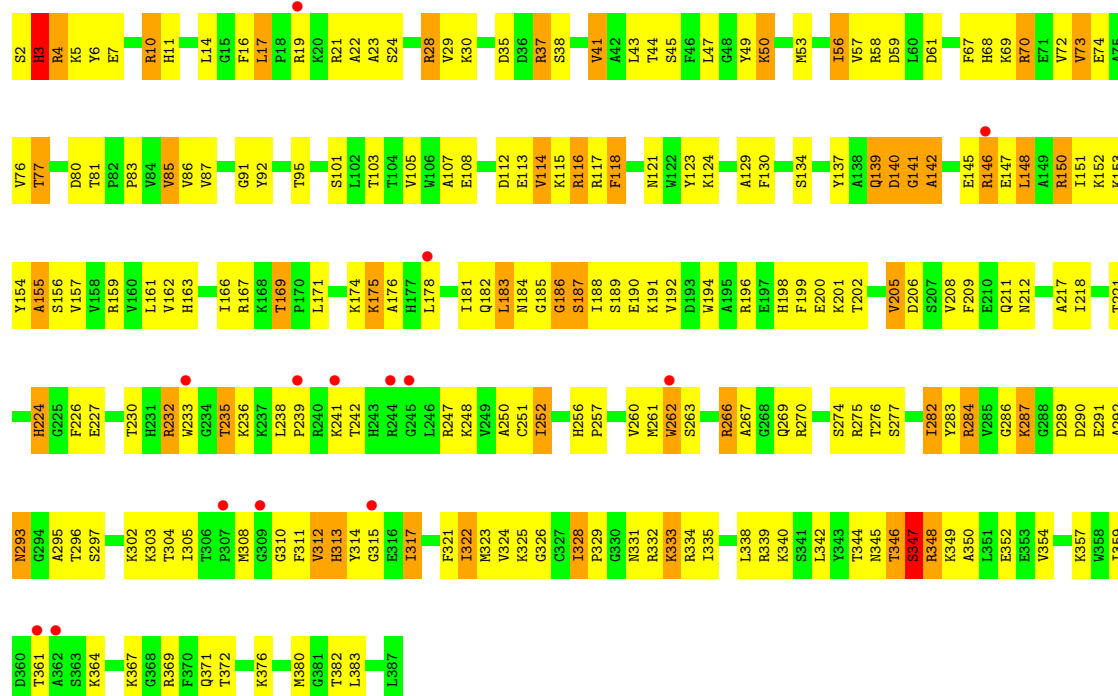


• Molecule 39: 60S ribosomal protein L2-A

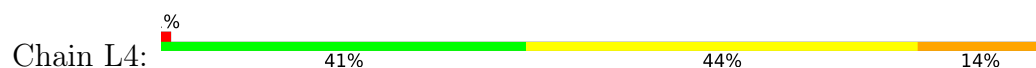


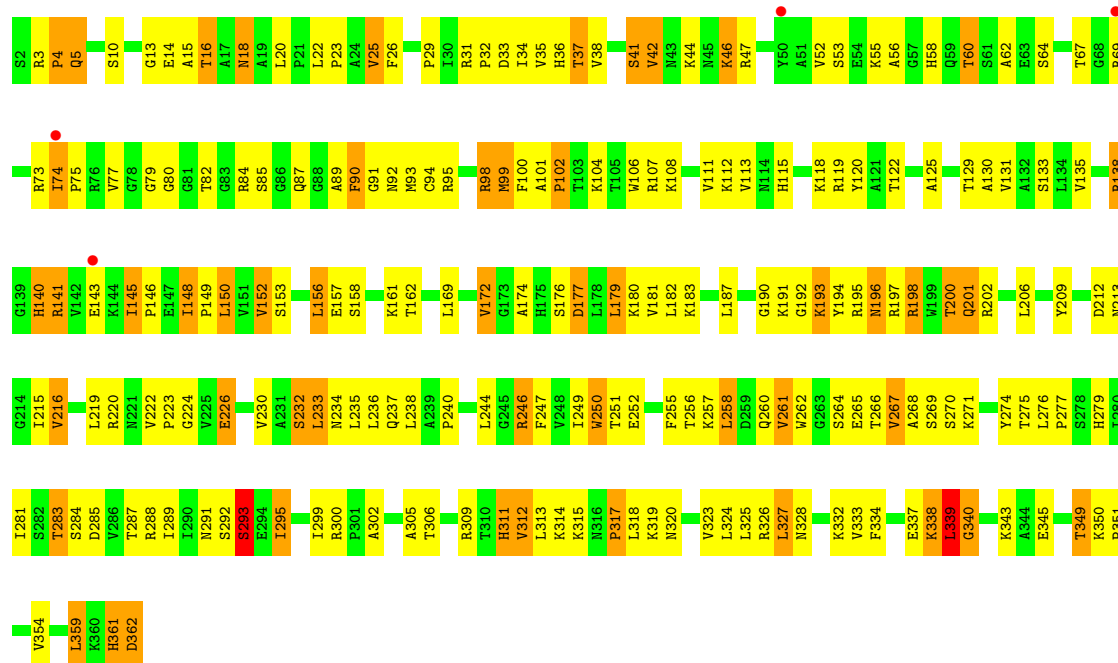


• Molecule 40: 60S ribosomal protein L3

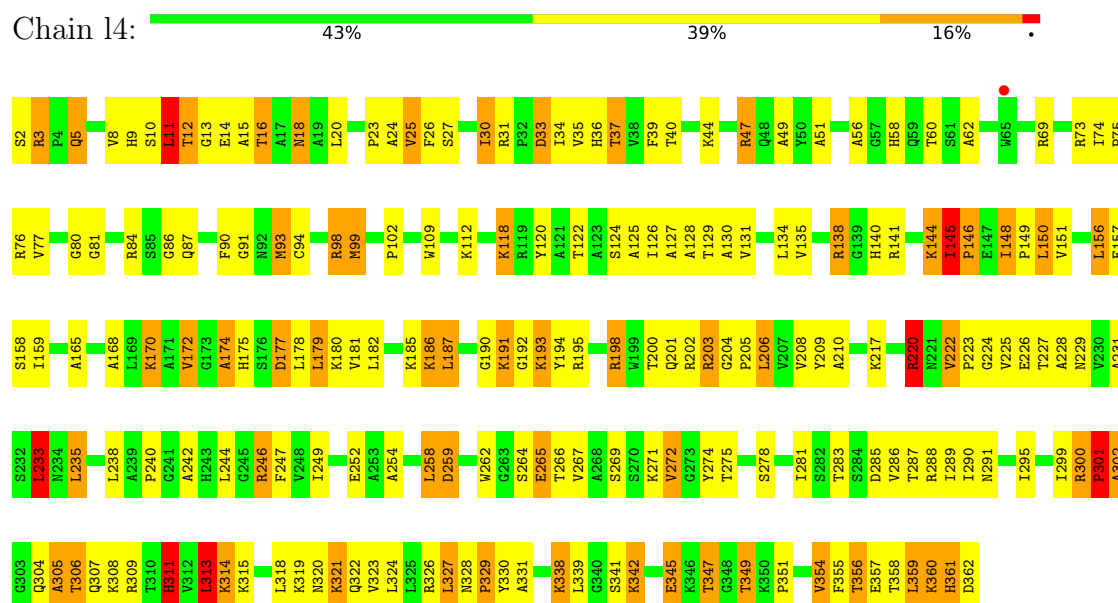


• Molecule 41: 60S ribosomal protein L4-A

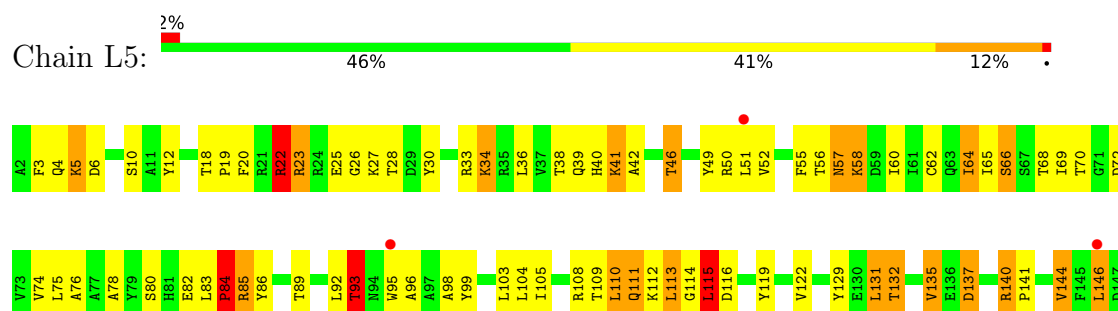


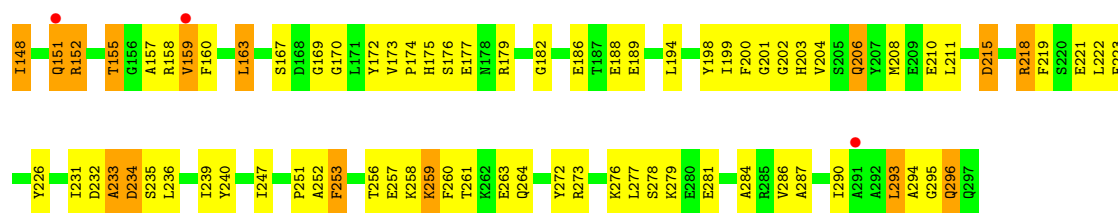


• Molecule 41: 60S ribosomal protein L4-A

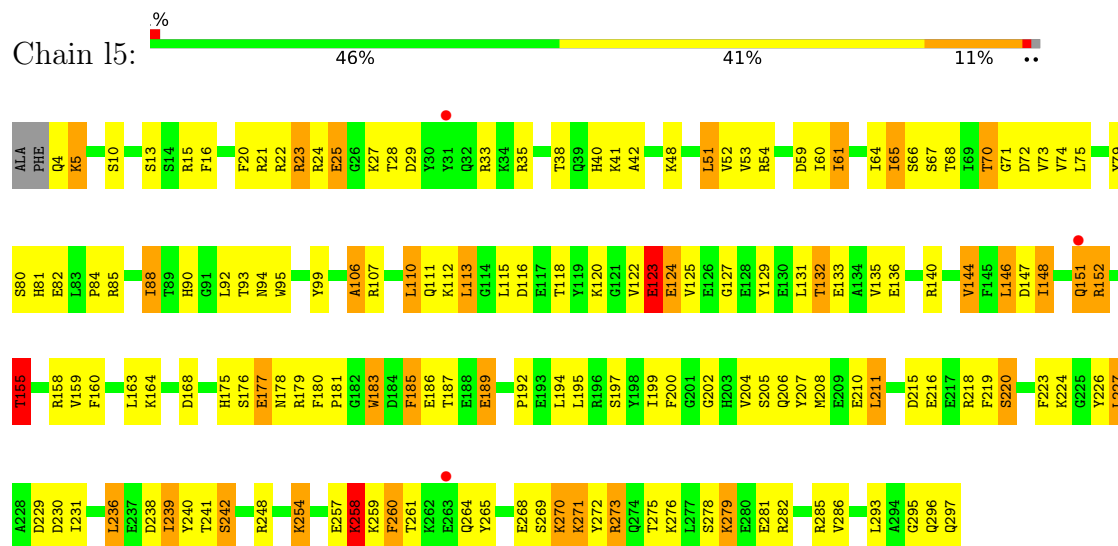


• Molecule 42: 60S ribosomal protein L5

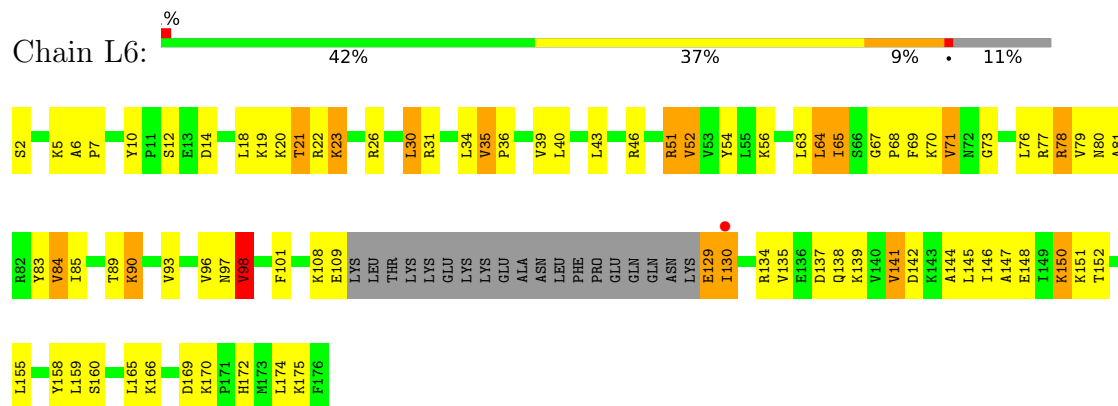




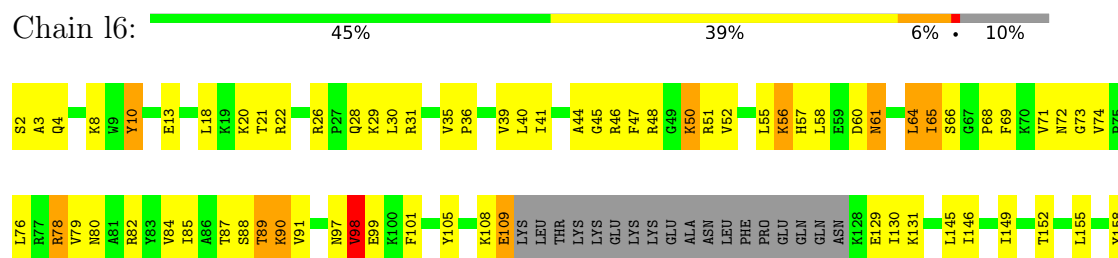
• Molecule 42: 60S ribosomal protein L5

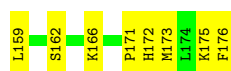


• Molecule 43: Large ribosomal subunit protein eL6A

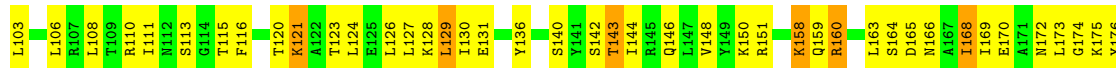
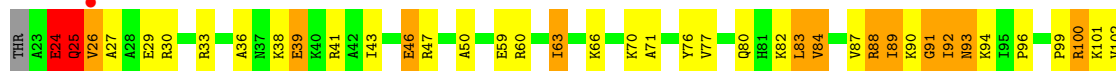


• Molecule 43: Large ribosomal subunit protein eL6A

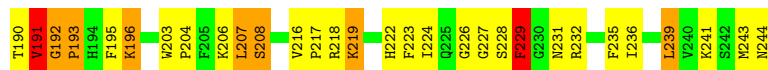
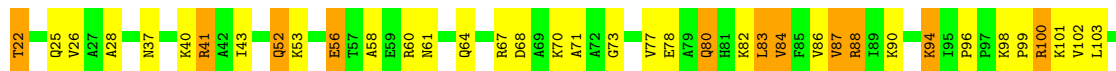




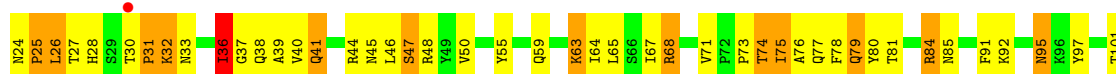
- Molecule 44: Large ribosomal subunit protein uL30A



- Molecule 44: Large ribosomal subunit protein uL30A

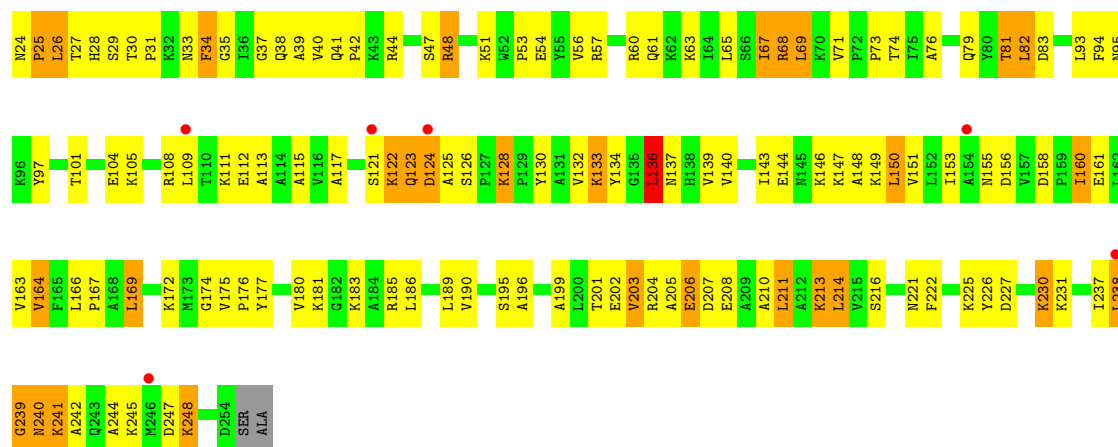


- Molecule 45: 60S ribosomal protein L8-A

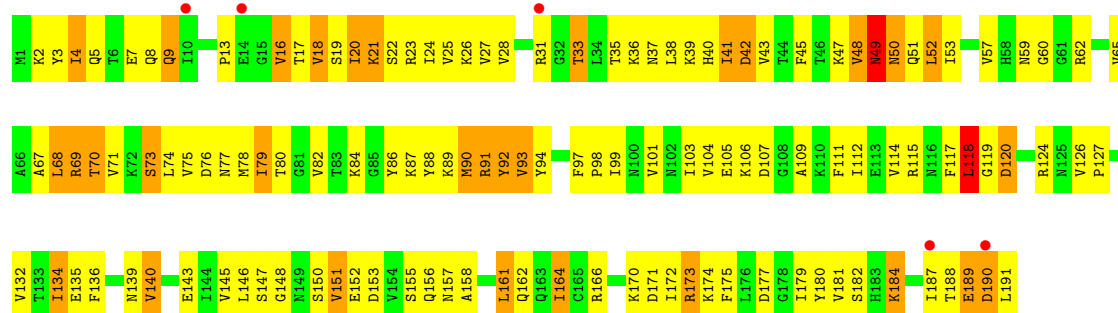


- Molecule 45: 60S ribosomal protein L8-A

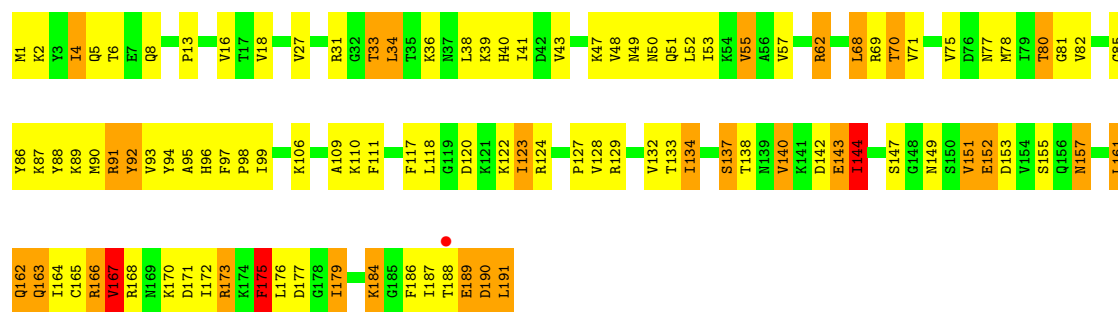
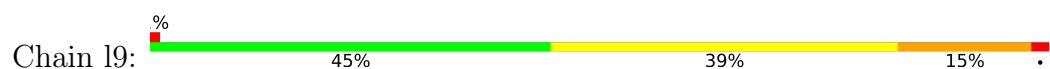




• Molecule 46: 60S ribosomal protein L9-A

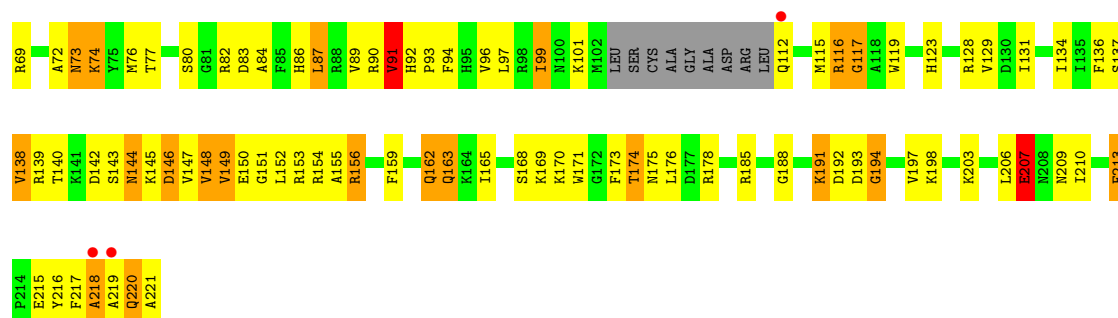


• Molecule 46: 60S ribosomal protein L9-A

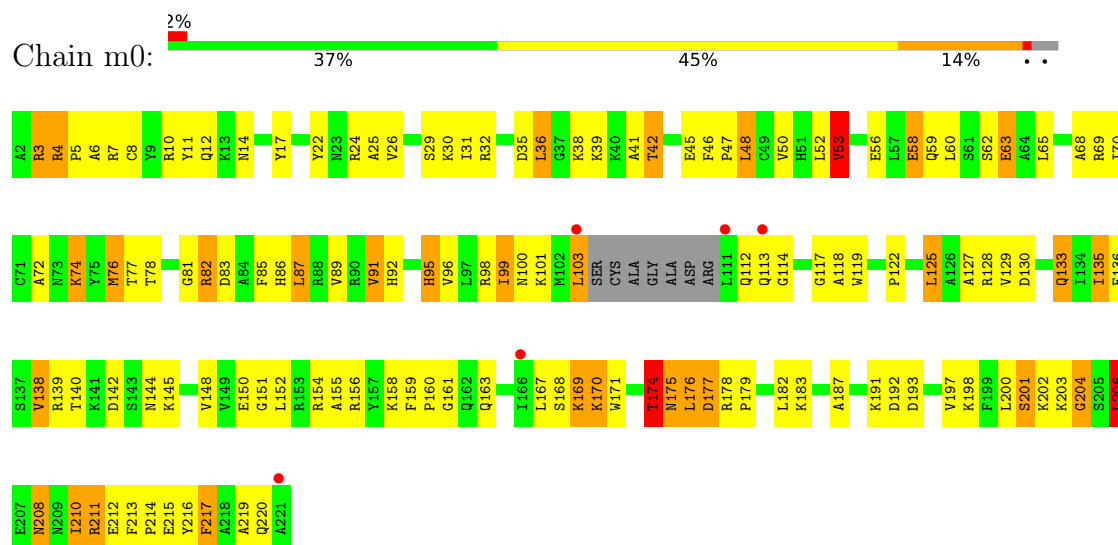


• Molecule 47: 60S ribosomal protein L10

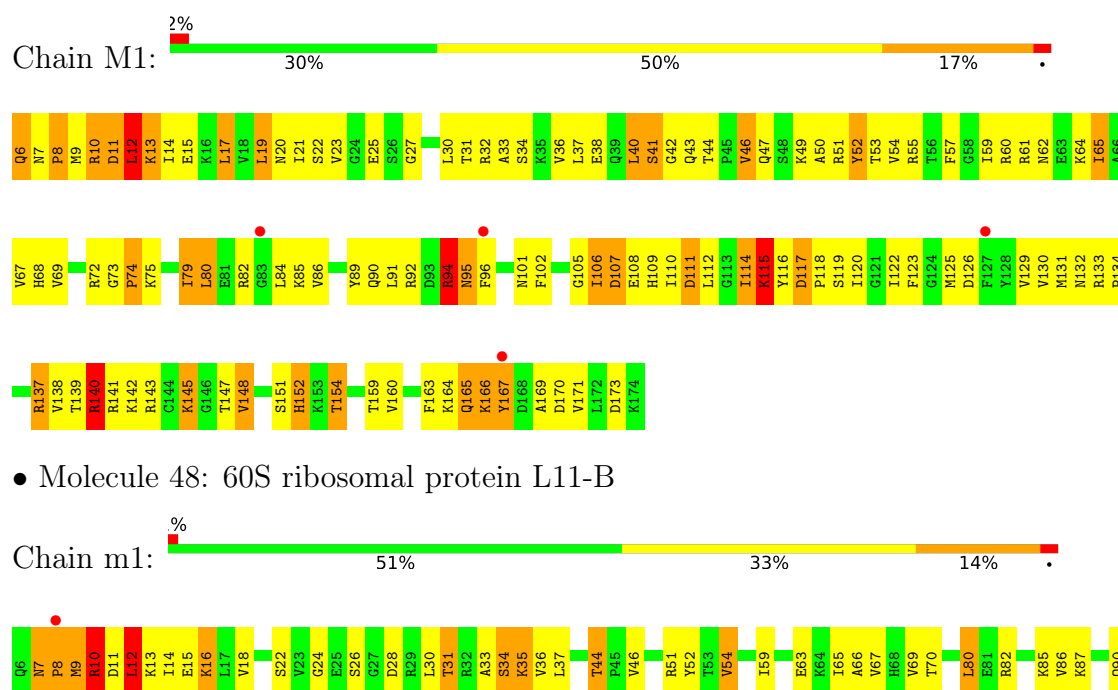




• Molecule 47: 60S ribosomal protein L10



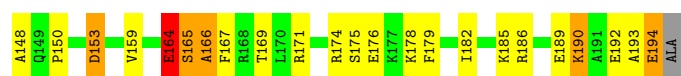
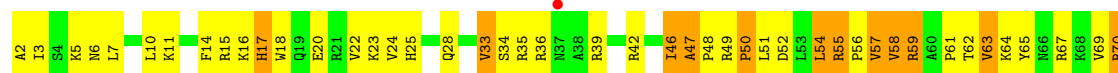
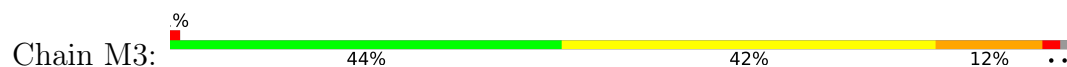
• Molecule 48: 60S ribosomal protein L11-B



• Molecule 48: 60S ribosomal protein L11-B



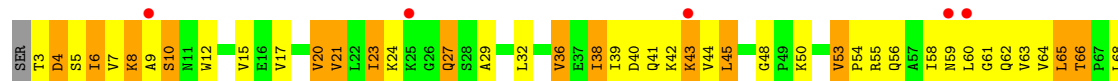
- Molecule 49: Large ribosomal subunit protein eL13A



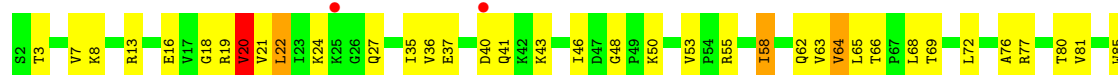
- Molecule 49: Large ribosomal subunit protein eL13A



- Molecule 50: Large ribosomal subunit protein eL14A



- Molecule 50: Large ribosomal subunit protein eL14A





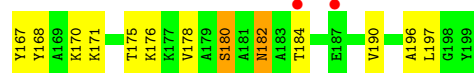
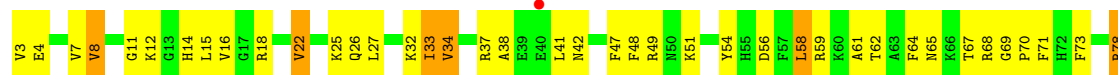
• Molecule 51: 60S ribosomal protein L15-A



• Molecule 51: 60S ribosomal protein L15-A

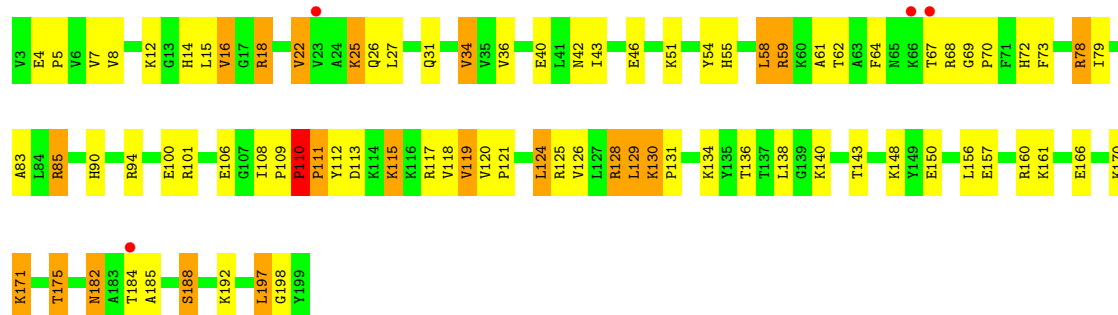


• Molecule 52: 60S ribosomal protein L16-A

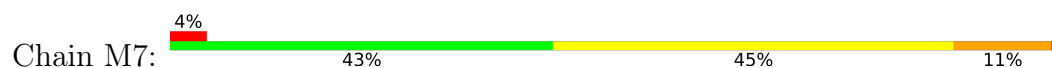


• Molecule 52: 60S ribosomal protein L16-A

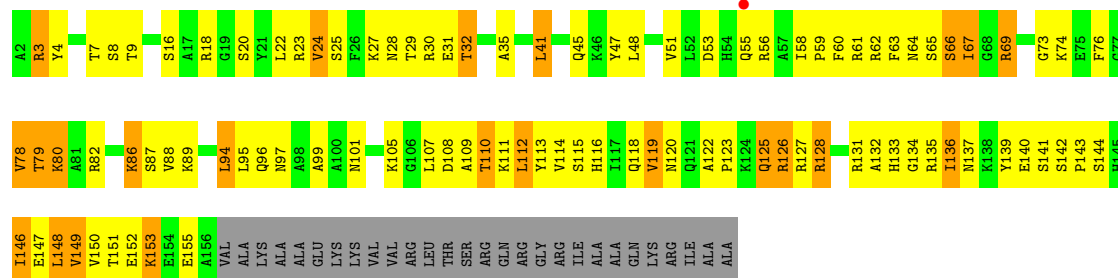




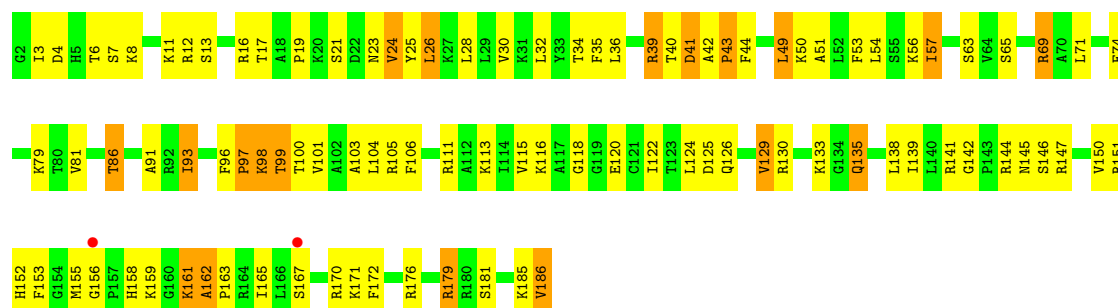
• Molecule 53: 60S ribosomal protein L17-A



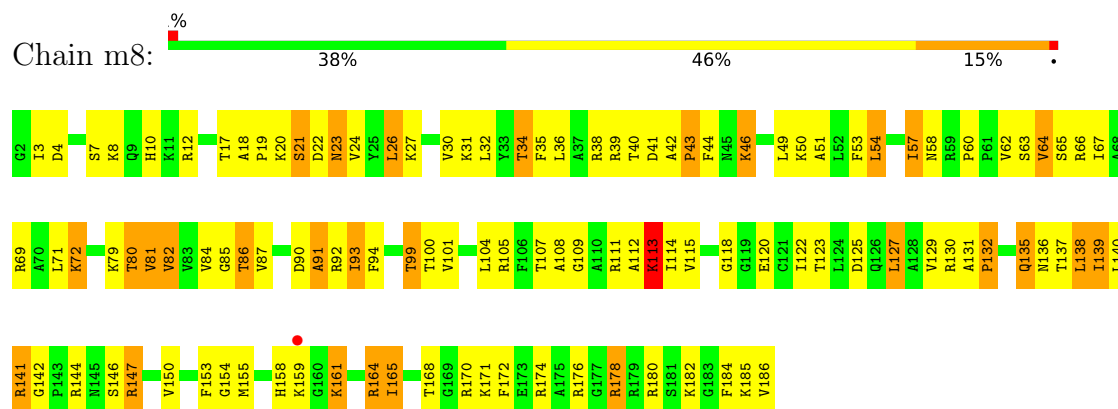
• Molecule 53: 60S ribosomal protein L17-A



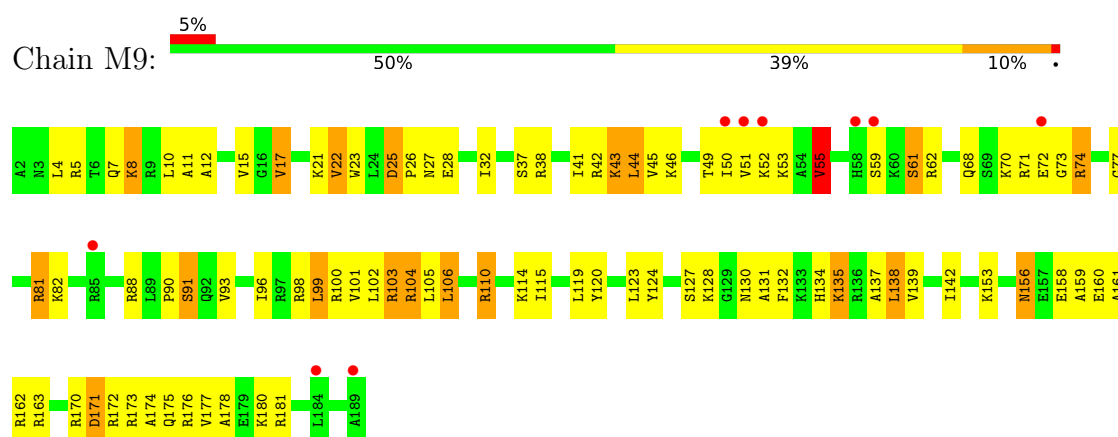
• Molecule 54: 60S ribosomal protein L18-A



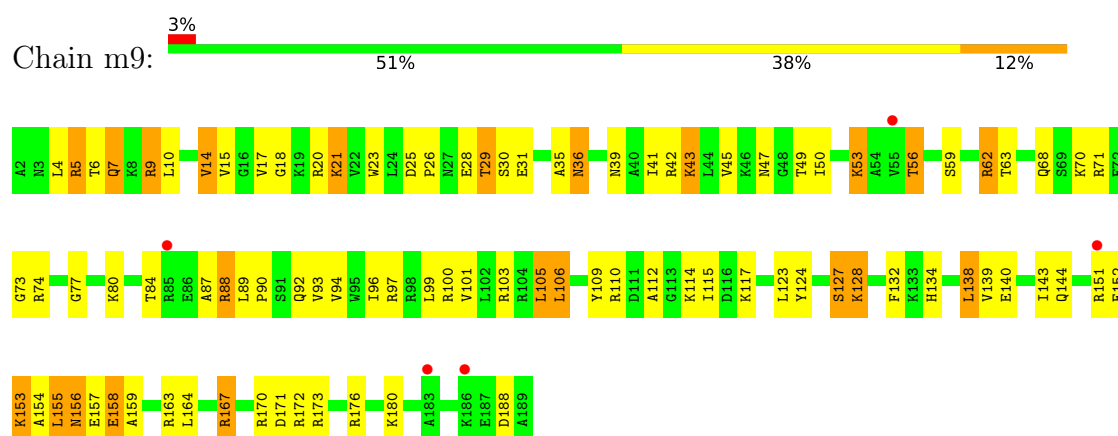
- Molecule 54: 60S ribosomal protein L18-A



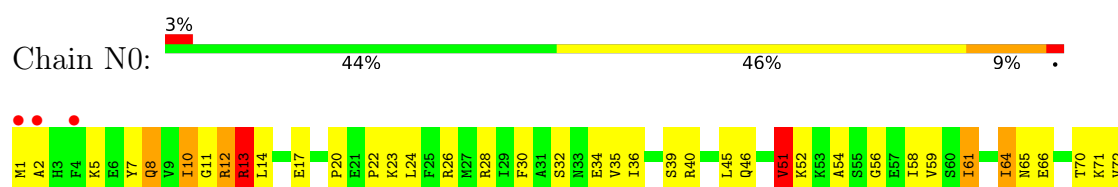
- Molecule 55: 60S ribosomal protein L19-A

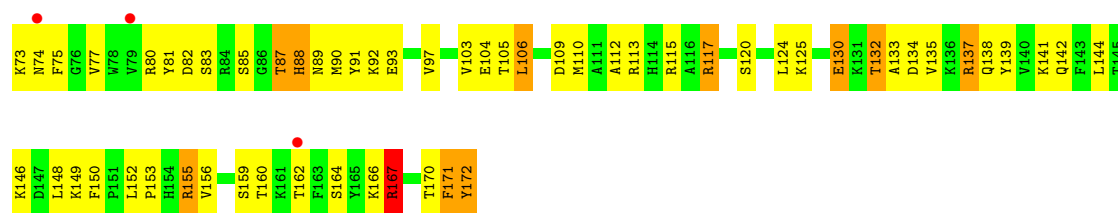


- Molecule 55: 60S ribosomal protein L19-A

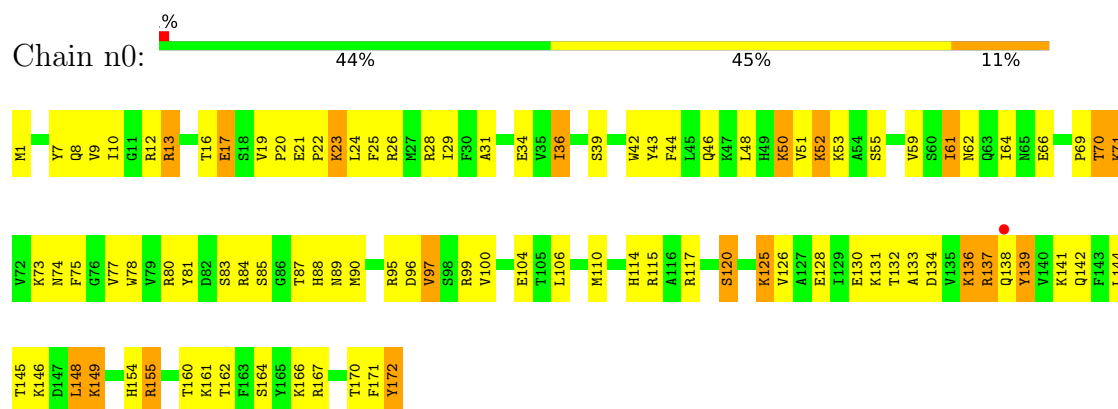


- Molecule 56: 60S ribosomal protein L20-A

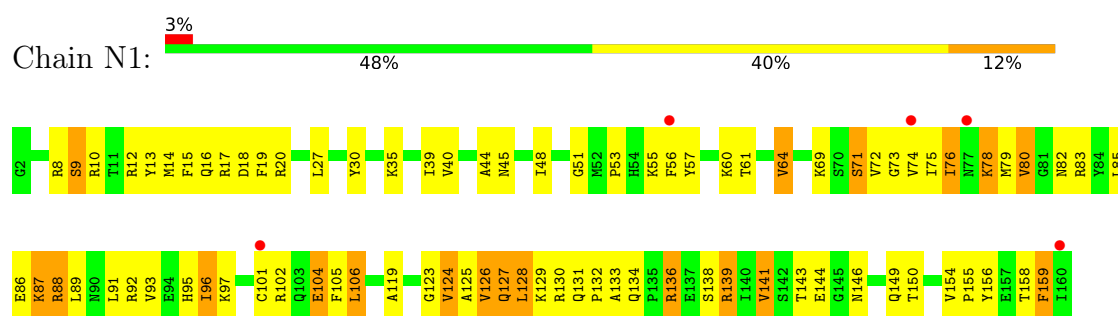




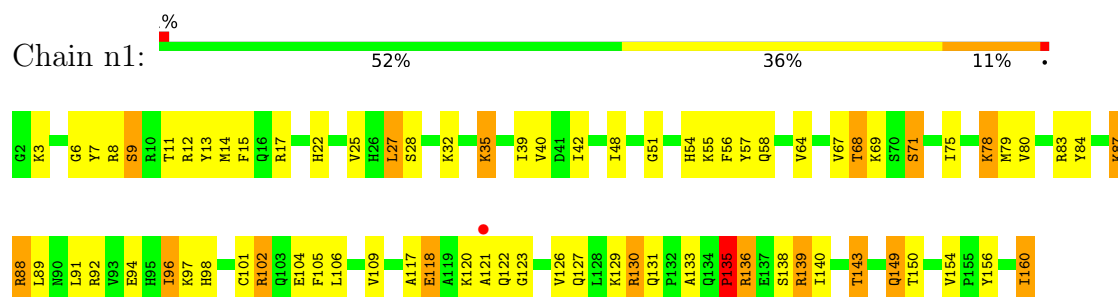
• Molecule 56: 60S ribosomal protein L20-A



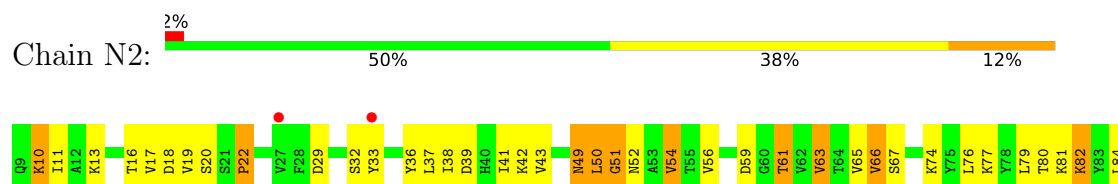
• Molecule 57: 60S ribosomal protein L21-A



• Molecule 57: 60S ribosomal protein L21-A

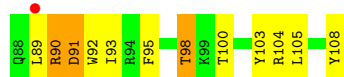
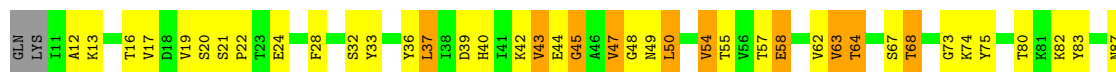


• Molecule 58: 60S ribosomal protein L22-A

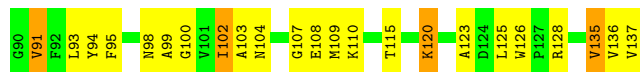
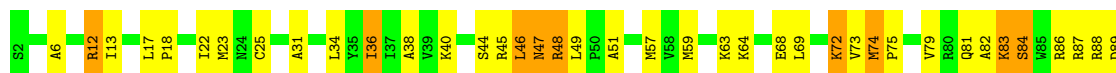




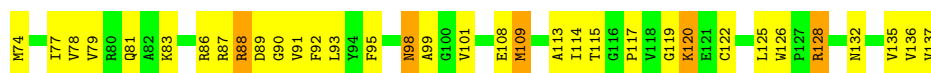
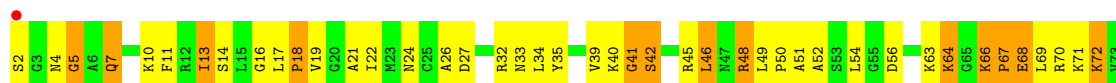
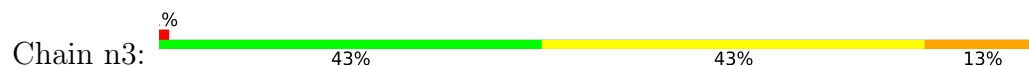
- Molecule 58: 60S ribosomal protein L22-A



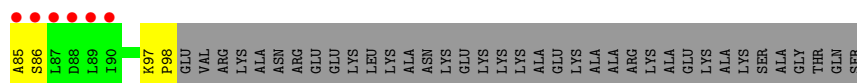
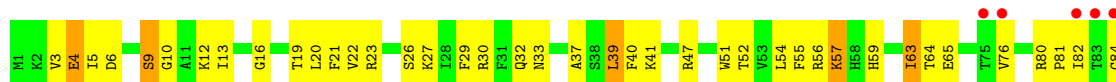
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 59: 60S ribosomal protein L23-A

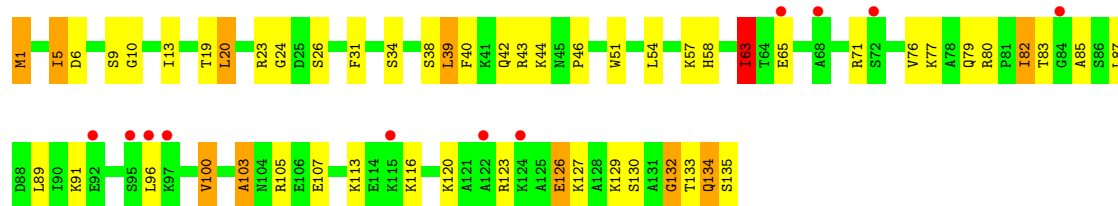


- Molecule 60: Large ribosomal subunit protein eL24A



- Molecule 60: Large ribosomal subunit protein eL24A

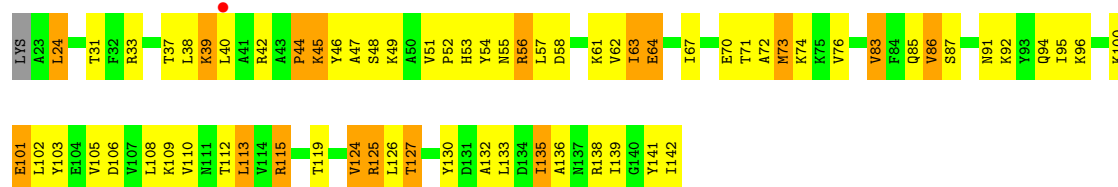
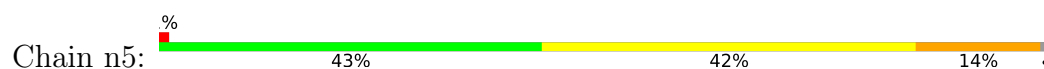




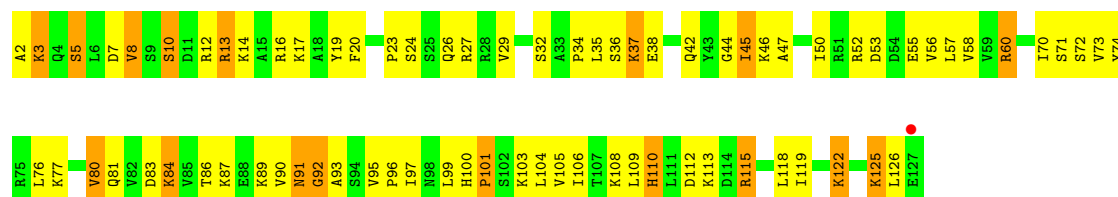
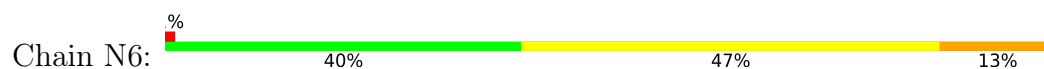
• Molecule 61: 60S ribosomal protein L25



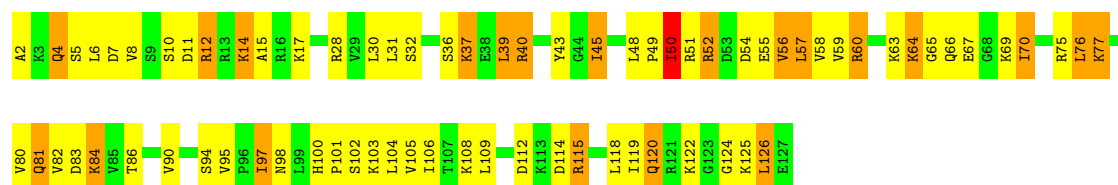
• Molecule 61: 60S ribosomal protein L25



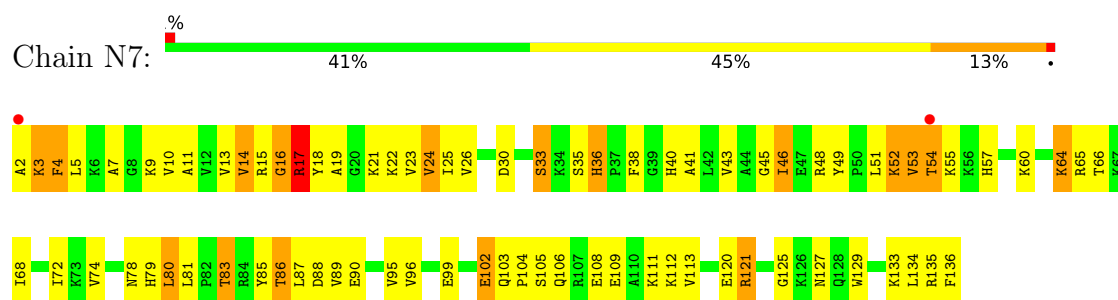
• Molecule 62: Large ribosomal subunit protein uL24A



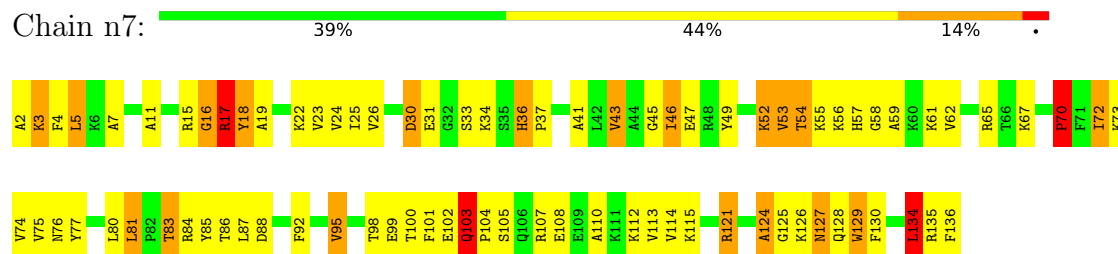
• Molecule 62: Large ribosomal subunit protein uL24A



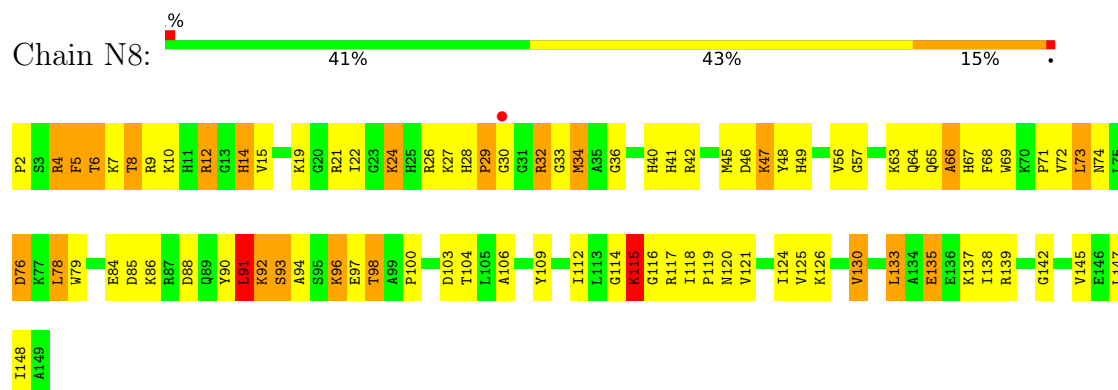
• Molecule 63: 60S ribosomal protein L27-A



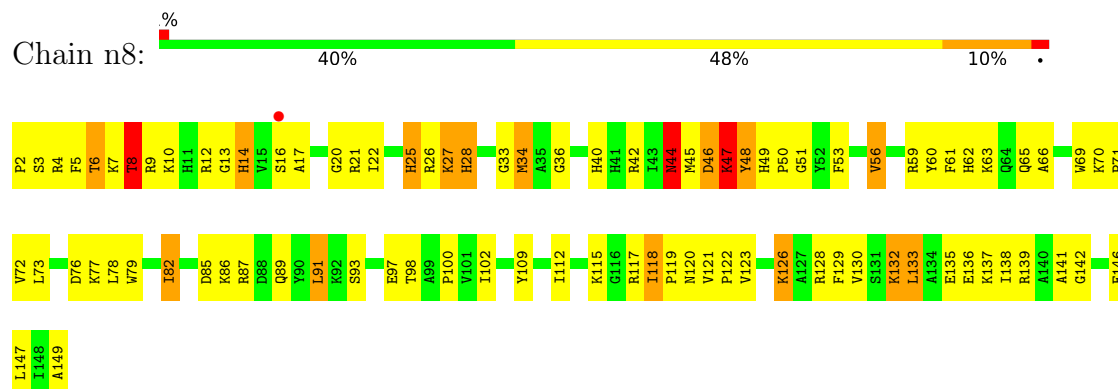
• Molecule 63: 60S ribosomal protein L27-A



• Molecule 64: 60S ribosomal protein L28



• Molecule 64: 60S ribosomal protein L28

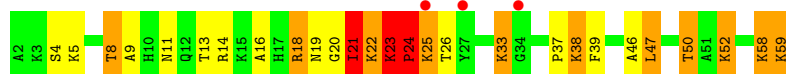


• Molecule 65: 60S ribosomal protein L29

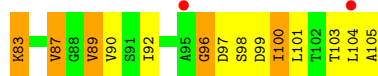




- Molecule 65: 60S ribosomal protein L29



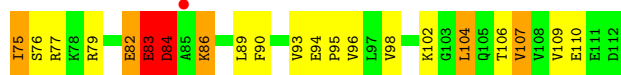
- Molecule 66: Large ribosomal subunit protein eL30



- Molecule 66: Large ribosomal subunit protein eL30



- Molecule 67: 60S ribosomal protein L31-A

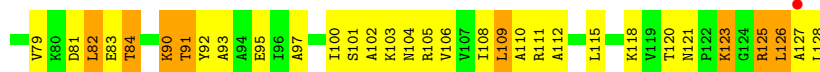
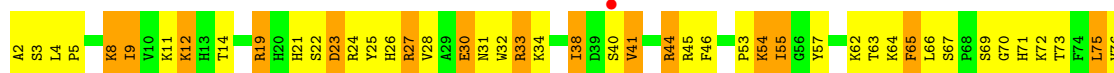


- Molecule 67: 60S ribosomal protein L31-A





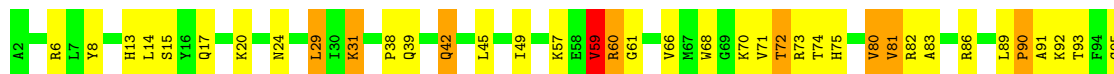
- Molecule 68: 60S ribosomal protein L32



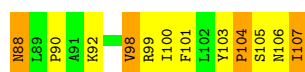
- Molecule 68: 60S ribosomal protein L32



- Molecule 69: 60S ribosomal protein L33-A

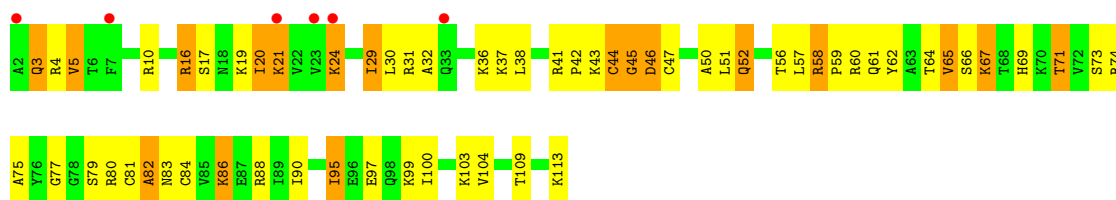


- Molecule 69: 60S ribosomal protein L33-A

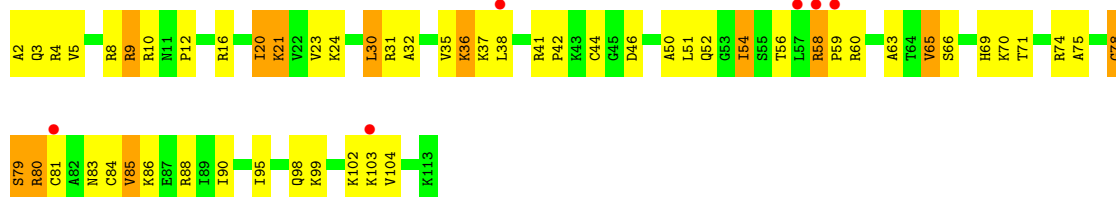


- Molecule 70: 60S ribosomal protein L34-A

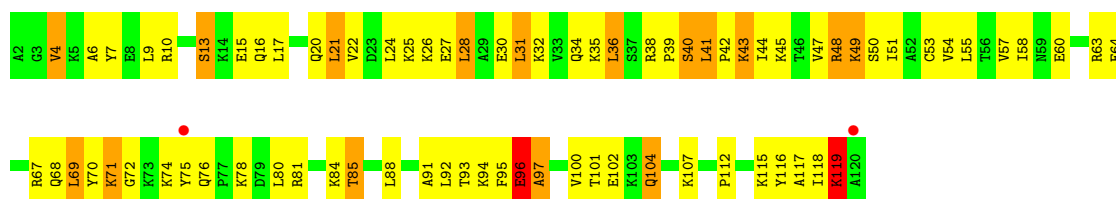




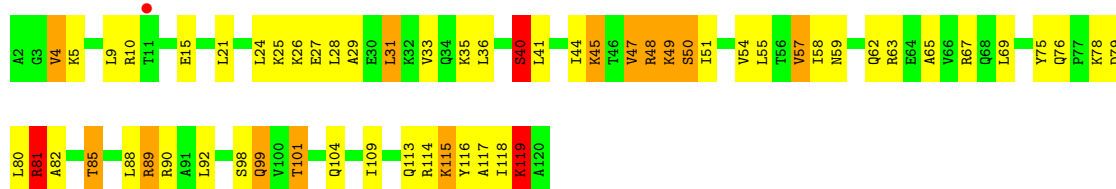
- Molecule 70: 60S ribosomal protein L34-A



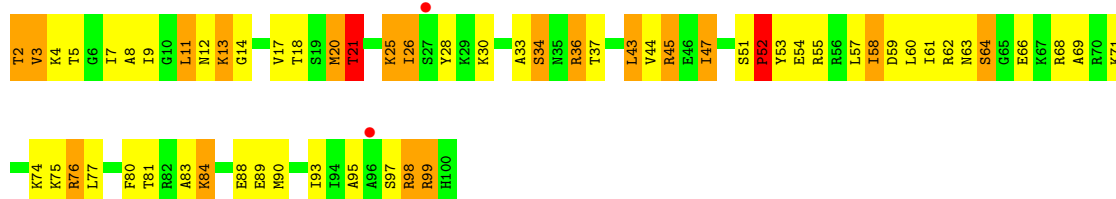
- Molecule 71: 60S ribosomal protein L35-A



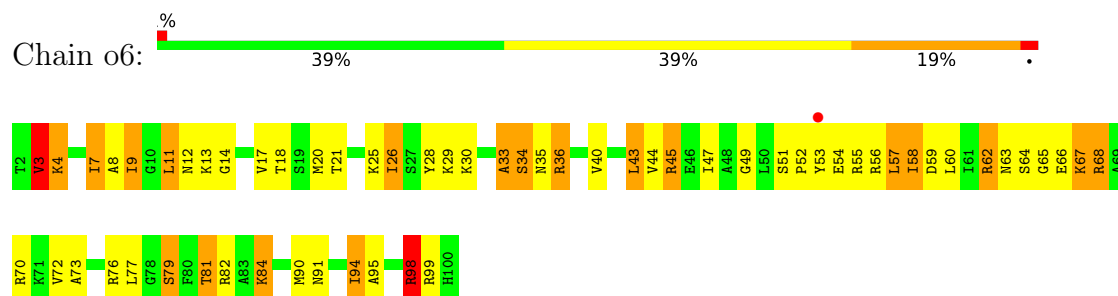
- Molecule 71: 60S ribosomal protein L35-A



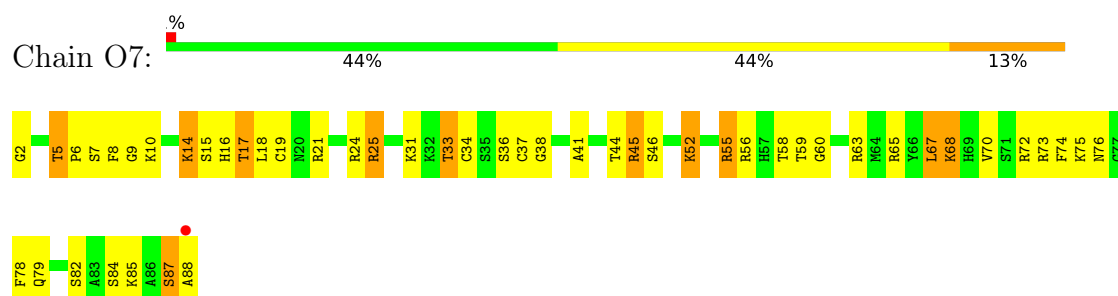
- Molecule 72: 60S ribosomal protein L36-A



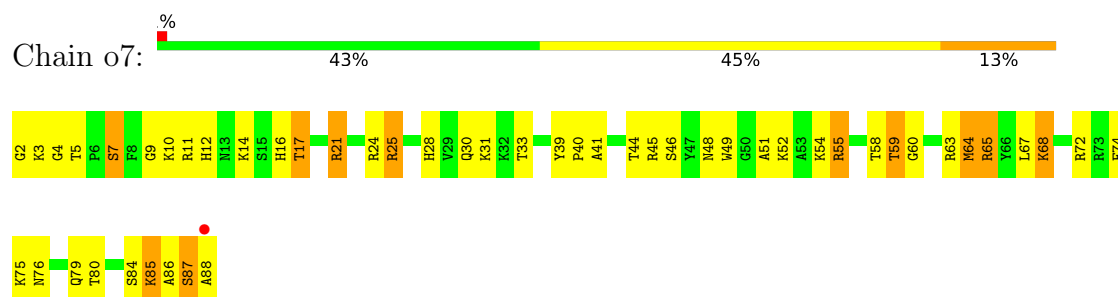
- Molecule 72: 60S ribosomal protein L36-A



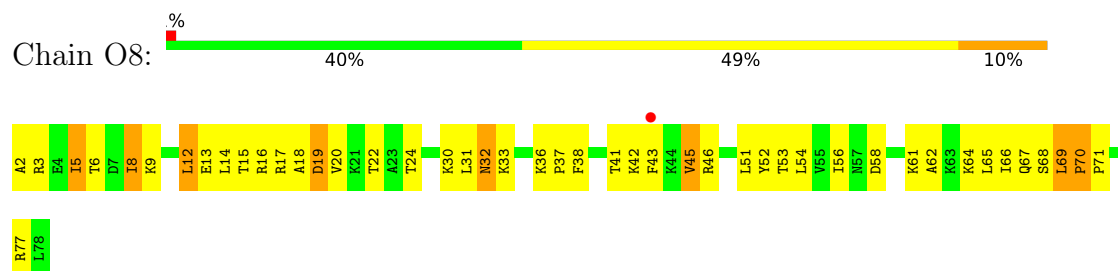
- Molecule 73: 60S ribosomal protein L37-A



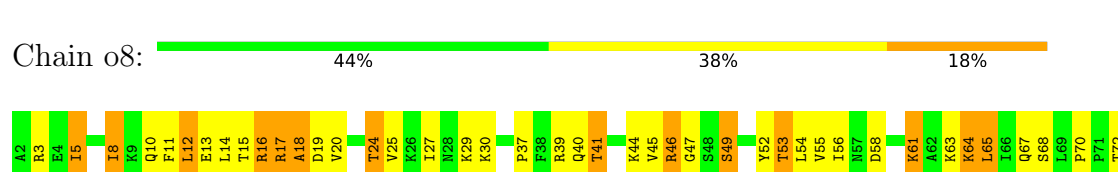
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



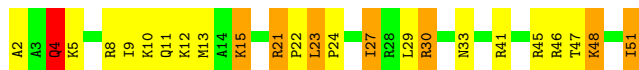
- Molecule 74: 60S ribosomal protein L38





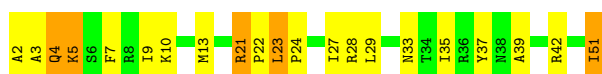
- Molecule 75: 60S ribosomal protein L39

Chain O9: 52% 32% 14% .



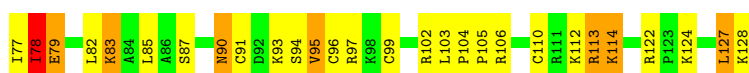
- Molecule 75: 60S ribosomal protein L39

Chain o9: 58% 32% 10% .



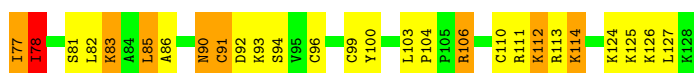
- Molecule 76: 60S ribosomal protein L40-A

Chain Q0: 46% 38% 13% .



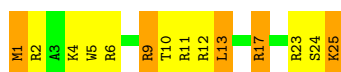
- Molecule 76: 60S ribosomal protein L40-A

Chain q0: 48% 35% 15% .



- Molecule 77: Large ribosomal subunit protein eL41B

Chain Q1: 44% 36% 20% .



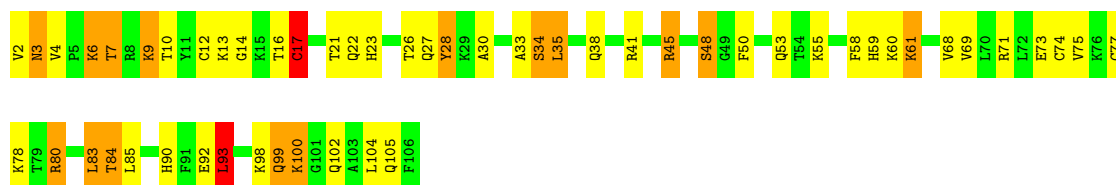
- Molecule 77: Large ribosomal subunit protein eL41B

Chain q1: 28% 56% 16% .



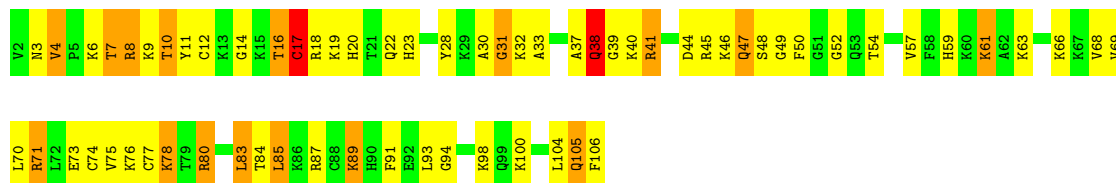
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 49% 35% 14% .



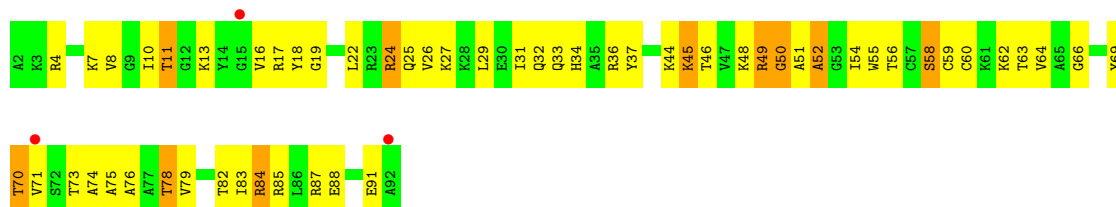
• Molecule 78: 60S ribosomal protein L42-A

Chain q2: 38% 45% 15% .



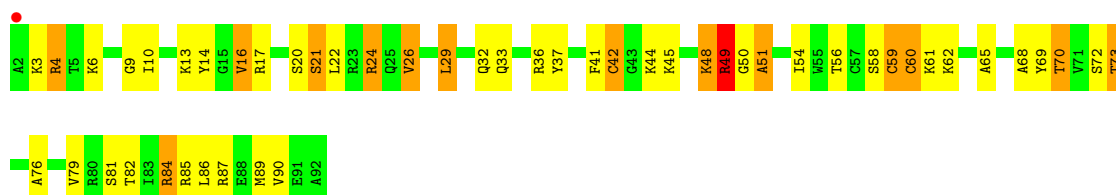
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3: 3% 38% 51% 11%



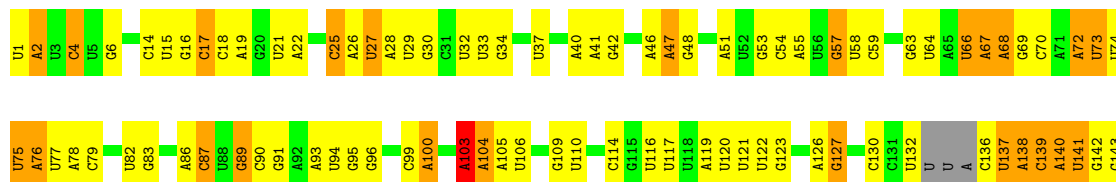
• Molecule 79: 60S ribosomal protein L43-A

Chain q3: % 45% 38% 15% .

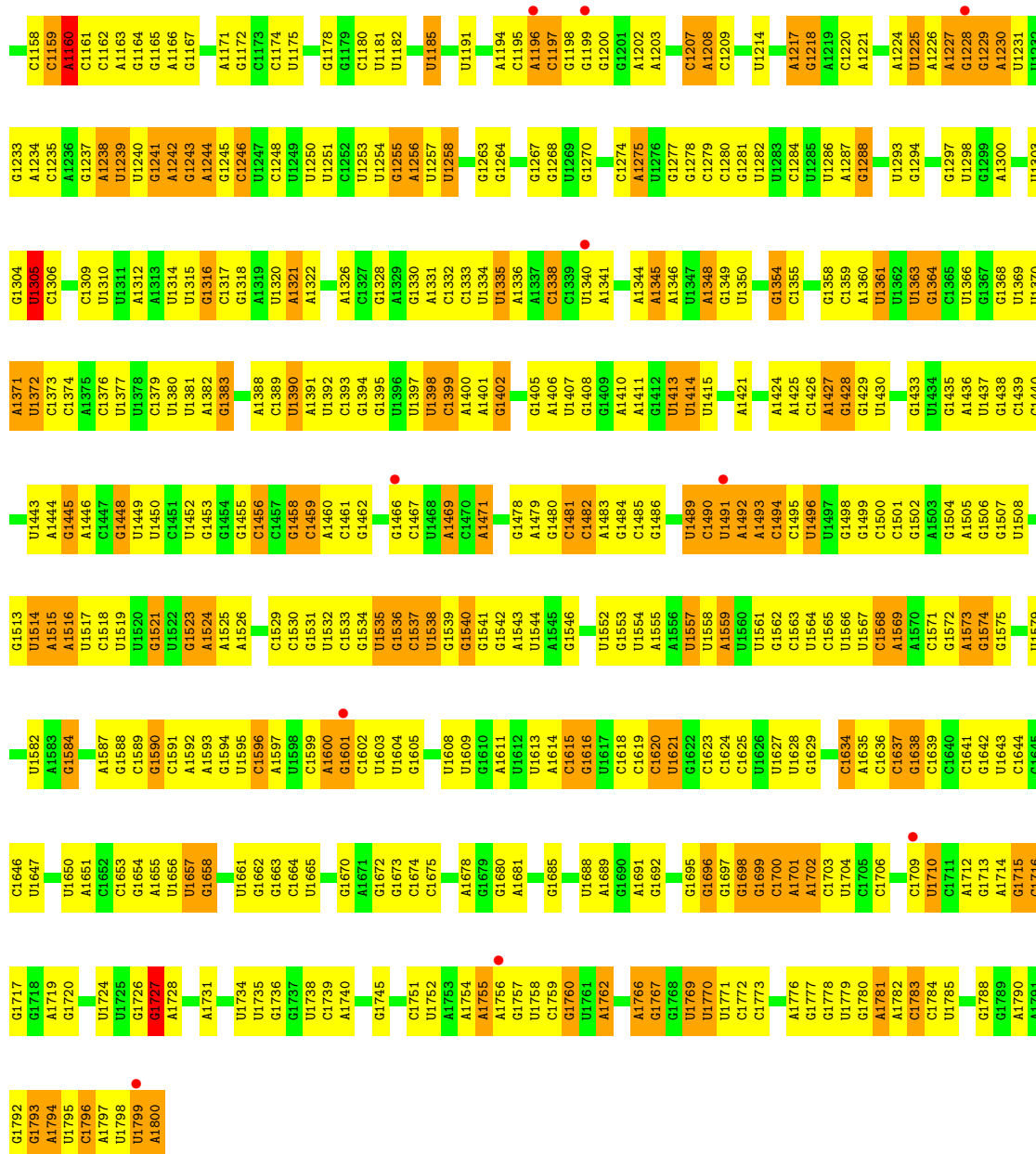


• Molecule 80: 18S ribosomal RNA

Chain 6: % 31% 49% 19% .



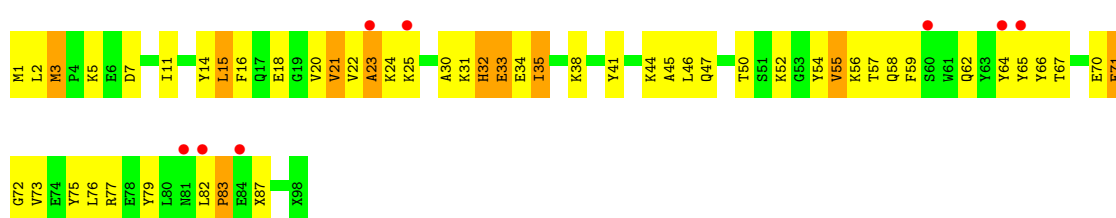
U1084	G1085	A1086	A1087	A1088	A1091	A1092	A1093	G1094	G1095	C1096	A1097	A1098	U1099	G1100	A1101	G1102	G1103	U1104	C1105	U1106	G1107	G1108	G1109	U1115	G1118	G1119	G1120	C1121	G1126	U1129	G1130	A1131	A1132	A1133	C1134	U1136	U1137	A1138	A1139	C1140	G1141	A1142	A1143	U1144	U1145	A1146	G1150	A1151	A1152	G1153	G1154	G1155																																																																																																																																																																																																																																																																																																																																																																																							
A1020	C1021	A1026	A1027	A1028	U1029	A1030	U1031	C1032	C1033	C1034	C1035	A1036	U1037	U1038	A1039	G1101	G1040	G1041	U1042	A1043	U1044	C1045	G1046	U1049	G1050	U1051	U1052	G1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	A1061	A1062	U1063	G1064	A1065	C1066	C1067	C1068	A1069	C1070	U1071	G1072	G1073	G1074	C1075	C1076	C1077	U1078	U1079	U1080	A1081	C1082	G1083																																																																																																																																																																																																																																																																																																																																																																																	
U958	U959	U960	U961	C962	A963	U964	U965	U966	U967	U968	C969	A970	A971	G972	A973	A974	G975	G976	A977	A978	A979	G980	U981	U982	A983	G987	A988	U989	G990	C991	A992	A993	A994	A995	U996	C997	A998	U999	C1000	A1001	G1002	A1003	U1004	A1005	C1006	C1007	G1008	U1009	C1010	G1011	U1012	A1013	C1014	U1015	G1016	U1017	U1018	A1019																																																																																																																																																																																																																																																																																																																																																																																	
U893	U894	G895	U898	U899	A900	G901	G902	A905	A906	G907	A907	U911	U912	U913	G914	G915	U916	U917	U918	A919	U920	U921	G922	A923	A924	G925	A926	U927	U928	A929	A930	C931	U932	A933	C934	U935	G936	C937	G938	A1001	A939	A940	A941	G942	C943	A944	U945	U946	U947	G948	C949	C950	A951	A952	A955	U956	U957	G958																																																																																																																																																																																																																																																																																																																																																																																	
U826	C827	U828	A829	U830	U831	U832	U833	U834	U835	U836	G837	G838	U839	U840	U841	C842	U843	A844	G845	A846	U847	U850	U851	C852	A856	U857	U858	U859	U860	U861	A862	U863	U864	G867	G868	G871	G872	U873	C874	G875	G876	G877	G878	G879	C880	A881	A884	G885	U886	A887	U888	A891	A892																																																																																																																																																																																																																																																																																																																																																																																						
A760	G761	A762	G765	U766	U767	C768	A769	A770	A771	C772	G773	A774	U775	U776	G777	G778	U779	A780	U781	U782	U783	U784	U785	C786	U787	U788	A789	U792	U793	A794	U795	A796	U800	G801	A804	U805	A806	U807	U808	A809	G810	A811	A812	U813	A814	G815	G816	G819	U820	U886	A887	U888	U891	U892	U893																																																																																																																																																																																																																																																																																																																																																																																				
C686	G687	G688	G689	G690	C691	U694	U695	U696	C697	U698	U699	C700	U701	U702	C703	C704	U709	U710	U711	U712	A713	G714	U717	U718	U719	U720	U721	U722	U723	U726	U727	U728	U729	U730	U731	U738	U739	U740	C741	U742	U745	U748	U751	A752	A753	U754	A755	A756	A757	U758	U759																																																																																																																																																																																																																																																																																																																																																																																								
A620	A621	A622	A623	G624	G625	U626	C627	G628	U632	U633	G634	A635	A636	C637	U638	U639	U640	C646	G647	G648	U649	U650	G651	G652	U653	U654	U655	U656	U657	C658	C659	G660	A661	U662	U663	U664	U665	U666	U667	G668	G669	U670	G	U	A673	C674	U675	G676	G677	U679	U680	U681	C682	C683	A684	A685																																																																																																																																																																																																																																																																																																																																																																																			
C586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	C614	U617	U618	A619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759																																																																																																																																																																																																																																																																		
U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619																																																																																																																																																																																																																																																																																																				
C484	A485	G486	C487	G488	U489	U490	C491	A492	U493	U494	C495	C496	G497	G498	C499	C500	U501	U502	U503	U504	A505	A506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619																																																																																																																																																																																																																																																																																																				
U409	A410	C411	C412	U413	U414	C415	A416	A417	C418	U419	C420	A421	C422	C423	C424	C425	C426	C427	A428	C434	A437	A438	U439	U440	C444	C445	U446	U447	C448	C449	A452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	C467	A468	C469	A470	A471	U472	A475	U476	A477	A478	C479	C480	A481	U482	A483																																																																																																																																																																																																																																																																																																																																																																																			
G336	G337	C338	C339	C340	A341	A344	U348	U349	U350	C351	A352	G355	C356	C357	U358	A359	A360	C361	C362	C363	A369	A370	U374	U375	C376	C377	U380	C381	C382	U383	U384	U385	U386	U387	U388	U389	U390	C393	A397	C398	A399	A400	A401	C402	G403	C404	C405	U406	A407	C408																																																																																																																																																																																																																																																																																																																																																																																									
U272	G273	G274	C275	C276	U277	U278	U279	U280	C281	C282	U283	C284	C285	C286	C287	C288	C289	C290	C291	U292	U293	C294	A295	A296	A297	A298	A299	A300	A301	U302	U303	U304	C305	U306	C307	C308	C309	C310	U311	U312	U313	C314	A315	A316	C317	U318	U319	U320	C321	C322	C323	C324	C325	C326	U327	A328	C329	G330	C331	C332	C333	U334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C



- Molecule 81: Small ribosomal subunit protein eS10A,40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10-A



Chain c0:



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

Chain A:  67% 33%

C3401
C3402
A3403

- Molecule 86: Peptidyl-tRNA analog ACCA-Pro

Chain B:  67% 33%

C3401
C3402
A3403

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	82.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OHX, 8AN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.43	0/42467	0.67	4/66169 (0.0%)
2	S0	0.54	1/1617 (0.1%)	0.69	0/2215
2	s0	0.49	0/1623	0.78	1/2222 (0.0%)
3	S1	0.34	0/1735	0.66	1/2335 (0.0%)
3	s1	0.45	0/1748	0.67	0/2352
4	S2	0.44	0/1665	0.72	0/2263
4	s2	0.59	0/1665	0.82	0/2263
5	S3	0.41	0/1759	0.65	0/2368
5	s3	0.43	0/1759	0.65	0/2368
6	S4	0.42	0/2109	0.74	0/2839
6	s4	0.52	0/2109	0.81	0/2839
7	S5	0.34	0/1629	0.63	0/2202
7	s5	0.40	0/1629	0.69	0/2202
8	S6	0.41	0/1823	0.65	0/2439
8	s6	0.50	0/1779	0.78	1/2379 (0.0%)
9	S7	0.40	0/1506	0.73	0/2028
9	s7	0.46	0/1516	0.73	0/2043
10	S8	0.46	0/1514	0.71	0/2021
10	s8	0.56	0/1514	0.82	0/2021
11	S9	0.44	0/1519	0.71	0/2035
11	s9	0.51	0/1519	0.77	0/2035
12	C0	0.35	0/789	0.85	3/1067 (0.3%)
13	C1	0.48	0/1239	0.71	0/1673
13	c1	0.58	0/1194	0.86	0/1610
14	C2	0.38	0/898	0.76	0/1220
14	c2	0.30	0/898	0.64	0/1220
15	C3	0.41	0/1215	0.69	5/1638 (0.3%)
15	c3	0.52	0/1215	0.75	0/1638
16	C4	0.34	0/901	0.67	0/1217
16	c4	0.46	0/960	0.70	0/1290
17	C5	0.43	0/998	0.71	0/1341
17	c5	0.48	0/1060	0.78	0/1426

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	C6	0.39	0/1125	0.74	3/1510 (0.2%)
18	c6	0.48	1/1131 (0.1%)	0.74	1/1518 (0.1%)
19	C7	0.42	0/935	0.74	2/1254 (0.2%)
19	c7	0.45	0/914	0.77	0/1224
20	C8	0.43	0/1211	0.71	0/1628
20	c8	0.42	0/1211	0.71	0/1628
21	C9	0.41	0/1130	0.71	0/1517
21	c9	0.43	0/1130	0.66	0/1517
22	D0	0.48	0/865	0.73	0/1169
22	d0	0.43	0/892	0.75	0/1205
23	D1	0.40	0/693	0.65	0/935
23	d1	0.56	0/693	0.83	0/935
24	D2	0.47	0/1038	0.74	0/1395
24	d2	0.57	0/1038	0.82	0/1395
25	D3	0.51	0/1139	0.79	0/1518
25	d3	0.61	0/1139	0.84	0/1518
26	D4	0.42	0/1087	0.69	0/1449
26	d4	0.52	0/1087	0.84	0/1449
27	D5	0.39	0/571	0.77	0/768
27	d5	0.42	0/566	0.64	0/761
28	D6	0.41	0/782	0.81	1/1047 (0.1%)
28	d6	0.52	0/782	0.75	0/1047
29	D7	0.41	0/620	0.65	0/838
29	d7	0.43	0/620	0.76	0/838
30	D8	0.34	0/499	0.63	0/670
30	d8	0.40	0/499	0.69	0/670
31	D9	0.50	0/452	0.79	0/600
31	d9	0.45	0/452	0.70	0/600
32	E0	0.43	0/483	0.63	0/643
32	e0	0.51	0/499	0.86	0/665
33	E1	0.42	0/577	0.91	0/770
33	e1	0.43	0/619	0.91	2/822 (0.2%)
34	SR	0.36	0/2490	0.60	0/3389
34	sR	0.35	0/2495	0.60	0/3395
35	SM	0.49	0/984	0.80	0/1323
36	1	0.59	0/75394	0.81	24/117545 (0.0%)
36	5	0.64	18/75414 (0.0%)	0.85	55/117575 (0.0%)
37	3	0.54	0/2883	0.74	0/4491
37	7	0.62	2/2883 (0.1%)	0.84	0/4491
38	4	0.58	0/3746	0.80	0/5832
38	8	0.56	1/3746 (0.0%)	0.77	0/5832
39	L2	0.56	0/1948	0.83	0/2617
39	l2	0.60	0/1946	0.90	0/2614

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	L3	0.61	1/3146 (0.0%)	0.88	0/4228
40	l3	0.69	0/3146	0.89	0/4228
41	L4	0.66	2/2800 (0.1%)	0.97	4/3790 (0.1%)
41	l4	0.63	1/2800 (0.0%)	0.89	0/3790
42	L5	0.50	0/2425	0.76	0/3271
42	l5	0.63	0/2408	0.84	0/3248
43	L6	0.58	0/1260	0.82	0/1694
43	l6	0.60	0/1269	0.84	0/1705
44	L7	0.62	0/1821	0.86	2/2451 (0.1%)
44	l7	0.65	0/1828	0.90	3/2461 (0.1%)
45	L8	0.43	0/1836	0.69	0/2481
45	l8	0.43	0/1795	0.70	0/2429
46	L9	0.53	0/1539	0.83	2/2073 (0.1%)
46	l9	0.64	0/1539	0.84	0/2073
47	M0	0.70	1/1741 (0.1%)	0.87	0/2335
47	m0	0.76	1/1758 (0.1%)	0.88	0/2358
48	M1	0.48	0/1374	0.76	0/1842
48	m1	0.61	0/1374	0.82	0/1842
49	M3	0.59	0/1568	0.86	0/2106
49	m3	0.57	0/1573	0.85	0/2113
50	M4	0.58	0/1068	0.83	0/1438
50	m4	0.65	0/1074	0.83	0/1446
51	M5	0.61	0/1757	0.85	1/2354 (0.0%)
51	m5	0.52	0/1757	0.81	2/2354 (0.1%)
52	M6	0.68	0/1585	0.89	2/2128 (0.1%)
52	m6	0.75	0/1585	0.91	0/2128
53	M7	0.64	0/1443	0.90	0/1944
53	m7	0.72	0/1250	0.89	0/1683
54	M8	0.61	0/1465	0.91	1/1965 (0.1%)
54	m8	0.62	0/1465	0.90	0/1965
55	M9	0.47	0/1538	0.71	0/2050
55	m9	0.53	0/1538	0.73	0/2050
56	N0	0.58	0/1481	0.81	1/1990 (0.1%)
56	n0	0.64	0/1481	0.87	0/1990
57	N1	0.58	0/1300	0.85	0/1743
57	n1	0.63	0/1300	0.81	0/1743
58	N2	0.39	0/812	0.64	0/1099
58	n2	0.46	0/794	0.70	0/1076
59	N3	0.62	0/1018	0.85	0/1369
59	n3	0.74	0/1018	0.98	3/1369 (0.2%)
60	N4	0.54	0/712	0.81	0/958
60	n4	0.61	0/1052	0.85	0/1398
61	N5	0.52	0/979	0.74	0/1321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	n5	0.50	0/974	0.76	0/1314
62	N6	0.60	0/1004	0.92	0/1341
62	n6	0.56	0/1004	0.80	0/1341
63	N7	0.40	0/1118	0.65	0/1497
63	n7	0.40	0/1118	0.66	0/1497
64	N8	0.65	0/1204	0.92	2/1612 (0.1%)
64	n8	0.69	1/1204 (0.1%)	0.93	2/1612 (0.1%)
65	N9	0.62	0/473	0.93	0/629
65	n9	0.68	0/473	1.03	0/629
66	O0	0.38	0/751	0.58	0/1008
66	o0	0.45	0/775	0.70	0/1040
67	O1	0.54	0/890	0.78	0/1196
67	o1	0.65	0/897	0.84	0/1205
68	O2	0.67	0/1041	0.98	0/1394
68	o2	0.65	0/1041	0.91	0/1394
69	O3	0.72	0/868	0.94	0/1168
69	o3	0.71	0/868	0.90	0/1168
70	O4	0.49	0/890	0.72	0/1189
70	o4	0.51	0/890	0.75	0/1189
71	O5	0.54	0/978	0.77	0/1301
71	o5	0.51	0/974	0.71	0/1297
72	O6	0.54	0/778	0.80	0/1034
72	o6	0.48	0/777	0.88	0/1033
73	O7	0.57	0/696	0.87	0/923
73	o7	0.61	0/696	0.90	0/923
74	O8	0.43	0/618	0.66	0/826
74	o8	0.43	0/614	0.67	0/822
75	O9	0.67	0/443	0.89	0/588
75	o9	0.66	0/443	0.78	0/588
76	Q0	0.59	0/423	0.83	0/562
76	q0	0.79	0/423	1.04	0/562
77	Q1	0.60	0/234	0.76	0/300
77	q1	0.69	0/234	0.92	0/300
78	Q2	0.72	1/860 (0.1%)	0.88	0/1136
78	q2	0.70	1/860 (0.1%)	0.85	3/1136 (0.3%)
79	Q3	0.58	0/701	0.84	0/934
79	q3	0.59	0/701	0.82	1/934 (0.1%)
80	6	0.53	8/42790 (0.0%)	0.76	26/66673 (0.0%)
81	c0	0.34	0/718	0.67	1/968 (0.1%)
82	sM	0.52	0/481	0.74	0/644
84	p0	0.37	0/1092	0.64	0/1474
86	A	0.56	0/43	0.77	0/64
86	B	0.56	0/43	0.77	0/64

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.56	40/430554 (0.0%)	0.79	159/632173 (0.0%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	m7	0	1
55	m9	0	1
56	N0	0	2
56	n0	0	2
59	n3	0	2
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 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S0	95	ALA	C-N	13.86	1.62	1.33
47	m0	92	HIS	C-N	-10.65	1.08	1.33
36	5	2707	C	C4-N4	9.91	1.53	1.33
41	l4	349	THR	C-N	8.99	1.52	1.33
78	Q2	17	CYS	CB-SG	8.62	2.09	1.81

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	3144	G	O5'-P-OP1	-15.50	61.49	108.00
80	6	403	G	P-O3'-C3'	-13.86	99.42	120.20
36	5	3083	G	OP1-P-O3'	10.37	139.11	108.00
12	C0	88	PRO	N-CA-CB	10.25	114.02	103.25
36	5	2246	G	P-O3'-C3'	-10.09	105.06	120.20

