



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 01:56 PM UTC

PDB ID : 4V7R / pdb_00004v7r
Title : Yeast 80S ribosome.
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Deposited on : 2010-07-23
Resolution : 4.00 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

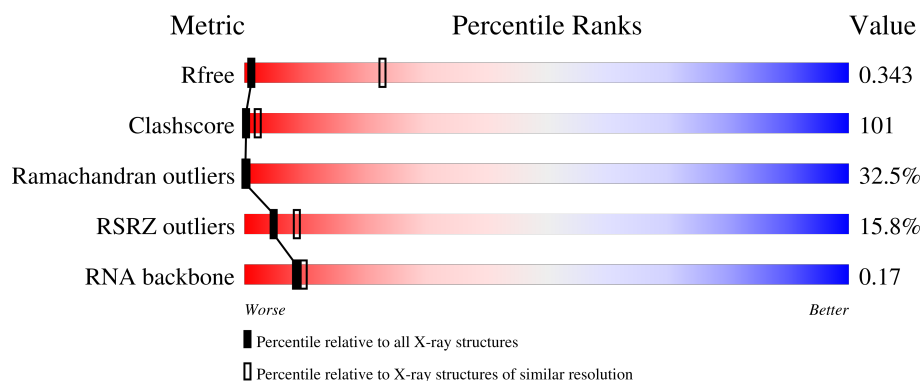
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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	A1	1800	8% 41% 55%
1	C1	1800	8% 42% 55%
2	AA	252	20% 19% 47% 17% 13%
2	CA	252	17% 19% 46% 19% 13%
3	AB	254	14% 23% 37% 22% 14%

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Mol	Chain	Length	Quality of chain
3	CB	254	
4	AC	240	
4	CC	240	
5	AD	225	
5	CD	225	
6	AE	197	
6	CE	197	
7	AF	156	
7	CF	156	
8	AG	151	
8	CG	151	
9	AH	137	
9	CH	137	
10	AI	142	
10	CI	142	
11	AJ	143	
11	CJ	143	
12	AK	136	
12	CK	136	
13	AL	146	
13	CL	146	
14	AM	144	
14	CM	144	
15	AN	121	
15	CN	121	

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Mol	Chain	Length	Quality of chain
16	AO	130	
16	CO	130	
17	AP	145	
17	CP	145	
18	AQ	108	
18	CQ	108	
19	AR	67	
19	CR	67	
20	AS	56	
20	CS	56	
21	AT	319	
21	CT	319	
22	Aa	20	
22	Bo	20	
22	Ca	20	
23	Ab	105	
23	Cb	105	
24	Ac	93	
24	Cc	93	
25	Ad	35	
25	Cd	35	
26	Ae	21	
26	Bj	21	
26	Dj	21	
27	Af	11	

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Mol	Chain	Length	Quality of chain
28	Ah	41	
28	Ch	41	
29	B1	3396	
29	D1	3396	
30	B2	121	
30	D2	121	
31	B3	158	
31	D3	158	
32	BA	217	
32	DA	217	
33	BB	254	
33	DB	254	
34	BC	387	
34	DC	387	
35	BD	362	
35	DD	362	
36	BE	297	
36	DE	297	
37	BF	176	
37	DF	176	
38	BG	244	
38	DG	244	
39	BH	256	
39	DH	256	
40	BI	191	

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Mol	Chain	Length	Quality of chain
40	DI	191	
41	BJ	221	
41	DJ	221	
42	BK	174	
42	DK	174	
43	BN	138	
43	DN	138	
44	BO	204	
44	DO	204	
45	BP	199	
45	DP	199	
46	BQ	184	
46	DQ	184	
47	BR	186	
47	DR	186	
48	BS	189	
48	DS	189	
49	BT	160	
49	DT	160	
50	BU	137	
50	DU	137	
51	BV	155	
51	DV	155	
52	BW	142	
52	DW	142	

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Mol	Chain	Length	Quality of chain
53	BX	127	
53	DX	127	
54	BY	149	
54	DY	149	
55	BZ	105	
55	DZ	105	
56	Ba	113	
56	Da	113	
57	Bb	130	
57	Db	130	
58	Bc	120	
58	Dc	120	
59	Bd	88	
59	Dd	88	
60	Be	51	
60	De	51	
61	Bf	106	
61	Df	106	
62	Bg	92	
62	Dg	92	
63	Bh	44	
63	Dh	44	
64	Bi	12	
64	Di	12	
65	Bk	16	

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Mol	Chain	Length	Quality of chain
65	Dk	16	
66	Bl	19	
67	Bm	9	
68	Bn	27	
69	Bp	8	
70	Bq	17	
71	Br	23	
72	DL	165	
73	DM	312	

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
74	OHX	A1	1901	-	-	X	-
74	OHX	A1	1910	-	-	X	-
74	OHX	A1	1913	-	-	X	-
74	OHX	A1	1915	-	-	X	-
74	OHX	A1	1916	-	-	X	-
74	OHX	A1	1917	-	-	X	-
74	OHX	A1	1931	-	-	X	-
74	OHX	A1	1943	-	-	X	-
74	OHX	A1	1949	-	-	X	-
74	OHX	A1	1953	-	-	-	X
74	OHX	A1	1966	-	-	-	X
74	OHX	A1	1974	-	-	-	X
74	OHX	A1	1975	-	-	X	-
74	OHX	A1	1976	-	-	X	-
74	OHX	A1	1978	-	-	-	X
74	OHX	A1	1983	-	-	-	X
74	OHX	A1	1986	-	-	X	-
74	OHX	A1	1988	-	-	-	X
74	OHX	A1	1993	-	-	-	X
74	OHX	A1	1995	-	-	-	X
74	OHX	A1	1996	-	-	-	X
74	OHX	A1	1998	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	AS	101	-	-	X	-
74	OHX	B1	3428	-	-	X	-
74	OHX	B1	3438	-	-	X	-
74	OHX	B1	3449	-	-	X	-
74	OHX	B1	3450	-	-	X	-
74	OHX	B1	3479	-	-	X	-
74	OHX	B1	3492	-	-	X	-
74	OHX	B1	3505	-	-	X	-
74	OHX	B1	3515	-	-	-	X
74	OHX	B1	3529	-	-	X	-
74	OHX	B1	3533	-	-	-	X
74	OHX	B1	3536	-	-	X	-
74	OHX	B1	3537	-	-	X	-
74	OHX	B1	3542	-	-	-	X
74	OHX	B1	3545	-	-	-	X
74	OHX	B1	3548	-	-	-	X
74	OHX	B1	3551	-	-	-	X
74	OHX	B1	3554	-	-	-	X
74	OHX	B1	3555	-	-	-	X
74	OHX	B1	3558	-	-	X	-
74	OHX	B1	3563	-	-	X	-
74	OHX	B1	3567	-	-	X	-
74	OHX	B1	3577	-	-	-	X
74	OHX	B1	3581	-	-	X	-
74	OHX	B1	3584	-	-	-	X
74	OHX	B1	3587	-	-	X	-
74	OHX	B1	3589	-	-	-	X
74	OHX	B1	3592	-	-	-	X
74	OHX	B1	3599	-	-	X	-
74	OHX	B1	3602	-	-	-	X
74	OHX	B1	3608	-	-	-	X
74	OHX	B1	3609	-	-	-	X
74	OHX	B1	3613	-	-	-	X
74	OHX	B1	3620	-	-	X	-
74	OHX	B2	201	-	-	X	-
74	OHX	B2	207	-	-	-	X
74	OHX	B2	208	-	-	-	X
74	OHX	B2	210	-	-	-	X
74	OHX	B3	206	-	-	X	-
74	OHX	BO	301	-	-	-	X
74	OHX	Bd	101	-	-	X	-
74	OHX	Bg	101	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	C1	1916	-	-	X	-
74	OHX	C1	1917	-	-	X	-
74	OHX	C1	1924	-	-	X	-
74	OHX	C1	1928	-	-	X	-
74	OHX	C1	1930	-	-	X	-
74	OHX	C1	1933	-	-	X	-
74	OHX	C1	1955	-	-	X	-
74	OHX	C1	1957	-	-	-	X
74	OHX	C1	1964	-	-	X	-
74	OHX	C1	1970	-	-	X	-
74	OHX	C1	1974	-	-	-	X
74	OHX	C1	1976	-	-	-	X
74	OHX	C1	1978	-	-	-	X
74	OHX	C1	1980	-	-	-	X
74	OHX	C1	1983	-	-	X	-
74	OHX	C1	1985	-	-	-	X
74	OHX	C1	1988	-	-	-	X
74	OHX	C1	1989	-	-	-	X
74	OHX	C1	1991	-	-	-	X
74	OHX	C1	1995	-	-	-	X
74	OHX	C1	1996	-	-	-	X
74	OHX	C1	1998	-	-	-	X
74	OHX	CS	101	-	-	X	-
74	OHX	D1	3408	-	-	X	-
74	OHX	D1	3415	-	-	X	-
74	OHX	D1	3430	-	-	X	-
74	OHX	D1	3431	-	-	X	-
74	OHX	D1	3452	-	-	X	-
74	OHX	D1	3463	-	-	X	-
74	OHX	D1	3473	-	-	X	-
74	OHX	D1	3480	-	-	X	-
74	OHX	D1	3502	-	-	X	-
74	OHX	D1	3506	-	-	-	X
74	OHX	D1	3509	-	-	-	X
74	OHX	D1	3516	-	-	-	X
74	OHX	D1	3519	-	-	-	X
74	OHX	D1	3522	-	-	-	X
74	OHX	D1	3535	-	-	-	X
74	OHX	D1	3541	-	-	-	X
74	OHX	D1	3543	-	-	X	-
74	OHX	D1	3545	-	-	-	X
74	OHX	D1	3555	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	OHX	D1	3567	-	-	X	-
74	OHX	D1	3568	-	-	X	X
74	OHX	D1	3573	-	-	-	X
74	OHX	D1	3574	-	-	X	-
74	OHX	D1	3578	-	-	-	X
74	OHX	D1	3582	-	-	X	-
74	OHX	D1	3583	-	-	X	-
74	OHX	D1	3586	-	-	-	X
74	OHX	D1	3587	-	-	-	X
74	OHX	D1	3588	-	-	X	-
74	OHX	D1	3593	-	-	-	X
74	OHX	D1	3595	-	-	-	X
74	OHX	D1	3601	-	-	-	X
74	OHX	D1	3603	-	-	-	X
74	OHX	D1	3605	-	-	-	X
74	OHX	D1	3610	-	-	-	X
74	OHX	D1	3616	-	-	-	X
74	OHX	D1	3623	-	-	-	X
74	OHX	D2	201	-	-	X	-
74	OHX	D2	207	-	-	X	-
74	OHX	D3	202	-	-	X	-
74	OHX	D3	205	-	-	X	-
74	OHX	D3	206	-	-	-	X
74	OHX	D3	212	-	-	X	-
74	OHX	DO	301	-	-	X	-
74	OHX	Dd	101	-	-	X	-
74	OHX	Dg	101	-	-	X	-