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide

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Mol	Chain	Res	Type	Group
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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37970	0	19103	1244	0
2	S0	1577	0	1567	99	0
2	s0	1583	0	1578	128	0
3	S1	1709	0	1784	135	0
3	s1	1722	0	1793	105	0
4	S2	1635	0	1723	97	0
4	s2	1635	0	1723	105	0
5	S3	1734	0	1817	84	0
5	s3	1734	0	1817	86	0
6	S4	2068	0	2154	105	0
6	s4	2068	0	2154	135	0
7	S5	1609	0	1675	85	0
7	s5	1609	0	1675	78	0
8	S6	1799	0	1879	91	0
8	s6	1755	0	1846	84	0
9	S7	1481	0	1572	92	0
9	s7	1491	0	1578	80	0
10	S8	1489	0	1525	67	0
10	s8	1489	0	1525	68	0
11	S9	1494	0	1573	89	0
11	s9	1494	0	1573	104	0
12	C0	772	0	727	41	0
13	C1	1213	0	1257	69	0
13	c1	1168	0	1233	70	0
14	C2	890	0	887	47	0
14	c2	890	0	887	33	0
15	C3	1192	0	1255	60	0
15	c3	1192	0	1255	61	0
16	C4	891	0	883	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	c4	949	0	985	67	0
17	C5	977	0	1002	64	0
17	c5	1039	0	1050	75	0
18	C6	1105	0	1166	79	0
18	c6	1111	0	1171	77	0
19	C7	926	0	930	49	0
19	c7	906	0	909	59	0
20	C8	1192	0	1222	77	0
20	c8	1192	0	1222	78	0
21	C9	1112	0	1124	74	0
21	c9	1112	0	1124	60	0
22	D0	855	0	917	53	0
22	d0	882	0	939	58	0
23	D1	684	0	672	41	0
23	d1	684	0	672	64	0
24	D2	1021	0	1060	53	0
24	d2	1021	0	1060	63	0
25	D3	1121	0	1196	66	0
25	d3	1121	0	1196	57	0
26	D4	1073	0	1132	47	0
26	d4	1073	0	1132	66	0
27	D5	563	0	603	42	0
27	d5	558	0	598	33	0
28	D6	769	0	814	64	0
28	d6	769	0	814	47	0
29	D7	610	0	631	27	0
29	d7	610	0	632	30	0
30	D8	497	0	535	27	0
30	d8	497	0	535	21	0
31	D9	442	0	428	24	0
31	d9	442	0	427	20	0
32	E0	475	0	525	21	0
32	e0	491	0	542	28	0
33	E1	566	0	601	38	0
33	e1	608	0	657	39	0
34	SR	2437	0	2386	104	0
34	sR	2442	0	2392	116	0
35	SM	1104	0	978	59	0
36	1	67355	0	33836	2003	0
36	5	67376	0	33839	1957	0
37	3	2579	0	1304	79	0
37	7	2579	0	1303	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	4	3353	0	1695	112	0
38	8	3353	0	1695	116	0
39	L2	1914	0	1981	115	0
39	l2	1912	0	1976	122	0
40	L3	3075	0	3142	169	0
40	l3	3075	0	3142	189	0
41	L4	2748	0	2858	182	0
41	l4	2748	0	2859	171	0
42	L5	2375	0	2325	124	0
42	l5	2359	0	2311	142	0
43	L6	1239	0	1326	66	0
43	l6	1248	0	1339	63	0
44	L7	1784	0	1862	114	0
44	l7	1791	0	1869	81	0
45	L8	1804	0	1877	88	0
45	l8	1763	0	1819	89	0
46	L9	1518	0	1587	105	0
46	l9	1518	0	1587	85	0
47	M0	1705	0	1736	113	0
47	m0	1722	0	1755	111	0
48	M1	1353	0	1383	88	0
48	m1	1353	0	1383	60	0
49	M3	1543	0	1608	93	0
49	m3	1548	0	1613	94	0
50	M4	1053	0	1149	72	0
50	m4	1059	0	1154	41	0
51	M5	1720	0	1779	93	0
51	m5	1720	0	1779	109	0
52	M6	1555	0	1658	75	0
52	m6	1555	0	1659	66	0
53	M7	1420	0	1437	81	0
53	m7	1227	0	1236	75	0
54	M8	1441	0	1542	79	0
54	m8	1441	0	1543	89	0
55	M9	1521	0	1617	71	0
55	m9	1521	0	1617	72	0
56	N0	1445	0	1487	81	0
56	n0	1445	0	1487	78	0
57	N1	1276	0	1323	64	0
57	n1	1276	0	1323	72	0
58	N2	796	0	812	35	0
58	n2	778	0	791	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	N3	1003	0	1047	50	0
59	n3	1003	0	1048	58	0
60	N4	699	0	640	26	0
60	n4	1038	0	1071	28	0
61	N5	964	0	1025	50	0
61	n5	959	0	1023	49	0
62	N6	993	0	1081	51	0
62	n6	993	0	1081	59	0
63	N7	1092	0	1155	65	0
63	n7	1092	0	1155	60	0
64	N8	1173	0	1215	73	0
64	n8	1173	0	1214	95	0
65	N9	462	0	491	25	0
65	n9	462	0	491	26	0
66	O0	743	0	797	40	0
66	o0	767	0	816	43	0
67	O1	876	0	911	44	0
67	o1	883	0	918	34	0
68	O2	1020	0	1090	62	0
68	o2	1020	0	1089	69	0
69	O3	850	0	880	44	0
69	o3	850	0	880	40	0
70	O4	880	0	945	58	0
70	o4	880	0	945	51	0
71	O5	969	0	1078	68	0
71	o5	965	0	1067	52	0
72	O6	771	0	849	49	0
72	o6	770	0	846	54	0
73	O7	681	0	683	43	0
73	o7	681	0	682	46	0
74	O8	612	0	682	28	0
74	o8	608	0	671	30	0
75	O9	436	0	475	28	0
75	o9	436	0	475	19	0
76	Q0	417	0	456	24	0
76	q0	417	0	456	26	0
77	Q1	233	0	284	7	0
77	q1	233	0	284	12	0
78	Q2	847	0	915	42	0
78	q2	847	0	914	58	0
79	Q3	694	0	734	45	0
79	q3	694	0	734	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	6	38260	0	19242	1256	0
81	c0	762	0	691	36	0
82	sM	681	0	544	30	0
83	m2	750	0	178	9	0
84	p0	1077	0	1041	45	0
85	p1	235	0	52	3	0
85	p2	230	0	49	0	0
86	A	62	0	33	16	0
86	B	62	0	32	12	0
87	1	2877	0	0	274	0
87	2	1323	0	0	121	0
87	3	84	0	0	5	0
87	4	119	0	0	8	0
87	5	2905	0	0	214	0
87	6	1386	0	0	115	0
87	7	84	0	0	1	0
87	8	147	0	0	17	0
87	C3	7	0	0	2	0
87	C5	7	0	0	3	0
87	C8	14	0	0	1	0
87	D9	7	0	0	1	0
87	L3	21	0	0	4	0
87	L4	7	0	0	2	0
87	L5	7	0	0	0	0
87	M0	28	0	0	11	0
87	M5	7	0	0	1	0
87	M7	7	0	0	0	0
87	M8	7	0	0	0	0
87	M9	21	0	0	2	0
87	N8	7	0	0	0	0
87	N9	7	0	0	1	0
87	O1	7	0	0	1	0
87	O3	7	0	0	0	0
87	O7	14	0	0	8	0
87	Q2	7	0	0	2	0
87	S2	7	0	0	2	0
87	S8	7	0	0	2	0
87	SR	7	0	0	0	0
87	c1	7	0	0	0	0
87	c3	7	0	0	2	0
87	c5	14	0	0	9	0
87	c8	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	d9	7	0	0	0	0
87	l2	7	0	0	0	0
87	l3	14	0	0	2	0
87	l4	14	0	0	3	0
87	l5	21	0	0	3	0
87	l9	7	0	0	0	0
87	m0	28	0	0	5	0
87	m1	7	0	0	1	0
87	m4	7	0	0	0	0
87	m5	14	0	0	0	0
87	m7	7	0	0	0	0
87	m9	7	0	0	0	0
87	n1	7	0	0	0	0
87	n3	14	0	0	2	0
87	n9	7	0	0	1	0
87	o3	7	0	0	0	0
87	o7	14	0	0	1	0
87	o9	7	0	0	0	0
87	q1	7	0	0	0	0
87	q2	7	0	0	3	0
87	s1	14	0	0	3	0
87	s4	7	0	0	1	0
87	s8	7	0	0	1	0
87	sR	7	0	0	0	0
88	1	698	0	0	0	0
88	2	170	0	0	0	0
88	3	18	0	0	0	0
88	4	28	0	0	0	0
88	5	759	0	0	0	0
88	6	235	0	0	0	0
88	7	28	0	0	0	0
88	8	19	0	0	0	0
88	C1	2	0	0	0	0
88	C5	1	0	0	0	0
88	C8	1	0	0	0	0
88	D0	1	0	0	0	0
88	D4	1	0	0	0	0
88	D6	1	0	0	0	0
88	D9	3	0	0	0	0
88	E1	1	0	0	0	0
88	L2	3	0	0	0	0
88	L3	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	L4	7	0	0	0	0
88	L7	3	0	0	0	0
88	L8	1	0	0	0	0
88	M0	5	0	0	0	0
88	M1	2	0	0	0	0
88	M3	3	0	0	0	0
88	M4	1	0	0	0	0
88	M5	4	0	0	0	0
88	M6	4	0	0	0	0
88	M7	10	0	0	0	0
88	M8	3	0	0	0	0
88	M9	2	0	0	0	0
88	N0	2	0	0	0	0
88	N1	1	0	0	0	0
88	N3	3	0	0	0	0
88	N6	2	0	0	0	0
88	N8	7	0	0	0	0
88	N9	1	0	0	0	0
88	O1	5	0	0	0	0
88	O2	4	0	0	0	0
88	O3	2	0	0	0	0
88	O4	1	0	0	0	0
88	O5	2	0	0	0	0
88	O7	6	0	0	0	0
88	Q0	2	0	0	0	0
88	Q2	3	0	0	0	0
88	S1	1	0	0	0	0
88	S2	1	0	0	0	0
88	S4	2	0	0	0	0
88	S6	1	0	0	0	0
88	S8	1	0	0	0	0
88	SM	1	0	0	0	0
88	c6	2	0	0	0	0
88	c7	1	0	0	0	0
88	c8	4	0	0	0	0
88	c9	3	0	0	0	0
88	d2	1	0	0	0	0
88	d3	2	0	0	0	0
88	d4	2	0	0	0	0
88	d5	1	0	0	0	0
88	d9	2	0	0	0	0
88	l2	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	l3	13	0	0	0	0
88	l4	1	0	0	0	0
88	l5	6	0	0	0	0
88	l7	7	0	0	0	0
88	l8	1	0	0	0	0
88	l9	3	0	0	0	0
88	m0	1	0	0	0	0
88	m3	1	0	0	0	0
88	m4	1	0	0	0	0
88	m5	3	0	0	0	0
88	m6	4	0	0	0	0
88	m7	8	0	0	0	0
88	m8	4	0	0	0	0
88	m9	1	0	0	0	0
88	n0	5	0	0	0	0
88	n1	3	0	0	0	0
88	n3	3	0	0	0	0
88	n6	1	0	0	0	0
88	n8	7	0	0	0	0
88	n9	2	0	0	0	0
88	o2	3	0	0	0	0
88	o3	4	0	0	0	0
88	o4	1	0	0	0	0
88	o6	1	0	0	0	0
88	o7	1	0	0	0	0
88	p0	1	0	0	0	0
88	q0	1	0	0	0	0
88	q1	2	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
88	s1	1	0	0	0	0
88	s4	1	0	0	0	0
88	s6	2	0	0	0	0
88	s8	4	0	0	0	0
88	sM	2	0	0	0	0
89	D6	1	0	0	0	0
89	D7	1	0	0	0	0
89	D9	1	0	0	0	0
89	E1	1	0	0	0	0
89	O7	1	0	0	0	0
89	Q0	1	0	0	1	0
89	Q2	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	Q3	1	0	0	0	0
89	d6	1	0	0	0	0
89	d7	1	0	0	0	0
89	d9	1	0	0	0	0
89	e1	1	0	0	0	0
89	o7	1	0	0	0	0
89	q0	1	0	0	1	0
89	q2	1	0	0	0	0
89	q3	1	0	0	0	0
90	A	7	0	7	0	0
90	B	7	0	7	2	0
All	All	414270	0	297569	14727	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 14727 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:q2:17:CYS:SG	78:q2:17:CYS:CB	2.01	1.47
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.09	1.39
73:O7:87:SER:O	87:O7:102:OHX:N3	1.78	1.16
78:Q2:17:CYS:SG	89:Q2:501:ZN:ZN	1.39	1.11
78:Q2:17:CYS:CB	89:Q2:501:ZN:ZN	1.30	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S0	204/206 (99%)	150 (74%)	34 (17%)	20 (10%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	9
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%)	1	12
10	s8	184/199 (92%)	150 (82%)	27 (15%)	7 (4%)	2	16
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
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	0
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	18
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	9
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	6
24	D2	127/129 (98%)	102 (80%)	21 (16%)	4 (3%)	3	20
24	d2	127/129 (98%)	100 (79%)	25 (20%)	2 (2%)	7	31
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	26
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
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%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	SR	316/318 (99%)	275 (87%)	31 (10%)	10 (3%)	3	19
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	13
39	l2	250/252 (99%)	201 (80%)	39 (16%)	10 (4%)	2	15
40	L3	384/386 (100%)	323 (84%)	44 (12%)	17 (4%)	2	13
40	l3	384/386 (100%)	331 (86%)	35 (9%)	18 (5%)	2	12
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%)	4	24
43	L6	152/175 (87%)	131 (86%)	18 (12%)	3 (2%)	6	27
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%)	2	17
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	14
46	l9	189/191 (99%)	156 (82%)	25 (13%)	8 (4%)	2	14
47	M0	207/220 (94%)	166 (80%)	30 (14%)	11 (5%)	1	10
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%)	0	5
50	m4	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	8	32
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	20
52	M6	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	12	40
52	m6	195/197 (99%)	179 (92%)	13 (7%)	3 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	M7	181/183 (99%)	144 (80%)	26 (14%)	11 (6%)	1	9
53	m7	153/183 (84%)	127 (83%)	24 (16%)	2 (1%)	9	35
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%)	24	55
56	N0	170/172 (99%)	149 (88%)	16 (9%)	5 (3%)	3	21
56	n0	170/172 (99%)	150 (88%)	17 (10%)	3 (2%)	6	29
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	23
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	14
59	N3	134/136 (98%)	118 (88%)	14 (10%)	2 (2%)	8	32
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	11
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	15
62	n6	124/126 (98%)	108 (87%)	7 (6%)	9 (7%)	1	6
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%)	2	17
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	26
66	o0	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	6	27
67	O1	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	2	12
67	o1	107/109 (98%)	91 (85%)	11 (10%)	5 (5%)	2	12
68	O2	125/127 (98%)	94 (75%)	22 (18%)	9 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	21
69	o3	104/106 (98%)	92 (88%)	6 (6%)	6 (6%)	1	9
70	O4	110/112 (98%)	94 (86%)	12 (11%)	4 (4%)	2	17
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	18
72	O6	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	0	2
72	o6	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	0	5
73	O7	85/87 (98%)	67 (79%)	17 (20%)	1 (1%)	10	37
73	o7	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	3	18
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	26
75	o9	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
76	Q0	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	2	15
76	q0	50/52 (96%)	41 (82%)	8 (16%)	1 (2%)	6	27
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%)	1	12
78	q2	103/105 (98%)	90 (87%)	8 (8%)	5 (5%)	1	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	18
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	11
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

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/173 (95%)	124 (76%)	40 (24%)	1	3
2	s0	165/173 (95%)	126 (76%)	39 (24%)	1	4
3	S1	191/192 (100%)	153 (80%)	38 (20%)	1	6
3	s1	192/192 (100%)	149 (78%)	43 (22%)	1	5
4	S2	176/176 (100%)	133 (76%)	43 (24%)	1	3
4	s2	176/176 (100%)	129 (73%)	47 (27%)	0	2
5	S3	182/182 (100%)	142 (78%)	40 (22%)	1	5
5	s3	182/182 (100%)	146 (80%)	36 (20%)	1	6
6	S4	221/221 (100%)	172 (78%)	49 (22%)	1	5
6	s4	221/221 (100%)	172 (78%)	49 (22%)	1	5
7	S5	173/173 (100%)	143 (83%)	30 (17%)	2	9
7	s5	173/173 (100%)	137 (79%)	36 (21%)	1	6
8	S6	188/193 (97%)	147 (78%)	41 (22%)	1	5
8	s6	187/193 (97%)	147 (79%)	40 (21%)	1	5
9	S7	165/166 (99%)	132 (80%)	33 (20%)	1	6
9	s7	165/166 (99%)	126 (76%)	39 (24%)	1	4
10	S8	150/160 (94%)	124 (83%)	26 (17%)	2	9
10	s8	150/160 (94%)	124 (83%)	26 (17%)	2	9
11	S9	158/158 (100%)	123 (78%)	35 (22%)	1	5
11	s9	158/158 (100%)	123 (78%)	35 (22%)	1	5
12	C0	77/89 (86%)	61 (79%)	16 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	C1	129/136 (95%)	110 (85%)	19 (15%)	3	14
13	c1	129/136 (95%)	100 (78%)	29 (22%)	1	5
14	C2	88/100 (88%)	62 (70%)	26 (30%)	0	2
14	c2	88/100 (88%)	67 (76%)	21 (24%)	1	4
15	C3	127/127 (100%)	96 (76%)	31 (24%)	1	3
15	c3	127/127 (100%)	100 (79%)	27 (21%)	1	5
16	C4	81/97 (84%)	58 (72%)	23 (28%)	0	2
16	c4	97/97 (100%)	63 (65%)	34 (35%)	0	1
17	C5	101/111 (91%)	78 (77%)	23 (23%)	1	4
17	c5	103/111 (93%)	87 (84%)	16 (16%)	2	12
18	C6	117/118 (99%)	93 (80%)	24 (20%)	1	6
18	c6	118/118 (100%)	92 (78%)	26 (22%)	1	5
19	C7	94/113 (83%)	74 (79%)	20 (21%)	1	5
19	c7	92/113 (81%)	75 (82%)	17 (18%)	1	7
20	C8	128/128 (100%)	93 (73%)	35 (27%)	0	2
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	5
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0	2
21	c9	115/115 (100%)	94 (82%)	21 (18%)	2	7
22	D0	100/103 (97%)	73 (73%)	27 (27%)	0	2
22	d0	103/103 (100%)	70 (68%)	33 (32%)	0	1
23	D1	74/74 (100%)	58 (78%)	16 (22%)	1	5
23	d1	74/74 (100%)	60 (81%)	14 (19%)	1	7
24	D2	110/110 (100%)	84 (76%)	26 (24%)	1	4
24	d2	110/110 (100%)	89 (81%)	21 (19%)	1	7
25	D3	119/119 (100%)	93 (78%)	26 (22%)	1	5
25	d3	119/119 (100%)	95 (80%)	24 (20%)	1	6
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1	7
26	d4	112/112 (100%)	85 (76%)	27 (24%)	1	3
27	D5	61/61 (100%)	43 (70%)	18 (30%)	0	2
27	d5	61/61 (100%)	49 (80%)	12 (20%)	1	6
28	D6	83/83 (100%)	64 (77%)	19 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	d6	83/83 (100%)	68 (82%)	15 (18%)	2	8
29	D7	70/70 (100%)	60 (86%)	10 (14%)	3	14
29	d7	70/70 (100%)	63 (90%)	7 (10%)	7	27
30	D8	56/56 (100%)	43 (77%)	13 (23%)	1	4
30	d8	56/56 (100%)	40 (71%)	16 (29%)	0	2
31	D9	47/47 (100%)	34 (72%)	13 (28%)	0	2
31	d9	47/47 (100%)	39 (83%)	8 (17%)	2	10
32	E0	51/53 (96%)	45 (88%)	6 (12%)	5	20
32	e0	53/53 (100%)	36 (68%)	17 (32%)	0	1
33	E1	62/66 (94%)	46 (74%)	16 (26%)	0	2
33	e1	66/66 (100%)	50 (76%)	16 (24%)	1	3
34	SR	259/261 (99%)	220 (85%)	39 (15%)	3	13
34	sR	260/261 (100%)	229 (88%)	31 (12%)	5	20
35	SM	97/107 (91%)	76 (78%)	21 (22%)	1	5
39	L2	193/194 (100%)	152 (79%)	41 (21%)	1	5
39	l2	192/194 (99%)	148 (77%)	44 (23%)	1	4
40	L3	319/322 (99%)	248 (78%)	71 (22%)	1	5
40	l3	321/322 (100%)	246 (77%)	75 (23%)	1	4
41	L4	288/288 (100%)	222 (77%)	66 (23%)	1	4
41	l4	288/288 (100%)	219 (76%)	69 (24%)	1	3
42	L5	244/244 (100%)	195 (80%)	49 (20%)	1	6
42	l5	243/244 (100%)	181 (74%)	62 (26%)	0	3
43	L6	134/152 (88%)	108 (81%)	26 (19%)	1	6
43	l6	135/152 (89%)	107 (79%)	28 (21%)	1	6
44	L7	186/187 (100%)	151 (81%)	35 (19%)	1	7
44	l7	187/187 (100%)	147 (79%)	40 (21%)	1	5
45	L8	187/191 (98%)	156 (83%)	31 (17%)	2	11
45	l8	177/191 (93%)	139 (78%)	38 (22%)	1	5
46	L9	171/171 (100%)	124 (72%)	47 (28%)	0	2
46	l9	171/171 (100%)	126 (74%)	45 (26%)	0	2
47	M0	177/186 (95%)	144 (81%)	33 (19%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	m0	179/186 (96%)	135 (75%)	44 (25%)	1	3
48	M1	147/147 (100%)	112 (76%)	35 (24%)	1	4
48	m1	147/147 (100%)	116 (79%)	31 (21%)	1	5
49	M3	154/154 (100%)	119 (77%)	35 (23%)	1	4
49	m3	154/154 (100%)	120 (78%)	34 (22%)	1	5
50	M4	107/108 (99%)	79 (74%)	28 (26%)	0	2
50	m4	108/108 (100%)	80 (74%)	28 (26%)	0	2
51	M5	175/175 (100%)	142 (81%)	33 (19%)	1	7
51	m5	175/175 (100%)	136 (78%)	39 (22%)	1	5
52	M6	160/160 (100%)	134 (84%)	26 (16%)	2	11
52	m6	160/160 (100%)	128 (80%)	32 (20%)	1	6
53	M7	140/145 (97%)	104 (74%)	36 (26%)	0	2
53	m7	125/145 (86%)	85 (68%)	40 (32%)	0	1
54	M8	150/150 (100%)	120 (80%)	30 (20%)	1	6
54	m8	150/150 (100%)	116 (77%)	34 (23%)	1	4
55	M9	153/153 (100%)	120 (78%)	33 (22%)	1	5
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	5
56	N0	156/156 (100%)	124 (80%)	32 (20%)	1	6
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	5
57	N1	136/136 (100%)	105 (77%)	31 (23%)	1	4
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	5
58	N2	87/87 (100%)	72 (83%)	15 (17%)	2	10
58	n2	85/87 (98%)	67 (79%)	18 (21%)	1	5
59	N3	104/104 (100%)	82 (79%)	22 (21%)	1	5
59	n3	104/104 (100%)	85 (82%)	19 (18%)	2	7
60	N4	57/114 (50%)	49 (86%)	8 (14%)	3	15
60	n4	100/114 (88%)	82 (82%)	18 (18%)	2	8
61	N5	104/105 (99%)	77 (74%)	27 (26%)	0	2
61	n5	104/105 (99%)	79 (76%)	25 (24%)	1	3
62	N6	109/109 (100%)	85 (78%)	24 (22%)	1	5
62	n6	109/109 (100%)	81 (74%)	28 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	N7	115/115 (100%)	92 (80%)	23 (20%)	1	6
63	n7	115/115 (100%)	87 (76%)	28 (24%)	1	3
64	N8	118/118 (100%)	89 (75%)	29 (25%)	1	3
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	6
65	N9	46/46 (100%)	34 (74%)	12 (26%)	0	2
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	1
66	O0	81/84 (96%)	67 (83%)	14 (17%)	2	9
66	o0	84/84 (100%)	67 (80%)	17 (20%)	1	6
67	O1	92/96 (96%)	65 (71%)	27 (29%)	0	2
67	o1	94/96 (98%)	65 (69%)	29 (31%)	0	1
68	O2	109/109 (100%)	80 (73%)	29 (27%)	0	2
68	o2	109/109 (100%)	88 (81%)	21 (19%)	1	6
69	O3	90/90 (100%)	73 (81%)	17 (19%)	1	7
69	o3	90/90 (100%)	76 (84%)	14 (16%)	2	12
70	O4	95/95 (100%)	76 (80%)	19 (20%)	1	6
70	o4	95/95 (100%)	79 (83%)	16 (17%)	2	11
71	O5	104/104 (100%)	77 (74%)	27 (26%)	0	2
71	o5	103/104 (99%)	79 (77%)	24 (23%)	1	4
72	O6	81/81 (100%)	56 (69%)	25 (31%)	0	1
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	52 (74%)	18 (26%)	0	2
73	o7	70/70 (100%)	53 (76%)	17 (24%)	1	3
74	O8	68/68 (100%)	51 (75%)	17 (25%)	0	3
74	o8	67/68 (98%)	48 (72%)	19 (28%)	0	2
75	O9	45/45 (100%)	34 (76%)	11 (24%)	1	3
75	o9	45/45 (100%)	39 (87%)	6 (13%)	4	17
76	Q0	47/47 (100%)	36 (77%)	11 (23%)	1	4
76	q0	47/47 (100%)	33 (70%)	14 (30%)	0	1
77	Q1	23/23 (100%)	12 (52%)	11 (48%)	0	0
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
78	Q2	90/90 (100%)	63 (70%)	27 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	q2	90/90 (100%)	67 (74%)	23 (26%)	0	2
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	14
79	q3	71/71 (100%)	51 (72%)	20 (28%)	0	2
81	c0	73/78 (94%)	63 (86%)	10 (14%)	3	16
82	sM	54/54 (100%)	36 (67%)	18 (33%)	0	1
84	p0	105/186 (56%)	83 (79%)	22 (21%)	1	5
All	All	18727/19202 (98%)	14586 (78%)	4141 (22%)	1	5

5 of 4141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
58	n2	63	VAL
63	n7	70	PRO
58	n2	55	THR
56	N0	45	LEU
54	M8	135	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 205 such sidechains are listed below:

Mol	Chain	Res	Type
2	s0	140	ASN
22	d0	72	ASN
78	q2	47	GLN
4	s2	201	ASN
7	s5	224	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1829 (97%)	521 (29%)	70 (3%)
36	1	3145/3394 (92%)	773 (24%)	87 (2%)
36	5	3145/3394 (92%)	780 (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%)	43 (27%)	4 (2%)
38	8	157/158 (99%)	40 (25%)	3 (1%)
80	6	1792/1800 (99%)	492 (27%)	67 (3%)
86	A	1/3 (33%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
86	B	1/3 (33%)	0	0
All	All	10414/10981 (94%)	2694 (25%)	327 (3%)

5 of 2694 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 ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	8AN	A	3403	36,86	21,24,25	1.57	4 (19%)	26,35,38	2.29	10 (38%)
86	8AN	B	3403	36,86	21,24,25	7.96	7 (33%)	26,35,38	1.60	6 (23%)

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
86	8AN	A	3403	36,86	-	0/7/25/26	0/3/3/3
86	8AN	B	3403	36,86	-	0/7/25/26	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	B	3403	8AN	C3'-N3'	-35.32	0.93	1.47
86	B	3403	8AN	O2'-C2'	5.58	1.56	1.43
86	A	3403	8AN	C5-C4	4.74	1.47	1.39
86	B	3403	8AN	C4-N9	4.47	1.47	1.37
86	B	3403	8AN	C5-C6	2.79	1.48	1.41

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	A	3403	8AN	C5-C4-N3	-5.84	118.68	126.72
86	A	3403	8AN	N3-C4-N9	4.58	134.96	127.17
86	A	3403	8AN	C2-N3-C4	3.70	120.86	111.83
86	A	3403	8AN	C4-C5-N7	-3.50	106.58	110.58
86	B	3403	8AN	N1-C2-N3	-3.22	123.70	128.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A	3403	8AN	12	0
86	B	3403	8AN	9	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3555 ligands modelled in this entry, 2208 are monoatomic - leaving 1347 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	$\# Z > 2$
87	OHX	1	3797	87	0,6,6	-	-	-		
87	OHX	6	2022	80,87	0,6,6	-	-	-		
87	OHX	6	2097	88,87	0,6,6	-	-	-		
87	OHX	5	3595	87	0,6,6	-	-	-		
87	OHX	5	3813	87	0,6,6	-	-	-		
87	OHX	5	3684	87	0,6,6	-	-	-		
87	OHX	6	1971	88,87	0,6,6	-	-	-		
87	OHX	6	2006	88	0,6,6	-	-	-		
87	OHX	6	1955	80	0,6,6	-	-	-		
87	OHX	5	3554	88,36	0,6,6	-	-	-		
87	OHX	1	3433	87	0,6,6	-	-	-		
87	OHX	1	3468	88,36	0,6,6	-	-	-		
87	OHX	8	209	-	0,6,6	-	-	-		
87	OHX	6	1903	-	0,6,6	-	-	-		
87	OHX	5	3564	88	0,6,6	-	-	-		
87	OHX	1	3732	-	0,6,6	-	-	-		
87	OHX	1	3638	88	0,6,6	-	-	-		
87	OHX	5	3583	87,36	0,6,6	-	-	-		
87	OHX	1	3785	87	0,6,6	-	-	-		
87	OHX	5	3605	88,87	0,6,6	-	-	-		
87	OHX	L3	402	-	0,6,6	-	-	-		
87	OHX	1	3763	87	0,6,6	-	-	-		
87	OHX	5	3639	-	0,6,6	-	-	-		
87	OHX	1	3539	-	0,6,6	-	-	-		
87	OHX	6	2094	80,87	0,6,6	-	-	-		
87	OHX	o7	503	87	0,6,6	-	-	-		
87	OHX	6	1962	80	0,6,6	-	-	-		
87	OHX	6	1917	80	0,6,6	-	-	-		
87	OHX	1	3616	88	0,6,6	-	-	-		
87	OHX	1	3485	87	0,6,6	-	-	-		
87	OHX	1	3722	88	0,6,6	-	-	-		
87	OHX	2	1918	88,87	0,6,6	-	-	-		
87	OHX	1	3451	87	0,6,6	-	-	-		
87	OHX	O7	103	-	0,6,6	-	-	-		
87	OHX	3	209	87	0,6,6	-	-	-		
87	OHX	o3	201	-	0,6,6	-	-	-		
87	OHX	6	2067	87	0,6,6	-	-	-		
87	OHX	1	3602	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3789	88	0,6,6	-	-	-		
87	OHX	1	3645	-	0,6,6	-	-	-		
87	OHX	1	3462	88	0,6,6	-	-	-		
87	OHX	2	2043	-	0,6,6	-	-	-		
87	OHX	5	3556	87,36	0,6,6	-	-	-		
87	OHX	q1	101	87	0,6,6	-	-	-		
87	OHX	5	3456	87,36	0,6,6	-	-	-		
87	OHX	1	3526	36	0,6,6	-	-	-		
87	OHX	1	3800	87	0,6,6	-	-	-		
87	OHX	1	3511	-	0,6,6	-	-	-		
87	OHX	5	3546	88	0,6,6	-	-	-		
87	OHX	1	3654	88	0,6,6	-	-	-		
87	OHX	1	3741	-	0,6,6	-	-	-		
87	OHX	2	2026	87	0,6,6	-	-	-		
87	OHX	6	1972	88	0,6,6	-	-	-		
87	OHX	5	3516	88	0,6,6	-	-	-		
87	OHX	5	3466	88	0,6,6	-	-	-		
87	OHX	6	2002	88,80,87	0,6,6	-	-	-		
87	OHX	1	3424	-	0,6,6	-	-	-		
87	OHX	5	3412	-	0,6,6	-	-	-		
87	OHX	5	3681	-	0,6,6	-	-	-		
87	OHX	5	3584	88	0,6,6	-	-	-		
87	OHX	6	1941	80	0,6,6	-	-	-		
87	OHX	1	3525	88	0,6,6	-	-	-		
87	OHX	6	1952	80,87	0,6,6	-	-	-		
87	OHX	6	2049	80	0,6,6	-	-	-		
87	OHX	6	1902	-	0,6,6	-	-	-		
87	OHX	1	3795	87	0,6,6	-	-	-		
87	OHX	5	3600	88	0,6,6	-	-	-		
87	OHX	2	2005	-	0,6,6	-	-	-		
87	OHX	6	1965	88,87	0,6,6	-	-	-		
87	OHX	5	3518	36	0,6,6	-	-	-		
87	OHX	6	2081	-	0,6,6	-	-	-		
87	OHX	5	3780	-	0,6,6	-	-	-		
87	OHX	5	3548	-	0,6,6	-	-	-		
87	OHX	5	3670	87,36	0,6,6	-	-	-		
87	OHX	5	3635	88	0,6,6	-	-	-		
87	OHX	O1	201	88,87	0,6,6	-	-	-		
87	OHX	5	3413	-	0,6,6	-	-	-		
87	OHX	1	3581	-	0,6,6	-	-	-		
87	OHX	5	3471	36	0,6,6	-	-	-		
87	OHX	6	2019	88	0,6,6	-	-	-		
87	OHX	5	3585	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	1985	-	0,6,6	-	-	-		
87	OHX	5	3586	87	0,6,6	-	-	-		
87	OHX	2	2031	87	0,6,6	-	-	-		
87	OHX	3	208	-	0,6,6	-	-	-		
87	OHX	1	3578	36	0,6,6	-	-	-		
87	OHX	5	3497	87	0,6,6	-	-	-		
87	OHX	2	2010	-	0,6,6	-	-	-		
87	OHX	1	3646	88	0,6,6	-	-	-		
87	OHX	5	3771	88	0,6,6	-	-	-		
87	OHX	5	3778	36	0,6,6	-	-	-		
87	OHX	5	3680	-	0,6,6	-	-	-		
87	OHX	1	3743	88,36	0,6,6	-	-	-		
87	OHX	1	3655	88	0,6,6	-	-	-		
87	OHX	6	2086	-	0,6,6	-	-	-		
87	OHX	1	3421	-	0,6,6	-	-	-		
87	OHX	6	2031	-	0,6,6	-	-	-		
87	OHX	4	204	-	0,6,6	-	-	-		
87	OHX	1	3580	36	0,6,6	-	-	-		
87	OHX	5	3698	36	0,6,6	-	-	-		
87	OHX	6	2015	87	0,6,6	-	-	-		
87	OHX	5	3528	88	0,6,6	-	-	-		
87	OHX	4	217	-	0,6,6	-	-	-		
87	OHX	6	1934	-	0,6,6	-	-	-		
87	OHX	5	3498	87,36	0,6,6	-	-	-		
87	OHX	M7	201	88	0,6,6	-	-	-		
87	OHX	1	3441	-	0,6,6	-	-	-		
87	OHX	6	1946	-	0,6,6	-	-	-		
87	OHX	6	2037	88,80	0,6,6	-	-	-		
87	OHX	5	3688	88	0,6,6	-	-	-		
87	OHX	C3	201	-	0,6,6	-	-	-		
87	OHX	7	211	88	0,6,6	-	-	-		
87	OHX	2	2082	1,87	0,6,6	-	-	-		
87	OHX	L3	401	-	0,6,6	-	-	-		
87	OHX	1	3631	-	0,6,6	-	-	-		
87	OHX	5	3811	87	0,6,6	-	-	-		
87	OHX	6	1939	87	0,6,6	-	-	-		
87	OHX	1	3432	88	0,6,6	-	-	-		
87	OHX	1	3494	88	0,6,6	-	-	-		
87	OHX	5	3462	36	0,6,6	-	-	-		
87	OHX	2	1969	1	0,6,6	-	-	-		
87	OHX	5	3565	87	0,6,6	-	-	-		
87	OHX	5	3436	-	0,6,6	-	-	-		
87	OHX	1	3772	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	1983	80	0,6,6	-	-	-		
87	OHX	1	3573	-	0,6,6	-	-	-		
87	OHX	1	3592	88,87	0,6,6	-	-	-		
87	OHX	7	210	88,87	0,6,6	-	-	-		
87	OHX	2	2025	88	0,6,6	-	-	-		
87	OHX	m1	201	-	0,6,6	-	-	-		
87	OHX	2	1936	88	0,6,6	-	-	-		
87	OHX	5	3526	88	0,6,6	-	-	-		
87	OHX	1	3693	-	0,6,6	-	-	-		
87	OHX	5	3759	-	0,6,6	-	-	-		
87	OHX	5	3474	87	0,6,6	-	-	-		
87	OHX	5	3442	88	0,6,6	-	-	-		
87	OHX	2	2004	-	0,6,6	-	-	-		
87	OHX	1	3725	88	0,6,6	-	-	-		
87	OHX	5	3449	-	0,6,6	-	-	-		
87	OHX	5	3463	88	0,6,6	-	-	-		
87	OHX	1	3717	87	0,6,6	-	-	-		
87	OHX	2	2012	-	0,6,6	-	-	-		
87	OHX	C5	201	17	0,6,6	-	-	-		
87	OHX	5	3673	88	0,6,6	-	-	-		
87	OHX	2	2054	88,87	0,6,6	-	-	-		
87	OHX	m0	302	87	0,6,6	-	-	-		
87	OHX	4	208	38	0,6,6	-	-	-		
87	OHX	8	214	-	0,6,6	-	-	-		
87	OHX	5	3588	88	0,6,6	-	-	-		
87	OHX	s1	302	-	0,6,6	-	-	-		
87	OHX	6	2012	80	0,6,6	-	-	-		
87	OHX	1	3782	87	0,6,6	-	-	-		
87	OHX	2	2021	-	0,6,6	-	-	-		
87	OHX	5	3686	-	0,6,6	-	-	-		
87	OHX	1	3550	-	0,6,6	-	-	-		
87	OHX	5	3499	36	0,6,6	-	-	-		
87	OHX	5	3803	87,36	0,6,6	-	-	-		
87	OHX	1	3403	-	0,6,6	-	-	-		
87	OHX	1	3604	-	0,6,6	-	-	-		
87	OHX	4	207	88	0,6,6	-	-	-		
87	OHX	6	2040	-	0,6,6	-	-	-		
87	OHX	2	1997	88	0,6,6	-	-	-		
87	OHX	5	3552	88	0,6,6	-	-	-		
87	OHX	6	2014	-	0,6,6	-	-	-		
87	OHX	2	1923	-	0,6,6	-	-	-		
87	OHX	2	1973	87	0,6,6	-	-	-		
87	OHX	5	3607	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3754	88,36	0,6,6	-	-	-		
87	OHX	5	3731	88,87	0,6,6	-	-	-		
87	OHX	5	3568	88,87	0,6,6	-	-	-		
87	OHX	n3	202	-	0,6,6	-	-	-		
87	OHX	5	3555	88	0,6,6	-	-	-		
87	OHX	6	2013	88	0,6,6	-	-	-		
87	OHX	1	3447	-	0,6,6	-	-	-		
87	OHX	l5	303	-	0,6,6	-	-	-		
87	OHX	5	3675	-	0,6,6	-	-	-		
87	OHX	1	3547	-	0,6,6	-	-	-		
87	OHX	2	2029	1	0,6,6	-	-	-		
87	OHX	1	3572	-	0,6,6	-	-	-		
87	OHX	m4	201	-	0,6,6	-	-	-		
87	OHX	6	2095	-	0,6,6	-	-	-		
87	OHX	5	3537	87	0,6,6	-	-	-		
87	OHX	5	3618	-	0,6,6	-	-	-		
87	OHX	1	3532	87	0,6,6	-	-	-		
87	OHX	5	3809	36	0,6,6	-	-	-		
87	OHX	5	3677	-	0,6,6	-	-	-		
87	OHX	1	3656	-	0,6,6	-	-	-		
87	OHX	6	1920	87	0,6,6	-	-	-		
87	OHX	5	3713	-	0,6,6	-	-	-		
87	OHX	6	2029	-	0,6,6	-	-	-		
87	OHX	4	205	-	0,6,6	-	-	-		
87	OHX	2	2022	87	0,6,6	-	-	-		
87	OHX	6	2090	87	0,6,6	-	-	-		
87	OHX	2	1956	-	0,6,6	-	-	-		
87	OHX	1	3734	87	0,6,6	-	-	-		
87	OHX	5	3502	87,36,88	0,6,6	-	-	-		
87	OHX	1	3660	-	0,6,6	-	-	-		
87	OHX	5	3666	36	0,6,6	-	-	-		
87	OHX	5	3446	88	0,6,6	-	-	-		
87	OHX	5	3567	88,36	0,6,6	-	-	-		
87	OHX	5	3467	87	0,6,6	-	-	-		
87	OHX	1	3410	-	0,6,6	-	-	-		
87	OHX	1	3630	-	0,6,6	-	-	-		
87	OHX	5	3517	-	0,6,6	-	-	-		
87	OHX	1	3802	88	0,6,6	-	-	-		
87	OHX	5	3617	-	0,6,6	-	-	-		
87	OHX	1	3607	-	0,6,6	-	-	-		
87	OHX	1	3629	88	0,6,6	-	-	-		
87	OHX	2	1991	1,87	0,6,6	-	-	-		
87	OHX	5	3763	87,36,88	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3728	-	0,6,6	-	-	-		
87	OHX	2	2068	87	0,6,6	-	-	-		
87	OHX	2	1987	-	0,6,6	-	-	-		
87	OHX	1	3701	87	0,6,6	-	-	-		
87	OHX	6	2000	88	0,6,6	-	-	-		
87	OHX	5	3477	-	0,6,6	-	-	-		
87	OHX	6	1998	80	0,6,6	-	-	-		
87	OHX	5	3591	-	0,6,6	-	-	-		
87	OHX	5	3514	36	0,6,6	-	-	-		
87	OHX	6	2068	80,87	0,6,6	-	-	-		
87	OHX	1	3487	-	0,6,6	-	-	-		
87	OHX	1	3498	87,36,88	0,6,6	-	-	-		
87	OHX	6	2025	-	0,6,6	-	-	-		
87	OHX	1	3598	87	0,6,6	-	-	-		
87	OHX	1	3542	87	0,6,6	-	-	-		
87	OHX	1	3600	-	0,6,6	-	-	-		
87	OHX	1	3537	-	0,6,6	-	-	-		
87	OHX	6	1938	80,87	0,6,6	-	-	-		
87	OHX	o7	502	-	0,6,6	-	-	-		
87	OHX	6	2044	-	0,6,6	-	-	-		
87	OHX	1	3408	88	0,6,6	-	-	-		
87	OHX	3	205	87	0,6,6	-	-	-		
87	OHX	1	3670	88	0,6,6	-	-	-		
87	OHX	7	202	-	0,6,6	-	-	-		
87	OHX	2	1915	1,87	0,6,6	-	-	-		
87	OHX	2	2037	88	0,6,6	-	-	-		
87	OHX	5	3714	-	0,6,6	-	-	-		
87	OHX	5	3530	88,36	0,6,6	-	-	-		
87	OHX	1	3606	-	0,6,6	-	-	-		
87	OHX	M9	201	-	0,6,6	-	-	-		
87	OHX	5	3628	87	0,6,6	-	-	-		
87	OHX	1	3703	-	0,6,6	-	-	-		
87	OHX	1	3593	88	0,6,6	-	-	-		
87	OHX	2	2027	87	0,6,6	-	-	-		
87	OHX	5	3627	-	0,6,6	-	-	-		
87	OHX	2	2046	1	0,6,6	-	-	-		
87	OHX	2	1979	87	0,6,6	-	-	-		
87	OHX	4	212	38	0,6,6	-	-	-		
87	OHX	1	3431	88	0,6,6	-	-	-		
87	OHX	5	3702	88	0,6,6	-	-	-		
87	OHX	1	3617	-	0,6,6	-	-	-		
87	OHX	1	3575	88,36	0,6,6	-	-	-		
87	OHX	1	3766	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3507	36	0,6,6	-	-	-		
87	OHX	1	3523	-	0,6,6	-	-	-		
87	OHX	1	3595	36	0,6,6	-	-	-		
87	OHX	5	3669	87,36	0,6,6	-	-	-		
87	OHX	1	3510	88	0,6,6	-	-	-		
87	OHX	1	3690	-	0,6,6	-	-	-		
87	OHX	6	2039	88	0,6,6	-	-	-		
87	OHX	5	3712	88,87	0,6,6	-	-	-		
87	OHX	c1	201	87	0,6,6	-	-	-		
87	OHX	7	208	88	0,6,6	-	-	-		
87	OHX	6	2066	88	0,6,6	-	-	-		
87	OHX	5	3638	87,36	0,6,6	-	-	-		
87	OHX	2	2001	-	0,6,6	-	-	-		
87	OHX	6	2075	80,87	0,6,6	-	-	-		
87	OHX	1	3810	87,36	0,6,6	-	-	-		
87	OHX	1	3760	87	0,6,6	-	-	-		
87	OHX	2	2064	87	0,6,6	-	-	-		
87	OHX	2	2066	-	0,6,6	-	-	-		
87	OHX	1	3514	87	0,6,6	-	-	-		
87	OHX	5	3746	36	0,6,6	-	-	-		
87	OHX	1	3768	-	0,6,6	-	-	-		
87	OHX	2	2083	-	0,6,6	-	-	-		
87	OHX	1	3407	87	0,6,6	-	-	-		
87	OHX	6	1948	80,87	0,6,6	-	-	-		
87	OHX	1	3705	87,36,88	0,6,6	-	-	-		
87	OHX	6	2035	-	0,6,6	-	-	-		
87	OHX	5	3645	88,36	0,6,6	-	-	-		
87	OHX	5	3551	88	0,6,6	-	-	-		
87	OHX	5	3640	88,36	0,6,6	-	-	-		
87	OHX	6	1925	80	0,6,6	-	-	-		
87	OHX	5	3741	88	0,6,6	-	-	-		
87	OHX	1	3762	-	0,6,6	-	-	-		
87	OHX	6	2059	87	0,6,6	-	-	-		
87	OHX	5	3800	87,36	0,6,6	-	-	-		
87	OHX	6	2065	-	0,6,6	-	-	-		
87	OHX	1	3755	88	0,6,6	-	-	-		
87	OHX	6	1986	88	0,6,6	-	-	-		
87	OHX	5	3704	87	0,6,6	-	-	-		
87	OHX	1	3778	-	0,6,6	-	-	-		
87	OHX	1	3422	-	0,6,6	-	-	-		
87	OHX	1	3445	88	0,6,6	-	-	-		
87	OHX	1	3712	87	0,6,6	-	-	-		
87	OHX	3	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	1953	88	0,6,6	-	-	-		
87	OHX	19	201	-	0,6,6	-	-	-		
87	OHX	1	3559	88	0,6,6	-	-	-		
87	OHX	1	3429	88	0,6,6	-	-	-		
87	OHX	1	3520	88	0,6,6	-	-	-		
87	OHX	1	3688	-	0,6,6	-	-	-		
87	OHX	2	2042	-	0,6,6	-	-	-		
87	OHX	s8	301	-	0,6,6	-	-	-		
87	OHX	2	2063	-	0,6,6	-	-	-		
87	OHX	1	3552	-	0,6,6	-	-	-		
87	OHX	5	3765	87	0,6,6	-	-	-		
87	OHX	1	3519	88	0,6,6	-	-	-		
87	OHX	1	3746	88,87	0,6,6	-	-	-		
87	OHX	5	3807	87	0,6,6	-	-	-		
87	OHX	6	2093	80,87	0,6,6	-	-	-		
87	OHX	5	3438	-	0,6,6	-	-	-		
87	OHX	6	2008	-	0,6,6	-	-	-		
87	OHX	2	1976	87	0,6,6	-	-	-		
87	OHX	6	2052	80	0,6,6	-	-	-		
87	OHX	1	3551	-	0,6,6	-	-	-		
87	OHX	5	3804	87	0,6,6	-	-	-		
87	OHX	2	1930	-	0,6,6	-	-	-		
87	OHX	1	3406	36	0,6,6	-	-	-		
87	OHX	6	1984	80	0,6,6	-	-	-		
87	OHX	1	3709	-	0,6,6	-	-	-		
87	OHX	1	3420	-	0,6,6	-	-	-		
87	OHX	1	3474	87	0,6,6	-	-	-		
87	OHX	1	3555	87	0,6,6	-	-	-		
87	OHX	2	2038	-	0,6,6	-	-	-		
87	OHX	6	2007	88,80	0,6,6	-	-	-		
87	OHX	6	1937	-	0,6,6	-	-	-		
87	OHX	6	1927	88,80	0,6,6	-	-	-		
87	OHX	1	3522	-	0,6,6	-	-	-		
87	OHX	5	3453	87	0,6,6	-	-	-		
87	OHX	5	3710	-	0,6,6	-	-	-		
87	OHX	2	1996	-	0,6,6	-	-	-		
87	OHX	1	3418	87,36	0,6,6	-	-	-		
87	OHX	5	3452	-	0,6,6	-	-	-		
87	OHX	5	3401	36	0,6,6	-	-	-		
87	OHX	5	3455	36	0,6,6	-	-	-		
87	OHX	1	3413	-	0,6,6	-	-	-		
87	OHX	1	3666	-	0,6,6	-	-	-		
87	OHX	5	3719	88	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3671	36	0,6,6	-	-	-		
87	OHX	1	3749	87	0,6,6	-	-	-		
87	OHX	1	3475	87	0,6,6	-	-	-		
87	OHX	5	3654	88,36	0,6,6	-	-	-		
87	OHX	2	1989	87	0,6,6	-	-	-		
87	OHX	6	1953	-	0,6,6	-	-	-		
87	OHX	1	3569	-	0,6,6	-	-	-		
87	OHX	M8	201	-	0,6,6	-	-	-		
87	OHX	1	3478	-	0,6,6	-	-	-		
87	OHX	1	3794	-	0,6,6	-	-	-		
87	OHX	1	3667	-	0,6,6	-	-	-		
87	OHX	1	3697	-	0,6,6	-	-	-		
87	OHX	5	3729	87	0,6,6	-	-	-		
87	OHX	1	3517	-	0,6,6	-	-	-		
87	OHX	1	3438	-	0,6,6	-	-	-		
87	OHX	1	3651	88	0,6,6	-	-	-		
87	OHX	M5	301	-	0,6,6	-	-	-		
87	OHX	6	1942	80	0,6,6	-	-	-		
87	OHX	1	3589	88	0,6,6	-	-	-		
87	OHX	5	3464	87	0,6,6	-	-	-		
87	OHX	8	205	88	0,6,6	-	-	-		
87	OHX	1	3482	-	0,6,6	-	-	-		
87	OHX	1	3648	88	0,6,6	-	-	-		
87	OHX	5	3482	87	0,6,6	-	-	-		
87	OHX	1	3591	87	0,6,6	-	-	-		
87	OHX	5	3616	87	0,6,6	-	-	-		
87	OHX	1	3599	-	0,6,6	-	-	-		
87	OHX	1	3737	87	0,6,6	-	-	-		
87	OHX	1	3490	87	0,6,6	-	-	-		
87	OHX	5	3428	-	0,6,6	-	-	-		
87	OHX	1	3562	-	0,6,6	-	-	-		
87	OHX	1	3676	-	0,6,6	-	-	-		
87	OHX	5	3451	87	0,6,6	-	-	-		
87	OHX	2	1963	-	0,6,6	-	-	-		
87	OHX	2	2023	-	0,6,6	-	-	-		
87	OHX	6	2034	80,87	0,6,6	-	-	-		
87	OHX	6	1961	-	0,6,6	-	-	-		
87	OHX	5	3427	-	0,6,6	-	-	-		
87	OHX	1	3796	88,87	0,6,6	-	-	-		
87	OHX	1	3700	-	0,6,6	-	-	-		
87	OHX	5	3679	87,36	0,6,6	-	-	-		
87	OHX	6	2048	-	0,6,6	-	-	-		
87	OHX	1	3545	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3748	-	0,6,6	-	-	-		
87	OHX	1	3521	88	0,6,6	-	-	-		
87	OHX	5	3779	36	0,6,6	-	-	-		
87	OHX	2	1978	-	0,6,6	-	-	-		
87	OHX	5	3460	87	0,6,6	-	-	-		
87	OHX	2	1916	1	0,6,6	-	-	-		
87	OHX	1	3723	-	0,6,6	-	-	-		
87	OHX	5	3683	-	0,6,6	-	-	-		
87	OHX	5	3784	87	0,6,6	-	-	-		
87	OHX	1	3472	87	0,6,6	-	-	-		
87	OHX	5	3511	88	0,6,6	-	-	-		
87	OHX	5	3421	-	0,6,6	-	-	-		
87	OHX	1	3619	-	0,6,6	-	-	-		
87	OHX	2	1902	-	0,6,6	-	-	-		
87	OHX	1	3750	-	0,6,6	-	-	-		
87	OHX	1	3627	88	0,6,6	-	-	-		
87	OHX	2	2045	-	0,6,6	-	-	-		
87	OHX	1	3707	87	0,6,6	-	-	-		
87	OHX	5	3650	87	0,6,6	-	-	-		
87	OHX	1	3672	-	0,6,6	-	-	-		
87	OHX	q2	502	88	0,6,6	-	-	-		
87	OHX	5	3487	88	0,6,6	-	-	-		
87	OHX	5	3764	36	0,6,6	-	-	-		
87	OHX	5	3547	36	0,6,6	-	-	-		
87	OHX	5	3491	88	0,6,6	-	-	-		
87	OHX	6	2053	80	0,6,6	-	-	-		
87	OHX	6	2003	80	0,6,6	-	-	-		
87	OHX	1	3535	87	0,6,6	-	-	-		
87	OHX	1	3658	-	0,6,6	-	-	-		
87	OHX	5	3788	87	0,6,6	-	-	-		
87	OHX	1	3469	-	0,6,6	-	-	-		
87	OHX	1	3477	-	0,6,6	-	-	-		
87	OHX	5	3541	-	0,6,6	-	-	-		
87	OHX	5	3776	-	0,6,6	-	-	-		
87	OHX	5	3716	88,36	0,6,6	-	-	-		
87	OHX	5	3814	87,36	0,6,6	-	-	-		
87	OHX	6	2058	87	0,6,6	-	-	-		
87	OHX	5	3469	88	0,6,6	-	-	-		
87	OHX	5	3572	88	0,6,6	-	-	-		
87	OHX	N9	101	-	0,6,6	-	-	-		
87	OHX	2	2073	87	0,6,6	-	-	-		
87	OHX	2	1977	87	0,6,6	-	-	-		
87	OHX	5	3582	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3734	-	0,6,6	-	-	-		
87	OHX	1	3685	87	0,6,6	-	-	-		
87	OHX	c3	201	-	0,6,6	-	-	-		
87	OHX	2	2086	88	0,6,6	-	-	-		
87	OHX	1	3419	-	0,6,6	-	-	-		
87	OHX	5	3602	88,36	0,6,6	-	-	-		
87	OHX	1	3556	36	0,6,6	-	-	-		
87	OHX	1	3496	-	0,6,6	-	-	-		
87	OHX	1	3459	-	0,6,6	-	-	-		
87	OHX	1	3457	88,87	0,6,6	-	-	-		
87	OHX	5	3646	88,36	0,6,6	-	-	-		
87	OHX	2	2085	87	0,6,6	-	-	-		
87	OHX	6	2079	88	0,6,6	-	-	-		
87	OHX	1	3460	87	0,6,6	-	-	-		
87	OHX	1	3529	-	0,6,6	-	-	-		
87	OHX	5	3473	36	0,6,6	-	-	-		
87	OHX	5	3743	36	0,6,6	-	-	-		
87	OHX	N8	201	-	0,6,6	-	-	-		
87	OHX	6	1974	80	0,6,6	-	-	-		
87	OHX	1	3640	88	0,6,6	-	-	-		
87	OHX	1	3516	-	0,6,6	-	-	-		
87	OHX	6	2028	80	0,6,6	-	-	-		
87	OHX	2	1935	-	0,6,6	-	-	-		
87	OHX	2	1932	-	0,6,6	-	-	-		
87	OHX	6	1923	88,80	0,6,6	-	-	-		
87	OHX	2	2051	-	0,6,6	-	-	-		
87	OHX	5	3589	87,36,88	0,6,6	-	-	-		
87	OHX	1	3682	-	0,6,6	-	-	-		
87	OHX	1	3570	-	0,6,6	-	-	-		
87	OHX	1	3561	-	0,6,6	-	-	-		
87	OHX	6	1910	88	0,6,6	-	-	-		
87	OHX	5	3678	-	0,6,6	-	-	-		
87	OHX	5	3533	36	0,6,6	-	-	-		
87	OHX	1	3669	88	0,6,6	-	-	-		
87	OHX	6	1951	-	0,6,6	-	-	-		
87	OHX	8	208	88	0,6,6	-	-	-		
87	OHX	1	3788	87	0,6,6	-	-	-		
87	OHX	1	3479	-	0,6,6	-	-	-		
87	OHX	5	3687	87	0,6,6	-	-	-		
87	OHX	5	3532	87	0,6,6	-	-	-		
87	OHX	1	3653	88	0,6,6	-	-	-		
87	OHX	6	1957	88,80	0,6,6	-	-	-		
87	OHX	8	213	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3461	87	0,6,6	-	-	-		
87	OHX	2	2039	87	0,6,6	-	-	-		
87	OHX	3	207	87	0,6,6	-	-	-		
87	OHX	13	401	-	0,6,6	-	-	-		
87	OHX	5	3662	-	0,6,6	-	-	-		
87	OHX	2	2024	-	0,6,6	-	-	-		
87	OHX	5	3775	87	0,6,6	-	-	-		
87	OHX	1	3601	87	0,6,6	-	-	-		
87	OHX	1	3585	-	0,6,6	-	-	-		
87	OHX	5	3606	-	0,6,6	-	-	-		
87	OHX	5	3806	87	0,6,6	-	-	-		
87	OHX	1	3513	87	0,6,6	-	-	-		
87	OHX	5	3717	36	0,6,6	-	-	-		
87	OHX	5	3718	87	0,6,6	-	-	-		
87	OHX	5	3766	-	0,6,6	-	-	-		
87	OHX	5	3501	87	0,6,6	-	-	-		
87	OHX	1	3641	88	0,6,6	-	-	-		
87	OHX	6	2080	88	0,6,6	-	-	-		
87	OHX	1	3804	87	0,6,6	-	-	-		
87	OHX	6	1950	88,80	0,6,6	-	-	-		
87	OHX	1	3652	88,87	0,6,6	-	-	-		
87	OHX	5	3782	88	0,6,6	-	-	-		
87	OHX	5	3660	87	0,6,6	-	-	-		
87	OHX	1	3610	-	0,6,6	-	-	-		
87	OHX	5	3520	87	0,6,6	-	-	-		
87	OHX	5	3550	-	0,6,6	-	-	-		
87	OHX	5	3636	-	0,6,6	-	-	-		
87	OHX	M0	301	87	0,6,6	-	-	-		
87	OHX	7	204	88	0,6,6	-	-	-		
87	OHX	5	3730	87	0,6,6	-	-	-		
87	OHX	5	3643	36	0,6,6	-	-	-		
87	OHX	5	3631	36	0,6,6	-	-	-		
87	OHX	3	206	-	0,6,6	-	-	-		
87	OHX	6	2030	-	0,6,6	-	-	-		
87	OHX	6	1970	-	0,6,6	-	-	-		
87	OHX	2	1911	88	0,6,6	-	-	-		
87	OHX	2	1944	88	0,6,6	-	-	-		
87	OHX	5	3723	88,87	0,6,6	-	-	-		
87	OHX	5	3484	36	0,6,6	-	-	-		
87	OHX	sR	401	-	0,6,6	-	-	-		
87	OHX	1	3671	87,36	0,6,6	-	-	-		
87	OHX	5	3735	36	0,6,6	-	-	-		
87	OHX	1	3613	87,36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3533	-	0,6,6	-	-	-		
87	OHX	5	3701	88	0,6,6	-	-	-		
87	OHX	1	3557	-	0,6,6	-	-	-		
87	OHX	1	3497	-	0,6,6	-	-	-		
87	OHX	1	3492	88	0,6,6	-	-	-		
87	OHX	5	3689	36	0,6,6	-	-	-		
87	OHX	2	2070	87	0,6,6	-	-	-		
87	OHX	1	3449	-	0,6,6	-	-	-		
87	OHX	6	2061	87	0,6,6	-	-	-		
87	OHX	5	3777	-	0,6,6	-	-	-		
87	OHX	1	3448	-	0,6,6	-	-	-		
87	OHX	5	3658	88	0,6,6	-	-	-		
87	OHX	5	3674	-	0,6,6	-	-	-		
87	OHX	1	3528	-	0,6,6	-	-	-		
87	OHX	5	3563	88	0,6,6	-	-	-		
87	OHX	1	3729	88	0,6,6	-	-	-		
87	OHX	5	3479	88,87	0,6,6	-	-	-		
87	OHX	5	3561	-	0,6,6	-	-	-		
87	OHX	6	2070	80,87	0,6,6	-	-	-		
87	OHX	5	3656	88,36	0,6,6	-	-	-		
87	OHX	6	1918	87	0,6,6	-	-	-		
87	OHX	2	2019	88	0,6,6	-	-	-		
87	OHX	2	2077	1,87	0,6,6	-	-	-		
87	OHX	n1	201	88	0,6,6	-	-	-		
87	OHX	1	3465	87	0,6,6	-	-	-		
87	OHX	2	2088	1,87	0,6,6	-	-	-		
87	OHX	1	3715	-	0,6,6	-	-	-		
87	OHX	5	3703	-	0,6,6	-	-	-		
87	OHX	1	3430	-	0,6,6	-	-	-		
87	OHX	2	1984	87	0,6,6	-	-	-		
87	OHX	1	3748	-	0,6,6	-	-	-		
87	OHX	1	3621	87	0,6,6	-	-	-		
87	OHX	6	2088	87	0,6,6	-	-	-		
87	OHX	1	3720	87	0,6,6	-	-	-		
87	OHX	1	3594	87	0,6,6	-	-	-		
87	OHX	5	3644	-	0,6,6	-	-	-		
87	OHX	4	214	38	0,6,6	-	-	-		
87	OHX	5	3629	36	0,6,6	-	-	-		
87	OHX	1	3801	87	0,6,6	-	-	-		
87	OHX	c5	202	17	0,6,6	-	-	-		
87	OHX	1	3735	-	0,6,6	-	-	-		
87	OHX	6	1996	-	0,6,6	-	-	-		
87	OHX	1	3439	88	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3731	-	0,6,6	-	-	-		
87	OHX	5	3797	87	0,6,6	-	-	-		
87	OHX	m5	502	88	0,6,6	-	-	-		
87	OHX	1	3784	87	0,6,6	-	-	-		
87	OHX	5	3667	88	0,6,6	-	-	-		
87	OHX	2	1912	-	0,6,6	-	-	-		
87	OHX	2	1964	-	0,6,6	-	-	-		
87	OHX	5	3524	-	0,6,6	-	-	-		
87	OHX	2	1901	-	0,6,6	-	-	-		
87	OHX	l5	301	-	0,6,6	-	-	-		
87	OHX	6	2089	80	0,6,6	-	-	-		
87	OHX	1	3704	88	0,6,6	-	-	-		
87	OHX	2	2084	87	0,6,6	-	-	-		
87	OHX	2	1906	88,87	0,6,6	-	-	-		
87	OHX	6	1912	-	0,6,6	-	-	-		
87	OHX	5	3406	36	0,6,6	-	-	-		
87	OHX	5	3774	-	0,6,6	-	-	-		
87	OHX	6	1901	80	0,6,6	-	-	-		
87	OHX	5	3426	36	0,6,6	-	-	-		
87	OHX	2	1913	88	0,6,6	-	-	-		
87	OHX	1	3713	87	0,6,6	-	-	-		
87	OHX	2	1967	-	0,6,6	-	-	-		
87	OHX	6	2084	88,87	0,6,6	-	-	-		
87	OHX	5	3632	87	0,6,6	-	-	-		
87	OHX	5	3522	-	0,6,6	-	-	-		
87	OHX	1	3483	88	0,6,6	-	-	-		
87	OHX	8	217	-	0,6,6	-	-	-		
87	OHX	O7	102	88,73	0,6,6	-	-	-		
87	OHX	3	212	-	0,6,6	-	-	-		
87	OHX	1	3661	88	0,6,6	-	-	-		
87	OHX	6	1985	88	0,6,6	-	-	-		
87	OHX	5	3612	-	0,6,6	-	-	-		
87	OHX	1	3417	88	0,6,6	-	-	-		
87	OHX	1	3751	36	0,6,6	-	-	-		
87	OHX	1	3783	-	0,6,6	-	-	-		
87	OHX	2	1958	-	0,6,6	-	-	-		
87	OHX	2	1962	-	0,6,6	-	-	-		
87	OHX	6	2072	-	0,6,6	-	-	-		
87	OHX	1	3798	88	0,6,6	-	-	-		
87	OHX	5	3431	-	0,6,6	-	-	-		
87	OHX	5	3772	-	0,6,6	-	-	-		
87	OHX	1	3644	-	0,6,6	-	-	-		
87	OHX	6	2009	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3444	87	0,6,6	-	-	-		
87	OHX	1	3455	88	0,6,6	-	-	-		
87	OHX	6	1958	80	0,6,6	-	-	-		
87	OHX	6	1914	80,87	0,6,6	-	-	-		
87	OHX	2	2020	-	0,6,6	-	-	-		
87	OHX	2	2087	87	0,6,6	-	-	-		
87	OHX	5	3706	87	0,6,6	-	-	-		
87	OHX	5	3416	88,36	0,6,6	-	-	-		
87	OHX	5	3651	87,36	0,6,6	-	-	-		
87	OHX	5	3663	-	0,6,6	-	-	-		
87	OHX	5	3757	87	0,6,6	-	-	-		
87	OHX	1	3437	87	0,6,6	-	-	-		
87	OHX	6	1966	-	0,6,6	-	-	-		
87	OHX	1	3576	88	0,6,6	-	-	-		
87	OHX	1	3402	-	0,6,6	-	-	-		
87	OHX	5	3732	87	0,6,6	-	-	-		
87	OHX	6	1989	88,80	0,6,6	-	-	-		
87	OHX	1	3414	-	0,6,6	-	-	-		
87	OHX	5	3795	-	0,6,6	-	-	-		
87	OHX	1	3799	-	0,6,6	-	-	-		
87	OHX	5	3458	36	0,6,6	-	-	-		
87	OHX	2	2017	-	0,6,6	-	-	-		
87	OHX	5	3770	-	0,6,6	-	-	-		
87	OHX	2	1929	88	0,6,6	-	-	-		
87	OHX	4	215	87	0,6,6	-	-	-		
87	OHX	5	3425	36	0,6,6	-	-	-		
87	OHX	5	3724	88	0,6,6	-	-	-		
87	OHX	1	3612	88,87	0,6,6	-	-	-		
87	OHX	C8	202	87,36	0,6,6	-	-	-		
87	OHX	2	2032	88	0,6,6	-	-	-		
87	OHX	5	3581	-	0,6,6	-	-	-		
87	OHX	6	2017	80	0,6,6	-	-	-		
90	PRO	B	3501	-	6,7,8	0.61	0	7,8,10	1.40	1 (14%)
87	OHX	6	2078	-	0,6,6	-	-	-		
87	OHX	2	1903	-	0,6,6	-	-	-		
87	OHX	6	1968	88	0,6,6	-	-	-		
87	OHX	5	3762	-	0,6,6	-	-	-		
87	OHX	6	1919	80,87	0,6,6	-	-	-		
87	OHX	5	3525	-	0,6,6	-	-	-		
87	OHX	1	3620	36	0,6,6	-	-	-		
87	OHX	5	3472	88	0,6,6	-	-	-		
87	OHX	2	2065	-	0,6,6	-	-	-		
87	OHX	5	3708	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2032	80,87	0,6,6	-	-	-		
87	OHX	5	3475	-	0,6,6	-	-	-		
87	OHX	1	3464	-	0,6,6	-	-	-		
87	OHX	M0	302	87	0,6,6	-	-	-		
87	OHX	5	3655	87,36	0,6,6	-	-	-		
87	OHX	2	1917	-	0,6,6	-	-	-		
87	OHX	5	3527	88,36	0,6,6	-	-	-		
87	OHX	1	3718	87	0,6,6	-	-	-		
87	OHX	6	2082	87	0,6,6	-	-	-		
87	OHX	6	2043	87	0,6,6	-	-	-		
87	OHX	5	3690	-	0,6,6	-	-	-		
87	OHX	2	1945	87	0,6,6	-	-	-		
87	OHX	2	1931	-	0,6,6	-	-	-		
87	OHX	6	1928	80	0,6,6	-	-	-		
87	OHX	6	2085	80	0,6,6	-	-	-		
87	OHX	1	3509	87	0,6,6	-	-	-		
87	OHX	5	3751	36	0,6,6	-	-	-		
87	OHX	5	3749	87,36	0,6,6	-	-	-		
87	OHX	5	3614	88	0,6,6	-	-	-		
87	OHX	5	3408	-	0,6,6	-	-	-		
87	OHX	1	3742	87	0,6,6	-	-	-		
87	OHX	1	3684	87	0,6,6	-	-	-		
87	OHX	2	1907	87	0,6,6	-	-	-		
87	OHX	1	3643	87	0,6,6	-	-	-		
87	OHX	5	3494	-	0,6,6	-	-	-		
87	OHX	2	1960	-	0,6,6	-	-	-		
87	OHX	5	3519	87	0,6,6	-	-	-		
87	OHX	7	201	37	0,6,6	-	-	-		
87	OHX	5	3794	88,36	0,6,6	-	-	-		
87	OHX	5	3626	-	0,6,6	-	-	-		
87	OHX	5	3630	88,87	0,6,6	-	-	-		
87	OHX	6	1975	80,87	0,6,6	-	-	-		
87	OHX	2	2015	1,87	0,6,6	-	-	-		
87	OHX	2	1934	-	0,6,6	-	-	-		
87	OHX	1	3543	87	0,6,6	-	-	-		
87	OHX	5	3615	88	0,6,6	-	-	-		
87	OHX	8	216	38	0,6,6	-	-	-		
87	OHX	M9	202	87	0,6,6	-	-	-		
87	OHX	1	3678	88	0,6,6	-	-	-		
87	OHX	5	3457	-	0,6,6	-	-	-		
87	OHX	5	3728	87	0,6,6	-	-	-		
87	OHX	2	1946	-	0,6,6	-	-	-		
87	OHX	5	3709	87,36,88	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3420	36	0,6,6	-	-	-		
87	OHX	6	2036	88,80	0,6,6	-	-	-		
87	OHX	5	3747	88	0,6,6	-	-	-		
87	OHX	2	1920	-	0,6,6	-	-	-		
87	OHX	2	1941	-	0,6,6	-	-	-		
87	OHX	8	202	38	0,6,6	-	-	-		
87	OHX	2	2049	-	0,6,6	-	-	-		
87	OHX	1	3553	-	0,6,6	-	-	-		
87	OHX	1	3708	-	0,6,6	-	-	-		
87	OHX	6	2062	-	0,6,6	-	-	-		
87	OHX	2	1965	87	0,6,6	-	-	-		
87	OHX	4	206	-	0,6,6	-	-	-		
87	OHX	5	3566	88,36	0,6,6	-	-	-		
87	OHX	5	3571	88	0,6,6	-	-	-		
87	OHX	6	2033	-	0,6,6	-	-	-		
87	OHX	1	3773	87	0,6,6	-	-	-		
87	OHX	1	3605	-	0,6,6	-	-	-		
87	OHX	1	3639	88	0,6,6	-	-	-		
87	OHX	5	3580	-	0,6,6	-	-	-		
87	OHX	1	3662	-	0,6,6	-	-	-		
87	OHX	6	1973	87	0,6,6	-	-	-		
87	OHX	1	3740	87	0,6,6	-	-	-		
87	OHX	8	204	-	0,6,6	-	-	-		
87	OHX	1	3699	36	0,6,6	-	-	-		
87	OHX	5	3429	88,36	0,6,6	-	-	-		
87	OHX	5	3812	87	0,6,6	-	-	-		
87	OHX	1	3696	88,87	0,6,6	-	-	-		
87	OHX	2	2047	-	0,6,6	-	-	-		
87	OHX	6	1932	88	0,6,6	-	-	-		
87	OHX	5	4574	88,87,37	0,6,6	-	-	-		
87	OHX	6	2051	-	0,6,6	-	-	-		
87	OHX	7	207	88	0,6,6	-	-	-		
87	OHX	1	3531	87	0,6,6	-	-	-		
87	OHX	1	3584	87	0,6,6	-	-	-		
87	OHX	6	1990	80	0,6,6	-	-	-		
87	OHX	3	203	88	0,6,6	-	-	-		
87	OHX	5	3450	87,36	0,6,6	-	-	-		
87	OHX	1	3524	-	0,6,6	-	-	-		
87	OHX	5	3448	-	0,6,6	-	-	-		
87	OHX	6	1929	88	0,6,6	-	-	-		
87	OHX	5	3465	-	0,6,6	-	-	-		
87	OHX	1	3476	87	0,6,6	-	-	-		
87	OHX	8	212	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3599	88,36	0,6,6	-	-	-		
87	OHX	1	3806	88,87	0,6,6	-	-	-		
87	OHX	5	3622	-	0,6,6	-	-	-		
87	OHX	5	3715	36	0,6,6	-	-	-		
87	OHX	5	3562	-	0,6,6	-	-	-		
87	OHX	5	3603	36	0,6,6	-	-	-		
87	OHX	5	3407	36	0,6,6	-	-	-		
87	OHX	M0	304	87	0,6,6	-	-	-		
87	OHX	2	1948	88,87	0,6,6	-	-	-		
87	OHX	2	2034	-	0,6,6	-	-	-		
87	OHX	1	3761	88	0,6,6	-	-	-		
87	OHX	1	3687	87,36	0,6,6	-	-	-		
87	OHX	5	3480	-	0,6,6	-	-	-		
87	OHX	8	221	87	0,6,6	-	-	-		
87	OHX	1	3698	88	0,6,6	-	-	-		
87	OHX	1	3452	87	0,6,6	-	-	-		
87	OHX	2	1992	-	0,6,6	-	-	-		
87	OHX	4	213	-	0,6,6	-	-	-		
87	OHX	2	2076	1,87	0,6,6	-	-	-		
87	OHX	5	3604	36	0,6,6	-	-	-		
87	OHX	1	3719	87	0,6,6	-	-	-		
87	OHX	2	1994	-	0,6,6	-	-	-		
87	OHX	5	3459	88	0,6,6	-	-	-		
87	OHX	1	3500	87	0,6,6	-	-	-		
87	OHX	1	3767	-	0,6,6	-	-	-		
87	OHX	5	3691	-	0,6,6	-	-	-		
87	OHX	2	1983	-	0,6,6	-	-	-		
87	OHX	2	2053	87	0,6,6	-	-	-		
87	OHX	1	3590	-	0,6,6	-	-	-		
87	OHX	M0	303	87	0,6,6	-	-	-		
87	OHX	5	3745	87	0,6,6	-	-	-		
87	OHX	6	1993	80	0,6,6	-	-	-		
87	OHX	1	3548	-	0,6,6	-	-	-		
87	OHX	M9	203	-	0,6,6	-	-	-		
87	OHX	1	3792	-	0,6,6	-	-	-		
87	OHX	2	1952	1	0,6,6	-	-	-		
87	OHX	2	2055	88	0,6,6	-	-	-		
87	OHX	5	3750	-	0,6,6	-	-	-		
87	OHX	6	2076	80	0,6,6	-	-	-		
87	OHX	1	3481	-	0,6,6	-	-	-		
87	OHX	2	2013	1	0,6,6	-	-	-		
87	OHX	2	1922	88,87	0,6,6	-	-	-		
87	OHX	6	1940	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	2041	80	0,6,6	-	-	-		
87	OHX	1	3633	-	0,6,6	-	-	-		
87	OHX	6	1954	87	0,6,6	-	-	-		
87	OHX	5	3433	36	0,6,6	-	-	-		
87	OHX	5	3613	-	0,6,6	-	-	-		
87	OHX	2	2061	-	0,6,6	-	-	-		
87	OHX	1	3512	88	0,6,6	-	-	-		
87	OHX	2	2081	87	0,6,6	-	-	-		
87	OHX	5	3793	36	0,6,6	-	-	-		
87	OHX	2	2058	-	0,6,6	-	-	-		
87	OHX	1	3647	36	0,6,6	-	-	-		
87	OHX	7	212	88	0,6,6	-	-	-		
87	OHX	5	3439	-	0,6,6	-	-	-		
87	OHX	5	3515	36	0,6,6	-	-	-		
87	OHX	1	3711	87	0,6,6	-	-	-		
87	OHX	1	3506	36	0,6,6	-	-	-		
87	OHX	6	1922	-	0,6,6	-	-	-		
87	OHX	1	4509	87	0,6,6	-	-	-		
87	OHX	6	2021	88	0,6,6	-	-	-		
87	OHX	5	3694	-	0,6,6	-	-	-		
87	OHX	5	3634	-	0,6,6	-	-	-		
87	OHX	2	2069	88,87	0,6,6	-	-	-		
87	OHX	1	3721	88,36	0,6,6	-	-	-		
87	OHX	6	1944	88,80	0,6,6	-	-	-		
87	OHX	6	1969	-	0,6,6	-	-	-		
87	OHX	2	1999	-	0,6,6	-	-	-		
87	OHX	2	1968	-	0,6,6	-	-	-		
87	OHX	1	3453	-	0,6,6	-	-	-		
87	OHX	6	2064	80	0,6,6	-	-	-		
87	OHX	5	3405	36	0,6,6	-	-	-		
87	OHX	5	3510	87,36	0,6,6	-	-	-		
87	OHX	1	3757	-	0,6,6	-	-	-		
87	OHX	4	203	-	0,6,6	-	-	-		
87	OHX	5	3432	-	0,6,6	-	-	-		
87	OHX	2	2036	-	0,6,6	-	-	-		
87	OHX	5	3490	-	0,6,6	-	-	-		
87	OHX	5	3742	36	0,6,6	-	-	-		
87	OHX	1	3427	87	0,6,6	-	-	-		
87	OHX	2	2079	-	0,6,6	-	-	-		
87	OHX	5	3685	88,36	0,6,6	-	-	-		
87	OHX	5	3559	-	0,6,6	-	-	-		
87	OHX	2	2060	-	0,6,6	-	-	-		
87	OHX	1	3435	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3558	-	0,6,6	-	-	-		
87	OHX	1	3480	-	0,6,6	-	-	-		
87	OHX	5	3574	-	0,6,6	-	-	-		
87	OHX	1	3493	-	0,6,6	-	-	-		
87	OHX	2	2089	87	0,6,6	-	-	-		
87	OHX	2	2028	1	0,6,6	-	-	-		
87	OHX	1	3770	-	0,6,6	-	-	-		
87	OHX	6	2026	80	0,6,6	-	-	-		
87	OHX	1	3488	-	0,6,6	-	-	-		
87	OHX	5	3659	-	0,6,6	-	-	-		
87	OHX	1	3769	88	0,6,6	-	-	-		
87	OHX	5	3410	88	0,6,6	-	-	-		
87	OHX	1	3808	87	0,6,6	-	-	-		
87	OHX	5	3529	87,36	0,6,6	-	-	-		
87	OHX	1	3745	-	0,6,6	-	-	-		
87	OHX	4	210	88	0,6,6	-	-	-		
87	OHX	2	2057	88	0,6,6	-	-	-		
87	OHX	1	3583	36	0,6,6	-	-	-		
87	OHX	8	211	38	0,6,6	-	-	-		
87	OHX	5	3664	-	0,6,6	-	-	-		
87	OHX	8	220	-	0,6,6	-	-	-		
87	OHX	6	2005	87	0,6,6	-	-	-		
87	OHX	L4	401	-	0,6,6	-	-	-		
87	OHX	6	2057	80,87	0,6,6	-	-	-		
87	OHX	1	3637	-	0,6,6	-	-	-		
87	OHX	1	3536	36	0,6,6	-	-	-		
87	OHX	5	3711	87,36	0,6,6	-	-	-		
87	OHX	6	1959	87	0,6,6	-	-	-		
87	OHX	m7	201	-	0,6,6	-	-	-		
87	OHX	1	3625	36	0,6,6	-	-	-		
87	OHX	3	204	-	0,6,6	-	-	-		
87	OHX	1	3786	88	0,6,6	-	-	-		
87	OHX	5	3423	-	0,6,6	-	-	-		
87	OHX	1	3673	-	0,6,6	-	-	-		
87	OHX	6	2063	-	0,6,6	-	-	-		
87	OHX	6	1976	80	0,6,6	-	-	-		
87	OHX	5	3505	87	0,6,6	-	-	-		
87	OHX	5	3810	87	0,6,6	-	-	-		
87	OHX	5	3727	88,87	0,6,6	-	-	-		
87	OHX	5	3792	87,36,88	0,6,6	-	-	-		
87	OHX	5	3440	36	0,6,6	-	-	-		
87	OHX	6	1987	-	0,6,6	-	-	-		
87	OHX	5	3696	87,36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	1957	-	0,6,6	-	-	-		
87	OHX	6	2010	80,87	0,6,6	-	-	-		
87	OHX	5	3557	87	0,6,6	-	-	-		
87	OHX	5	3781	-	0,6,6	-	-	-		
87	OHX	6	2083	87	0,6,6	-	-	-		
87	OHX	6	2069	87	0,6,6	-	-	-		
87	OHX	5	3461	88,87	0,6,6	-	-	-		
87	OHX	4	211	88	0,6,6	-	-	-		
87	OHX	6	1964	88,80	0,6,6	-	-	-		
87	OHX	5	3791	88	0,6,6	-	-	-		
87	OHX	6	2038	-	0,6,6	-	-	-		
87	OHX	5	3601	36	0,6,6	-	-	-		
87	OHX	1	3568	-	0,6,6	-	-	-		
87	OHX	1	3458	-	0,6,6	-	-	-		
87	OHX	1	3428	88	0,6,6	-	-	-		
87	OHX	2	2071	87	0,6,6	-	-	-		
87	OHX	5	3768	87,36	0,6,6	-	-	-		
87	OHX	5	3417	88,36	0,6,6	-	-	-		
87	OHX	5	3623	-	0,6,6	-	-	-		
87	OHX	1	3756	88	0,6,6	-	-	-		
87	OHX	1	3502	87	0,6,6	-	-	-		
87	OHX	3	202	88	0,6,6	-	-	-		
87	OHX	5	3454	88	0,6,6	-	-	-		
87	OHX	5	3577	36	0,6,6	-	-	-		
87	OHX	S2	301	87	0,6,6	-	-	-		
87	OHX	2	2007	-	0,6,6	-	-	-		
87	OHX	6	1967	88	0,6,6	-	-	-		
87	OHX	m0	303	87	0,6,6	-	-	-		
87	OHX	5	3652	-	0,6,6	-	-	-		
87	OHX	2	1939	-	0,6,6	-	-	-		
87	OHX	1	3664	88	0,6,6	-	-	-		
87	OHX	5	3587	88	0,6,6	-	-	-		
87	OHX	2	1966	88	0,6,6	-	-	-		
87	OHX	1	3579	-	0,6,6	-	-	-		
87	OHX	1	3747	87,36	0,6,6	-	-	-		
87	OHX	1	3787	87	0,6,6	-	-	-		
87	OHX	1	3440	88	0,6,6	-	-	-		
87	OHX	1	3733	36	0,6,6	-	-	-		
87	OHX	5	3682	88	0,6,6	-	-	-		
87	OHX	5	3570	-	0,6,6	-	-	-		
87	OHX	1	3467	88	0,6,6	-	-	-		
87	OHX	1	3695	87	0,6,6	-	-	-		
87	OHX	1	3571	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2044	88	0,6,6	-	-	-		
87	OHX	6	1956	-	0,6,6	-	-	-		
87	OHX	6	1979	88,80	0,6,6	-	-	-		
87	OHX	1	3425	88	0,6,6	-	-	-		
87	OHX	5	3489	36	0,6,6	-	-	-		
87	OHX	5	3594	87,36	0,6,6	-	-	-		
87	OHX	1	3582	88	0,6,6	-	-	-		
87	OHX	5	3752	36	0,6,6	-	-	-		
87	OHX	5	3796	-	0,6,6	-	-	-		
87	OHX	1	3423	88	0,6,6	-	-	-		
87	OHX	5	3785	-	0,6,6	-	-	-		
87	OHX	5	3649	-	0,6,6	-	-	-		
87	OHX	6	2004	-	0,6,6	-	-	-		
87	OHX	1	3663	87,36,88	0,6,6	-	-	-		
87	OHX	1	3727	87	0,6,6	-	-	-		
87	OHX	5	3799	88,87	0,6,6	-	-	-		
87	OHX	2	1925	-	0,6,6	-	-	-		
87	OHX	2	1982	-	0,6,6	-	-	-		
87	OHX	5	3609	-	0,6,6	-	-	-		
87	OHX	5	3758	36	0,6,6	-	-	-		
87	OHX	6	1945	88,80	0,6,6	-	-	-		
87	OHX	5	3485	36	0,6,6	-	-	-		
87	OHX	6	2001	-	0,6,6	-	-	-		
87	OHX	1	3628	-	0,6,6	-	-	-		
87	OHX	2	1942	1,88	0,6,6	-	-	-		
87	OHX	2	1986	-	0,6,6	-	-	-		
87	OHX	1	3505	-	0,6,6	-	-	-		
87	OHX	5	3536	87	0,6,6	-	-	-		
87	OHX	1	3739	87	0,6,6	-	-	-		
87	OHX	1	3623	88	0,6,6	-	-	-		
87	OHX	6	1930	80	0,6,6	-	-	-		
87	OHX	5	3657	87,36,88	0,6,6	-	-	-		
87	OHX	5	3445	87	0,6,6	-	-	-		
87	OHX	8	206	-	0,6,6	-	-	-		
87	OHX	1	3534	88,36	0,6,6	-	-	-		
87	OHX	1	3668	88	0,6,6	-	-	-		
87	OHX	1	3764	87,36,88	0,6,6	-	-	-		
87	OHX	5	3697	36	0,6,6	-	-	-		
87	OHX	Q2	502	88	0,6,6	-	-	-		
87	OHX	1	3738	88	0,6,6	-	-	-		
87	OHX	6	2071	87	0,6,6	-	-	-		
87	OHX	5	3641	87	0,6,6	-	-	-		
87	OHX	6	1963	80	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2048	87	0,6,6	-	-	-		
87	OHX	1	3587	-	0,6,6	-	-	-		
87	OHX	5	3504	36	0,6,6	-	-	-		
87	OHX	1	3624	88	0,6,6	-	-	-		
87	OHX	5	3486	-	0,6,6	-	-	-		
87	OHX	7	203	88,87	0,6,6	-	-	-		
87	OHX	1	3554	-	0,6,6	-	-	-		
87	OHX	5	3661	-	0,6,6	-	-	-		
87	OHX	2	2040	-	0,6,6	-	-	-		
87	OHX	4	201	-	0,6,6	-	-	-		
87	OHX	5	3549	-	0,6,6	-	-	-		
87	OHX	4	216	88,87	0,6,6	-	-	-		
87	OHX	5	3437	88	0,6,6	-	-	-		
87	OHX	5	3608	36	0,6,6	-	-	-		
87	OHX	2	2050	1	0,6,6	-	-	-		
87	OHX	5	3418	-	0,6,6	-	-	-		
87	OHX	5	3424	-	0,6,6	-	-	-		
87	OHX	2	1981	-	0,6,6	-	-	-		
87	OHX	5	3621	36	0,6,6	-	-	-		
87	OHX	2	1926	-	0,6,6	-	-	-		
87	OHX	6	1915	-	0,6,6	-	-	-		
87	OHX	5	3720	-	0,6,6	-	-	-		
87	OHX	6	1936	80	0,6,6	-	-	-		
87	OHX	5	3597	-	0,6,6	-	-	-		
87	OHX	5	3760	-	0,6,6	-	-	-		
87	OHX	1	3691	87	0,6,6	-	-	-		
87	OHX	2	1908	-	0,6,6	-	-	-		
87	OHX	5	3699	36	0,6,6	-	-	-		
87	OHX	6	2050	80	0,6,6	-	-	-		
87	OHX	2	2011	88	0,6,6	-	-	-		
87	OHX	5	3593	-	0,6,6	-	-	-		
87	OHX	D9	102	87	0,6,6	-	-	-		
87	OHX	6	2045	88,80	0,6,6	-	-	-		
87	OHX	c8	201	-	0,6,6	-	-	-		
87	OHX	2	2056	-	0,6,6	-	-	-		
87	OHX	6	1981	-	0,6,6	-	-	-		
87	OHX	5	3496	-	0,6,6	-	-	-		
87	OHX	6	1931	80,87	0,6,6	-	-	-		
87	OHX	1	3714	87	0,6,6	-	-	-		
87	OHX	5	3538	36	0,6,6	-	-	-		
87	OHX	6	2011	88	0,6,6	-	-	-		
87	OHX	5	3738	-	0,6,6	-	-	-		
87	OHX	5	3543	36	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	1	3793	87,36	0,6,6	-	-	-		
87	OHX	1	3563	88	0,6,6	-	-	-		
87	OHX	6	1909	88,80,87	0,6,6	-	-	-		
87	OHX	1	3626	-	0,6,6	-	-	-		
87	OHX	6	1907	80	0,6,6	-	-	-		
87	OHX	5	3576	-	0,6,6	-	-	-		
87	OHX	6	2018	87	0,6,6	-	-	-		
87	OHX	5	3573	36	0,6,6	-	-	-		
87	OHX	4	209	-	0,6,6	-	-	-		
87	OHX	6	1977	88	0,6,6	-	-	-		
87	OHX	5	3404	88	0,6,6	-	-	-		
87	OHX	2	1904	-	0,6,6	-	-	-		
87	OHX	5	3553	36	0,6,6	-	-	-		
87	OHX	5	3483	-	0,6,6	-	-	-		
87	OHX	1	3541	-	0,6,6	-	-	-		
87	OHX	8	210	-	0,6,6	-	-	-		
87	OHX	2	2018	87	0,6,6	-	-	-		
87	OHX	1	3549	87	0,6,6	-	-	-		
87	OHX	6	1935	80	0,6,6	-	-	-		
87	OHX	6	1906	-	0,6,6	-	-	-		
87	OHX	1	3412	-	0,6,6	-	-	-		
87	OHX	5	3700	87	0,6,6	-	-	-		
87	OHX	1	3608	87	0,6,6	-	-	-		
87	OHX	1	3564	88	0,6,6	-	-	-		
87	OHX	6	2074	80	0,6,6	-	-	-		
87	OHX	1	3504	87	0,6,6	-	-	-		
87	OHX	1	3597	87	0,6,6	-	-	-		
87	OHX	5	3620	87,36	0,6,6	-	-	-		
87	OHX	2	2075	-	0,6,6	-	-	-		
87	OHX	1	3692	87	0,6,6	-	-	-		
87	OHX	1	3665	88,87	0,6,6	-	-	-		
87	OHX	2	1937	88	0,6,6	-	-	-		
87	OHX	2	1990	1,87	0,6,6	-	-	-		
87	OHX	5	3569	88,87	0,6,6	-	-	-		
87	OHX	5	3443	87	0,6,6	-	-	-		
87	OHX	5	3478	87	0,6,6	-	-	-		
87	OHX	5	3403	36	0,6,6	-	-	-		
87	OHX	1	3411	-	0,6,6	-	-	-		
87	OHX	5	3531	-	0,6,6	-	-	-		
87	OHX	5	3619	88	0,6,6	-	-	-		
87	OHX	1	3603	-	0,6,6	-	-	-		
87	OHX	6	1994	-	0,6,6	-	-	-		
87	OHX	1	3635	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3707	-	0,6,6	-	-	-		
87	OHX	5	3672	36	0,6,6	-	-	-		
87	OHX	2	1951	-	0,6,6	-	-	-		
87	OHX	5	3642	-	0,6,6	-	-	-		
87	OHX	2	1927	88	0,6,6	-	-	-		
87	OHX	5	3503	87	0,6,6	-	-	-		
87	OHX	2	1947	88	0,6,6	-	-	-		
87	OHX	5	3447	88,87	0,6,6	-	-	-		
87	OHX	2	2078	87	0,6,6	-	-	-		
87	OHX	6	2042	80,87	0,6,6	-	-	-		
87	OHX	2	1980	87	0,6,6	-	-	-		
87	OHX	6	2056	88,80	0,6,6	-	-	-		
87	OHX	1	3473	88,87	0,6,6	-	-	-		
87	OHX	5	3693	-	0,6,6	-	-	-		
87	OHX	m9	201	-	0,6,6	-	-	-		
87	OHX	5	3414	88	0,6,6	-	-	-		
87	OHX	1	3586	87	0,6,6	-	-	-		
87	OHX	5	3535	87	0,6,6	-	-	-		
87	OHX	5	3737	88	0,6,6	-	-	-		
87	OHX	5	3725	88,87	0,6,6	-	-	-		
87	OHX	1	3507	87	0,6,6	-	-	-		
87	OHX	1	3680	-	0,6,6	-	-	-		
87	OHX	5	3508	87	0,6,6	-	-	-		
87	OHX	2	1919	1	0,6,6	-	-	-		
87	OHX	2	2059	87	0,6,6	-	-	-		
87	OHX	6	2024	80	0,6,6	-	-	-		
87	OHX	1	3527	-	0,6,6	-	-	-		
87	OHX	2	1971	-	0,6,6	-	-	-		
87	OHX	1	3752	87,36	0,6,6	-	-	-		
87	OHX	d9	102	87	0,6,6	-	-	-		
87	OHX	1	3415	-	0,6,6	-	-	-		
87	OHX	1	3730	87	0,6,6	-	-	-		
87	OHX	2	1954	87	0,6,6	-	-	-		
87	OHX	5	3783	-	0,6,6	-	-	-		
87	OHX	o9	101	88	0,6,6	-	-	-		
87	OHX	5	3668	-	0,6,6	-	-	-		
87	OHX	8	219	38	0,6,6	-	-	-		
87	OHX	1	3444	-	0,6,6	-	-	-		
87	OHX	1	3642	88	0,6,6	-	-	-		
87	OHX	5	3808	-	0,6,6	-	-	-		
90	PRO	A	3501	-	6,7,8	0.61	0	7,8,10	1.40	1 (14%)
87	OHX	1	3659	87	0,6,6	-	-	-		
87	OHX	6	2023	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2002	-	0,6,6	-	-	-		
87	OHX	1	3765	-	0,6,6	-	-	-		
87	OHX	5	3633	36	0,6,6	-	-	-		
87	OHX	1	3454	-	0,6,6	-	-	-		
87	OHX	1	3450	88	0,6,6	-	-	-		
87	OHX	1	3518	88	0,6,6	-	-	-		
87	OHX	1	3706	88	0,6,6	-	-	-		
87	OHX	1	3443	88	0,6,6	-	-	-		
87	OHX	6	1924	88	0,6,6	-	-	-		
87	OHX	5	3647	87	0,6,6	-	-	-		
87	OHX	1	3416	-	0,6,6	-	-	-		
87	OHX	1	3565	-	0,6,6	-	-	-		
87	OHX	4	202	-	0,6,6	-	-	-		
87	OHX	6	1992	88	0,6,6	-	-	-		
87	OHX	1	3436	-	0,6,6	-	-	-		
87	OHX	l3	402	-	0,6,6	-	-	-		
87	OHX	1	3774	-	0,6,6	-	-	-		
87	OHX	1	3503	88	0,6,6	-	-	-		
87	OHX	m5	501	-	0,6,6	-	-	-		
87	OHX	6	2091	87	0,6,6	-	-	-		
87	OHX	5	3509	36	0,6,6	-	-	-		
87	OHX	6	2016	80	0,6,6	-	-	-		
87	OHX	2	1970	87	0,6,6	-	-	-		
87	OHX	8	218	38	0,6,6	-	-	-		
87	OHX	6	1978	80	0,6,6	-	-	-		
87	OHX	1	3744	87	0,6,6	-	-	-		
87	OHX	5	3470	36	0,6,6	-	-	-		
87	OHX	2	1961	87	0,6,6	-	-	-		
87	OHX	5	3726	36	0,6,6	-	-	-		
87	OHX	5	3560	87	0,6,6	-	-	-		
87	OHX	5	3721	87,36	0,6,6	-	-	-		
87	OHX	5	3434	88,36	0,6,6	-	-	-		
87	OHX	1	3442	88	0,6,6	-	-	-		
87	OHX	2	2052	1	0,6,6	-	-	-		
87	OHX	6	1947	88	0,6,6	-	-	-		
87	OHX	5	3736	-	0,6,6	-	-	-		
87	OHX	6	1943	-	0,6,6	-	-	-		
87	OHX	1	3724	88	0,6,6	-	-	-		
87	OHX	5	3435	-	0,6,6	-	-	-		
87	OHX	1	3649	-	0,6,6	-	-	-		
87	OHX	7	206	-	0,6,6	-	-	-		
87	OHX	5	3419	88,36	0,6,6	-	-	-		
87	OHX	5	3493	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3598	87	0,6,6	-	-	-		
87	OHX	1	3609	88	0,6,6	-	-	-		
87	OHX	1	3401	-	0,6,6	-	-	-		
87	OHX	2	1972	1	0,6,6	-	-	-		
87	OHX	1	3538	88	0,6,6	-	-	-		
87	OHX	5	3611	87,36,86	0,6,6	-	-	-		
87	OHX	2	1995	-	0,6,6	-	-	-		
87	OHX	6	1999	-	0,6,6	-	-	-		
87	OHX	2	2033	-	0,6,6	-	-	-		
87	OHX	5	3544	-	0,6,6	-	-	-		
87	OHX	1	3515	36	0,6,6	-	-	-		
87	OHX	2	1988	87	0,6,6	-	-	-		
87	OHX	1	3803	-	0,6,6	-	-	-		
87	OHX	7	209	88	0,6,6	-	-	-		
87	OHX	5	3575	36	0,6,6	-	-	-		
87	OHX	5	3513	88,87	0,6,6	-	-	-		
87	OHX	8	201	-	0,6,6	-	-	-		
87	OHX	1	3694	-	0,6,6	-	-	-		
87	OHX	2	2003	1	0,6,6	-	-	-		
87	OHX	1	3657	87	0,6,6	-	-	-		
87	OHX	6	2060	-	0,6,6	-	-	-		
87	OHX	5	3761	88,87	0,6,6	-	-	-		
87	OHX	6	1988	-	0,6,6	-	-	-		
87	OHX	5	3790	87	0,6,6	-	-	-		
87	OHX	8	215	88	0,6,6	-	-	-		
87	OHX	5	3773	-	0,6,6	-	-	-		
87	OHX	1	3405	36	0,6,6	-	-	-		
87	OHX	1	3546	88	0,6,6	-	-	-		
87	OHX	L5	301	-	0,6,6	-	-	-		
87	OHX	5	3637	-	0,6,6	-	-	-		
87	OHX	5	3789	-	0,6,6	-	-	-		
87	OHX	6	1997	-	0,6,6	-	-	-		
87	OHX	1	3681	87,36	0,6,6	-	-	-		
87	OHX	1	3726	-	0,6,6	-	-	-		
87	OHX	1	3560	88	0,6,6	-	-	-		
87	OHX	5	3740	-	0,6,6	-	-	-		
87	OHX	2	2080	88,87	0,6,6	-	-	-		
87	OHX	l5	302	-	0,6,6	-	-	-		
87	OHX	1	3434	87	0,6,6	-	-	-		
87	OHX	6	2092	88,87	0,6,6	-	-	-		
87	OHX	5	3692	88,36	0,6,6	-	-	-		
87	OHX	5	3409	88,36	0,6,6	-	-	-		
87	OHX	1	3675	88	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	1949	88,87	0,6,6	-	-	-		
87	OHX	n9	101	-	0,6,6	-	-	-		
87	OHX	5	3596	88	0,6,6	-	-	-		
87	OHX	5	3653	88,87	0,6,6	-	-	-		
87	OHX	5	3739	-	0,6,6	-	-	-		
87	OHX	1	3491	87	0,6,6	-	-	-		
87	OHX	5	3705	36	0,6,6	-	-	-		
87	OHX	5	3542	-	0,6,6	-	-	-		
87	OHX	1	3615	36	0,6,6	-	-	-		
87	OHX	1	3686	-	0,6,6	-	-	-		
87	OHX	1	3758	88	0,6,6	-	-	-		
87	OHX	1	3771	87	0,6,6	-	-	-		
87	OHX	1	3544	88	0,6,6	-	-	-		
87	OHX	1	3446	88,87	0,6,6	-	-	-		
87	OHX	2	1910	1	0,6,6	-	-	-		
87	OHX	5	3476	87	0,6,6	-	-	-		
87	OHX	6	2073	-	0,6,6	-	-	-		
87	OHX	3	210	88	0,6,6	-	-	-		
87	OHX	O3	201	88	0,6,6	-	-	-		
87	OHX	1	3463	-	0,6,6	-	-	-		
87	OHX	1	3566	88	0,6,6	-	-	-		
87	OHX	6	2077	87	0,6,6	-	-	-		
87	OHX	5	3441	88	0,6,6	-	-	-		
87	OHX	5	3468	-	0,6,6	-	-	-		
87	OHX	1	3404	88	0,6,6	-	-	-		
87	OHX	1	3790	87	0,6,6	-	-	-		
87	OHX	8	207	38,87	0,6,6	-	-	-		
87	OHX	1	3636	88	0,6,6	-	-	-		
87	OHX	5	3523	87,36	0,6,6	-	-	-		
87	OHX	5	3769	36	0,6,6	-	-	-		
87	OHX	S8	301	-	0,6,6	-	-	-		
87	OHX	1	3466	-	0,6,6	-	-	-		
87	OHX	5	3500	-	0,6,6	-	-	-		
87	OHX	5	3767	87	0,6,6	-	-	-		
87	OHX	8	203	87	0,6,6	-	-	-		
87	OHX	1	3614	88	0,6,6	-	-	-		
87	OHX	1	3716	-	0,6,6	-	-	-		
87	OHX	5	3590	88,36	0,6,6	-	-	-		
87	OHX	2	1993	1,88	0,6,6	-	-	-		
87	OHX	5	3422	-	0,6,6	-	-	-		
87	OHX	2	2009	88	0,6,6	-	-	-		
87	OHX	6	1991	80	0,6,6	-	-	-		
87	OHX	5	3481	88	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	2041	-	0,6,6	-	-	-		
87	OHX	5	3512	-	0,6,6	-	-	-		
87	OHX	2	1924	88	0,6,6	-	-	-		
87	OHX	2	1933	87	0,6,6	-	-	-		
87	OHX	n3	201	-	0,6,6	-	-	-		
87	OHX	1	3484	88,87	0,6,6	-	-	-		
87	OHX	5	3801	87	0,6,6	-	-	-		
87	OHX	2	1928	-	0,6,6	-	-	-		
87	OHX	5	3506	-	0,6,6	-	-	-		
87	OHX	m0	301	87	0,6,6	-	-	-		
87	OHX	1	3618	-	0,6,6	-	-	-		
87	OHX	1	3809	87	0,6,6	-	-	-		
87	OHX	6	2098	87	0,6,6	-	-	-		
87	OHX	1	3409	-	0,6,6	-	-	-		
87	OHX	5	3744	-	0,6,6	-	-	-		
87	OHX	1	3530	88	0,6,6	-	-	-		
87	OHX	1	3650	88	0,6,6	-	-	-		
87	OHX	1	3622	-	0,6,6	-	-	-		
87	OHX	6	2055	-	0,6,6	-	-	-		
87	OHX	1	3702	-	0,6,6	-	-	-		
87	OHX	1	3501	87	0,6,6	-	-	-		
87	OHX	2	2030	87	0,6,6	-	-	-		
87	OHX	1	3471	-	0,6,6	-	-	-		
87	OHX	2	2014	-	0,6,6	-	-	-		
87	OHX	6	1995	-	0,6,6	-	-	-		
87	OHX	2	1975	87	0,6,6	-	-	-		
87	OHX	6	2027	88	0,6,6	-	-	-		
87	OHX	7	205	-	0,6,6	-	-	-		
87	OHX	SR	401	-	0,6,6	-	-	-		
87	OHX	5	3488	36	0,6,6	-	-	-		
87	OHX	5	3753	87	0,6,6	-	-	-		
87	OHX	5	3430	88,87	0,6,6	-	-	-		
87	OHX	6	2046	87	0,6,6	-	-	-		
87	OHX	5	3540	88	0,6,6	-	-	-		
87	OHX	5	3411	-	0,6,6	-	-	-		
87	OHX	1	3499	-	0,6,6	-	-	-		
87	OHX	1	3508	-	0,6,6	-	-	-		
87	OHX	2	2035	87	0,6,6	-	-	-		
87	OHX	2	1905	-	0,6,6	-	-	-		
87	OHX	L3	403	-	0,6,6	-	-	-		
87	OHX	1	3588	88	0,6,6	-	-	-		
87	OHX	14	402	-	0,6,6	-	-	-		
87	OHX	1	3710	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	2	1959	-	0,6,6	-	-	-		
87	OHX	6	2054	88,80,87	0,6,6	-	-	-		
87	OHX	2	1921	88,87	0,6,6	-	-	-		
87	OHX	5	3592	87	0,6,6	-	-	-		
87	OHX	2	1909	87	0,6,6	-	-	-		
87	OHX	5	3579	87	0,6,6	-	-	-		
87	OHX	2	1943	87	0,6,6	-	-	-		
87	OHX	1	3779	87	0,6,6	-	-	-		
87	OHX	5	3787	-	0,6,6	-	-	-		
87	OHX	c5	201	-	0,6,6	-	-	-		
87	OHX	5	3578	87	0,6,6	-	-	-		
87	OHX	5	3492	88	0,6,6	-	-	-		
87	OHX	1	3634	88	0,6,6	-	-	-		
87	OHX	5	3625	88,36	0,6,6	-	-	-		
87	OHX	6	1921	-	0,6,6	-	-	-		
87	OHX	6	1926	-	0,6,6	-	-	-		
87	OHX	6	1911	80	0,6,6	-	-	-		
87	OHX	1	3805	87,36	0,6,6	-	-	-		
87	OHX	6	1982	87	0,6,6	-	-	-		
87	OHX	6	1933	-	0,6,6	-	-	-		
87	OHX	5	3786	88	0,6,6	-	-	-		
87	OHX	2	1938	-	0,6,6	-	-	-		
87	OHX	5	3805	87	0,6,6	-	-	-		
87	OHX	6	1908	-	0,6,6	-	-	-		
87	OHX	3	211	87	0,6,6	-	-	-		
87	OHX	1	3674	87	0,6,6	-	-	-		
87	OHX	l2	301	87	0,6,6	-	-	-		
87	OHX	5	3495	88	0,6,6	-	-	-		
87	OHX	1	3759	87	0,6,6	-	-	-		
87	OHX	2	1974	-	0,6,6	-	-	-		
87	OHX	2	2074	87	0,6,6	-	-	-		
87	OHX	1	3689	-	0,6,6	-	-	-		
87	OHX	2	1950	-	0,6,6	-	-	-		
87	OHX	1	3776	-	0,6,6	-	-	-		
87	OHX	5	3648	87	0,6,6	-	-	-		
87	OHX	2	2008	87	0,6,6	-	-	-		
87	OHX	6	2096	80,87	0,6,6	-	-	-		
87	OHX	5	3756	87	0,6,6	-	-	-		
87	OHX	1	3753	87,36,88	0,6,6	-	-	-		
87	OHX	5	3534	-	0,6,6	-	-	-		
87	OHX	2	2000	-	0,6,6	-	-	-		
87	OHX	C8	201	88,87	0,6,6	-	-	-		
87	OHX	1	3489	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	6	1913	80	0,6,6	-	-	-		
87	OHX	1	3567	87	0,6,6	-	-	-		
87	OHX	m0	304	87	0,6,6	-	-	-		
87	OHX	1	3611	87	0,6,6	-	-	-		
87	OHX	5	3665	88	0,6,6	-	-	-		
87	OHX	5	3521	-	0,6,6	-	-	-		
87	OHX	2	2062	1	0,6,6	-	-	-		
87	OHX	2	1949	-	0,6,6	-	-	-		
87	OHX	1	3679	-	0,6,6	-	-	-		
87	OHX	5	3624	88	0,6,6	-	-	-		
87	OHX	s4	301	-	0,6,6	-	-	-		
87	OHX	1	3540	-	0,6,6	-	-	-		
87	OHX	2	1998	87	0,6,6	-	-	-		
87	OHX	5	3798	88,87	0,6,6	-	-	-		
87	OHX	6	1905	-	0,6,6	-	-	-		
87	OHX	5	3755	-	0,6,6	-	-	-		
87	OHX	5	3733	36	0,6,6	-	-	-		
87	OHX	1	3807	87	0,6,6	-	-	-		
87	OHX	5	3695	88,36	0,6,6	-	-	-		
87	OHX	1	3777	-	0,6,6	-	-	-		
87	OHX	1	3486	-	0,6,6	-	-	-		
87	OHX	5	3610	88	0,6,6	-	-	-		
87	OHX	2	1940	87	0,6,6	-	-	-		
87	OHX	5	3402	88,36	0,6,6	-	-	-		
87	OHX	5	3802	87,36,88	0,6,6	-	-	-		
87	OHX	1	3470	-	0,6,6	-	-	-		
87	OHX	5	3539	87	0,6,6	-	-	-		
87	OHX	6	1960	-	0,6,6	-	-	-		
87	OHX	6	2047	-	0,6,6	-	-	-		
87	OHX	6	2020	88,80	0,6,6	-	-	-		
87	OHX	1	3558	87	0,6,6	-	-	-		
87	OHX	1	3456	-	0,6,6	-	-	-		
87	OHX	6	1916	-	0,6,6	-	-	-		
87	OHX	1	3781	87	0,6,6	-	-	-		
87	OHX	6	2087	-	0,6,6	-	-	-		
87	OHX	2	2067	-	0,6,6	-	-	-		
87	OHX	2	2072	-	0,6,6	-	-	-		
87	OHX	1	3791	88	0,6,6	-	-	-		
87	OHX	5	3722	88,36	0,6,6	-	-	-		
87	OHX	1	3596	87	0,6,6	-	-	-		
87	OHX	1	3780	88	0,6,6	-	-	-		
87	OHX	1	3736	88	0,6,6	-	-	-		
87	OHX	2	2016	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	5	3676	88	0,6,6	-	-	-		
87	OHX	2	1914	1	0,6,6	-	-	-		
87	OHX	6	1904	80	0,6,6	-	-	-		
87	OHX	1	3577	88,87	0,6,6	-	-	-		
87	OHX	6	1980	80	0,6,6	-	-	-		
87	OHX	5	3415	-	0,6,6	-	-	-		
87	OHX	s1	301	88	0,6,6	-	-	-		
87	OHX	1	3574	88	0,6,6	-	-	-		
87	OHX	1	3495	88	0,6,6	-	-	-		
87	OHX	14	401	-	0,6,6	-	-	-		
87	OHX	2	2006	-	0,6,6	-	-	-		
87	OHX	2	1955	-	0,6,6	-	-	-		
87	OHX	1	3677	87	0,6,6	-	-	-		
87	OHX	5	3545	-	0,6,6	-	-	-		
87	OHX	1	3426	-	0,6,6	-	-	-		
87	OHX	1	3683	88,36	0,6,6	-	-	-		
87	OHX	1	3632	-	0,6,6	-	-	-		
87	OHX	5	3754	88,36	0,6,6	-	-	-		
87	OHX	1	3775	87	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
90	PRO	B	3501	-	-	0/0/9/11	0/1/1/1
90	PRO	A	3501	-	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	A	3501	PRO	O-C-CA	-2.25	118.98	124.77
90	B	3501	PRO	O-C-CA	-2.25	118.99	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

570 monomers are involved in 836 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3684	OHX	4	0
87	6	2006	OHX	1	0
87	6	1955	OHX	1	0
87	5	3554	OHX	1	0
87	1	3433	OHX	5	0
87	6	1903	OHX	1	0
87	1	3732	OHX	1	0
87	1	3638	OHX	1	0
87	5	3605	OHX	1	0
87	L3	402	OHX	3	0
87	1	3539	OHX	2	0
87	6	2094	OHX	1	0
87	o7	503	OHX	1	0
87	1	3616	OHX	1	0
87	O7	103	OHX	1	0
87	1	3602	OHX	2	0
87	1	3645	OHX	1	0
87	2	2043	OHX	1	0
87	1	3526	OHX	1	0
87	5	3466	OHX	1	0
87	6	2002	OHX	1	0
87	5	3681	OHX	1	0
87	6	1952	OHX	1	0
87	1	3795	OHX	1	0
87	5	3635	OHX	2	0
87	O1	201	OHX	1	0
87	5	3413	OHX	1	0
87	6	2019	OHX	1	0
87	5	3586	OHX	2	0
87	2	2010	OHX	1	0
87	5	3771	OHX	1	0
87	1	3580	OHX	2	0
87	6	2015	OHX	2	0
87	5	3528	OHX	1	0
87	6	1934	OHX	1	0
87	5	3688	OHX	1	0
87	C3	201	OHX	2	0
87	L3	401	OHX	1	0
87	6	1939	OHX	2	0
87	2	1969	OHX	4	0
87	1	3772	OHX	4	0
87	6	1983	OHX	1	0
87	1	3573	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	7	210	OHX	1	0
87	m1	201	OHX	1	0
87	2	1936	OHX	1	0
87	2	2004	OHX	1	0
87	1	3725	OHX	2	0
87	5	3449	OHX	4	0
87	5	3463	OHX	3	0
87	1	3717	OHX	1	0
87	C5	201	OHX	3	0
87	m0	302	OHX	3	0
87	5	3588	OHX	1	0
87	s1	302	OHX	1	0
87	2	2021	OHX	1	0
87	5	3803	OHX	1	0
87	1	3403	OHX	2	0
87	2	1997	OHX	2	0
87	5	3552	OHX	1	0
87	2	1923	OHX	1	0
87	2	1973	OHX	1	0
87	5	3607	OHX	1	0
87	1	3754	OHX	2	0
87	5	3731	OHX	1	0
87	5	3568	OHX	2	0
87	n3	202	OHX	1	0
87	5	3675	OHX	1	0
87	1	3547	OHX	1	0
87	1	3572	OHX	1	0
87	5	3537	OHX	1	0
87	1	3656	OHX	1	0
87	6	1920	OHX	4	0
87	5	3713	OHX	2	0
87	4	205	OHX	1	0
87	6	2090	OHX	2	0
87	2	1956	OHX	1	0
87	5	3502	OHX	1	0
87	5	3446	OHX	1	0
87	5	3567	OHX	1	0
87	1	3410	OHX	1	0
87	1	3630	OHX	1	0
87	5	3517	OHX	2	0
87	1	3607	OHX	1	0
87	1	3701	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2068	OHX	1	0
87	1	3598	OHX	2	0
87	1	3542	OHX	1	0
87	1	3537	OHX	3	0
87	6	1938	OHX	1	0
87	3	205	OHX	1	0
87	2	1915	OHX	1	0
87	2	2037	OHX	2	0
87	5	3714	OHX	1	0
87	1	3703	OHX	1	0
87	5	3627	OHX	1	0
87	5	3702	OHX	1	0
87	5	3507	OHX	1	0
87	1	3595	OHX	1	0
87	5	3712	OHX	2	0
87	6	2066	OHX	1	0
87	6	2075	OHX	1	0
87	1	3810	OHX	3	0
87	2	2064	OHX	3	0
87	1	3514	OHX	1	0
87	1	3407	OHX	3	0
87	6	2035	OHX	2	0
87	5	3551	OHX	1	0
87	6	1925	OHX	1	0
87	5	3741	OHX	1	0
87	6	2065	OHX	1	0
87	5	3704	OHX	1	0
87	3	201	OHX	1	0
87	2	1953	OHX	2	0
87	1	3429	OHX	1	0
87	1	3520	OHX	2	0
87	2	2042	OHX	1	0
87	s8	301	OHX	1	0
87	2	2063	OHX	1	0
87	1	3552	OHX	1	0
87	1	3519	OHX	1	0
87	5	3807	OHX	1	0
87	6	2008	OHX	1	0
87	2	1976	OHX	1	0
87	5	3804	OHX	4	0
87	1	3406	OHX	1	0
87	6	1984	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3420	OHX	2	0
87	1	3474	OHX	1	0
87	5	3453	OHX	1	0
87	5	3401	OHX	1	0
87	5	3455	OHX	1	0
87	1	3413	OHX	1	0
87	1	3666	OHX	1	0
87	1	3749	OHX	2	0
87	1	3475	OHX	1	0
87	1	3478	OHX	1	0
87	1	3438	OHX	1	0
87	M5	301	OHX	1	0
87	5	3464	OHX	1	0
87	1	3648	OHX	1	0
87	1	3591	OHX	1	0
87	1	3737	OHX	2	0
87	1	3490	OHX	1	0
87	1	3562	OHX	2	0
87	5	3451	OHX	1	0
87	2	1963	OHX	2	0
87	2	2023	OHX	1	0
87	6	2034	OHX	1	0
87	6	1961	OHX	1	0
87	1	3796	OHX	2	0
87	1	3700	OHX	1	0
87	5	3779	OHX	1	0
87	5	3460	OHX	2	0
87	1	3472	OHX	1	0
87	5	3511	OHX	1	0
87	1	3750	OHX	1	0
87	1	3627	OHX	1	0
87	1	3707	OHX	1	0
87	5	3650	OHX	1	0
87	1	3672	OHX	1	0
87	q2	502	OHX	3	0
87	5	3487	OHX	1	0
87	5	3491	OHX	1	0
87	6	2053	OHX	1	0
87	1	3535	OHX	2	0
87	1	3658	OHX	1	0
87	5	3541	OHX	1	0
87	5	3716	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	2058	OHX	2	0
87	N9	101	OHX	1	0
87	2	1977	OHX	3	0
87	5	3582	OHX	1	0
87	1	3685	OHX	1	0
87	c3	201	OHX	2	0
87	1	3419	OHX	1	0
87	1	3496	OHX	5	0
87	1	3459	OHX	2	0
87	1	3457	OHX	1	0
87	2	2085	OHX	2	0
87	6	2079	OHX	1	0
87	1	3529	OHX	1	0
87	5	3473	OHX	2	0
87	6	1974	OHX	1	0
87	6	2028	OHX	1	0
87	2	1935	OHX	1	0
87	2	1932	OHX	1	0
87	2	2051	OHX	1	0
87	1	3682	OHX	1	0
87	1	3570	OHX	1	0
87	6	1910	OHX	2	0
87	5	3533	OHX	1	0
87	6	1951	OHX	3	0
87	1	3788	OHX	1	0
87	1	3479	OHX	1	0
87	5	3687	OHX	1	0
87	6	1957	OHX	1	0
87	8	213	OHX	2	0
87	1	3461	OHX	1	0
87	l3	401	OHX	2	0
87	5	3806	OHX	2	0
87	5	3718	OHX	1	0
87	5	3766	OHX	1	0
87	1	3804	OHX	1	0
87	1	3652	OHX	1	0
87	5	3782	OHX	1	0
87	1	3610	OHX	1	0
87	5	3520	OHX	1	0
87	3	206	OHX	1	0
87	2	1944	OHX	1	0
87	5	3701	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3492	OHX	1	0
87	5	3689	OHX	2	0
87	1	3449	OHX	3	0
87	6	2061	OHX	1	0
87	5	3777	OHX	1	0
87	5	3658	OHX	1	0
87	5	3563	OHX	1	0
87	5	3561	OHX	2	0
87	5	3656	OHX	1	0
87	2	2088	OHX	1	0
87	1	3430	OHX	1	0
87	2	1984	OHX	2	0
87	1	3621	OHX	1	0
87	1	3594	OHX	1	0
87	5	3644	OHX	2	0
87	5	3629	OHX	1	0
87	1	3801	OHX	1	0
87	c5	202	OHX	6	0
87	5	3797	OHX	1	0
87	5	3667	OHX	1	0
87	2	1912	OHX	1	0
87	2	1964	OHX	4	0
87	2	1901	OHX	1	0
87	2	2084	OHX	1	0
87	2	1906	OHX	1	0
87	6	1912	OHX	2	0
87	6	1901	OHX	1	0
87	5	3426	OHX	1	0
87	2	1913	OHX	1	0
87	6	2084	OHX	1	0
87	5	3632	OHX	3	0
87	O7	102	OHX	7	0
87	3	212	OHX	1	0
87	1	3661	OHX	1	0
87	6	1985	OHX	1	0
87	1	3417	OHX	1	0
87	1	3751	OHX	1	0
87	1	3783	OHX	2	0
87	2	1962	OHX	4	0
87	1	3798	OHX	1	0
87	5	3772	OHX	1	0
87	6	2009	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	2087	OHX	1	0
87	5	3663	OHX	1	0
87	5	3757	OHX	1	0
87	6	1966	OHX	2	0
87	5	3732	OHX	1	0
87	1	3414	OHX	1	0
87	5	3795	OHX	1	0
87	2	2017	OHX	1	0
87	5	3425	OHX	2	0
87	C8	202	OHX	1	0
87	5	3581	OHX	1	0
90	B	3501	PRO	2	0
87	6	1968	OHX	1	0
87	5	3525	OHX	1	0
87	6	2032	OHX	1	0
87	1	3464	OHX	1	0
87	5	3655	OHX	2	0
87	2	1917	OHX	1	0
87	5	3527	OHX	1	0
87	6	2082	OHX	2	0
87	6	2043	OHX	2	0
87	2	1945	OHX	1	0
87	6	1928	OHX	1	0
87	1	3509	OHX	1	0
87	5	3408	OHX	1	0
87	1	3742	OHX	2	0
87	1	3684	OHX	2	0
87	1	3643	OHX	1	0
87	5	3494	OHX	1	0
87	5	3519	OHX	1	0
87	6	1975	OHX	1	0
87	5	3615	OHX	1	0
87	8	216	OHX	1	0
87	5	3457	OHX	2	0
87	2	1946	OHX	1	0
87	5	3709	OHX	2	0
87	2	1941	OHX	1	0
87	8	202	OHX	1	0
87	2	1965	OHX	1	0
87	4	206	OHX	2	0
87	1	3773	OHX	1	0
87	1	3662	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3740	OHX	3	0
87	8	204	OHX	1	0
87	1	3699	OHX	1	0
87	2	2047	OHX	1	0
87	6	2051	OHX	2	0
87	1	3531	OHX	3	0
87	1	3524	OHX	1	0
87	6	1929	OHX	1	0
87	1	3476	OHX	1	0
87	8	212	OHX	3	0
87	1	3806	OHX	5	0
87	5	3622	OHX	1	0
87	M0	304	OHX	6	0
87	2	2034	OHX	1	0
87	5	3480	OHX	1	0
87	1	3698	OHX	1	0
87	2	1992	OHX	1	0
87	4	213	OHX	3	0
87	2	2076	OHX	3	0
87	5	3604	OHX	1	0
87	1	3500	OHX	1	0
87	M0	303	OHX	5	0
87	M9	203	OHX	2	0
87	2	1952	OHX	1	0
87	2	2013	OHX	1	0
87	6	2041	OHX	1	0
87	5	3613	OHX	1	0
87	2	2061	OHX	1	0
87	1	3512	OHX	2	0
87	2	2081	OHX	1	0
87	1	3647	OHX	1	0
87	5	3439	OHX	1	0
87	1	3711	OHX	1	0
87	6	1922	OHX	1	0
87	1	4509	OHX	1	0
87	6	2021	OHX	1	0
87	5	3634	OHX	1	0
87	6	1969	OHX	1	0
87	1	3453	OHX	1	0
87	5	3510	OHX	1	0
87	5	3432	OHX	1	0
87	1	3427	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3558	OHX	1	0
87	1	3480	OHX	2	0
87	5	3574	OHX	1	0
87	1	3770	OHX	1	0
87	4	210	OHX	1	0
87	2	2057	OHX	1	0
87	1	3583	OHX	2	0
87	8	211	OHX	1	0
87	6	2005	OHX	3	0
87	L4	401	OHX	2	0
87	6	2057	OHX	1	0
87	1	3786	OHX	1	0
87	5	3792	OHX	1	0
87	6	2083	OHX	1	0
87	6	2069	OHX	3	0
87	5	3461	OHX	2	0
87	6	2038	OHX	1	0
87	1	3428	OHX	1	0
87	2	2071	OHX	2	0
87	5	3768	OHX	1	0
87	5	3417	OHX	2	0
87	3	202	OHX	1	0
87	5	3454	OHX	1	0
87	S2	301	OHX	2	0
87	6	1967	OHX	1	0
87	2	1966	OHX	1	0
87	1	3579	OHX	2	0
87	1	3747	OHX	9	0
87	1	3787	OHX	1	0
87	1	3733	OHX	11	0
87	5	3570	OHX	1	0
87	1	3695	OHX	1	0
87	2	2044	OHX	2	0
87	6	1956	OHX	1	0
87	5	3594	OHX	1	0
87	1	3582	OHX	2	0
87	5	3785	OHX	1	0
87	5	3649	OHX	2	0
87	6	2004	OHX	1	0
87	1	3663	OHX	1	0
87	1	3727	OHX	1	0
87	5	3799	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	1925	OHX	1	0
87	5	3609	OHX	2	0
87	5	3758	OHX	1	0
87	5	3485	OHX	2	0
87	1	3628	OHX	1	0
87	1	3505	OHX	1	0
87	1	3623	OHX	1	0
87	5	3445	OHX	1	0
87	8	206	OHX	1	0
87	1	3534	OHX	1	0
87	1	3668	OHX	1	0
87	1	3764	OHX	1	0
87	5	3697	OHX	1	0
87	Q2	502	OHX	2	0
87	1	3738	OHX	2	0
87	6	2071	OHX	1	0
87	5	3641	OHX	1	0
87	6	1963	OHX	1	0
87	5	3504	OHX	3	0
87	5	3486	OHX	1	0
87	5	3608	OHX	2	0
87	2	2050	OHX	1	0
87	2	1981	OHX	1	0
87	5	3621	OHX	1	0
87	2	1926	OHX	1	0
87	6	1915	OHX	1	0
87	5	3720	OHX	3	0
87	5	3597	OHX	1	0
87	1	3691	OHX	4	0
87	2	2011	OHX	1	0
87	5	3593	OHX	4	0
87	D9	102	OHX	1	0
87	1	3714	OHX	1	0
87	5	3543	OHX	2	0
87	1	3793	OHX	4	0
87	6	1909	OHX	1	0
87	5	3576	OHX	3	0
87	4	209	OHX	1	0
87	2	1904	OHX	1	0
87	5	3553	OHX	1	0
87	1	3541	OHX	2	0
87	2	2018	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	1	3549	OHX	1	0
87	5	3700	OHX	1	0
87	6	2074	OHX	2	0
87	2	1937	OHX	1	0
87	2	1990	OHX	3	0
87	5	3443	OHX	1	0
87	5	3403	OHX	2	0
87	1	3411	OHX	1	0
87	5	3531	OHX	1	0
87	5	3619	OHX	1	0
87	1	3603	OHX	1	0
87	1	3635	OHX	1	0
87	5	3707	OHX	1	0
87	5	3672	OHX	1	0
87	2	1927	OHX	1	0
87	5	3447	OHX	1	0
87	2	2078	OHX	2	0
87	6	2056	OHX	3	0
87	1	3586	OHX	2	0
87	5	3535	OHX	1	0
87	5	3737	OHX	1	0
87	5	3725	OHX	3	0
87	1	3680	OHX	1	0
87	2	1971	OHX	1	0
87	1	3415	OHX	1	0
87	1	3730	OHX	1	0
87	2	1954	OHX	1	0
87	8	219	OHX	2	0
87	1	3444	OHX	1	0
87	1	3659	OHX	2	0
87	6	2023	OHX	1	0
87	1	3518	OHX	1	0
87	1	3706	OHX	2	0
87	1	3443	OHX	1	0
87	1	3416	OHX	1	0
87	6	1992	OHX	1	0
87	1	3436	OHX	1	0
87	1	3774	OHX	1	0
87	1	3503	OHX	1	0
87	6	2091	OHX	1	0
87	6	2016	OHX	3	0
87	2	1970	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	6	1978	OHX	2	0
87	2	1961	OHX	1	0
87	5	3726	OHX	1	0
87	5	3434	OHX	1	0
87	1	3442	OHX	1	0
87	1	3724	OHX	2	0
87	5	3435	OHX	1	0
87	1	3649	OHX	1	0
87	5	3419	OHX	1	0
87	5	3493	OHX	2	0
87	1	3538	OHX	1	0
87	2	1995	OHX	1	0
87	2	2033	OHX	1	0
87	1	3515	OHX	1	0
87	2	1988	OHX	1	0
87	5	3513	OHX	1	0
87	8	201	OHX	2	0
87	1	3694	OHX	1	0
87	2	2003	OHX	3	0
87	8	215	OHX	1	0
87	5	3773	OHX	1	0
87	5	3789	OHX	1	0
87	6	1997	OHX	2	0
87	1	3681	OHX	3	0
87	1	3726	OHX	3	0
87	15	302	OHX	3	0
87	6	2092	OHX	1	0
87	5	3409	OHX	2	0
87	n9	101	OHX	1	0
87	5	3705	OHX	3	0
87	1	3686	OHX	1	0
87	1	3758	OHX	3	0
87	1	3771	OHX	1	0
87	1	3544	OHX	1	0
87	1	3446	OHX	1	0
87	1	3463	OHX	1	0
87	1	3566	OHX	2	0
87	6	2077	OHX	1	0
87	1	3636	OHX	2	0
87	5	3769	OHX	1	0
87	S8	301	OHX	2	0
87	5	3500	OHX	1	0

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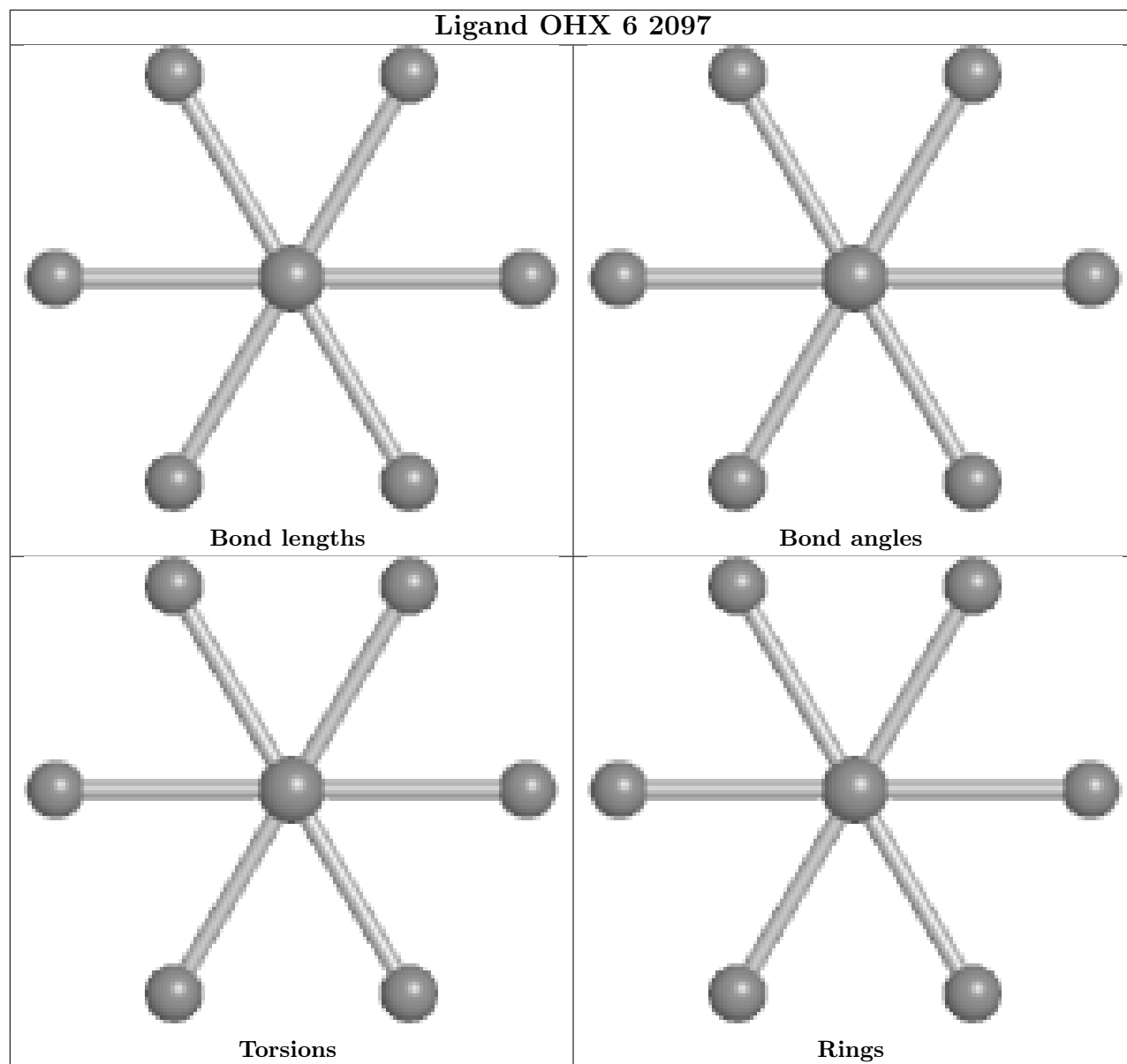
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	8	203	OHX	2	0
87	2	1993	OHX	1	0
87	5	3422	OHX	1	0
87	2	2009	OHX	2	0
87	6	1991	OHX	2	0
87	2	1924	OHX	1	0
87	n3	201	OHX	1	0
87	2	1928	OHX	1	0
87	m0	301	OHX	1	0
87	1	3809	OHX	1	0
87	6	2098	OHX	5	0
87	1	3409	OHX	1	0
87	1	3650	OHX	1	0
87	2	2030	OHX	2	0
87	1	3471	OHX	3	0
87	2	1975	OHX	2	0
87	5	3753	OHX	1	0
87	5	3411	OHX	1	0
87	2	2035	OHX	4	0
87	6	2054	OHX	1	0
87	5	3592	OHX	1	0
87	2	1909	OHX	5	0
87	2	1943	OHX	1	0
87	c5	201	OHX	3	0
87	5	3492	OHX	1	0
87	6	1921	OHX	3	0
87	6	1926	OHX	1	0
87	6	1911	OHX	3	0
87	1	3805	OHX	6	0
87	2	1938	OHX	1	0
87	2	1974	OHX	1	0
87	2	1950	OHX	1	0
87	1	3776	OHX	2	0
87	1	3753	OHX	2	0
87	5	3534	OHX	2	0
87	m0	304	OHX	1	0
87	5	3665	OHX	1	0
87	5	3521	OHX	1	0
87	2	2062	OHX	1	0
87	2	1949	OHX	2	0
87	s4	301	OHX	1	0
87	1	3540	OHX	2	0

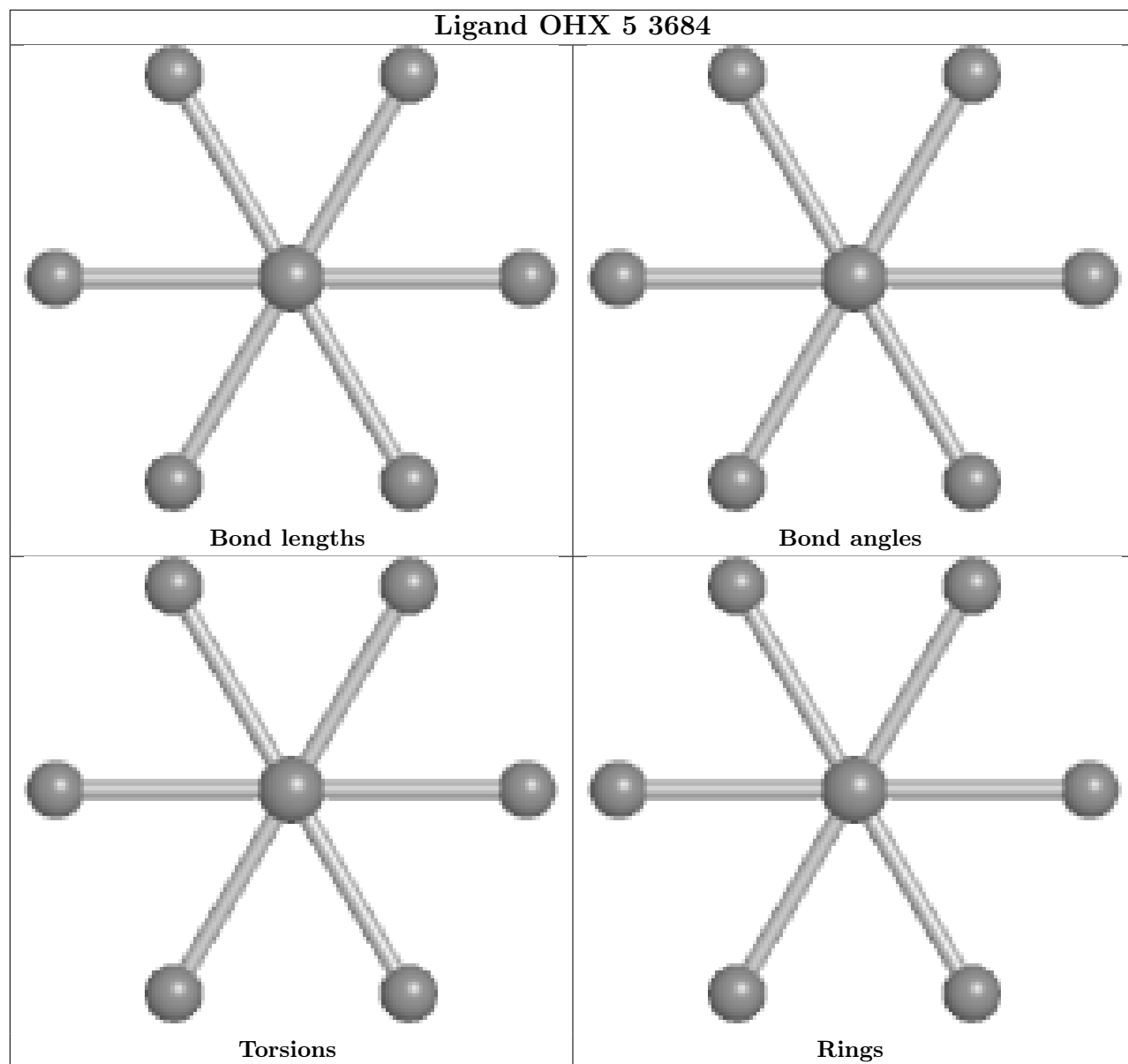
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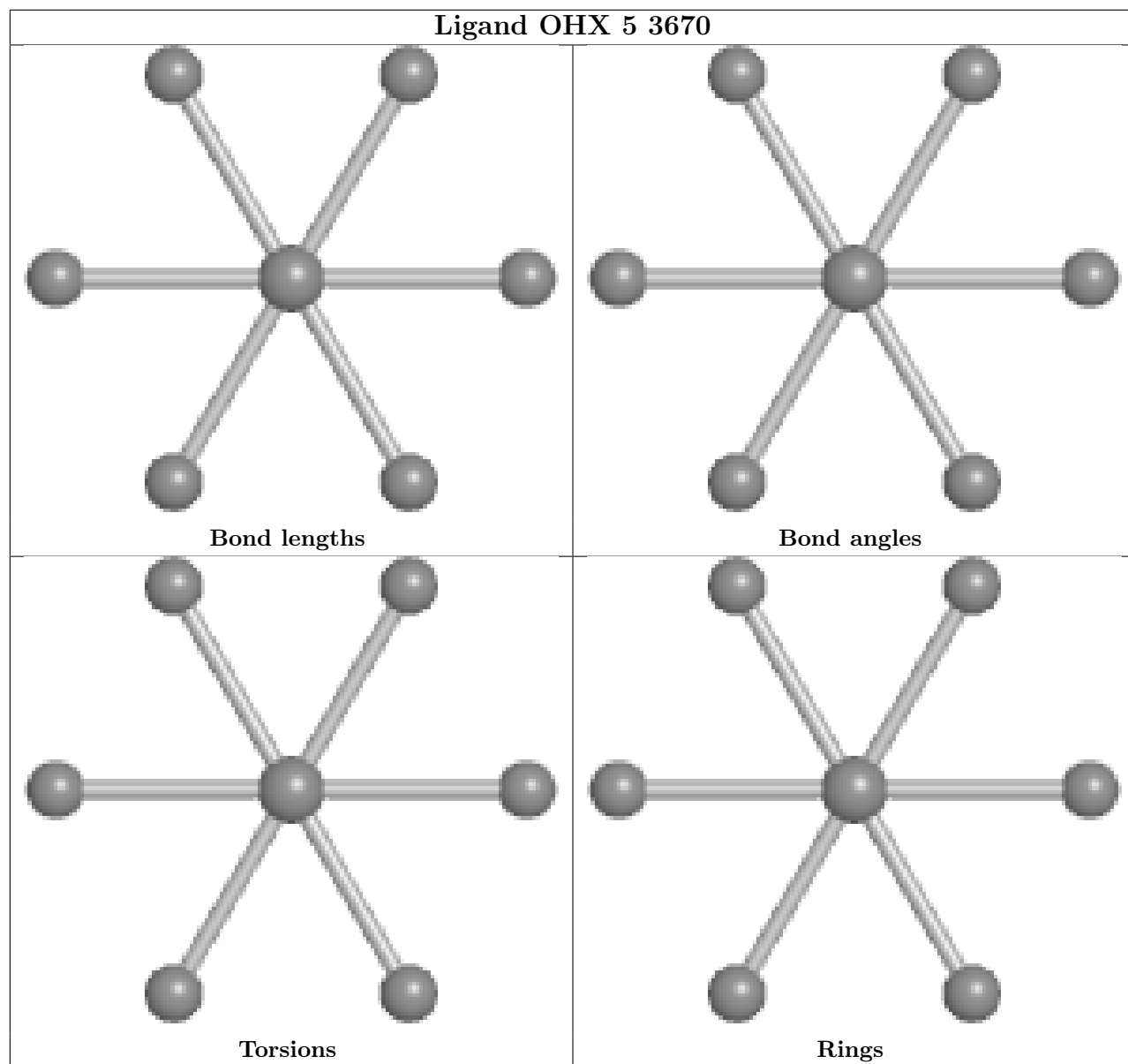
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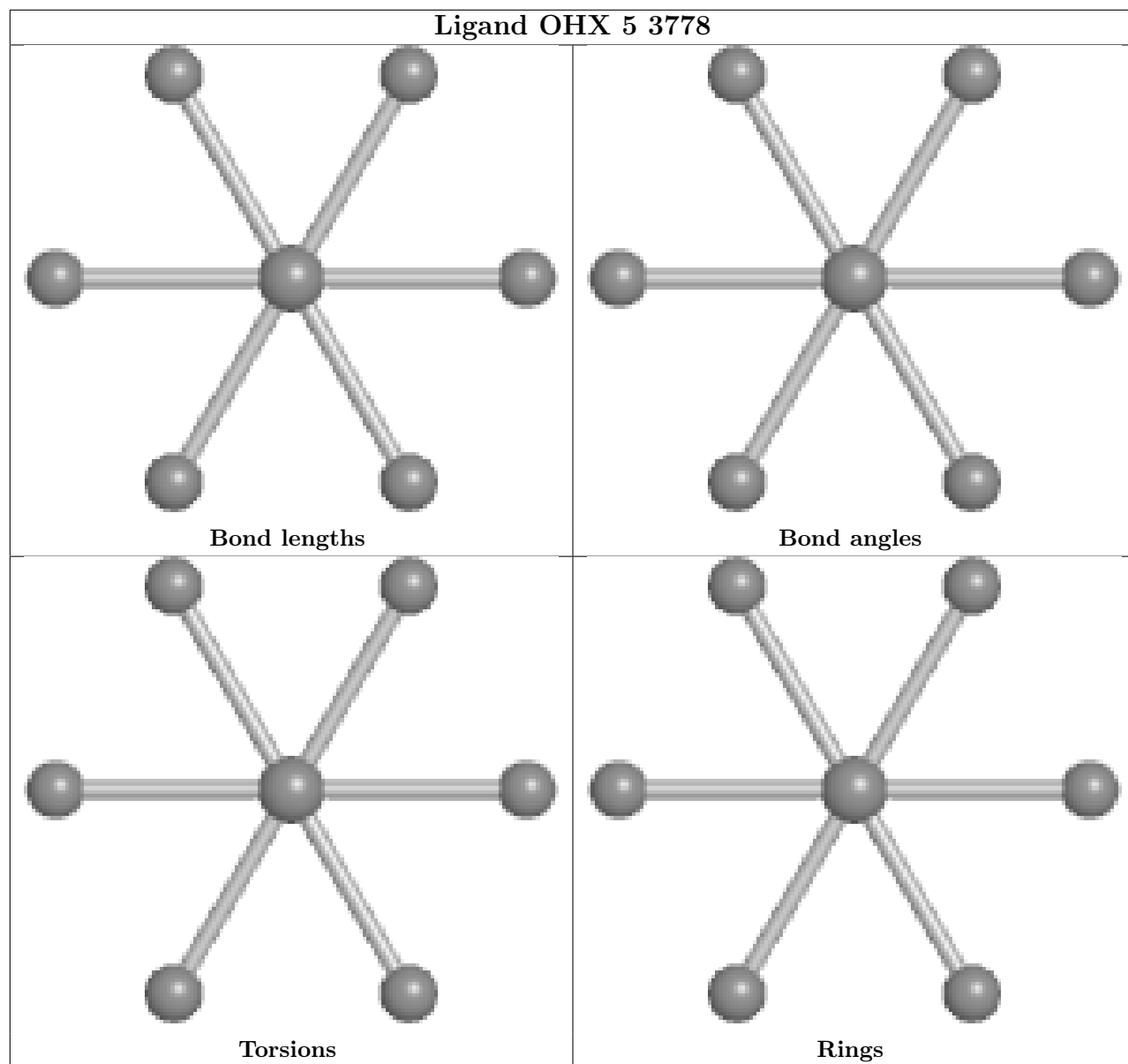
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	5	3755	OHX	1	0
87	1	3777	OHX	2	0
87	5	3802	OHX	3	0
87	1	3470	OHX	2	0
87	1	3558	OHX	2	0
87	1	3456	OHX	1	0
87	6	1916	OHX	2	0
87	2	2067	OHX	1	0
87	1	3736	OHX	1	0
87	2	2016	OHX	1	0
87	5	3676	OHX	1	0
87	2	1914	OHX	2	0
87	6	1980	OHX	1	0
87	s1	301	OHX	2	0
87	1	3574	OHX	1	0
87	1	3495	OHX	1	0
87	14	401	OHX	3	0
87	2	1955	OHX	1	0
87	1	3426	OHX	1	0
87	1	3683	OHX	1	0
87	1	3632	OHX	1	0
87	5	3754	OHX	1	0
87	1	3775	OHX	1	0

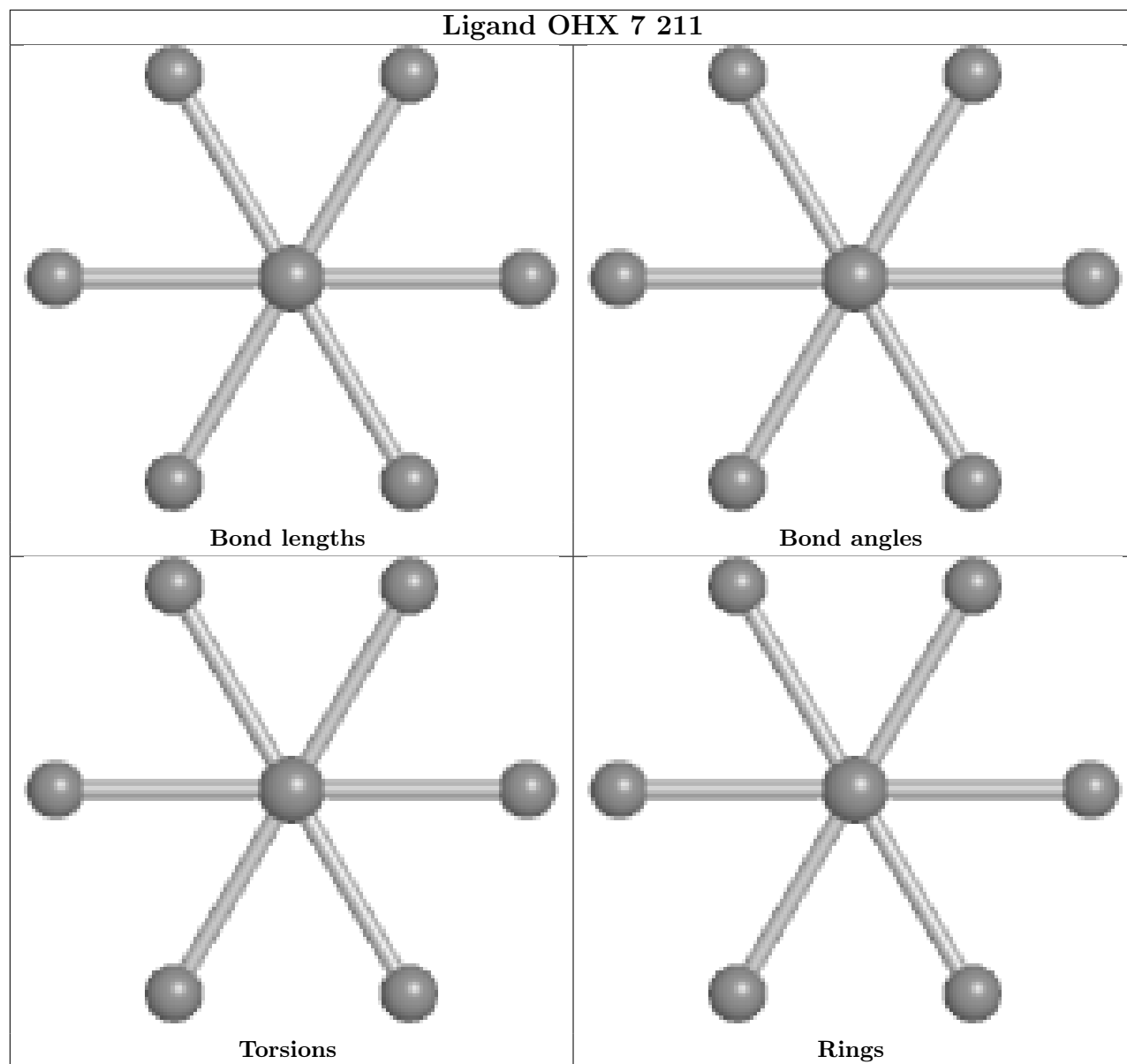
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