2 Entry composition

There are 74 unique types of molecules in this entry. The entry contains 309610 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	A1	1789	Total	C	N	O	P	0	0	0
			38107	17037	6732	12549	1789			
1	C1	1789	Total	C	N	O	P	0	0	0
			38107	17037	6732	12549	1789			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AA	220	Total	C	N	O	0	0	0
			1090	650	220	220			
2	CA	220	Total	C	N	O	0	0	0
			1090	650	220	220			

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AB	219	Total	C	N	O	0	0	0
			1074	636	219	219			
3	CB	219	Total	C	N	O	0	0	0
			1074	636	219	219			

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AC	189	Total	C	N	O	0	0	0
			928	550	189	189			
4	CC	189	Total	C	N	O	0	0	0
			928	550	189	189			

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AD	169	Total	C	N	O	0	0	0
			836	498	169	169			
5	CD	169	Total	C	N	O	0	0	0
			836	498	169	169			

- Molecule 6 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	AE	157	Total	C	N	O	0	0	0
			777	463	157	157			
6	CE	157	Total	C	N	O	0	0	0
			777	463	157	157			

- Molecule 7 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	AF	77	Total	C	N	O	0	0	0
			382	228	77	77			
7	CF	77	Total	C	N	O	0	0	0
			382	228	77	77			

- Molecule 8 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AG	117	Total	C	N	O	0	0	0
			580	346	117	117			
8	CG	117	Total	C	N	O	0	0	0
			580	346	117	117			

- Molecule 9 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AH	128	Total	C	N	O	0	0	0
			627	371	128	128			
9	CH	128	Total	C	N	O	0	0	0
			627	371	128	128			

- Molecule 10 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AI	121	Total	C	N	O	0	0	0
			596	354	121	121			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CI	121	Total	C	N	O	0	0	0
			596	354	121	121			

- Molecule 11 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AJ	134	Total	C	N	O	0	0	0
			658	390	134	134			
11	CJ	134	Total	C	N	O	0	0	0
			658	390	134	134			

- Molecule 12 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AK	67	Total	C	N	O	0	0	0
			332	198	67	67			
12	CK	67	Total	C	N	O	0	0	0
			332	198	67	67			

- Molecule 13 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AL	120	Total	C	N	O	0	0	0
			591	351	120	120			
13	CL	120	Total	C	N	O	0	0	0
			591	351	120	120			

- Molecule 14 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AM	106	Total	C	N	O	0	0	0
			521	309	106	106			
14	CM	106	Total	C	N	O	0	0	0
			521	309	106	106			

- Molecule 15 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AN	111	Total	C	N	O	0	0	0
			551	329	111	111			
15	CN	111	Total	C	N	O	0	0	0
			551	329	111	111			

- Molecule 16 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AO	127	Total	C	N	O	0	0	0
			622	368	127	127			
16	CO	127	Total	C	N	O	0	0	0
			622	368	127	127			

- Molecule 17 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AP	116	Total	C	N	O	0	0	0
			566	334	116	116			
17	CP	116	Total	C	N	O	0	0	0
			566	334	116	116			

- Molecule 18 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AQ	67	Total	C	N	O	0	0	0
			332	198	67	67			
18	CQ	63	Total	C	N	O	0	0	0
			312	186	63	63			

- Molecule 19 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AR	47	Total	C	N	O	0	0	0
			230	136	47	47			
19	CR	47	Total	C	N	O	0	0	0
			230	136	47	47			

- Molecule 20 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AS	39	Total	C	N	O	0	0	0
			190	112	39	39			
20	CS	39	Total	C	N	O	0	0	0
			190	112	39	39			

- Molecule 21 is a protein called Guanine nucleotide-binding protein subunit beta-like protein; RACK-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AT	313	Total	C	N	O	0	0	0
			1543	917	313	313			
21	CT	313	Total	C	N	O	0	0	0
			1543	917	313	313			

- Molecule 22 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	Aa	20	Total	C	N	O	0	0	0
			100	60	20	20			
22	Bo	20	Total	C	N	O	0	0	0
			100	60	20	20			
22	Ca	20	Total	C	N	O	0	0	0
			100	60	20	20			

- Molecule 23 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	Ab	105	Total	C	N	O	0	0	0
			525	315	105	105			
23	Cb	105	Total	C	N	O	0	0	0
			525	315	105	105			

- Molecule 24 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	Ac	93	Total	C	N	O	0	0	0
			465	279	93	93			
24	Cc	93	Total	C	N	O	0	0	0
			465	279	93	93			

- Molecule 25 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Ad	35	Total	C	N	O	0	0	0
			175	105	35	35			
25	Cd	35	Total	C	N	O	0	0	0
			175	105	35	35			

- Molecule 26 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Ae	21	Total	C	N	O	0	0	0
			105	63	21	21			
26	Bj	21	Total	C	N	O	0	0	0
			105	63	21	21			
26	Dj	21	Total	C	N	O	0	0	0
			105	63	21	21			

- Molecule 27 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	Af	11	Total	C	N	O	0	0	0
			55	33	11	11			

- Molecule 28 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	Ah	41	Total	C	N	O	0	0	0
			205	123	41	41			
28	Ch	41	Total	C	N	O	0	0	0
			205	123	41	41			

- Molecule 29 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B1	3206	Total	C	N	O	P	0	0	0
			68577	30632	12365	22374	3206			
29	D1	3206	Total	C	N	O	P	0	0	0
			68577	30632	12365	22374	3206			

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B2	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
30	D2	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 31 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B3	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D3	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 32 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	BA	213	Total	C	N	O	0	0	0
			1055	629	213	213			
32	DA	213	Total	C	N	O	0	0	0
			1055	629	213	213			

- Molecule 33 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	BB	234	Total	C	N	O	0	0	0
			1106	638	234	234			
33	DB	234	Total	C	N	O	0	0	0
			1106	638	234	234			

- Molecule 34 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	BC	364	Total	C	N	O	0	0	0
			1791	1063	364	364			
34	DC	364	Total	C	N	O	0	0	0
			1791	1063	364	364			

- Molecule 35 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	BD	268	Total	C	N	O	0	0	0
			1312	776	268	268			
35	DD	268	Total	C	N	O	0	0	0
			1312	776	268	268			

- Molecule 36 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BE	287	Total	C	N	O	0	0	0
			1412	838	287	287			
36	DE	287	Total	C	N	O	0	0	0
			1412	838	287	287			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BE	112	ARG	LYS	conflict	UNP P26321
DE	112	ARG	LYS	conflict	UNP P26321

- Molecule 37 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BF	176	Total	C	N	O	0	0	0
			873	521	176	176			
37	DF	176	Total	C	N	O	0	0	0
			873	521	176	176			

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BG	215	Total	C	N	O	0	0	0
			1061	631	215	215			
38	DG	215	Total	C	N	O	0	0	0
			1061	631	215	215			

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BH	173	Total	C	N	O	0	0	0
			856	510	173	173			
39	DH	173	Total	C	N	O	0	0	0
			856	510	173	173			