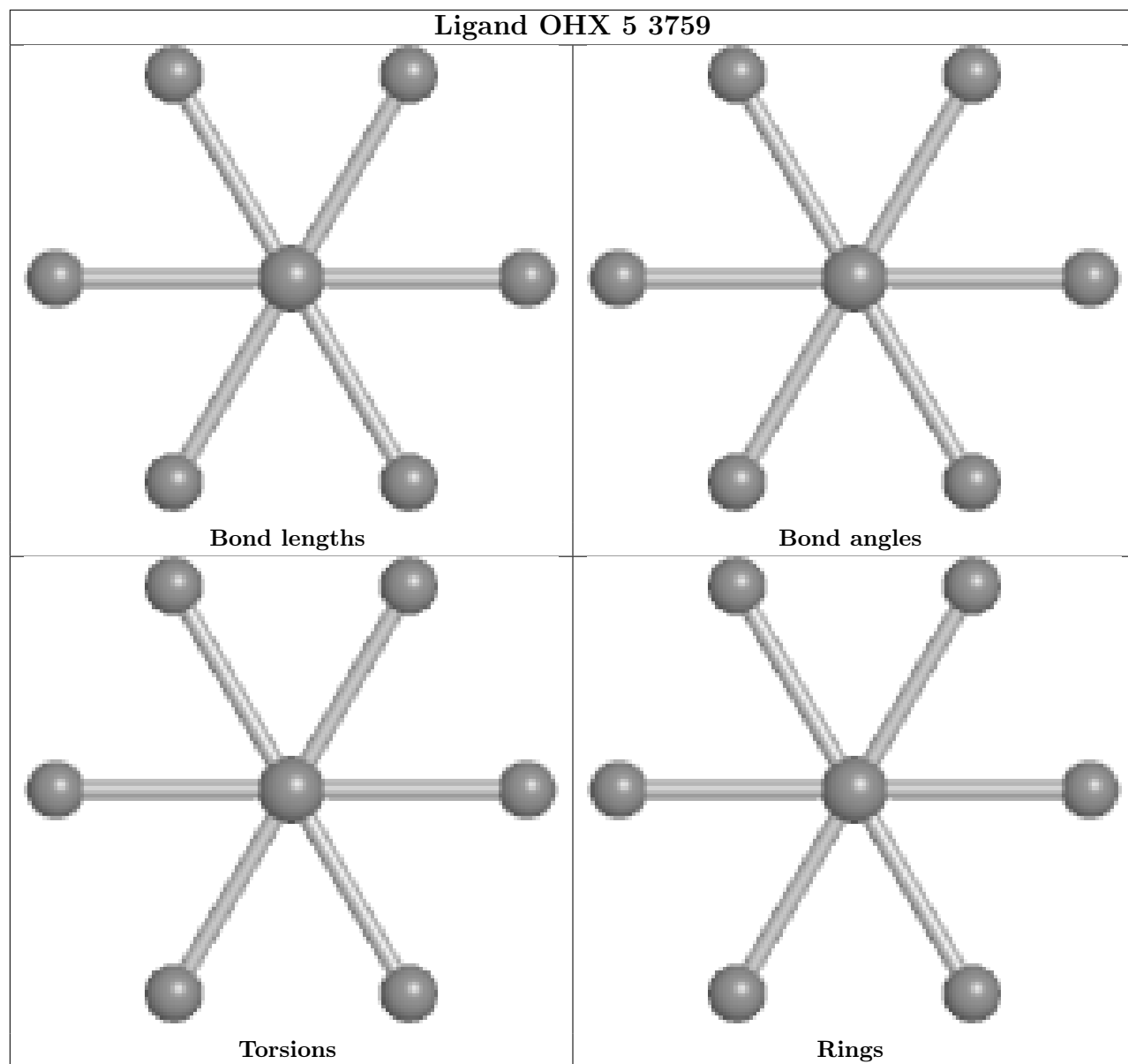


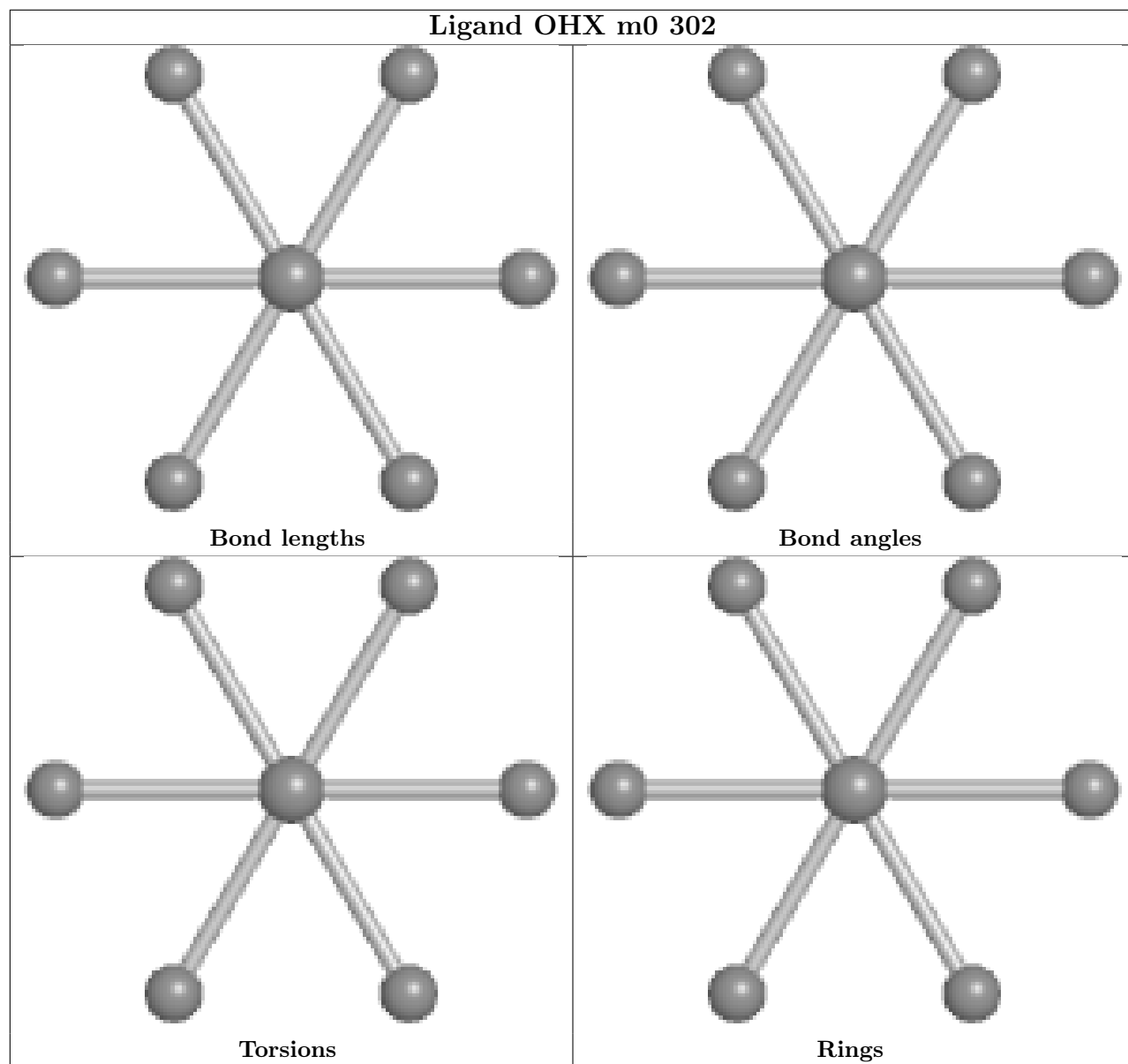


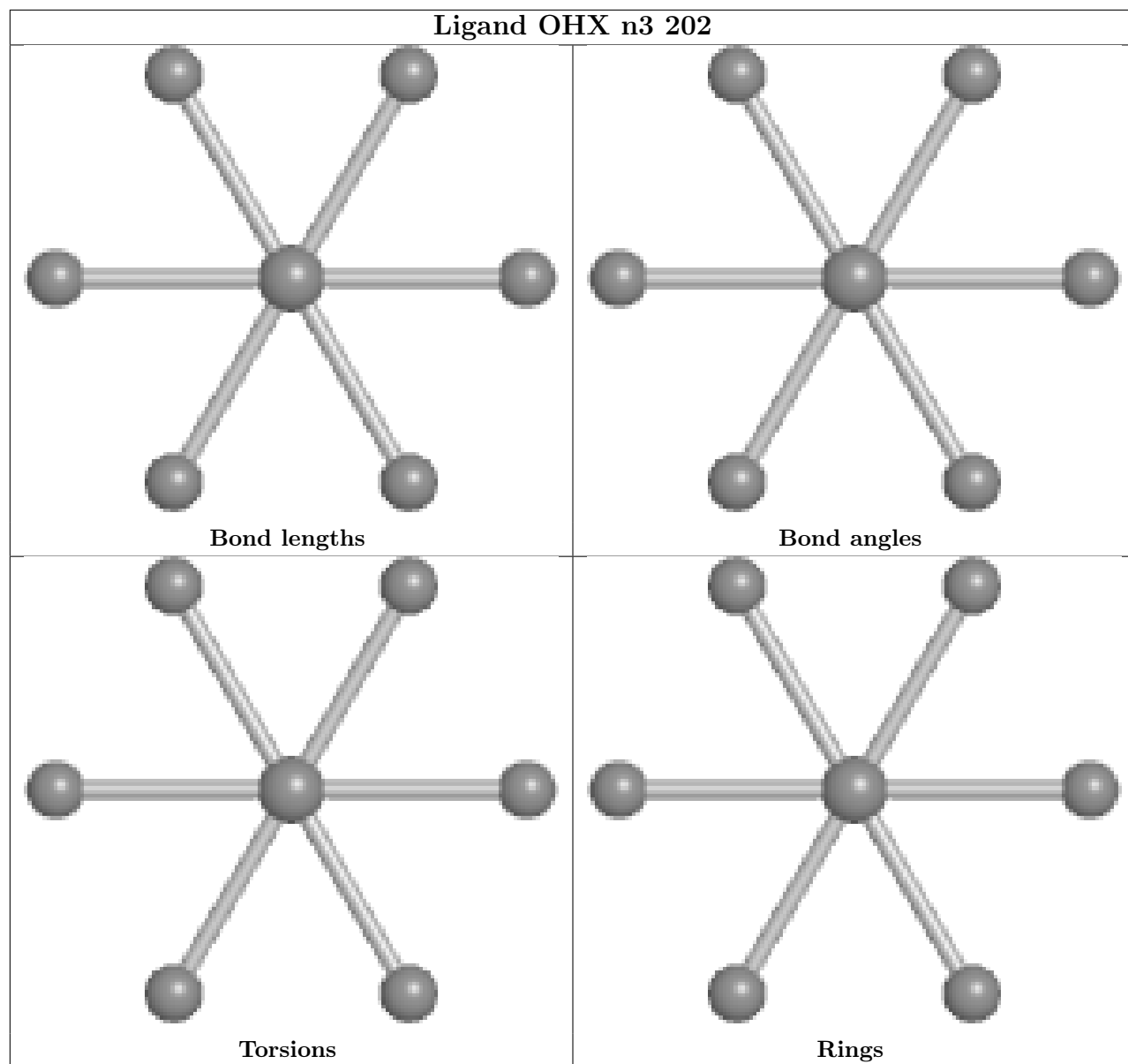


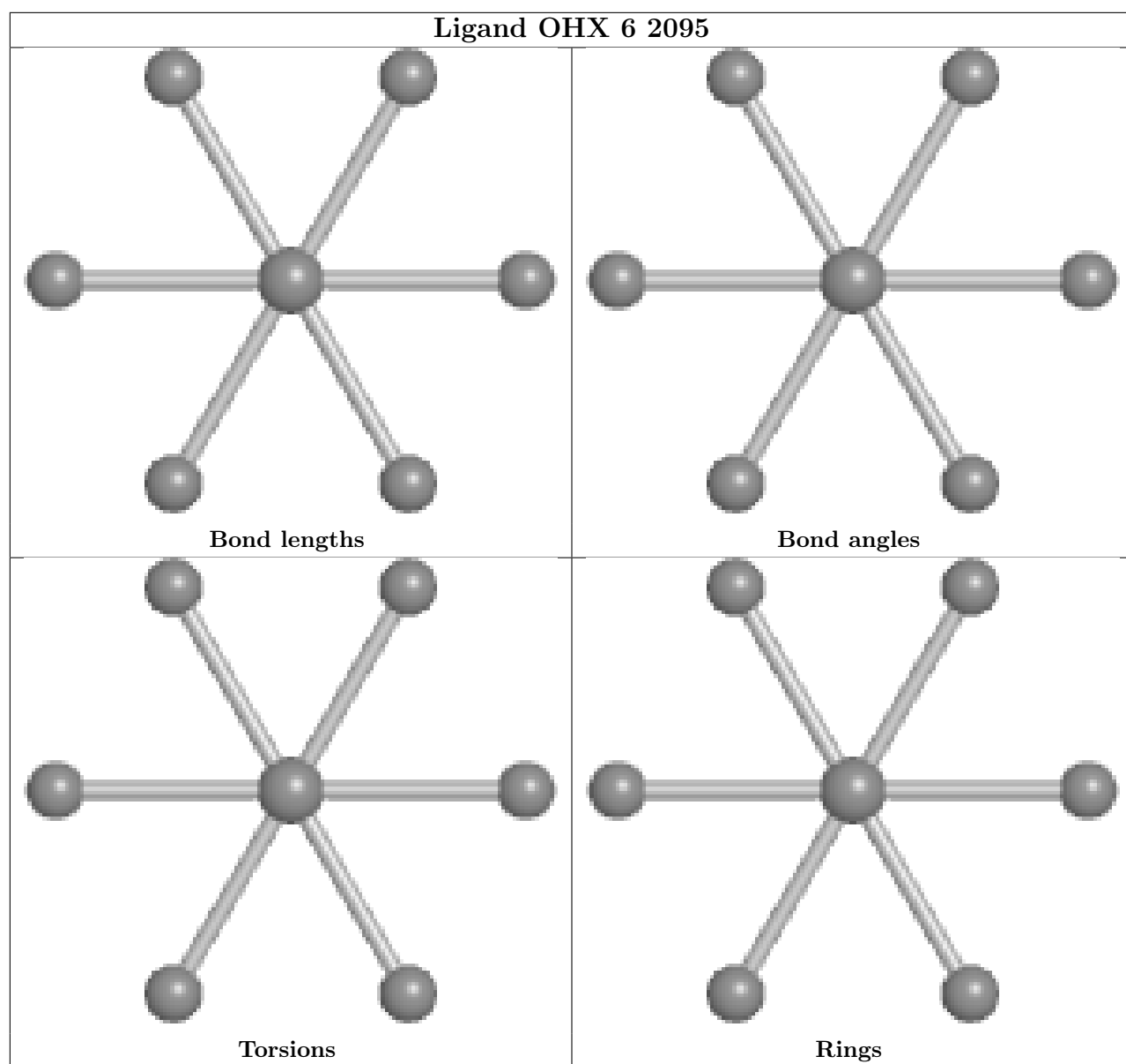


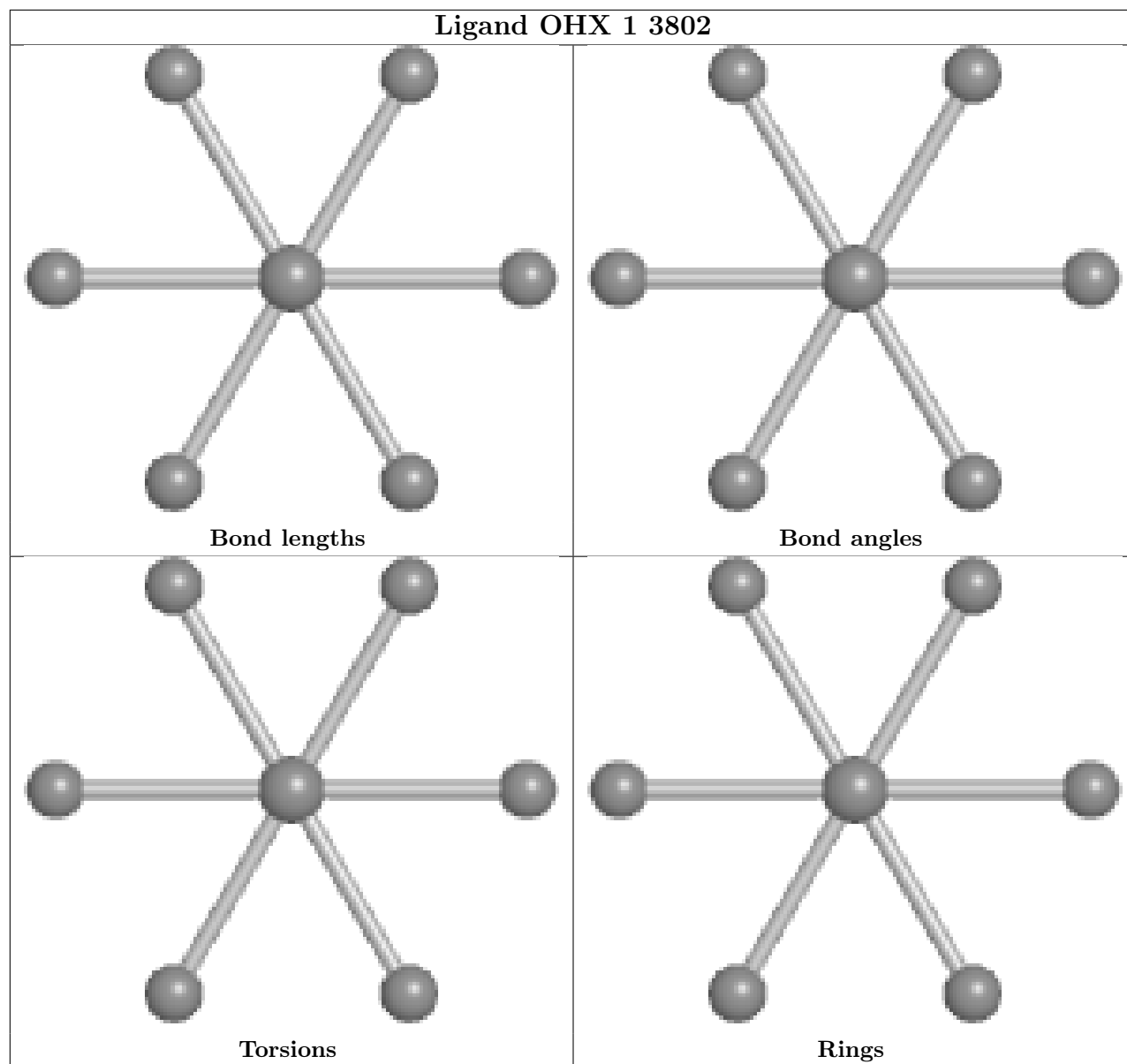


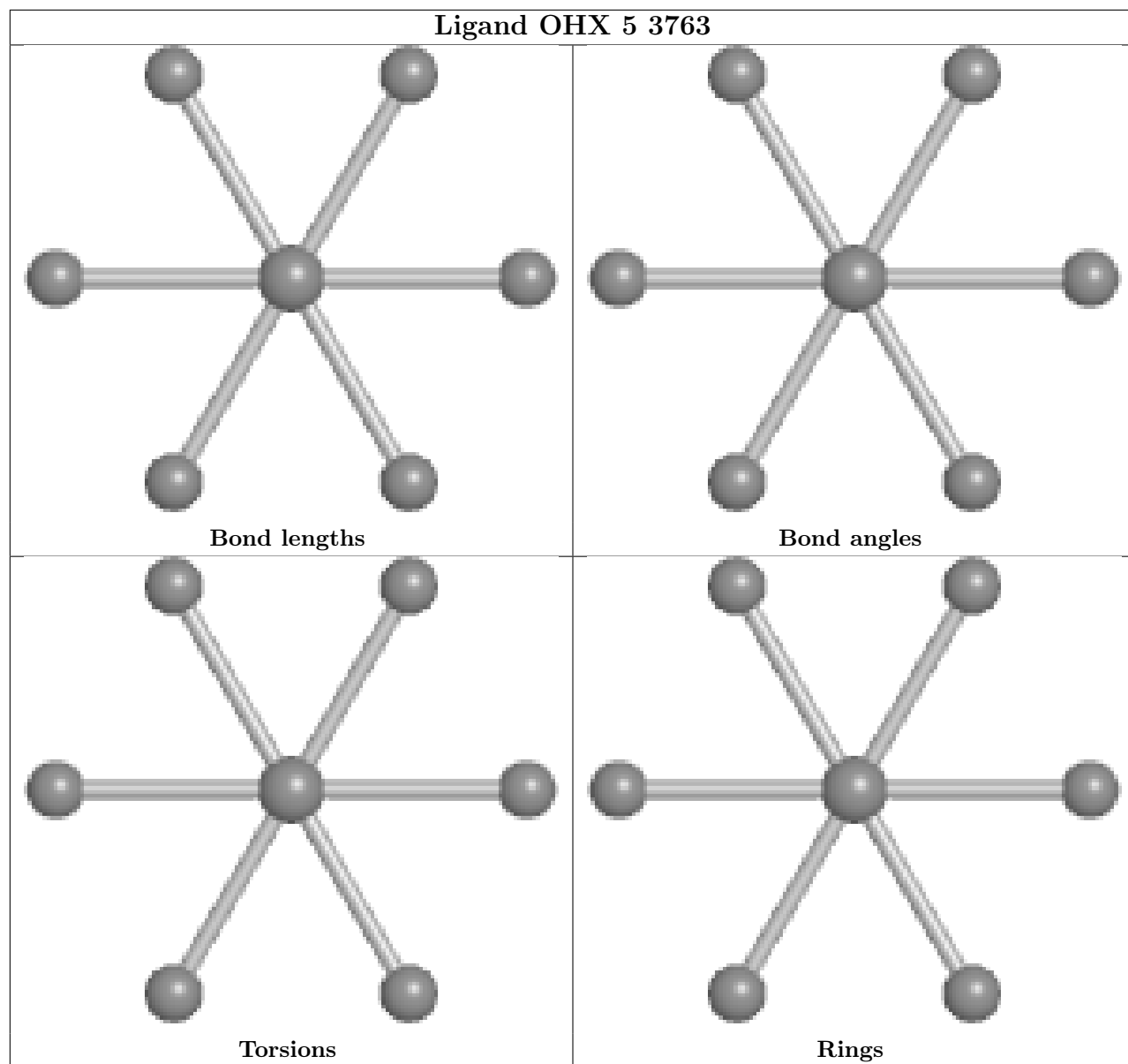


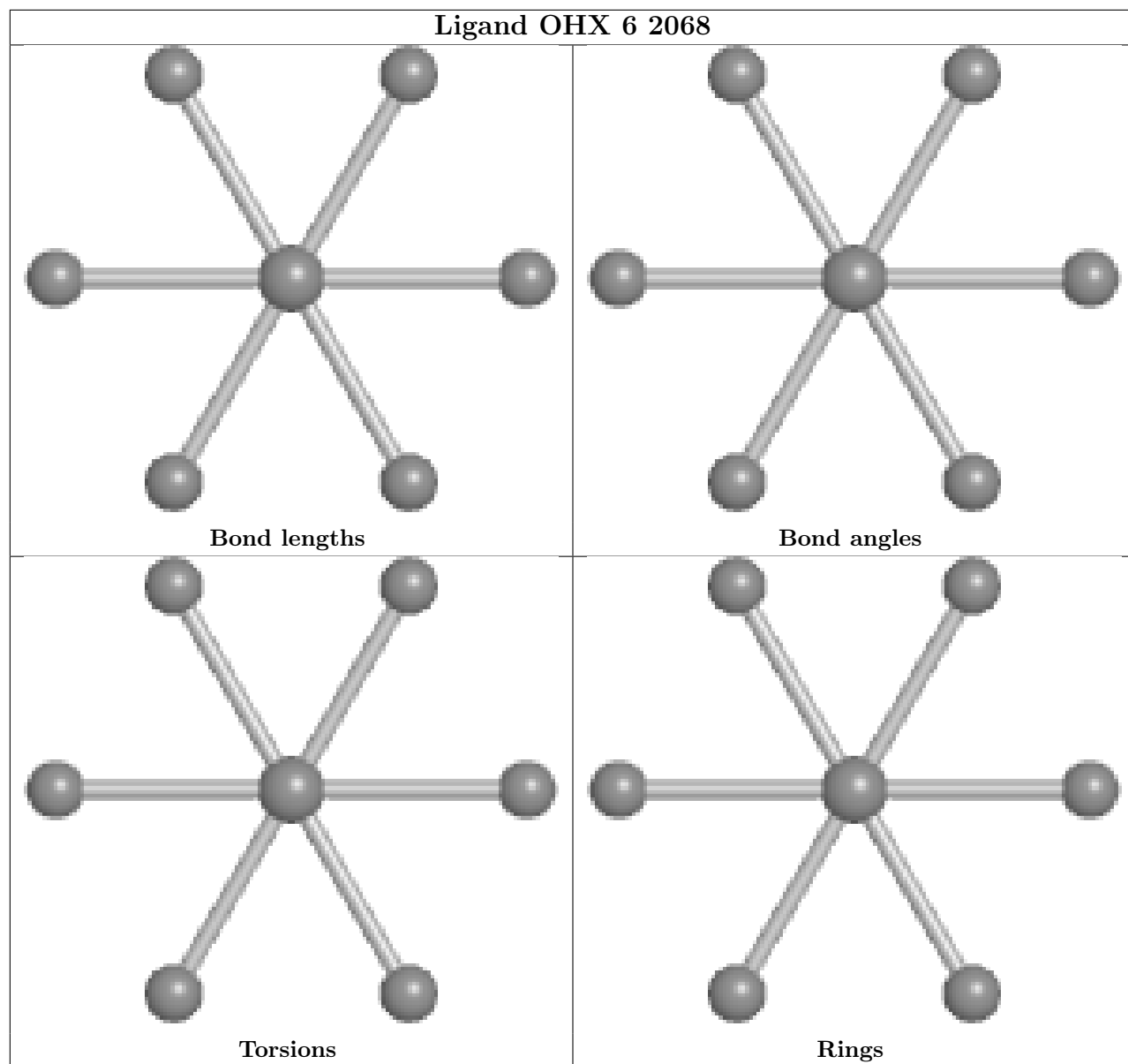


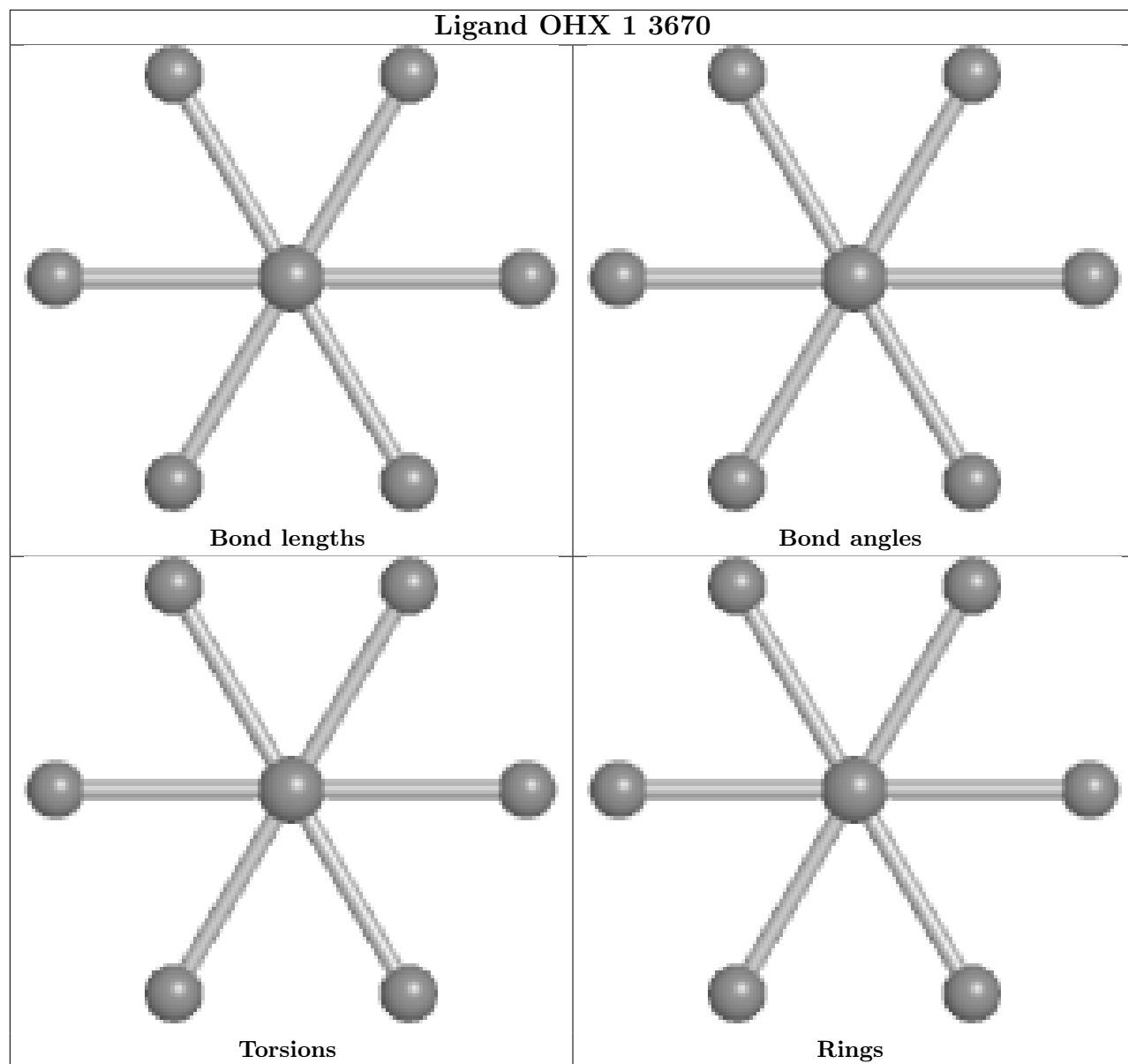


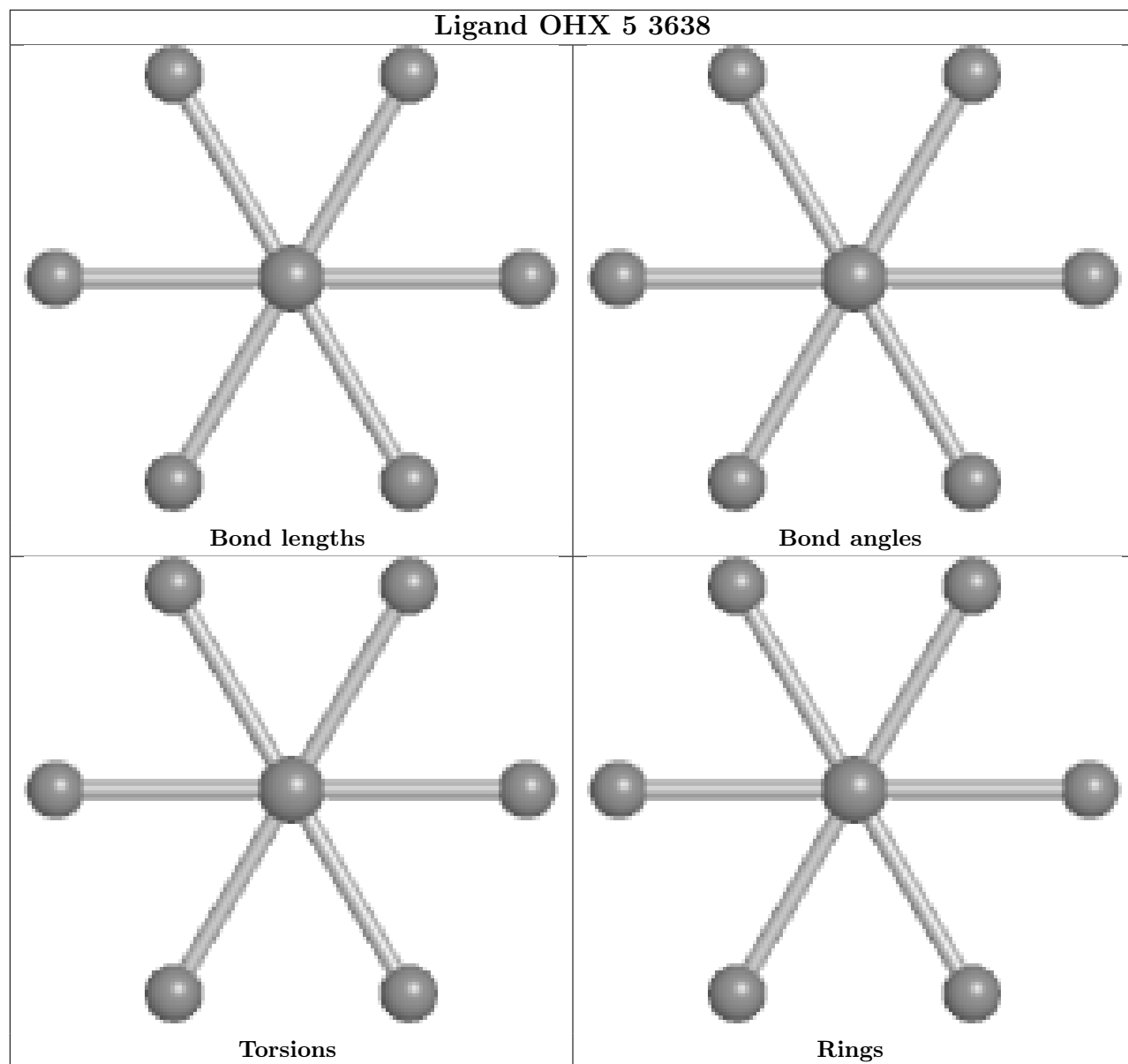


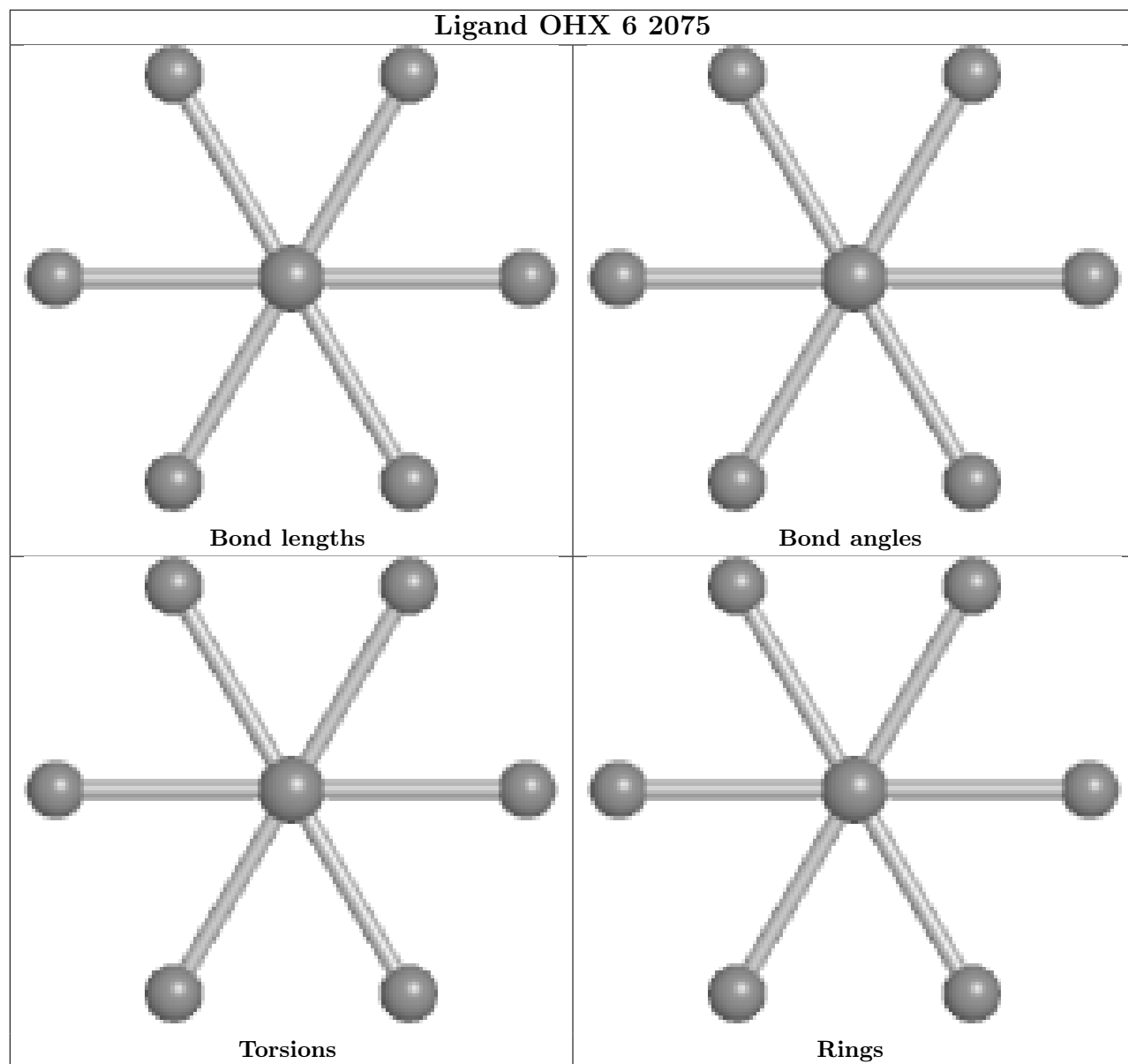


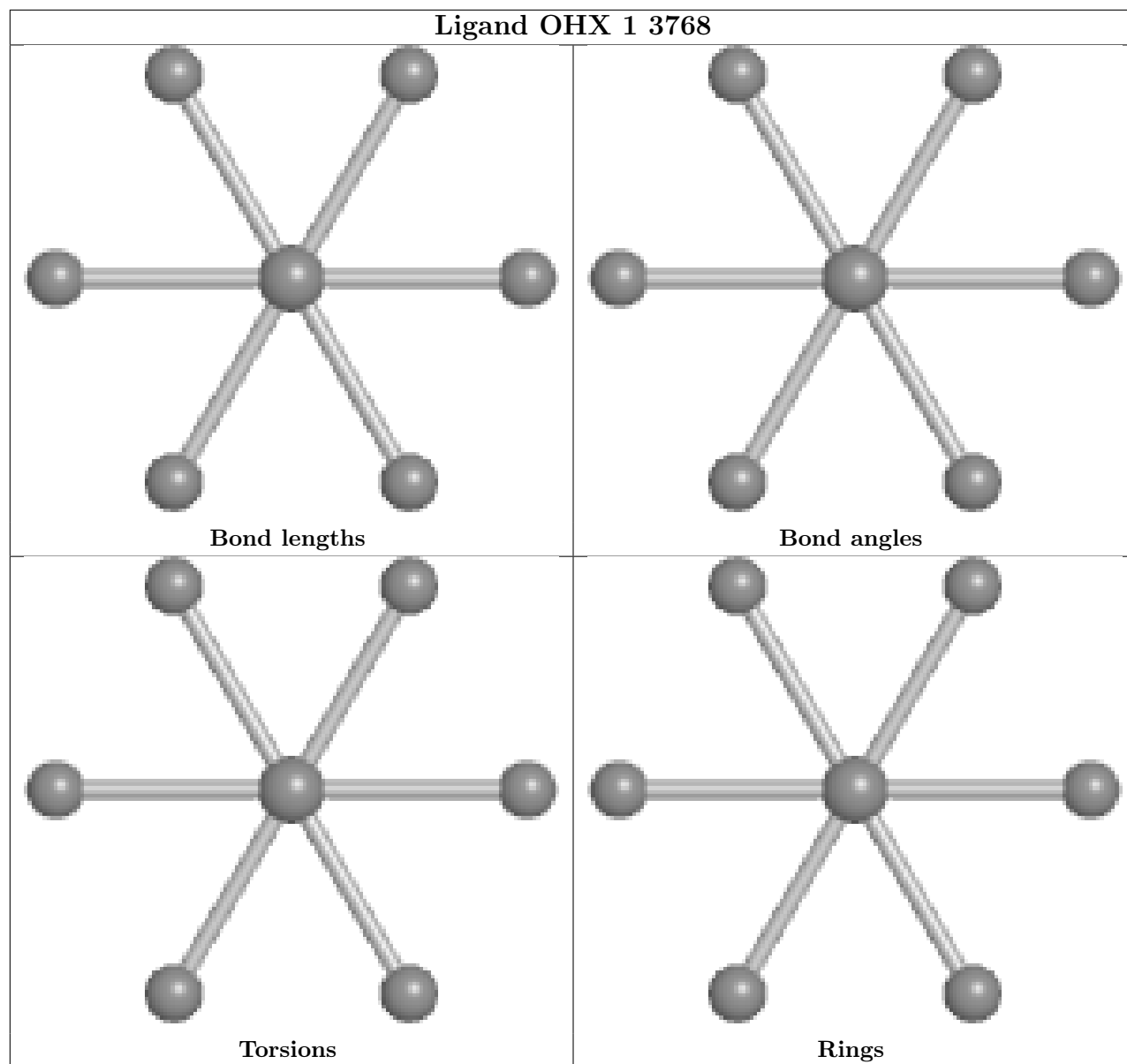


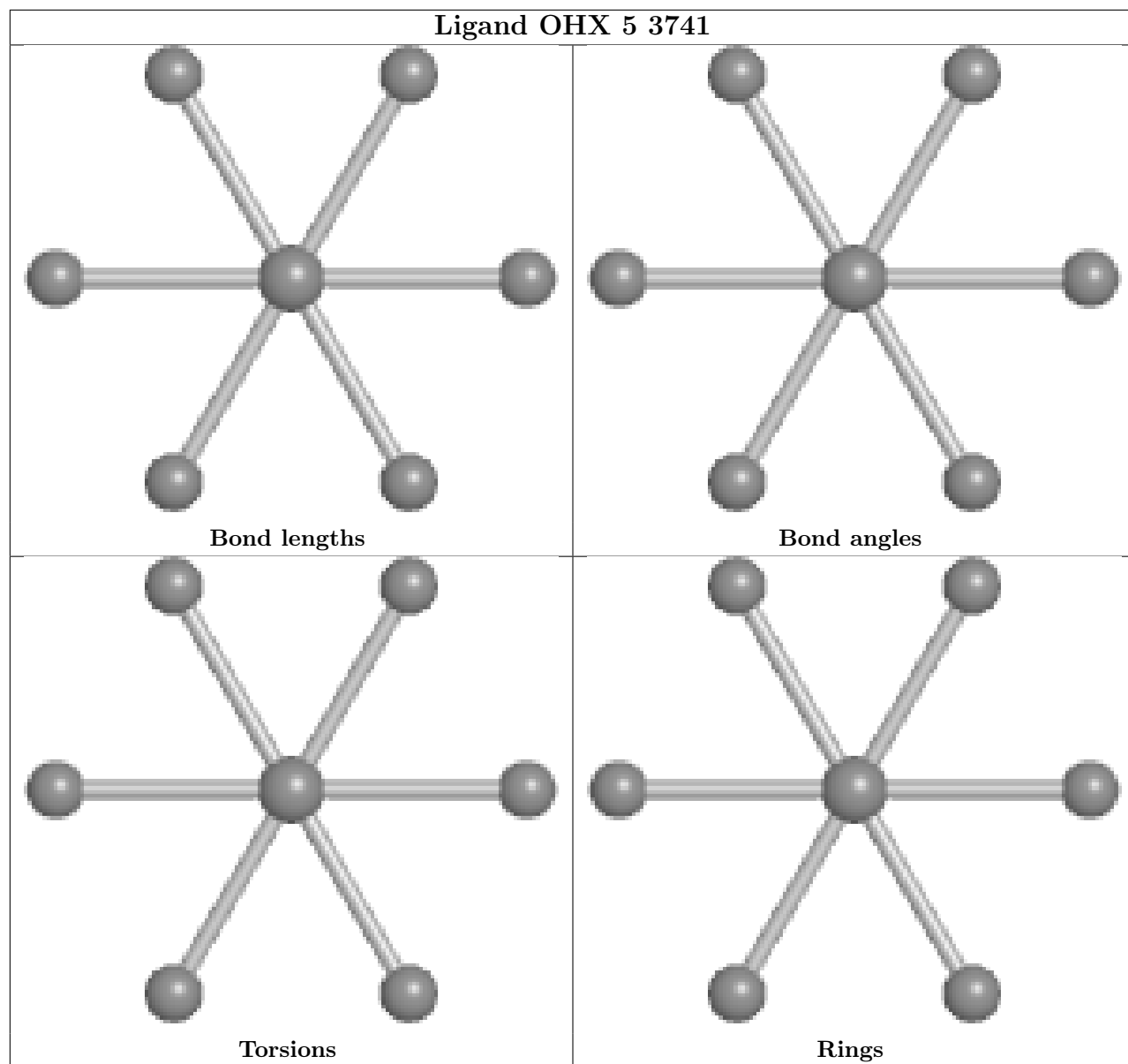


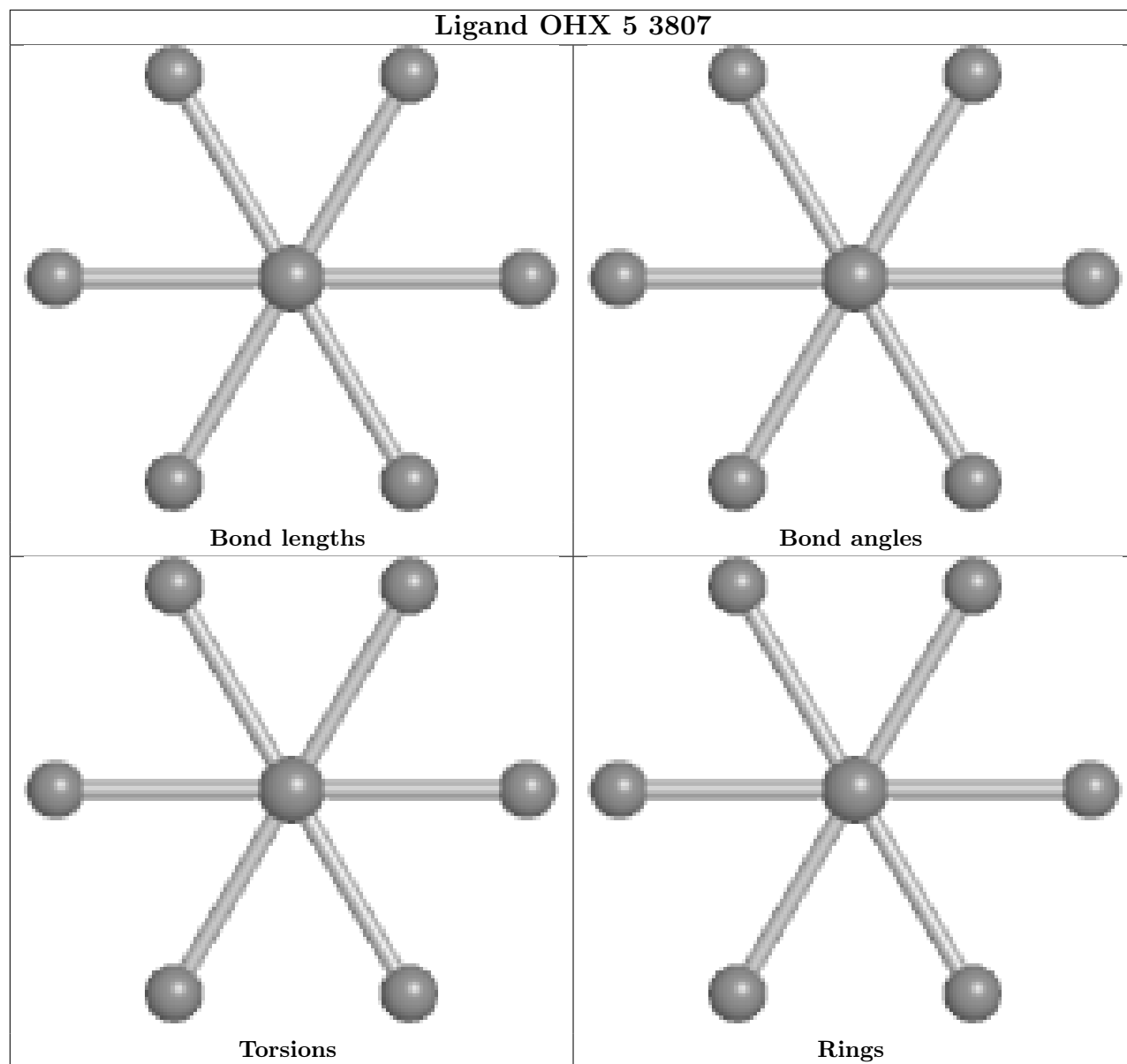


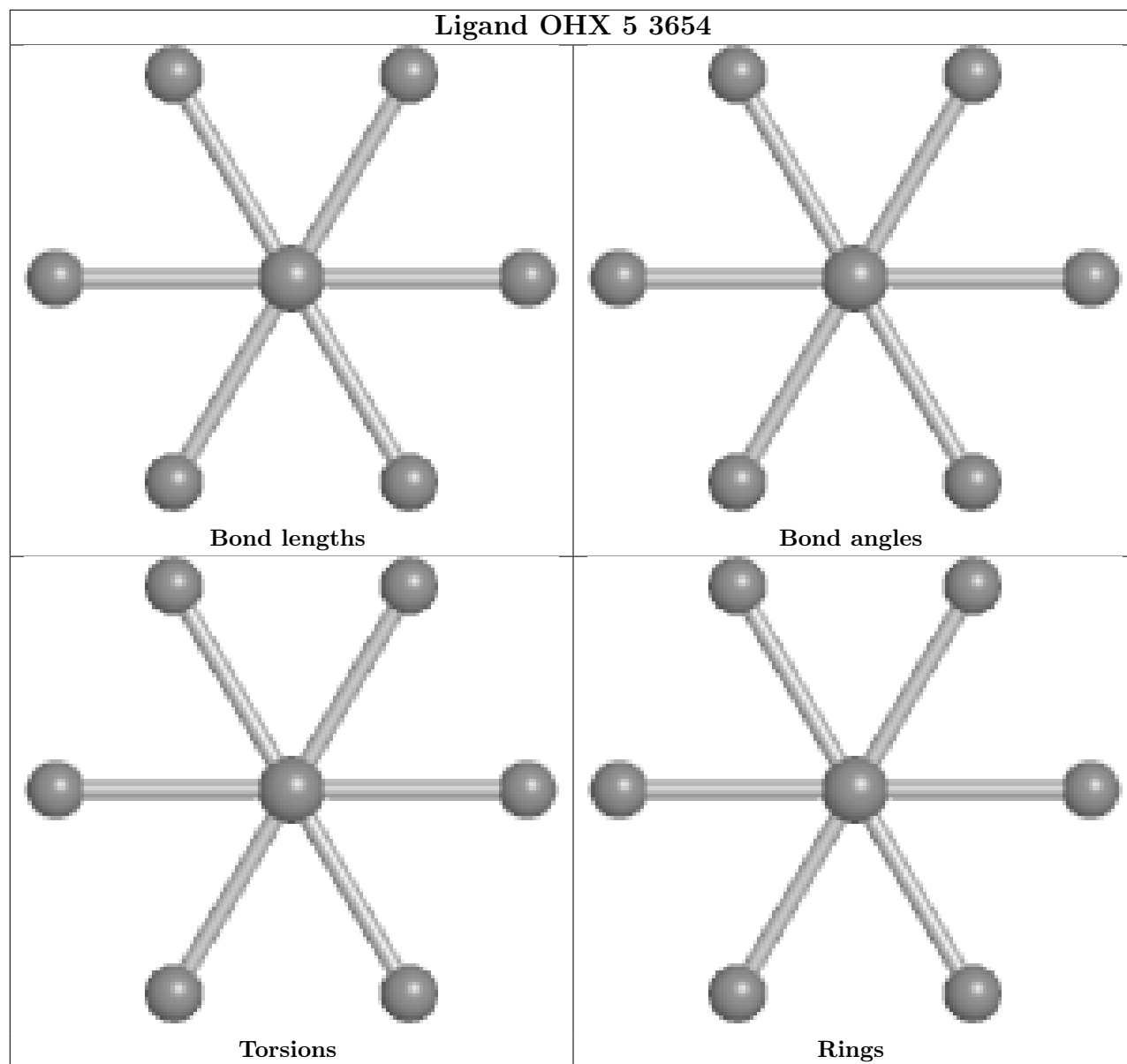


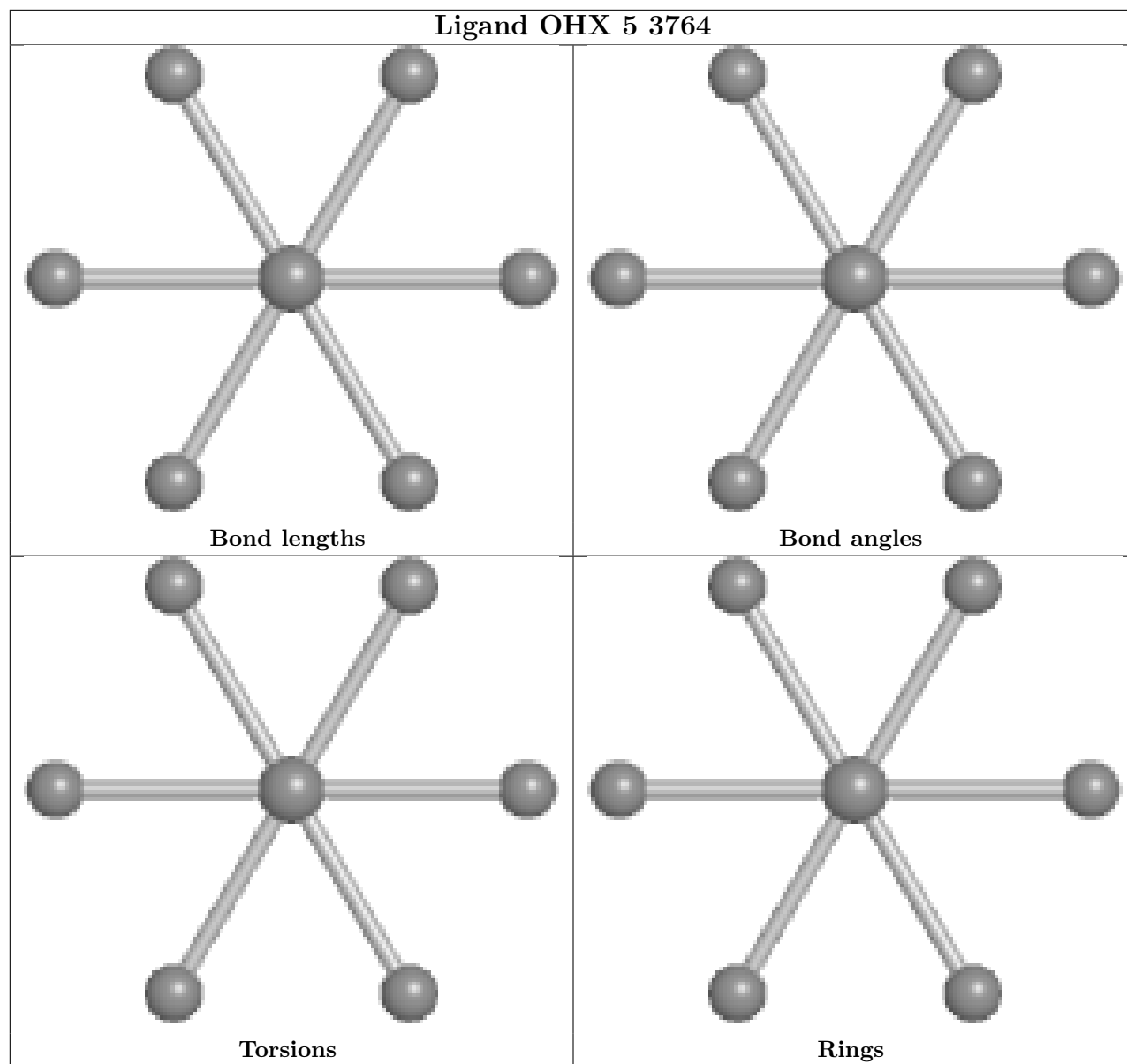


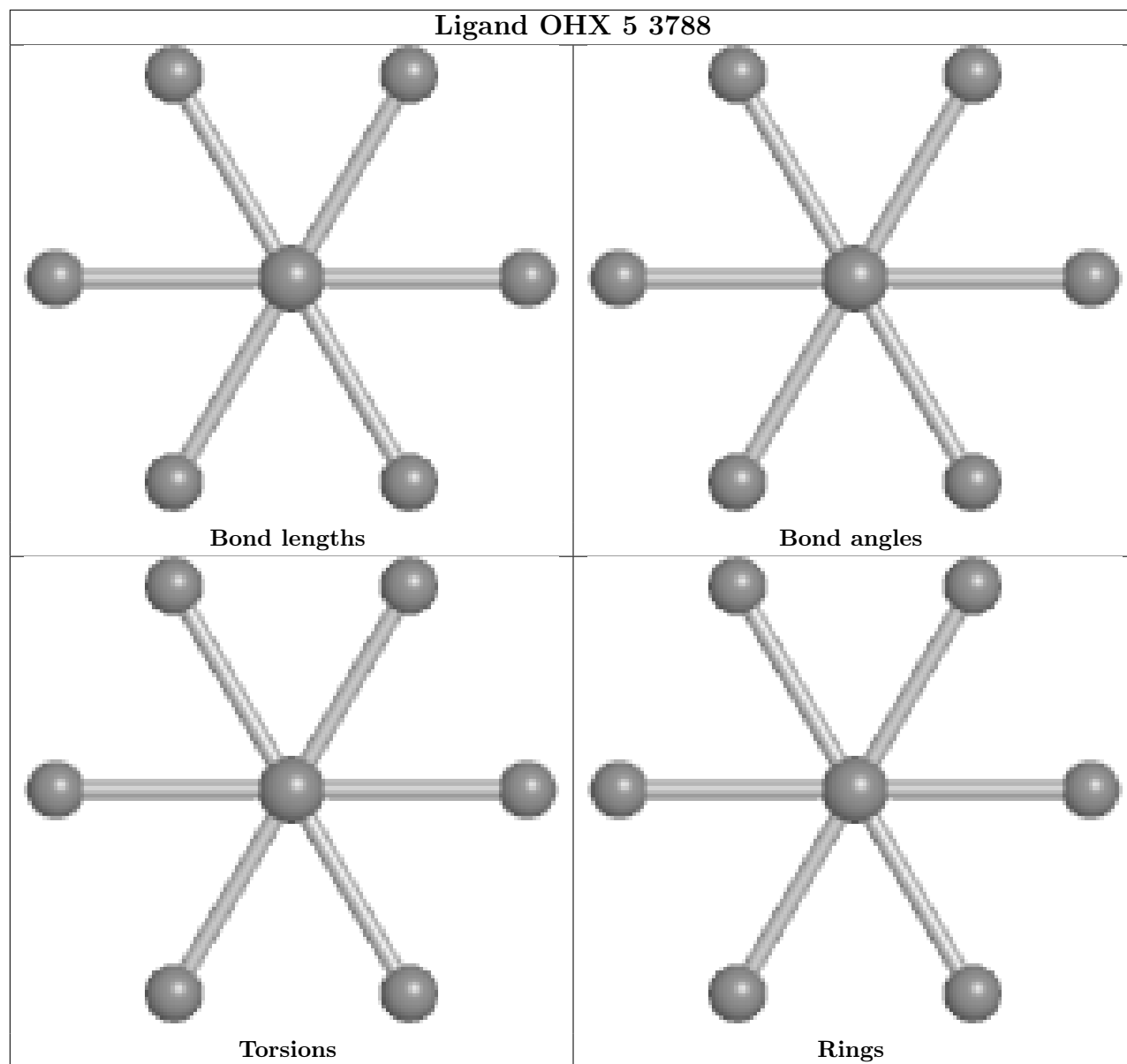


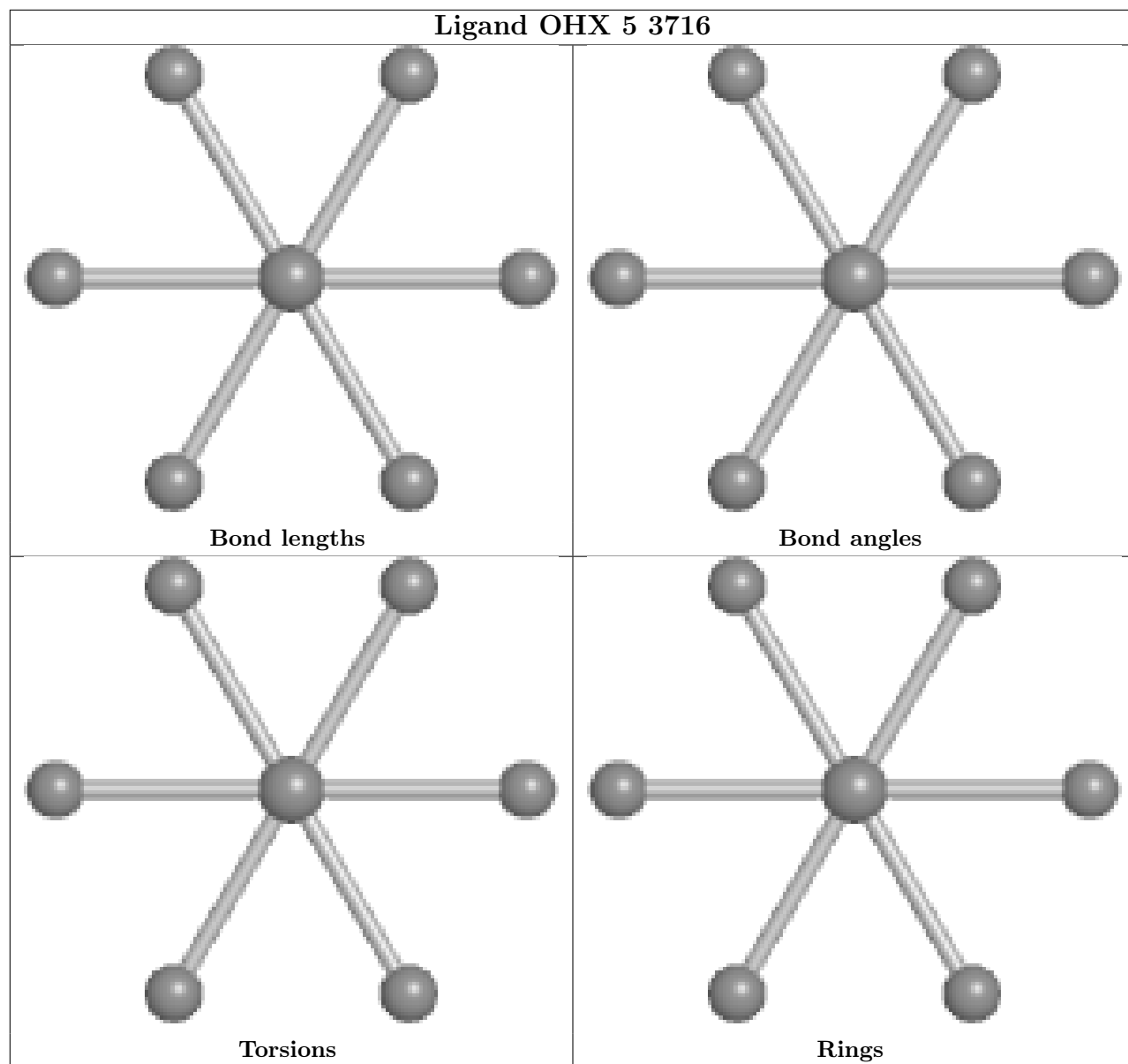


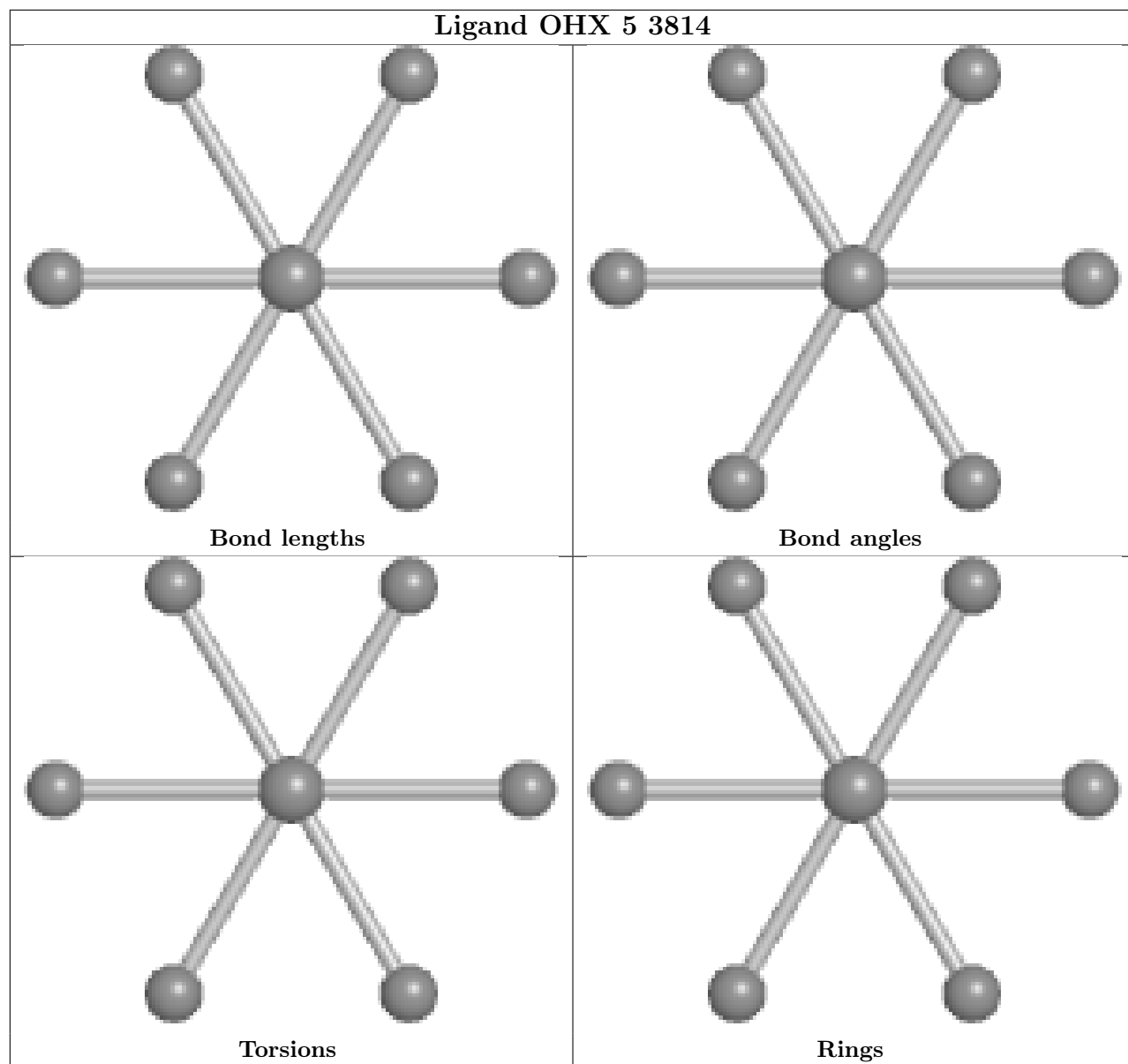


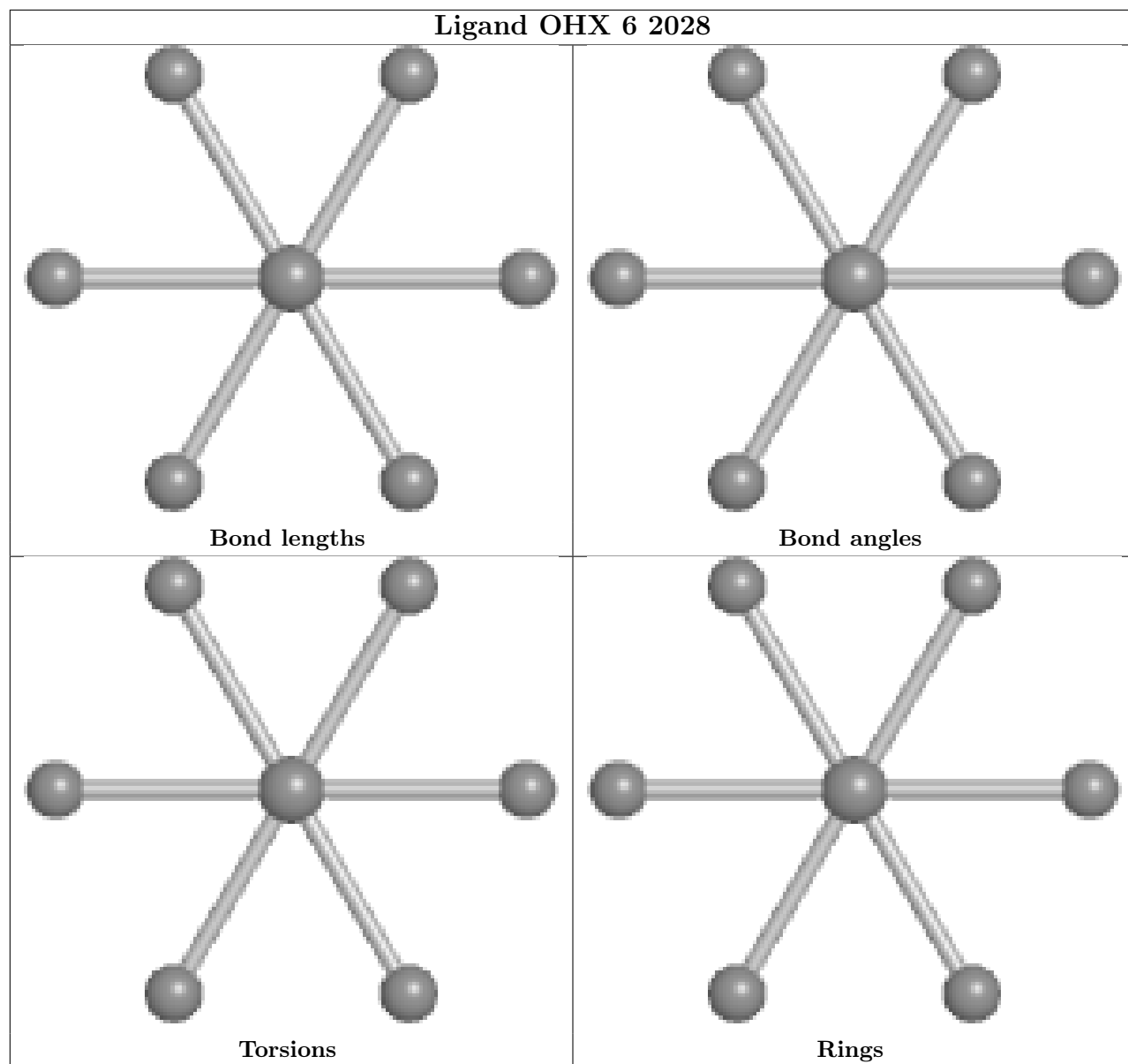


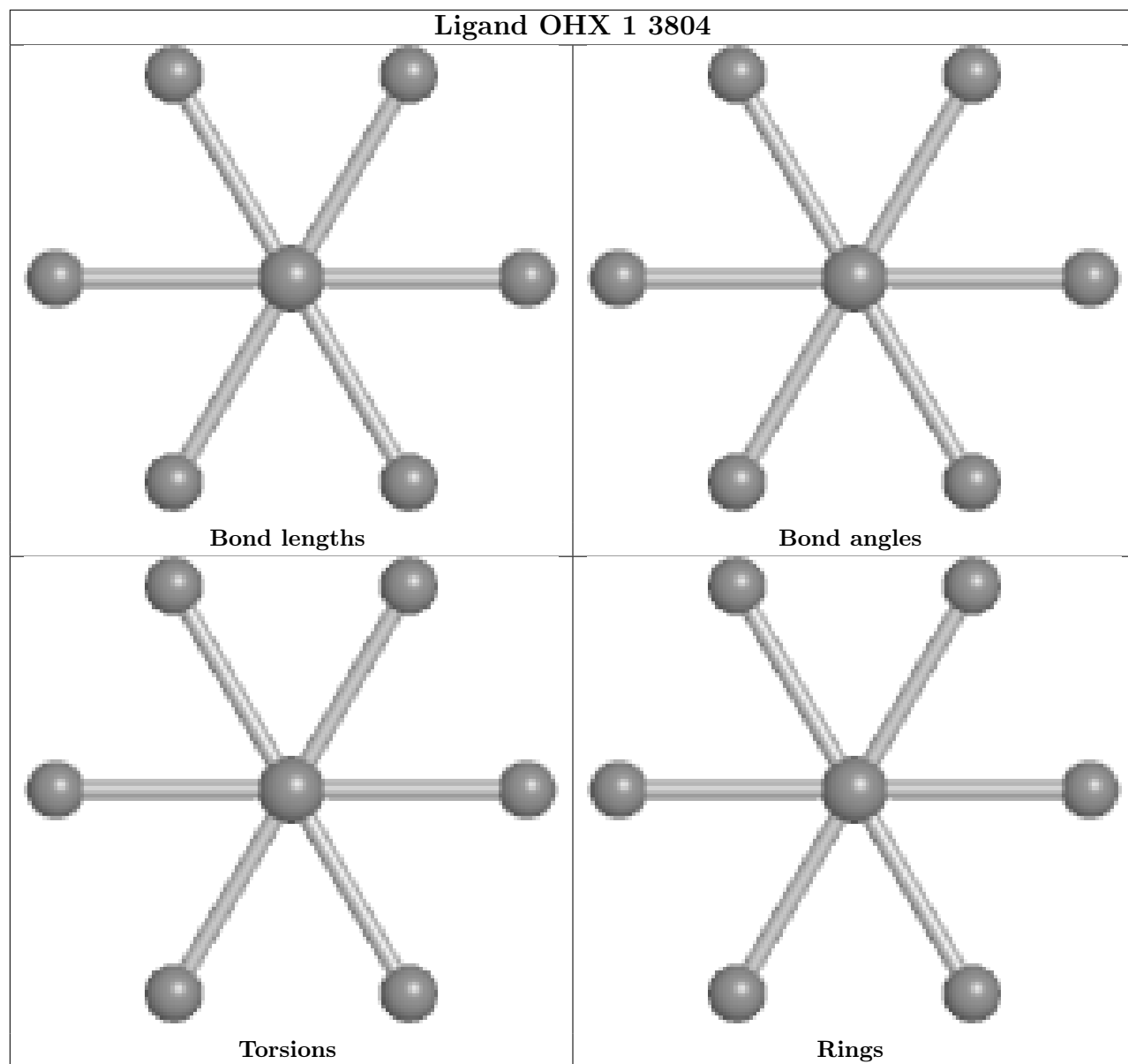


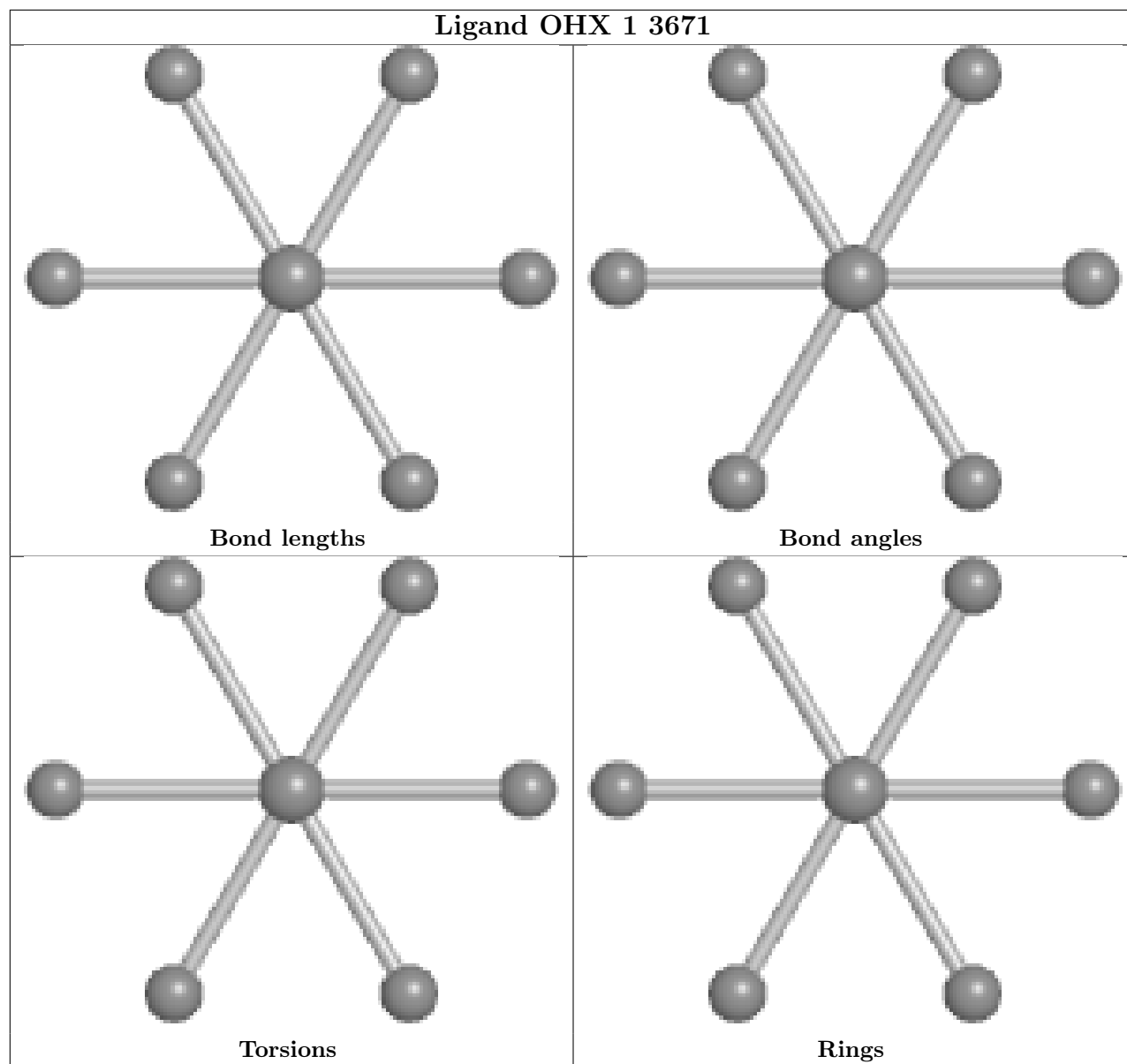


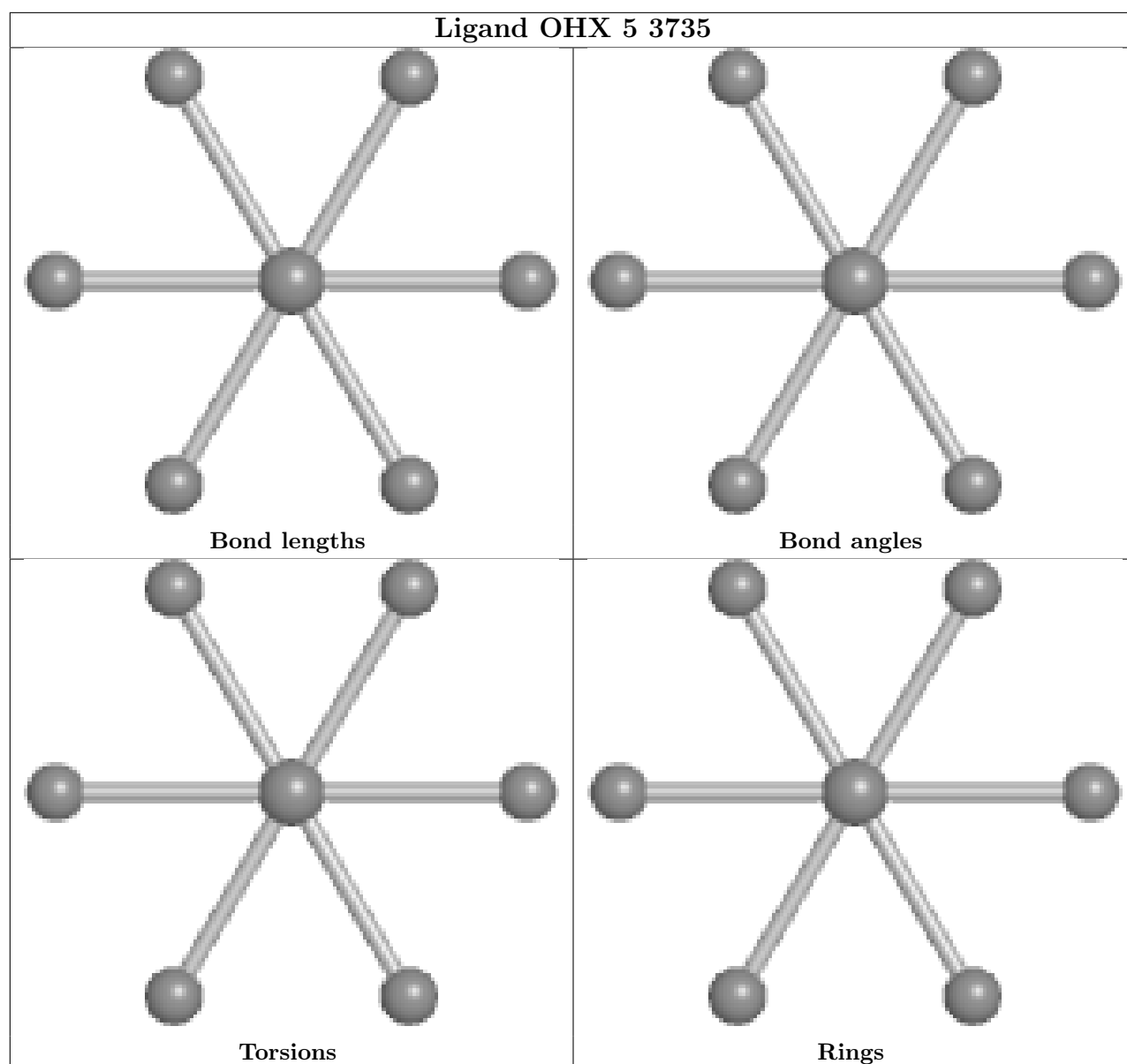


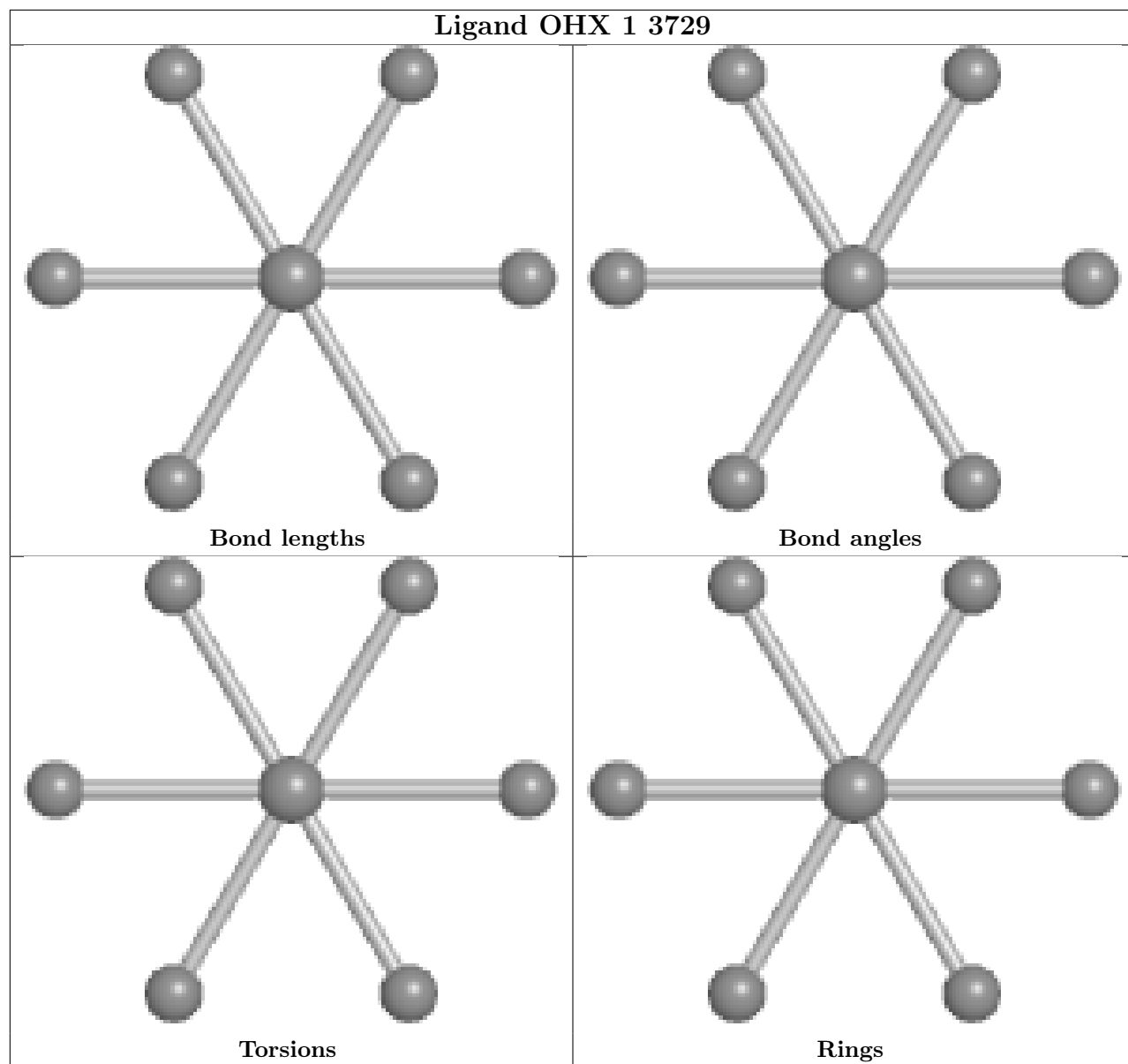


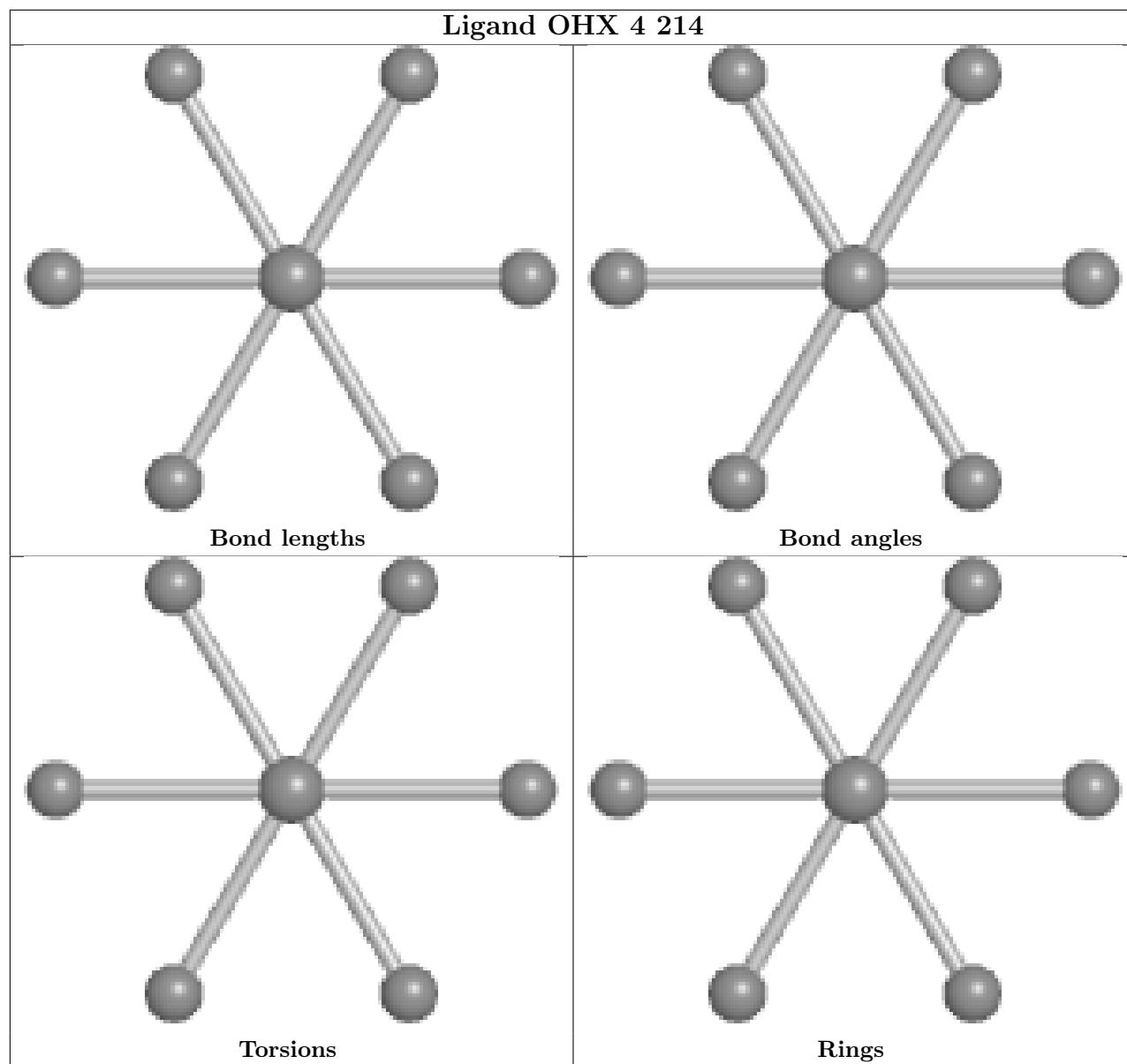


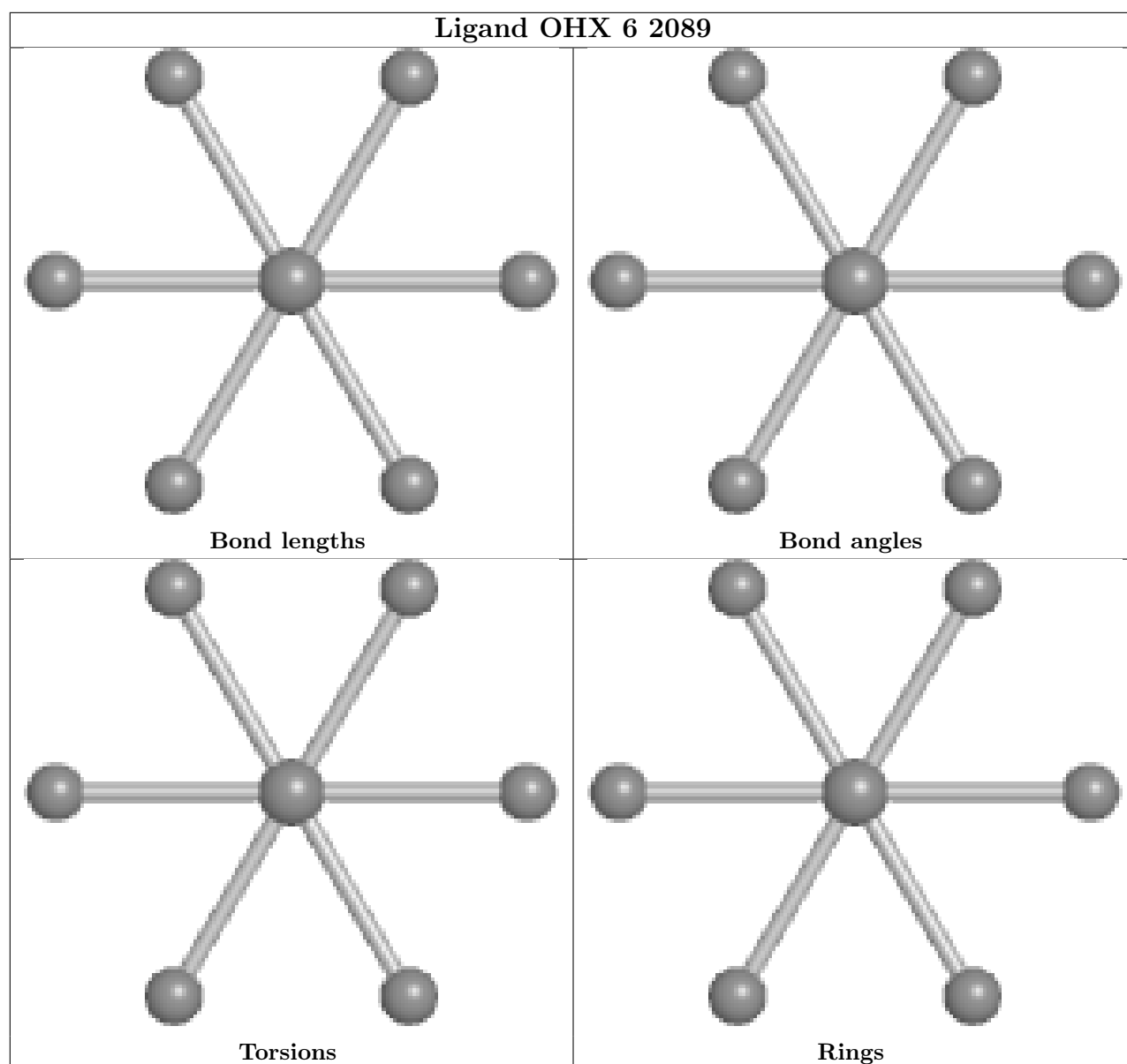


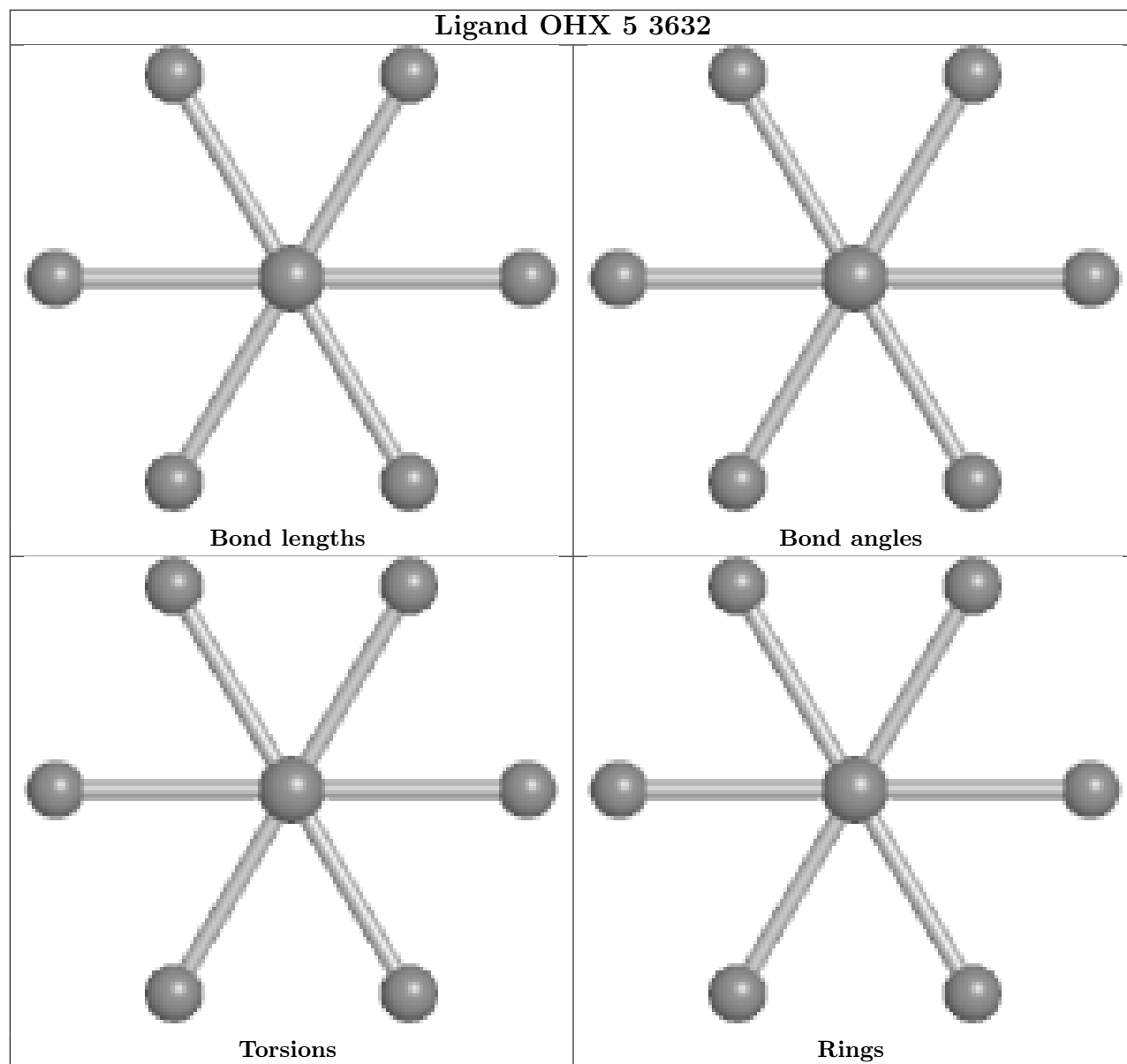


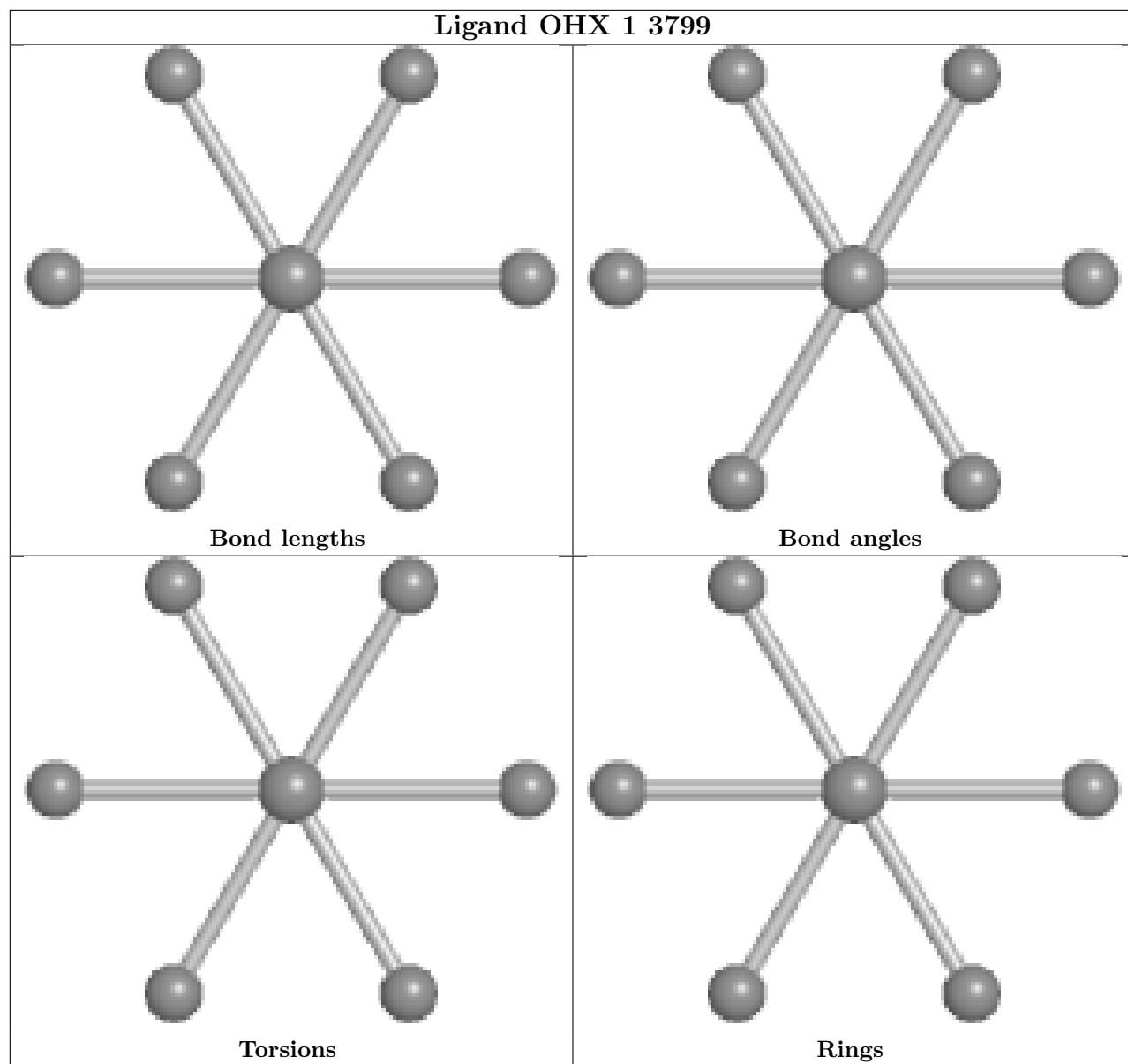


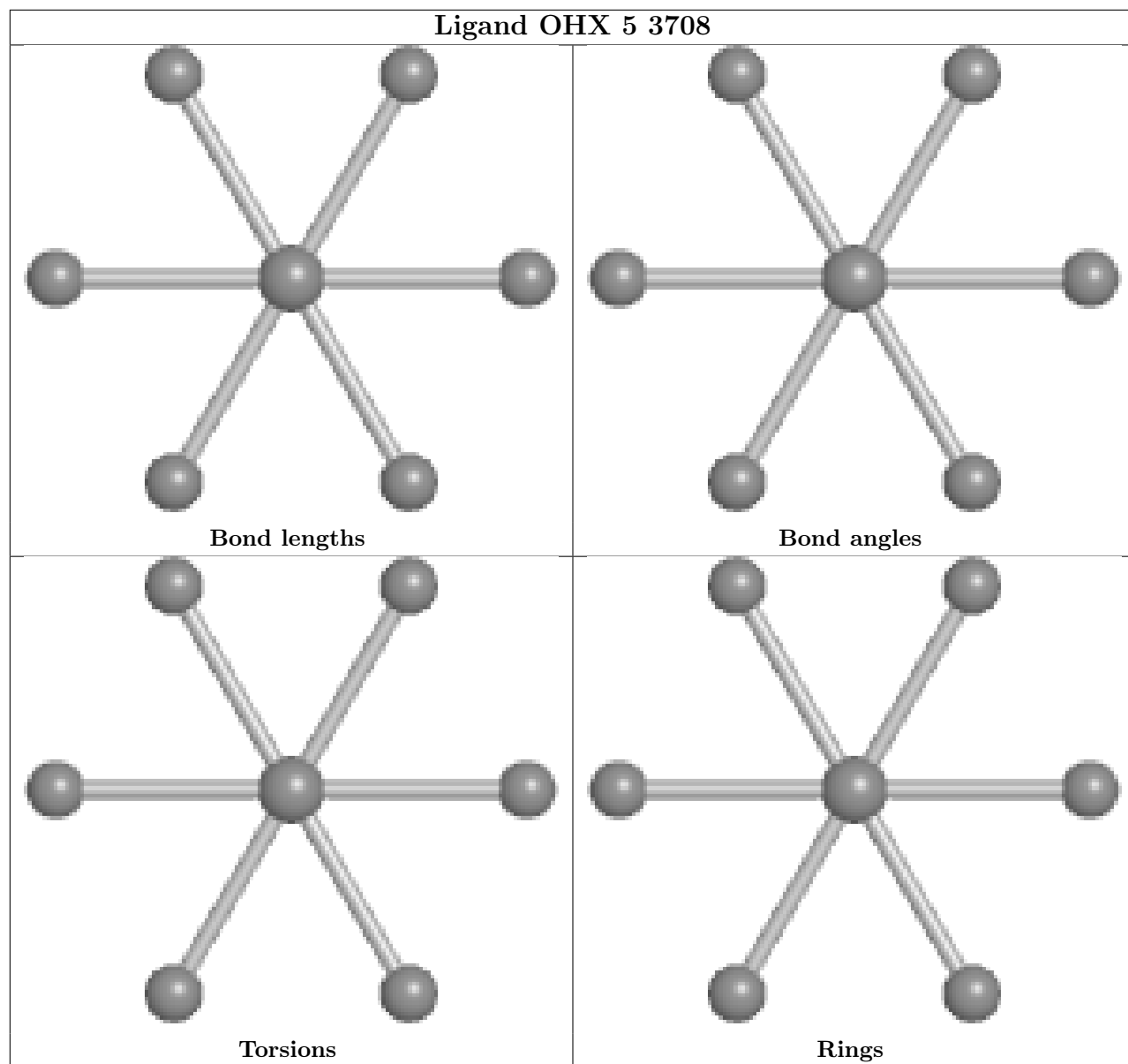


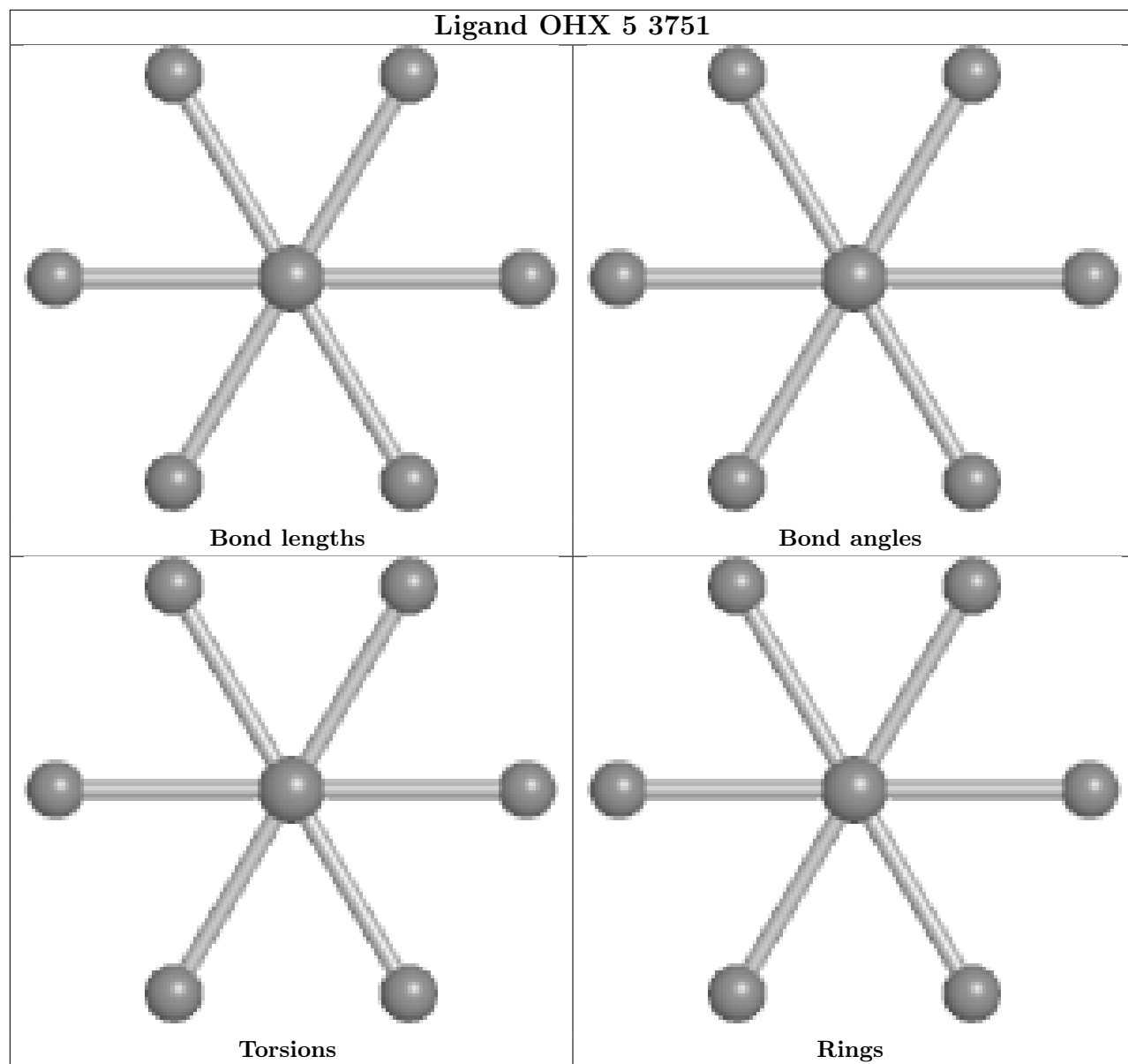


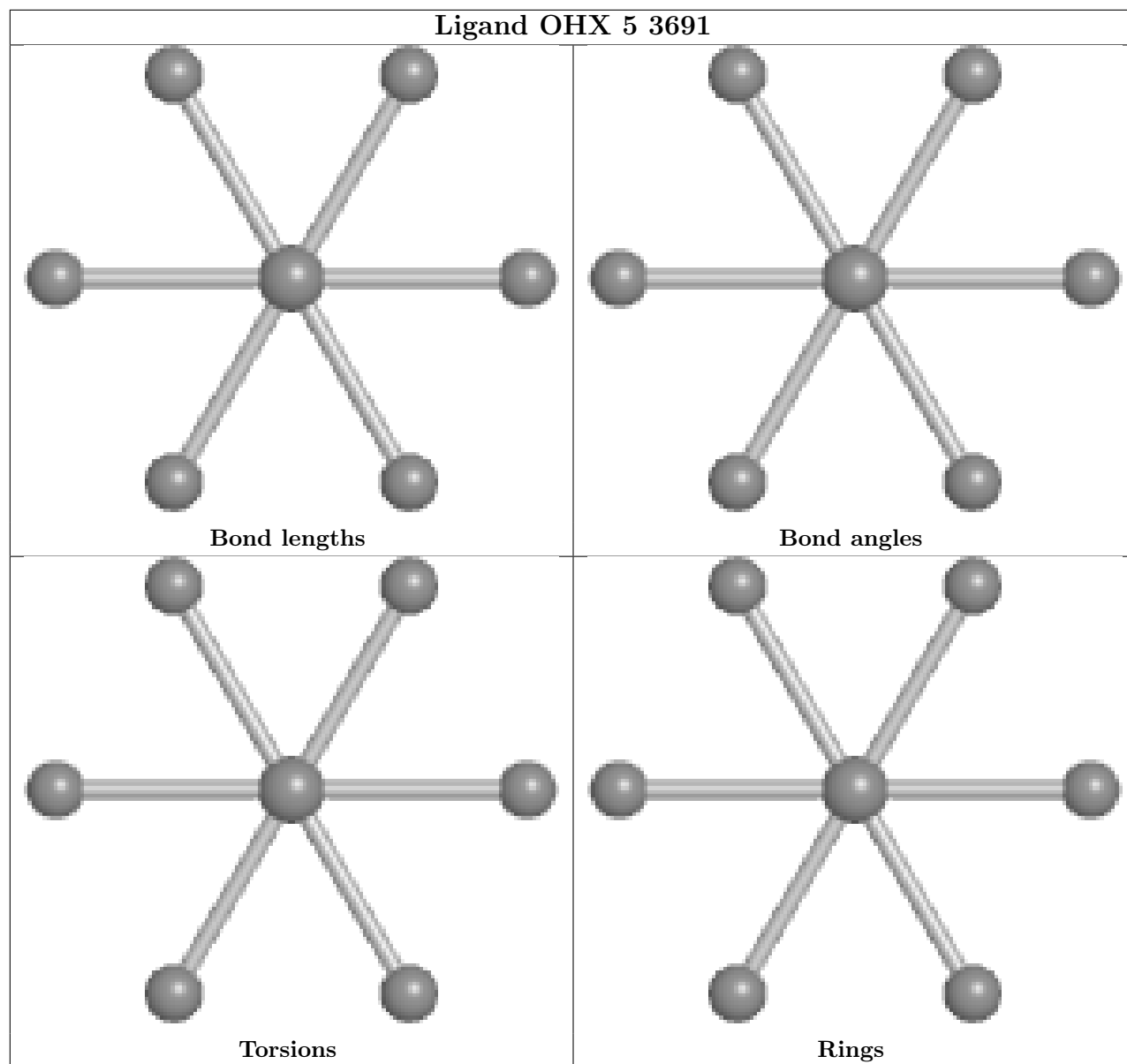


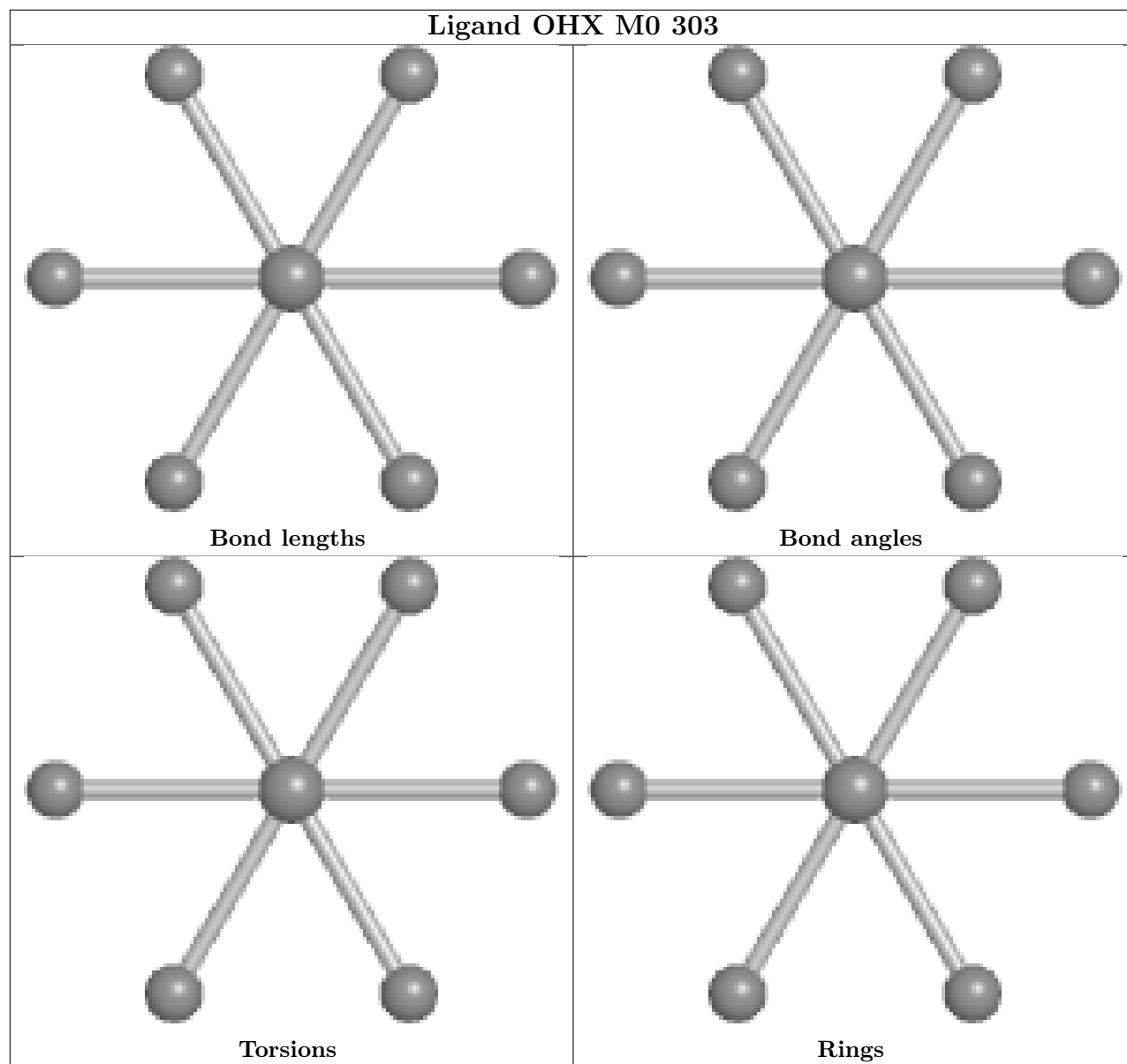


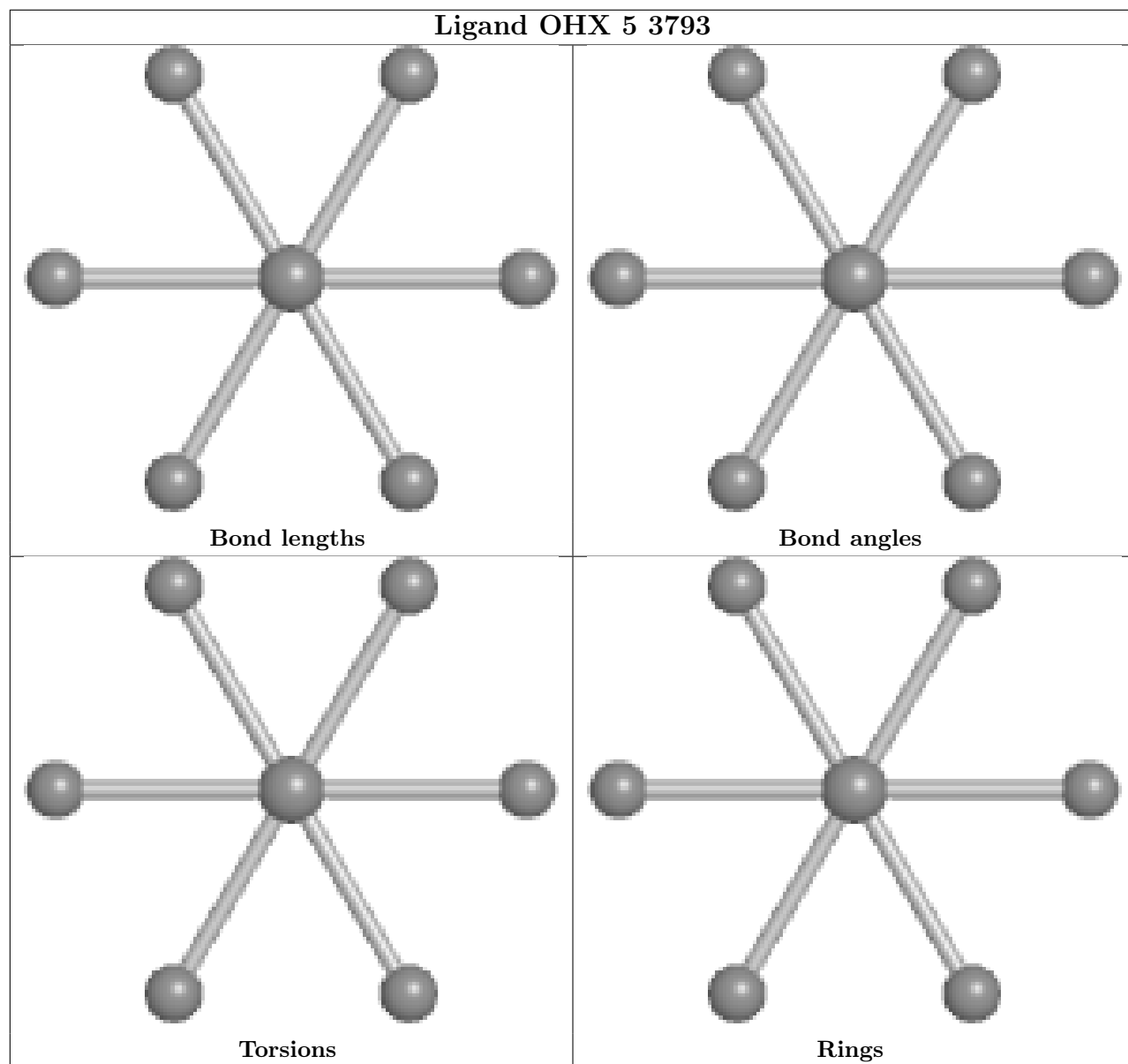


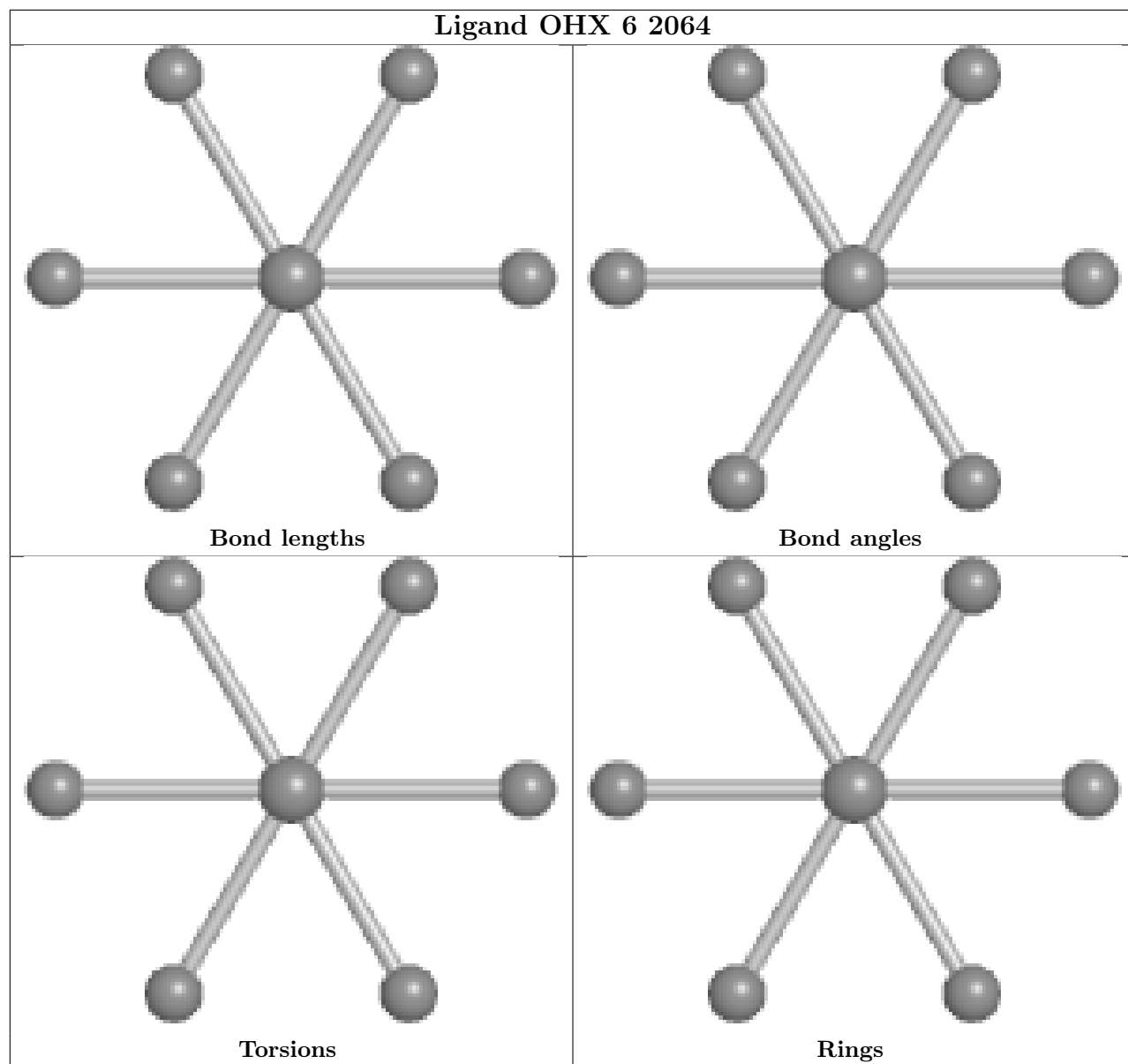


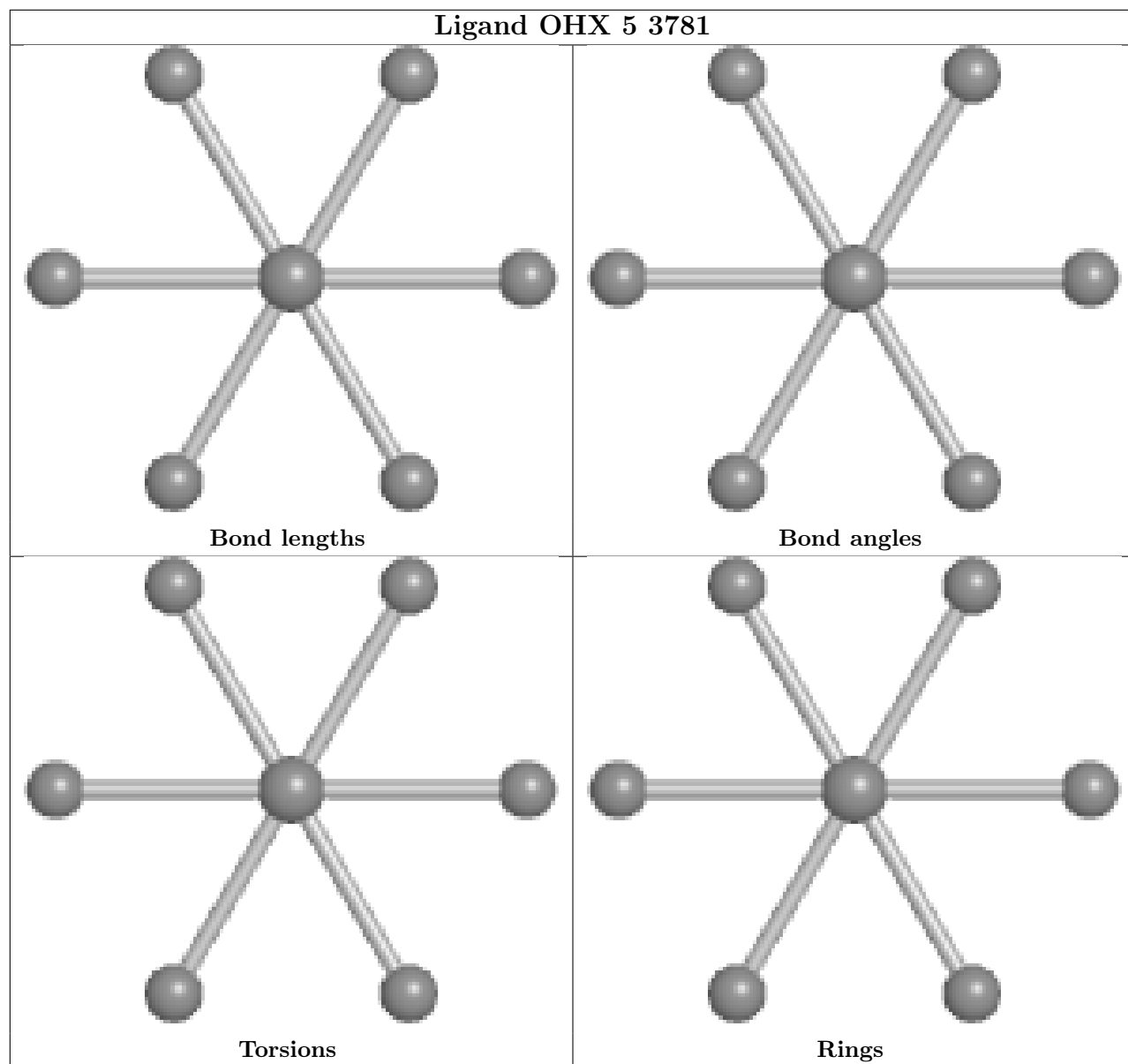


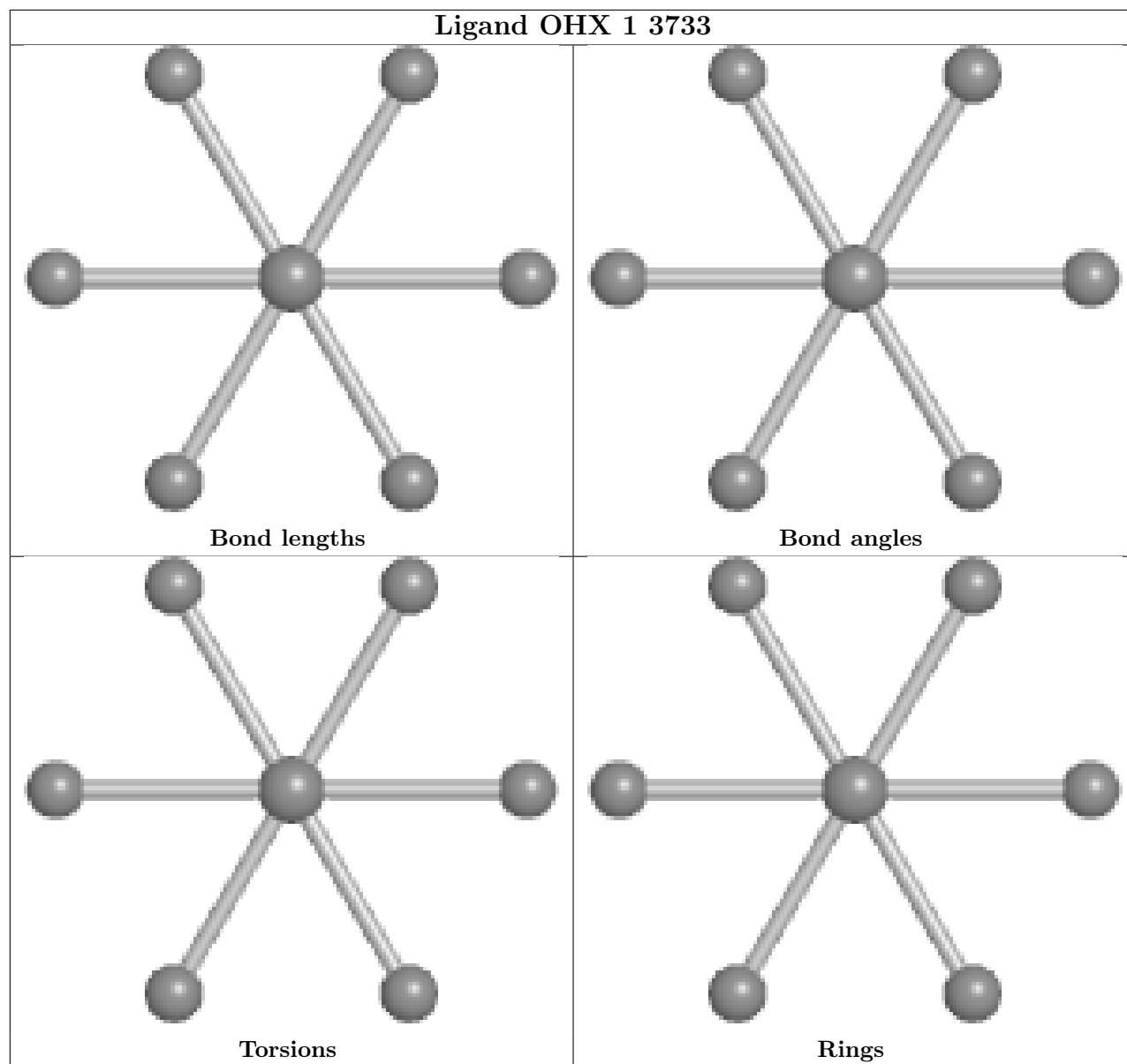


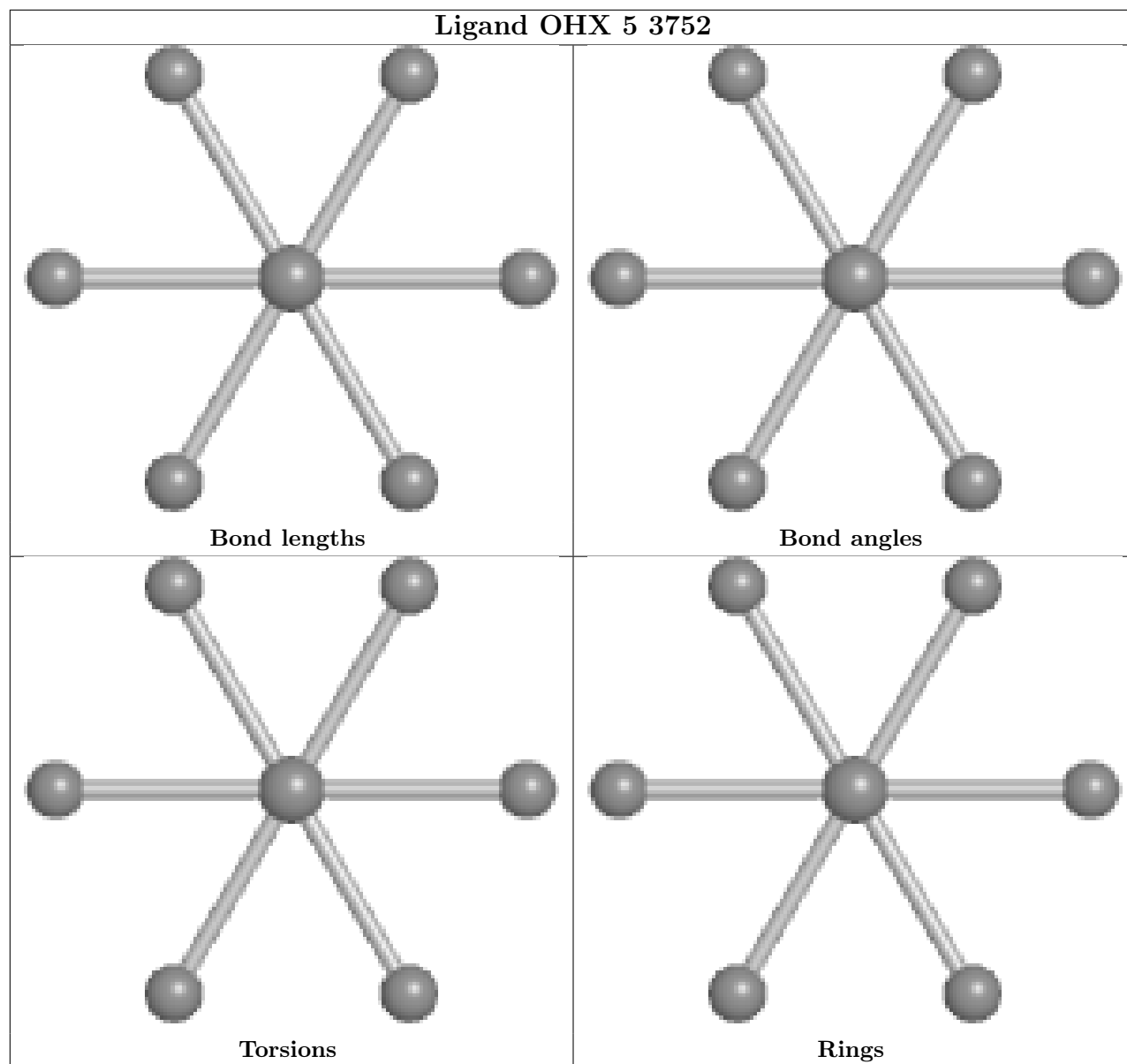


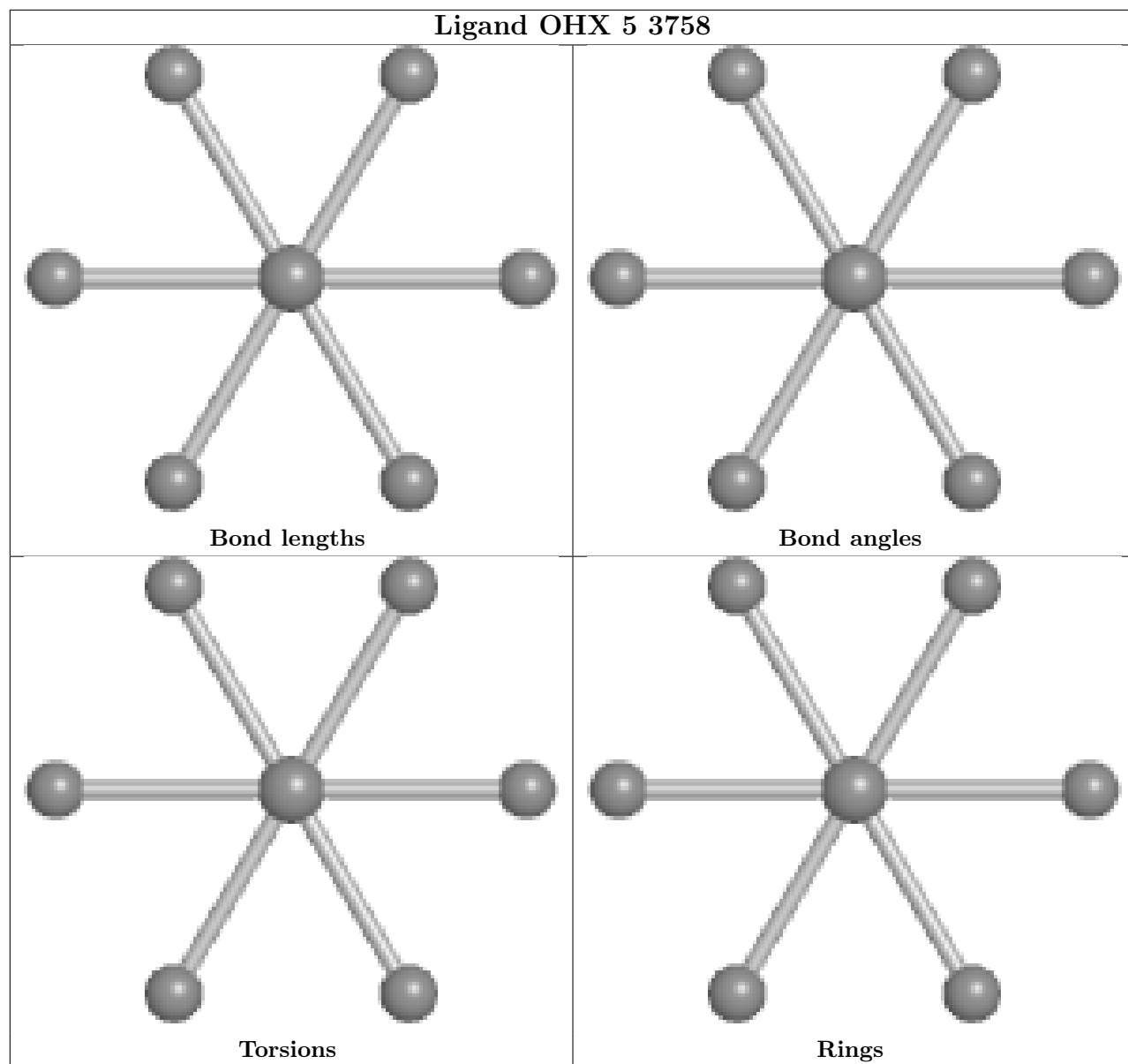


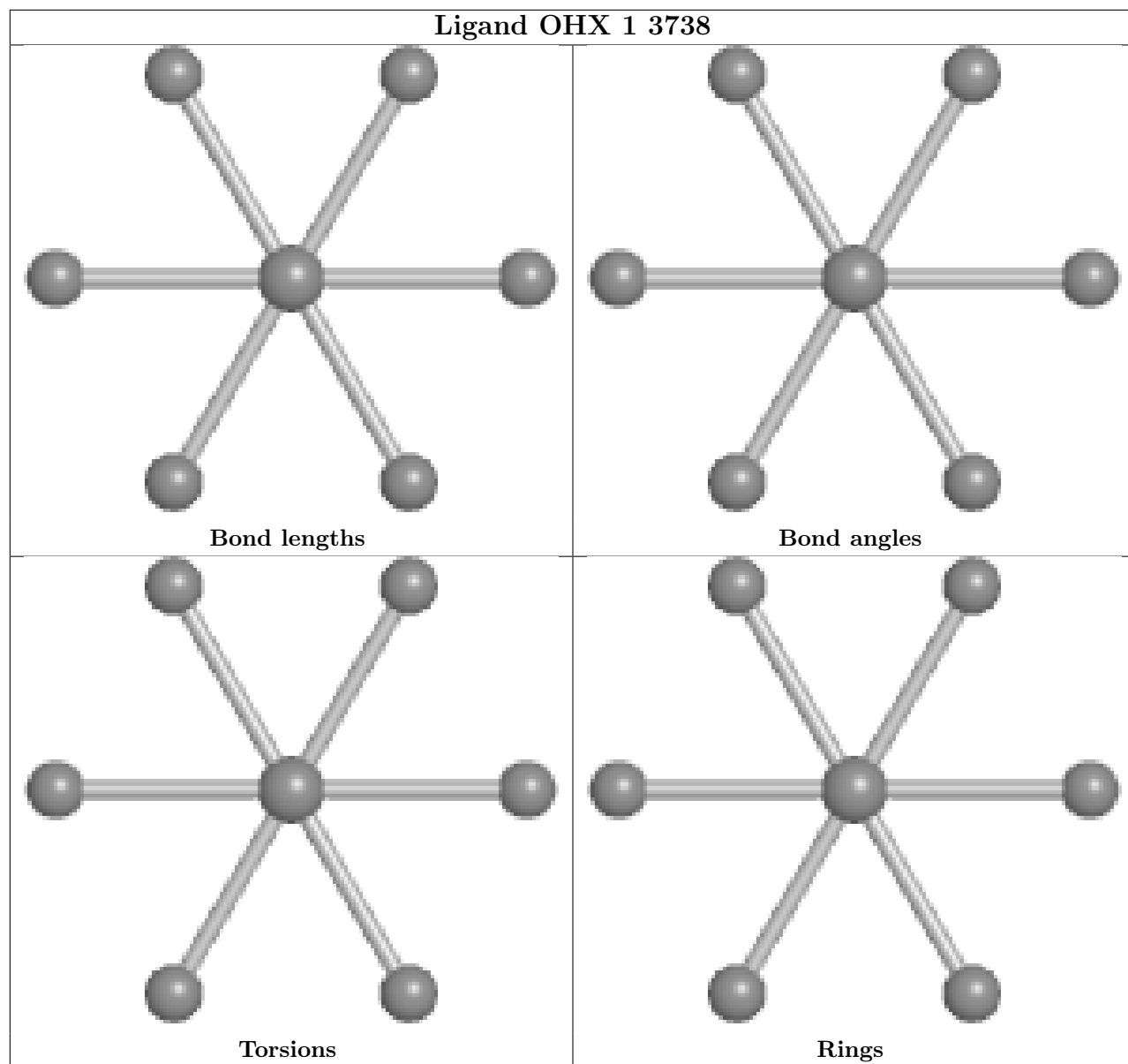


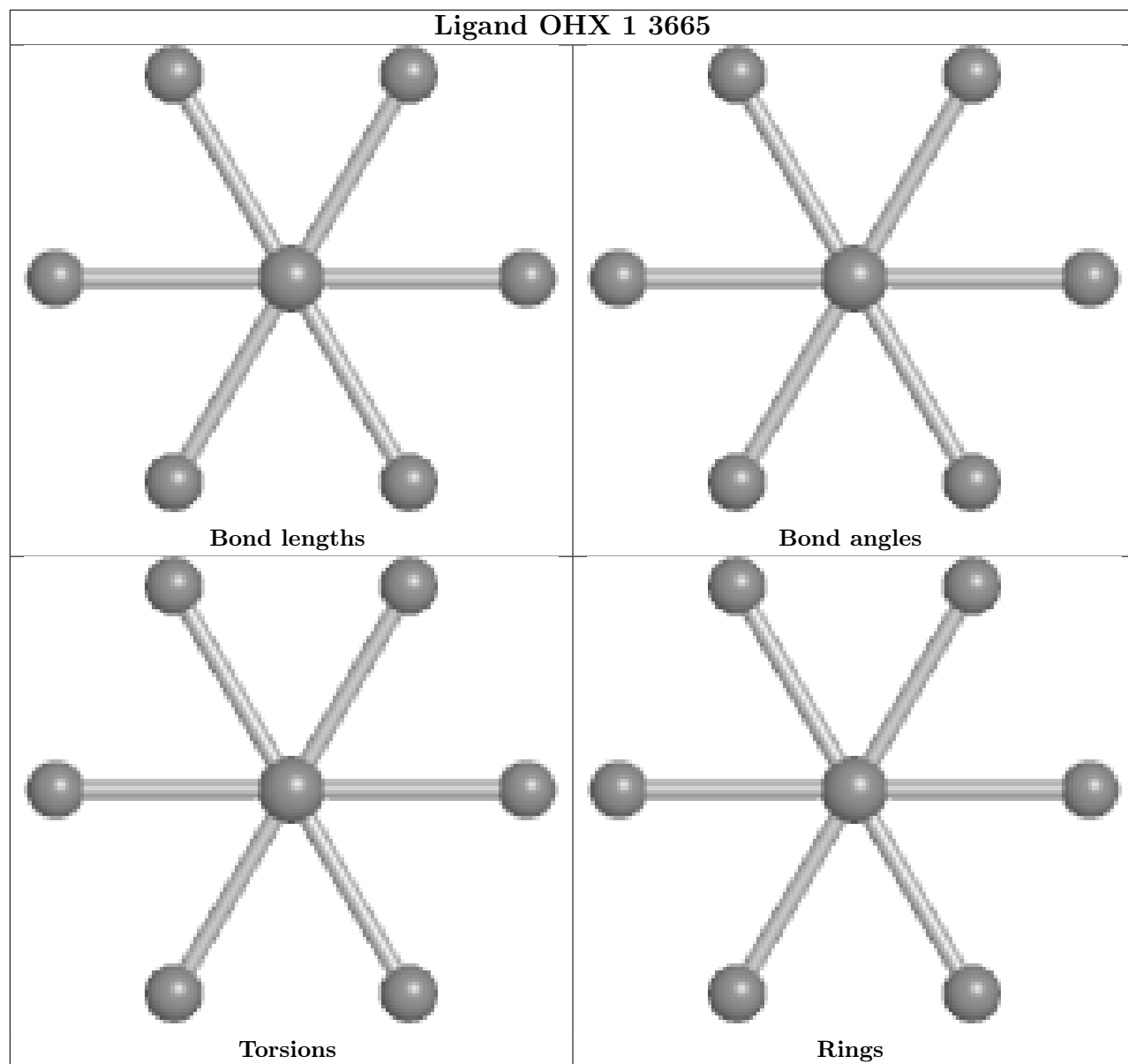


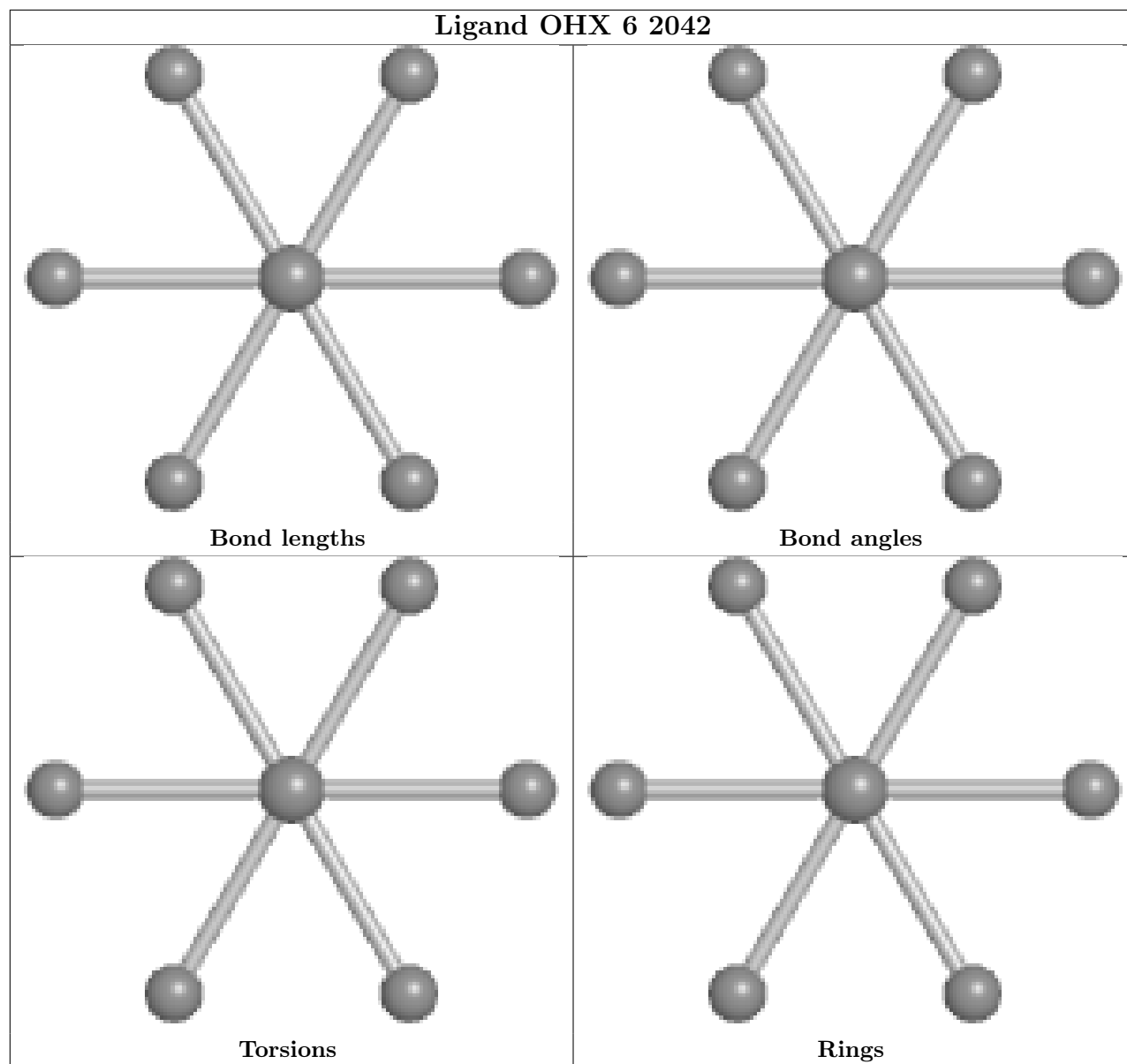


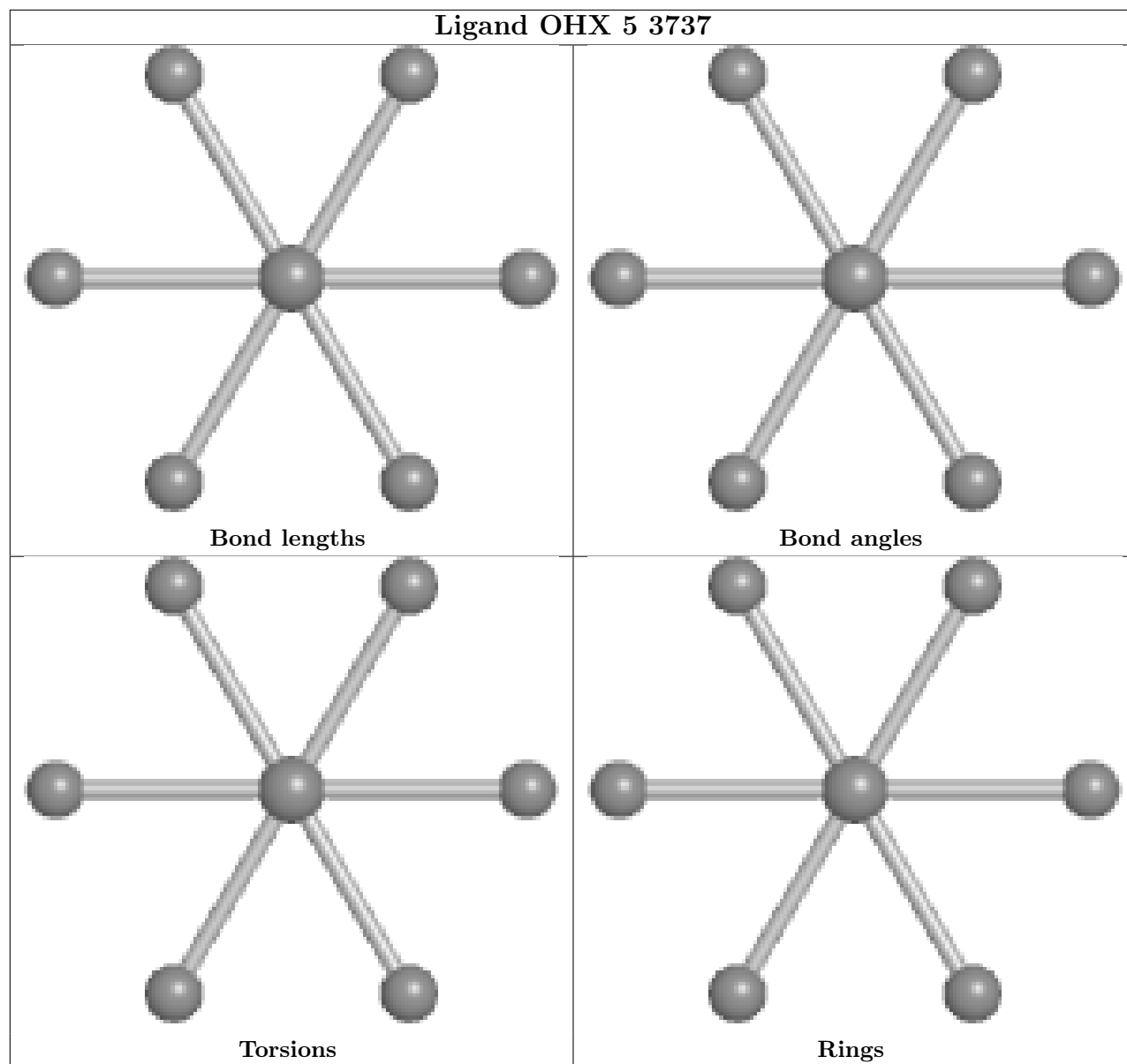


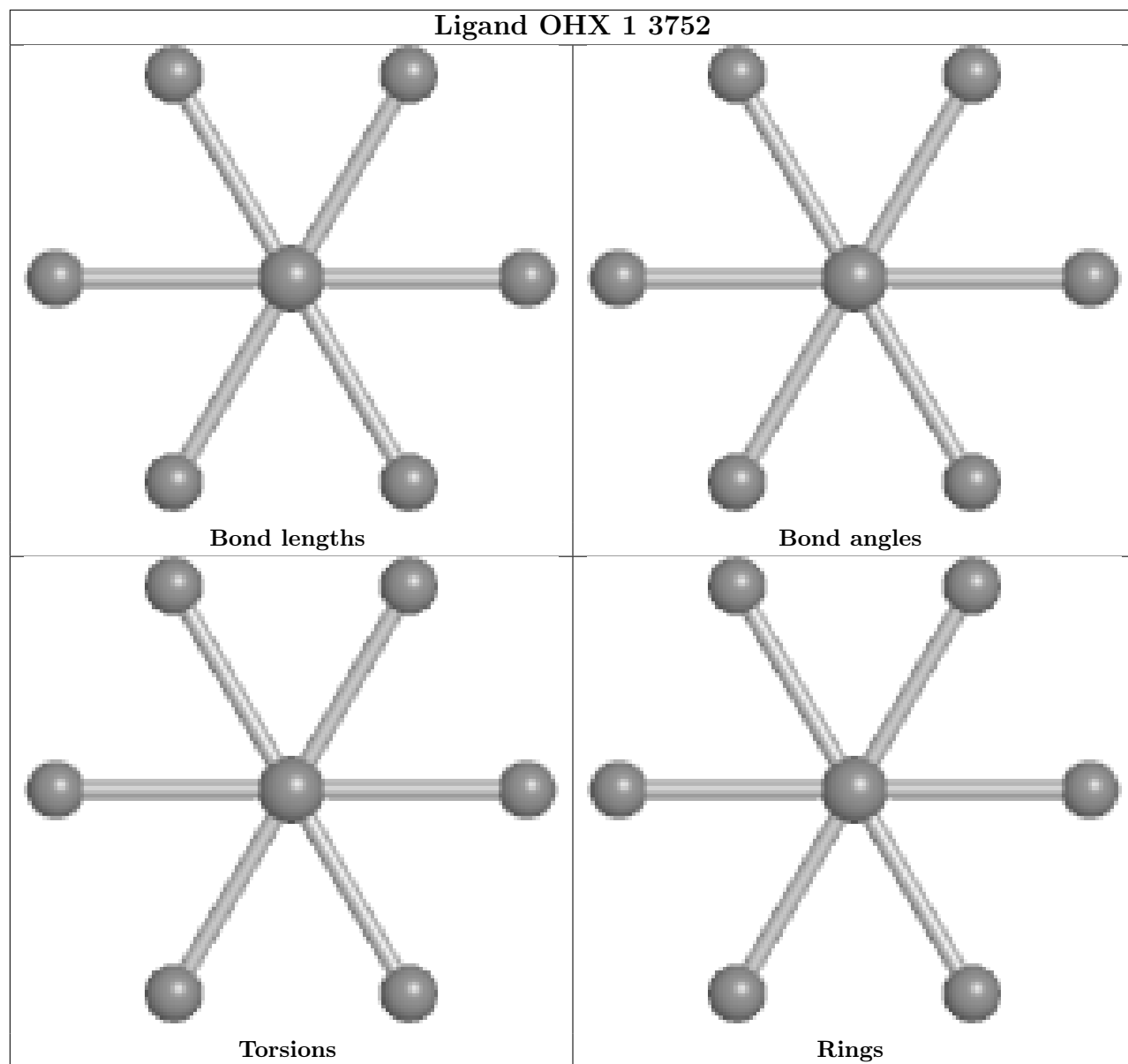


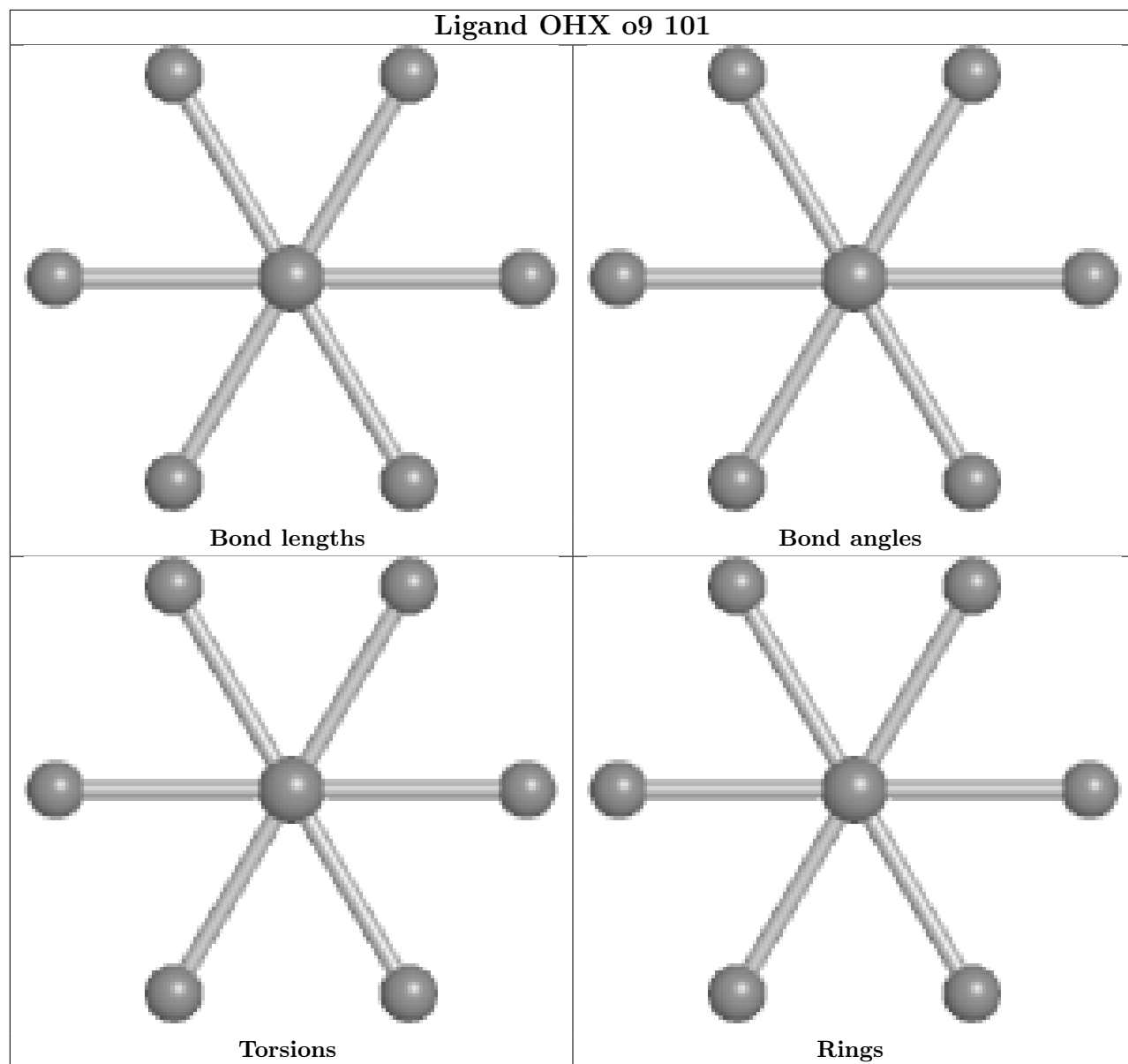


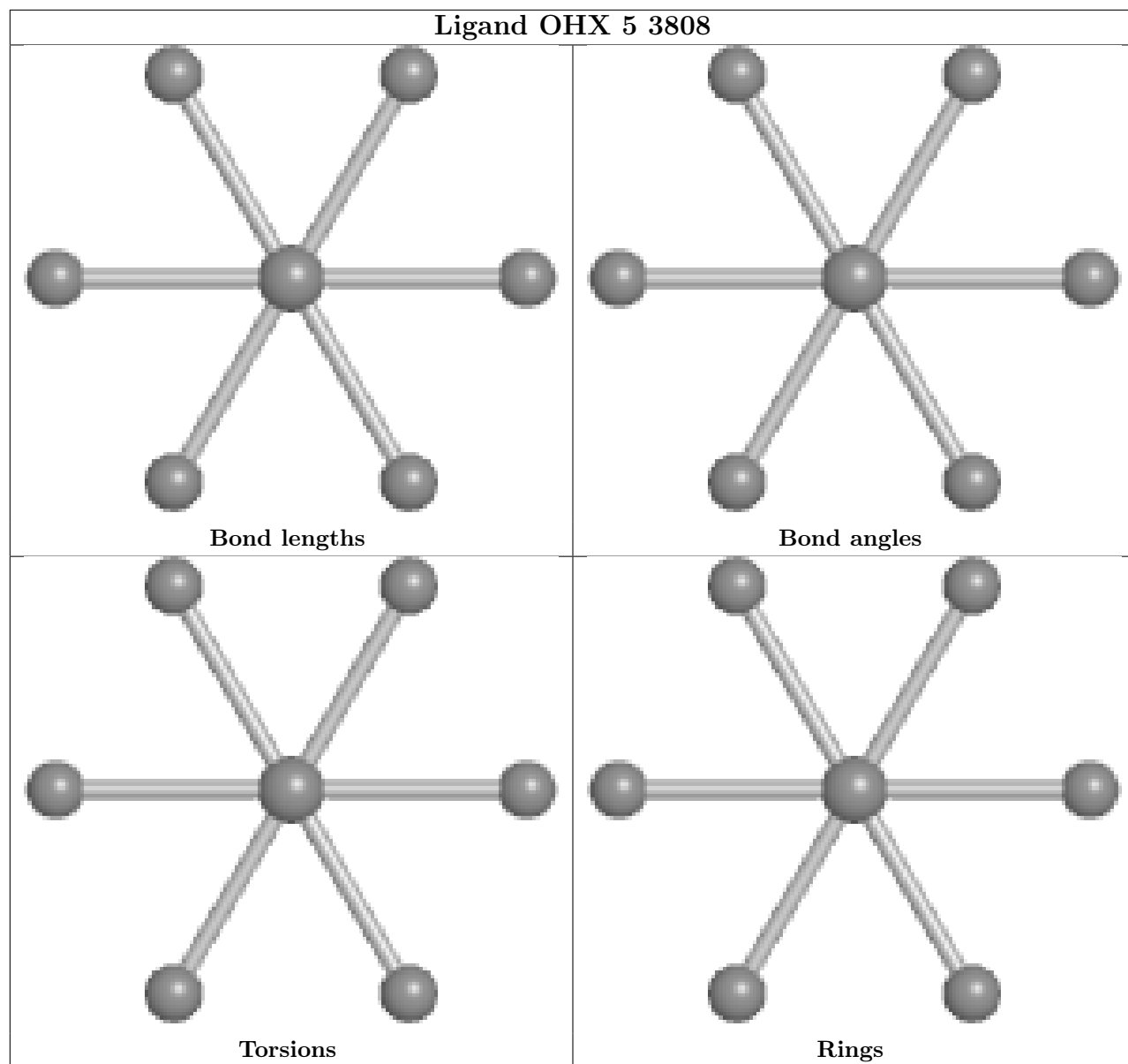


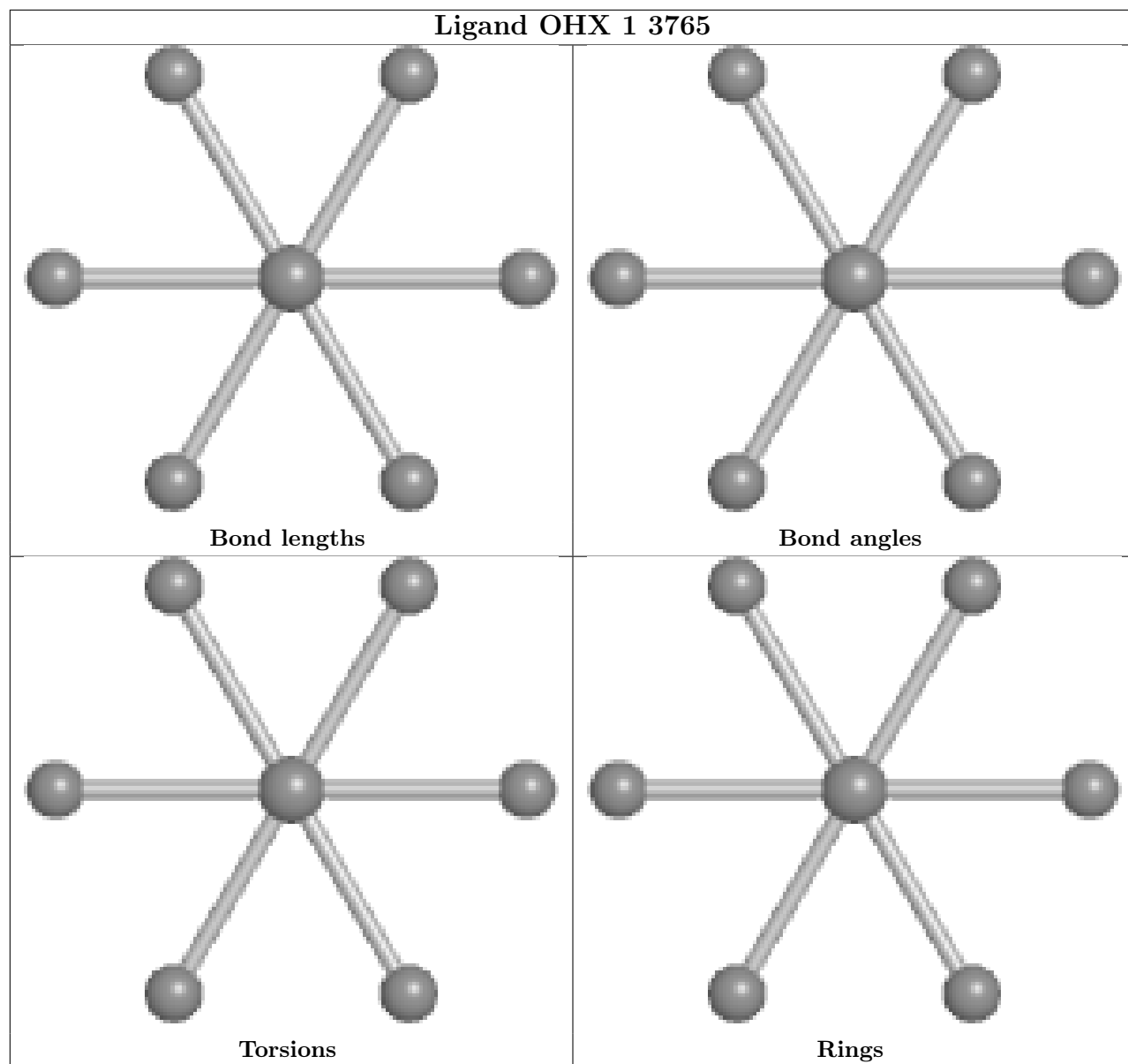


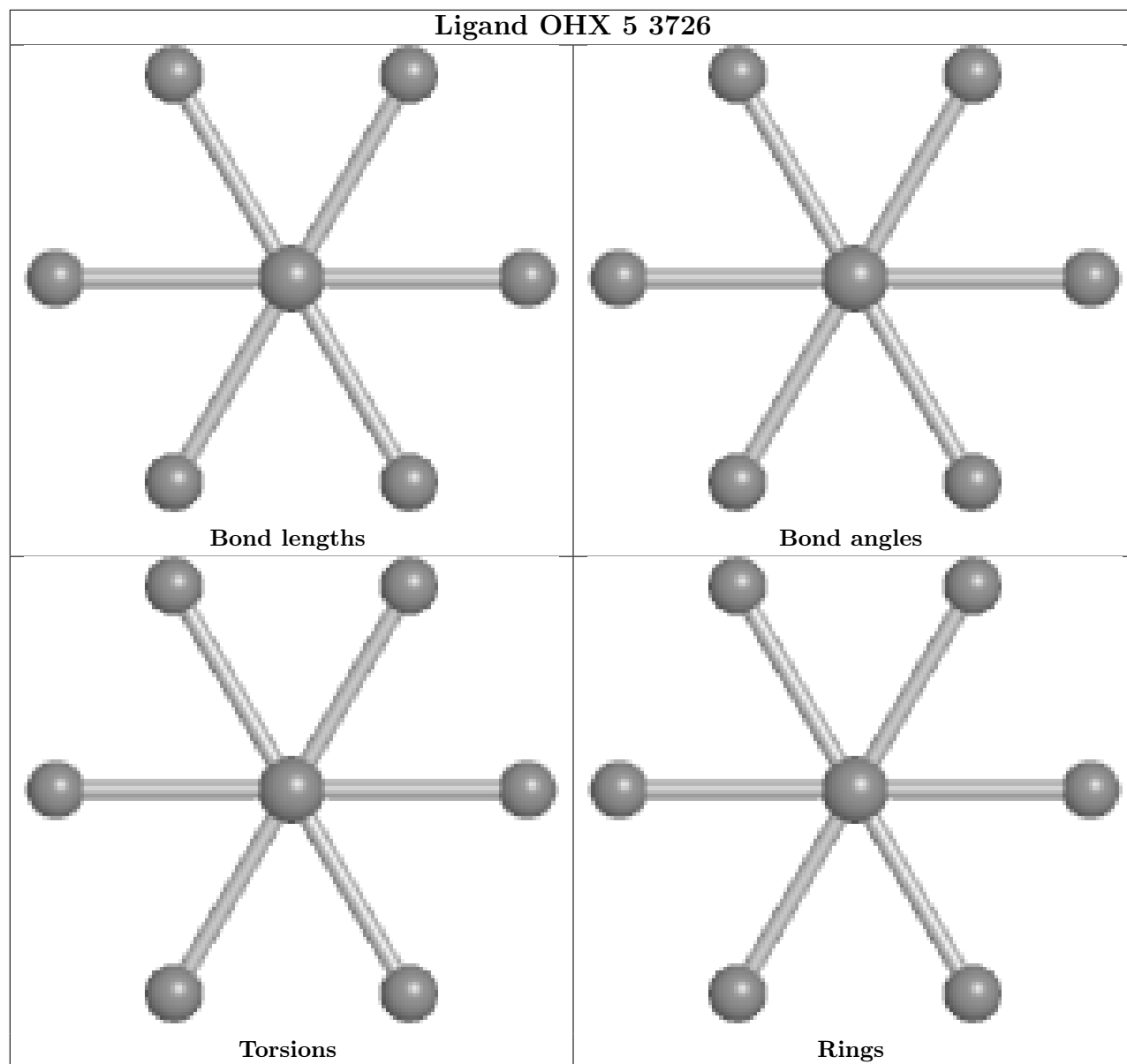


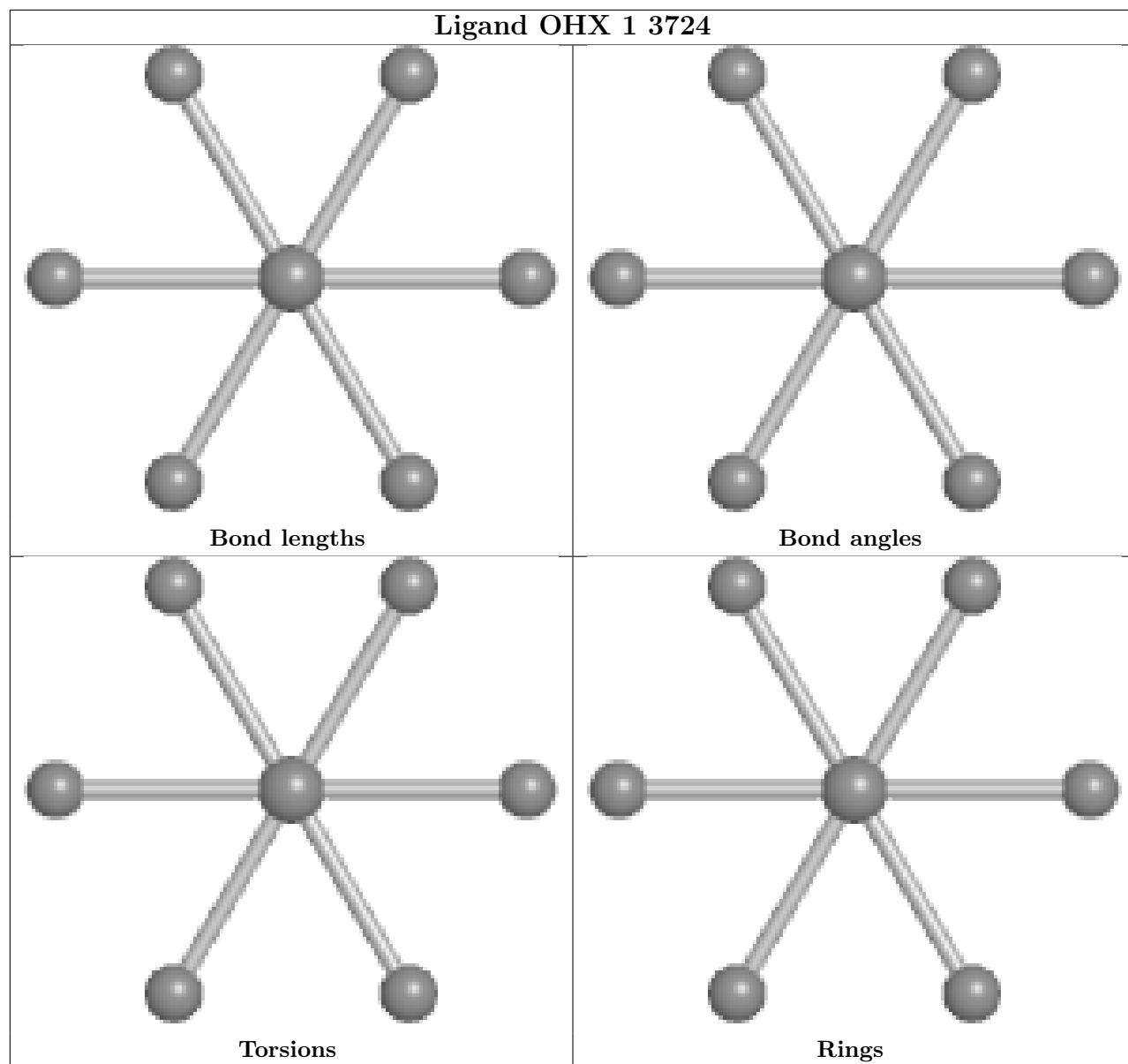


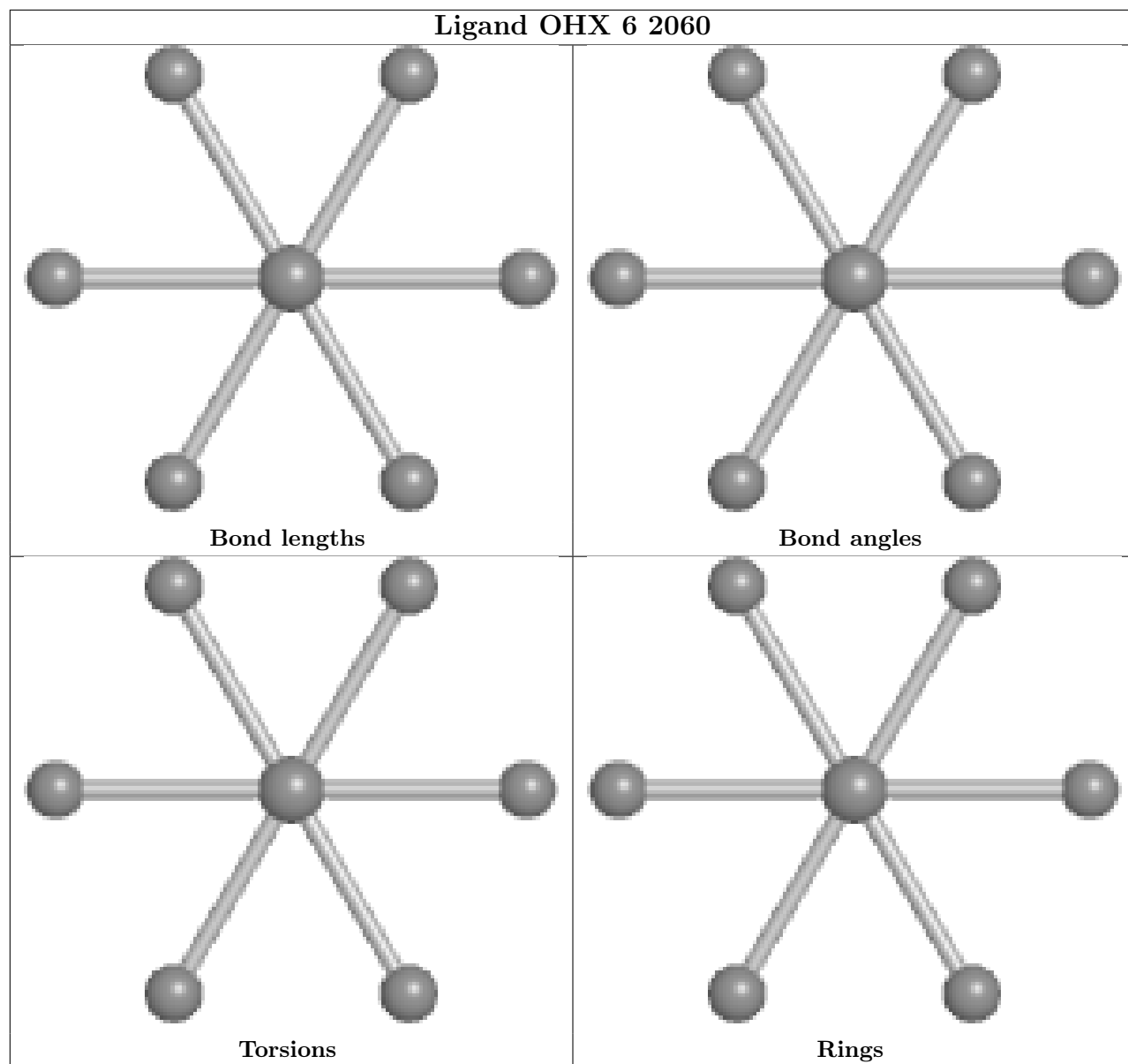


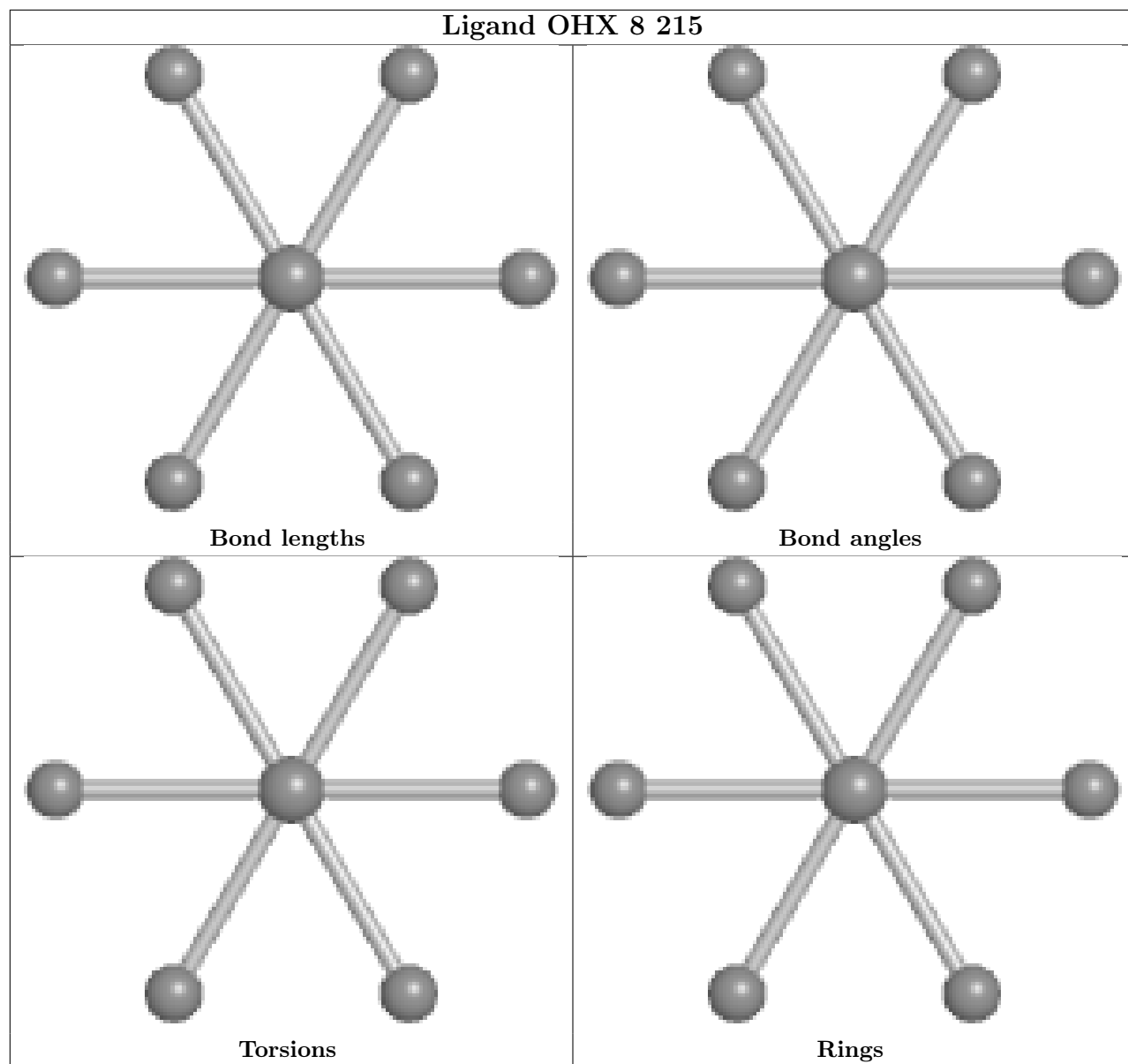


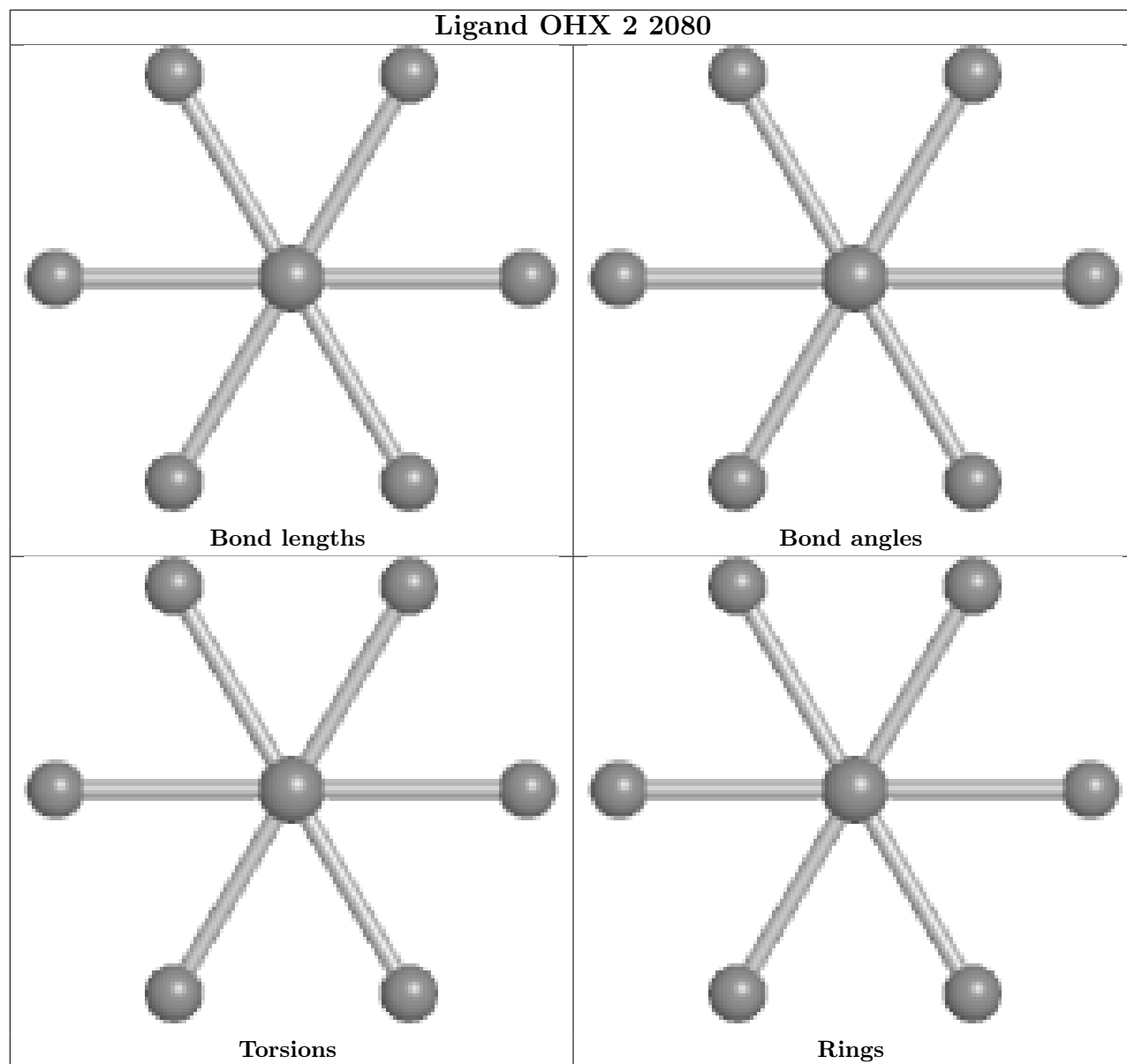


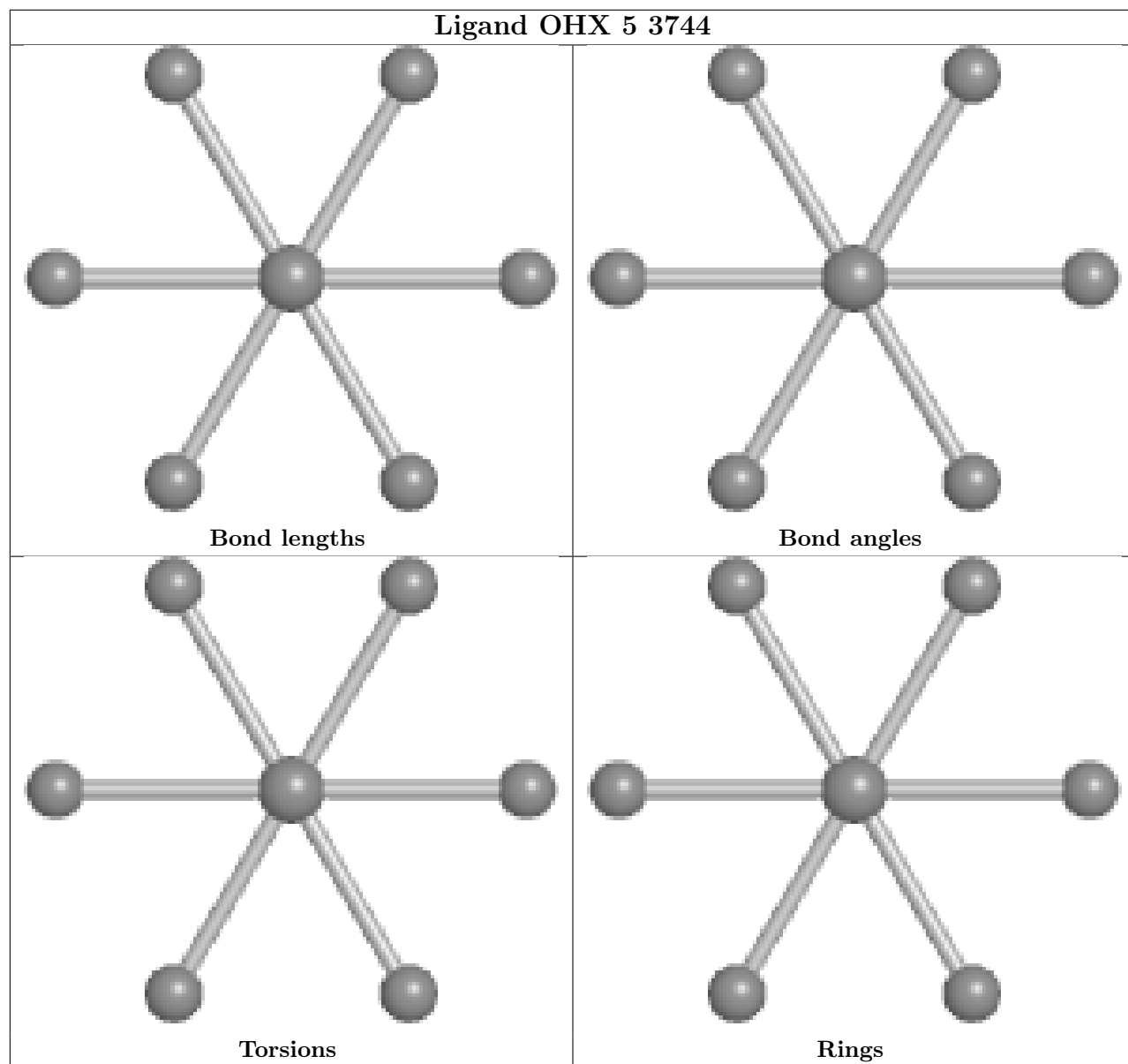


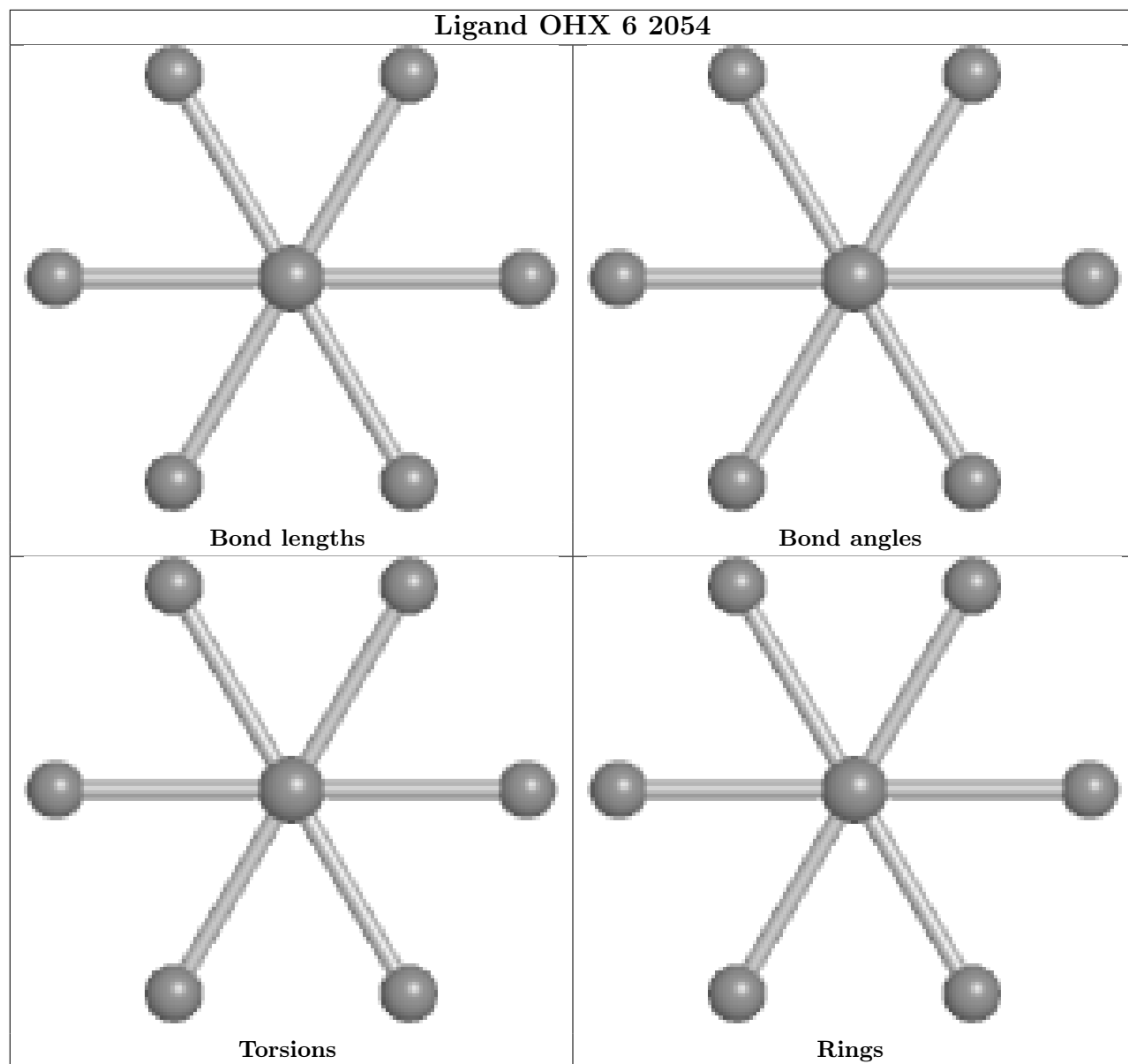


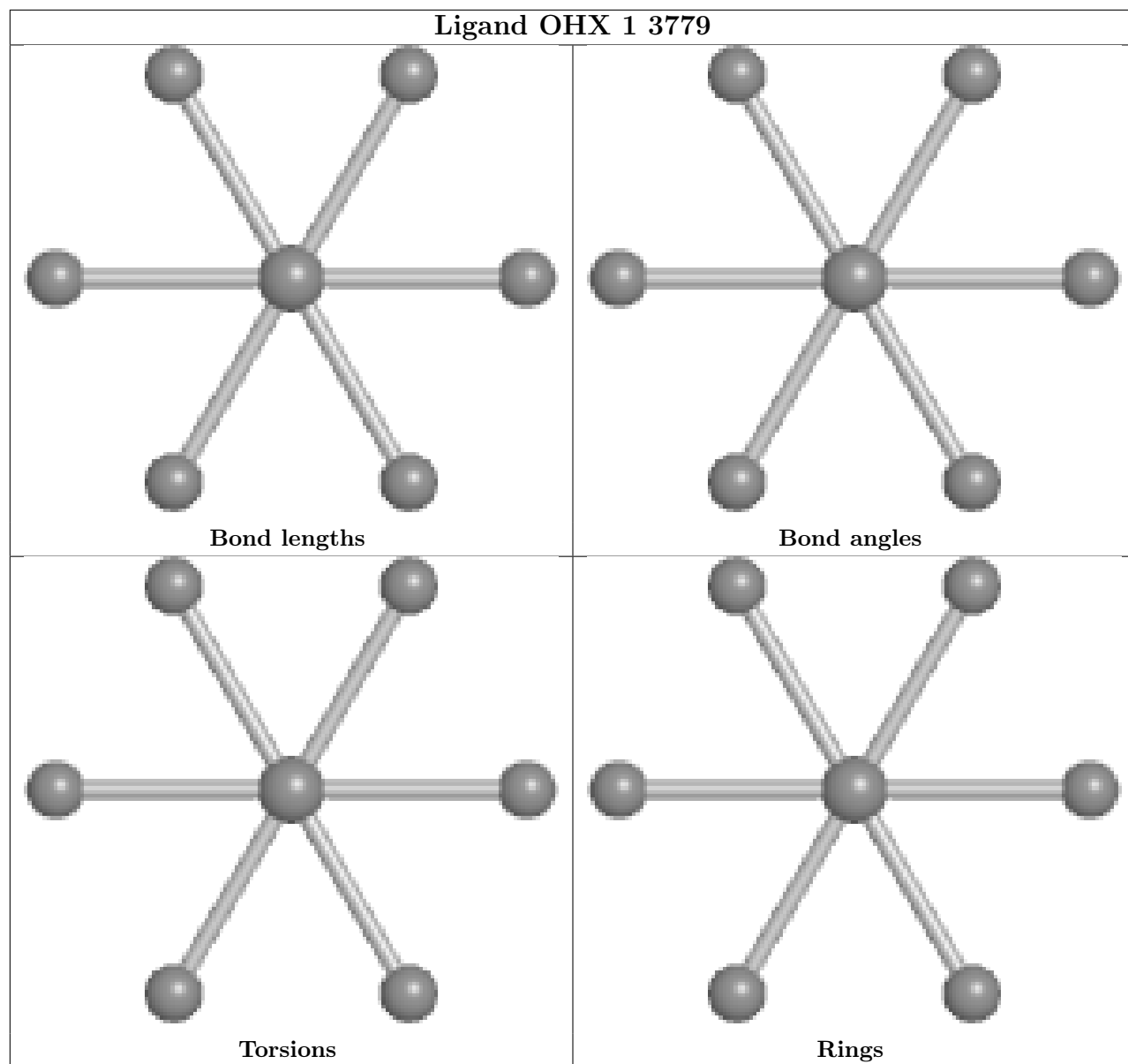


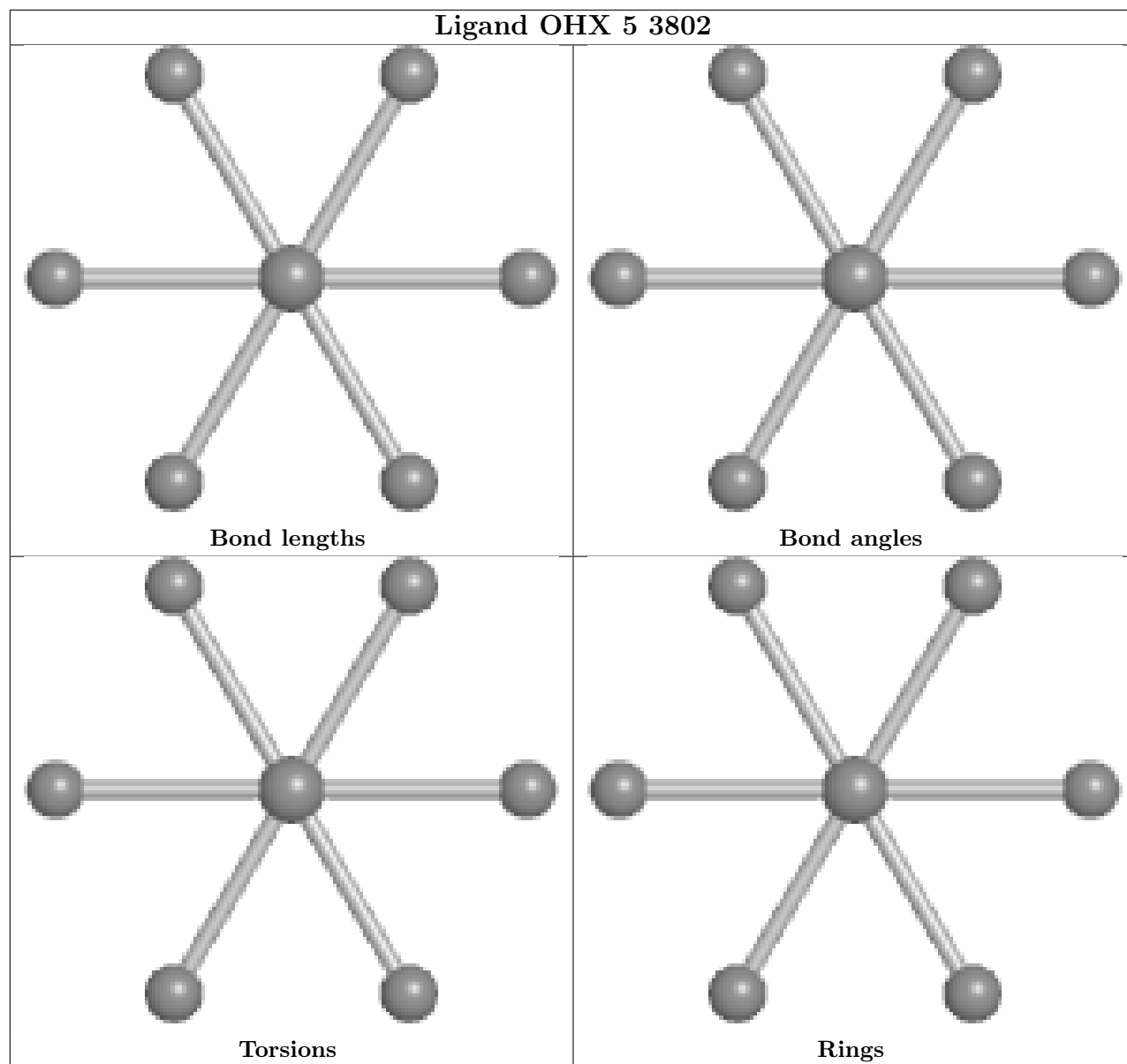


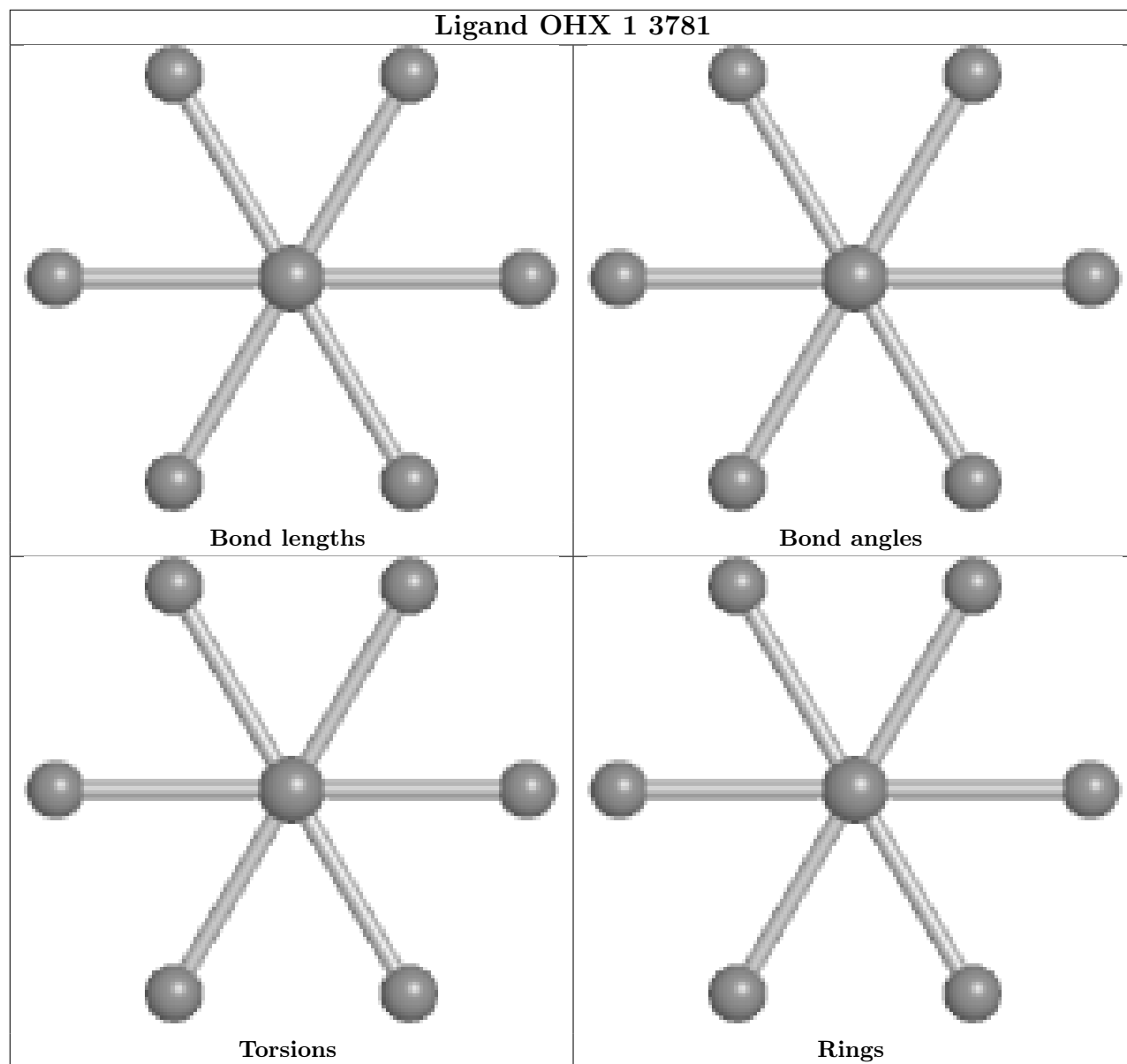


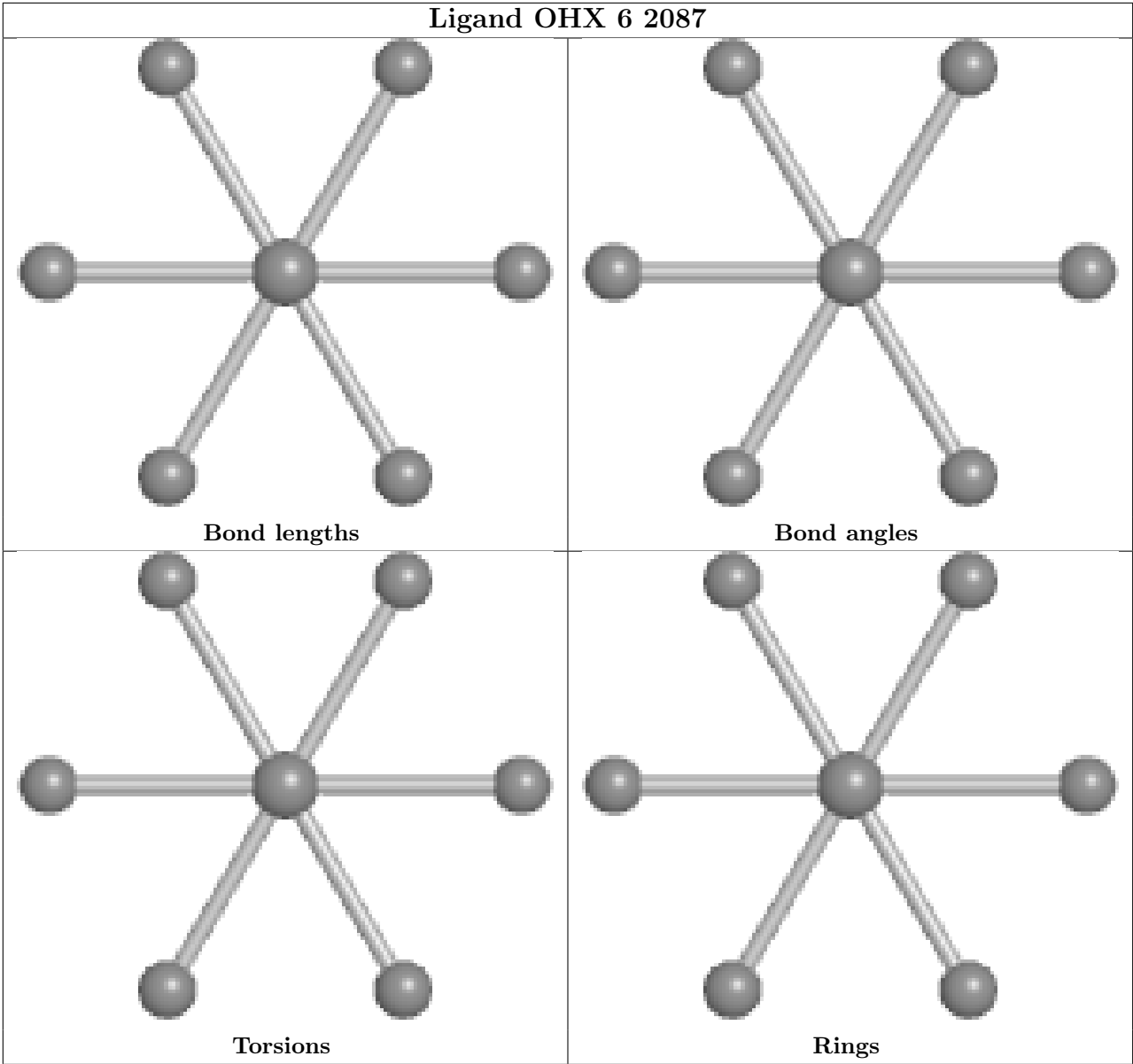












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
82	sM	2
83	m2	2
1	2	1

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Mol	Chain	Number of breaks
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1781/1829 (97%)	0.01	31 (1%) 69 50	38, 90, 174, 223	1 (0%)
2	S0	206/206 (100%)	0.62	11 (5%) 32 22	91, 107, 116, 121	0
2	s0	206/206 (100%)	0.41	5 (2%) 59 40	68, 84, 96, 105	0
3	S1	214/216 (99%)	0.73	19 (8%) 15 12	104, 134, 158, 165	0
3	s1	216/216 (100%)	0.16	4 (1%) 66 48	72, 84, 102, 115	0
4	S2	217/217 (100%)	0.58	7 (3%) 50 34	75, 86, 98, 108	0
4	s2	217/217 (100%)	0.24	6 (2%) 55 36	55, 68, 78, 87	0
5	S3	223/223 (100%)	0.50	5 (2%) 62 43	82, 93, 112, 124	0
5	s3	223/223 (100%)	0.48	7 (3%) 51 35	74, 99, 116, 124	0
6	S4	260/260 (100%)	0.46	2 (0%) 82 68	69, 91, 98, 119	0
6	s4	260/260 (100%)	0.13	1 (0%) 88 79	47, 69, 82, 106	0
7	S5	206/206 (100%)	0.83	18 (8%) 16 12	96, 112, 124, 132	0
7	s5	206/206 (100%)	0.54	10 (4%) 35 23	79, 97, 113, 121	0
8	S6	226/226 (100%)	0.88	24 (10%) 11 9	72, 106, 120, 125	0
8	s6	218/226 (96%)	0.36	11 (5%) 34 23	49, 77, 94, 110	0
9	S7	184/186 (98%)	0.66	7 (3%) 44 30	90, 114, 139, 144	0
9	s7	186/186 (100%)	0.41	9 (4%) 35 24	65, 96, 124, 132	0
10	S8	188/199 (94%)	0.34	3 (1%) 70 52	63, 79, 113, 125	0
10	s8	188/199 (94%)	0.40	7 (3%) 45 31	46, 66, 107, 124	0
11	S9	185/185 (100%)	0.48	3 (1%) 70 52	81, 95, 126, 141	0
11	s9	185/185 (100%)	0.31	4 (2%) 62 43	57, 74, 104, 122	0
12	C0	96/96 (100%)	0.69	6 (6%) 26 17	84, 105, 126, 135	0
13	C1	155/155 (100%)	0.54	13 (8%) 17 13	64, 76, 112, 121	0
13	c1	146/155 (94%)	0.46	9 (6%) 26 18	48, 61, 89, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	C2	124/124 (100%)	0.73	8 (6%) 25 17	133, 139, 151, 157	0
14	c2	124/124 (100%)	1.06	19 (15%) 5 5	167, 183, 195, 200	0
15	C3	150/150 (100%)	0.48	6 (4%) 42 28	75, 88, 104, 108	0
15	c3	150/150 (100%)	0.16	2 (1%) 75 56	57, 70, 86, 88	0
16	C4	127/128 (99%)	0.82	8 (6%) 26 17	75, 129, 142, 144	0
16	c4	128/128 (100%)	0.30	4 (3%) 51 35	54, 86, 94, 104	0
17	C5	124/135 (91%)	0.47	4 (3%) 50 34	79, 94, 110, 126	0
17	c5	135/135 (100%)	0.47	8 (5%) 28 19	67, 97, 112, 115	0
18	C6	141/142 (99%)	0.78	9 (6%) 25 17	82, 102, 107, 110	0
18	c6	142/142 (100%)	0.68	13 (9%) 14 11	73, 91, 104, 121	0
19	C7	120/125 (96%)	0.54	2 (1%) 69 50	91, 105, 124, 126	0
19	c7	117/125 (93%)	0.48	6 (5%) 33 22	78, 91, 105, 112	0
20	C8	145/145 (100%)	0.47	3 (2%) 63 44	77, 97, 120, 127	0
20	c8	145/145 (100%)	0.42	8 (5%) 30 21	73, 89, 109, 114	0
21	C9	143/143 (100%)	0.66	9 (6%) 26 17	85, 99, 111, 120	0
21	c9	143/143 (100%)	0.29	4 (2%) 55 36	76, 85, 99, 107	0
22	D0	107/110 (97%)	0.90	10 (9%) 14 11	77, 105, 124, 127	0
22	d0	110/110 (100%)	0.66	7 (6%) 25 17	74, 102, 127, 134	0
23	D1	87/87 (100%)	0.42	2 (2%) 61 42	87, 95, 109, 115	0
23	d1	87/87 (100%)	0.14	0 100 100	65, 73, 93, 100	0
24	D2	129/129 (100%)	0.52	3 (2%) 61 42	73, 84, 90, 100	0
24	d2	129/129 (100%)	-0.05	0 100 100	53, 61, 68, 76	0
25	D3	144/144 (100%)	0.41	10 (6%) 23 16	64, 71, 83, 97	0
25	d3	144/144 (100%)	0.29	7 (4%) 35 23	45, 52, 62, 77	0
26	D4	134/134 (100%)	0.41	2 (1%) 72 53	81, 102, 113, 118	0
26	d4	134/134 (100%)	0.26	2 (1%) 72 53	56, 76, 87, 91	0
27	D5	70/70 (100%)	0.45	2 (2%) 53 35	108, 118, 124, 125	0
27	d5	69/70 (98%)	0.39	1 (1%) 73 55	89, 104, 111, 113	0
28	D6	97/97 (100%)	1.17	16 (16%) 4 4	79, 94, 142, 143	0
28	d6	97/97 (100%)	0.43	2 (2%) 63 44	58, 72, 97, 100	0
29	D7	81/81 (100%)	0.69	2 (2%) 58 39	90, 106, 133, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	d7	81/81 (100%)	0.36	2 (2%) 58 39	66, 83, 117, 120	0
30	D8	63/63 (100%)	1.06	10 (15%) 5 4	106, 122, 129, 131	0
30	d8	63/63 (100%)	0.58	1 (1%) 70 52	96, 110, 117, 119	0
31	D9	53/53 (100%)	0.39	1 (1%) 66 48	75, 80, 100, 104	0
31	d9	53/53 (100%)	0.29	0 100 100	71, 83, 117, 130	0
32	E0	60/62 (96%)	0.59	4 (6%) 24 16	70, 100, 125, 128	0
32	e0	62/62 (100%)	0.25	3 (4%) 35 24	55, 79, 104, 105	0
33	E1	71/76 (93%)	0.62	4 (5%) 30 20	96, 129, 140, 142	0
33	e1	76/76 (100%)	1.06	14 (18%) 3 3	100, 155, 176, 178	0
34	SR	318/318 (100%)	0.54	12 (3%) 44 30	100, 111, 126, 148	0
34	sR	318/318 (100%)	0.77	22 (6%) 23 16	96, 110, 122, 137	0
35	SM	133/159 (83%)	0.83	15 (11%) 10 8	54, 86, 117, 122	0
36	1	3149/3394 (92%)	-0.37	26 (0%) 82 68	30, 54, 125, 221	0
36	5	3150/3394 (92%)	-0.45	21 (0%) 84 70	31, 50, 117, 193	0
37	3	121/121 (100%)	-0.42	0 100 100	40, 70, 86, 94	0
37	7	121/121 (100%)	-0.67	1 (0%) 82 68	35, 53, 64, 71	0
38	4	158/158 (100%)	-0.48	1 (0%) 85 73	40, 60, 96, 129	0
38	8	158/158 (100%)	-0.40	1 (0%) 85 73	42, 64, 97, 126	0
39	L2	252/252 (100%)	0.18	5 (1%) 65 46	40, 57, 74, 83	0
39	l2	252/252 (100%)	0.09	5 (1%) 65 46	38, 56, 74, 87	0
40	L3	386/386 (100%)	0.07	4 (1%) 79 63	38, 57, 69, 83	0
40	l3	386/386 (100%)	-0.06	14 (3%) 46 31	30, 42, 56, 76	0
41	L4	361/361 (100%)	-0.11	4 (1%) 78 60	34, 48, 63, 70	0
41	l4	361/361 (100%)	-0.09	1 (0%) 90 82	37, 52, 70, 76	0
42	L5	296/296 (100%)	0.28	6 (2%) 65 46	51, 76, 94, 108	0
42	l5	294/296 (99%)	-0.06	3 (1%) 79 63	42, 54, 75, 94	0
43	L6	156/175 (89%)	-0.08	1 (0%) 85 73	44, 53, 66, 77	0
43	l6	157/175 (89%)	-0.16	0 100 100	44, 54, 71, 83	0
44	L7	222/223 (99%)	-0.16	2 (0%) 81 65	35, 45, 70, 99	0
44	l7	223/223 (100%)	-0.11	0 100 100	35, 43, 74, 102	0
45	L8	233/233 (100%)	0.41	4 (1%) 69 50	65, 83, 108, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	l8	231/233 (99%)	0.40	6 (2%) 57 38	72, 87, 109, 112	0
46	L9	191/191 (100%)	0.16	5 (2%) 57 38	57, 65, 74, 85	0
46	l9	191/191 (100%)	-0.19	1 (0%) 87 76	39, 48, 63, 72	0
47	M0	211/220 (95%)	0.11	3 (1%) 73 55	41, 54, 88, 102	0
47	m0	213/220 (96%)	0.10	5 (2%) 61 42	36, 50, 74, 87	0
48	M1	169/169 (100%)	0.21	4 (2%) 59 40	62, 77, 87, 93	0
48	m1	169/169 (100%)	-0.08	1 (0%) 85 73	45, 61, 68, 72	0
49	M3	193/194 (99%)	-0.01	2 (1%) 79 63	35, 58, 94, 119	0
49	m3	194/194 (100%)	0.13	3 (1%) 72 53	38, 67, 100, 109	0
50	M4	136/137 (99%)	-0.01	5 (3%) 45 31	50, 59, 70, 74	0
50	m4	137/137 (100%)	-0.15	2 (1%) 72 53	44, 50, 66, 72	0
51	M5	203/203 (100%)	0.15	3 (1%) 72 53	38, 55, 66, 68	0
51	m5	203/203 (100%)	0.24	3 (1%) 72 53	42, 61, 73, 76	0
52	M6	197/197 (100%)	0.04	4 (2%) 65 46	38, 45, 63, 65	0
52	m6	197/197 (100%)	-0.04	4 (2%) 65 46	31, 37, 63, 68	0
53	M7	183/183 (100%)	0.16	7 (3%) 44 30	41, 47, 96, 121	0
53	m7	155/183 (84%)	-0.18	1 (0%) 85 73	37, 42, 52, 70	0
54	M8	185/185 (100%)	-0.07	2 (1%) 78 60	37, 48, 61, 75	0
54	m8	185/185 (100%)	-0.04	1 (0%) 87 76	37, 52, 62, 69	0
55	M9	188/188 (100%)	0.40	9 (4%) 35 24	61, 73, 137, 144	0
55	m9	188/188 (100%)	0.15	5 (2%) 56 37	49, 63, 121, 132	0
56	N0	172/172 (100%)	0.21	6 (3%) 47 31	46, 54, 65, 73	0
56	n0	172/172 (100%)	-0.22	1 (0%) 85 73	38, 45, 55, 63	0
57	N1	159/159 (100%)	0.06	5 (3%) 51 35	37, 51, 92, 98	0
57	n1	159/159 (100%)	0.05	1 (0%) 85 73	36, 44, 78, 83	0
58	N2	100/100 (100%)	0.48	2 (2%) 65 46	92, 102, 107, 115	0
58	n2	98/100 (98%)	0.28	1 (1%) 79 63	74, 85, 91, 93	0
59	N3	136/136 (100%)	0.06	0 100 100	44, 54, 64, 69	0
59	n3	136/136 (100%)	-0.07	1 (0%) 84 70	31, 38, 47, 50	0
60	N4	98/135 (72%)	0.82	11 (11%) 10 9	55, 67, 134, 136	0
60	n4	135/135 (100%)	0.54	11 (8%) 18 13	39, 83, 109, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	N5	121/121 (100%)	0.19	2 (1%) 69 50	57, 69, 85, 106	0
61	n5	120/121 (99%)	0.18	1 (0%) 82 68	56, 69, 87, 93	0
62	N6	126/126 (100%)	0.06	1 (0%) 82 68	44, 61, 70, 79	0
62	n6	126/126 (100%)	0.05	0 100 100	50, 66, 80, 83	0
63	N7	135/135 (100%)	0.37	2 (1%) 72 53	83, 96, 107, 111	0
63	n7	135/135 (100%)	0.38	0 100 100	82, 96, 113, 117	0
64	N8	148/148 (100%)	-0.13	1 (0%) 84 70	31, 49, 67, 75	0
64	n8	148/148 (100%)	0.01	1 (0%) 84 70	33, 54, 68, 71	0
65	N9	58/58 (100%)	0.08	1 (1%) 69 50	34, 54, 89, 101	0
65	n9	58/58 (100%)	0.21	3 (5%) 33 22	35, 52, 73, 77	0
66	O0	97/100 (97%)	0.28	4 (4%) 41 27	80, 88, 103, 106	0
66	o0	100/100 (100%)	0.24	1 (1%) 79 63	72, 83, 100, 103	0
67	O1	109/109 (100%)	0.35	2 (1%) 67 49	55, 65, 88, 92	0
67	o1	109/109 (100%)	-0.03	0 100 100	43, 53, 80, 96	0
68	O2	127/127 (100%)	-0.09	2 (1%) 70 52	33, 44, 55, 67	0
68	o2	127/127 (100%)	-0.10	0 100 100	34, 49, 59, 64	0
69	O3	106/106 (100%)	-0.04	0 100 100	37, 45, 66, 74	0
69	o3	106/106 (100%)	-0.11	0 100 100	36, 42, 64, 74	0
70	O4	112/112 (100%)	0.58	6 (5%) 31 21	54, 74, 103, 109	0
70	o4	112/112 (100%)	0.59	6 (5%) 31 21	51, 73, 105, 111	0
71	O5	119/119 (100%)	0.24	2 (1%) 69 50	55, 70, 77, 80	0
71	o5	119/119 (100%)	0.24	1 (0%) 82 68	63, 71, 86, 95	0
72	O6	99/99 (100%)	0.05	2 (2%) 65 46	55, 67, 92, 100	0
72	o6	99/99 (100%)	0.04	1 (1%) 79 63	61, 72, 86, 99	0
73	O7	87/87 (100%)	0.05	1 (1%) 78 60	41, 46, 67, 75	0
73	o7	87/87 (100%)	0.08	1 (1%) 78 60	37, 49, 77, 91	0
74	O8	77/77 (100%)	0.35	1 (1%) 75 56	82, 92, 103, 106	0
74	o8	77/77 (100%)	0.25	0 100 100	81, 89, 97, 99	0
75	O9	50/50 (100%)	0.19	0 100 100	47, 55, 57, 57	0
75	o9	50/50 (100%)	0.18	0 100 100	48, 55, 60, 62	0
76	Q0	52/52 (100%)	0.02	0 100 100	49, 53, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	q0	52/52 (100%)	-0.41	0 100 100	36, 40, 49, 54	0
77	Q1	25/25 (100%)	0.47	0 100 100	57, 62, 66, 66	0
77	q1	25/25 (100%)	-0.06	0 100 100	45, 47, 48, 50	0
78	Q2	105/105 (100%)	-0.11	0 100 100	41, 51, 72, 93	0
78	q2	105/105 (100%)	-0.18	0 100 100	42, 50, 64, 85	0
79	Q3	91/91 (100%)	0.18	3 (3%) 49 33	46, 59, 74, 81	0
79	q3	91/91 (100%)	0.11	1 (1%) 78 60	42, 55, 67, 73	0
80	6	1795/1800 (99%)	-0.23	23 (1%) 75 56	29, 75, 157, 226	1 (0%)
81	c0	84/96 (87%)	0.87	8 (9%) 14 11	94, 126, 139, 141	0
82	sM	63/104 (60%)	0.55	6 (9%) 14 11	47, 97, 105, 110	0
83	m2	0/150	-	-	-	-
84	p0	143/219 (65%)	0.59	10 (6%) 22 15	88, 109, 177, 181	0
85	p1	0/47	-	-	-	-
85	p2	0/47	-	-	-	-
86	A	2/3 (66%)	1.20	0 100 100	85, 85, 85, 89	0
86	B	2/3 (66%)	0.45	0 100 100	78, 78, 78, 83	0
All	All	33019/34173 (96%)	0.09	796 (2%) 59 40	29, 69, 125, 226	2 (0%)