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BI	191	Total	C	N	O	0	0	0
			942	560	191	191			
40	DI	191	Total	C	N	O	0	0	0
			942	560	191	191			

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BJ	208	Total	C	N	O	0	0	0
			1027	611	208	208			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	DJ	208	Total	C	N	O	0	0	0
			1027	611	208	208			

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BK	165	Total	C	N	O	0	0	0
			810	480	165	165			
42	DK	165	Total	C	N	O	0	0	0
			810	480	165	165			

- Molecule 43 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BN	120	Total	C	N	O	0	0	0
			593	353	120	120			
43	DN	120	Total	C	N	O	0	0	0
			593	353	120	120			

- Molecule 44 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BO	187	Total	C	N	O	0	0	0
			923	549	187	187			
44	DO	187	Total	C	N	O	0	0	0
			923	549	187	187			

- Molecule 45 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BP	196	Total	C	N	O	0	0	0
			967	575	196	196			
45	DP	196	Total	C	N	O	0	0	0
			967	575	196	196			

- Molecule 46 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BQ	154	Total	C	N	O	0	0	0
			761	453	154	154			
46	DQ	154	Total	C	N	O	0	0	0
			761	453	154	154			

- Molecule 47 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	BR	143	Total	C	N	O	0	0	0
			706	420	143	143			
47	DR	143	Total	C	N	O	0	0	0
			706	420	143	143			

- Molecule 48 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BS	188	Total	C	N	O	0	0	0
			931	555	188	188			
48	DS	188	Total	C	N	O	0	0	0
			931	555	188	188			

- Molecule 49 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BT	119	Total	C	N	O	0	0	0
			586	348	119	119			
49	DT	119	Total	C	N	O	0	0	0
			586	348	119	119			

- Molecule 50 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BU	129	Total	C	N	O	0	0	0
			631	373	129	129			
50	DU	129	Total	C	N	O	0	0	0
			631	373	129	129			

- Molecule 51 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BV	59	Total	C	N	O	0	0	0
			291	173	59	59			
51	DV	59	Total	C	N	O	0	0	0
			291	173	59	59			

- Molecule 52 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BW	94	Total	C	N	O	0	0	0
			468	280	94	94			
52	DW	94	Total	C	N	O	0	0	0
			468	280	94	94			

- Molecule 53 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	BX	107	Total	C	N	O	0	0	0
			530	316	107	107			
53	DX	107	Total	C	N	O	0	0	0
			530	316	107	107			

- Molecule 54 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BY	149	Total	C	N	O	0	0	0
			727	429	149	149			
54	DY	149	Total	C	N	O	0	0	0
			727	429	149	149			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BY	38	GLU	GLN	conflict	UNP P02406
DY	38	GLU	GLN	conflict	UNP P02406

- Molecule 55 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BZ	98	Total	C	N	O	0	0	0
			481	285	98	98			
55	DZ	98	Total	C	N	O	0	0	0
			481	285	98	98			

- Molecule 56 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	Ba	86	Total	C	N	O	0	0	0
			425	253	86	86			
56	Da	86	Total	C	N	O	0	0	0
			425	253	86	86			

- Molecule 57 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	Bb	125	Total	C	N	O	0	0	0
			618	368	125	125			
57	Db	125	Total	C	N	O	0	0	0
			618	368	125	125			

- Molecule 58 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	Bc	68	Total	C	N	O	0	0	0
			339	203	68	68			
58	Dc	68	Total	C	N	O	0	0	0
			339	203	68	68			

- Molecule 59 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
59	Bd	72	Total	C	N	O	0	0	0
			352	208	72	72			
59	Dd	72	Total	C	N	O	0	0	0
			352	208	72	72			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
60	Be	48	Total	C	N	O	0	0	0
			240	144	48	48			
60	De	48	Total	C	N	O	0	0	0
			240	144	48	48			

- Molecule 61 is a protein called 60S ribosomal protein L42.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
61	Bf	95	Total	C	N	O	0	0	0
			467	277	95	95			
61	Df	95	Total	C	N	O	0	0	0
			467	277	95	95			

- Molecule 62 is a protein called 60S ribosomal protein L43.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	Bg	83	Total	C	N	O	0	0	0
			407	241	83	83			
62	Dg	83	Total	C	N	O	0	0	0
			407	241	83	83			

- Molecule 63 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	Bh	44	Total	C	N	O	0	0	0
			220	132	44	44			
63	Dh	44	Total	C	N	O	0	0	0
			220	132	44	44			

- Molecule 64 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
64	Bi	12	Total	C	N	O	0	0	0
			60	36	12	12			
64	Di	12	Total	C	N	O	0	0	0
			60	36	12	12			

- Molecule 65 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	Bk	16	Total	C	N	O	0	0	0
			80	48	16	16			
65	Dk	16	Total	C	N	O	0	0	0
			80	48	16	16			

- Molecule 66 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
66	Bl	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 67 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
67	Bm	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 68 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
68	Bn	27	Total	C	N	O	0	0	0
			135	81	27	27			

- Molecule 69 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
69	Bp	8	Total	C	N	O	0	0	0
			40	24	8	8			

- Molecule 70 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
70	Bq	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 71 is a protein called Unassigned secondary structure.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
71	Br	23	Total	C	N	O	0	0	0
			115	69	23	23			

- Molecule 72 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
72	DL	138	Total	C	N	O	0	0	0
			679	403	138	138			

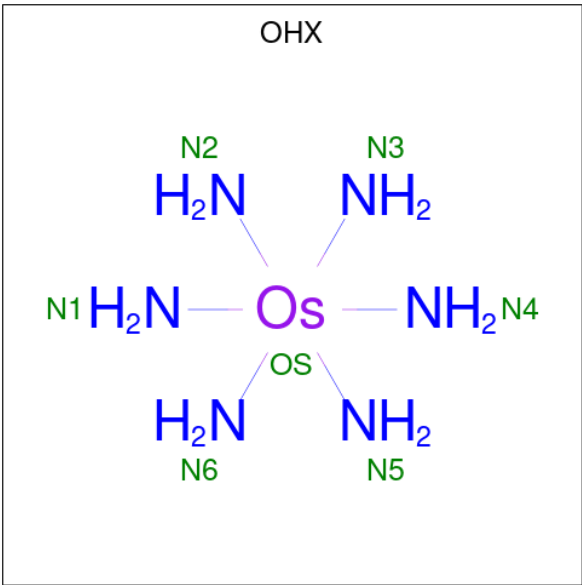
- Molecule 73 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
73	DM	130	Total	C	N	O	0	0	0
			641	381	130	130			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DM	83	TYR	ASN	conflict	UNP P05317

- Molecule 74 is osmium (III) hexamine (CCD ID: OHX) (formula: H₁₂N₆Os).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	A1	1	Total	N	Os	0	0
			7	6	1		
74	AL	1	Total	N	Os	0	0
			7	6	1		
74	AS	1	Total	N	Os	0	0
			7	6	1		
74	AT	1	Total	N	Os	0	0
			7	6	1		
74	Ac	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
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74	B1	1	Total	N	Os	0	0
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74	B1	1	Total	N	Os	0	0
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74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
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74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B1	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B2	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	B3	1	Total	N	Os	0	0
			7	6	1		
74	BC	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	BO	1	Total	N	Os	0	0
			7	6	1		
74	BT	1	Total	N	Os	0	0
			7	6	1		
74	Bd	1	Total	N	Os	0	0
			7	6	1		
74	Bd	1	Total	N	Os	0	0
			7	6	1		
74	Bg	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	C1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	C1	1	Total	N	Os	0	0
			7	6	1		
74	CI	1	Total	N	Os	0	0
			7	6	1		
74	CS	1	Total	N	Os	0	0
			7	6	1		
74	CS	1	Total	N	Os	0	0
			7	6	1		
74	CT	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D1	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D2	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	D3	1	Total	N	Os	0	0
			7	6	1		
74	DC	1	Total	N	Os	0	0
			7	6	1		