The worst 5 of 796 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	86	SER	8.4
13	c1	3	THR	8.2
8	s6	162	VAL	6.6
53	M7	161	ALA	6.0
7	s5	37	GLN	6.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	8AN	A	3403	22/23	0.76	0.20	48,103,107,107	0
86	8AN	B	3403	22/23	0.81	0.18	42,97,101,102	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
88	MG	1	4344	1/1	-0.14	0.25	191,191,191,191	0
88	MG	6	2332	1/1	-0.13	0.23	213,213,213,213	0
88	MG	2	2198	1/1	-0.01	0.36	120,120,120,120	0
88	MG	2	2173	1/1	0.01	0.42	116,116,116,116	0
88	MG	2	2230	1/1	0.08	0.28	124,124,124,124	0
88	MG	1	4289	1/1	0.13	0.26	127,127,127,127	0
88	MG	5	4182	1/1	0.15	0.44	123,123,123,123	0
88	MG	2	2247	1/1	0.18	0.25	115,115,115,115	0
88	MG	5	4388	1/1	0.18	0.25	134,134,134,134	0
88	MG	6	2281	1/1	0.21	0.34	124,124,124,124	0
87	OHX	8	219	7/7	0.22	0.36	92,92,92,92	7
88	MG	2	2148	1/1	0.23	0.28	130,130,130,130	0
88	MG	1	4302	1/1	0.27	0.17	126,126,126,126	0
87	OHX	5	3802	7/7	0.31	0.47	76,76,76,76	7
88	MG	2	2156	1/1	0.32	0.43	86,86,86,86	0
88	MG	2	2224	1/1	0.33	0.40	99,99,99,99	0
88	MG	2	2204	1/1	0.33	0.31	106,106,106,106	0
88	MG	2	2147	1/1	0.35	0.28	100,100,100,100	0
88	MG	1	4461	1/1	0.35	0.34	109,109,109,109	0
87	OHX	m1	201	7/7	0.36	0.35	73,73,73,73	7
87	OHX	5	3716	7/7	0.37	0.43	73,73,73,73	7
87	OHX	5	3735	7/7	0.37	0.42	72,72,72,72	7
87	OHX	M0	303	7/7	0.39	0.41	96,96,96,96	7
88	MG	2	2162	1/1	0.39	0.60	85,85,85,85	0
87	OHX	6	2068	7/7	0.41	0.41	83,83,83,83	7
88	MG	5	4524	1/1	0.41	0.19	83,83,83,83	1
88	MG	5	4134	1/1	0.43	0.24	100,100,100,100	0
88	MG	1	4149	1/1	0.43	0.33	101,101,101,101	0
88	MG	6	2305	1/1	0.45	0.42	98,98,98,98	0
88	MG	E1	502	1/1	0.46	0.48	125,125,125,125	0
88	MG	1	4363	1/1	0.47	0.39	92,92,92,92	0
88	MG	6	2333	1/1	0.47	0.21	59,59,59,59	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4314	1/1	0.47	0.28	115,115,115,115	0
88	MG	2	2157	1/1	0.48	0.35	103,103,103,103	0
88	MG	2	2211	1/1	0.49	0.32	106,106,106,106	0
87	OHX	6	2089	7/7	0.50	0.49	74,74,74,74	7
88	MG	5	4419	1/1	0.50	0.15	59,59,59,59	0
88	MG	6	2169	1/1	0.50	0.31	85,85,85,85	0
88	MG	5	4565	1/1	0.50	0.15	117,117,117,117	0
88	MG	M1	201	1/1	0.51	0.13	73,73,73,73	0
87	OHX	2	2072	7/7	0.51	0.33	104,104,104,104	7
87	OHX	6	2093	7/7	0.52	0.32	83,83,83,83	7
88	MG	5	3907	1/1	0.52	0.24	53,53,53,53	1
87	OHX	5	3763	7/7	0.52	0.66	39,39,39,39	7
88	MG	1	4050	1/1	0.52	0.25	105,105,105,105	0
87	OHX	6	2064	7/7	0.53	0.51	68,68,68,68	7
88	MG	2	2137	1/1	0.53	0.27	126,126,126,126	0
87	OHX	2	2079	7/7	0.53	0.27	103,103,103,103	7
87	OHX	5	3758	7/7	0.53	0.46	53,53,53,53	7
88	MG	1	3855	1/1	0.54	0.31	89,89,89,89	0
88	MG	2	2191	1/1	0.54	0.37	99,99,99,99	0
87	OHX	5	3765	7/7	0.55	0.36	78,78,78,78	7
88	MG	1	4327	1/1	0.55	0.23	86,86,86,86	0
88	MG	6	2295	1/1	0.56	0.25	58,58,58,58	1
88	MG	6	2302	1/1	0.56	0.29	106,106,106,106	0
87	OHX	5	3781	7/7	0.56	0.66	53,53,53,53	7
88	MG	1	4205	1/1	0.56	0.21	67,67,67,67	1
88	MG	2	2252	1/1	0.57	0.14	126,126,126,126	0
87	OHX	5	3654	7/7	0.57	0.50	51,51,51,51	7
88	MG	p0	301	1/1	0.57	0.34	93,93,93,93	0
88	MG	2	2119	1/1	0.58	0.34	92,92,92,92	0
88	MG	2	2101	1/1	0.58	0.40	73,73,73,73	0
88	MG	6	2262	1/1	0.58	0.39	114,114,114,114	0
88	MG	1	4486	1/1	0.58	0.33	100,100,100,100	0
88	MG	5	4313	1/1	0.58	0.20	102,102,102,102	0
88	MG	5	4355	1/1	0.59	0.30	73,73,73,73	0
88	MG	6	2191	1/1	0.59	0.29	86,86,86,86	0
88	MG	D9	103	1/1	0.59	0.24	94,94,94,94	0
89	ZN	d7	101	1/1	0.59	0.16	135,135,135,135	0
87	OHX	6	2087	7/7	0.60	0.50	71,71,71,71	7
88	MG	5	4481	1/1	0.60	0.31	95,95,95,95	0
87	OHX	2	2060	7/7	0.60	0.27	98,98,98,98	7
88	MG	2	2149	1/1	0.60	0.30	92,92,92,92	0
88	MG	5	3885	1/1	0.60	0.19	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	OHX	5	3796	7/7	0.60	0.33	87,87,87,87	7
87	OHX	5	3726	7/7	0.61	0.63	42,42,42,42	7
88	MG	2	2250	1/1	0.61	0.16	79,79,79,79	0
88	MG	1	4009	1/1	0.61	0.39	47,47,47,47	0
88	MG	2	2164	1/1	0.61	0.27	122,122,122,122	0
88	MG	d5	201	1/1	0.61	0.26	124,124,124,124	0
87	OHX	2	2029	7/7	0.61	0.35	95,95,95,95	7
88	MG	d9	104	1/1	0.62	0.25	109,109,109,109	0
88	MG	2	2142	1/1	0.62	0.39	61,61,61,61	0
87	OHX	5	3778	7/7	0.62	0.53	45,45,45,45	7
87	OHX	5	3737	7/7	0.62	0.62	53,53,53,53	7
88	MG	1	4083	1/1	0.62	0.34	101,101,101,101	0
88	MG	c9	203	1/1	0.62	0.35	87,87,87,87	0
87	OHX	1	3771	7/7	0.62	0.32	84,84,84,84	7
87	OHX	5	3772	7/7	0.63	0.36	80,80,80,80	7
88	MG	2	2212	1/1	0.63	0.28	86,86,86,86	0
88	MG	2	2217	1/1	0.63	0.26	103,103,103,103	0
88	MG	1	4177	1/1	0.63	0.29	75,75,75,75	0
88	MG	5	4452	1/1	0.63	0.26	100,100,100,100	0
87	OHX	6	2054	7/7	0.63	0.41	65,65,65,65	7
88	MG	1	4482	1/1	0.63	0.14	53,53,53,53	0
88	MG	5	4131	1/1	0.63	0.32	69,69,69,69	0
87	OHX	6	2095	7/7	0.63	0.48	73,73,73,73	7
88	MG	2	2169	1/1	0.63	0.18	101,101,101,101	0
87	OHX	5	3751	7/7	0.64	0.43	49,49,49,49	7
88	MG	2	2214	1/1	0.64	0.18	78,78,78,78	0
88	MG	5	4341	1/1	0.64	0.10	95,95,95,95	0
87	OHX	2	2030	7/7	0.64	0.21	112,112,112,112	7
88	MG	6	2164	1/1	0.64	0.35	87,87,87,87	0
88	MG	1	4477	1/1	0.64	0.13	82,82,82,82	0
88	MG	O4	201	1/1	0.65	0.36	77,77,77,77	0
88	MG	6	2108	1/1	0.65	0.28	98,98,98,98	0
88	MG	6	2154	1/1	0.65	0.29	76,76,76,76	0
88	MG	2	2242	1/1	0.65	0.24	85,85,85,85	0
88	MG	6	2166	1/1	0.65	0.26	88,88,88,88	0
87	OHX	5	3752	7/7	0.65	0.76	42,42,42,42	7
88	MG	5	4294	1/1	0.65	0.14	106,106,106,106	0
87	OHX	1	3733	7/7	0.65	0.50	42,42,42,42	7
87	OHX	1	3656	7/7	0.65	0.16	127,127,127,127	7
87	OHX	6	2036	7/7	0.66	0.40	48,48,48,48	7
88	MG	1	3896	1/1	0.66	0.24	104,104,104,104	0
88	MG	6	2203	1/1	0.66	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	2019	7/7	0.66	0.30	105,105,105,105	7
87	OHX	5	3779	7/7	0.66	0.35	56,56,56,56	7
88	MG	2	2150	1/1	0.66	0.16	74,74,74,74	0
88	MG	5	3882	1/1	0.66	0.27	97,97,97,97	0
87	OHX	6	2010	7/7	0.66	0.37	84,84,84,84	7
87	OHX	5	3809	7/7	0.67	0.13	173,173,173,173	7
88	MG	1	3912	1/1	0.67	0.24	86,86,86,86	0
88	MG	2	2216	1/1	0.67	0.29	69,69,69,69	0
88	MG	2	2143	1/1	0.67	0.24	91,91,91,91	0
88	MG	3	226	1/1	0.67	0.16	65,65,65,65	0
87	OHX	1	3680	7/7	0.67	0.34	81,81,81,81	7
87	OHX	1	3792	7/7	0.67	0.34	71,71,71,71	7
88	MG	2	2176	1/1	0.67	0.14	84,84,84,84	0
88	MG	5	3850	1/1	0.67	0.31	72,72,72,72	0
88	MG	2	2190	1/1	0.68	0.14	78,78,78,78	0
88	MG	1	3815	1/1	0.68	0.35	106,106,106,106	0
87	OHX	1	3699	7/7	0.68	0.28	101,101,101,101	7
88	MG	6	2202	1/1	0.68	0.24	81,81,81,81	0
88	MG	1	4502	1/1	0.68	0.21	94,94,94,94	0
88	MG	2	2090	1/1	0.68	0.30	83,83,83,83	0
87	OHX	6	2074	7/7	0.68	0.24	108,108,108,108	7
87	OHX	6	2081	7/7	0.68	0.34	91,91,91,91	7
87	OHX	O1	201	7/7	0.68	0.34	77,77,77,77	7
87	OHX	3	212	7/7	0.68	0.24	79,79,79,79	7
88	MG	2	2181	1/1	0.68	0.28	80,80,80,80	0
89	ZN	D7	101	1/1	0.68	0.19	147,147,147,147	0
88	MG	5	4199	1/1	0.68	0.17	36,36,36,36	1
88	MG	5	3901	1/1	0.69	0.20	71,71,71,71	0
87	OHX	6	2075	7/7	0.69	0.42	54,54,54,54	7
88	MG	6	2207	1/1	0.69	0.20	93,93,93,93	0
88	MG	2	2186	1/1	0.69	0.29	65,65,65,65	0
88	MG	6	2274	1/1	0.69	0.34	42,42,42,42	1
87	OHX	1	3798	7/7	0.69	0.37	63,63,63,63	7
88	MG	5	4238	1/1	0.69	0.26	44,44,44,44	0
88	MG	6	2184	1/1	0.69	0.17	69,69,69,69	0
87	OHX	1	3731	7/7	0.69	0.40	71,71,71,71	7
87	OHX	6	2096	7/7	0.69	0.33	78,78,78,78	7
88	MG	2	2105	1/1	0.70	0.37	72,72,72,72	0
88	MG	6	2278	1/1	0.70	0.12	83,83,83,83	0
87	OHX	5	3794	7/7	0.70	0.39	73,73,73,73	7
87	OHX	5	3764	7/7	0.70	0.43	47,47,47,47	7
88	MG	2	2255	1/1	0.70	0.22	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4100	1/1	0.70	0.19	45,45,45,45	1
87	OHX	o9	101	7/7	0.70	0.61	52,52,52,52	7
87	OHX	1	3693	7/7	0.70	0.12	169,169,169,169	7
88	MG	4	239	1/1	0.70	0.15	57,57,57,57	0
87	OHX	2	2053	7/7	0.70	0.32	80,80,80,80	7
88	MG	1	4174	1/1	0.70	0.14	93,93,93,93	0
88	MG	1	4368	1/1	0.70	0.18	76,76,76,76	0
87	OHX	5	3804	7/7	0.71	0.29	83,83,83,83	7
88	MG	1	4029	1/1	0.71	0.37	73,73,73,73	0
88	MG	2	2154	1/1	0.71	0.27	68,68,68,68	0
88	MG	6	2153	1/1	0.71	0.35	44,44,44,44	0
87	OHX	6	2042	7/7	0.71	0.47	54,54,54,54	7
88	MG	S4	302	1/1	0.71	0.19	87,87,87,87	0
88	MG	2	2098	1/1	0.71	0.28	80,80,80,80	0
87	OHX	6	2028	7/7	0.71	0.46	58,58,58,58	7
87	OHX	2	2075	7/7	0.71	0.35	87,87,87,87	7
88	MG	2	2192	1/1	0.71	0.33	64,64,64,64	0
88	MG	2	2165	1/1	0.71	0.13	98,98,98,98	0
87	OHX	m4	201	7/7	0.71	0.21	101,101,101,101	7
88	MG	5	4261	1/1	0.71	0.21	61,61,61,61	0
88	MG	1	3820	1/1	0.72	0.28	55,55,55,55	0
88	MG	1	3838	1/1	0.72	0.31	45,45,45,45	0
87	OHX	1	3768	7/7	0.72	0.42	61,61,61,61	7
88	MG	5	4321	1/1	0.72	0.15	74,74,74,74	0
87	OHX	5	3677	7/7	0.72	0.40	80,80,80,80	7
87	OHX	8	218	7/7	0.72	0.39	48,48,48,48	7
87	OHX	5	3684	7/7	0.72	0.53	37,37,37,37	7
87	OHX	5	3795	7/7	0.72	0.32	72,72,72,72	7
88	MG	2	2134	1/1	0.72	0.24	76,76,76,76	0
87	OHX	1	3802	7/7	0.72	0.41	54,54,54,54	7
88	MG	1	4138	1/1	0.72	0.16	45,45,45,45	1
87	OHX	n3	202	7/7	0.72	0.44	44,44,44,44	7
88	MG	6	2326	1/1	0.72	0.15	79,79,79,79	0
88	MG	1	4481	1/1	0.72	0.17	63,63,63,63	0
87	OHX	6	2077	7/7	0.72	0.26	85,85,85,85	7
87	OHX	6	2051	7/7	0.73	0.31	82,82,82,82	7
88	MG	2	2225	1/1	0.73	0.43	58,58,58,58	1
88	MG	1	4043	1/1	0.73	0.17	83,83,83,83	0
88	MG	6	2273	1/1	0.73	0.19	80,80,80,80	0
87	OHX	1	3750	7/7	0.73	0.18	99,99,99,99	7
87	OHX	8	217	7/7	0.73	0.31	82,82,82,82	7
88	MG	2	2140	1/1	0.73	0.49	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	6	2063	7/7	0.73	0.36	77,77,77,77	7
87	OHX	1	3752	7/7	0.73	0.43	59,59,59,59	7
88	MG	M5	305	1/1	0.73	0.41	69,69,69,69	0
87	OHX	6	2066	7/7	0.73	0.37	70,70,70,70	7
87	OHX	1	3757	7/7	0.73	0.22	117,117,117,117	7
88	MG	6	2117	1/1	0.73	0.34	61,61,61,61	0
87	OHX	5	3744	7/7	0.73	0.46	54,54,54,54	7
87	OHX	5	3788	7/7	0.73	0.52	51,51,51,51	7
87	OHX	1	3679	7/7	0.73	0.40	61,61,61,61	7
87	OHX	1	3691	7/7	0.73	0.40	56,56,56,56	7
87	OHX	5	3670	7/7	0.73	0.43	39,39,39,39	7
88	MG	2	2161	1/1	0.73	0.27	63,63,63,63	0
87	OHX	5	3759	7/7	0.73	0.44	56,56,56,56	7
88	MG	2	2116	1/1	0.73	0.26	89,89,89,89	0
88	MG	2	2124	1/1	0.74	0.30	77,77,77,77	0
87	OHX	N8	201	7/7	0.74	0.23	94,94,94,94	7
87	OHX	1	3667	7/7	0.74	0.35	85,85,85,85	7
88	MG	6	2301	1/1	0.74	0.20	57,57,57,57	0
87	OHX	1	3807	7/7	0.74	0.24	89,89,89,89	7
87	OHX	5	3708	7/7	0.74	0.65	36,36,36,36	7
87	OHX	6	2094	7/7	0.74	0.22	102,102,102,102	7
88	MG	1	3852	1/1	0.74	0.41	63,63,63,63	0
87	OHX	6	2060	7/7	0.74	0.42	58,58,58,58	7
88	MG	5	4328	1/1	0.74	0.11	106,106,106,106	0
88	MG	1	4229	1/1	0.74	0.14	63,63,63,63	0
88	MG	1	4254	1/1	0.74	0.20	77,77,77,77	0
88	MG	2	2111	1/1	0.74	0.35	63,63,63,63	0
87	OHX	2	2081	7/7	0.74	0.15	120,120,120,120	7
88	MG	6	2216	1/1	0.74	0.19	86,86,86,86	0
88	MG	2	2254	1/1	0.74	0.13	97,97,97,97	0
88	MG	6	2272	1/1	0.74	0.30	98,98,98,98	0
87	OHX	2	2034	7/7	0.74	0.28	86,86,86,86	7
88	MG	5	4067	1/1	0.74	0.43	89,89,89,89	0
88	MG	Q2	503	1/1	0.74	0.32	62,62,62,62	0
88	MG	5	4117	1/1	0.74	0.21	52,52,52,52	0
88	MG	4	235	1/1	0.75	0.24	98,98,98,98	0
88	MG	2	2193	1/1	0.75	0.29	71,71,71,71	0
88	MG	5	4125	1/1	0.75	0.34	82,82,82,82	0
87	OHX	1	3725	7/7	0.75	0.39	57,57,57,57	7
87	OHX	1	3727	7/7	0.75	0.20	100,100,100,100	7
88	MG	5	4151	1/1	0.75	0.26	80,80,80,80	0
88	MG	1	3921	1/1	0.75	0.42	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	6	2283	1/1	0.75	0.17	69,69,69,69	1
87	OHX	C3	201	7/7	0.75	0.29	99,99,99,99	7
88	MG	1	4324	1/1	0.75	0.18	70,70,70,70	0
87	OHX	5	3808	7/7	0.75	0.60	54,54,54,54	7
88	MG	1	4341	1/1	0.75	0.18	44,44,44,44	1
88	MG	2	2257	1/1	0.75	0.13	121,121,121,121	0
87	OHX	2	2084	7/7	0.75	0.13	183,183,183,183	7
88	MG	2	2178	1/1	0.75	0.25	79,79,79,79	0
87	OHX	5	3811	7/7	0.75	0.40	66,66,66,66	7
88	MG	1	4145	1/1	0.75	0.17	82,82,82,82	0
87	OHX	7	211	7/7	0.75	0.45	61,61,61,61	7
88	MG	sM	201	1/1	0.75	0.19	48,48,48,48	0
87	OHX	1	3700	7/7	0.75	0.40	55,55,55,55	7
87	OHX	5	3755	7/7	0.75	0.18	110,110,110,110	7
88	MG	1	4488	1/1	0.75	0.25	65,65,65,65	0
88	MG	5	4568	1/1	0.75	0.36	69,69,69,69	0
88	MG	8	230	1/1	0.75	0.17	72,72,72,72	0
88	MG	8	233	1/1	0.75	0.17	88,88,88,88	0
88	MG	12	305	1/1	0.75	0.11	71,71,71,71	0
88	MG	1	4193	1/1	0.75	0.23	56,56,56,56	0
88	MG	6	2251	1/1	0.75	0.29	74,74,74,74	0
88	MG	2	2163	1/1	0.75	0.31	70,70,70,70	0
88	MG	5	4270	1/1	0.76	0.12	46,46,46,46	0
87	OHX	2	2086	7/7	0.76	0.20	105,105,105,105	7
88	MG	2	2189	1/1	0.76	0.27	94,94,94,94	0
87	OHX	2	2066	7/7	0.76	0.39	80,80,80,80	7
87	OHX	1	3799	7/7	0.76	0.51	48,48,48,48	7
87	OHX	5	3741	7/7	0.76	0.64	37,37,37,37	7
87	OHX	6	2049	7/7	0.76	0.33	70,70,70,70	7
88	MG	1	4089	1/1	0.76	0.39	43,43,43,43	0
88	MG	5	3909	1/1	0.76	0.19	55,55,55,55	0
88	MG	1	4099	1/1	0.76	0.41	88,88,88,88	0
88	MG	6	2175	1/1	0.76	0.21	56,56,56,56	0
88	MG	6	2178	1/1	0.76	0.21	54,54,54,54	0
87	OHX	1	3738	7/7	0.76	0.55	41,41,41,41	7
88	MG	6	2304	1/1	0.76	0.33	52,52,52,52	1
88	MG	4	236	1/1	0.76	0.17	67,67,67,67	0
87	OHX	6	2052	7/7	0.76	0.13	127,127,127,127	7
88	MG	2	2125	1/1	0.76	0.27	85,85,85,85	0
88	MG	12	306	1/1	0.76	0.37	53,53,53,53	1
87	OHX	5	3754	7/7	0.76	0.38	42,42,42,42	7
87	OHX	2	2058	7/7	0.76	0.10	193,193,193,193	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	6	2229	1/1	0.76	0.23	45,45,45,45	0
88	MG	1	4180	1/1	0.77	0.17	63,63,63,63	0
87	OHX	5	3814	7/7	0.77	0.42	63,63,63,63	7
88	MG	2	2188	1/1	0.77	0.09	84,84,84,84	0
87	OHX	1	3741	7/7	0.77	0.33	72,72,72,72	7
88	MG	5	4251	1/1	0.77	0.14	37,37,37,37	0
87	OHX	7	212	7/7	0.77	0.26	56,56,56,56	7
88	MG	s4	302	1/1	0.77	0.29	55,55,55,55	0
88	MG	c8	205	1/1	0.77	0.21	93,93,93,93	0
88	MG	2	2249	1/1	0.77	0.38	97,97,97,97	0
87	OHX	6	2012	7/7	0.77	0.28	64,64,64,64	7
87	OHX	1	3804	7/7	0.77	0.41	60,60,60,60	7
88	MG	6	2222	1/1	0.77	0.19	81,81,81,81	0
87	OHX	5	3699	7/7	0.77	0.21	86,86,86,86	7
87	OHX	19	201	7/7	0.77	0.33	62,62,62,62	7
87	OHX	1	3671	7/7	0.77	0.57	49,49,49,49	7
88	MG	S1	301	1/1	0.77	0.17	105,105,105,105	0
88	MG	5	3904	1/1	0.77	0.30	76,76,76,76	0
87	OHX	1	3791	7/7	0.77	0.28	79,79,79,79	7
88	MG	6	2129	1/1	0.77	0.29	59,59,59,59	0
88	MG	5	4063	1/1	0.77	0.14	54,54,54,54	0
88	MG	6	2139	1/1	0.77	0.39	63,63,63,63	0
87	OHX	1	3665	7/7	0.77	0.55	54,54,54,54	7
87	OHX	2	2078	7/7	0.77	0.25	102,102,102,102	7
87	OHX	1	3765	7/7	0.77	0.60	49,49,49,49	7
87	OHX	5	3644	7/7	0.77	0.28	69,69,69,69	7
88	MG	5	4133	1/1	0.77	0.33	63,63,63,63	0
87	OHX	6	2076	7/7	0.77	0.27	74,74,74,74	7
88	MG	5	4158	1/1	0.78	0.28	49,49,49,49	0
87	OHX	2	2063	7/7	0.78	0.33	81,81,81,81	7
87	OHX	5	3715	7/7	0.78	0.26	64,64,64,64	7
87	OHX	1	3766	7/7	0.78	0.17	141,141,141,141	7
88	MG	2	2139	1/1	0.78	0.40	70,70,70,70	0
87	OHX	6	2023	7/7	0.78	0.26	80,80,80,80	7
88	MG	1	4210	1/1	0.78	0.13	36,36,36,36	0
87	OHX	4	214	7/7	0.78	0.50	46,46,46,46	7
87	OHX	1	3702	7/7	0.78	0.34	60,60,60,60	7
88	MG	6	2234	1/1	0.78	0.17	79,79,79,79	0
88	MG	2	2232	1/1	0.78	0.14	90,90,90,90	0
88	MG	6	2256	1/1	0.78	0.28	73,73,73,73	0
88	MG	2	2093	1/1	0.78	0.41	74,74,74,74	0
88	MG	5	4372	1/1	0.78	0.21	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	3672	7/7	0.78	0.37	42,42,42,42	7
87	OHX	1	3724	7/7	0.78	0.53	37,37,37,37	7
87	OHX	5	3682	7/7	0.78	0.37	56,56,56,56	7
88	MG	5	3942	1/1	0.78	0.33	33,33,33,33	0
88	MG	5	4490	1/1	0.78	0.19	69,69,69,69	0
88	MG	5	4512	1/1	0.78	0.40	62,62,62,62	1
87	OHX	8	215	7/7	0.78	0.43	48,48,48,48	7
88	MG	1	4072	1/1	0.78	0.27	76,76,76,76	0
88	MG	2	2114	1/1	0.78	0.53	79,79,79,79	0
88	MG	5	4572	1/1	0.78	0.12	53,53,53,53	0
88	MG	5	4103	1/1	0.78	0.28	59,59,59,59	0
87	OHX	1	3670	7/7	0.78	0.43	64,64,64,64	7
88	MG	1	4400	1/1	0.78	0.24	57,57,57,57	0
88	MG	2	2117	1/1	0.78	0.21	74,74,74,74	0
88	MG	2	2203	1/1	0.78	0.13	85,85,85,85	0
87	OHX	5	3692	7/7	0.78	0.31	49,49,49,49	7
87	OHX	6	1993	7/7	0.78	0.26	78,78,78,78	7
87	OHX	M9	203	7/7	0.79	0.18	78,78,78,78	7
88	MG	5	3977	1/1	0.79	0.32	50,50,50,50	0
88	MG	5	4011	1/1	0.79	0.39	38,38,38,38	0
87	OHX	1	3726	7/7	0.79	0.35	59,59,59,59	7
87	OHX	1	3779	7/7	0.79	0.48	48,48,48,48	7
88	MG	5	4095	1/1	0.79	0.27	61,61,61,61	0
87	OHX	1	3783	7/7	0.79	0.37	69,69,69,69	7
88	MG	6	2208	1/1	0.79	0.09	67,67,67,67	0
88	MG	6	2212	1/1	0.79	0.10	84,84,84,84	0
88	MG	1	4431	1/1	0.79	0.22	41,41,41,41	1
87	OHX	6	2097	7/7	0.79	0.41	70,70,70,70	7
88	MG	1	4464	1/1	0.79	0.10	70,70,70,70	1
88	MG	2	2126	1/1	0.79	0.38	69,69,69,69	0
88	MG	2	2244	1/1	0.79	0.21	78,78,78,78	0
88	MG	2	2175	1/1	0.79	0.29	87,87,87,87	0
88	MG	2	2128	1/1	0.79	0.46	60,60,60,60	0
88	MG	1	4122	1/1	0.79	0.10	66,66,66,66	0
87	OHX	5	3722	7/7	0.79	0.32	62,62,62,62	7
88	MG	5	4248	1/1	0.79	0.22	58,58,58,58	0
88	MG	2	2136	1/1	0.79	0.26	71,71,71,71	0
88	MG	3	229	1/1	0.79	0.48	52,52,52,52	1
88	MG	1	4147	1/1	0.79	0.19	50,50,50,50	0
87	OHX	5	3569	7/7	0.79	0.40	64,64,64,64	7
88	MG	1	4172	1/1	0.79	0.13	72,72,72,72	0
88	MG	L8	301	1/1	0.79	0.13	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	3638	7/7	0.79	0.50	39,39,39,39	7
87	OHX	5	3793	7/7	0.79	0.51	42,42,42,42	7
88	MG	5	4342	1/1	0.79	0.36	68,68,68,68	1
88	MG	5	4345	1/1	0.79	0.11	41,41,41,41	1
88	MG	M9	204	1/1	0.79	0.12	70,70,70,70	0
88	MG	6	2306	1/1	0.79	0.17	79,79,79,79	0
88	MG	N6	201	1/1	0.79	0.24	63,63,63,63	0
87	OHX	1	3785	7/7	0.79	0.39	56,56,56,56	7
88	MG	O7	108	1/1	0.79	0.33	69,69,69,69	0
87	OHX	5	3651	7/7	0.79	0.31	47,47,47,47	7
88	MG	2	2146	1/1	0.79	0.27	86,86,86,86	0
88	MG	5	4509	1/1	0.79	0.12	97,97,97,97	0
88	MG	c9	201	1/1	0.79	0.14	78,78,78,78	0
87	OHX	2	1989	7/7	0.79	0.24	104,104,104,104	7
87	OHX	6	2056	7/7	0.79	0.14	97,97,97,97	7
88	MG	2	2096	1/1	0.79	0.40	61,61,61,61	0
88	MG	1	4258	1/1	0.79	0.14	74,74,74,74	0
88	MG	1	4278	1/1	0.79	0.14	47,47,47,47	1
87	OHX	2	2041	7/7	0.79	0.33	83,83,83,83	7
87	OHX	6	2085	7/7	0.79	0.13	128,128,128,128	7
87	OHX	6	2062	7/7	0.79	0.29	74,74,74,74	7
88	MG	1	3868	1/1	0.79	0.30	54,54,54,54	0
87	OHX	2	2049	7/7	0.79	0.29	84,84,84,84	7
87	OHX	5	3691	7/7	0.79	0.61	55,55,55,55	7
88	MG	1	4472	1/1	0.80	0.16	81,81,81,81	0
88	MG	6	2214	1/1	0.80	0.09	79,79,79,79	0
87	OHX	5	3700	7/7	0.80	0.30	67,67,67,67	7
87	OHX	5	3782	7/7	0.80	0.44	42,42,42,42	7
87	OHX	1	3721	7/7	0.80	0.28	68,68,68,68	7
87	OHX	1	3767	7/7	0.80	0.45	52,52,52,52	7
88	MG	6	2240	1/1	0.80	0.18	74,74,74,74	0
88	MG	6	2242	1/1	0.80	0.37	55,55,55,55	1
88	MG	5	4130	1/1	0.80	0.09	37,37,37,37	0
87	OHX	1	3735	7/7	0.80	0.45	52,52,52,52	7
88	MG	6	2255	1/1	0.80	0.32	54,54,54,54	0
88	MG	1	4127	1/1	0.80	0.23	63,63,63,63	0
88	MG	5	4150	1/1	0.80	0.18	44,44,44,44	0
87	OHX	1	3808	7/7	0.80	0.26	88,88,88,88	7
88	MG	1	4144	1/1	0.80	0.12	69,69,69,69	0
88	MG	5	4160	1/1	0.80	0.13	83,83,83,83	0
87	OHX	1	3810	7/7	0.80	0.14	149,149,149,149	7
87	OHX	1	3736	7/7	0.80	0.27	70,70,70,70	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	2080	7/7	0.80	0.60	66,66,66,66	7
87	OHX	5	3807	7/7	0.80	0.42	44,44,44,44	7
87	OHX	1	3781	7/7	0.80	0.68	47,47,47,47	7
87	OHX	5	3632	7/7	0.80	0.49	44,44,44,44	7
88	MG	6	2300	1/1	0.80	0.17	82,82,82,82	0
87	OHX	1	3703	7/7	0.80	0.21	106,106,106,106	7
88	MG	5	4304	1/1	0.80	0.21	58,58,58,58	0
88	MG	5	4306	1/1	0.80	0.08	50,50,50,50	0
88	MG	2	2182	1/1	0.80	0.38	87,87,87,87	0
88	MG	S4	301	1/1	0.80	0.30	76,76,76,76	0
88	MG	2	2185	1/1	0.80	0.38	74,74,74,74	0
87	OHX	1	3709	7/7	0.80	0.41	58,58,58,58	7
88	MG	6	2323	1/1	0.80	0.32	70,70,70,70	0
87	OHX	6	2065	7/7	0.80	0.14	129,129,129,129	7
88	MG	1	3811	1/1	0.80	0.29	44,44,44,44	0
87	OHX	1	3786	7/7	0.80	0.25	69,69,69,69	7
88	MG	5	4385	1/1	0.80	0.18	63,63,63,63	0
87	OHX	5	3756	7/7	0.80	0.21	89,89,89,89	7
88	MG	c8	204	1/1	0.80	0.22	81,81,81,81	0
88	MG	6	2143	1/1	0.80	0.44	86,86,86,86	0
87	OHX	1	3789	7/7	0.80	0.54	46,46,46,46	7
87	OHX	1	3717	7/7	0.80	0.25	96,96,96,96	7
87	OHX	1	3729	7/7	0.80	0.70	46,46,46,46	7
87	OHX	1	3794	7/7	0.80	0.25	93,93,93,93	7
88	MG	1	3885	1/1	0.80	0.28	37,37,37,37	0
88	MG	5	4537	1/1	0.80	0.10	56,56,56,56	0
88	MG	6	2171	1/1	0.80	0.18	79,79,79,79	0
87	OHX	m0	302	7/7	0.80	0.53	45,45,45,45	7
88	MG	1	4356	1/1	0.80	0.40	55,55,55,55	1
87	OHX	6	2024	7/7	0.80	0.24	86,86,86,86	7
87	OHX	1	3760	7/7	0.80	0.49	49,49,49,49	7
88	MG	5	3906	1/1	0.80	0.34	88,88,88,88	0
87	OHX	1	3718	7/7	0.80	0.34	69,69,69,69	7
87	OHX	6	2086	7/7	0.80	0.15	147,147,147,147	7
87	OHX	5	3780	7/7	0.80	0.56	55,55,55,55	7
88	MG	2	2155	1/1	0.80	0.32	60,60,60,60	0
88	MG	4	240	1/1	0.81	0.22	53,53,53,53	0
88	MG	1	4194	1/1	0.81	0.41	47,47,47,47	0
87	OHX	6	2079	7/7	0.81	0.32	60,60,60,60	7
87	OHX	5	3701	7/7	0.81	0.43	46,46,46,46	7
88	MG	1	4220	1/1	0.81	0.20	74,74,74,74	0
88	MG	1	4222	1/1	0.81	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4136	1/1	0.81	0.23	82,82,82,82	0
88	MG	1	4225	1/1	0.81	0.22	64,64,64,64	0
88	MG	6	2287	1/1	0.81	0.26	62,62,62,62	0
87	OHX	m5	502	7/7	0.81	0.41	78,78,78,78	7
87	OHX	1	3734	7/7	0.81	0.29	68,68,68,68	7
88	MG	5	4181	1/1	0.81	0.13	50,50,50,50	0
88	MG	1	3919	1/1	0.81	0.31	75,75,75,75	0
87	OHX	1	3751	7/7	0.81	0.30	79,79,79,79	7
88	MG	1	3935	1/1	0.81	0.38	37,37,37,37	0
88	MG	1	3996	1/1	0.81	0.18	39,39,39,39	0
87	OHX	4	216	7/7	0.81	0.29	73,73,73,73	7
88	MG	6	2320	1/1	0.81	0.13	62,62,62,62	0
87	OHX	1	3659	7/7	0.81	0.47	48,48,48,48	7
88	MG	6	2325	1/1	0.81	0.18	59,59,59,59	0
88	MG	1	4042	1/1	0.81	0.17	59,59,59,59	0
88	MG	6	2156	1/1	0.81	0.57	66,66,66,66	0
88	MG	2	2145	1/1	0.81	0.43	97,97,97,97	0
88	MG	2	2251	1/1	0.81	0.14	59,59,59,59	1
88	MG	1	4063	1/1	0.81	0.34	71,71,71,71	0
88	MG	1	4064	1/1	0.81	0.17	62,62,62,62	0
88	MG	2	2095	1/1	0.81	0.27	63,63,63,63	0
87	OHX	1	3770	7/7	0.81	0.35	53,53,53,53	7
87	OHX	5	3766	7/7	0.81	0.26	96,96,96,96	7
88	MG	1	4436	1/1	0.81	0.14	43,43,43,43	0
88	MG	2	2099	1/1	0.81	0.32	63,63,63,63	0
87	OHX	S8	301	7/7	0.81	0.19	108,108,108,108	7
88	MG	5	4409	1/1	0.81	0.08	72,72,72,72	0
88	MG	5	3856	1/1	0.81	0.24	39,39,39,39	0
88	MG	5	4424	1/1	0.81	0.12	69,69,69,69	0
88	MG	1	4124	1/1	0.81	0.20	55,55,55,55	0
87	OHX	2	2045	7/7	0.81	0.30	73,73,73,73	7
88	MG	5	3891	1/1	0.81	0.21	59,59,59,59	0
87	OHX	2	2083	7/7	0.81	0.19	106,106,106,106	7
87	OHX	5	3742	7/7	0.81	0.12	149,149,149,149	7
87	OHX	6	2003	7/7	0.81	0.33	61,61,61,61	7
87	OHX	6	2007	7/7	0.81	0.28	62,62,62,62	7
87	OHX	5	3785	7/7	0.81	0.17	90,90,90,90	7
88	MG	6	2233	1/1	0.81	0.36	83,83,83,83	0
87	OHX	5	3786	7/7	0.81	0.58	40,40,40,40	7
87	OHX	8	220	7/7	0.81	0.28	77,77,77,77	7
88	MG	4	220	1/1	0.81	0.37	65,65,65,65	0
88	MG	6	2248	1/1	0.81	0.37	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4094	1/1	0.81	0.23	50,50,50,50	0
88	MG	n0	201	1/1	0.81	0.39	49,49,49,49	1
87	OHX	c3	201	7/7	0.81	0.28	79,79,79,79	7
88	MG	1	3853	1/1	0.81	0.19	51,51,51,51	0
87	OHX	3	209	7/7	0.81	0.31	82,82,82,82	7
88	MG	6	2217	1/1	0.82	0.11	66,66,66,66	0
87	OHX	6	2078	7/7	0.82	0.23	93,93,93,93	7
88	MG	1	4463	1/1	0.82	0.24	58,58,58,58	0
88	MG	2	2122	1/1	0.82	0.41	68,68,68,68	0
88	MG	1	4465	1/1	0.82	0.12	55,55,55,55	0
87	OHX	1	3777	7/7	0.82	0.23	63,63,63,63	7
87	OHX	6	2080	7/7	0.82	0.18	126,126,126,126	7
88	MG	1	4117	1/1	0.82	0.17	37,37,37,37	0
88	MG	2	2179	1/1	0.82	0.25	85,85,85,85	0
87	OHX	1	3778	7/7	0.82	0.36	55,55,55,55	7
87	OHX	5	3688	7/7	0.82	0.51	38,38,38,38	7
88	MG	6	2260	1/1	0.82	0.21	55,55,55,55	0
87	OHX	6	1989	7/7	0.82	0.29	84,84,84,84	7
88	MG	6	2268	1/1	0.82	0.40	84,84,84,84	0
88	MG	1	4143	1/1	0.82	0.24	48,48,48,48	0
87	OHX	6	2053	7/7	0.82	0.23	85,85,85,85	7
87	OHX	1	3755	7/7	0.82	0.35	45,45,45,45	7
87	OHX	2	2046	7/7	0.82	0.15	114,114,114,114	7
87	OHX	6	2092	7/7	0.82	0.20	104,104,104,104	7
88	MG	1	4169	1/1	0.82	0.40	52,52,52,52	0
87	OHX	6	2059	7/7	0.82	0.20	104,104,104,104	7
87	OHX	2	2055	7/7	0.82	0.34	72,72,72,72	7
88	MG	1	3834	1/1	0.82	0.23	59,59,59,59	0
88	MG	1	3835	1/1	0.82	0.29	46,46,46,46	0
87	OHX	1	3762	7/7	0.82	0.54	59,59,59,59	7
87	OHX	2	2077	7/7	0.82	0.17	139,139,139,139	7
87	OHX	5	3723	7/7	0.82	0.47	53,53,53,53	7
88	MG	O7	104	1/1	0.82	0.24	81,81,81,81	0
87	OHX	6	2018	7/7	0.82	0.42	54,54,54,54	7
88	MG	2	2209	1/1	0.82	0.23	71,71,71,71	0
88	MG	5	4318	1/1	0.82	0.10	62,62,62,62	0
87	OHX	1	3744	7/7	0.82	0.28	89,89,89,89	7
88	MG	5	4323	1/1	0.82	0.38	82,82,82,82	0
88	MG	1	3890	1/1	0.82	0.29	53,53,53,53	0
87	OHX	1	3745	7/7	0.82	0.38	62,62,62,62	7
88	MG	1	4240	1/1	0.82	0.15	72,72,72,72	0
88	MG	1	3899	1/1	0.82	0.29	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	c6	201	1/1	0.82	0.25	97,97,97,97	0
87	OHX	5	3629	7/7	0.82	0.34	43,43,43,43	7
88	MG	1	3913	1/1	0.82	0.19	49,49,49,49	0
87	OHX	2	2065	7/7	0.82	0.20	110,110,110,110	7
87	OHX	6	2073	7/7	0.82	0.31	64,64,64,64	7
88	MG	2	2102	1/1	0.82	0.29	84,84,84,84	0
88	MG	1	3970	1/1	0.82	0.22	54,54,54,54	0
87	OHX	5	3640	7/7	0.82	0.35	47,47,47,47	7
88	MG	5	4460	1/1	0.82	0.16	66,66,66,66	0
88	MG	5	3842	1/1	0.82	0.16	43,43,43,43	0
88	MG	2	2229	1/1	0.82	0.18	84,84,84,84	0
88	MG	1	4020	1/1	0.82	0.27	37,37,37,37	0
88	MG	1	4345	1/1	0.82	0.10	69,69,69,69	0
88	MG	1	4352	1/1	0.82	0.11	88,88,88,88	0
88	MG	6	2192	1/1	0.82	0.35	75,75,75,75	0
88	MG	1	4355	1/1	0.82	0.16	51,51,51,51	1
88	MG	2	2109	1/1	0.82	0.37	73,73,73,73	0
87	OHX	6	2034	7/7	0.82	0.10	134,134,134,134	7
87	OHX	1	3661	7/7	0.82	0.38	59,59,59,59	7
87	OHX	2	2039	7/7	0.82	0.23	103,103,103,103	7
88	MG	5	3931	1/1	0.82	0.24	54,54,54,54	0
87	OHX	6	2044	7/7	0.82	0.24	78,78,78,78	7
88	MG	15	304	1/1	0.82	0.21	61,61,61,61	0
88	MG	5	3943	1/1	0.82	0.25	43,43,43,43	0
88	MG	5	3961	1/1	0.82	0.16	55,55,55,55	0
88	MG	2	2170	1/1	0.82	0.17	78,78,78,78	0
88	MG	5	3978	1/1	0.82	0.33	57,57,57,57	0
88	MG	1	3875	1/1	0.83	0.24	61,61,61,61	0
88	MG	2	2159	1/1	0.83	0.23	75,75,75,75	0
87	OHX	6	2022	7/7	0.83	0.14	139,139,139,139	7
88	MG	6	2258	1/1	0.83	0.25	84,84,84,84	0
88	MG	1	3895	1/1	0.83	0.17	40,40,40,40	0
88	MG	2	2218	1/1	0.83	0.14	82,82,82,82	0
87	OHX	5	3680	7/7	0.83	0.41	43,43,43,43	7
88	MG	4	244	1/1	0.83	0.14	95,95,95,95	0
87	OHX	2	2061	7/7	0.83	0.26	78,78,78,78	7
87	OHX	4	215	7/7	0.83	0.27	74,74,74,74	7
88	MG	1	3917	1/1	0.83	0.33	37,37,37,37	0
87	OHX	2	2027	7/7	0.83	0.18	111,111,111,111	7
87	OHX	1	3773	7/7	0.83	0.30	68,68,68,68	7
87	OHX	6	2070	7/7	0.83	0.28	71,71,71,71	7
88	MG	1	3955	1/1	0.83	0.23	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	OHX	1	3774	7/7	0.83	0.36	56,56,56,56	7
88	MG	2	2245	1/1	0.83	0.17	71,71,71,71	0
88	MG	6	2105	1/1	0.83	0.28	49,49,49,49	0
87	OHX	2	2052	7/7	0.83	0.10	189,189,189,189	7
88	MG	5	4207	1/1	0.83	0.20	46,46,46,46	0
88	MG	5	4222	1/1	0.83	0.12	36,36,36,36	0
88	MG	5	4226	1/1	0.83	0.15	55,55,55,55	0
87	OHX	2	2047	7/7	0.83	0.20	106,106,106,106	7
88	MG	6	2128	1/1	0.83	0.21	68,68,68,68	0
88	MG	1	4028	1/1	0.83	0.29	49,49,49,49	0
88	MG	6	2138	1/1	0.83	0.12	73,73,73,73	0
87	OHX	5	3620	7/7	0.83	0.24	51,51,51,51	7
87	OHX	5	3710	7/7	0.83	0.29	82,82,82,82	7
87	OHX	5	3711	7/7	0.83	0.31	69,69,69,69	7
88	MG	2	2253	1/1	0.83	0.26	76,76,76,76	0
88	MG	6	2155	1/1	0.83	0.23	72,72,72,72	0
88	MG	1	4346	1/1	0.83	0.18	40,40,40,40	1
87	OHX	2	2067	7/7	0.83	0.27	92,92,92,92	7
87	OHX	2	2069	7/7	0.83	0.28	78,78,78,78	7
87	OHX	1	3600	7/7	0.83	0.32	62,62,62,62	7
88	MG	5	4336	1/1	0.83	0.32	34,34,34,34	0
88	MG	1	4361	1/1	0.83	0.33	38,38,38,38	1
87	OHX	1	3809	7/7	0.83	0.57	60,60,60,60	7
87	OHX	m9	201	7/7	0.83	0.22	70,70,70,70	7
87	OHX	1	3706	7/7	0.83	0.41	55,55,55,55	7
87	OHX	1	3748	7/7	0.83	0.09	180,180,180,180	7
87	OHX	5	3736	7/7	0.83	0.32	62,62,62,62	7
88	MG	6	2200	1/1	0.83	0.21	74,74,74,74	0
88	MG	5	4396	1/1	0.83	0.14	43,43,43,43	1
88	MG	5	3872	1/1	0.83	0.24	33,33,33,33	0
88	MG	5	4414	1/1	0.83	0.22	64,64,64,64	0
87	OHX	6	2013	7/7	0.83	0.27	82,82,82,82	7
88	MG	1	4126	1/1	0.83	0.32	58,58,58,58	0
88	MG	6	2205	1/1	0.83	0.21	84,84,84,84	0
88	MG	2	2194	1/1	0.83	0.26	72,72,72,72	0
88	MG	2	2197	1/1	0.83	0.31	76,76,76,76	0
88	MG	2	2094	1/1	0.83	0.33	62,62,62,62	0
88	MG	1	4473	1/1	0.83	0.14	47,47,47,47	0
87	OHX	5	3668	7/7	0.83	0.29	71,71,71,71	7
88	MG	5	3917	1/1	0.83	0.10	51,51,51,51	0
88	MG	5	3922	1/1	0.83	0.25	65,65,65,65	0
87	OHX	6	2015	7/7	0.83	0.38	65,65,65,65	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	3602	7/7	0.83	0.27	68,68,68,68	7
87	OHX	5	3746	7/7	0.83	0.12	131,131,131,131	7
88	MG	7	221	1/1	0.83	0.13	61,61,61,61	0
88	MG	7	224	1/1	0.83	0.20	39,39,39,39	0
88	MG	5	3954	1/1	0.83	0.59	61,61,61,61	0
87	OHX	5	3747	7/7	0.83	0.35	61,61,61,61	7
88	MG	5	3967	1/1	0.83	0.30	27,27,27,27	0
88	MG	5	3972	1/1	0.83	0.25	41,41,41,41	0
88	MG	1	4490	1/1	0.83	0.25	58,58,58,58	0
88	MG	l5	306	1/1	0.83	0.11	54,54,54,54	0
88	MG	m6	203	1/1	0.83	0.15	41,41,41,41	1
88	MG	1	4499	1/1	0.83	0.15	47,47,47,47	0
88	MG	n6	201	1/1	0.83	0.17	54,54,54,54	0
88	MG	1	3864	1/1	0.83	0.23	70,70,70,70	0
88	MG	5	4051	1/1	0.83	0.13	33,33,33,33	0
87	OHX	5	3806	7/7	0.83	0.31	63,63,63,63	7
88	MG	4	237	1/1	0.84	0.13	59,59,59,59	0
87	OHX	M0	302	7/7	0.84	0.38	48,48,48,48	7
88	MG	1	3947	1/1	0.84	0.38	35,35,35,35	0
87	OHX	5	3738	7/7	0.84	0.35	49,49,49,49	7
88	MG	1	3960	1/1	0.84	0.23	51,51,51,51	0
88	MG	1	3966	1/1	0.84	0.31	66,66,66,66	0
87	OHX	5	3740	7/7	0.84	0.33	56,56,56,56	7
87	OHX	1	3759	7/7	0.84	0.30	64,64,64,64	7
88	MG	1	4002	1/1	0.84	0.23	39,39,39,39	0
87	OHX	2	2042	7/7	0.84	0.16	113,113,113,113	7
88	MG	1	4019	1/1	0.84	0.25	45,45,45,45	0
87	OHX	1	3761	7/7	0.84	0.23	93,93,93,93	7
87	OHX	2	2070	7/7	0.84	0.37	78,78,78,78	7
88	MG	5	4187	1/1	0.84	0.22	44,44,44,44	1
88	MG	6	2099	1/1	0.84	0.41	43,43,43,43	0
88	MG	6	2102	1/1	0.84	0.15	81,81,81,81	0
88	MG	5	4221	1/1	0.84	0.32	71,71,71,71	0
87	OHX	6	2029	7/7	0.84	0.30	82,82,82,82	7
88	MG	1	4039	1/1	0.84	0.15	66,66,66,66	0
88	MG	6	2109	1/1	0.84	0.22	47,47,47,47	0
88	MG	6	2312	1/1	0.84	0.18	75,75,75,75	0
87	OHX	6	1984	7/7	0.84	0.21	82,82,82,82	7
88	MG	6	2121	1/1	0.84	0.28	61,61,61,61	0
88	MG	6	2124	1/1	0.84	0.42	71,71,71,71	0
88	MG	6	2125	1/1	0.84	0.36	40,40,40,40	0
87	OHX	2	2064	7/7	0.84	0.10	130,130,130,130	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	2	2100	1/1	0.84	0.35	66,66,66,66	0
88	MG	5	4307	1/1	0.84	0.16	37,37,37,37	1
88	MG	6	2137	1/1	0.84	0.14	83,83,83,83	0
87	OHX	6	2037	7/7	0.84	0.26	75,75,75,75	7
88	MG	1	3817	1/1	0.84	0.22	55,55,55,55	0
88	MG	2	2205	1/1	0.84	0.24	76,76,76,76	0
88	MG	1	3830	1/1	0.84	0.38	71,71,71,71	0
88	MG	5	4331	1/1	0.84	0.10	35,35,35,35	0
87	OHX	6	2041	7/7	0.84	0.28	62,62,62,62	7
87	OHX	5	3698	7/7	0.84	0.18	86,86,86,86	7
88	MG	1	4369	1/1	0.84	0.21	69,69,69,69	0
88	MG	6	2161	1/1	0.84	0.29	59,59,59,59	0
88	MG	5	3834	1/1	0.84	0.28	40,40,40,40	0
88	MG	2	2158	1/1	0.84	0.30	68,68,68,68	0
88	MG	1	4424	1/1	0.84	0.37	67,67,67,67	0
88	MG	1	4430	1/1	0.84	0.28	38,38,38,38	1
87	OHX	2	2044	7/7	0.84	0.14	134,134,134,134	7
87	OHX	5	3610	7/7	0.84	0.39	60,60,60,60	7
87	OHX	5	3611	7/7	0.84	0.27	51,51,51,51	7
87	OHX	1	3677	7/7	0.84	0.34	56,56,56,56	7
88	MG	1	4129	1/1	0.84	0.12	83,83,83,83	0
88	MG	1	3866	1/1	0.84	0.24	34,34,34,34	0
87	OHX	5	3625	7/7	0.84	0.27	67,67,67,67	7
87	OHX	6	2048	7/7	0.84	0.43	51,51,51,51	7
87	OHX	5	3631	7/7	0.84	0.20	81,81,81,81	7
87	OHX	1	3652	7/7	0.84	0.32	69,69,69,69	7
87	OHX	8	221	7/7	0.84	0.26	74,74,74,74	7
87	OHX	6	2008	7/7	0.84	0.25	82,82,82,82	7
88	MG	5	4535	1/1	0.84	0.17	56,56,56,56	0
88	MG	6	2210	1/1	0.84	0.34	79,79,79,79	0
88	MG	5	4545	1/1	0.84	0.22	77,77,77,77	0
87	OHX	1	3714	7/7	0.84	0.30	73,73,73,73	7
88	MG	1	3904	1/1	0.84	0.28	43,43,43,43	0
88	MG	2	2130	1/1	0.84	0.27	75,75,75,75	0
87	OHX	2	2018	7/7	0.84	0.23	102,102,102,102	7
88	MG	3	214	1/1	0.84	0.19	46,46,46,46	0
88	MG	3	220	1/1	0.84	0.23	55,55,55,55	0
88	MG	2	2135	1/1	0.84	0.18	72,72,72,72	0
88	MG	8	239	1/1	0.84	0.31	71,71,71,71	0
87	OHX	2	2020	7/7	0.84	0.22	84,84,84,84	7
88	MG	5	4021	1/1	0.84	0.49	32,32,32,32	0
88	MG	3	230	1/1	0.84	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	l5	305	1/1	0.84	0.14	62,62,62,62	0
88	MG	1	4203	1/1	0.84	0.14	58,58,58,58	0
88	MG	4	226	1/1	0.84	0.20	58,58,58,58	0
88	MG	5	4084	1/1	0.84	0.19	42,42,42,42	1
88	MG	6	2249	1/1	0.84	0.09	53,53,53,53	0
88	MG	4	227	1/1	0.84	0.10	58,58,58,58	0
87	OHX	2	2089	7/7	0.84	0.18	121,121,121,121	7
88	MG	1	3923	1/1	0.84	0.29	40,40,40,40	0
87	OHX	6	2055	7/7	0.85	0.37	59,59,59,59	7
88	MG	6	2279	1/1	0.85	0.16	80,80,80,80	0
87	OHX	1	3754	7/7	0.85	0.34	55,55,55,55	7
87	OHX	1	3803	7/7	0.85	0.14	112,112,112,112	7
88	MG	2	2177	1/1	0.85	0.28	69,69,69,69	0
87	OHX	1	3610	7/7	0.85	0.39	53,53,53,53	7
87	OHX	5	3724	7/7	0.85	0.35	57,57,57,57	7
87	OHX	5	3805	7/7	0.85	0.22	86,86,86,86	7
88	MG	5	4172	1/1	0.85	0.19	45,45,45,45	0
87	OHX	1	3769	7/7	0.85	0.22	71,71,71,71	7
88	MG	1	4135	1/1	0.85	0.34	44,44,44,44	0
87	OHX	6	2014	7/7	0.85	0.31	74,74,74,74	7
88	MG	5	4192	1/1	0.85	0.13	52,52,52,52	0
88	MG	6	2131	1/1	0.85	0.36	53,53,53,53	0
88	MG	6	2132	1/1	0.85	0.28	69,69,69,69	0
87	OHX	5	3686	7/7	0.85	0.25	90,90,90,90	7
88	MG	1	4444	1/1	0.85	0.49	37,37,37,37	1
88	MG	2	2144	1/1	0.85	0.17	66,66,66,66	0
88	MG	6	2142	1/1	0.85	0.19	73,73,73,73	0
88	MG	2	2097	1/1	0.85	0.22	82,82,82,82	0
87	OHX	6	2043	7/7	0.85	0.22	86,86,86,86	7
88	MG	1	3933	1/1	0.85	0.26	33,33,33,33	0
88	MG	s6	302	1/1	0.85	0.31	75,75,75,75	0
88	MG	5	4285	1/1	0.85	0.43	57,57,57,57	1
88	MG	5	4286	1/1	0.85	0.10	72,72,72,72	0
88	MG	1	4168	1/1	0.85	0.27	53,53,53,53	0
87	OHX	5	3769	7/7	0.85	0.10	145,145,145,145	7
88	MG	1	3942	1/1	0.85	0.39	39,39,39,39	0
88	MG	1	4480	1/1	0.85	0.18	49,49,49,49	1
88	MG	c9	202	1/1	0.85	0.22	80,80,80,80	0
87	OHX	5	3813	7/7	0.85	0.21	85,85,85,85	7
88	MG	d4	201	1/1	0.85	0.26	68,68,68,68	0
87	OHX	1	3743	7/7	0.85	0.45	46,46,46,46	7
87	OHX	5	3776	7/7	0.85	0.16	110,110,110,110	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	2	2104	1/1	0.85	0.29	70,70,70,70	0
88	MG	6	2176	1/1	0.85	0.15	73,73,73,73	0
88	MG	1	4489	1/1	0.85	0.16	46,46,46,46	0
88	MG	1	3968	1/1	0.85	0.26	41,41,41,41	0
88	MG	1	4497	1/1	0.85	0.14	66,66,66,66	0
87	OHX	5	3777	7/7	0.85	0.33	53,53,53,53	7
88	MG	1	3972	1/1	0.85	0.34	44,44,44,44	0
88	MG	3	213	1/1	0.85	0.19	78,78,78,78	0
88	MG	1	3981	1/1	0.85	0.44	28,28,28,28	0
88	MG	6	2204	1/1	0.85	0.13	47,47,47,47	0
87	OHX	8	213	7/7	0.85	0.18	77,77,77,77	7
87	OHX	6	2045	7/7	0.85	0.26	61,61,61,61	7
87	OHX	2	2005	7/7	0.85	0.24	86,86,86,86	7
88	MG	1	4228	1/1	0.85	0.32	61,61,61,61	0
88	MG	1	4012	1/1	0.85	0.24	38,38,38,38	0
87	OHX	1	3556	7/7	0.85	0.26	72,72,72,72	7
88	MG	5	4477	1/1	0.85	0.13	44,44,44,44	1
87	OHX	2	2016	7/7	0.85	0.21	101,101,101,101	7
87	OHX	5	3745	7/7	0.85	0.54	39,39,39,39	7
88	MG	6	2218	1/1	0.85	0.06	81,81,81,81	0
88	MG	5	3944	1/1	0.85	0.31	24,24,24,24	0
87	OHX	1	3697	7/7	0.85	0.23	68,68,68,68	7
88	MG	5	4525	1/1	0.85	0.35	37,37,37,37	1
87	OHX	1	3712	7/7	0.85	0.39	61,61,61,61	7
88	MG	1	4291	1/1	0.85	0.49	41,41,41,41	1
88	MG	1	4293	1/1	0.85	0.17	46,46,46,46	0
88	MG	5	4552	1/1	0.85	0.16	43,43,43,43	0
88	MG	5	3973	1/1	0.85	0.35	55,55,55,55	0
88	MG	1	4300	1/1	0.85	0.18	44,44,44,44	1
87	OHX	5	3660	7/7	0.85	0.29	63,63,63,63	7
88	MG	2	2168	1/1	0.85	0.45	68,68,68,68	0
88	MG	1	4048	1/1	0.85	0.29	49,49,49,49	0
88	MG	5	4035	1/1	0.85	0.21	57,57,57,57	0
88	MG	M7	211	1/1	0.85	0.18	75,75,75,75	0
88	MG	8	237	1/1	0.85	0.10	71,71,71,71	0
88	MG	5	4054	1/1	0.85	0.18	37,37,37,37	0
88	MG	8	240	1/1	0.85	0.13	72,72,72,72	0
88	MG	2	2219	1/1	0.85	0.22	62,62,62,62	0
88	MG	N3	202	1/1	0.85	0.15	67,67,67,67	0
88	MG	1	4062	1/1	0.85	0.26	55,55,55,55	0
88	MG	5	4091	1/1	0.85	0.23	60,60,60,60	0
88	MG	O3	203	1/1	0.85	0.25	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4343	1/1	0.85	0.10	41,41,41,41	1
88	MG	1	3860	1/1	0.85	0.41	55,55,55,55	0
87	OHX	5	3789	7/7	0.85	0.37	58,58,58,58	7
88	MG	n8	201	1/1	0.85	0.22	33,33,33,33	0
87	OHX	2	2071	7/7	0.85	0.20	94,94,94,94	7
88	MG	2	2171	1/1	0.85	0.17	90,90,90,90	0
88	MG	6	2275	1/1	0.85	0.24	67,67,67,67	1
90	PRO	A	3501	7/8	0.85	0.25	75,75,75,75	0
87	OHX	1	3758	7/7	0.86	0.17	63,63,63,63	7
87	OHX	6	2017	7/7	0.86	0.29	50,50,50,50	7
88	MG	1	4292	1/1	0.86	0.24	72,72,72,72	0
87	OHX	3	211	7/7	0.86	0.23	81,81,81,81	7
87	OHX	5	3695	7/7	0.86	0.34	39,39,39,39	7
87	OHX	8	216	7/7	0.86	0.23	67,67,67,67	7
88	MG	2	2132	1/1	0.86	0.22	70,70,70,70	0
88	MG	1	4318	1/1	0.86	0.09	65,65,65,65	0
88	MG	5	4163	1/1	0.86	0.38	39,39,39,39	0
88	MG	5	4169	1/1	0.86	0.27	82,82,82,82	0
88	MG	1	4323	1/1	0.86	0.27	51,51,51,51	0
87	OHX	sR	401	7/7	0.86	0.15	122,122,122,122	7
87	OHX	2	1981	7/7	0.86	0.24	106,106,106,106	7
87	OHX	5	3581	7/7	0.86	0.42	44,44,44,44	7
88	MG	6	2106	1/1	0.86	0.23	68,68,68,68	0
88	MG	1	4046	1/1	0.86	0.16	35,35,35,35	0
87	OHX	5	3601	7/7	0.86	0.35	44,44,44,44	7
88	MG	6	2116	1/1	0.86	0.22	61,61,61,61	0
88	MG	2	2138	1/1	0.86	0.12	76,76,76,76	0
88	MG	1	4054	1/1	0.86	0.08	44,44,44,44	0
88	MG	6	2123	1/1	0.86	0.28	67,67,67,67	0
88	MG	5	4239	1/1	0.86	0.20	58,58,58,58	0
87	OHX	5	3705	7/7	0.86	0.58	41,41,41,41	7
88	MG	2	2196	1/1	0.86	0.17	82,82,82,82	0
87	OHX	5	3774	7/7	0.86	0.15	109,109,109,109	7
88	MG	1	4070	1/1	0.86	0.21	50,50,50,50	0
87	OHX	5	3608	7/7	0.86	0.29	39,39,39,39	7
88	MG	1	4078	1/1	0.86	0.59	52,52,52,52	1
87	OHX	1	3784	7/7	0.86	0.20	105,105,105,105	7
88	MG	5	4300	1/1	0.86	0.25	70,70,70,70	0
88	MG	c6	202	1/1	0.86	0.29	87,87,87,87	0
88	MG	1	4391	1/1	0.86	0.28	34,34,34,34	1
87	OHX	1	3678	7/7	0.86	0.19	75,75,75,75	7
88	MG	1	4092	1/1	0.86	0.29	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4095	1/1	0.86	0.23	59,59,59,59	0
88	MG	6	2150	1/1	0.86	0.46	59,59,59,59	0
87	OHX	1	3658	7/7	0.86	0.28	60,60,60,60	7
88	MG	1	4435	1/1	0.86	0.15	200,200,200,200	0
88	MG	1	4103	1/1	0.86	0.22	69,69,69,69	0
87	OHX	1	3788	7/7	0.86	0.12	147,147,147,147	7
88	MG	5	3815	1/1	0.86	0.42	36,36,36,36	0
88	MG	1	4449	1/1	0.86	0.18	82,82,82,82	0
88	MG	1	3872	1/1	0.86	0.21	30,30,30,30	0
88	MG	5	3844	1/1	0.86	0.20	33,33,33,33	0
88	MG	2	2210	1/1	0.86	0.27	69,69,69,69	0
88	MG	5	4382	1/1	0.86	0.17	37,37,37,37	1
87	OHX	5	3720	7/7	0.86	0.28	58,58,58,58	7
87	OHX	2	2087	7/7	0.86	0.33	71,71,71,71	7
88	MG	5	4390	1/1	0.86	0.34	62,62,62,62	0
88	MG	6	2172	1/1	0.86	0.23	76,76,76,76	0
88	MG	1	3892	1/1	0.86	0.34	66,66,66,66	0
88	MG	5	4410	1/1	0.86	0.23	38,38,38,38	1
87	OHX	5	3783	7/7	0.86	0.15	111,111,111,111	7
87	OHX	1	3684	7/7	0.86	0.33	54,54,54,54	7
88	MG	5	4420	1/1	0.86	0.12	63,63,63,63	0
88	MG	1	3897	1/1	0.86	0.21	66,66,66,66	0
87	OHX	1	3688	7/7	0.86	0.27	65,65,65,65	7
87	OHX	1	3719	7/7	0.86	0.34	57,57,57,57	7
88	MG	5	4470	1/1	0.86	0.09	62,62,62,62	0
88	MG	6	2198	1/1	0.86	0.11	90,90,90,90	0
87	OHX	1	3720	7/7	0.86	0.17	100,100,100,100	7
87	OHX	5	3643	7/7	0.86	0.32	35,35,35,35	7
88	MG	1	4167	1/1	0.86	0.14	46,46,46,46	0
88	MG	5	3941	1/1	0.86	0.21	41,41,41,41	0
88	MG	5	4523	1/1	0.86	0.20	55,55,55,55	0
87	OHX	2	2056	7/7	0.86	0.09	155,155,155,155	7
87	OHX	6	1990	7/7	0.86	0.24	65,65,65,65	7
88	MG	2	2160	1/1	0.86	0.07	67,67,67,67	0
87	OHX	1	3723	7/7	0.86	0.10	141,141,141,141	7
88	MG	5	4543	1/1	0.86	0.32	46,46,46,46	0
88	MG	1	3929	1/1	0.86	0.28	49,49,49,49	0
88	MG	5	3966	1/1	0.86	0.30	38,38,38,38	0
87	OHX	6	1998	7/7	0.86	0.23	64,64,64,64	7
88	MG	1	3934	1/1	0.86	0.39	36,36,36,36	0
88	MG	3	225	1/1	0.86	0.30	68,68,68,68	0
87	OHX	5	3667	7/7	0.86	0.31	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	OHX	1	3662	7/7	0.86	0.26	62,62,62,62	7
88	MG	5	3998	1/1	0.86	0.24	37,37,37,37	0
87	OHX	6	2005	7/7	0.86	0.23	80,80,80,80	7
87	OHX	2	2062	7/7	0.86	0.22	85,85,85,85	7
87	OHX	1	3623	7/7	0.86	0.41	45,45,45,45	7
87	OHX	1	3642	7/7	0.86	0.35	54,54,54,54	7
87	OHX	2	2010	7/7	0.86	0.16	101,101,101,101	7
87	OHX	1	3676	7/7	0.86	0.30	60,60,60,60	7
88	MG	l3	414	1/1	0.86	0.11	32,32,32,32	1
88	MG	6	2243	1/1	0.86	0.30	68,68,68,68	0
88	MG	5	4070	1/1	0.86	0.27	86,86,86,86	0
87	OHX	1	4509	7/7	0.86	0.34	51,51,51,51	7
88	MG	1	3975	1/1	0.86	0.36	45,45,45,45	0
88	MG	m7	205	1/1	0.86	0.08	50,50,50,50	0
88	MG	2	2120	1/1	0.86	0.16	70,70,70,70	0
88	MG	1	4255	1/1	0.86	0.22	61,61,61,61	0
87	OHX	7	209	7/7	0.86	0.24	63,63,63,63	7
88	MG	n8	205	1/1	0.86	0.21	39,39,39,39	0
88	MG	1	4267	1/1	0.86	0.15	48,48,48,48	0
88	MG	M4	201	1/1	0.86	0.09	53,53,53,53	0
88	MG	M5	302	1/1	0.86	0.27	42,42,42,42	1
88	MG	2	2123	1/1	0.86	0.16	68,68,68,68	0
88	MG	3	223	1/1	0.87	0.12	62,62,62,62	0
88	MG	5	4115	1/1	0.87	0.31	61,61,61,61	0
88	MG	1	3938	1/1	0.87	0.34	32,32,32,32	0
87	OHX	6	2072	7/7	0.87	0.27	66,66,66,66	7
88	MG	1	4202	1/1	0.87	0.10	48,48,48,48	0
88	MG	1	3946	1/1	0.87	0.26	31,31,31,31	0
87	OHX	1	3682	7/7	0.87	0.19	117,117,117,117	7
88	MG	4	223	1/1	0.87	0.18	37,37,37,37	0
88	MG	1	3948	1/1	0.87	0.22	48,48,48,48	0
88	MG	5	4140	1/1	0.87	0.17	44,44,44,44	0
88	MG	1	4218	1/1	0.87	0.11	45,45,45,45	0
88	MG	4	231	1/1	0.87	0.14	42,42,42,42	0
87	OHX	5	3621	7/7	0.87	0.26	52,52,52,52	7
87	OHX	2	2051	7/7	0.87	0.23	86,86,86,86	7
88	MG	1	4223	1/1	0.87	0.13	45,45,45,45	0
88	MG	5	4167	1/1	0.87	0.07	115,115,115,115	0
88	MG	1	3961	1/1	0.87	0.29	31,31,31,31	0
87	OHX	5	3719	7/7	0.87	0.26	62,62,62,62	7
88	MG	5	4178	1/1	0.87	0.34	66,66,66,66	0
87	OHX	1	3635	7/7	0.87	0.24	85,85,85,85	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	6	2000	7/7	0.87	0.36	63,63,63,63	7
88	MG	5	4183	1/1	0.87	0.26	53,53,53,53	0
88	MG	1	3971	1/1	0.87	0.31	41,41,41,41	0
87	OHX	6	2001	7/7	0.87	0.29	68,68,68,68	7
87	OHX	1	3666	7/7	0.87	0.27	50,50,50,50	7
88	MG	5	4205	1/1	0.87	0.15	50,50,50,50	0
88	MG	1	3977	1/1	0.87	0.20	51,51,51,51	0
88	MG	5	4210	1/1	0.87	0.12	52,52,52,52	0
88	MG	5	4213	1/1	0.87	0.34	66,66,66,66	0
88	MG	1	4276	1/1	0.87	0.13	76,76,76,76	0
88	MG	2	2166	1/1	0.87	0.24	55,55,55,55	0
87	OHX	5	3791	7/7	0.87	0.33	54,54,54,54	7
88	MG	1	4290	1/1	0.87	0.21	58,58,58,58	0
87	OHX	5	3725	7/7	0.87	0.33	58,58,58,58	7
87	OHX	3	210	7/7	0.87	0.36	53,53,53,53	7
88	MG	1	4011	1/1	0.87	0.36	53,53,53,53	0
88	MG	5	4257	1/1	0.87	0.07	44,44,44,44	0
87	OHX	2	2024	7/7	0.87	0.18	91,91,91,91	7
88	MG	2	2110	1/1	0.87	0.20	66,66,66,66	0
88	MG	1	4307	1/1	0.87	0.17	57,57,57,57	1
87	OHX	1	3669	7/7	0.87	0.33	47,47,47,47	7
87	OHX	5	3647	7/7	0.87	0.29	63,63,63,63	7
88	MG	2	2115	1/1	0.87	0.44	71,71,71,71	0
87	OHX	5	3650	7/7	0.87	0.37	55,55,55,55	7
88	MG	1	4326	1/1	0.87	0.11	59,59,59,59	0
88	MG	6	2113	1/1	0.87	0.14	75,75,75,75	0
88	MG	s6	301	1/1	0.87	0.15	71,71,71,71	0
87	OHX	6	2082	7/7	0.87	0.34	54,54,54,54	7
88	MG	1	4336	1/1	0.87	0.13	49,49,49,49	1
87	OHX	6	2050	7/7	0.87	0.11	132,132,132,132	7
88	MG	5	4327	1/1	0.87	0.14	62,62,62,62	0
88	MG	1	3823	1/1	0.87	0.18	67,67,67,67	0
88	MG	5	4330	1/1	0.87	0.17	37,37,37,37	0
87	OHX	4	212	7/7	0.87	0.35	42,42,42,42	7
87	OHX	1	3698	7/7	0.87	0.39	42,42,42,42	7
88	MG	5	4338	1/1	0.87	0.21	34,34,34,34	0
87	OHX	1	3567	7/7	0.87	0.24	64,64,64,64	7
87	OHX	2	1960	7/7	0.87	0.19	97,97,97,97	7
88	MG	1	3845	1/1	0.87	0.19	44,44,44,44	0
87	OHX	4	217	7/7	0.87	0.32	70,70,70,70	7
88	MG	5	4364	1/1	0.87	0.18	53,53,53,53	1
88	MG	1	4067	1/1	0.87	0.35	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	3749	7/7	0.87	0.29	49,49,49,49	7
87	OHX	1	3657	7/7	0.87	0.44	45,45,45,45	7
87	OHX	7	210	7/7	0.87	0.32	52,52,52,52	7
87	OHX	5	3679	7/7	0.87	0.31	60,60,60,60	7
88	MG	1	4395	1/1	0.87	0.12	54,54,54,54	0
88	MG	5	4404	1/1	0.87	0.12	57,57,57,57	0
88	MG	5	3845	1/1	0.87	0.18	34,34,34,34	0
88	MG	1	4084	1/1	0.87	0.18	52,52,52,52	0
88	MG	1	4419	1/1	0.87	0.76	40,40,40,40	1
88	MG	1	4422	1/1	0.87	0.20	63,63,63,63	0
88	MG	5	3874	1/1	0.87	0.26	54,54,54,54	0
88	MG	2	2133	1/1	0.87	0.26	76,76,76,76	0
88	MG	5	4440	1/1	0.87	0.08	39,39,39,39	0
88	MG	5	4451	1/1	0.87	0.22	37,37,37,37	1
87	OHX	6	2057	7/7	0.87	0.27	78,78,78,78	7
88	MG	5	4453	1/1	0.87	0.12	54,54,54,54	0
87	OHX	2	2043	7/7	0.87	0.14	119,119,119,119	7
87	OHX	M7	201	7/7	0.87	0.57	42,42,42,42	7
87	OHX	s1	302	7/7	0.87	0.17	93,93,93,93	7
87	OHX	1	3608	7/7	0.87	0.40	46,46,46,46	7
87	OHX	5	3760	7/7	0.87	0.23	71,71,71,71	7
88	MG	5	4495	1/1	0.87	0.23	55,55,55,55	0
88	MG	1	4451	1/1	0.87	0.20	43,43,43,43	0
88	MG	5	3914	1/1	0.87	0.16	50,50,50,50	0
88	MG	1	4458	1/1	0.87	0.23	53,53,53,53	0
88	MG	1	4123	1/1	0.87	0.18	49,49,49,49	0
88	MG	6	2179	1/1	0.87	0.17	67,67,67,67	0
88	MG	6	2180	1/1	0.87	0.17	52,52,52,52	0
87	OHX	1	3756	7/7	0.87	0.36	52,52,52,52	7
88	MG	6	2185	1/1	0.87	0.23	44,44,44,44	0
87	OHX	5	3532	7/7	0.87	0.34	53,53,53,53	7
88	MG	5	4549	1/1	0.87	1.05	50,50,50,50	1
88	MG	5	4551	1/1	0.87	0.08	53,53,53,53	0
87	OHX	6	2027	7/7	0.87	0.27	83,83,83,83	7
88	MG	6	2194	1/1	0.87	0.17	52,52,52,52	0
87	OHX	5	3696	7/7	0.87	0.31	43,43,43,43	7
88	MG	6	2199	1/1	0.87	0.38	83,83,83,83	0
88	MG	7	219	1/1	0.87	0.18	58,58,58,58	0
88	MG	5	3971	1/1	0.87	0.22	74,74,74,74	0
87	OHX	1	3660	7/7	0.87	0.29	65,65,65,65	7
88	MG	7	234	1/1	0.87	0.26	60,60,60,60	0
88	MG	1	3907	1/1	0.87	0.24	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	8	232	1/1	0.87	0.28	64,64,64,64	0
87	OHX	m0	304	7/7	0.87	0.47	43,43,43,43	7
87	OHX	5	3597	7/7	0.87	0.23	89,89,89,89	7
88	MG	5	3988	1/1	0.87	0.33	33,33,33,33	0
87	OHX	5	3773	7/7	0.87	0.43	38,38,38,38	7
88	MG	5	4009	1/1	0.87	0.27	39,39,39,39	0
88	MG	1	3918	1/1	0.87	0.20	58,58,58,58	0
87	OHX	2	1994	7/7	0.87	0.17	111,111,111,111	7
88	MG	5	4022	1/1	0.87	0.33	37,37,37,37	0
88	MG	1	4152	1/1	0.87	0.08	60,60,60,60	0
88	MG	2	2223	1/1	0.87	0.26	69,69,69,69	0
88	MG	1	4493	1/1	0.87	0.11	51,51,51,51	0
87	OHX	5	3775	7/7	0.87	0.17	122,122,122,122	7
88	MG	2	2151	1/1	0.87	0.28	58,58,58,58	0
87	OHX	5	3603	7/7	0.87	0.18	112,112,112,112	7
88	MG	5	4072	1/1	0.87	0.25	56,56,56,56	0
87	OHX	6	2031	7/7	0.87	0.21	81,81,81,81	7
87	OHX	1	3681	7/7	0.87	0.18	95,95,95,95	7
88	MG	6	2230	1/1	0.87	0.29	59,59,59,59	0
88	MG	6	2232	1/1	0.87	0.14	53,53,53,53	0
88	MG	1	3937	1/1	0.87	0.30	36,36,36,36	0
90	PRO	B	3501	7/8	0.87	0.27	71,71,71,71	0
88	MG	S8	302	1/1	0.88	0.09	69,69,69,69	1
88	MG	6	2174	1/1	0.88	0.25	58,58,58,58	0
87	OHX	5	3576	7/7	0.88	0.34	63,63,63,63	7
88	MG	1	4487	1/1	0.88	0.13	36,36,36,36	0
88	MG	5	3825	1/1	0.88	0.23	39,39,39,39	0
88	MG	5	3830	1/1	0.88	0.21	46,46,46,46	0
88	MG	1	4207	1/1	0.88	0.17	58,58,58,58	0
88	MG	5	4245	1/1	0.88	0.15	60,60,60,60	0
87	OHX	5	3685	7/7	0.88	0.15	116,116,116,116	7
88	MG	1	3990	1/1	0.88	0.46	56,56,56,56	0
87	OHX	6	2067	7/7	0.88	0.35	70,70,70,70	7
88	MG	5	3846	1/1	0.88	0.20	65,65,65,65	0
88	MG	5	3847	1/1	0.88	0.12	36,36,36,36	0
87	OHX	6	2033	7/7	0.88	0.24	67,67,67,67	7
87	OHX	1	3732	7/7	0.88	0.15	113,113,113,113	7
88	MG	5	3867	1/1	0.88	0.26	36,36,36,36	0
87	OHX	6	2035	7/7	0.88	0.19	82,82,82,82	7
87	OHX	5	3693	7/7	0.88	0.49	44,44,44,44	7
87	OHX	1	3780	7/7	0.88	0.28	66,66,66,66	7
88	MG	5	3883	1/1	0.88	0.15	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	6	1997	7/7	0.88	0.19	94,94,94,94	7
88	MG	3	221	1/1	0.88	0.11	70,70,70,70	0
88	MG	1	4021	1/1	0.88	0.18	39,39,39,39	0
87	OHX	6	2038	7/7	0.88	0.17	88,88,88,88	7
87	OHX	1	3668	7/7	0.88	0.36	46,46,46,46	7
87	OHX	2	2085	7/7	0.88	0.25	93,93,93,93	7
88	MG	6	2206	1/1	0.88	0.25	67,67,67,67	0
88	MG	1	3847	1/1	0.88	0.19	53,53,53,53	0
88	MG	5	4332	1/1	0.88	0.24	69,69,69,69	0
87	OHX	1	3715	7/7	0.88	0.23	86,86,86,86	7
87	OHX	1	3689	7/7	0.88	0.17	81,81,81,81	7
88	MG	5	3925	1/1	0.88	0.22	39,39,39,39	0
88	MG	5	3927	1/1	0.88	0.18	42,42,42,42	0
88	MG	5	4344	1/1	0.88	0.29	46,46,46,46	1
87	OHX	13	402	7/7	0.88	0.21	73,73,73,73	7
88	MG	5	4350	1/1	0.88	0.17	61,61,61,61	0
88	MG	5	4351	1/1	0.88	0.11	53,53,53,53	0
87	OHX	14	401	7/7	0.88	0.22	69,69,69,69	7
87	OHX	1	3501	7/7	0.88	0.34	50,50,50,50	7
88	MG	5	4365	1/1	0.88	0.21	52,52,52,52	1
88	MG	2	2202	1/1	0.88	0.15	69,69,69,69	0
88	MG	1	4296	1/1	0.88	0.16	46,46,46,46	0
88	MG	6	2220	1/1	0.88	0.14	47,47,47,47	0
88	MG	5	3960	1/1	0.88	0.26	33,33,33,33	0
87	OHX	5	3709	7/7	0.88	0.28	70,70,70,70	7
88	MG	5	3965	1/1	0.88	0.27	41,41,41,41	0
88	MG	6	2223	1/1	0.88	0.14	52,52,52,52	0
87	OHX	1	3740	7/7	0.88	0.37	60,60,60,60	7
87	OHX	1	3615	7/7	0.88	0.24	70,70,70,70	7
87	OHX	1	3673	7/7	0.88	0.25	74,74,74,74	7
87	OHX	1	3620	7/7	0.88	0.20	63,63,63,63	7
87	OHX	m7	201	7/7	0.88	0.29	49,49,49,49	7
88	MG	1	4079	1/1	0.88	0.20	29,29,29,29	0
88	MG	5	4430	1/1	0.88	0.15	93,93,93,93	0
87	OHX	5	3718	7/7	0.88	0.21	76,76,76,76	7
87	OHX	2	2002	7/7	0.88	0.25	86,86,86,86	7
88	MG	5	4002	1/1	0.88	0.32	37,37,37,37	0
88	MG	2	2215	1/1	0.88	0.30	78,78,78,78	0
87	OHX	o7	503	7/7	0.88	0.39	53,53,53,53	7
88	MG	5	4469	1/1	0.88	0.11	49,49,49,49	0
88	MG	5	4018	1/1	0.88	0.30	31,31,31,31	0
87	OHX	5	3645	7/7	0.88	0.32	41,41,41,41	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	L3	403	7/7	0.88	0.17	85,85,85,85	7
88	MG	5	4026	1/1	0.88	0.39	34,34,34,34	0
87	OHX	L5	301	7/7	0.88	0.23	78,78,78,78	7
88	MG	1	4111	1/1	0.88	0.22	49,49,49,49	0
88	MG	2	2222	1/1	0.88	0.10	80,80,80,80	0
88	MG	5	4056	1/1	0.88	0.15	45,45,45,45	0
88	MG	1	4119	1/1	0.88	0.29	56,56,56,56	0
87	OHX	1	3633	7/7	0.88	0.26	76,76,76,76	7
87	OHX	2	2040	7/7	0.88	0.23	88,88,88,88	7
87	OHX	5	3787	7/7	0.88	0.33	68,68,68,68	7
88	MG	6	2104	1/1	0.88	0.27	52,52,52,52	0
88	MG	2	2228	1/1	0.88	0.27	56,56,56,56	0
87	OHX	M0	304	7/7	0.88	0.21	96,96,96,96	7
87	OHX	5	3731	7/7	0.88	0.24	62,62,62,62	7
88	MG	5	4096	1/1	0.88	0.20	32,32,32,32	0
88	MG	5	4555	1/1	0.88	0.25	73,73,73,73	1
88	MG	5	4559	1/1	0.88	0.24	85,85,85,85	0
88	MG	1	4394	1/1	0.88	0.10	72,72,72,72	0
87	OHX	5	3734	7/7	0.88	0.26	53,53,53,53	7
88	MG	1	4396	1/1	0.88	0.27	59,59,59,59	0
87	OHX	1	3800	7/7	0.88	0.31	67,67,67,67	7
88	MG	1	4401	1/1	0.88	0.12	44,44,44,44	0
88	MG	5	4127	1/1	0.88	0.15	35,35,35,35	1
88	MG	1	4418	1/1	0.88	0.28	60,60,60,60	0
87	OHX	2	1968	7/7	0.88	0.24	77,77,77,77	7
87	OHX	5	3669	7/7	0.88	0.33	44,44,44,44	7
87	OHX	6	2025	7/7	0.88	0.12	113,113,113,113	7
88	MG	1	4146	1/1	0.88	0.20	73,73,73,73	0
88	MG	2	2248	1/1	0.88	0.20	78,78,78,78	0
88	MG	5	4147	1/1	0.88	0.18	52,52,52,52	0
88	MG	1	3945	1/1	0.88	0.23	31,31,31,31	0
87	OHX	5	3671	7/7	0.88	0.32	49,49,49,49	7
88	MG	1	4155	1/1	0.88	0.23	45,45,45,45	0
88	MG	1	4165	1/1	0.88	0.33	72,72,72,72	0
87	OHX	1	3704	7/7	0.88	0.17	103,103,103,103	7
87	OHX	5	3674	7/7	0.88	0.28	51,51,51,51	7
88	MG	18	301	1/1	0.88	0.28	70,70,70,70	0
87	OHX	1	3753	7/7	0.88	0.60	49,49,49,49	7
88	MG	2	2112	1/1	0.88	0.20	69,69,69,69	0
88	MG	m7	206	1/1	0.88	0.19	35,35,35,35	0
87	OHX	1	3650	7/7	0.88	0.26	65,65,65,65	7
88	MG	2	2172	1/1	0.88	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4468	1/1	0.88	0.28	61,61,61,61	0
88	MG	1	4178	1/1	0.88	0.10	55,55,55,55	0
88	MG	6	2163	1/1	0.88	0.33	40,40,40,40	0
87	OHX	5	3538	7/7	0.88	0.22	84,84,84,84	7
88	MG	2	2174	1/1	0.88	0.27	68,68,68,68	0
87	OHX	5	3681	7/7	0.88	0.15	88,88,88,88	7
87	OHX	2	2038	7/7	0.88	0.28	85,85,85,85	7
87	OHX	5	3797	7/7	0.89	0.27	66,66,66,66	7
88	MG	1	4420	1/1	0.89	0.09	54,54,54,54	0
87	OHX	2	1961	7/7	0.89	0.16	112,112,112,112	7
88	MG	6	2130	1/1	0.89	0.11	55,55,55,55	0
87	OHX	5	3642	7/7	0.89	0.26	52,52,52,52	7
88	MG	5	4194	1/1	0.89	0.27	43,43,43,43	0
88	MG	1	4428	1/1	0.89	0.13	47,47,47,47	1
88	MG	6	2133	1/1	0.89	0.07	39,39,39,39	0
88	MG	1	3988	1/1	0.89	0.29	27,27,27,27	0
87	OHX	s8	301	7/7	0.89	0.17	104,104,104,104	7
88	MG	1	4434	1/1	0.89	0.16	64,64,64,64	0
87	OHX	1	3555	7/7	0.89	0.20	90,90,90,90	7
88	MG	1	3999	1/1	0.89	0.30	44,44,44,44	0
88	MG	5	4224	1/1	0.89	0.12	44,44,44,44	0
88	MG	5	4225	1/1	0.89	0.17	43,43,43,43	0
88	MG	6	2144	1/1	0.89	0.17	55,55,55,55	0
88	MG	6	2146	1/1	0.89	0.34	37,37,37,37	0
87	OHX	c5	202	7/7	0.89	0.15	98,98,98,98	7
88	MG	5	3817	1/1	0.89	0.26	54,54,54,54	0
88	MG	5	3819	1/1	0.89	0.28	33,33,33,33	0
88	MG	1	4004	1/1	0.89	0.26	52,52,52,52	0
88	MG	1	4005	1/1	0.89	0.35	48,48,48,48	0
88	MG	1	4456	1/1	0.89	0.16	75,75,75,75	0
88	MG	1	4008	1/1	0.89	0.29	35,35,35,35	0
88	MG	1	4460	1/1	0.89	0.33	60,60,60,60	0
88	MG	1	4187	1/1	0.89	0.14	90,90,90,90	0
88	MG	1	4191	1/1	0.89	0.42	52,52,52,52	0
88	MG	1	4192	1/1	0.89	0.20	55,55,55,55	0
88	MG	2	2103	1/1	0.89	0.12	65,65,65,65	0
88	MG	6	2170	1/1	0.89	0.07	49,49,49,49	0
88	MG	5	3864	1/1	0.89	0.21	36,36,36,36	0
88	MG	5	3865	1/1	0.89	0.20	62,62,62,62	0
88	MG	5	3866	1/1	0.89	0.21	34,34,34,34	0
88	MG	1	4010	1/1	0.89	0.28	49,49,49,49	0
87	OHX	5	3646	7/7	0.89	0.25	46,46,46,46	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4325	1/1	0.89	0.18	47,47,47,47	0
87	OHX	1	3612	7/7	0.89	0.32	60,60,60,60	7
87	OHX	2	2088	7/7	0.89	0.14	94,94,94,94	7
87	OHX	5	3706	7/7	0.89	0.31	79,79,79,79	7
87	OHX	5	3707	7/7	0.89	0.22	83,83,83,83	7
88	MG	1	4212	1/1	0.89	0.38	52,52,52,52	1
88	MG	5	3892	1/1	0.89	0.10	50,50,50,50	0
88	MG	5	3900	1/1	0.89	0.25	44,44,44,44	0
87	OHX	1	3692	7/7	0.89	0.23	63,63,63,63	7