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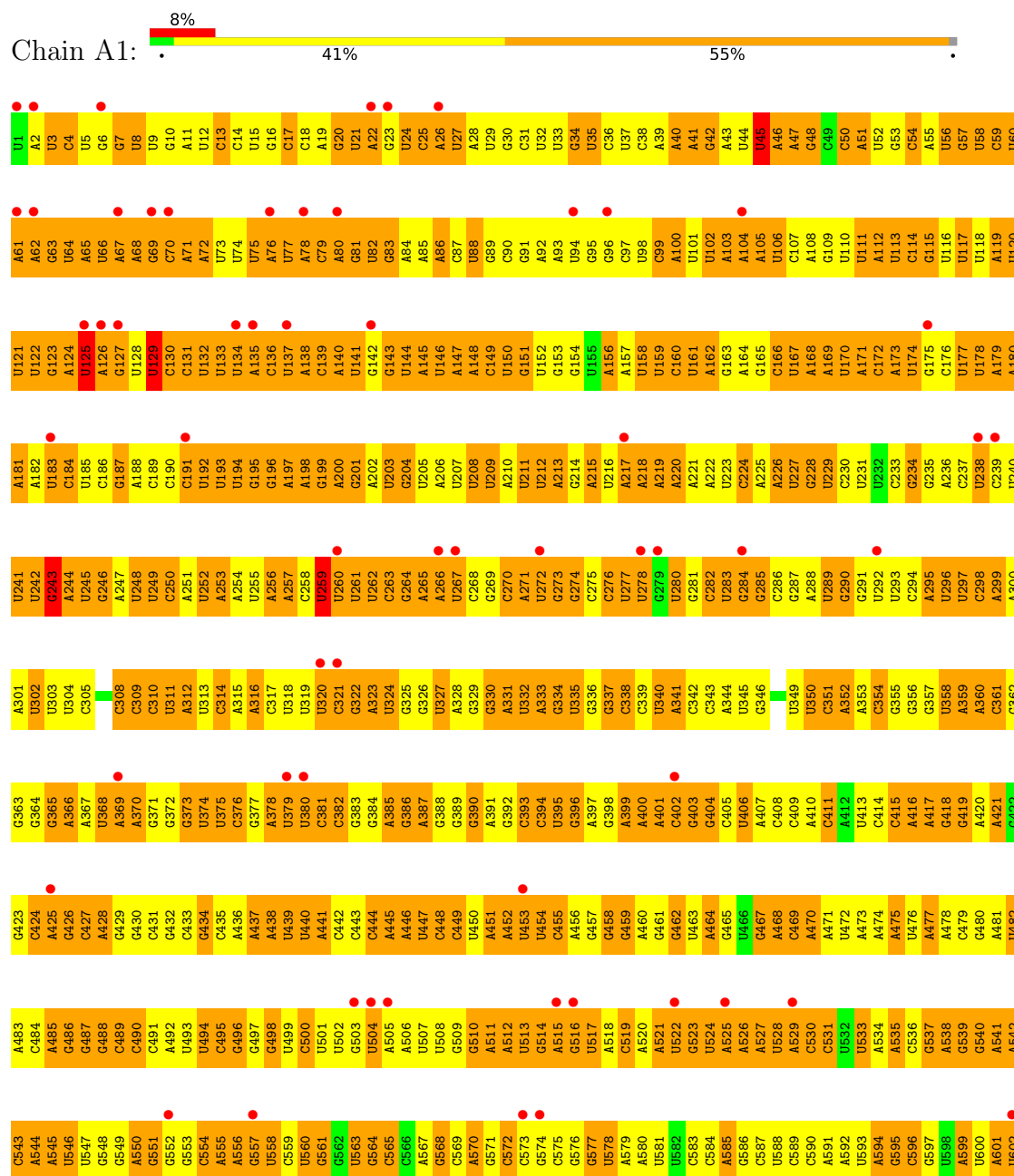
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
74	DE	1	Total	N	Os	0	0
			7	6	1		
74	DJ	1	Total	N	Os	0	0
			7	6	1		
74	DO	1	Total	N	Os	0	0
			7	6	1		
74	DO	1	Total	N	Os	0	0
			7	6	1		
74	DT	1	Total	N	Os	0	0
			7	6	1		
74	Dd	1	Total	N	Os	0	0
			7	6	1		
74	Dd	1	Total	N	Os	0	0
			7	6	1		
74	Dg	1	Total	N	Os	0	0
			7	6	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.

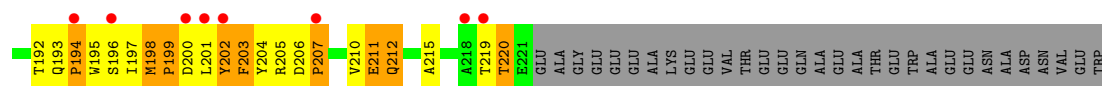
• Molecule 1: 18S ribosomal RNA



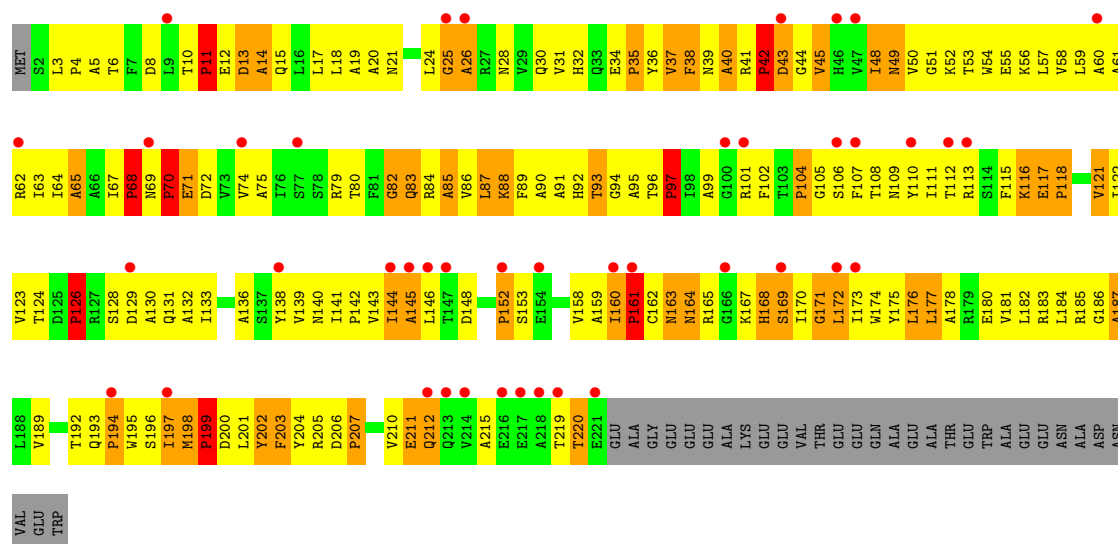
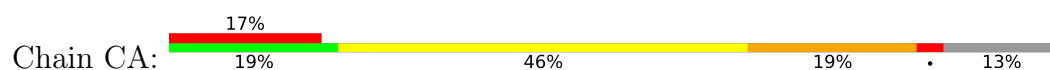
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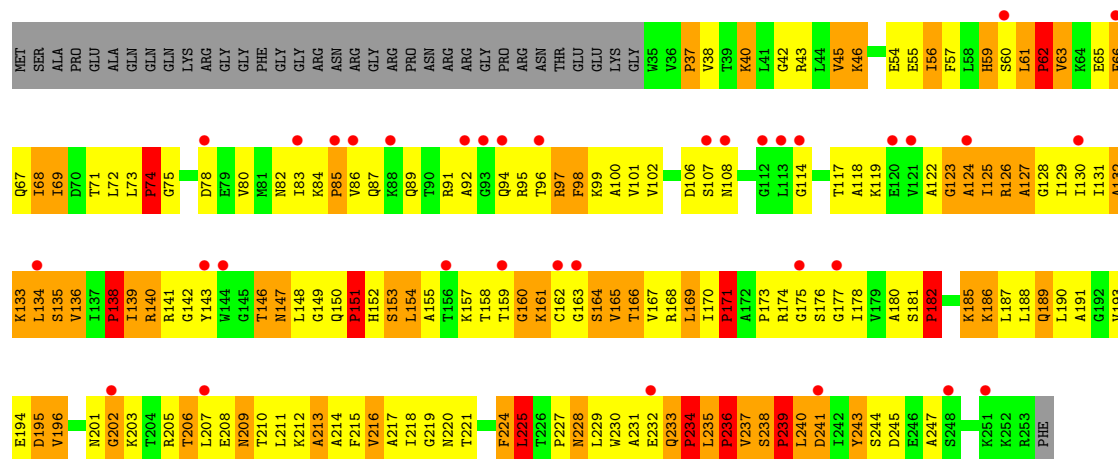
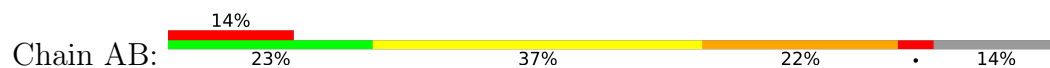
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A1202	C1202	A1142	C1082	C1022	C962	G902	U782	G722	U662	U602	A542	U482
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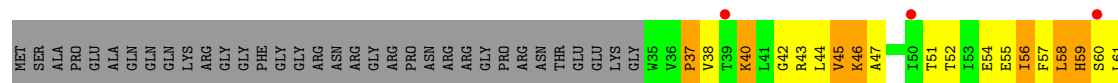
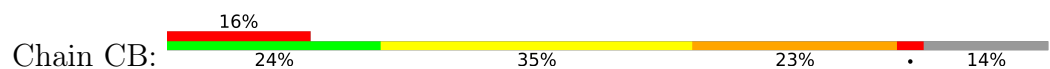
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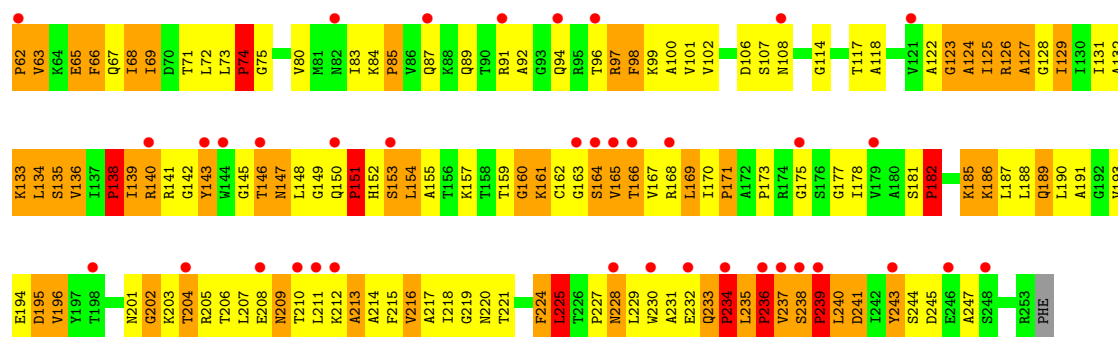


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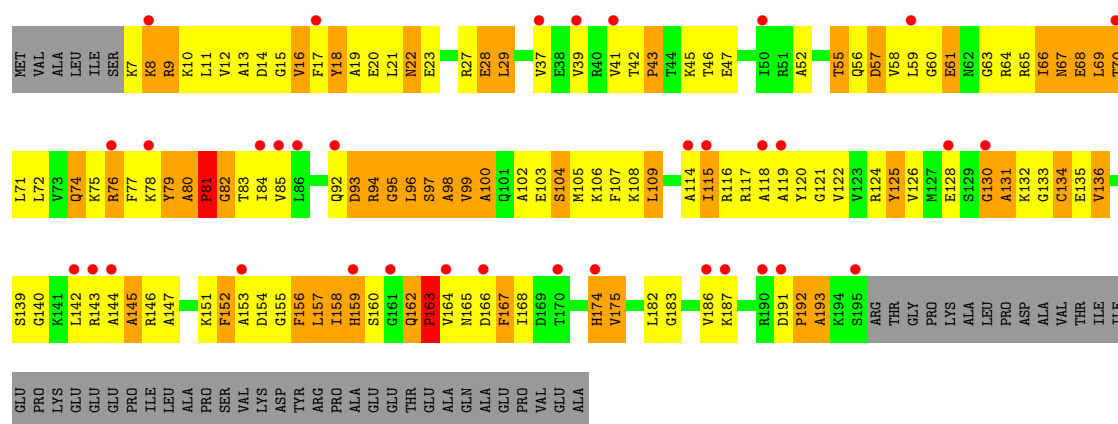
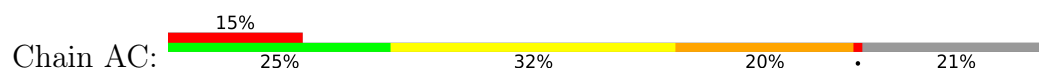


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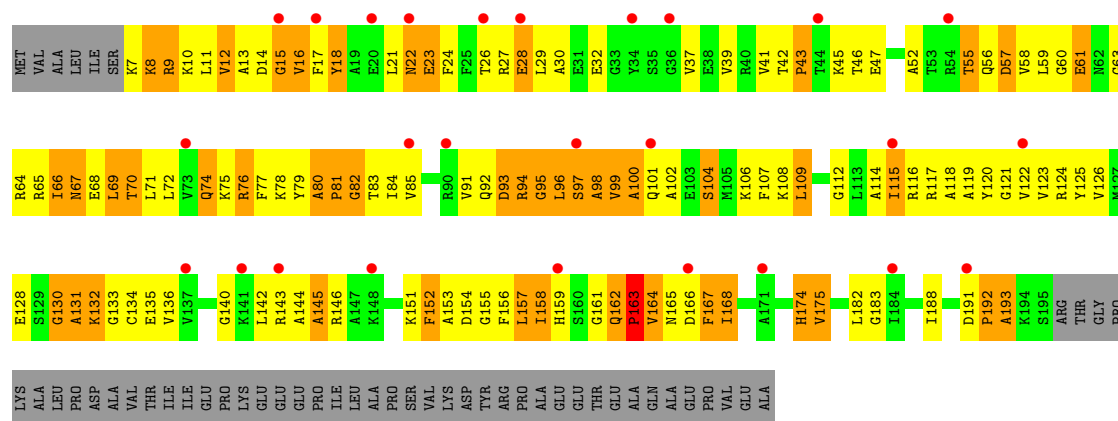
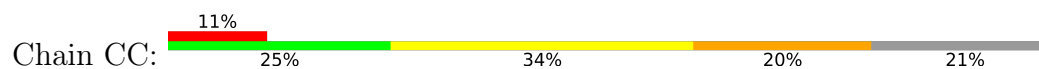




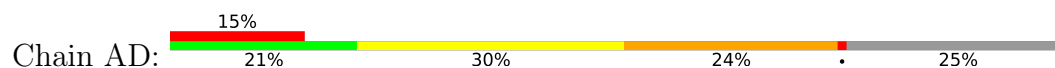
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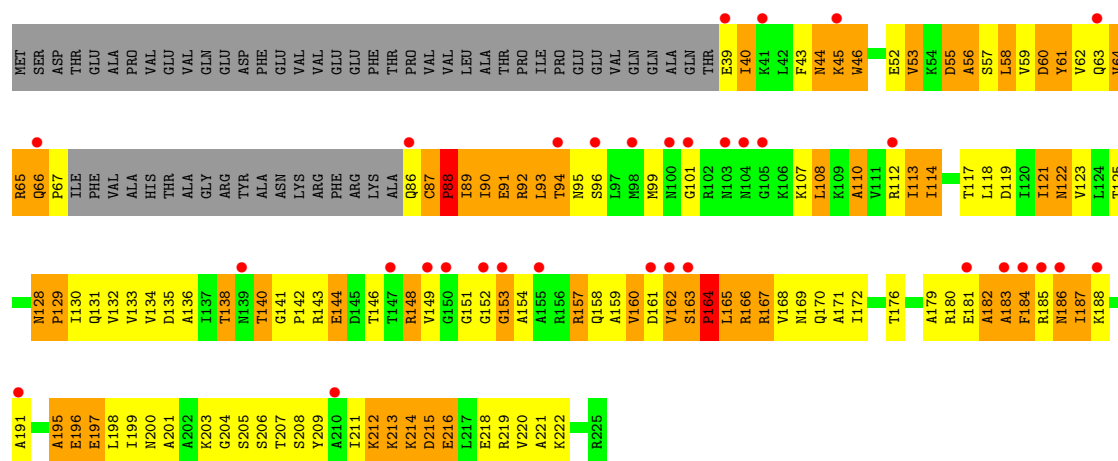


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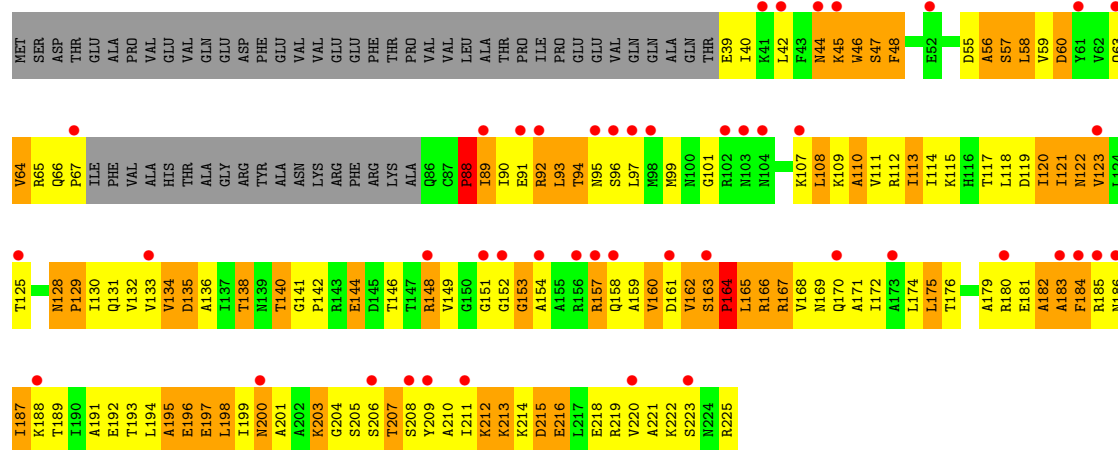