87	OHX	5	3762	7/7	0.89	0.24	66,66,66,66	7
88	MG	5	4343	1/1	0.89	0.09	60,60,60,60	0
88	MG	1	3877	1/1	0.89	0.20	47,47,47,47	0
88	MG	6	2187	1/1	0.89	0.08	77,77,77,77	0
88	MG	5	4347	1/1	0.89	0.19	59,59,59,59	0
88	MG	1	3879	1/1	0.89	0.24	48,48,48,48	0
87	OHX	5	3653	7/7	0.89	0.37	41,41,41,41	7
88	MG	5	3916	1/1	0.89	0.13	41,41,41,41	0
88	MG	2	2167	1/1	0.89	0.18	84,84,84,84	0
87	OHX	5	3545	7/7	0.89	0.34	55,55,55,55	7
88	MG	1	4237	1/1	0.89	0.22	57,57,57,57	0
88	MG	5	4377	1/1	0.89	0.28	79,79,79,79	0
87	OHX	5	3658	7/7	0.89	0.34	45,45,45,45	7
88	MG	5	3930	1/1	0.89	0.30	35,35,35,35	0
88	MG	1	4245	1/1	0.89	0.12	54,54,54,54	0
88	MG	1	4051	1/1	0.89	0.20	51,51,51,51	0
88	MG	3	219	1/1	0.89	0.37	63,63,63,63	0
87	OHX	5	3659	7/7	0.89	0.30	57,57,57,57	7
88	MG	2	2231	1/1	0.89	0.23	82,82,82,82	0
87	OHX	6	2030	7/7	0.89	0.11	105,105,105,105	7
88	MG	5	3959	1/1	0.89	0.20	43,43,43,43	0
88	MG	2	2239	1/1	0.89	0.19	86,86,86,86	0
88	MG	1	4066	1/1	0.89	0.14	70,70,70,70	0
88	MG	3	227	1/1	0.89	0.16	78,78,78,78	0
88	MG	1	4284	1/1	0.89	0.18	52,52,52,52	0
88	MG	5	4438	1/1	0.89	0.69	34,34,34,34	1
87	OHX	1	3563	7/7	0.89	0.39	48,48,48,48	7
88	MG	4	219	1/1	0.89	0.14	64,64,64,64	0
88	MG	1	3908	1/1	0.89	0.07	52,52,52,52	0
88	MG	6	2219	1/1	0.89	0.30	60,60,60,60	0
87	OHX	1	3566	7/7	0.89	0.33	41,41,41,41	7
87	OHX	M9	202	7/7	0.89	0.23	78,78,78,78	7
88	MG	5	3979	1/1	0.89	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4472	1/1	0.89	0.11	46,46,46,46	0
88	MG	5	4475	1/1	0.89	0.23	56,56,56,56	1
88	MG	5	3981	1/1	0.89	0.40	50,50,50,50	0
88	MG	5	4478	1/1	0.89	0.21	45,45,45,45	1
87	OHX	5	3721	7/7	0.89	0.23	75,75,75,75	7
87	OHX	1	3627	7/7	0.89	0.34	51,51,51,51	7
87	OHX	1	3629	7/7	0.89	0.19	79,79,79,79	7
87	OHX	5	3606	7/7	0.89	0.31	60,60,60,60	7
87	OHX	2	2022	7/7	0.89	0.27	66,66,66,66	7
88	MG	5	4014	1/1	0.89	0.11	34,34,34,34	0
87	OHX	6	1968	7/7	0.89	0.28	74,74,74,74	7
87	OHX	m0	303	7/7	0.89	0.20	86,86,86,86	7
88	MG	5	4531	1/1	0.89	0.22	56,56,56,56	0
88	MG	4	242	1/1	0.89	0.11	57,57,57,57	1
87	OHX	6	2040	7/7	0.89	0.34	58,58,58,58	7
88	MG	5	4030	1/1	0.89	0.09	45,45,45,45	0
88	MG	1	4104	1/1	0.89	0.11	56,56,56,56	0
88	MG	5	4038	1/1	0.89	0.27	35,35,35,35	0
88	MG	5	4550	1/1	0.89	0.14	43,43,43,43	0
88	MG	M0	306	1/1	0.89	0.10	53,53,53,53	0
88	MG	1	4110	1/1	0.89	0.07	67,67,67,67	0
87	OHX	5	3732	7/7	0.89	0.18	93,93,93,93	7
87	OHX	5	3616	7/7	0.89	0.35	42,42,42,42	7
87	OHX	6	1981	7/7	0.89	0.30	45,45,45,45	7
88	MG	1	4120	1/1	0.89	0.08	46,46,46,46	0
87	OHX	1	3701	7/7	0.89	0.25	64,64,64,64	7
87	OHX	2	2000	7/7	0.89	0.20	110,110,110,110	7
88	MG	5	4089	1/1	0.89	0.14	34,34,34,34	0
87	OHX	2	2082	7/7	0.89	0.10	137,137,137,137	7
88	MG	N8	202	1/1	0.89	0.20	37,37,37,37	0
88	MG	8	224	1/1	0.89	0.25	52,52,52,52	0
88	MG	1	4348	1/1	0.89	0.14	52,52,52,52	0
88	MG	8	231	1/1	0.89	0.18	50,50,50,50	0
88	MG	D6	102	1/1	0.89	0.15	77,77,77,77	0
88	MG	O5	201	1/1	0.89	0.09	58,58,58,58	0
87	OHX	1	3644	7/7	0.89	0.29	65,65,65,65	7
87	OHX	6	2046	7/7	0.89	0.19	100,100,100,100	7
88	MG	1	4357	1/1	0.89	0.25	67,67,67,67	0
88	MG	SM	201	1/1	0.89	0.24	55,55,55,55	0
88	MG	6	2289	1/1	0.89	0.19	57,57,57,57	0
88	MG	l3	403	1/1	0.89	0.34	26,26,26,26	0
88	MG	1	4136	1/1	0.89	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4365	1/1	0.89	0.10	43,43,43,43	0
87	OHX	5	3792	7/7	0.89	0.27	63,63,63,63	7
88	MG	1	4140	1/1	0.89	0.09	41,41,41,41	0
88	MG	1	4374	1/1	0.89	0.25	41,41,41,41	1
88	MG	m4	202	1/1	0.89	0.12	53,53,53,53	1
88	MG	1	3963	1/1	0.89	0.29	40,40,40,40	0
88	MG	6	2110	1/1	0.89	0.18	82,82,82,82	0
87	OHX	5	3690	7/7	0.89	0.30	55,55,55,55	7
88	MG	6	2313	1/1	0.89	0.13	71,71,71,71	0
88	MG	6	2114	1/1	0.89	0.23	49,49,49,49	0
87	OHX	5	3743	7/7	0.89	0.20	66,66,66,66	7
88	MG	2	2201	1/1	0.89	0.12	61,61,61,61	0
88	MG	q2	503	1/1	0.89	0.09	42,42,42,42	1
87	OHX	5	3634	7/7	0.89	0.25	73,73,73,73	7
88	MG	6	2331	1/1	0.89	0.10	76,76,76,76	0
87	OHX	6	2071	7/7	0.89	0.35	55,55,55,55	7
88	MG	5	4174	1/1	0.89	0.17	38,38,38,38	1
88	MG	1	4150	1/1	0.89	0.21	81,81,81,81	0
87	OHX	6	1985	7/7	0.90	0.23	90,90,90,90	7
88	MG	5	4156	1/1	0.90	0.08	67,67,67,67	0
88	MG	1	3976	1/1	0.90	0.20	54,54,54,54	0
87	OHX	5	3604	7/7	0.90	0.32	44,44,44,44	7
88	MG	1	3979	1/1	0.90	0.25	40,40,40,40	0
88	MG	6	2321	1/1	0.90	0.09	72,72,72,72	0
88	MG	1	3841	1/1	0.90	0.19	44,44,44,44	0
88	MG	1	4393	1/1	0.90	0.16	38,38,38,38	1
87	OHX	1	3722	7/7	0.90	0.34	54,54,54,54	7
88	MG	6	2112	1/1	0.90	0.25	42,42,42,42	0
88	MG	2	2118	1/1	0.90	0.26	46,46,46,46	0
88	MG	1	3849	1/1	0.90	0.30	41,41,41,41	0
88	MG	1	4157	1/1	0.90	0.17	47,47,47,47	0
87	OHX	1	3541	7/7	0.90	0.21	91,91,91,91	7
88	MG	5	4191	1/1	0.90	0.41	35,35,35,35	1
88	MG	6	2119	1/1	0.90	0.31	59,59,59,59	0
88	MG	s8	303	1/1	0.90	0.22	46,46,46,46	0
88	MG	5	4198	1/1	0.90	0.16	32,32,32,32	1
88	MG	s8	305	1/1	0.90	0.14	56,56,56,56	0
88	MG	1	4404	1/1	0.90	0.09	56,56,56,56	1
87	OHX	1	3636	7/7	0.90	0.19	83,83,83,83	7
88	MG	5	4209	1/1	0.90	0.10	59,59,59,59	0
88	MG	c8	202	1/1	0.90	0.33	81,81,81,81	0
88	MG	1	4003	1/1	0.90	0.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	2	2121	1/1	0.90	0.14	73,73,73,73	0
88	MG	1	4171	1/1	0.90	0.26	46,46,46,46	0
88	MG	5	4223	1/1	0.90	0.11	48,48,48,48	0
88	MG	1	3859	1/1	0.90	0.19	38,38,38,38	0
87	OHX	2	2009	7/7	0.90	0.27	70,70,70,70	7
88	MG	d2	201	1/1	0.90	0.20	46,46,46,46	0
88	MG	5	4232	1/1	0.90	0.16	42,42,42,42	0
88	MG	d3	201	1/1	0.90	0.18	47,47,47,47	0
87	OHX	l5	301	7/7	0.90	0.18	90,90,90,90	7
87	OHX	4	213	7/7	0.90	0.25	64,64,64,64	7
88	MG	2	2227	1/1	0.90	0.08	63,63,63,63	0
88	MG	1	4184	1/1	0.90	0.23	47,47,47,47	0
87	OHX	5	3748	7/7	0.90	0.29	49,49,49,49	7
87	OHX	5	3618	7/7	0.90	0.24	74,74,74,74	7
87	OHX	5	3750	7/7	0.90	0.08	161,161,161,161	7
88	MG	2	2129	1/1	0.90	0.17	66,66,66,66	0
88	MG	1	4455	1/1	0.90	0.35	46,46,46,46	1
88	MG	5	4289	1/1	0.90	0.13	43,43,43,43	0
88	MG	1	4023	1/1	0.90	0.21	43,43,43,43	0
88	MG	5	3837	1/1	0.90	0.31	43,43,43,43	0
88	MG	5	3839	1/1	0.90	0.21	62,62,62,62	0
88	MG	1	4195	1/1	0.90	0.23	46,46,46,46	0
88	MG	1	4196	1/1	0.90	0.14	51,51,51,51	0
88	MG	1	3882	1/1	0.90	0.19	39,39,39,39	0
88	MG	5	4315	1/1	0.90	0.16	59,59,59,59	0
87	OHX	2	1988	7/7	0.90	0.22	80,80,80,80	7
88	MG	1	4204	1/1	0.90	0.16	47,47,47,47	1
88	MG	5	4322	1/1	0.90	0.15	53,53,53,53	0
88	MG	6	2158	1/1	0.90	0.34	40,40,40,40	0
88	MG	1	4031	1/1	0.90	0.13	44,44,44,44	0
88	MG	2	2234	1/1	0.90	0.14	76,76,76,76	0
88	MG	1	4469	1/1	0.90	0.21	51,51,51,51	0
88	MG	1	4040	1/1	0.90	0.28	69,69,69,69	0
88	MG	6	2167	1/1	0.90	0.19	55,55,55,55	0
87	OHX	5	3714	7/7	0.90	0.10	136,136,136,136	7
88	MG	1	3893	1/1	0.90	0.20	43,43,43,43	0
87	OHX	5	3753	7/7	0.90	0.20	75,75,75,75	7
87	OHX	1	3611	7/7	0.90	0.23	68,68,68,68	7
87	OHX	1	3796	7/7	0.90	0.45	41,41,41,41	7
88	MG	1	4224	1/1	0.90	0.16	62,62,62,62	0
87	OHX	5	3678	7/7	0.90	0.22	75,75,75,75	7
88	MG	5	3894	1/1	0.90	0.30	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4346	1/1	0.90	0.15	44,44,44,44	1
88	MG	5	3898	1/1	0.90	0.22	71,71,71,71	0
88	MG	6	2177	1/1	0.90	0.10	80,80,80,80	0
87	OHX	5	3757	7/7	0.90	0.31	69,69,69,69	7
88	MG	2	2183	1/1	0.90	0.30	66,66,66,66	0
88	MG	5	4361	1/1	0.90	0.31	45,45,45,45	0
88	MG	1	4232	1/1	0.90	0.13	52,52,52,52	0
87	OHX	1	3797	7/7	0.90	0.25	57,57,57,57	7
87	OHX	1	3728	7/7	0.90	0.28	55,55,55,55	7
88	MG	1	4065	1/1	0.90	0.18	56,56,56,56	0
88	MG	6	2188	1/1	0.90	0.15	52,52,52,52	0
88	MG	1	4252	1/1	0.90	0.17	58,58,58,58	0
88	MG	1	4505	1/1	0.90	0.14	90,90,90,90	0
88	MG	1	4508	1/1	0.90	0.07	41,41,41,41	0
87	OHX	1	3710	7/7	0.90	0.31	45,45,45,45	7
87	OHX	2	2021	7/7	0.90	0.23	72,72,72,72	7
88	MG	3	215	1/1	0.90	0.35	51,51,51,51	0
88	MG	5	3936	1/1	0.90	0.31	34,34,34,34	0
87	OHX	1	3776	7/7	0.90	0.37	45,45,45,45	7
88	MG	1	4260	1/1	0.90	0.36	53,53,53,53	0
87	OHX	2	1992	7/7	0.90	0.25	75,75,75,75	7
88	MG	3	222	1/1	0.90	0.23	45,45,45,45	0
88	MG	5	3952	1/1	0.90	0.28	47,47,47,47	0
88	MG	1	4272	1/1	0.90	0.29	37,37,37,37	0
88	MG	1	4077	1/1	0.90	0.22	46,46,46,46	0
88	MG	1	3920	1/1	0.90	0.20	36,36,36,36	0
88	MG	1	4281	1/1	0.90	0.15	52,52,52,52	0
88	MG	5	3962	1/1	0.90	0.23	39,39,39,39	0
88	MG	3	228	1/1	0.90	0.17	78,78,78,78	0
88	MG	5	4464	1/1	0.90	0.21	43,43,43,43	0
88	MG	2	2256	1/1	0.90	0.10	66,66,66,66	0
87	OHX	C5	201	7/7	0.90	0.14	112,112,112,112	7
88	MG	5	3969	1/1	0.90	0.32	34,34,34,34	0
88	MG	1	3928	1/1	0.90	0.23	28,28,28,28	0
87	OHX	5	3810	7/7	0.90	0.17	70,70,70,70	7
88	MG	1	4091	1/1	0.90	0.08	41,41,41,41	0
88	MG	4	225	1/1	0.90	0.08	61,61,61,61	0
87	OHX	1	3716	7/7	0.90	0.13	104,104,104,104	7
87	OHX	5	3812	7/7	0.90	0.31	43,43,43,43	7
88	MG	5	4503	1/1	0.90	0.23	46,46,46,46	1
88	MG	1	4097	1/1	0.90	0.10	57,57,57,57	0
88	MG	4	233	1/1	0.90	0.20	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4514	1/1	0.90	0.17	41,41,41,41	0
88	MG	5	3991	1/1	0.90	0.36	34,34,34,34	0
88	MG	5	3992	1/1	0.90	0.30	31,31,31,31	0
88	MG	1	4301	1/1	0.90	0.16	59,59,59,59	0
88	MG	5	4001	1/1	0.90	0.23	30,30,30,30	0
88	MG	5	4532	1/1	0.90	0.43	42,42,42,42	1
87	OHX	5	3535	7/7	0.90	0.31	54,54,54,54	7
88	MG	5	4008	1/1	0.90	0.27	33,33,33,33	0
88	MG	5	4539	1/1	0.90	0.24	41,41,41,41	1
88	MG	1	4304	1/1	0.90	0.35	55,55,55,55	0
88	MG	1	4101	1/1	0.90	0.18	47,47,47,47	0
88	MG	6	2241	1/1	0.90	0.16	70,70,70,70	0
88	MG	C5	202	1/1	0.90	0.17	76,76,76,76	0
87	OHX	5	3770	7/7	0.90	0.21	66,66,66,66	7
88	MG	6	2247	1/1	0.90	0.14	50,50,50,50	0
88	MG	5	4023	1/1	0.90	0.24	41,41,41,41	0
87	OHX	5	3771	7/7	0.90	0.29	59,59,59,59	7
88	MG	5	4560	1/1	0.90	0.25	34,34,34,34	1
88	MG	L3	407	1/1	0.90	0.33	51,51,51,51	1
88	MG	L4	407	1/1	0.90	0.11	55,55,55,55	1
88	MG	1	3943	1/1	0.90	0.20	37,37,37,37	0
88	MG	7	213	1/1	0.90	0.19	46,46,46,46	0
88	MG	2	2152	1/1	0.90	0.12	88,88,88,88	0
88	MG	1	4118	1/1	0.90	0.11	45,45,45,45	0
88	MG	1	4335	1/1	0.90	0.14	73,73,73,73	1
88	MG	7	226	1/1	0.90	0.24	50,50,50,50	1
88	MG	7	233	1/1	0.90	0.07	45,45,45,45	0
88	MG	5	4058	1/1	0.90	0.22	39,39,39,39	0
88	MG	7	235	1/1	0.90	0.11	44,44,44,44	0
88	MG	6	2261	1/1	0.90	0.10	60,60,60,60	0
87	OHX	1	3570	7/7	0.90	0.30	56,56,56,56	7
88	MG	5	4068	1/1	0.90	0.17	55,55,55,55	0
88	MG	6	2263	1/1	0.90	0.17	40,40,40,40	0
88	MG	6	2266	1/1	0.90	0.10	71,71,71,71	0
88	MG	8	236	1/1	0.90	0.24	57,57,57,57	0
88	MG	5	4075	1/1	0.90	0.15	44,44,44,44	0
88	MG	5	4082	1/1	0.90	0.17	48,48,48,48	0
88	MG	6	2267	1/1	0.90	0.14	54,54,54,54	0
88	MG	5	4086	1/1	0.90	0.09	52,52,52,52	0
87	OHX	1	3626	7/7	0.90	0.30	57,57,57,57	7
88	MG	6	2271	1/1	0.90	0.16	42,42,42,42	0
88	MG	5	4093	1/1	0.90	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	M7	202	1/1	0.90	0.41	52,52,52,52	0
87	OHX	1	3589	7/7	0.90	0.30	56,56,56,56	7
88	MG	1	3816	1/1	0.90	0.15	44,44,44,44	0
88	MG	17	304	1/1	0.90	0.19	49,49,49,49	1
87	OHX	6	1961	7/7	0.90	0.24	65,65,65,65	7
88	MG	m0	305	1/1	0.90	0.26	32,32,32,32	0
88	MG	6	2277	1/1	0.90	0.07	48,48,48,48	0
87	OHX	2	2007	7/7	0.90	0.19	101,101,101,101	7
87	OHX	3	208	7/7	0.90	0.20	85,85,85,85	7
88	MG	O1	204	1/1	0.90	0.31	63,63,63,63	0
88	MG	1	4350	1/1	0.90	0.09	62,62,62,62	0
88	MG	n1	204	1/1	0.90	0.23	56,56,56,56	0
88	MG	n3	203	1/1	0.90	0.26	29,29,29,29	0
88	MG	1	3964	1/1	0.90	0.34	43,43,43,43	0
88	MG	1	3826	1/1	0.90	0.24	40,40,40,40	0
88	MG	n8	204	1/1	0.90	0.13	55,55,55,55	1
88	MG	O5	202	1/1	0.90	0.27	54,54,54,54	1
88	MG	o2	202	1/1	0.90	0.09	49,49,49,49	0
88	MG	o3	202	1/1	0.90	0.10	53,53,53,53	0
88	MG	o6	201	1/1	0.90	0.14	69,69,69,69	1
88	MG	1	3827	1/1	0.90	0.21	44,44,44,44	0
88	MG	1	3828	1/1	0.90	0.16	39,39,39,39	0
88	MG	Q0	203	1/1	0.90	0.30	52,52,52,52	0
87	OHX	1	3601	7/7	0.90	0.15	107,107,107,107	7
88	MG	5	4149	1/1	0.90	0.26	41,41,41,41	0
88	MG	2	2213	1/1	0.90	0.13	55,55,55,55	0
87	OHX	8	208	7/7	0.91	0.26	63,63,63,63	7
87	OHX	5	3583	7/7	0.91	0.26	53,53,53,53	7
88	MG	5	4203	1/1	0.91	0.38	62,62,62,62	0
88	MG	2	2208	1/1	0.91	0.13	72,72,72,72	0
88	MG	1	4440	1/1	0.91	0.24	41,41,41,41	1
88	MG	6	2141	1/1	0.91	0.16	40,40,40,40	0
87	OHX	5	3590	7/7	0.91	0.30	42,42,42,42	7
87	OHX	1	3749	7/7	0.91	0.26	51,51,51,51	7
88	MG	5	4219	1/1	0.91	0.10	53,53,53,53	0
87	OHX	6	1982	7/7	0.91	0.16	98,98,98,98	7
88	MG	5	3821	1/1	0.91	0.18	48,48,48,48	0
88	MG	1	4453	1/1	0.91	0.17	43,43,43,43	0
88	MG	6	2147	1/1	0.91	0.34	58,58,58,58	0
87	OHX	2	2006	7/7	0.91	0.28	72,72,72,72	7
88	MG	6	2152	1/1	0.91	0.20	50,50,50,50	0
88	MG	5	4231	1/1	0.91	0.24	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	OHX	2	1980	7/7	0.91	0.22	93,93,93,93	7
88	MG	1	4199	1/1	0.91	0.78	42,42,42,42	1
87	OHX	1	3695	7/7	0.91	0.38	44,44,44,44	7
88	MG	5	4243	1/1	0.91	0.22	37,37,37,37	0
87	OHX	2	2057	7/7	0.91	0.28	67,67,67,67	7
88	MG	6	2157	1/1	0.91	0.34	46,46,46,46	0
87	OHX	2	2003	7/7	0.91	0.14	103,103,103,103	7
88	MG	5	4252	1/1	0.91	0.17	44,44,44,44	0
88	MG	1	4030	1/1	0.91	0.15	54,54,54,54	0
88	MG	1	3876	1/1	0.91	0.18	49,49,49,49	0
88	MG	5	4264	1/1	0.91	0.18	46,46,46,46	0
88	MG	1	4467	1/1	0.91	0.38	33,33,33,33	1
88	MG	5	4278	1/1	0.91	0.10	39,39,39,39	0
88	MG	1	4037	1/1	0.91	0.19	33,33,33,33	0
87	OHX	1	3578	7/7	0.91	0.21	67,67,67,67	7
88	MG	5	4288	1/1	0.91	0.18	37,37,37,37	0
88	MG	1	4214	1/1	0.91	0.13	50,50,50,50	0
87	OHX	5	3613	7/7	0.91	0.21	74,74,74,74	7
88	MG	1	3880	1/1	0.91	0.11	50,50,50,50	0
88	MG	1	4479	1/1	0.91	0.22	59,59,59,59	0
88	MG	5	4305	1/1	0.91	0.11	74,74,74,74	0
87	OHX	15	302	7/7	0.91	0.19	88,88,88,88	7
87	OHX	15	303	7/7	0.91	0.20	69,69,69,69	7
88	MG	5	4309	1/1	0.91	0.21	57,57,57,57	0
87	OHX	2	2074	7/7	0.91	0.22	92,92,92,92	7
88	MG	1	4049	1/1	0.91	0.18	44,44,44,44	0
88	MG	1	4227	1/1	0.91	0.08	44,44,44,44	0
88	MG	5	3896	1/1	0.91	0.30	41,41,41,41	0
87	OHX	5	3617	7/7	0.91	0.24	43,43,43,43	7
87	OHX	5	3768	7/7	0.91	0.15	115,115,115,115	7
88	MG	6	2181	1/1	0.91	0.19	55,55,55,55	0
87	OHX	6	1999	7/7	0.91	0.18	85,85,85,85	7
88	MG	1	4491	1/1	0.91	0.29	71,71,71,71	0
88	MG	1	4059	1/1	0.91	0.30	53,53,53,53	0
87	OHX	1	3672	7/7	0.91	0.22	71,71,71,71	7
88	MG	5	3912	1/1	0.91	0.23	57,57,57,57	0
87	OHX	2	2032	7/7	0.91	0.19	82,82,82,82	7
88	MG	1	4248	1/1	0.91	0.13	58,58,58,58	0
88	MG	1	4504	1/1	0.91	0.33	37,37,37,37	1
88	MG	5	3919	1/1	0.91	0.13	35,35,35,35	0
88	MG	6	2196	1/1	0.91	0.15	45,45,45,45	1
88	MG	6	2197	1/1	0.91	0.28	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	OHX	5	3622	7/7	0.91	0.22	69,69,69,69	7
88	MG	5	3929	1/1	0.91	0.18	46,46,46,46	0
88	MG	1	4507	1/1	0.91	0.11	52,52,52,52	0
87	OHX	2	2001	7/7	0.91	0.18	82,82,82,82	7
88	MG	5	3934	1/1	0.91	0.43	28,28,28,28	0
87	OHX	5	3627	7/7	0.91	0.17	89,89,89,89	7
87	OHX	2	2036	7/7	0.91	0.11	123,123,123,123	7
88	MG	5	4362	1/1	0.91	0.21	41,41,41,41	0
88	MG	5	4363	1/1	0.91	0.16	44,44,44,44	0
87	OHX	6	2047	7/7	0.91	0.23	67,67,67,67	7
87	OHX	2	2011	7/7	0.91	0.22	69,69,69,69	7
88	MG	1	4073	1/1	0.91	0.16	54,54,54,54	0
88	MG	1	3914	1/1	0.91	0.16	57,57,57,57	0
88	MG	5	4381	1/1	0.91	0.25	34,34,34,34	1
87	OHX	5	3633	7/7	0.91	0.15	109,109,109,109	7
87	OHX	2	2050	7/7	0.91	0.16	96,96,96,96	7
88	MG	3	224	1/1	0.91	0.12	47,47,47,47	0
87	OHX	5	3637	7/7	0.91	0.31	52,52,52,52	7
88	MG	1	4285	1/1	0.91	0.21	57,57,57,57	0
88	MG	5	4400	1/1	0.91	0.23	38,38,38,38	1
87	OHX	1	3763	7/7	0.91	0.34	45,45,45,45	7
87	OHX	5	3717	7/7	0.91	0.25	50,50,50,50	7
87	OHX	1	3764	7/7	0.91	0.44	50,50,50,50	7
88	MG	5	4412	1/1	0.91	0.13	38,38,38,38	0
88	MG	1	3927	1/1	0.91	0.23	41,41,41,41	0
88	MG	6	2221	1/1	0.91	0.07	53,53,53,53	1
87	OHX	1	3517	7/7	0.91	0.29	59,59,59,59	7
87	OHX	2	2012	7/7	0.91	0.14	102,102,102,102	7
88	MG	6	2228	1/1	0.91	0.13	59,59,59,59	1
88	MG	1	4298	1/1	0.91	0.24	48,48,48,48	0
87	OHX	1	3613	7/7	0.91	0.39	36,36,36,36	7
87	OHX	6	2016	7/7	0.91	0.14	91,91,91,91	7
88	MG	5	3987	1/1	0.91	0.23	34,34,34,34	0
87	OHX	1	3543	7/7	0.91	0.32	56,56,56,56	7
88	MG	5	3989	1/1	0.91	0.34	29,29,29,29	0
88	MG	5	4463	1/1	0.91	0.09	37,37,37,37	0
88	MG	1	3936	1/1	0.91	0.23	38,38,38,38	0
88	MG	6	2238	1/1	0.91	0.10	66,66,66,66	0
88	MG	1	4105	1/1	0.91	0.08	46,46,46,46	0
88	MG	5	3999	1/1	0.91	0.28	27,27,27,27	0
88	MG	5	4000	1/1	0.91	0.27	42,42,42,42	0
88	MG	1	4308	1/1	0.91	0.19	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4109	1/1	0.91	0.15	49,49,49,49	0
88	MG	5	4006	1/1	0.91	0.41	46,46,46,46	0
88	MG	5	4488	1/1	0.91	0.15	41,41,41,41	1
87	OHX	s4	301	7/7	0.91	0.23	79,79,79,79	7
88	MG	6	2244	1/1	0.91	0.17	53,53,53,53	0
88	MG	1	4321	1/1	0.91	0.27	52,52,52,52	0
87	OHX	1	3801	7/7	0.91	0.23	73,73,73,73	7
88	MG	5	4016	1/1	0.91	0.25	30,30,30,30	0
87	OHX	6	2019	7/7	0.91	0.25	55,55,55,55	7
88	MG	5	4520	1/1	0.91	0.06	47,47,47,47	0
88	MG	2	2107	1/1	0.91	0.26	60,60,60,60	0
87	OHX	5	3652	7/7	0.91	0.33	58,58,58,58	7
88	MG	1	4328	1/1	0.91	0.28	37,37,37,37	1
87	OHX	1	3686	7/7	0.91	0.29	66,66,66,66	7
88	MG	M0	305	1/1	0.91	0.23	62,62,62,62	0
88	MG	1	4121	1/1	0.91	0.18	35,35,35,35	0
88	MG	1	4338	1/1	0.91	0.17	58,58,58,58	0
88	MG	5	4039	1/1	0.91	0.22	37,37,37,37	0
88	MG	5	4049	1/1	0.91	0.32	44,44,44,44	0
87	OHX	2	2015	7/7	0.91	0.17	87,87,87,87	7
88	MG	1	4342	1/1	0.91	0.14	48,48,48,48	1
87	OHX	5	3656	7/7	0.91	0.71	42,42,42,42	7
88	MG	1	3951	1/1	0.91	0.21	36,36,36,36	0
88	MG	5	4060	1/1	0.91	0.08	64,64,64,64	0
88	MG	6	2269	1/1	0.91	0.15	89,89,89,89	0
88	MG	1	3953	1/1	0.91	0.16	34,34,34,34	0
87	OHX	5	3657	7/7	0.91	0.25	50,50,50,50	7
88	MG	N3	201	1/1	0.91	0.33	39,39,39,39	0
88	MG	1	4347	1/1	0.91	0.15	43,43,43,43	0
88	MG	5	4074	1/1	0.91	0.09	41,41,41,41	0
87	OHX	5	3505	7/7	0.91	0.24	66,66,66,66	7
88	MG	7	215	1/1	0.91	0.30	53,53,53,53	0
88	MG	1	4132	1/1	0.91	0.19	58,58,58,58	0
88	MG	N8	203	1/1	0.91	0.21	33,33,33,33	0
88	MG	O1	203	1/1	0.91	0.26	57,57,57,57	0
87	OHX	5	3519	7/7	0.91	0.15	120,120,120,120	7
88	MG	7	228	1/1	0.91	0.07	38,38,38,38	0
88	MG	O2	202	1/1	0.91	0.27	32,32,32,32	0
88	MG	O2	204	1/1	0.91	0.18	33,33,33,33	0
88	MG	1	4354	1/1	0.91	0.17	51,51,51,51	0
88	MG	7	239	1/1	0.91	0.11	53,53,53,53	1
88	MG	8	223	1/1	0.91	0.14	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	OHX	1	3621	7/7	0.91	0.33	61,61,61,61	7
88	MG	8	229	1/1	0.91	0.09	52,52,52,52	0
88	MG	6	2296	1/1	0.91	0.14	54,54,54,54	1
87	OHX	5	3665	7/7	0.91	0.32	37,37,37,37	7
87	OHX	O3	201	7/7	0.91	0.31	49,49,49,49	7
88	MG	5	4106	1/1	0.91	0.27	50,50,50,50	0
88	MG	1	4142	1/1	0.91	0.13	50,50,50,50	0
87	OHX	1	3690	7/7	0.91	0.18	85,85,85,85	7
88	MG	5	4121	1/1	0.91	0.18	38,38,38,38	0
88	MG	1	3818	1/1	0.91	0.28	34,34,34,34	0
88	MG	12	303	1/1	0.91	0.20	55,55,55,55	1
87	OHX	5	3544	7/7	0.91	0.26	48,48,48,48	7
88	MG	6	2307	1/1	0.91	0.17	68,68,68,68	0
87	OHX	6	1966	7/7	0.91	0.29	56,56,56,56	7
88	MG	1	4370	1/1	0.91	0.15	44,44,44,44	0
88	MG	13	415	1/1	0.91	0.13	36,36,36,36	1
88	MG	6	2317	1/1	0.91	0.20	59,59,59,59	0
88	MG	1	3974	1/1	0.91	0.37	28,28,28,28	0
88	MG	5	4138	1/1	0.91	0.08	40,40,40,40	0
88	MG	1	4390	1/1	0.91	0.17	41,41,41,41	1
88	MG	1	4148	1/1	0.91	0.20	75,75,75,75	0
87	OHX	5	3557	7/7	0.91	0.31	51,51,51,51	7
87	OHX	5	3560	7/7	0.91	0.25	89,89,89,89	7
87	OHX	2	2025	7/7	0.91	0.17	94,94,94,94	7
88	MG	5	4152	1/1	0.91	0.17	41,41,41,41	0
87	OHX	5	4574	7/7	0.91	0.28	40,40,40,40	7
88	MG	m8	1503	1/1	0.91	0.13	52,52,52,52	0
88	MG	1	3831	1/1	0.91	0.20	41,41,41,41	0
88	MG	n0	203	1/1	0.91	0.19	41,41,41,41	0
88	MG	1	3982	1/1	0.91	0.14	54,54,54,54	0
88	MG	6	2115	1/1	0.91	0.26	75,75,75,75	0
88	MG	1	4402	1/1	0.91	0.11	46,46,46,46	1
88	MG	1	3833	1/1	0.91	0.25	41,41,41,41	0
88	MG	1	4409	1/1	0.91	0.10	52,52,52,52	1
88	MG	1	4410	1/1	0.91	0.16	50,50,50,50	1
88	MG	5	4175	1/1	0.91	0.25	44,44,44,44	0
88	MG	o2	203	1/1	0.91	0.42	34,34,34,34	1
88	MG	1	3989	1/1	0.91	0.23	28,28,28,28	0
88	MG	2	2127	1/1	0.91	0.26	60,60,60,60	0
87	OHX	5	3571	7/7	0.91	0.23	66,66,66,66	7
88	MG	2	2200	1/1	0.91	0.23	65,65,65,65	0
87	OHX	6	1971	7/7	0.91	0.22	85,85,85,85	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	3844	1/1	0.91	0.21	46,46,46,46	0
87	OHX	5	3579	7/7	0.91	0.12	148,148,148,148	7
87	OHX	6	2069	7/7	0.91	0.19	78,78,78,78	7
88	MG	1	4134	1/1	0.92	0.11	46,46,46,46	0
88	MG	2	2235	1/1	0.92	0.14	102,102,102,102	1
88	MG	1	3995	1/1	0.92	0.26	32,32,32,32	0
88	MG	1	4137	1/1	0.92	0.10	51,51,51,51	0
88	MG	2	2108	1/1	0.92	0.47	59,59,59,59	0
88	MG	2	2240	1/1	0.92	0.25	66,66,66,66	0
88	MG	5	4259	1/1	0.92	0.23	32,32,32,32	1
88	MG	6	2201	1/1	0.92	0.10	83,83,83,83	0
88	MG	5	4263	1/1	0.92	0.09	38,38,38,38	0
88	MG	4	218	1/1	0.92	0.34	54,54,54,54	0
88	MG	1	4141	1/1	0.92	0.15	47,47,47,47	0
87	OHX	1	3559	7/7	0.92	0.29	50,50,50,50	7
87	OHX	5	3694	7/7	0.92	0.18	66,66,66,66	7
87	OHX	1	3561	7/7	0.92	0.20	84,84,84,84	7
88	MG	1	3891	1/1	0.92	0.19	44,44,44,44	0
88	MG	2	2246	1/1	0.92	0.19	77,77,77,77	0
88	MG	5	4291	1/1	0.92	0.31	43,43,43,43	0
88	MG	4	229	1/1	0.92	0.13	47,47,47,47	0
87	OHX	2	2048	7/7	0.92	0.21	83,83,83,83	7
88	MG	4	232	1/1	0.92	0.15	43,43,43,43	1
87	OHX	5	3697	7/7	0.92	0.10	120,120,120,120	7
87	OHX	1	3507	7/7	0.92	0.24	66,66,66,66	7
88	MG	5	3932	1/1	0.92	0.21	28,28,28,28	0
87	OHX	2	2028	7/7	0.92	0.11	134,134,134,134	7
88	MG	5	4311	1/1	0.92	0.59	31,31,31,31	1
88	MG	1	3898	1/1	0.92	0.19	43,43,43,43	0
88	MG	5	3937	1/1	0.92	0.35	30,30,30,30	0
88	MG	5	3940	1/1	0.92	0.31	32,32,32,32	0
88	MG	5	4319	1/1	0.92	0.20	36,36,36,36	1
88	MG	5	4320	1/1	0.92	0.15	42,42,42,42	1
87	OHX	1	3795	7/7	0.92	0.26	54,54,54,54	7
87	OHX	5	3561	7/7	0.92	0.21	72,72,72,72	7
87	OHX	5	3703	7/7	0.92	0.23	46,46,46,46	7
88	MG	5	4324	1/1	0.92	0.16	53,53,53,53	0
87	OHX	5	3565	7/7	0.92	0.21	78,78,78,78	7
88	MG	5	3948	1/1	0.92	0.29	34,34,34,34	0
88	MG	6	2226	1/1	0.92	0.11	107,107,107,107	0
88	MG	1	3910	1/1	0.92	0.27	34,34,34,34	0
88	MG	1	4359	1/1	0.92	0.20	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4360	1/1	0.92	0.17	70,70,70,70	0
88	MG	6	2231	1/1	0.92	0.18	86,86,86,86	0
88	MG	1	3911	1/1	0.92	0.18	48,48,48,48	0
87	OHX	8	206	7/7	0.92	0.16	94,94,94,94	7
88	MG	1	4034	1/1	0.92	0.21	45,45,45,45	0
88	MG	6	2235	1/1	0.92	0.16	76,76,76,76	0
88	MG	1	4366	1/1	0.92	0.07	41,41,41,41	1
87	OHX	L4	401	7/7	0.92	0.22	59,59,59,59	7
88	MG	1	4176	1/1	0.92	0.08	58,58,58,58	0
88	MG	M6	204	1/1	0.92	0.19	39,39,39,39	1
88	MG	1	4038	1/1	0.92	0.15	50,50,50,50	0
88	MG	M7	203	1/1	0.92	0.37	36,36,36,36	0
88	MG	5	4352	1/1	0.92	0.15	45,45,45,45	0
87	OHX	1	3531	7/7	0.92	0.32	47,47,47,47	7
88	MG	5	4356	1/1	0.92	0.19	50,50,50,50	0
88	MG	1	4376	1/1	0.92	0.13	30,30,30,30	0
88	MG	5	3982	1/1	0.92	0.24	35,35,35,35	0
88	MG	1	4386	1/1	0.92	0.17	36,36,36,36	1
87	OHX	5	3573	7/7	0.92	0.22	53,53,53,53	7
88	MG	N3	203	1/1	0.92	0.21	51,51,51,51	0
87	OHX	6	2006	7/7	0.92	0.27	54,54,54,54	7
87	OHX	M0	301	7/7	0.92	0.31	49,49,49,49	7
88	MG	5	4378	1/1	0.92	0.14	47,47,47,47	0
88	MG	5	3995	1/1	0.92	0.47	32,32,32,32	0
87	OHX	5	3767	7/7	0.92	0.27	60,60,60,60	7
87	OHX	1	3539	7/7	0.92	0.18	64,64,64,64	7
87	OHX	5	3712	7/7	0.92	0.26	60,60,60,60	7
87	OHX	1	3581	7/7	0.92	0.29	54,54,54,54	7
88	MG	5	4391	1/1	0.92	0.09	41,41,41,41	0
88	MG	O2	203	1/1	0.92	0.14	44,44,44,44	1
87	OHX	2	2008	7/7	0.92	0.24	83,83,83,83	7
88	MG	1	4052	1/1	0.92	0.12	44,44,44,44	0
88	MG	5	4405	1/1	0.92	0.28	39,39,39,39	0
87	OHX	1	3632	7/7	0.92	0.20	75,75,75,75	7
88	MG	1	4200	1/1	0.92	0.13	60,60,60,60	0
88	MG	5	4411	1/1	0.92	0.12	33,33,33,33	1
87	OHX	14	402	7/7	0.92	0.25	55,55,55,55	7
88	MG	1	4417	1/1	0.92	0.33	41,41,41,41	1
88	MG	5	4417	1/1	0.92	0.15	46,46,46,46	0
88	MG	1	4060	1/1	0.92	0.19	56,56,56,56	0
88	MG	Q0	202	1/1	0.92	0.15	54,54,54,54	0
87	OHX	5	3598	7/7	0.92	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	OHX	5	3600	7/7	0.92	0.23	70,70,70,70	7
88	MG	5	4024	1/1	0.92	0.31	38,38,38,38	0
88	MG	1	4421	1/1	0.92	0.24	46,46,46,46	1
88	MG	6	2100	1/1	0.92	0.07	60,60,60,60	0
87	OHX	M8	201	7/7	0.92	0.28	53,53,53,53	7
88	MG	5	4036	1/1	0.92	0.20	35,35,35,35	0
87	OHX	5	3661	7/7	0.92	0.37	47,47,47,47	7
88	MG	6	2288	1/1	0.92	0.12	65,65,65,65	0
88	MG	5	4046	1/1	0.92	0.11	42,42,42,42	0
87	OHX	5	3662	7/7	0.92	0.27	65,65,65,65	7
87	OHX	1	3592	7/7	0.92	0.22	70,70,70,70	7
88	MG	5	4052	1/1	0.92	0.21	40,40,40,40	0
88	MG	6	2107	1/1	0.92	0.19	47,47,47,47	0
87	OHX	6	2088	7/7	0.92	0.24	71,71,71,71	7
88	MG	5	4057	1/1	0.92	0.17	51,51,51,51	0
88	MG	5	4480	1/1	0.92	0.09	39,39,39,39	1
88	MG	1	4219	1/1	0.92	0.29	37,37,37,37	1
88	MG	1	3944	1/1	0.92	0.20	34,34,34,34	0
87	OHX	1	3598	7/7	0.92	0.09	152,152,152,152	7
88	MG	5	4064	1/1	0.92	0.28	42,42,42,42	0
88	MG	5	4500	1/1	0.92	0.16	39,39,39,39	1
88	MG	1	4439	1/1	0.92	0.22	41,41,41,41	1
87	OHX	1	3775	7/7	0.92	0.28	50,50,50,50	7
88	MG	1	4441	1/1	0.92	0.15	41,41,41,41	0
87	OHX	2	1998	7/7	0.92	0.18	94,94,94,94	7
87	OHX	1	3549	7/7	0.92	0.23	60,60,60,60	7
88	MG	6	2118	1/1	0.92	0.23	38,38,38,38	0
88	MG	5	4081	1/1	0.92	0.07	57,57,57,57	0
88	MG	6	2319	1/1	0.92	0.22	57,57,57,57	0
88	MG	1	4226	1/1	0.92	0.27	41,41,41,41	1
88	MG	6	2120	1/1	0.92	0.30	43,43,43,43	0
88	MG	5	4087	1/1	0.92	0.24	53,53,53,53	0
88	MG	1	4082	1/1	0.92	0.07	57,57,57,57	0
88	MG	1	4454	1/1	0.92	0.13	47,47,47,47	0
87	OHX	1	3551	7/7	0.92	0.21	89,89,89,89	7
87	OHX	5	3733	7/7	0.92	0.22	73,73,73,73	7
88	MG	1	4085	1/1	0.92	0.08	44,44,44,44	0
88	MG	1	4236	1/1	0.92	0.15	46,46,46,46	0
88	MG	5	4097	1/1	0.92	0.06	49,49,49,49	0
88	MG	1	4087	1/1	0.92	0.10	39,39,39,39	0
87	OHX	1	3645	7/7	0.92	0.24	52,52,52,52	7
88	MG	1	4090	1/1	0.92	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	3956	1/1	0.92	0.27	43,43,43,43	0
88	MG	5	4561	1/1	0.92	0.10	37,37,37,37	0
88	MG	s8	304	1/1	0.92	0.12	56,56,56,56	0
88	MG	1	4251	1/1	0.92	0.21	48,48,48,48	0
88	MG	1	3957	1/1	0.92	0.35	37,37,37,37	0
88	MG	1	4094	1/1	0.92	0.17	46,46,46,46	0
88	MG	7	214	1/1	0.92	0.29	27,27,27,27	0
88	MG	1	4470	1/1	0.92	0.22	55,55,55,55	0
88	MG	7	217	1/1	0.92	0.24	30,30,30,30	0
88	MG	1	3958	1/1	0.92	0.11	46,46,46,46	0
88	MG	1	4096	1/1	0.92	0.19	44,44,44,44	1
88	MG	1	4475	1/1	0.92	0.18	41,41,41,41	1
87	OHX	5	3676	7/7	0.92	0.30	38,38,38,38	7
87	OHX	1	3604	7/7	0.92	0.22	51,51,51,51	7
88	MG	6	2149	1/1	0.92	0.35	65,65,65,65	0
88	MG	5	4142	1/1	0.92	0.07	43,43,43,43	0
88	MG	1	4270	1/1	0.92	0.13	43,43,43,43	1
88	MG	7	238	1/1	0.92	0.14	50,50,50,50	1
88	MG	1	4100	1/1	0.92	0.28	52,52,52,52	0
88	MG	1	3843	1/1	0.92	0.19	49,49,49,49	0
87	OHX	2	1984	7/7	0.92	0.09	177,177,177,177	7
88	MG	1	3965	1/1	0.92	0.28	41,41,41,41	0
88	MG	1	4283	1/1	0.92	0.48	40,40,40,40	1
87	OHX	6	1980	7/7	0.92	0.24	61,61,61,61	7
88	MG	5	4159	1/1	0.92	0.16	59,59,59,59	0
88	MG	1	4107	1/1	0.92	0.21	40,40,40,40	1
88	MG	5	4161	1/1	0.92	0.05	54,54,54,54	0
88	MG	5	3820	1/1	0.92	0.15	39,39,39,39	0
87	OHX	5	3739	7/7	0.92	0.16	105,105,105,105	7
87	OHX	1	3782	7/7	0.92	0.26	73,73,73,73	7
88	MG	5	4171	1/1	0.92	0.12	86,86,86,86	0
88	MG	5	3828	1/1	0.92	0.26	35,35,35,35	0
88	MG	1	4494	1/1	0.92	0.13	41,41,41,41	0
88	MG	5	3833	1/1	0.92	0.29	33,33,33,33	0
88	MG	l3	407	1/1	0.92	0.31	38,38,38,38	1
88	MG	l3	412	1/1	0.92	0.14	34,34,34,34	0
88	MG	1	4495	1/1	0.92	0.15	60,60,60,60	0
87	OHX	1	3705	7/7	0.92	0.26	59,59,59,59	7
88	MG	1	4114	1/1	0.92	0.22	42,42,42,42	0
87	OHX	5	3624	7/7	0.92	0.23	66,66,66,66	7
88	MG	5	4186	1/1	0.92	0.16	44,44,44,44	1
88	MG	l7	303	1/1	0.92	0.17	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4503	1/1	0.92	0.32	36,36,36,36	1
88	MG	17	306	1/1	0.92	0.21	37,37,37,37	1
88	MG	1	3973	1/1	0.92	0.26	41,41,41,41	0
88	MG	6	2173	1/1	0.92	0.20	56,56,56,56	0
87	OHX	c5	201	7/7	0.92	0.11	118,118,118,118	7
87	OHX	5	3800	7/7	0.92	0.20	52,52,52,52	7
88	MG	5	3852	1/1	0.92	0.17	35,35,35,35	0
88	MG	5	4201	1/1	0.92	0.13	60,60,60,60	0
87	OHX	SR	401	7/7	0.92	0.11	130,130,130,130	7
88	MG	5	3859	1/1	0.92	0.23	35,35,35,35	0
88	MG	5	3862	1/1	0.92	0.05	34,34,34,34	0
88	MG	5	4208	1/1	0.92	0.10	41,41,41,41	0
87	OHX	1	3707	7/7	0.92	0.22	67,67,67,67	7
87	OHX	5	3630	7/7	0.92	0.26	42,42,42,42	7
88	MG	1	4305	1/1	0.92	0.51	44,44,44,44	1
88	MG	5	4215	1/1	0.92	0.11	39,39,39,39	0
88	MG	3	216	1/1	0.92	0.30	55,55,55,55	0
88	MG	n8	206	1/1	0.92	0.15	37,37,37,37	1
88	MG	3	218	1/1	0.92	0.29	35,35,35,35	0
87	OHX	6	2032	7/7	0.92	0.22	61,61,61,61	7
87	OHX	1	3557	7/7	0.92	0.17	76,76,76,76	7
88	MG	1	3985	1/1	0.92	0.35	37,37,37,37	0
88	MG	2	2106	1/1	0.92	0.11	60,60,60,60	0
88	MG	5	3887	1/1	0.92	0.23	39,39,39,39	0
88	MG	5	3890	1/1	0.92	0.12	40,40,40,40	1
88	MG	1	4320	1/1	0.92	0.15	54,54,54,54	0
87	OHX	1	3787	7/7	0.92	0.27	68,68,68,68	7
88	MG	6	2193	1/1	0.92	0.12	57,57,57,57	0
87	OHX	1	3674	7/7	0.93	0.25	44,44,44,44	7
88	MG	5	4254	1/1	0.93	0.09	57,57,57,57	0
88	MG	O1	205	1/1	0.93	0.17	65,65,65,65	0
88	MG	5	4258	1/1	0.93	0.12	39,39,39,39	0
88	MG	1	4425	1/1	0.93	0.15	49,49,49,49	1
88	MG	1	4233	1/1	0.93	0.38	54,54,54,54	0
88	MG	1	4234	1/1	0.93	0.11	46,46,46,46	0
87	OHX	5	3635	7/7	0.93	0.10	138,138,138,138	7
88	MG	5	4267	1/1	0.93	0.20	40,40,40,40	1
88	MG	5	3945	1/1	0.93	0.24	28,28,28,28	0
88	MG	5	4275	1/1	0.93	0.31	36,36,36,36	1
88	MG	5	4276	1/1	0.93	0.08	39,39,39,39	0
88	MG	1	3840	1/1	0.93	0.22	39,39,39,39	0
88	MG	1	4098	1/1	0.93	0.31	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	OHX	1	3675	7/7	0.93	0.30	42,42,42,42	7
88	MG	5	3955	1/1	0.93	0.28	35,35,35,35	0
88	MG	5	3956	1/1	0.93	0.26	37,37,37,37	0
88	MG	5	3958	1/1	0.93	0.25	44,44,44,44	0
87	OHX	1	3548	7/7	0.93	0.26	60,60,60,60	7
88	MG	5	4295	1/1	0.93	0.12	47,47,47,47	0
88	MG	O7	105	1/1	0.93	0.11	51,51,51,51	0
88	MG	O7	106	1/1	0.93	0.12	59,59,59,59	0
87	OHX	5	3639	7/7	0.93	0.30	53,53,53,53	7
87	OHX	1	3594	7/7	0.93	0.19	100,100,100,100	7
87	OHX	6	2009	7/7	0.93	0.27	56,56,56,56	7
87	OHX	2	1950	7/7	0.93	0.18	97,97,97,97	7
88	MG	5	3968	1/1	0.93	0.26	31,31,31,31	0
87	OHX	1	3599	7/7	0.93	0.10	128,128,128,128	7
88	MG	5	3970	1/1	0.93	0.23	36,36,36,36	0
87	OHX	6	2061	7/7	0.93	0.14	102,102,102,102	7
88	MG	1	4266	1/1	0.93	0.11	77,77,77,77	0
87	OHX	1	3637	7/7	0.93	0.19	89,89,89,89	7
88	MG	5	3974	1/1	0.93	0.32	40,40,40,40	0
88	MG	5	3976	1/1	0.93	0.29	58,58,58,58	0
88	MG	2	2221	1/1	0.93	0.11	61,61,61,61	0
88	MG	1	4457	1/1	0.93	0.16	54,54,54,54	1
87	OHX	1	3640	7/7	0.93	0.17	91,91,91,91	7
88	MG	1	4274	1/1	0.93	0.30	46,46,46,46	1
88	MG	1	3862	1/1	0.93	0.23	49,49,49,49	0
88	MG	5	3984	1/1	0.93	0.14	28,28,28,28	0
88	MG	5	3986	1/1	0.93	0.19	57,57,57,57	0
88	MG	1	4277	1/1	0.93	0.10	40,40,40,40	0
87	OHX	5	3648	7/7	0.93	0.18	65,65,65,65	7
88	MG	6	2284	1/1	0.93	0.27	59,59,59,59	0
88	MG	1	4280	1/1	0.93	0.13	50,50,50,50	0
88	MG	1	3865	1/1	0.93	0.34	62,62,62,62	0
87	OHX	5	3649	7/7	0.93	0.20	64,64,64,64	7
88	MG	1	3984	1/1	0.93	0.09	42,42,42,42	0
87	OHX	2	2031	7/7	0.93	0.17	90,90,90,90	7
88	MG	6	2299	1/1	0.93	0.25	59,59,59,59	0
88	MG	1	4471	1/1	0.93	0.13	62,62,62,62	0
88	MG	5	4348	1/1	0.93	0.10	54,54,54,54	1
88	MG	1	3870	1/1	0.93	0.26	31,31,31,31	0
88	MG	1	3871	1/1	0.93	0.23	35,35,35,35	0
87	OHX	1	3683	7/7	0.93	0.19	61,61,61,61	7
88	MG	1	4476	1/1	0.93	0.14	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	OHX	2	1999	7/7	0.93	0.17	94,94,94,94	7
88	MG	5	4357	1/1	0.93	0.19	37,37,37,37	1
88	MG	1	4128	1/1	0.93	0.15	51,51,51,51	0
88	MG	1	4294	1/1	0.93	0.14	53,53,53,53	0
88	MG	2	2091	1/1	0.93	0.23	44,44,44,44	0
88	MG	5	4019	1/1	0.93	0.23	32,32,32,32	0
87	OHX	5	3562	7/7	0.93	0.20	96,96,96,96	7
88	MG	5	4369	1/1	0.93	0.27	38,38,38,38	1
88	MG	5	4370	1/1	0.93	0.10	45,45,45,45	1
88	MG	1	4484	1/1	0.93	0.10	55,55,55,55	0
88	MG	1	4133	1/1	0.93	0.10	38,38,38,38	0
88	MG	1	4001	1/1	0.93	0.18	29,29,29,29	0
88	MG	6	2135	1/1	0.93	0.33	50,50,50,50	0
88	MG	5	4027	1/1	0.93	0.52	30,30,30,30	0
88	MG	5	4028	1/1	0.93	0.08	49,49,49,49	0
88	MG	5	4387	1/1	0.93	0.12	52,52,52,52	0
88	MG	5	4029	1/1	0.93	0.17	43,43,43,43	0
87	OHX	2	1986	7/7	0.93	0.21	80,80,80,80	7
88	MG	5	4033	1/1	0.93	0.23	35,35,35,35	0
88	MG	5	4392	1/1	0.93	0.16	52,52,52,52	1
88	MG	5	4393	1/1	0.93	0.37	38,38,38,38	1
88	MG	5	4395	1/1	0.93	0.12	46,46,46,46	1
87	OHX	5	3567	7/7	0.93	0.22	62,62,62,62	7
87	OHX	1	3648	7/7	0.93	0.27	58,58,58,58	7
88	MG	5	4037	1/1	0.93	0.16	51,51,51,51	0
88	MG	1	3883	1/1	0.93	0.28	31,31,31,31	0
87	OHX	1	3603	7/7	0.93	0.27	55,55,55,55	7
88	MG	5	4041	1/1	0.93	0.14	40,40,40,40	0
88	MG	5	4044	1/1	0.93	0.13	34,34,34,34	0
88	MG	1	4310	1/1	0.93	0.50	40,40,40,40	1
88	MG	1	3889	1/1	0.93	0.29	51,51,51,51	0
88	MG	5	4050	1/1	0.93	0.22	50,50,50,50	0
88	MG	1	4496	1/1	0.93	0.15	49,49,49,49	0
88	MG	2	2237	1/1	0.93	0.15	80,80,80,80	0
87	OHX	1	3447	7/7	0.93	0.22	77,77,77,77	7
88	MG	5	4425	1/1	0.93	0.27	37,37,37,37	1
88	MG	5	4426	1/1	0.93	0.12	45,45,45,45	0
88	MG	1	4501	1/1	0.93	0.09	51,51,51,51	0
87	OHX	5	3575	7/7	0.93	0.17	55,55,55,55	7
88	MG	1	4013	1/1	0.93	0.19	35,35,35,35	0
88	MG	5	4450	1/1	0.93	0.19	47,47,47,47	0
88	MG	5	4059	1/1	0.93	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	1971	7/7	0.93	0.25	80,80,80,80	7
88	MG	c8	203	1/1	0.93	0.05	86,86,86,86	0
87	OHX	1	3609	7/7	0.93	0.24	62,62,62,62	7
87	OHX	2	2059	7/7	0.93	0.28	66,66,66,66	7
87	OHX	2	1979	7/7	0.93	0.18	75,75,75,75	7
88	MG	5	4468	1/1	0.93	0.07	42,42,42,42	0
88	MG	1	4331	1/1	0.93	0.31	45,45,45,45	1
88	MG	1	4333	1/1	0.93	0.18	42,42,42,42	0
88	MG	5	4471	1/1	0.93	0.07	39,39,39,39	0
87	OHX	5	3586	7/7	0.93	0.17	83,83,83,83	7
88	MG	1	4151	1/1	0.93	0.11	54,54,54,54	0
88	MG	5	4080	1/1	0.93	0.17	41,41,41,41	0
87	OHX	6	1945	7/7	0.93	0.24	58,58,58,58	7
87	OHX	5	3592	7/7	0.93	0.25	43,43,43,43	7
88	MG	5	4083	1/1	0.93	0.14	36,36,36,36	0
88	MG	5	4485	1/1	0.93	0.08	57,57,57,57	0
87	OHX	1	3526	7/7	0.93	0.17	67,67,67,67	7
87	OHX	2	1935	7/7	0.93	0.13	98,98,98,98	7
87	OHX	1	3806	7/7	0.93	0.18	62,62,62,62	7
88	MG	5	4499	1/1	0.93	0.15	46,46,46,46	0
87	OHX	5	3675	7/7	0.93	0.29	47,47,47,47	7
88	MG	5	3818	1/1	0.93	0.10	48,48,48,48	0
88	MG	5	4506	1/1	0.93	0.17	33,33,33,33	0
88	MG	5	4092	1/1	0.93	0.12	34,34,34,34	0
87	OHX	1	3535	7/7	0.93	0.12	147,147,147,147	7
87	OHX	6	1979	7/7	0.93	0.16	79,79,79,79	7
88	MG	2	2113	1/1	0.93	0.35	68,68,68,68	0
88	MG	5	3824	1/1	0.93	0.24	54,54,54,54	0
87	OHX	1	3617	7/7	0.93	0.19	73,73,73,73	7
88	MG	5	4098	1/1	0.93	0.21	44,44,44,44	0
88	MG	5	3827	1/1	0.93	0.27	43,43,43,43	0
88	MG	5	4102	1/1	0.93	0.17	35,35,35,35	0
88	MG	1	4351	1/1	0.93	0.25	67,67,67,67	0
88	MG	5	3829	1/1	0.93	0.29	59,59,59,59	0
88	MG	5	4111	1/1	0.93	0.12	35,35,35,35	0
88	MG	1	4175	1/1	0.93	0.18	53,53,53,53	1
88	MG	5	3831	1/1	0.93	0.19	37,37,37,37	0
88	MG	1	4353	1/1	0.93	0.07	49,49,49,49	0
87	OHX	5	3605	7/7	0.93	0.18	96,96,96,96	7
88	MG	5	4126	1/1	0.93	0.11	35,35,35,35	1
87	OHX	1	3575	7/7	0.93	0.29	53,53,53,53	7
88	MG	5	4129	1/1	0.93	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4558	1/1	0.93	0.12	68,68,68,68	0
87	OHX	6	2083	7/7	0.93	0.20	82,82,82,82	7
88	MG	S6	301	1/1	0.93	0.08	103,103,103,103	0
88	MG	1	3922	1/1	0.93	0.25	34,34,34,34	0
87	OHX	2	2004	7/7	0.93	0.15	89,89,89,89	7
88	MG	6	2190	1/1	0.93	0.09	44,44,44,44	0
88	MG	5	4137	1/1	0.93	0.15	54,54,54,54	0
88	MG	5	4573	1/1	0.93	0.19	44,44,44,44	0
87	OHX	1	3622	7/7	0.93	0.18	84,84,84,84	7
88	MG	5	3848	1/1	0.93	0.25	40,40,40,40	0
88	MG	C8	203	1/1	0.93	0.12	96,96,96,96	0
88	MG	D0	201	1/1	0.93	0.32	71,71,71,71	0
88	MG	5	3853	1/1	0.93	0.10	47,47,47,47	0
88	MG	1	3932	1/1	0.93	0.36	31,31,31,31	0
88	MG	6	2195	1/1	0.93	0.25	46,46,46,46	0
88	MG	7	225	1/1	0.93	0.20	64,64,64,64	0
87	OHX	3	202	7/7	0.93	0.28	48,48,48,48	7
88	MG	5	4153	1/1	0.93	0.29	51,51,51,51	0
88	MG	7	231	1/1	0.93	0.10	50,50,50,50	0
88	MG	5	4154	1/1	0.93	0.06	45,45,45,45	0
88	MG	4	234	1/1	0.93	0.13	90,90,90,90	1
87	OHX	6	1988	7/7	0.93	0.25	57,57,57,57	7
87	OHX	3	206	7/7	0.93	0.21	81,81,81,81	7
87	OHX	6	2091	7/7	0.93	0.13	96,96,96,96	7
88	MG	1	4375	1/1	0.93	0.12	33,33,33,33	0
88	MG	5	3873	1/1	0.93	0.25	38,38,38,38	0
88	MG	8	225	1/1	0.93	0.19	55,55,55,55	0
88	MG	8	226	1/1	0.93	0.11	63,63,63,63	0
88	MG	5	4165	1/1	0.93	0.08	43,43,43,43	0
87	OHX	1	3580	7/7	0.93	0.14	106,106,106,106	7
88	MG	5	3875	1/1	0.93	0.21	33,33,33,33	0
88	MG	1	4382	1/1	0.93	0.12	53,53,53,53	0
88	MG	4	243	1/1	0.93	0.73	41,41,41,41	1
88	MG	1	4384	1/1	0.93	0.26	35,35,35,35	1
88	MG	L2	303	1/1	0.93	0.07	53,53,53,53	0
88	MG	8	238	1/1	0.93	0.15	45,45,45,45	0
88	MG	5	4177	1/1	0.93	0.13	55,55,55,55	0
88	MG	5	3889	1/1	0.93	0.16	47,47,47,47	0
88	MG	5	4179	1/1	0.93	0.12	54,54,54,54	0
88	MG	L3	404	1/1	0.93	0.17	42,42,42,42	1
88	MG	1	4069	1/1	0.93	0.11	37,37,37,37	0
88	MG	1	4389	1/1	0.93	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	l3	405	1/1	0.93	0.09	35,35,35,35	0
87	OHX	8	210	7/7	0.93	0.29	49,49,49,49	7
88	MG	l3	409	1/1	0.93	0.08	41,41,41,41	1
88	MG	5	3895	1/1	0.93	0.21	32,32,32,32	0
88	MG	1	4071	1/1	0.93	0.15	43,43,43,43	0
87	OHX	2	1993	7/7	0.93	0.19	80,80,80,80	7
88	MG	5	3899	1/1	0.93	0.13	61,61,61,61	0
87	OHX	8	214	7/7	0.93	0.18	100,100,100,100	7
88	MG	M1	202	1/1	0.93	0.21	72,72,72,72	0
88	MG	5	3902	1/1	0.93	0.20	48,48,48,48	0
88	MG	5	4202	1/1	0.93	0.10	40,40,40,40	0
88	MG	1	4211	1/1	0.93	0.32	37,37,37,37	0
88	MG	l7	307	1/1	0.93	0.11	38,38,38,38	1
87	OHX	6	1994	7/7	0.93	0.16	76,76,76,76	7
88	MG	1	4399	1/1	0.93	0.21	65,65,65,65	0
88	MG	m3	201	1/1	0.93	0.52	55,55,55,55	1
87	OHX	6	1996	7/7	0.93	0.15	90,90,90,90	7
88	MG	5	3910	1/1	0.93	0.33	33,33,33,33	0
88	MG	5	3911	1/1	0.93	0.11	39,39,39,39	0
88	MG	1	3821	1/1	0.93	0.23	38,38,38,38	0
87	OHX	2	1947	7/7	0.93	0.10	130,130,130,130	7
88	MG	5	4218	1/1	0.93	0.10	49,49,49,49	0
87	OHX	1	3591	7/7	0.93	0.17	95,95,95,95	7
88	MG	n0	205	1/1	0.93	0.18	41,41,41,41	1
87	OHX	1	3746	7/7	0.93	0.27	46,46,46,46	7
88	MG	N1	201	1/1	0.93	0.22	42,42,42,42	1
87	OHX	4	208	7/7	0.93	0.15	85,85,85,85	7
88	MG	5	3923	1/1	0.93	0.19	38,38,38,38	0
88	MG	1	3954	1/1	0.93	0.33	32,32,32,32	0
88	MG	5	3926	1/1	0.93	0.17	34,34,34,34	0
88	MG	5	4229	1/1	0.93	0.28	58,58,58,58	1
88	MG	n9	102	1/1	0.93	0.10	37,37,37,37	0
87	OHX	4	210	7/7	0.93	0.16	101,101,101,101	7
87	OHX	c1	201	7/7	0.93	0.21	79,79,79,79	7
88	MG	2	2206	1/1	0.93	0.10	58,58,58,58	0
88	MG	o3	204	1/1	0.93	0.18	37,37,37,37	1
87	OHX	1	3631	7/7	0.93	0.29	45,45,45,45	7
88	MG	5	4240	1/1	0.93	0.21	58,58,58,58	0
88	MG	5	4241	1/1	0.93	0.07	65,65,65,65	0
88	MG	N8	207	1/1	0.93	0.41	39,39,39,39	1
88	MG	N9	102	1/1	0.93	0.12	38,38,38,38	0
88	MG	5	3935	1/1	0.93	0.25	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	3959	1/1	0.93	0.26	31,31,31,31	0
88	MG	5	3980	1/1	0.94	0.15	50,50,50,50	0
88	MG	1	4264	1/1	0.94	0.18	32,32,32,32	0
88	MG	6	2101	1/1	0.94	0.31	39,39,39,39	0
87	OHX	1	3528	7/7	0.94	0.25	59,59,59,59	7
88	MG	6	2292	1/1	0.94	0.68	50,50,50,50	1
88	MG	6	2103	1/1	0.94	0.16	66,66,66,66	0
87	OHX	4	209	7/7	0.94	0.25	45,45,45,45	7
87	OHX	1	3562	7/7	0.94	0.15	92,92,92,92	7
88	MG	1	4112	1/1	0.94	0.21	36,36,36,36	0
88	MG	1	4273	1/1	0.94	0.11	37,37,37,37	0
88	MG	5	3993	1/1	0.94	0.20	31,31,31,31	0
88	MG	5	4312	1/1	0.94	0.10	74,74,74,74	0
87	OHX	4	211	7/7	0.94	0.13	99,99,99,99	7
88	MG	5	4314	1/1	0.94	0.25	64,64,64,64	0
88	MG	5	3996	1/1	0.94	0.23	34,34,34,34	0
88	MG	5	3997	1/1	0.94	0.23	36,36,36,36	0
88	MG	1	4115	1/1	0.94	0.20	52,52,52,52	0
87	OHX	2	1949	7/7	0.94	0.12	108,108,108,108	7
88	MG	1	4466	1/1	0.94	0.35	35,35,35,35	1
87	OHX	5	3587	7/7	0.94	0.21	52,52,52,52	7
88	MG	1	3873	1/1	0.94	0.24	39,39,39,39	0
88	MG	1	3986	1/1	0.94	0.19	31,31,31,31	0
88	MG	6	2315	1/1	0.94	0.09	54,54,54,54	0
88	MG	6	2316	1/1	0.94	0.18	60,60,60,60	1
88	MG	5	4010	1/1	0.94	0.18	30,30,30,30	0
87	OHX	5	3589	7/7	0.94	0.28	44,44,44,44	7
87	OHX	6	1992	7/7	0.94	0.16	71,71,71,71	7
87	OHX	5	3790	7/7	0.94	0.20	57,57,57,57	7
88	MG	5	4335	1/1	0.94	0.22	43,43,43,43	0
88	MG	5	4017	1/1	0.94	0.38	36,36,36,36	0
88	MG	1	3993	1/1	0.94	0.35	43,43,43,43	0
87	OHX	5	3728	7/7	0.94	0.20	49,49,49,49	7
88	MG	6	2324	1/1	0.94	0.21	47,47,47,47	1
87	OHX	5	3729	7/7	0.94	0.19	57,57,57,57	7
88	MG	6	2122	1/1	0.94	0.15	49,49,49,49	0
88	MG	1	3998	1/1	0.94	0.34	36,36,36,36	0
87	OHX	5	3730	7/7	0.94	0.21	70,70,70,70	7
87	OHX	2	1955	7/7	0.94	0.17	91,91,91,91	7
87	OHX	2	1983	7/7	0.94	0.16	70,70,70,70	7
87	OHX	1	3793	7/7	0.94	0.15	85,85,85,85	7
88	MG	1	4483	1/1	0.94	0.18	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4031	1/1	0.94	0.10	46,46,46,46	0
87	OHX	2	2033	7/7	0.94	0.10	113,113,113,113	7
87	OHX	5	3798	7/7	0.94	0.22	55,55,55,55	7
87	OHX	1	3542	7/7	0.94	0.20	52,52,52,52	7
88	MG	5	4359	1/1	0.94	0.08	42,42,42,42	0
88	MG	6	2134	1/1	0.94	0.22	42,42,42,42	0
88	MG	1	4303	1/1	0.94	0.11	58,58,58,58	1
87	OHX	1	3638	7/7	0.94	0.21	52,52,52,52	7
87	OHX	1	3639	7/7	0.94	0.21	52,52,52,52	7
87	OHX	2	1974	7/7	0.94	0.09	137,137,137,137	7
88	MG	5	4367	1/1	0.94	0.12	38,38,38,38	1
88	MG	5	4045	1/1	0.94	0.13	48,48,48,48	0
88	MG	1	4492	1/1	0.94	0.10	56,56,56,56	1
87	OHX	6	2002	7/7	0.94	0.21	52,52,52,52	7
87	OHX	5	3607	7/7	0.94	0.24	52,52,52,52	7
88	MG	1	4017	1/1	0.94	0.31	37,37,37,37	0
88	MG	1	4317	1/1	0.94	0.62	44,44,44,44	1
88	MG	2	2258	1/1	0.94	0.14	74,74,74,74	1
88	MG	5	4383	1/1	0.94	0.12	45,45,45,45	0
88	MG	6	2148	1/1	0.94	0.39	45,45,45,45	0
88	MG	1	4498	1/1	0.94	0.10	46,46,46,46	0
88	MG	d9	103	1/1	0.94	0.15	83,83,83,83	1
88	MG	1	4319	1/1	0.94	0.34	42,42,42,42	1
87	OHX	1	3579	7/7	0.94	0.24	54,54,54,54	7
88	MG	5	4061	1/1	0.94	0.12	39,39,39,39	0
87	OHX	5	3609	7/7	0.94	0.20	70,70,70,70	7
88	MG	5	3816	1/1	0.94	0.17	32,32,32,32	0
87	OHX	6	2004	7/7	0.94	0.25	54,54,54,54	7
88	MG	5	4398	1/1	0.94	0.17	42,42,42,42	1
88	MG	1	4024	1/1	0.94	0.16	48,48,48,48	0
88	MG	1	4026	1/1	0.94	0.20	46,46,46,46	0
88	MG	5	4071	1/1	0.94	0.24	36,36,36,36	0
88	MG	5	4408	1/1	0.94	0.22	39,39,39,39	0
88	MG	1	4506	1/1	0.94	0.07	50,50,50,50	0
88	MG	5	4073	1/1	0.94	0.06	34,34,34,34	0
87	OHX	1	3547	7/7	0.94	0.18	65,65,65,65	7
88	MG	5	3823	1/1	0.94	0.32	46,46,46,46	0
88	MG	5	4076	1/1	0.94	0.13	37,37,37,37	0
88	MG	5	4416	1/1	0.94	0.18	40,40,40,40	1
88	MG	5	4078	1/1	0.94	0.17	62,62,62,62	0
88	MG	5	4079	1/1	0.94	0.20	36,36,36,36	1
87	OHX	1	3739	7/7	0.94	0.17	76,76,76,76	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4422	1/1	0.94	0.08	62,62,62,62	0
88	MG	5	4423	1/1	0.94	0.23	39,39,39,39	1
87	OHX	2	1996	7/7	0.94	0.15	93,93,93,93	7
87	OHX	2	1985	7/7	0.94	0.19	59,59,59,59	7
88	MG	1	4159	1/1	0.94	0.28	52,52,52,52	0
88	MG	1	4033	1/1	0.94	0.31	45,45,45,45	0
87	OHX	1	3711	7/7	0.94	0.20	77,77,77,77	7
88	MG	1	4339	1/1	0.94	0.17	62,62,62,62	0
88	MG	5	4441	1/1	0.94	0.19	32,32,32,32	1
88	MG	5	4445	1/1	0.94	0.18	48,48,48,48	0
88	MG	1	4035	1/1	0.94	0.14	32,32,32,32	0
88	MG	D4	201	1/1	0.94	0.21	83,83,83,83	0
88	MG	5	3836	1/1	0.94	0.27	60,60,60,60	0
87	OHX	7	208	7/7	0.94	0.25	54,54,54,54	7
88	MG	5	4455	1/1	0.94	0.12	36,36,36,36	1
88	MG	5	4458	1/1	0.94	0.10	54,54,54,54	0
87	OHX	1	3616	7/7	0.94	0.25	60,60,60,60	7
88	MG	D9	104	1/1	0.94	0.11	85,85,85,85	0
88	MG	D9	105	1/1	0.94	0.08	76,76,76,76	0
87	OHX	6	2011	7/7	0.94	0.25	57,57,57,57	7
87	OHX	2	1976	7/7	0.94	0.21	92,92,92,92	7
88	MG	5	4099	1/1	0.94	0.29	35,35,35,35	0
88	MG	1	3924	1/1	0.94	0.22	43,43,43,43	0
88	MG	1	4179	1/1	0.94	0.25	37,37,37,37	0
88	MG	5	3849	1/1	0.94	0.28	43,43,43,43	0
88	MG	1	3925	1/1	0.94	0.33	40,40,40,40	0
88	MG	5	4107	1/1	0.94	0.17	36,36,36,36	0
88	MG	5	4108	1/1	0.94	0.11	28,28,28,28	0
88	MG	5	4110	1/1	0.94	0.28	43,43,43,43	0
88	MG	6	2182	1/1	0.94	0.12	51,51,51,51	0
88	MG	5	4114	1/1	0.94	0.12	32,32,32,32	1
88	MG	1	4182	1/1	0.94	0.10	43,43,43,43	0
88	MG	2	2195	1/1	0.94	0.34	65,65,65,65	0
87	OHX	6	2058	7/7	0.94	0.10	148,148,148,148	7
88	MG	5	3861	1/1	0.94	0.24	44,44,44,44	0
88	MG	4	221	1/1	0.94	0.36	46,46,46,46	0
87	OHX	1	3653	7/7	0.94	0.24	40,40,40,40	7
88	MG	5	4508	1/1	0.94	0.08	53,53,53,53	1
88	MG	4	224	1/1	0.94	0.39	55,55,55,55	0
87	OHX	1	3747	7/7	0.94	0.09	146,146,146,146	7
88	MG	1	4358	1/1	0.94	0.20	42,42,42,42	0
88	MG	5	4515	1/1	0.94	0.11	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	3870	1/1	0.94	0.17	43,43,43,43	0
88	MG	5	4522	1/1	0.94	0.18	51,51,51,51	1
87	OHX	5	3628	7/7	0.94	0.18	63,63,63,63	7
87	OHX	8	211	7/7	0.94	0.15	105,105,105,105	7
88	MG	4	230	1/1	0.94	0.19	56,56,56,56	0
88	MG	1	4061	1/1	0.94	0.17	50,50,50,50	0
88	MG	5	3876	1/1	0.94	0.25	34,34,34,34	0
88	MG	5	3879	1/1	0.94	0.27	41,41,41,41	0
88	MG	5	4145	1/1	0.94	0.15	50,50,50,50	0
88	MG	5	4146	1/1	0.94	0.13	41,41,41,41	1
88	MG	5	4540	1/1	0.94	0.19	37,37,37,37	0
88	MG	5	4541	1/1	0.94	0.34	34,34,34,34	1
88	MG	5	3880	1/1	0.94	0.17	40,40,40,40	0
88	MG	5	3881	1/1	0.94	0.29	58,58,58,58	0
87	OHX	5	3507	7/7	0.94	0.20	61,61,61,61	7
88	MG	1	4364	1/1	0.94	0.09	38,38,38,38	0
87	OHX	1	3655	7/7	0.94	0.28	48,48,48,48	7
88	MG	1	3824	1/1	0.94	0.17	40,40,40,40	0
87	OHX	5	3522	7/7	0.94	0.26	46,46,46,46	7
88	MG	1	3940	1/1	0.94	0.21	35,35,35,35	0
87	OHX	5	3527	7/7	0.94	0.19	57,57,57,57	7
87	OHX	6	1944	7/7	0.94	0.16	60,60,60,60	7
88	MG	5	3893	1/1	0.94	0.24	52,52,52,52	0
88	MG	5	4562	1/1	0.94	0.11	40,40,40,40	0
88	MG	1	3829	1/1	0.94	0.22	84,84,84,84	0
87	OHX	5	3761	7/7	0.94	0.19	42,42,42,42	7
88	MG	1	4378	1/1	0.94	0.14	70,70,70,70	0
88	MG	5	3897	1/1	0.94	0.11	67,67,67,67	0
88	MG	5	4168	1/1	0.94	0.21	40,40,40,40	0
88	MG	6	2209	1/1	0.94	0.09	46,46,46,46	0
88	MG	1	4380	1/1	0.94	0.10	64,64,64,64	0
88	MG	7	216	1/1	0.94	0.38	43,43,43,43	0
88	MG	6	2211	1/1	0.94	0.06	50,50,50,50	0
87	OHX	1	3618	7/7	0.94	0.20	56,56,56,56	7
88	MG	7	220	1/1	0.94	0.08	41,41,41,41	0
87	OHX	5	3537	7/7	0.94	0.26	55,55,55,55	7
88	MG	7	223	1/1	0.94	0.07	55,55,55,55	0
88	MG	1	4213	1/1	0.94	0.26	39,39,39,39	1
88	MG	L4	408	1/1	0.94	0.22	34,34,34,34	1
88	MG	L7	302	1/1	0.94	0.09	44,44,44,44	0
87	OHX	6	1959	7/7	0.94	0.24	57,57,57,57	7
88	MG	1	4216	1/1	0.94	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4217	1/1	0.94	0.21	43,43,43,43	0
88	MG	5	4184	1/1	0.94	0.13	45,45,45,45	0
88	MG	M0	307	1/1	0.94	0.18	45,45,45,45	0
88	MG	1	3950	1/1	0.94	0.22	47,47,47,47	0
88	MG	5	3915	1/1	0.94	0.14	44,44,44,44	0
87	OHX	1	3519	7/7	0.94	0.18	95,95,95,95	7
88	MG	6	2227	1/1	0.94	0.11	52,52,52,52	0
88	MG	5	4195	1/1	0.94	0.14	41,41,41,41	0
88	MG	1	3837	1/1	0.94	0.14	55,55,55,55	0
88	MG	8	227	1/1	0.94	0.18	61,61,61,61	0
87	OHX	5	3704	7/7	0.94	0.26	43,43,43,43	7
87	OHX	6	2021	7/7	0.94	0.19	53,53,53,53	7
88	MG	M6	201	1/1	0.94	0.26	40,40,40,40	1
87	OHX	5	3550	7/7	0.94	0.18	57,57,57,57	7
88	MG	5	4204	1/1	0.94	0.30	32,32,32,32	0
88	MG	8	234	1/1	0.94	0.18	41,41,41,41	1
88	MG	1	3842	1/1	0.94	0.14	35,35,35,35	0
87	OHX	5	3553	7/7	0.94	0.19	49,49,49,49	7
88	MG	1	4403	1/1	0.94	0.42	47,47,47,47	1
88	MG	6	2237	1/1	0.94	0.17	55,55,55,55	0
87	OHX	6	1963	7/7	0.94	0.18	72,72,72,72	7
88	MG	6	2239	1/1	0.94	0.15	56,56,56,56	1
88	MG	l2	304	1/1	0.94	0.27	44,44,44,44	1
88	MG	N0	202	1/1	0.94	0.20	51,51,51,51	1
88	MG	5	4216	1/1	0.94	0.18	49,49,49,49	1
88	MG	1	4408	1/1	0.94	0.24	32,32,32,32	1
87	OHX	1	3525	7/7	0.94	0.24	66,66,66,66	7
88	MG	5	3938	1/1	0.94	0.20	40,40,40,40	0
88	MG	1	3846	1/1	0.94	0.16	37,37,37,37	0
88	MG	1	4413	1/1	0.94	0.17	44,44,44,44	1
88	MG	1	4231	1/1	0.94	0.13	49,49,49,49	1
87	OHX	3	207	7/7	0.94	0.14	85,85,85,85	7
88	MG	1	3848	1/1	0.94	0.31	30,30,30,30	0
88	MG	5	4227	1/1	0.94	0.17	35,35,35,35	1
88	MG	N8	204	1/1	0.94	0.10	48,48,48,48	0
88	MG	5	3946	1/1	0.94	0.40	36,36,36,36	0
88	MG	N8	206	1/1	0.94	0.24	39,39,39,39	0
88	MG	5	3950	1/1	0.94	0.25	40,40,40,40	0
87	OHX	6	1969	7/7	0.94	0.18	68,68,68,68	7
88	MG	6	2257	1/1	0.94	0.14	72,72,72,72	0
88	MG	l9	204	1/1	0.94	0.17	41,41,41,41	1
88	MG	1	4235	1/1	0.94	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4242	1/1	0.94	0.16	45,45,45,45	0
88	MG	1	3851	1/1	0.94	0.17	32,32,32,32	0
88	MG	m5	505	1/1	0.94	0.12	58,58,58,58	0
88	MG	m6	202	1/1	0.94	0.18	36,36,36,36	1
88	MG	5	4244	1/1	0.94	0.23	39,39,39,39	1
88	MG	m7	202	1/1	0.94	0.33	36,36,36,36	0
88	MG	1	3967	1/1	0.94	0.15	43,43,43,43	0
88	MG	1	4239	1/1	0.94	0.19	45,45,45,45	0
88	MG	5	4249	1/1	0.94	0.06	44,44,44,44	0
88	MG	5	4250	1/1	0.94	0.06	38,38,38,38	1
87	OHX	6	2026	7/7	0.94	0.10	151,151,151,151	7
88	MG	1	4244	1/1	0.94	0.26	55,55,55,55	0
87	OHX	5	3713	7/7	0.94	0.24	56,56,56,56	7
88	MG	O3	202	1/1	0.94	0.25	38,38,38,38	1
88	MG	n3	204	1/1	0.94	0.17	42,42,42,42	0
88	MG	1	4246	1/1	0.94	0.09	53,53,53,53	1
88	MG	1	4247	1/1	0.94	0.57	45,45,45,45	1
88	MG	5	4260	1/1	0.94	0.24	63,63,63,63	0
87	OHX	1	3595	7/7	0.94	0.21	42,42,42,42	7
88	MG	1	4102	1/1	0.94	0.11	45,45,45,45	0
87	OHX	1	3597	7/7	0.94	0.26	49,49,49,49	7
88	MG	o2	201	1/1	0.94	0.14	35,35,35,35	1
87	OHX	1	3624	7/7	0.94	0.15	74,74,74,74	7
88	MG	5	4268	1/1	0.94	0.20	48,48,48,48	0
88	MG	1	4443	1/1	0.94	0.15	44,44,44,44	0
88	MG	o3	203	1/1	0.94	0.10	40,40,40,40	1
88	MG	5	4271	1/1	0.94	0.48	36,36,36,36	1
88	MG	5	4273	1/1	0.94	0.14	35,35,35,35	1
87	OHX	2	1963	7/7	0.94	0.19	83,83,83,83	7
88	MG	1	4256	1/1	0.94	0.08	40,40,40,40	0
88	MG	1	4106	1/1	0.94	0.29	51,51,51,51	0
88	MG	1	4259	1/1	0.94	0.06	45,45,45,45	1
87	OHX	1	3527	7/7	0.94	0.23	49,49,49,49	7
88	MG	6	2285	1/1	0.94	0.21	68,68,68,68	1
88	MG	6	2246	1/1	0.95	0.11	50,50,50,50	1
87	OHX	2	1932	7/7	0.95	0.12	92,92,92,92	7
88	MG	5	4277	1/1	0.95	0.44	44,44,44,44	1
87	OHX	1	3583	7/7	0.95	0.18	77,77,77,77	7
88	MG	5	4283	1/1	0.95	0.16	39,39,39,39	1
88	MG	L7	303	1/1	0.95	0.11	42,42,42,42	0
88	MG	1	4349	1/1	0.95	0.10	59,59,59,59	0
87	OHX	1	3585	7/7	0.95	0.18	50,50,50,50	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	3539	7/7	0.95	0.21	60,60,60,60	7
88	MG	5	4290	1/1	0.95	0.09	39,39,39,39	0
87	OHX	5	3540	7/7	0.95	0.16	99,99,99,99	7
87	OHX	5	3673	7/7	0.95	0.18	48,48,48,48	7
87	OHX	1	3654	7/7	0.95	0.20	49,49,49,49	7
88	MG	5	4296	1/1	0.95	0.09	32,32,32,32	0
88	MG	5	3975	1/1	0.95	0.26	48,48,48,48	0
88	MG	2	2141	1/1	0.95	0.23	67,67,67,67	0
87	OHX	1	3512	7/7	0.95	0.17	65,65,65,65	7
87	OHX	5	3547	7/7	0.95	0.16	66,66,66,66	7
87	OHX	5	3548	7/7	0.95	0.18	47,47,47,47	7
87	OHX	5	3549	7/7	0.95	0.14	84,84,84,84	7
87	OHX	1	3513	7/7	0.95	0.23	61,61,61,61	7
88	MG	1	4154	1/1	0.95	0.37	42,42,42,42	1
88	MG	M7	205	1/1	0.95	0.20	42,42,42,42	0
88	MG	M7	209	1/1	0.95	0.09	42,42,42,42	0
87	OHX	5	3552	7/7	0.95	0.14	107,107,107,107	7
88	MG	5	4316	1/1	0.95	0.23	35,35,35,35	1
88	MG	1	4156	1/1	0.95	0.12	46,46,46,46	0
88	MG	M9	205	1/1	0.95	0.19	68,68,68,68	1
88	MG	6	2276	1/1	0.95	0.25	40,40,40,40	0
87	OHX	2	1969	7/7	0.95	0.16	62,62,62,62	7
88	MG	1	4158	1/1	0.95	0.07	42,42,42,42	0
87	OHX	5	3555	7/7	0.95	0.22	53,53,53,53	7
88	MG	1	4160	1/1	0.95	0.22	62,62,62,62	0
88	MG	6	2282	1/1	0.95	0.24	55,55,55,55	0
88	MG	1	4162	1/1	0.95	0.14	36,36,36,36	0
88	MG	1	3983	1/1	0.95	0.17	40,40,40,40	0
88	MG	5	4329	1/1	0.95	0.10	43,43,43,43	0
88	MG	1	4166	1/1	0.95	0.18	45,45,45,45	0
88	MG	6	2286	1/1	0.95	0.17	65,65,65,65	0
87	OHX	5	3683	7/7	0.95	0.24	46,46,46,46	7
88	MG	5	4005	1/1	0.95	0.21	38,38,38,38	0
87	OHX	2	1933	7/7	0.95	0.22	71,71,71,71	7
88	MG	5	4007	1/1	0.95	0.20	33,33,33,33	0
88	MG	N8	205	1/1	0.95	0.18	31,31,31,31	1
88	MG	6	2291	1/1	0.95	0.07	65,65,65,65	0
88	MG	1	3822	1/1	0.95	0.18	43,43,43,43	0
88	MG	6	2293	1/1	0.95	0.20	46,46,46,46	1
88	MG	1	4170	1/1	0.95	0.35	35,35,35,35	0
88	MG	5	4015	1/1	0.95	0.51	30,30,30,30	0
88	MG	N8	208	1/1	0.95	0.16	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	6	2297	1/1	0.95	0.19	70,70,70,70	1
88	MG	6	2298	1/1	0.95	0.12	86,86,86,86	0
87	OHX	5	3558	7/7	0.95	0.20	51,51,51,51	7
87	OHX	5	3559	7/7	0.95	0.15	93,93,93,93	7
88	MG	1	3825	1/1	0.95	0.12	58,58,58,58	0
87	OHX	5	3803	7/7	0.95	0.10	147,147,147,147	7
88	MG	1	3994	1/1	0.95	0.24	27,27,27,27	0
88	MG	5	4025	1/1	0.95	0.24	26,26,26,26	0
87	OHX	6	1950	7/7	0.95	0.11	100,100,100,100	7
87	OHX	6	1953	7/7	0.95	0.09	137,137,137,137	7
87	OHX	6	1954	7/7	0.95	0.10	149,149,149,149	7
88	MG	6	2309	1/1	0.95	0.24	65,65,65,65	0
88	MG	6	2311	1/1	0.95	0.07	60,60,60,60	1
87	OHX	5	3564	7/7	0.95	0.25	53,53,53,53	7
87	OHX	1	3521	7/7	0.95	0.27	44,44,44,44	7
87	OHX	1	3596	7/7	0.95	0.18	68,68,68,68	7
88	MG	5	4371	1/1	0.95	0.17	61,61,61,61	0
87	OHX	6	1962	7/7	0.95	0.21	62,62,62,62	7
88	MG	5	4375	1/1	0.95	0.12	37,37,37,37	1
88	MG	5	4376	1/1	0.95	0.09	45,45,45,45	0
87	OHX	5	3570	7/7	0.95	0.19	53,53,53,53	7
88	MG	1	3836	1/1	0.95	0.20	43,43,43,43	0
87	OHX	2	1972	7/7	0.95	0.20	81,81,81,81	7
88	MG	1	4405	1/1	0.95	0.15	46,46,46,46	0
88	MG	5	4043	1/1	0.95	0.10	40,40,40,40	1
88	MG	6	2322	1/1	0.95	0.13	62,62,62,62	0
87	OHX	5	3572	7/7	0.95	0.18	56,56,56,56	7
87	OHX	2	2073	7/7	0.95	0.18	89,89,89,89	7
88	MG	5	4389	1/1	0.95	0.15	34,34,34,34	0
88	MG	5	4048	1/1	0.95	0.20	39,39,39,39	0