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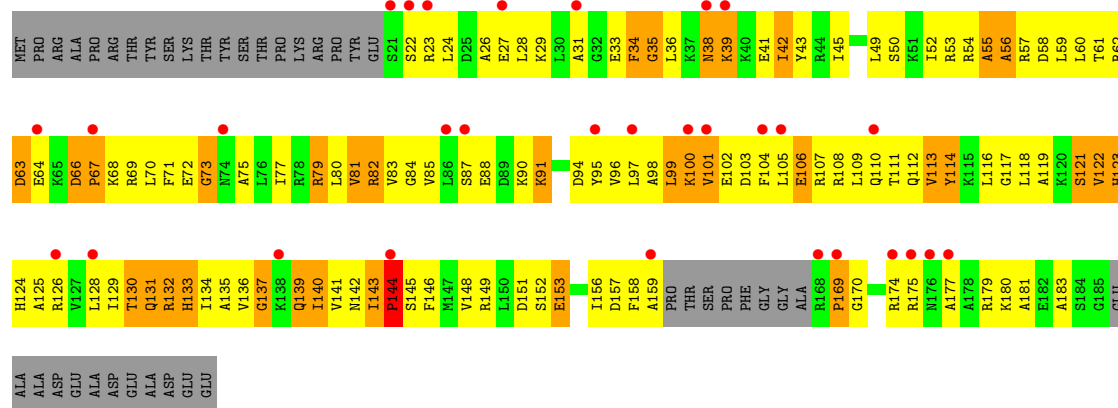
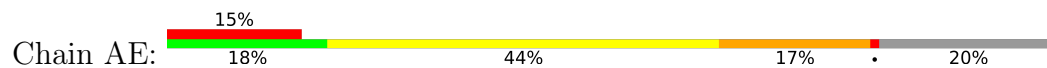




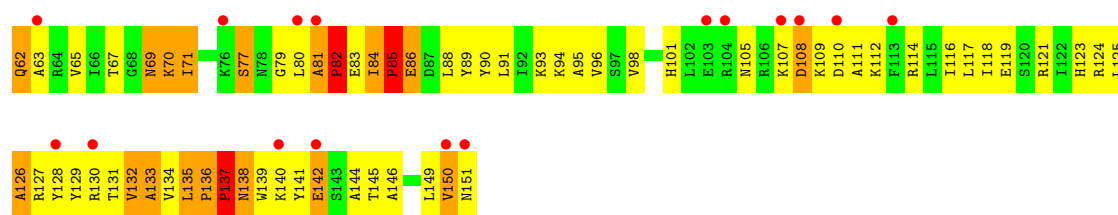
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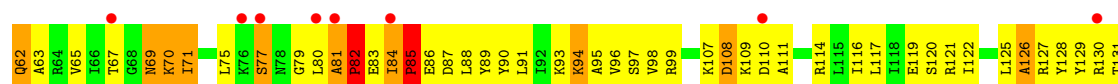
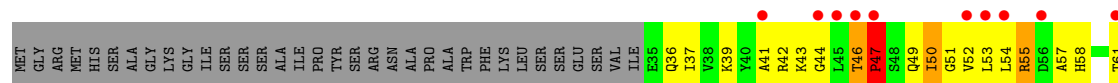
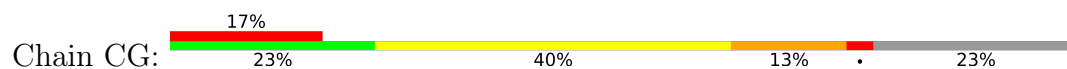
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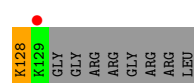
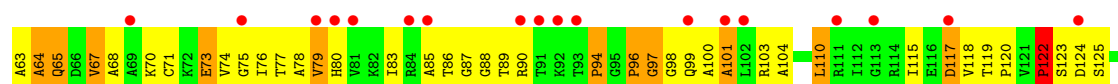
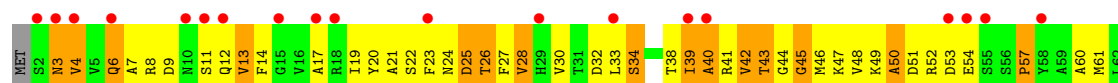
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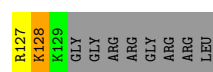
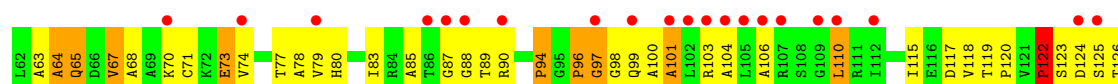
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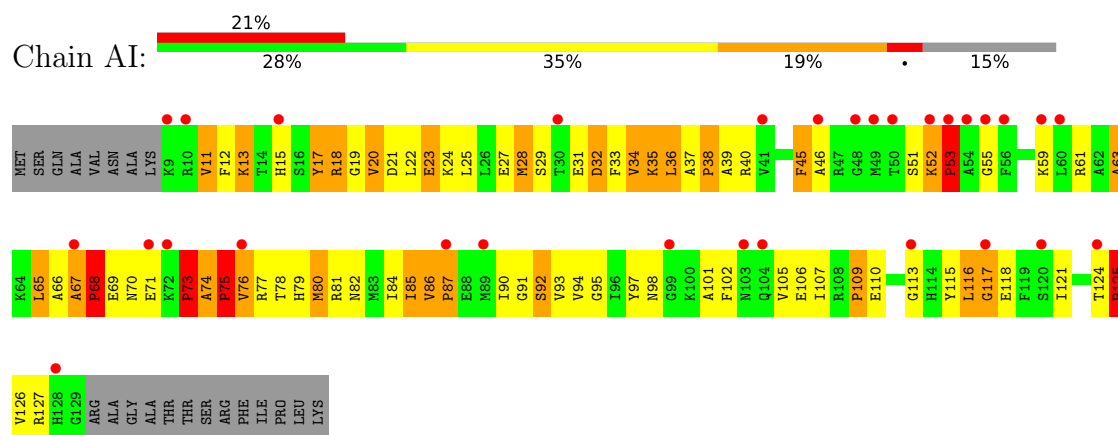
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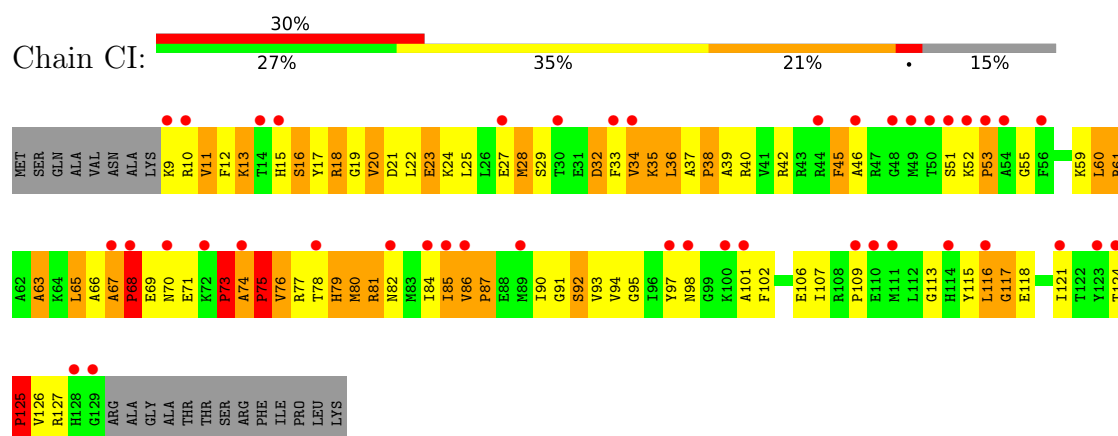
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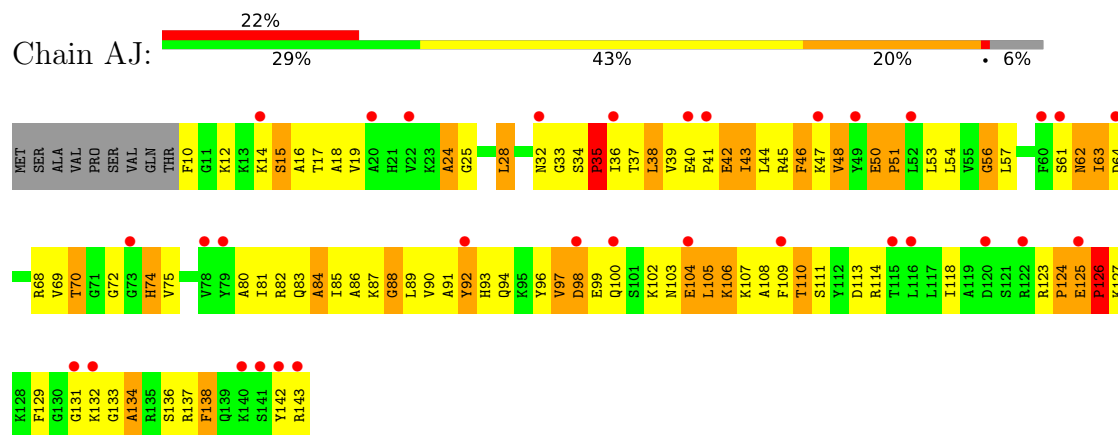
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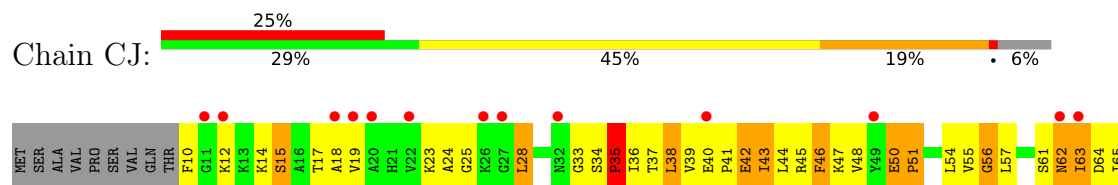
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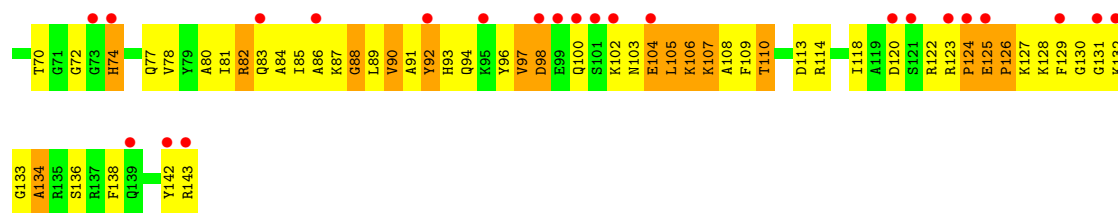


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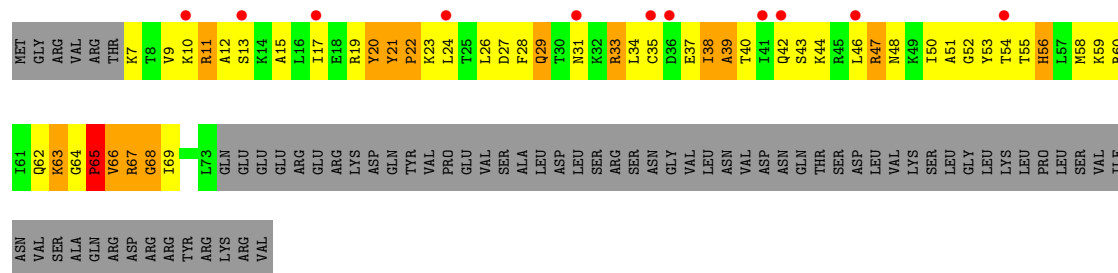
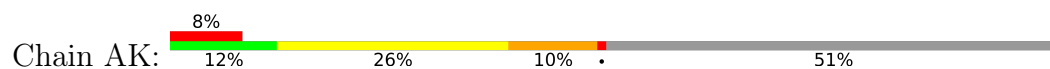


• Molecule 11: 40S ribosomal protein S16

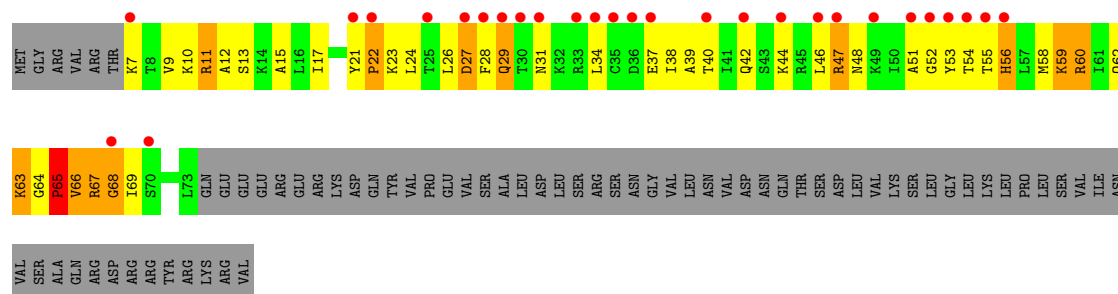
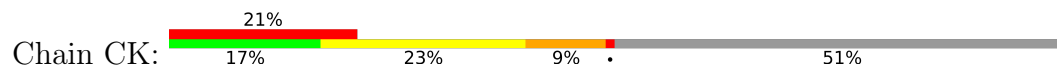




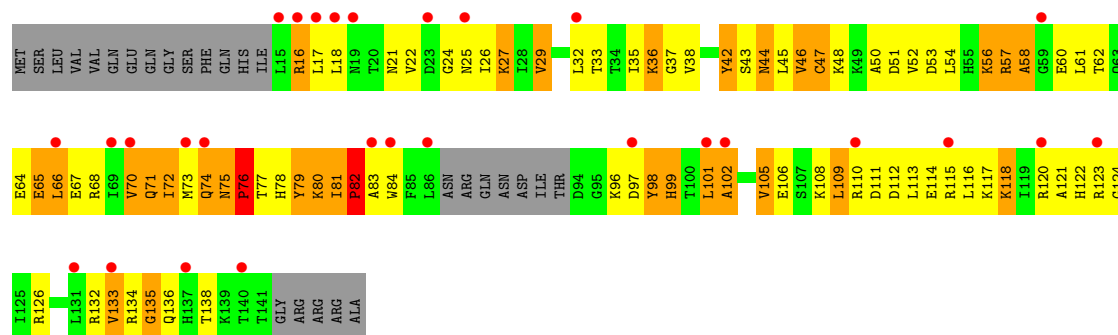
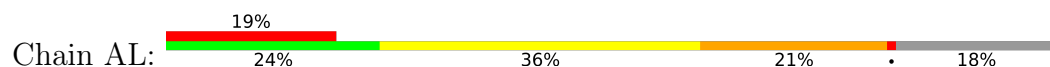
• Molecule 12: 40S ribosomal protein S17-A



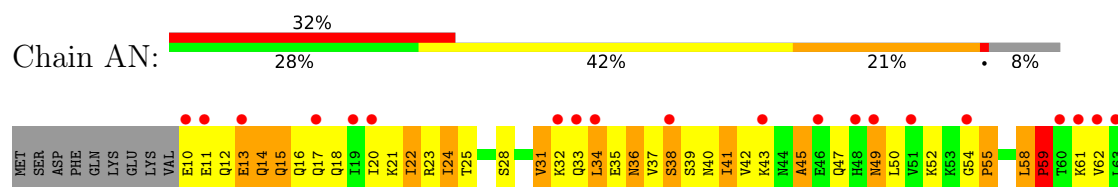
• Molecule 12: 40S ribosomal protein S17-A



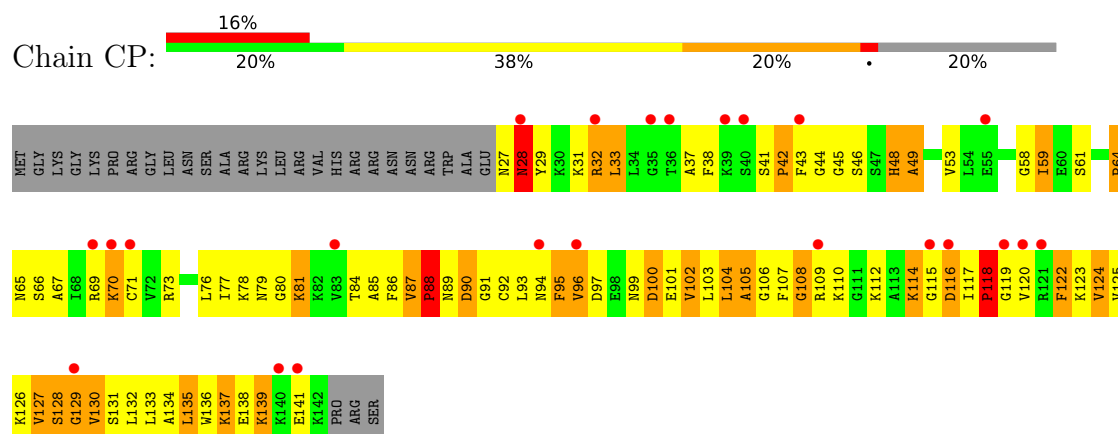
• Molecule 13: 40S ribosomal protein S18



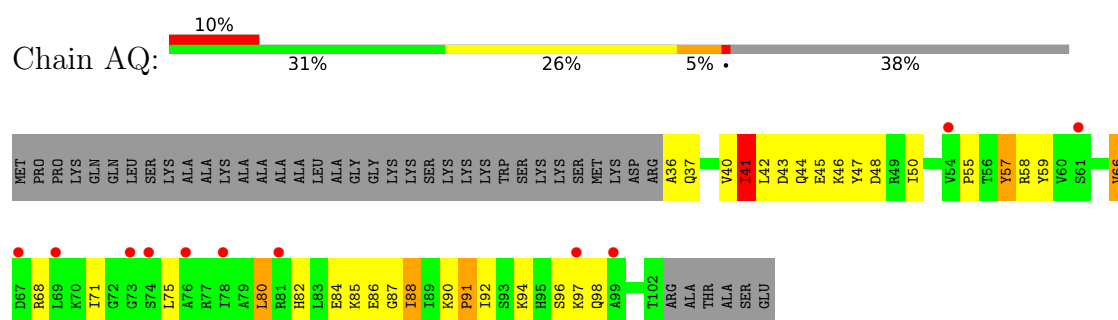
• Molecule 13: 40S ribosomal protein S18