87	OHX	1	3663	7/7	0.95	0.18	49,49,49,49	7
88	MG	Q2	505	1/1	0.95	0.09	45,45,45,45	1
88	MG	6	2329	1/1	0.95	0.08	48,48,48,48	0
88	MG	6	2330	1/1	0.95	0.27	55,55,55,55	1
88	MG	5	4053	1/1	0.95	0.07	45,45,45,45	0
88	MG	5	4397	1/1	0.95	0.24	48,48,48,48	0
88	MG	1	4412	1/1	0.95	0.21	60,60,60,60	0
87	OHX	7	205	7/7	0.95	0.21	68,68,68,68	7
88	MG	1	4414	1/1	0.95	0.16	60,60,60,60	1
88	MG	1	4415	1/1	0.95	0.13	34,34,34,34	1
88	MG	5	4407	1/1	0.95	0.09	55,55,55,55	0
87	OHX	2	1973	7/7	0.95	0.15	103,103,103,103	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4016	1/1	0.95	0.33	32,32,32,32	0
87	OHX	5	3578	7/7	0.95	0.19	67,67,67,67	7
88	MG	5	4062	1/1	0.95	0.12	53,53,53,53	0
88	MG	1	4018	1/1	0.95	0.35	22,22,22,22	0
88	MG	5	4413	1/1	0.95	0.13	56,56,56,56	0
87	OHX	2	2023	7/7	0.95	0.15	71,71,71,71	7
88	MG	5	4065	1/1	0.95	0.12	50,50,50,50	0
87	OHX	6	1976	7/7	0.95	0.11	95,95,95,95	7
87	OHX	1	3790	7/7	0.95	0.18	68,68,68,68	7
88	MG	5	4069	1/1	0.95	0.08	36,36,36,36	0
88	MG	c7	201	1/1	0.95	0.14	81,81,81,81	1
87	OHX	8	204	7/7	0.95	0.17	66,66,66,66	7
87	OHX	1	3529	7/7	0.95	0.09	129,129,129,129	7
87	OHX	1	3530	7/7	0.95	0.19	65,65,65,65	7
88	MG	1	4027	1/1	0.95	0.31	44,44,44,44	0
87	OHX	8	209	7/7	0.95	0.18	88,88,88,88	7
87	OHX	5	3588	7/7	0.95	0.18	63,63,63,63	7
88	MG	5	4439	1/1	0.95	0.12	32,32,32,32	0
88	MG	5	4077	1/1	0.95	0.15	48,48,48,48	0
87	OHX	1	3730	7/7	0.95	0.20	52,52,52,52	7
88	MG	5	4442	1/1	0.95	0.14	45,45,45,45	0
88	MG	1	3857	1/1	0.95	0.19	40,40,40,40	0
87	OHX	6	1983	7/7	0.95	0.16	95,95,95,95	7
88	MG	1	4221	1/1	0.95	0.20	37,37,37,37	1
88	MG	d4	202	1/1	0.95	0.12	55,55,55,55	0
87	OHX	2	1931	7/7	0.95	0.12	116,116,116,116	7
88	MG	5	4454	1/1	0.95	0.23	38,38,38,38	1
87	OHX	5	3593	7/7	0.95	0.22	46,46,46,46	7
88	MG	2	2184	1/1	0.95	0.12	59,59,59,59	0
87	OHX	5	3595	7/7	0.95	0.18	56,56,56,56	7
88	MG	sM	202	1/1	0.95	0.09	44,44,44,44	0
88	MG	5	4090	1/1	0.95	0.17	52,52,52,52	0
88	MG	5	4467	1/1	0.95	0.12	55,55,55,55	0
88	MG	1	4452	1/1	0.95	0.18	56,56,56,56	1
88	MG	6	2126	1/1	0.95	0.31	43,43,43,43	0
87	OHX	5	3596	7/7	0.95	0.20	57,57,57,57	7
88	MG	1	3867	1/1	0.95	0.22	46,46,46,46	0
87	OHX	1	3533	7/7	0.95	0.10	112,112,112,112	7
88	MG	5	4474	1/1	0.95	0.23	33,33,33,33	0
87	OHX	1	3607	7/7	0.95	0.25	42,42,42,42	7
88	MG	1	4230	1/1	0.95	0.08	51,51,51,51	0
87	OHX	5	3599	7/7	0.95	0.18	43,43,43,43	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	1951	7/7	0.95	0.19	87,87,87,87	7
87	OHX	12	301	7/7	0.95	0.20	63,63,63,63	7
87	OHX	2	2026	7/7	0.95	0.18	93,93,93,93	7
87	OHX	2	1952	7/7	0.95	0.09	131,131,131,131	7
88	MG	5	4105	1/1	0.95	0.08	40,40,40,40	0
87	OHX	2	1954	7/7	0.95	0.17	88,88,88,88	7
88	MG	5	4497	1/1	0.95	0.14	33,33,33,33	1
88	MG	6	2140	1/1	0.95	0.28	44,44,44,44	0
87	OHX	2	1938	7/7	0.95	0.20	70,70,70,70	7
88	MG	5	4501	1/1	0.95	0.24	49,49,49,49	0
88	MG	1	4238	1/1	0.95	0.18	37,37,37,37	0
88	MG	1	4056	1/1	0.95	0.06	44,44,44,44	0
88	MG	1	4057	1/1	0.95	0.14	32,32,32,32	0
88	MG	1	4242	1/1	0.95	0.14	41,41,41,41	1
88	MG	5	4511	1/1	0.95	0.10	34,34,34,34	0
88	MG	5	4116	1/1	0.95	0.28	39,39,39,39	0
88	MG	1	4058	1/1	0.95	0.07	33,33,33,33	1
88	MG	5	4120	1/1	0.95	0.20	57,57,57,57	0
88	MG	5	4519	1/1	0.95	0.16	43,43,43,43	1
87	OHX	1	3544	7/7	0.95	0.23	59,59,59,59	7
88	MG	5	4521	1/1	0.95	0.08	41,41,41,41	0
88	MG	5	4123	1/1	0.95	0.09	44,44,44,44	1
87	OHX	1	3614	7/7	0.95	0.14	78,78,78,78	7
88	MG	2	2199	1/1	0.95	0.17	81,81,81,81	0
88	MG	1	3884	1/1	0.95	0.22	66,66,66,66	0
88	MG	5	4128	1/1	0.95	0.17	33,33,33,33	1
88	MG	1	4249	1/1	0.95	0.23	66,66,66,66	0
88	MG	1	4478	1/1	0.95	0.24	46,46,46,46	0
87	OHX	1	3742	7/7	0.95	0.13	71,71,71,71	7
88	MG	5	4132	1/1	0.95	0.26	48,48,48,48	0
87	OHX	1	3805	7/7	0.95	0.15	83,83,83,83	7
88	MG	5	3851	1/1	0.95	0.19	36,36,36,36	0
87	OHX	1	3545	7/7	0.95	0.23	54,54,54,54	7
87	OHX	2	1982	7/7	0.95	0.12	100,100,100,100	7
88	MG	6	2159	1/1	0.95	0.41	45,45,45,45	0
88	MG	6	2160	1/1	0.95	0.34	59,59,59,59	0
88	MG	5	3860	1/1	0.95	0.13	35,35,35,35	0
88	MG	5	4143	1/1	0.95	0.15	36,36,36,36	0
87	OHX	5	3612	7/7	0.95	0.24	46,46,46,46	7
88	MG	5	4556	1/1	0.95	0.11	40,40,40,40	0
88	MG	1	4257	1/1	0.95	0.15	41,41,41,41	1
88	MG	1	4485	1/1	0.95	0.32	56,56,56,56	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	6	2165	1/1	0.95	0.11	45,45,45,45	0
87	OHX	2	1957	7/7	0.95	0.16	79,79,79,79	7
87	OHX	5	3614	7/7	0.95	0.23	52,52,52,52	7
88	MG	5	4564	1/1	0.95	0.16	38,38,38,38	1
88	MG	6	2168	1/1	0.95	0.14	59,59,59,59	0
87	OHX	5	3615	7/7	0.95	0.27	38,38,38,38	7
88	MG	5	4569	1/1	0.95	0.12	30,30,30,30	0
88	MG	5	4570	1/1	0.95	0.09	49,49,49,49	0
87	OHX	2	1940	7/7	0.95	0.15	85,85,85,85	7
88	MG	5	4155	1/1	0.95	0.18	37,37,37,37	0
88	MG	1	4265	1/1	0.95	0.12	68,68,68,68	0
88	MG	5	4157	1/1	0.95	0.18	38,38,38,38	0
87	OHX	1	3550	7/7	0.95	0.15	78,78,78,78	7
88	MG	1	4076	1/1	0.95	0.24	51,51,51,51	0
88	MG	5	3877	1/1	0.95	0.15	41,41,41,41	0
88	MG	5	3878	1/1	0.95	0.11	37,37,37,37	0
87	OHX	o3	201	7/7	0.95	0.26	51,51,51,51	7
88	MG	1	3902	1/1	0.95	0.19	42,42,42,42	1
88	MG	7	222	1/1	0.95	0.14	52,52,52,52	0
87	OHX	2	1943	7/7	0.95	0.16	95,95,95,95	7
87	OHX	2	1962	7/7	0.95	0.15	97,97,97,97	7
88	MG	1	4275	1/1	0.95	0.08	58,58,58,58	0
88	MG	5	3884	1/1	0.95	0.08	37,37,37,37	0
87	OHX	3	203	7/7	0.95	0.24	56,56,56,56	7
88	MG	7	229	1/1	0.95	0.39	37,37,37,37	1
88	MG	7	230	1/1	0.95	0.10	43,43,43,43	0
88	MG	5	4173	1/1	0.95	0.21	42,42,42,42	0
87	OHX	3	204	7/7	0.95	0.17	85,85,85,85	7
88	MG	5	3888	1/1	0.95	0.23	46,46,46,46	0
87	OHX	1	3687	7/7	0.95	0.19	67,67,67,67	7
88	MG	7	236	1/1	0.95	0.21	53,53,53,53	1
87	OHX	2	1987	7/7	0.95	0.17	75,75,75,75	7
87	OHX	5	3626	7/7	0.95	0.14	75,75,75,75	7
88	MG	1	4282	1/1	0.95	0.20	40,40,40,40	0
88	MG	6	2186	1/1	0.95	0.18	53,53,53,53	0
87	OHX	2	2037	7/7	0.95	0.16	60,60,60,60	7
88	MG	1	3915	1/1	0.95	0.20	42,42,42,42	0
87	OHX	S2	301	7/7	0.95	0.17	81,81,81,81	7
88	MG	8	228	1/1	0.95	0.27	46,46,46,46	1
88	MG	1	4286	1/1	0.95	0.22	40,40,40,40	1
88	MG	1	4287	1/1	0.95	0.17	41,41,41,41	0
87	OHX	2	1946	7/7	0.95	0.12	110,110,110,110	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	1965	7/7	0.95	0.14	91,91,91,91	7
87	OHX	6	2090	7/7	0.95	0.15	68,68,68,68	7
88	MG	5	4196	1/1	0.95	0.27	43,43,43,43	1
88	MG	3	217	1/1	0.95	0.30	36,36,36,36	0
88	MG	5	3903	1/1	0.95	0.26	28,28,28,28	0
88	MG	5	4200	1/1	0.95	0.24	60,60,60,60	0
87	OHX	1	3630	7/7	0.95	0.07	121,121,121,121	7
88	MG	2	2226	1/1	0.95	0.11	76,76,76,76	0
87	OHX	4	207	7/7	0.95	0.20	61,61,61,61	7
87	OHX	2	2013	7/7	0.95	0.08	158,158,158,158	7
88	MG	1	4297	1/1	0.95	0.11	52,52,52,52	0
87	OHX	1	3696	7/7	0.95	0.33	47,47,47,47	7
88	MG	1	3926	1/1	0.95	0.12	41,41,41,41	0
87	OHX	1	3564	7/7	0.95	0.14	79,79,79,79	7
87	OHX	6	2020	7/7	0.95	0.15	49,49,49,49	7
87	OHX	2	1991	7/7	0.95	0.10	104,104,104,104	7
87	OHX	2	1967	7/7	0.95	0.18	92,92,92,92	7
88	MG	5	3918	1/1	0.95	0.17	33,33,33,33	0
88	MG	5	4217	1/1	0.95	0.21	54,54,54,54	0
87	OHX	1	3568	7/7	0.95	0.13	95,95,95,95	7
88	MG	5	3920	1/1	0.95	0.15	42,42,42,42	0
88	MG	5	3921	1/1	0.95	0.16	43,43,43,43	1
88	MG	17	301	1/1	0.95	0.23	36,36,36,36	1
87	OHX	1	3569	7/7	0.95	0.26	58,58,58,58	7
87	OHX	1	3469	7/7	0.95	0.18	60,60,60,60	7
88	MG	17	305	1/1	0.95	0.10	40,40,40,40	0
88	MG	5	3924	1/1	0.95	0.26	38,38,38,38	0
87	OHX	1	3571	7/7	0.95	0.22	47,47,47,47	7
88	MG	2	2241	1/1	0.95	0.25	60,60,60,60	0
87	OHX	1	3573	7/7	0.95	0.14	114,114,114,114	7
87	OHX	1	3641	7/7	0.95	0.21	58,58,58,58	7
87	OHX	d9	102	7/7	0.95	0.12	97,97,97,97	7
87	OHX	1	3486	7/7	0.95	0.26	54,54,54,54	7
88	MG	m5	504	1/1	0.95	0.08	45,45,45,45	0
88	MG	5	4235	1/1	0.95	0.36	34,34,34,34	1
88	MG	5	4236	1/1	0.95	0.25	37,37,37,37	1
87	OHX	5	3502	7/7	0.95	0.24	41,41,41,41	7
87	OHX	1	3498	7/7	0.95	0.20	63,63,63,63	7
88	MG	4	228	1/1	0.95	0.28	66,66,66,66	0
87	OHX	1	3708	7/7	0.95	0.19	62,62,62,62	7
87	OHX	5	3508	7/7	0.95	0.23	69,69,69,69	7
88	MG	m8	1504	1/1	0.95	0.32	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	6	2224	1/1	0.95	0.11	47,47,47,47	0
87	OHX	5	3511	7/7	0.95	0.25	40,40,40,40	7
88	MG	n0	204	1/1	0.95	0.26	45,45,45,45	0
87	OHX	5	3517	7/7	0.95	0.17	56,56,56,56	7
88	MG	5	4247	1/1	0.95	0.06	51,51,51,51	0
87	OHX	2	2068	7/7	0.95	0.22	66,66,66,66	7
88	MG	1	4332	1/1	0.95	0.13	43,43,43,43	0
87	OHX	5	3521	7/7	0.95	0.28	42,42,42,42	7
88	MG	1	4334	1/1	0.95	0.31	37,37,37,37	1
88	MG	n8	202	1/1	0.95	0.13	51,51,51,51	0
87	OHX	1	3772	7/7	0.95	0.17	59,59,59,59	7
87	OHX	5	3525	7/7	0.95	0.18	51,51,51,51	7
88	MG	5	4256	1/1	0.95	0.14	59,59,59,59	0
88	MG	n8	207	1/1	0.95	0.12	39,39,39,39	1
88	MG	5	3949	1/1	0.95	0.38	45,45,45,45	0
88	MG	n9	103	1/1	0.95	0.17	40,40,40,40	1
88	MG	1	4130	1/1	0.95	0.04	49,49,49,49	1
88	MG	4	241	1/1	0.95	0.19	45,45,45,45	0
87	OHX	1	3506	7/7	0.95	0.15	93,93,93,93	7
87	OHX	5	3528	7/7	0.95	0.20	38,38,38,38	7
88	MG	5	4262	1/1	0.95	0.21	42,42,42,42	1
88	MG	2	2259	1/1	0.95	0.15	74,74,74,74	1
88	MG	L2	301	1/1	0.95	0.13	39,39,39,39	0
88	MG	q1	102	1/1	0.95	0.19	43,43,43,43	0
87	OHX	5	3664	7/7	0.95	0.25	39,39,39,39	7
87	OHX	5	3531	7/7	0.95	0.24	42,42,42,42	7
88	MG	5	4269	1/1	0.95	0.12	34,34,34,34	1
87	OHX	5	3666	7/7	0.95	0.21	51,51,51,51	7
87	OHX	1	3649	7/7	0.95	0.17	59,59,59,59	7
88	MG	5	3964	1/1	0.95	0.22	27,27,27,27	0
88	MG	5	4354	1/1	0.96	0.10	54,54,54,54	0
88	MG	5	4066	1/1	0.96	0.12	49,49,49,49	0
87	OHX	1	3651	7/7	0.96	0.17	64,64,64,64	7
88	MG	5	3826	1/1	0.96	0.23	31,31,31,31	0
87	OHX	2	1970	7/7	0.96	0.16	89,89,89,89	7
87	OHX	1	3505	7/7	0.96	0.24	42,42,42,42	7
88	MG	1	3916	1/1	0.96	0.18	52,52,52,52	0
87	OHX	5	3523	7/7	0.96	0.18	49,49,49,49	7
88	MG	1	4088	1/1	0.96	0.28	42,42,42,42	0
87	OHX	6	1965	7/7	0.96	0.14	83,83,83,83	7
87	OHX	1	3554	7/7	0.96	0.16	62,62,62,62	7
88	MG	5	3835	1/1	0.96	0.20	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	OHX	2	1997	7/7	0.96	0.14	88,88,88,88	7
88	MG	2	2233	1/1	0.96	0.20	72,72,72,72	0
88	MG	5	3838	1/1	0.96	0.13	45,45,45,45	0
88	MG	5	4374	1/1	0.96	0.14	55,55,55,55	0
88	MG	6	2162	1/1	0.96	0.29	53,53,53,53	0
88	MG	5	3840	1/1	0.96	0.14	36,36,36,36	0
88	MG	5	3841	1/1	0.96	0.24	46,46,46,46	0
87	OHX	5	3529	7/7	0.96	0.16	47,47,47,47	7
88	MG	5	4379	1/1	0.96	0.11	53,53,53,53	0
87	OHX	2	1944	7/7	0.96	0.18	72,72,72,72	7
87	OHX	1	3605	7/7	0.96	0.21	49,49,49,49	7
87	OHX	5	3533	7/7	0.96	0.10	114,114,114,114	7
87	OHX	5	3534	7/7	0.96	0.20	42,42,42,42	7
88	MG	5	4386	1/1	0.96	0.10	39,39,39,39	1
87	OHX	6	1974	7/7	0.96	0.16	67,67,67,67	7
87	OHX	5	3655	7/7	0.96	0.14	58,58,58,58	7
88	MG	2	2243	1/1	0.96	0.09	61,61,61,61	0
88	MG	1	3930	1/1	0.96	0.15	40,40,40,40	0
88	MG	1	3931	1/1	0.96	0.35	32,32,32,32	0
87	OHX	1	3606	7/7	0.96	0.09	110,110,110,110	7
87	OHX	1	3509	7/7	0.96	0.21	49,49,49,49	7
88	MG	5	3857	1/1	0.96	0.16	36,36,36,36	0
87	OHX	1	3558	7/7	0.96	0.18	71,71,71,71	7
87	OHX	2	1927	7/7	0.96	0.15	94,94,94,94	7
88	MG	1	4108	1/1	0.96	0.12	48,48,48,48	0
88	MG	5	4101	1/1	0.96	0.16	38,38,38,38	0
88	MG	5	4401	1/1	0.96	0.08	70,70,70,70	1
88	MG	5	4402	1/1	0.96	0.16	37,37,37,37	0
87	OHX	5	3543	7/7	0.96	0.09	136,136,136,136	7
87	OHX	2	2014	7/7	0.96	0.12	80,80,80,80	7
87	OHX	1	3516	7/7	0.96	0.18	52,52,52,52	7
87	OHX	5	3663	7/7	0.96	0.18	41,41,41,41	7
88	MG	1	3941	1/1	0.96	0.15	43,43,43,43	0
88	MG	6	2183	1/1	0.96	0.16	54,54,54,54	1
88	MG	5	4109	1/1	0.96	0.07	39,39,39,39	0
88	MG	5	3871	1/1	0.96	0.21	31,31,31,31	0
87	OHX	1	3713	7/7	0.96	0.16	50,50,50,50	7
88	MG	5	4113	1/1	0.96	0.16	46,46,46,46	0
87	OHX	1	3664	7/7	0.96	0.17	50,50,50,50	7
87	OHX	6	1987	7/7	0.96	0.15	70,70,70,70	7
87	OHX	2	1953	7/7	0.96	0.12	64,64,64,64	7
87	OHX	5	3551	7/7	0.96	0.18	60,60,60,60	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	1941	7/7	0.96	0.11	92,92,92,92	7
87	OHX	1	3565	7/7	0.96	0.13	79,79,79,79	7
87	OHX	6	1991	7/7	0.96	0.12	83,83,83,83	7
88	MG	5	4124	1/1	0.96	0.12	40,40,40,40	0
87	OHX	5	3784	7/7	0.96	0.18	58,58,58,58	7
88	MG	5	4428	1/1	0.96	0.09	36,36,36,36	1
88	MG	5	4429	1/1	0.96	0.17	45,45,45,45	1
88	MG	1	3952	1/1	0.96	0.32	40,40,40,40	0
88	MG	5	4432	1/1	0.96	0.08	39,39,39,39	0
88	MG	S2	302	1/1	0.96	0.10	75,75,75,75	0
88	MG	1	4322	1/1	0.96	0.14	42,42,42,42	0
87	OHX	1	3520	7/7	0.96	0.16	55,55,55,55	7
87	OHX	2	2017	7/7	0.96	0.10	108,108,108,108	7
87	OHX	1	3522	7/7	0.96	0.21	47,47,47,47	7
87	OHX	6	1995	7/7	0.96	0.11	113,113,113,113	7
88	MG	C1	202	1/1	0.96	0.13	72,72,72,72	1
88	MG	4	222	1/1	0.96	0.31	32,32,32,32	0
87	OHX	1	3523	7/7	0.96	0.15	81,81,81,81	7
87	OHX	1	3524	7/7	0.96	0.15	68,68,68,68	7
87	OHX	5	3563	7/7	0.96	0.22	39,39,39,39	7
88	MG	1	3962	1/1	0.96	0.15	41,41,41,41	0
88	MG	5	4141	1/1	0.96	0.16	49,49,49,49	0
87	OHX	2	1964	7/7	0.96	0.14	101,101,101,101	7
88	MG	1	4139	1/1	0.96	0.12	54,54,54,54	0
88	MG	1	4337	1/1	0.96	0.17	38,38,38,38	1
87	OHX	2	2035	7/7	0.96	0.13	95,95,95,95	7
87	OHX	2	1977	7/7	0.96	0.08	138,138,138,138	7
87	OHX	1	3576	7/7	0.96	0.14	89,89,89,89	7
87	OHX	2	2054	7/7	0.96	0.14	87,87,87,87	7
87	OHX	2	1990	7/7	0.96	0.10	111,111,111,111	7
87	OHX	2	1942	7/7	0.96	0.14	74,74,74,74	7
87	OHX	5	3799	7/7	0.96	0.21	69,69,69,69	7
88	MG	5	3905	1/1	0.96	0.14	49,49,49,49	0
88	MG	5	4476	1/1	0.96	0.16	50,50,50,50	1
88	MG	1	3813	1/1	0.96	0.28	40,40,40,40	0
88	MG	1	3814	1/1	0.96	0.20	58,58,58,58	0
88	MG	5	3908	1/1	0.96	0.16	40,40,40,40	0
87	OHX	D9	102	7/7	0.96	0.12	83,83,83,83	7
88	MG	5	4483	1/1	0.96	0.08	37,37,37,37	0
88	MG	5	4484	1/1	0.96	0.10	46,46,46,46	0
87	OHX	5	3801	7/7	0.96	0.15	88,88,88,88	7
87	OHX	5	3687	7/7	0.96	0.21	54,54,54,54	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	L3	401	7/7	0.96	0.15	56,56,56,56	7
88	MG	5	4494	1/1	0.96	0.15	45,45,45,45	1
88	MG	5	4162	1/1	0.96	0.19	44,44,44,44	0
88	MG	5	4496	1/1	0.96	0.19	54,54,54,54	0
88	MG	6	2225	1/1	0.96	0.32	55,55,55,55	0
87	OHX	1	3582	7/7	0.96	0.16	50,50,50,50	7
88	MG	5	4166	1/1	0.96	0.12	36,36,36,36	1
87	OHX	5	3577	7/7	0.96	0.16	46,46,46,46	7
88	MG	L2	302	1/1	0.96	0.20	46,46,46,46	0
88	MG	2	2153	1/1	0.96	0.11	72,72,72,72	0
87	OHX	2	1923	7/7	0.96	0.14	80,80,80,80	7
87	OHX	1	3584	7/7	0.96	0.18	47,47,47,47	7
88	MG	L4	405	1/1	0.96	0.26	38,38,38,38	1
87	OHX	2	2076	7/7	0.96	0.10	122,122,122,122	7
87	OHX	5	3582	7/7	0.96	0.15	83,83,83,83	7
88	MG	5	4176	1/1	0.96	0.15	51,51,51,51	0
88	MG	5	4517	1/1	0.96	0.28	59,59,59,59	0
87	OHX	1	3685	7/7	0.96	0.17	55,55,55,55	7
87	OHX	5	3584	7/7	0.96	0.19	43,43,43,43	7
87	OHX	1	3587	7/7	0.96	0.10	90,90,90,90	7
88	MG	5	4180	1/1	0.96	0.11	40,40,40,40	1
88	MG	1	3991	1/1	0.96	0.18	36,36,36,36	0
88	MG	1	3992	1/1	0.96	0.25	32,32,32,32	0
87	OHX	1	3737	7/7	0.96	0.20	56,56,56,56	7
88	MG	5	4530	1/1	0.96	0.12	54,54,54,54	0
87	OHX	M5	301	7/7	0.96	0.17	75,75,75,75	7
88	MG	1	4367	1/1	0.96	0.07	43,43,43,43	1
88	MG	5	4533	1/1	0.96	0.15	38,38,38,38	0
88	MG	5	3933	1/1	0.96	0.34	33,33,33,33	0
88	MG	5	4189	1/1	0.96	0.12	39,39,39,39	1
88	MG	5	4538	1/1	0.96	0.21	45,45,45,45	0
88	MG	M3	201	1/1	0.96	0.11	45,45,45,45	0
87	OHX	1	3588	7/7	0.96	0.20	52,52,52,52	7
87	OHX	7	203	7/7	0.96	0.21	54,54,54,54	7
88	MG	1	4173	1/1	0.96	0.12	49,49,49,49	1
88	MG	1	4372	1/1	0.96	0.26	34,34,34,34	1
88	MG	M6	203	1/1	0.96	0.35	40,40,40,40	1
88	MG	1	3997	1/1	0.96	0.34	28,28,28,28	0
87	OHX	2	1958	7/7	0.96	0.18	75,75,75,75	7
87	OHX	7	206	7/7	0.96	0.16	67,67,67,67	7
88	MG	5	4554	1/1	0.96	0.10	50,50,50,50	1
88	MG	1	4000	1/1	0.96	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
88	MG	M7	206	1/1	0.96	0.16	43,43,43,43	0
88	MG	M7	207	1/1	0.96	0.18	43,43,43,43	0
88	MG	5	3947	1/1	0.96	0.34	39,39,39,39	0
87	OHX	7	207	7/7	0.96	0.17	78,78,78,78	7
88	MG	1	4381	1/1	0.96	0.10	32,32,32,32	1
88	MG	6	2265	1/1	0.96	0.10	48,48,48,48	0
88	MG	5	3951	1/1	0.96	0.30	32,32,32,32	0
88	MG	M8	203	1/1	0.96	0.16	41,41,41,41	0
88	MG	5	4566	1/1	0.96	0.27	50,50,50,50	0
88	MG	M8	204	1/1	0.96	0.19	46,46,46,46	1
87	OHX	1	3590	7/7	0.96	0.15	74,74,74,74	7
87	OHX	1	3477	7/7	0.96	0.13	88,88,88,88	7
88	MG	6	2270	1/1	0.96	0.16	61,61,61,61	0
88	MG	1	4181	1/1	0.96	0.15	40,40,40,40	1
88	MG	5	4220	1/1	0.96	0.18	38,38,38,38	0
88	MG	1	4387	1/1	0.96	0.10	37,37,37,37	1
87	OHX	5	3594	7/7	0.96	0.14	73,73,73,73	7
87	OHX	1	3482	7/7	0.96	0.20	65,65,65,65	7
88	MG	5	3963	1/1	0.96	0.30	28,28,28,28	0
88	MG	1	4186	1/1	0.96	0.10	65,65,65,65	0
87	OHX	1	3484	7/7	0.96	0.19	49,49,49,49	7
88	MG	N6	202	1/1	0.96	0.07	58,58,58,58	1
88	MG	5	4228	1/1	0.96	0.14	35,35,35,35	1
87	OHX	8	203	7/7	0.96	0.16	86,86,86,86	7
87	OHX	1	3643	7/7	0.96	0.17	64,64,64,64	7
87	OHX	8	205	7/7	0.96	0.18	64,64,64,64	7
88	MG	5	4234	1/1	0.96	0.08	33,33,33,33	1
88	MG	1	4397	1/1	0.96	0.21	36,36,36,36	1
87	OHX	O7	102	7/7	0.96	0.17	73,73,73,73	7
87	OHX	Q2	502	7/7	0.96	0.20	45,45,45,45	7
88	MG	1	4014	1/1	0.96	0.32	30,30,30,30	0
87	OHX	6	1921	7/7	0.96	0.20	51,51,51,51	7
87	OHX	6	1925	7/7	0.96	0.11	87,87,87,87	7
87	OHX	5	3602	7/7	0.96	0.13	74,74,74,74	7
87	OHX	6	2098	7/7	0.96	0.10	113,113,113,113	7
88	MG	7	237	1/1	0.96	0.10	51,51,51,51	1
87	OHX	6	1931	7/7	0.96	0.18	71,71,71,71	7
88	MG	1	3856	1/1	0.96	0.23	49,49,49,49	0
88	MG	8	222	1/1	0.96	0.17	41,41,41,41	0
87	OHX	6	1938	7/7	0.96	0.13	69,69,69,69	7
88	MG	1	4208	1/1	0.96	0.15	41,41,41,41	1
88	MG	1	4209	1/1	0.96	0.31	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	3983	1/1	0.96	0.26	45,45,45,45	0
88	MG	1	3858	1/1	0.96	0.15	41,41,41,41	0
88	MG	5	3985	1/1	0.96	0.26	32,32,32,32	0
87	OHX	6	1939	7/7	0.96	0.16	103,103,103,103	7
88	MG	5	4255	1/1	0.96	0.07	54,54,54,54	0
87	OHX	6	1940	7/7	0.96	0.15	64,64,64,64	7
87	OHX	1	3694	7/7	0.96	0.17	51,51,51,51	7
87	OHX	2	1959	7/7	0.96	0.08	127,127,127,127	7
87	OHX	6	1949	7/7	0.96	0.16	73,73,73,73	7
88	MG	6	2303	1/1	0.96	0.08	78,78,78,78	0
87	OHX	1	3487	7/7	0.96	0.10	118,118,118,118	7
88	MG	O7	109	1/1	0.96	0.33	46,46,46,46	1
87	OHX	2	1995	7/7	0.96	0.16	86,86,86,86	7
87	OHX	l3	401	7/7	0.96	0.21	52,52,52,52	7
87	OHX	5	3430	7/7	0.96	0.24	38,38,38,38	7
88	MG	6	2310	1/1	0.96	0.40	48,48,48,48	1
88	MG	Q2	504	1/1	0.96	0.10	50,50,50,50	0
87	OHX	5	3440	7/7	0.96	0.15	70,70,70,70	7
88	MG	l2	307	1/1	0.96	0.58	46,46,46,46	1
87	OHX	5	3461	7/7	0.96	0.22	40,40,40,40	7
88	MG	5	4004	1/1	0.96	0.26	48,48,48,48	0
88	MG	l3	406	1/1	0.96	0.15	31,31,31,31	1
87	OHX	5	3474	7/7	0.96	0.24	45,45,45,45	7
87	OHX	5	3475	7/7	0.96	0.15	79,79,79,79	7
88	MG	l3	411	1/1	0.96	0.14	33,33,33,33	1
87	OHX	5	3479	7/7	0.96	0.23	49,49,49,49	7
87	OHX	5	3619	7/7	0.96	0.19	46,46,46,46	7
88	MG	1	4437	1/1	0.96	0.07	43,43,43,43	1
88	MG	1	4044	1/1	0.96	0.23	44,44,44,44	0
87	OHX	5	3480	7/7	0.96	0.17	57,57,57,57	7
88	MG	5	4013	1/1	0.96	0.33	33,33,33,33	0
88	MG	l5	308	1/1	0.96	0.19	49,49,49,49	1
87	OHX	5	3483	7/7	0.96	0.20	48,48,48,48	7
88	MG	l7	302	1/1	0.96	0.15	35,35,35,35	1
88	MG	1	4442	1/1	0.96	0.09	45,45,45,45	1
88	MG	1	3881	1/1	0.96	0.15	41,41,41,41	0
87	OHX	5	3484	7/7	0.96	0.17	48,48,48,48	7
88	MG	1	4445	1/1	0.96	0.10	49,49,49,49	1
88	MG	1	4447	1/1	0.96	0.20	58,58,58,58	1
88	MG	5	4297	1/1	0.96	0.05	37,37,37,37	0
88	MG	l9	202	1/1	0.96	0.15	38,38,38,38	0
87	OHX	5	3623	7/7	0.96	0.14	81,81,81,81	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4301	1/1	0.96	0.14	34,34,34,34	1
88	MG	1	4450	1/1	0.96	0.15	50,50,50,50	0
87	OHX	5	3487	7/7	0.96	0.24	51,51,51,51	7
88	MG	m5	503	1/1	0.96	0.13	48,48,48,48	0
88	MG	1	4053	1/1	0.96	0.15	38,38,38,38	0
87	OHX	m5	501	7/7	0.96	0.16	81,81,81,81	7
88	MG	m6	201	1/1	0.96	0.13	38,38,38,38	1
88	MG	1	3887	1/1	0.96	0.14	45,45,45,45	0
88	MG	s8	302	1/1	0.96	0.20	45,45,45,45	0
87	OHX	5	3489	7/7	0.96	0.16	67,67,67,67	7
88	MG	m7	203	1/1	0.96	0.21	33,33,33,33	0
87	OHX	5	3490	7/7	0.96	0.17	89,89,89,89	7
87	OHX	5	3492	7/7	0.96	0.19	48,48,48,48	7
88	MG	m8	1501	1/1	0.96	0.31	42,42,42,42	1
87	OHX	5	3496	7/7	0.96	0.14	75,75,75,75	7
88	MG	1	4459	1/1	0.96	0.08	51,51,51,51	0
88	MG	m9	202	1/1	0.96	0.17	54,54,54,54	1
88	MG	5	4317	1/1	0.96	0.41	66,66,66,66	1
88	MG	1	4241	1/1	0.96	0.17	47,47,47,47	1
87	OHX	1	3499	7/7	0.96	0.17	57,57,57,57	7
88	MG	1	4462	1/1	0.96	0.12	43,43,43,43	0
88	MG	n1	202	1/1	0.96	0.07	40,40,40,40	1
88	MG	1	3894	1/1	0.96	0.23	48,48,48,48	0
87	OHX	5	3503	7/7	0.96	0.21	62,62,62,62	7
87	OHX	6	1955	7/7	0.96	0.09	145,145,145,145	7
87	OHX	6	1958	7/7	0.96	0.17	77,77,77,77	7
87	OHX	1	3500	7/7	0.96	0.14	90,90,90,90	7
88	MG	5	4326	1/1	0.96	0.07	79,79,79,79	0
88	MG	2	2092	1/1	0.96	0.28	40,40,40,40	0
87	OHX	6	2039	7/7	0.96	0.17	46,46,46,46	7
88	MG	6	2136	1/1	0.96	0.18	54,54,54,54	0
88	MG	1	3903	1/1	0.96	0.14	59,59,59,59	0
87	OHX	5	3513	7/7	0.96	0.18	56,56,56,56	7
87	OHX	5	3515	7/7	0.96	0.07	132,132,132,132	7
87	OHX	5	3516	7/7	0.96	0.22	42,42,42,42	7
88	MG	1	4474	1/1	0.96	0.25	47,47,47,47	1
88	MG	1	4075	1/1	0.96	0.08	43,43,43,43	0
88	MG	5	4055	1/1	0.96	0.19	39,39,39,39	0
88	MG	1	3909	1/1	0.96	0.19	49,49,49,49	0
87	OHX	6	1960	7/7	0.96	0.18	72,72,72,72	7
88	MG	6	2145	1/1	0.96	0.20	33,33,33,33	0
87	OHX	5	3518	7/7	0.96	0.17	56,56,56,56	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4262	1/1	0.96	0.11	33,33,33,33	0
87	OHX	5	3641	7/7	0.96	0.19	68,68,68,68	7
88	MG	1	4080	1/1	0.96	0.10	49,49,49,49	0
89	ZN	Q2	501	1/1	0.96	0.15	73,73,73,73	0
88	MG	5	3822	1/1	0.96	0.06	35,35,35,35	0
89	ZN	e1	501	1/1	0.96	0.06	163,163,163,163	0
88	MG	1	4081	1/1	0.96	0.14	46,46,46,46	0
88	MG	6	2151	1/1	0.96	0.32	47,47,47,47	0
88	MG	1	4025	1/1	0.97	0.08	62,62,62,62	0
88	MG	1	4188	1/1	0.97	0.15	38,38,38,38	0
88	MG	L7	301	1/1	0.97	0.06	39,39,39,39	0
88	MG	5	4394	1/1	0.97	0.23	38,38,38,38	1
88	MG	1	4189	1/1	0.97	0.09	40,40,40,40	1
87	OHX	5	3510	7/7	0.97	0.19	39,39,39,39	7
87	OHX	q1	101	7/7	0.97	0.18	46,46,46,46	7
87	OHX	1	3488	7/7	0.97	0.09	113,113,113,113	7
87	OHX	1	3491	7/7	0.97	0.19	44,44,44,44	7
87	OHX	1	3546	7/7	0.97	0.15	55,55,55,55	7
88	MG	M0	308	1/1	0.97	0.18	44,44,44,44	1
88	MG	5	4403	1/1	0.97	0.07	48,48,48,48	0
88	MG	M0	309	1/1	0.97	0.07	46,46,46,46	1
87	OHX	3	205	7/7	0.97	0.13	80,80,80,80	7
88	MG	1	4032	1/1	0.97	0.15	41,41,41,41	0
87	OHX	6	1964	7/7	0.97	0.14	49,49,49,49	7
88	MG	M3	203	1/1	0.97	0.10	46,46,46,46	1
88	MG	1	4388	1/1	0.97	0.13	37,37,37,37	1
88	MG	5	4135	1/1	0.97	0.08	38,38,38,38	0
88	MG	1	3886	1/1	0.97	0.15	49,49,49,49	0
88	MG	M5	303	1/1	0.97	0.10	41,41,41,41	1
88	MG	M5	304	1/1	0.97	0.14	40,40,40,40	1
88	MG	5	4139	1/1	0.97	0.10	34,34,34,34	1
87	OHX	1	3492	7/7	0.97	0.21	45,45,45,45	7
88	MG	5	4418	1/1	0.97	0.08	35,35,35,35	0
88	MG	1	4036	1/1	0.97	0.31	47,47,47,47	0
87	OHX	1	3495	7/7	0.97	0.14	54,54,54,54	7
87	OHX	6	1967	7/7	0.97	0.15	47,47,47,47	7
87	OHX	1	3497	7/7	0.97	0.13	83,83,83,83	7
87	OHX	2	1936	7/7	0.97	0.17	72,72,72,72	7
87	OHX	5	3524	7/7	0.97	0.14	62,62,62,62	7
88	MG	5	4148	1/1	0.97	0.12	40,40,40,40	0
88	MG	1	4398	1/1	0.97	0.10	48,48,48,48	0
87	OHX	6	1970	7/7	0.97	0.12	88,88,88,88	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	6	2245	1/1	0.97	0.11	60,60,60,60	0
88	MG	5	4431	1/1	0.97	0.23	50,50,50,50	0
88	MG	M7	208	1/1	0.97	0.10	40,40,40,40	0
88	MG	5	4433	1/1	0.97	0.23	37,37,37,37	1
88	MG	5	4434	1/1	0.97	0.25	40,40,40,40	0
88	MG	5	4435	1/1	0.97	0.08	40,40,40,40	0
87	OHX	2	1908	7/7	0.97	0.09	104,104,104,104	0
88	MG	1	4045	1/1	0.97	0.10	42,42,42,42	0
88	MG	M8	202	1/1	0.97	0.37	39,39,39,39	1
88	MG	6	2250	1/1	0.97	0.26	47,47,47,47	0
87	OHX	6	1972	7/7	0.97	0.16	59,59,59,59	7
88	MG	5	4444	1/1	0.97	0.12	42,42,42,42	1
88	MG	6	2252	1/1	0.97	0.21	47,47,47,47	0
88	MG	5	4448	1/1	0.97	0.13	38,38,38,38	1
88	MG	6	2253	1/1	0.97	0.12	47,47,47,47	0
88	MG	6	2254	1/1	0.97	0.08	53,53,53,53	0
88	MG	1	4215	1/1	0.97	0.10	54,54,54,54	0
87	OHX	6	1973	7/7	0.97	0.15	86,86,86,86	7
88	MG	5	3928	1/1	0.97	0.07	39,39,39,39	0
88	MG	5	4164	1/1	0.97	0.13	45,45,45,45	0
88	MG	5	4456	1/1	0.97	0.14	62,62,62,62	0
87	OHX	5	3530	7/7	0.97	0.16	42,42,42,42	7
88	MG	1	4406	1/1	0.97	0.10	56,56,56,56	0
88	MG	5	4462	1/1	0.97	0.08	39,39,39,39	0
88	MG	6	2259	1/1	0.97	0.04	48,48,48,48	0
88	MG	1	4407	1/1	0.97	0.19	42,42,42,42	1
88	MG	5	4466	1/1	0.97	0.26	36,36,36,36	1
87	OHX	1	3553	7/7	0.97	0.15	87,87,87,87	7
88	MG	1	3900	1/1	0.97	0.33	42,42,42,42	0
87	OHX	6	1975	7/7	0.97	0.15	61,61,61,61	7
87	OHX	2	1939	7/7	0.97	0.10	98,98,98,98	7
87	OHX	6	1977	7/7	0.97	0.13	86,86,86,86	7
88	MG	1	3905	1/1	0.97	0.08	43,43,43,43	0
88	MG	5	4473	1/1	0.97	0.08	38,38,38,38	1
88	MG	5	3939	1/1	0.97	0.17	48,48,48,48	0
87	OHX	4	203	7/7	0.97	0.15	61,61,61,61	7
87	OHX	5	3536	7/7	0.97	0.19	54,54,54,54	7
87	OHX	4	206	7/7	0.97	0.14	88,88,88,88	7
88	MG	2	2236	1/1	0.97	0.08	64,64,64,64	0
88	MG	5	4479	1/1	0.97	0.26	34,34,34,34	1
87	OHX	2	1924	7/7	0.97	0.13	89,89,89,89	7
88	MG	2	2238	1/1	0.97	0.05	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	4482	1/1	0.97	0.18	46,46,46,46	0
87	OHX	1	3503	7/7	0.97	0.15	60,60,60,60	7
88	MG	O1	202	1/1	0.97	0.20	60,60,60,60	1
88	MG	5	4185	1/1	0.97	0.16	35,35,35,35	1
88	MG	5	4487	1/1	0.97	0.30	35,35,35,35	1
87	OHX	2	1909	7/7	0.97	0.11	94,94,94,94	7
88	MG	5	4489	1/1	0.97	0.05	38,38,38,38	0
87	OHX	5	3541	7/7	0.97	0.16	46,46,46,46	7
87	OHX	5	3542	7/7	0.97	0.15	52,52,52,52	7
88	MG	5	4190	1/1	0.97	0.10	39,39,39,39	0
88	MG	1	4429	1/1	0.97	0.13	43,43,43,43	0
88	MG	6	2280	1/1	0.97	0.10	46,46,46,46	0
88	MG	5	4193	1/1	0.97	0.17	36,36,36,36	0
88	MG	5	3953	1/1	0.97	0.23	30,30,30,30	0
87	OHX	2	1956	7/7	0.97	0.12	91,91,91,91	7
88	MG	5	4502	1/1	0.97	0.32	38,38,38,38	1
87	OHX	2	1928	7/7	0.97	0.14	75,75,75,75	7
88	MG	5	4505	1/1	0.97	0.08	33,33,33,33	0
88	MG	5	4197	1/1	0.97	0.09	43,43,43,43	0
88	MG	1	4432	1/1	0.97	0.07	41,41,41,41	0
88	MG	1	4433	1/1	0.97	0.17	39,39,39,39	1
87	OHX	2	1930	7/7	0.97	0.14	77,77,77,77	7
87	OHX	5	3546	7/7	0.97	0.21	47,47,47,47	7
88	MG	5	4513	1/1	0.97	0.08	54,54,54,54	0
87	OHX	1	3510	7/7	0.97	0.16	50,50,50,50	7
87	OHX	1	3511	7/7	0.97	0.13	98,98,98,98	7
88	MG	5	4516	1/1	0.97	0.09	43,43,43,43	0
88	MG	1	4438	1/1	0.97	0.19	51,51,51,51	0
88	MG	5	4518	1/1	0.97	0.05	35,35,35,35	1
88	MG	6	2290	1/1	0.97	0.10	52,52,52,52	0
88	MG	1	4074	1/1	0.97	0.17	31,31,31,31	0
88	MG	O7	107	1/1	0.97	0.38	42,42,42,42	1
87	OHX	C8	202	7/7	0.97	0.09	94,94,94,94	7
88	MG	6	2294	1/1	0.97	0.08	43,43,43,43	0
88	MG	5	4211	1/1	0.97	0.10	38,38,38,38	0
87	OHX	2	1975	7/7	0.97	0.08	112,112,112,112	7
88	MG	5	4214	1/1	0.97	0.18	41,41,41,41	0
88	MG	1	4243	1/1	0.97	0.14	44,44,44,44	1
87	OHX	1	3514	7/7	0.97	0.19	41,41,41,41	7
87	OHX	1	3515	7/7	0.97	0.15	50,50,50,50	7
87	OHX	L3	402	7/7	0.97	0.16	67,67,67,67	7
87	OHX	5	3554	7/7	0.97	0.13	45,45,45,45	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	1	4448	1/1	0.97	0.19	44,44,44,44	0
87	OHX	2	1912	7/7	0.97	0.10	109,109,109,109	0
88	MG	2	2131	1/1	0.97	0.10	73,73,73,73	0
87	OHX	5	3556	7/7	0.97	0.13	50,50,50,50	7
88	MG	5	4542	1/1	0.97	0.15	34,34,34,34	1
87	OHX	1	3432	7/7	0.97	0.18	46,46,46,46	7
87	OHX	1	3518	7/7	0.97	0.20	40,40,40,40	7
88	MG	5	4548	1/1	0.97	0.06	39,39,39,39	0
87	OHX	1	3441	7/7	0.97	0.16	51,51,51,51	7
87	OHX	1	3625	7/7	0.97	0.07	186,186,186,186	7
87	OHX	1	3572	7/7	0.97	0.14	53,53,53,53	7
87	OHX	2	1945	7/7	0.97	0.10	110,110,110,110	7
87	OHX	1	3448	7/7	0.97	0.15	70,70,70,70	7
88	MG	1	3939	1/1	0.97	0.19	38,38,38,38	0
88	MG	6	2314	1/1	0.97	0.18	48,48,48,48	0
88	MG	5	4557	1/1	0.97	0.06	41,41,41,41	0
88	MG	6	2111	1/1	0.97	0.31	49,49,49,49	0
88	MG	1	4261	1/1	0.97	0.13	56,56,56,56	0
87	OHX	1	3452	7/7	0.97	0.13	85,85,85,85	7
88	MG	1	4263	1/1	0.97	0.06	36,36,36,36	0
87	OHX	1	3453	7/7	0.97	0.17	50,50,50,50	7
88	MG	5	3994	1/1	0.97	0.36	41,41,41,41	0
87	OHX	5	3566	7/7	0.97	0.09	98,98,98,98	7
87	OHX	M9	201	7/7	0.97	0.14	68,68,68,68	7
87	OHX	5	3568	7/7	0.97	0.16	66,66,66,66	7
88	MG	1	4268	1/1	0.97	0.29	46,46,46,46	1
88	MG	5	4246	1/1	0.97	0.21	58,58,58,58	0
88	MG	1	4269	1/1	0.97	0.16	45,45,45,45	1
87	OHX	1	3454	7/7	0.97	0.13	79,79,79,79	7
88	MG	6	2327	1/1	0.97	0.12	78,78,78,78	0
88	MG	6	2328	1/1	0.97	0.11	54,54,54,54	1
87	OHX	1	3460	7/7	0.97	0.22	50,50,50,50	7
87	OHX	1	3634	7/7	0.97	0.09	82,82,82,82	7
88	MG	5	4253	1/1	0.97	0.13	29,29,29,29	0
88	MG	7	218	1/1	0.97	0.12	39,39,39,39	0
87	OHX	1	3466	7/7	0.97	0.14	88,88,88,88	7
88	MG	1	3949	1/1	0.97	0.27	38,38,38,38	0
87	OHX	5	3689	7/7	0.97	0.16	45,45,45,45	7
88	MG	s1	303	1/1	0.97	0.09	77,77,77,77	0
88	MG	6	2127	1/1	0.97	0.24	45,45,45,45	0
87	OHX	2	1978	7/7	0.97	0.07	121,121,121,121	7
87	OHX	5	3574	7/7	0.97	0.16	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	OHX	1	3470	7/7	0.97	0.16	90,90,90,90	7
87	OHX	O7	103	7/7	0.97	0.16	60,60,60,60	7
87	OHX	1	3475	7/7	0.97	0.19	55,55,55,55	7
87	OHX	6	1914	7/7	0.97	0.14	52,52,52,52	7
88	MG	5	4266	1/1	0.97	0.20	45,45,45,45	0
88	MG	7	232	1/1	0.97	0.13	52,52,52,52	0
87	OHX	6	1918	7/7	0.97	0.19	56,56,56,56	7
87	OHX	6	1919	7/7	0.97	0.12	68,68,68,68	7
88	MG	5	4020	1/1	0.97	0.32	37,37,37,37	0
88	MG	1	4113	1/1	0.97	0.11	59,59,59,59	0
87	OHX	1	3476	7/7	0.97	0.20	75,75,75,75	7
88	MG	1	4288	1/1	0.97	0.08	39,39,39,39	0
88	MG	5	4274	1/1	0.97	0.11	35,35,35,35	1
88	MG	1	3819	1/1	0.97	0.18	31,31,31,31	0
87	OHX	2	1913	7/7	0.97	0.15	87,87,87,87	7
87	OHX	6	1929	7/7	0.97	0.20	53,53,53,53	7
87	OHX	5	3585	7/7	0.97	0.20	46,46,46,46	7
88	MG	5	4280	1/1	0.97	0.16	44,44,44,44	1
87	OHX	5	3702	7/7	0.97	0.14	74,74,74,74	7
87	OHX	6	1930	7/7	0.97	0.15	59,59,59,59	7
87	OHX	1	3481	7/7	0.97	0.15	87,87,87,87	7
88	MG	d3	202	1/1	0.97	0.14	49,49,49,49	1
87	OHX	6	1933	7/7	0.97	0.11	82,82,82,82	7
87	OHX	c8	201	7/7	0.97	0.10	95,95,95,95	7
88	MG	1	4299	1/1	0.97	0.17	41,41,41,41	1
88	MG	5	4292	1/1	0.97	0.07	48,48,48,48	1
88	MG	8	235	1/1	0.97	0.13	61,61,61,61	1
88	MG	1	4125	1/1	0.97	0.06	36,36,36,36	0
88	MG	1	3969	1/1	0.97	0.16	29,29,29,29	0
87	OHX	6	1937	7/7	0.97	0.10	88,88,88,88	7
88	MG	5	4040	1/1	0.97	0.15	35,35,35,35	0
87	OHX	5	3591	7/7	0.97	0.21	46,46,46,46	7
88	MG	12	302	1/1	0.97	0.15	36,36,36,36	0
88	MG	5	4042	1/1	0.97	0.38	51,51,51,51	0
88	MG	5	4303	1/1	0.97	0.09	41,41,41,41	1
87	OHX	2	1916	7/7	0.97	0.11	89,89,89,89	7
87	OHX	1	3537	7/7	0.97	0.16	54,54,54,54	7
87	OHX	5	3434	7/7	0.97	0.15	48,48,48,48	7
87	OHX	1	3538	7/7	0.97	0.20	49,49,49,49	7
88	MG	5	4308	1/1	0.97	0.07	29,29,29,29	0
88	MG	5	4047	1/1	0.97	0.16	33,33,33,33	0
88	MG	1	4309	1/1	0.97	0.15	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	OHX	5	3441	7/7	0.97	0.16	63,63,63,63	7
88	MG	l3	410	1/1	0.97	0.13	31,31,31,31	1
87	OHX	5	3453	7/7	0.97	0.17	67,67,67,67	7
88	MG	1	3978	1/1	0.97	0.28	31,31,31,31	0
88	MG	l3	413	1/1	0.97	0.12	32,32,32,32	1
87	OHX	5	3457	7/7	0.97	0.16	72,72,72,72	7
88	MG	1	3980	1/1	0.97	0.30	37,37,37,37	0
87	OHX	8	212	7/7	0.97	0.13	85,85,85,85	7
88	MG	1	3839	1/1	0.97	0.26	43,43,43,43	0
87	OHX	5	3458	7/7	0.97	0.13	56,56,56,56	7
87	OHX	5	3459	7/7	0.97	0.16	58,58,58,58	7
87	OHX	6	1942	7/7	0.97	0.12	70,70,70,70	7
88	MG	2	2180	1/1	0.97	0.19	68,68,68,68	0
88	MG	1	3987	1/1	0.97	0.19	36,36,36,36	0
87	OHX	5	3469	7/7	0.97	0.15	61,61,61,61	7
88	MG	1	4329	1/1	0.97	0.07	49,49,49,49	0
88	MG	1	4330	1/1	0.97	0.08	56,56,56,56	0
87	OHX	5	3470	7/7	0.97	0.12	78,78,78,78	7
87	OHX	5	3471	7/7	0.97	0.14	81,81,81,81	7
87	OHX	5	3473	7/7	0.97	0.13	44,44,44,44	7
87	OHX	6	1943	7/7	0.97	0.11	108,108,108,108	7
87	OHX	1	3483	7/7	0.97	0.14	74,74,74,74	7
88	MG	1	3850	1/1	0.97	0.12	48,48,48,48	0
88	MG	5	4334	1/1	0.97	0.15	39,39,39,39	1
88	MG	1	4153	1/1	0.97	0.08	42,42,42,42	0
88	MG	2	2187	1/1	0.97	0.12	87,87,87,87	0
88	MG	5	4337	1/1	0.97	0.17	46,46,46,46	0
87	OHX	1	3646	7/7	0.97	0.13	96,96,96,96	7
88	MG	5	4340	1/1	0.97	0.10	35,35,35,35	1
87	OHX	6	1946	7/7	0.97	0.13	71,71,71,71	7
88	MG	m6	204	1/1	0.97	0.06	40,40,40,40	0
87	OHX	5	3481	7/7	0.97	0.17	46,46,46,46	7
87	OHX	6	1947	7/7	0.97	0.17	59,59,59,59	7
88	MG	m7	204	1/1	0.97	0.16	40,40,40,40	1
87	OHX	6	1948	7/7	0.97	0.12	86,86,86,86	7
87	OHX	5	3485	7/7	0.97	0.13	51,51,51,51	7
88	MG	1	4161	1/1	0.97	0.23	54,54,54,54	0
87	OHX	1	3647	7/7	0.97	0.07	199,199,199,199	7
88	MG	6	2189	1/1	0.97	0.23	47,47,47,47	0
88	MG	5	3855	1/1	0.97	0.26	32,32,32,32	0
88	MG	1	4163	1/1	0.97	0.17	42,42,42,42	1
87	OHX	5	3488	7/7	0.97	0.16	42,42,42,42	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
88	MG	5	3858	1/1	0.97	0.27	35,35,35,35	0
88	MG	5	4085	1/1	0.97	0.18	37,37,37,37	0
88	MG	1	3861	1/1	0.97	0.09	42,42,42,42	0
87	OHX	1	3593	7/7	0.97	0.17	37,37,37,37	7
88	MG	5	4358	1/1	0.97	0.06	49,49,49,49	1
88	MG	1	4006	1/1	0.97	0.34	41,41,41,41	0
88	MG	1	3863	1/1	0.97	0.21	42,42,42,42	0
87	OHX	6	1952	7/7	0.97	0.13	84,84,84,84	7
87	OHX	1	3540	7/7	0.97	0.15	52,52,52,52	7
88	MG	n8	203	1/1	0.97	0.03	41,41,41,41	0
87	OHX	2	1948	7/7	0.97	0.17	67,67,67,67	7
87	OHX	5	3497	7/7	0.97	0.15	57,57,57,57	7
88	MG	5	3868	1/1	0.97	0.10	32,32,32,32	0
88	MG	5	3869	1/1	0.97	0.28	45,45,45,45	0
87	OHX	5	3501	7/7	0.97	0.15	59,59,59,59	7
88	MG	1	3869	1/1	0.97	0.26	39,39,39,39	0
88	MG	1	4015	1/1	0.97	0.55	27,27,27,27	0
87	OHX	2	1934	7/7	0.97	0.11	103,103,103,103	7
87	OHX	6	1956	7/7	0.97	0.12	90,90,90,90	7
87	OHX	5	3504	7/7	0.97	0.17	38,38,38,38	7
87	OHX	6	1957	7/7	0.97	0.14	63,63,63,63	7
88	MG	5	4104	1/1	0.97	0.08	49,49,49,49	0
88	MG	o4	201	1/1	0.97	0.16	70,70,70,70	1
87	OHX	2	1922	7/7	0.97	0.11	75,75,75,75	7
87	OHX	3	201	7/7	0.97	0.13	71,71,71,71	7
88	MG	1	4183	1/1	0.97	0.15	47,47,47,47	1
88	MG	L3	405	1/1	0.97	0.11	42,42,42,42	0
87	OHX	5	3509	7/7	0.97	0.09	107,107,107,107	7
88	MG	L4	403	1/1	0.97	0.20	34,34,34,34	0
88	MG	6	2213	1/1	0.97	0.12	68,68,68,68	1
88	MG	1	3878	1/1	0.97	0.09	49,49,49,49	0
88	MG	6	2215	1/1	0.97	0.31	52,52,52,52	0
88	MG	5	3886	1/1	0.97	0.26	46,46,46,46	0
87	OHX	6	1911	7/7	0.98	0.09	59,59,59,59	7
87	OHX	8	207	7/7	0.98	0.13	74,74,74,74	7
87	OHX	6	1913	7/7	0.98	0.08	85,85,85,85	7
88	MG	1	4068	1/1	0.98	0.28	40,40,40,40	0
88	MG	1	4206	1/1	0.98	0.08	47,47,47,47	0
88	MG	5	4265	1/1	0.98	0.17	39,39,39,39	1
87	OHX	C8	201	7/7	0.98	0.09	94,94,94,94	7
87	OHX	5	3512	7/7	0.98	0.11	60,60,60,60	7
87	OHX	6	1915	7/7	0.98	0.16	63,63,63,63	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	3514	7/7	0.98	0.11	60,60,60,60	7
87	OHX	5	3727	7/7	0.98	0.19	48,48,48,48	7
88	MG	5	4491	1/1	0.98	0.27	53,53,53,53	0
88	MG	5	4492	1/1	0.98	0.07	57,57,57,57	0
88	MG	5	4493	1/1	0.98	0.13	41,41,41,41	1
87	OHX	1	3574	7/7	0.98	0.17	40,40,40,40	7
88	MG	5	4272	1/1	0.98	0.08	33,33,33,33	1
87	OHX	1	3471	7/7	0.98	0.14	49,49,49,49	7
88	MG	5	3913	1/1	0.98	0.11	39,39,39,39	0
88	MG	5	4498	1/1	0.98	0.15	42,42,42,42	1
87	OHX	6	1920	7/7	0.98	0.08	114,114,114,114	7
88	MG	5	4088	1/1	0.98	0.20	36,36,36,36	1
87	OHX	1	3472	7/7	0.98	0.12	70,70,70,70	7
87	OHX	6	1923	7/7	0.98	0.12	71,71,71,71	7
87	OHX	5	3520	7/7	0.98	0.12	88,88,88,88	7
88	MG	5	4504	1/1	0.98	0.10	40,40,40,40	1
88	MG	5	4282	1/1	0.98	0.11	34,34,34,34	1
87	OHX	1	3577	7/7	0.98	0.13	54,54,54,54	7
88	MG	5	4507	1/1	0.98	0.08	52,52,52,52	1
87	OHX	6	1926	7/7	0.98	0.14	55,55,55,55	7
87	OHX	6	1927	7/7	0.98	0.08	109,109,109,109	7
88	MG	5	4510	1/1	0.98	0.21	30,30,30,30	1
88	MG	5	4287	1/1	0.98	0.15	35,35,35,35	1
87	OHX	6	1928	7/7	0.98	0.08	118,118,118,118	7
87	OHX	1	3473	7/7	0.98	0.14	62,62,62,62	7
88	MG	1	4371	1/1	0.98	0.08	43,43,43,43	1
87	OHX	5	3526	7/7	0.98	0.11	94,94,94,94	7
88	MG	1	4373	1/1	0.98	0.18	35,35,35,35	1
88	MG	1	4086	1/1	0.98	0.14	50,50,50,50	0
87	OHX	2	1915	7/7	0.98	0.09	122,122,122,122	7
88	MG	6	2308	1/1	0.98	0.13	51,51,51,51	1
87	OHX	2	1929	7/7	0.98	0.13	66,66,66,66	7
88	MG	5	4298	1/1	0.98	0.11	40,40,40,40	0
88	MG	5	4299	1/1	0.98	0.06	43,43,43,43	1
88	MG	1	4377	1/1	0.98	0.10	60,60,60,60	0
87	OHX	6	2084	7/7	0.98	0.11	79,79,79,79	7
88	MG	5	4302	1/1	0.98	0.16	35,35,35,35	1
88	MG	5	4526	1/1	0.98	0.07	43,43,43,43	0
88	MG	5	4528	1/1	0.98	0.13	43,43,43,43	0
88	MG	5	4529	1/1	0.98	0.21	36,36,36,36	1
88	MG	1	4379	1/1	0.98	0.08	33,33,33,33	1
87	OHX	5	3636	7/7	0.98	0.09	73,73,73,73	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	2	1966	7/7	0.98	0.11	61,61,61,61	7
87	OHX	m0	301	7/7	0.98	0.12	86,86,86,86	7
88	MG	5	4534	1/1	0.98	0.28	48,48,48,48	1
88	MG	1	4093	1/1	0.98	0.10	42,42,42,42	0
88	MG	5	4536	1/1	0.98	0.18	39,39,39,39	1
87	OHX	6	1934	7/7	0.98	0.15	57,57,57,57	7
88	MG	5	4112	1/1	0.98	0.20	36,36,36,36	1
88	MG	5	4310	1/1	0.98	0.04	33,33,33,33	0
88	MG	6	2318	1/1	0.98	0.07	54,54,54,54	0
87	OHX	6	1935	7/7	0.98	0.11	56,56,56,56	7
87	OHX	6	1936	7/7	0.98	0.13	57,57,57,57	7
87	OHX	1	3478	7/7	0.98	0.14	59,59,59,59	7
88	MG	5	4544	1/1	0.98	0.16	42,42,42,42	1
87	OHX	1	3479	7/7	0.98	0.15	55,55,55,55	7
88	MG	5	4546	1/1	0.98	0.07	49,49,49,49	1
88	MG	5	4118	1/1	0.98	0.26	48,48,48,48	1
88	MG	5	4119	1/1	0.98	0.08	42,42,42,42	0
87	OHX	1	3480	7/7	0.98	0.15	62,62,62,62	7
87	OHX	1	3415	7/7	0.98	0.10	66,66,66,66	7
88	MG	5	4122	1/1	0.98	0.14	55,55,55,55	0
88	MG	5	4553	1/1	0.98	0.08	50,50,50,50	0
88	MG	4	238	1/1	0.98	0.08	40,40,40,40	1
87	OHX	1	3586	7/7	0.98	0.11	91,91,91,91	7
87	OHX	1	3416	7/7	0.98	0.11	59,59,59,59	7
87	OHX	1	3532	7/7	0.98	0.13	54,54,54,54	7
87	OHX	1	3417	7/7	0.98	0.15	48,48,48,48	7
87	OHX	o7	502	7/7	0.98	0.18	64,64,64,64	7
87	OHX	1	3534	7/7	0.98	0.14	62,62,62,62	7
88	MG	4	245	1/1	0.98	0.22	51,51,51,51	0
87	OHX	1	3418	7/7	0.98	0.14	56,56,56,56	7
88	MG	5	4563	1/1	0.98	0.07	48,48,48,48	1
88	MG	1	3854	1/1	0.98	0.10	51,51,51,51	0
87	OHX	1	3536	7/7	0.98	0.07	128,128,128,128	7
87	OHX	q2	502	7/7	0.98	0.14	51,51,51,51	7
88	MG	5	4567	1/1	0.98	0.09	34,34,34,34	1
88	MG	5	3957	1/1	0.98	0.35	29,29,29,29	0
87	OHX	1	3485	7/7	0.98	0.10	89,89,89,89	7
88	MG	L3	406	1/1	0.98	0.15	39,39,39,39	1
88	MG	5	4571	1/1	0.98	0.25	48,48,48,48	1
88	MG	1	4250	1/1	0.98	0.10	51,51,51,51	0
88	MG	L3	408	1/1	0.98	0.20	53,53,53,53	1
88	MG	5	4339	1/1	0.98	0.10	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	3431	7/7	0.98	0.13	45,45,45,45	7
88	MG	L4	404	1/1	0.98	0.11	42,42,42,42	1
87	OHX	6	1951	7/7	0.98	0.06	133,133,133,133	7
88	MG	2	2207	1/1	0.98	0.13	61,61,61,61	0
87	OHX	2	1906	7/7	0.98	0.10	82,82,82,82	7
87	OHX	1	3435	7/7	0.98	0.10	69,69,69,69	7
88	MG	1	4411	1/1	0.98	0.05	60,60,60,60	1
87	OHX	4	204	7/7	0.98	0.13	57,57,57,57	7
87	OHX	4	205	7/7	0.98	0.11	75,75,75,75	7
87	OHX	1	3489	7/7	0.98	0.14	56,56,56,56	7
87	OHX	1	3439	7/7	0.98	0.16	61,61,61,61	7
88	MG	1	4416	1/1	0.98	0.11	56,56,56,56	0
87	OHX	5	3427	7/7	0.98	0.10	61,61,61,61	7
87	OHX	5	3429	7/7	0.98	0.10	47,47,47,47	7
87	OHX	2	1917	7/7	0.98	0.13	85,85,85,85	7
87	OHX	1	3493	7/7	0.98	0.15	50,50,50,50	7
87	OHX	5	3436	7/7	0.98	0.14	51,51,51,51	7
87	OHX	1	3494	7/7	0.98	0.12	62,62,62,62	7
88	MG	5	4360	1/1	0.98	0.06	35,35,35,35	1
88	MG	2	2220	1/1	0.98	0.06	70,70,70,70	1
88	MG	1	3874	1/1	0.98	0.19	46,46,46,46	0
88	MG	1	4426	1/1	0.98	0.23	49,49,49,49	0
87	OHX	1	3442	7/7	0.98	0.12	65,65,65,65	7
87	OHX	5	3443	7/7	0.98	0.14	60,60,60,60	7
88	MG	1	4271	1/1	0.98	0.04	46,46,46,46	0
88	MG	7	240	1/1	0.98	0.11	47,47,47,47	1
88	MG	5	4368	1/1	0.98	0.16	38,38,38,38	1
88	MG	M6	202	1/1	0.98	0.19	41,41,41,41	1
87	OHX	5	3444	7/7	0.98	0.16	46,46,46,46	7
87	OHX	5	3445	7/7	0.98	0.11	72,72,72,72	7
87	OHX	5	3447	7/7	0.98	0.15	43,43,43,43	7
88	MG	5	4373	1/1	0.98	0.07	36,36,36,36	1
88	MG	5	3990	1/1	0.98	0.21	21,21,21,21	0
88	MG	5	4170	1/1	0.98	0.05	41,41,41,41	0
87	OHX	5	3448	7/7	0.98	0.13	70,70,70,70	7
88	MG	M7	204	1/1	0.98	0.24	40,40,40,40	0
87	OHX	5	3449	7/7	0.98	0.12	79,79,79,79	7
87	OHX	5	3451	7/7	0.98	0.15	54,54,54,54	7
87	OHX	5	3452	7/7	0.98	0.09	115,115,115,115	0
88	MG	1	4279	1/1	0.98	0.08	38,38,38,38	1
87	OHX	1	3496	7/7	0.98	0.15	41,41,41,41	7
87	OHX	5	3454	7/7	0.98	0.18	42,42,42,42	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	3444	7/7	0.98	0.12	59,59,59,59	7
87	OHX	1	3445	7/7	0.98	0.10	88,88,88,88	7
88	MG	5	3832	1/1	0.98	0.09	34,34,34,34	0
88	MG	1	3888	1/1	0.98	0.17	41,41,41,41	0
88	MG	5	4003	1/1	0.98	0.23	28,28,28,28	0
87	OHX	2	1918	7/7	0.98	0.14	80,80,80,80	7
87	OHX	2	1921	7/7	0.98	0.10	88,88,88,88	7
88	MG	1	4446	1/1	0.98	0.08	54,54,54,54	0
87	OHX	1	3552	7/7	0.98	0.13	70,70,70,70	7
88	MG	5	4188	1/1	0.98	0.04	36,36,36,36	0
88	MG	l3	404	1/1	0.98	0.04	33,33,33,33	0
87	OHX	1	3450	7/7	0.98	0.14	61,61,61,61	7
87	OHX	1	3502	7/7	0.98	0.22	38,38,38,38	7
87	OHX	5	3472	7/7	0.98	0.15	46,46,46,46	7
88	MG	l3	408	1/1	0.98	0.08	31,31,31,31	0
88	MG	5	4399	1/1	0.98	0.09	40,40,40,40	1
87	OHX	1	3451	7/7	0.98	0.13	70,70,70,70	7
88	MG	5	4012	1/1	0.98	0.31	29,29,29,29	0
87	OHX	1	3504	7/7	0.98	0.11	71,71,71,71	7
88	MG	5	3843	1/1	0.98	0.31	38,38,38,38	0
87	OHX	2	1911	7/7	0.98	0.08	109,109,109,109	0
87	OHX	5	3476	7/7	0.98	0.13	63,63,63,63	7
88	MG	l4	403	1/1	0.98	0.06	39,39,39,39	0
88	MG	5	4406	1/1	0.98	0.09	47,47,47,47	1
87	OHX	5	3477	7/7	0.98	0.11	69,69,69,69	7
87	OHX	5	3478	7/7	0.98	0.16	54,54,54,54	7
88	MG	l5	307	1/1	0.98	0.05	46,46,46,46	1
88	MG	1	3901	1/1	0.98	0.06	48,48,48,48	0
88	MG	l5	309	1/1	0.98	0.07	54,54,54,54	1
87	OHX	2	1907	7/7	0.98	0.08	93,93,93,93	7
87	OHX	2	1903	7/7	0.98	0.10	90,90,90,90	0
87	OHX	1	3508	7/7	0.98	0.13	74,74,74,74	7
87	OHX	5	3482	7/7	0.98	0.13	64,64,64,64	7
88	MG	1	3906	1/1	0.98	0.41	44,44,44,44	0
88	MG	5	4415	1/1	0.98	0.15	39,39,39,39	1
88	MG	5	4206	1/1	0.98	0.11	35,35,35,35	1
88	MG	5	3854	1/1	0.98	0.17	58,58,58,58	0
88	MG	6	2236	1/1	0.98	0.10	54,54,54,54	0
88	MG	l9	203	1/1	0.98	0.06	46,46,46,46	1
87	OHX	1	3456	7/7	0.98	0.18	60,60,60,60	7
88	MG	1	4164	1/1	0.98	0.07	35,35,35,35	1
88	MG	O2	201	1/1	0.98	0.19	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	3457	7/7	0.98	0.11	96,96,96,96	7
87	OHX	6	1978	7/7	0.98	0.11	52,52,52,52	7
88	MG	5	4032	1/1	0.98	0.07	34,34,34,34	0
87	OHX	5	3486	7/7	0.98	0.14	50,50,50,50	7
88	MG	5	4427	1/1	0.98	0.24	44,44,44,44	1
88	MG	5	4034	1/1	0.98	0.17	29,29,29,29	0
87	OHX	1	3619	7/7	0.98	0.12	51,51,51,51	7
88	MG	5	3863	1/1	0.98	0.16	41,41,41,41	0
88	MG	1	4311	1/1	0.98	0.07	35,35,35,35	1
88	MG	1	4312	1/1	0.98	0.15	51,51,51,51	0
87	OHX	1	3458	7/7	0.98	0.11	59,59,59,59	7
88	MG	1	4315	1/1	0.98	0.09	59,59,59,59	0
88	MG	1	4316	1/1	0.98	0.17	36,36,36,36	1
88	MG	m7	207	1/1	0.98	0.08	41,41,41,41	1
88	MG	m7	208	1/1	0.98	0.12	40,40,40,40	1
88	MG	m7	209	1/1	0.98	0.14	42,42,42,42	1
88	MG	5	4436	1/1	0.98	0.11	33,33,33,33	0
88	MG	m8	1502	1/1	0.98	0.06	47,47,47,47	0
87	OHX	2	1937	7/7	0.98	0.10	94,94,94,94	7
87	OHX	1	3461	7/7	0.98	0.14	62,62,62,62	7
87	OHX	1	3462	7/7	0.98	0.12	45,45,45,45	7
88	MG	1	4041	1/1	0.98	0.15	35,35,35,35	0
88	MG	n0	202	1/1	0.98	0.17	38,38,38,38	1
87	OHX	5	3493	7/7	0.98	0.14	62,62,62,62	7
87	OHX	5	3494	7/7	0.98	0.11	66,66,66,66	7
87	OHX	5	3495	7/7	0.98	0.16	46,46,46,46	7
88	MG	5	4446	1/1	0.98	0.08	44,44,44,44	0
88	MG	5	4447	1/1	0.98	0.07	39,39,39,39	1
88	MG	5	4233	1/1	0.98	0.09	36,36,36,36	1
88	MG	5	4449	1/1	0.98	0.11	33,33,33,33	1
87	OHX	1	3463	7/7	0.98	0.10	113,113,113,113	7
88	MG	1	4325	1/1	0.98	0.31	60,60,60,60	0
87	OHX	7	201	7/7	0.98	0.13	70,70,70,70	7
88	MG	1	4047	1/1	0.98	0.16	41,41,41,41	0
87	OHX	7	202	7/7	0.98	0.11	60,60,60,60	7
87	OHX	1	3465	7/7	0.98	0.15	75,75,75,75	7
88	MG	C1	201	1/1	0.98	0.16	69,69,69,69	0
87	OHX	7	204	7/7	0.98	0.14	43,43,43,43	7
88	MG	5	4459	1/1	0.98	0.27	36,36,36,36	1
87	OHX	5	3498	7/7	0.98	0.13	46,46,46,46	7
88	MG	5	4461	1/1	0.98	0.06	44,44,44,44	0
87	OHX	5	3499	7/7	0.98	0.13	104,104,104,104	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	5	3500	7/7	0.98	0.10	75,75,75,75	7
88	MG	1	4055	1/1	0.98	0.20	38,38,38,38	0
87	OHX	6	1986	7/7	0.98	0.12	73,73,73,73	7
88	MG	1	4190	1/1	0.98	0.07	47,47,47,47	1
88	MG	o3	205	1/1	0.98	0.21	35,35,35,35	1
87	OHX	2	1926	7/7	0.98	0.10	81,81,81,81	7
87	OHX	1	3467	7/7	0.98	0.17	43,43,43,43	7
87	OHX	1	3628	7/7	0.98	0.14	43,43,43,43	7
88	MG	q1	103	1/1	0.98	0.15	46,46,46,46	1
87	OHX	2	1914	7/7	0.98	0.14	69,69,69,69	7
88	MG	q3	502	1/1	0.98	0.25	43,43,43,43	1
87	OHX	5	3506	7/7	0.98	0.18	48,48,48,48	7
88	MG	1	4500	1/1	0.98	0.11	60,60,60,60	0
89	ZN	E1	501	1/1	0.98	0.04	132,132,132,132	0
87	OHX	6	1905	7/7	0.98	0.10	74,74,74,74	0
88	MG	1	4197	1/1	0.98	0.07	38,38,38,38	0
87	OHX	6	1907	7/7	0.98	0.09	76,76,76,76	0
89	ZN	q2	501	1/1	0.98	0.12	69,69,69,69	0
88	MG	1	3812	1/1	0.98	0.34	49,49,49,49	0
88	MG	1	4201	1/1	0.98	0.10	52,52,52,52	1
87	OHX	1	3421	7/7	0.99	0.09	71,71,71,71	7
87	OHX	1	3422	7/7	0.99	0.08	71,71,71,71	7
87	OHX	6	1916	7/7	0.99	0.10	65,65,65,65	7
87	OHX	6	1917	7/7	0.99	0.08	55,55,55,55	7
87	OHX	1	3423	7/7	0.99	0.13	65,65,65,65	7
87	OHX	1	3464	7/7	0.99	0.13	65,65,65,65	7
87	OHX	5	3404	7/7	0.99	0.10	42,42,42,42	2
87	OHX	5	3405	7/7	0.99	0.10	57,57,57,57	1
87	OHX	5	3407	7/7	0.99	0.10	50,50,50,50	7
87	OHX	5	3408	7/7	0.99	0.10	64,64,64,64	7
87	OHX	5	3409	7/7	0.99	0.08	51,51,51,51	7
87	OHX	5	3410	7/7	0.99	0.10	43,43,43,43	7
87	OHX	5	3411	7/7	0.99	0.09	74,74,74,74	1
87	OHX	5	3412	7/7	0.99	0.10	46,46,46,46	7
87	OHX	5	3413	7/7	0.99	0.09	63,63,63,63	0
87	OHX	5	3414	7/7	0.99	0.11	58,58,58,58	7
87	OHX	5	3415	7/7	0.99	0.10	55,55,55,55	7
88	MG	6	2264	1/1	0.99	0.09	46,46,46,46	1
88	MG	5	4421	1/1	0.99	0.06	48,48,48,48	1
87	OHX	5	3416	7/7	0.99	0.08	56,56,56,56	7
87	OHX	5	3417	7/7	0.99	0.07	45,45,45,45	7
87	OHX	5	3418	7/7	0.99	0.10	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	OHX	5	3419	7/7	0.99	0.06	56,56,56,56	7
87	OHX	5	3420	7/7	0.99	0.08	70,70,70,70	0
87	OHX	5	3421	7/7	0.99	0.09	49,49,49,49	7
87	OHX	5	3422	7/7	0.99	0.07	59,59,59,59	7
88	MG	7	227	1/1	0.99	0.13	41,41,41,41	1
87	OHX	5	3423	7/7	0.99	0.07	66,66,66,66	7
87	OHX	5	3424	7/7	0.99	0.09	64,64,64,64	0
88	MG	5	4279	1/1	0.99	0.10	41,41,41,41	0
87	OHX	5	3425	7/7	0.99	0.10	49,49,49,49	7
88	MG	5	4281	1/1	0.99	0.12	38,38,38,38	1
87	OHX	5	3426	7/7	0.99	0.10	40,40,40,40	7
88	MG	1	4423	1/1	0.99	0.07	55,55,55,55	1
88	MG	5	4284	1/1	0.99	0.09	39,39,39,39	1
88	MG	5	4437	1/1	0.99	0.04	33,33,33,33	0
88	MG	1	4295	1/1	0.99	0.09	44,44,44,44	1
87	OHX	1	3424	7/7	0.99	0.08	79,79,79,79	0
87	OHX	5	3428	7/7	0.99	0.09	59,59,59,59	7
88	MG	5	4144	1/1	0.99	0.06	32,32,32,32	1
88	MG	1	4427	1/1	0.99	0.15	42,42,42,42	1
88	MG	5	4443	1/1	0.99	0.08	34,34,34,34	1
88	MG	1	3832	1/1	0.99	0.11	38,38,38,38	1
87	OHX	4	201	7/7	0.99	0.15	52,52,52,52	2
87	OHX	6	1922	7/7	0.99	0.07	58,58,58,58	7
88	MG	5	4293	1/1	0.99	0.19	33,33,33,33	1
87	OHX	5	3432	7/7	0.99	0.12	54,54,54,54	7
87	OHX	5	3433	7/7	0.99	0.07	100,100,100,100	0
88	MG	L4	402	1/1	0.99	0.12	43,43,43,43	0
87	OHX	4	202	7/7	0.99	0.09	55,55,55,55	7
87	OHX	n1	201	7/7	0.99	0.10	48,48,48,48	7
87	OHX	n3	201	7/7	0.99	0.11	55,55,55,55	7
88	MG	L4	406	1/1	0.99	0.11	38,38,38,38	1
88	MG	1	4306	1/1	0.99	0.04	45,45,45,45	1
88	MG	1	4185	1/1	0.99	0.06	46,46,46,46	0
88	MG	5	4457	1/1	0.99	0.08	45,45,45,45	1
87	OHX	5	3435	7/7	0.99	0.12	57,57,57,57	7
87	OHX	n9	101	7/7	0.99	0.11	59,59,59,59	7
87	OHX	6	1924	7/7	0.99	0.10	54,54,54,54	7
87	OHX	5	3437	7/7	0.99	0.09	54,54,54,54	7
87	OHX	5	3438	7/7	0.99	0.11	56,56,56,56	7
88	MG	1	4313	1/1	0.99	0.13	38,38,38,38	1
87	OHX	5	3439	7/7	0.99	0.07	82,82,82,82	7
88	MG	5	4465	1/1	0.99	0.09	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	OHX	1	3425	7/7	0.99	0.11	62,62,62,62	7
87	OHX	1	3426	7/7	0.99	0.12	55,55,55,55	7
87	OHX	5	3442	7/7	0.99	0.11	56,56,56,56	7
87	OHX	1	3468	7/7	0.99	0.09	54,54,54,54	7
87	OHX	1	3427	7/7	0.99	0.08	86,86,86,86	7
88	MG	M3	202	1/1	0.99	0.08	49,49,49,49	1
87	OHX	1	3428	7/7	0.99	0.09	64,64,64,64	7
88	MG	1	4198	1/1	0.99	0.07	59,59,59,59	1
87	OHX	5	3446	7/7	0.99	0.12	41,41,41,41	7
87	OHX	1	3429	7/7	0.99	0.09	53,53,53,53	7
87	OHX	1	3560	7/7	0.99	0.10	54,54,54,54	7
87	OHX	6	1932	7/7	0.99	0.09	47,47,47,47	7
87	OHX	5	3450	7/7	0.99	0.10	77,77,77,77	7
87	OHX	1	3430	7/7	0.99	0.08	68,68,68,68	7
87	OHX	2	1904	7/7	0.99	0.10	89,89,89,89	7
87	OHX	1	3474	7/7	0.99	0.09	58,58,58,58	7
87	OHX	2	1919	7/7	0.99	0.06	78,78,78,78	7
87	OHX	5	3455	7/7	0.99	0.10	80,80,80,80	7
87	OHX	5	3456	7/7	0.99	0.12	68,68,68,68	7
87	OHX	1	3433	7/7	0.99	0.10	61,61,61,61	7
88	MG	5	4486	1/1	0.99	0.11	46,46,46,46	0
87	OHX	1	3434	7/7	0.99	0.12	59,59,59,59	7
87	OHX	2	1920	7/7	0.99	0.12	84,84,84,84	7
87	OHX	5	3460	7/7	0.99	0.10	45,45,45,45	7
88	MG	5	4333	1/1	0.99	0.07	47,47,47,47	0
87	OHX	1	3436	7/7	0.99	0.10	75,75,75,75	7
88	MG	M7	210	1/1	0.99	0.05	45,45,45,45	1
87	OHX	5	3462	7/7	0.99	0.08	63,63,63,63	7
87	OHX	5	3463	7/7	0.99	0.11	66,66,66,66	7
88	MG	1	4340	1/1	0.99	0.09	40,40,40,40	0
87	OHX	5	3464	7/7	0.99	0.12	63,63,63,63	7
87	OHX	5	3465	7/7	0.99	0.13	49,49,49,49	7
87	OHX	5	3466	7/7	0.99	0.06	90,90,90,90	7
88	MG	N0	201	1/1	0.99	0.11	49,49,49,49	1
87	OHX	5	3467	7/7	0.99	0.09	76,76,76,76	7
87	OHX	5	3468	7/7	0.99	0.12	53,53,53,53	7
87	OHX	6	1941	7/7	0.99	0.09	79,79,79,79	7
87	OHX	1	3437	7/7	0.99	0.12	52,52,52,52	7
87	OHX	1	3438	7/7	0.99	0.10	55,55,55,55	7
87	OHX	2	1905	7/7	0.99	0.11	71,71,71,71	7
88	MG	5	4349	1/1	0.99	0.09	39,39,39,39	1
87	OHX	5	3580	7/7	0.99	0.14	52,52,52,52	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
87	OHX	1	3440	7/7	0.99	0.10	61,61,61,61	7
87	OHX	1	3401	7/7	0.99	0.08	48,48,48,48	0
88	MG	5	4353	1/1	0.99	0.06	36,36,36,36	1
87	OHX	1	3402	7/7	0.99	0.09	58,58,58,58	2
87	OHX	1	3443	7/7	0.99	0.12	69,69,69,69	7
87	OHX	1	3404	7/7	0.99	0.07	59,59,59,59	2
87	OHX	1	3405	7/7	0.99	0.09	58,58,58,58	1
87	OHX	1	3446	7/7	0.99	0.09	46,46,46,46	7
87	OHX	1	3490	7/7	0.99	0.11	66,66,66,66	7
88	MG	5	4212	1/1	0.99	0.11	44,44,44,44	0
88	MG	1	4116	1/1	0.99	0.39	51,51,51,51	0
87	OHX	1	3407	7/7	0.99	0.09	64,64,64,64	0
87	OHX	1	3409	7/7	0.99	0.07	55,55,55,55	1
88	MG	1	4362	1/1	0.99	0.08	42,42,42,42	1
88	MG	O1	206	1/1	0.99	0.13	59,59,59,59	1
88	MG	5	4366	1/1	0.99	0.30	47,47,47,47	1
87	OHX	1	3449	7/7	0.99	0.08	74,74,74,74	7
87	OHX	1	3411	7/7	0.99	0.11	53,53,53,53	7
87	OHX	1	3413	7/7	0.99	0.08	56,56,56,56	7
88	MG	n1	203	1/1	0.99	0.05	37,37,37,37	1
88	MG	5	4527	1/1	0.99	0.10	39,39,39,39	0
87	OHX	N9	101	7/7	0.99	0.11	58,58,58,58	7
88	MG	1	4007	1/1	0.99	0.26	31,31,31,31	0
88	MG	n3	205	1/1	0.99	0.13	34,34,34,34	1
87	OHX	1	3414	7/7	0.99	0.13	49,49,49,49	7
87	OHX	2	1910	7/7	0.99	0.08	94,94,94,94	7
87	OHX	2	1902	7/7	0.99	0.08	86,86,86,86	0
87	OHX	1	3455	7/7	0.99	0.10	81,81,81,81	7
87	OHX	5	3491	7/7	0.99	0.13	47,47,47,47	7
87	OHX	2	1901	7/7	0.99	0.10	81,81,81,81	0
87	OHX	6	1901	7/7	0.99	0.09	62,62,62,62	0
88	MG	5	4230	1/1	0.99	0.10	44,44,44,44	0
88	MG	5	4380	1/1	0.99	0.06	34,34,34,34	1
88	MG	1	4131	1/1	0.99	0.09	41,41,41,41	0
87	OHX	6	1902	7/7	0.99	0.08	77,77,77,77	2
87	OHX	6	1903	7/7	0.99	0.10	63,63,63,63	3
88	MG	5	4384	1/1	0.99	0.04	40,40,40,40	0
88	MG	1	4253	1/1	0.99	0.11	44,44,44,44	1
87	OHX	6	1904	7/7	0.99	0.08	71,71,71,71	7
87	OHX	2	1925	7/7	0.99	0.06	112,112,112,112	7
88	MG	5	4237	1/1	0.99	0.09	38,38,38,38	1
88	MG	5	4547	1/1	0.99	0.12	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	OHX	6	1906	7/7	0.99	0.11	55,55,55,55	7
88	MG	o7	504	1/1	0.99	0.10	37,37,37,37	1
88	MG	q0	202	1/1	0.99	0.12	42,42,42,42	0
87	OHX	1	3419	7/7	0.99	0.10	62,62,62,62	7
88	MG	1	4383	1/1	0.99	0.07	51,51,51,51	1
87	OHX	6	1908	7/7	0.99	0.09	71,71,71,71	7
88	MG	1	4385	1/1	0.99	0.06	59,59,59,59	1
88	MG	1	4022	1/1	0.99	0.07	40,40,40,40	0
89	ZN	D6	101	1/1	0.99	0.04	88,88,88,88	0
87	OHX	6	1909	7/7	0.99	0.10	79,79,79,79	7
87	OHX	s1	301	7/7	0.99	0.06	80,80,80,80	0
87	OHX	6	1910	7/7	0.99	0.07	60,60,60,60	7
89	ZN	d6	500	1/1	0.99	0.04	67,67,67,67	0
87	OHX	8	202	7/7	0.99	0.12	49,49,49,49	2
89	ZN	d9	101	1/1	0.99	0.03	81,81,81,81	0
87	OHX	1	3459	7/7	0.99	0.10	74,74,74,74	7
88	MG	1	4392	1/1	0.99	0.09	45,45,45,45	1
87	OHX	6	1912	7/7	0.99	0.09	72,72,72,72	7
87	OHX	1	3420	7/7	0.99	0.11	49,49,49,49	7
87	OHX	1	3410	7/7	1.00	0.04	67,67,67,67	0
87	OHX	1	3403	7/7	1.00	0.09	48,48,48,48	2
89	ZN	D9	101	1/1	1.00	0.02	79,79,79,79	0
87	OHX	8	201	7/7	1.00	0.07	55,55,55,55	7
89	ZN	O7	101	1/1	1.00	0.02	47,47,47,47	0
89	ZN	Q0	201	1/1	1.00	0.03	53,53,53,53	0
87	OHX	5	3401	7/7	1.00	0.07	48,48,48,48	3
89	ZN	Q3	501	1/1	1.00	0.01	73,73,73,73	0
87	OHX	5	3402	7/7	1.00	0.07	48,48,48,48	0
87	OHX	5	3403	7/7	1.00	0.09	44,44,44,44	2
87	OHX	5	3431	7/7	1.00	0.08	50,50,50,50	7
87	OHX	1	3412	7/7	1.00	0.09	69,69,69,69	0
89	ZN	o7	501	1/1	1.00	0.01	53,53,53,53	0
89	ZN	q0	201	1/1	1.00	0.01	40,40,40,40	0
87	OHX	1	3408	7/7	1.00	0.07	47,47,47,47	7
89	ZN	q3	501	1/1	1.00	0.03	64,64,64,64	0
87	OHX	5	3406	7/7	1.00	0.08	58,58,58,58	2
87	OHX	1	3406	7/7	1.00	0.07	53,53,53,53	3

6.5 Other polymers ⓘ

There are no such residues in this entry.