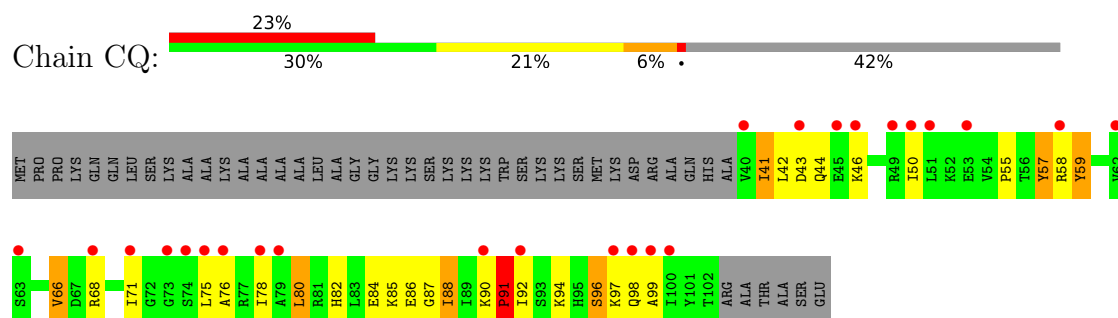
- Molecule 17: 40S ribosomal protein S23



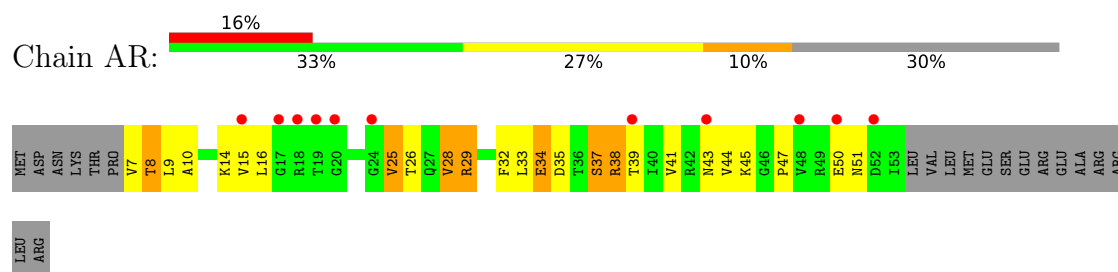
- Molecule 18: 40S ribosomal protein S25-A



- Molecule 18: 40S ribosomal protein S25-A

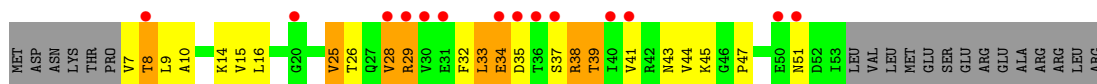


- Molecule 19: 40S ribosomal protein S28-A

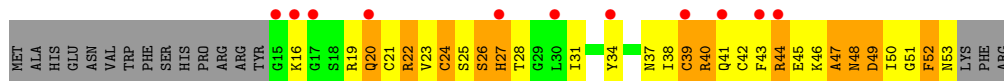


- Molecule 19: 40S ribosomal protein S28-A

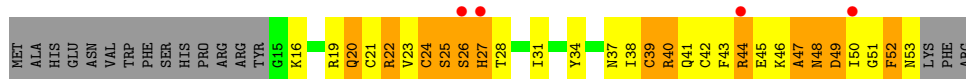




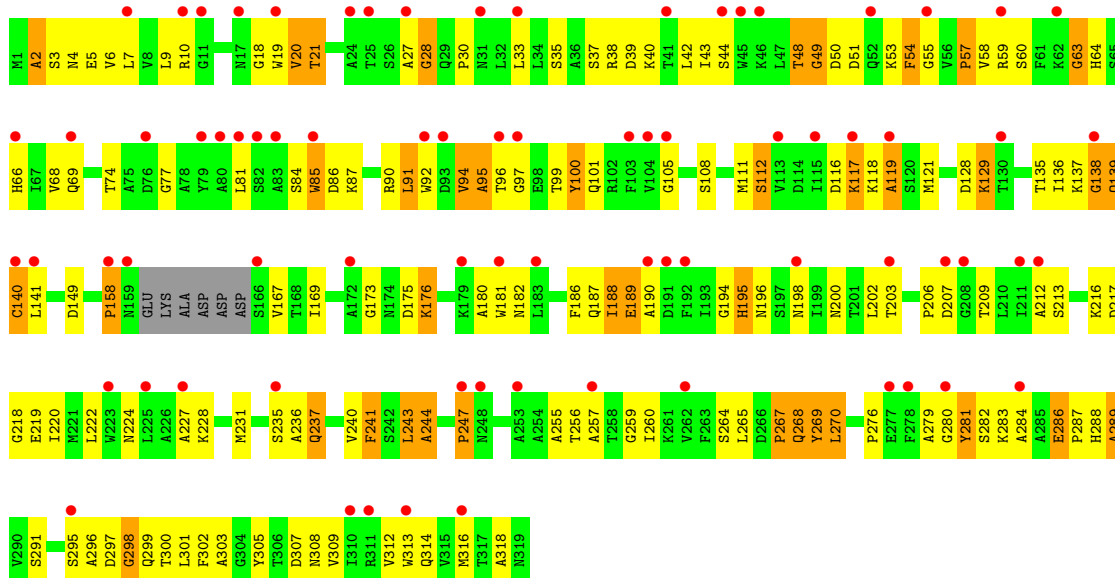
- Molecule 20: 40S ribosomal protein S29-A



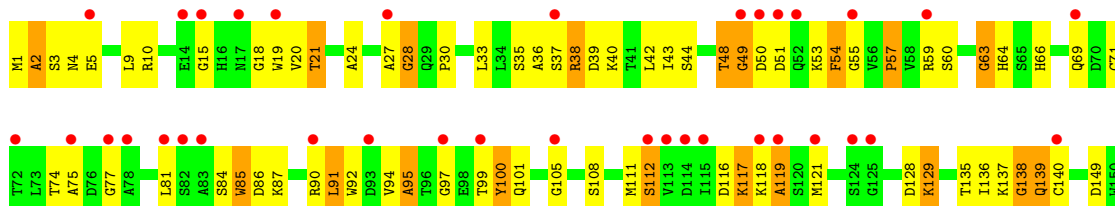
- Molecule 20: 40S ribosomal protein S29-A

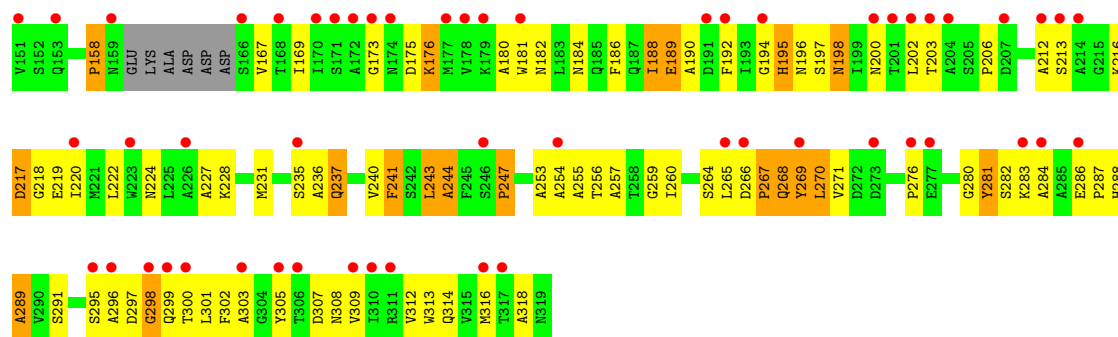


- Molecule 21: Guanine nucleotide-binding protein subunit beta-like protein; RACK-1



- Molecule 21: Guanine nucleotide-binding protein subunit beta-like protein; RACK-1





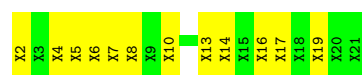
• Molecule 22: Unassigned secondary structure



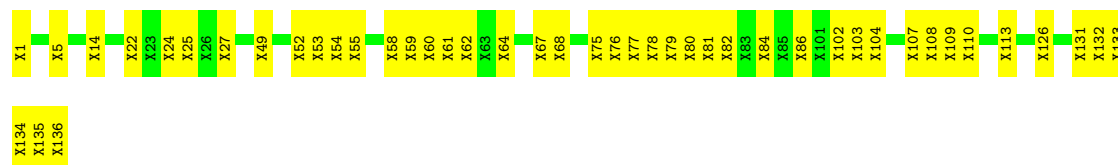
• Molecule 22: Unassigned secondary structure



• Molecule 22: Unassigned secondary structure

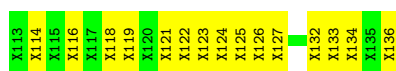


• Molecule 23: Unassigned secondary structure



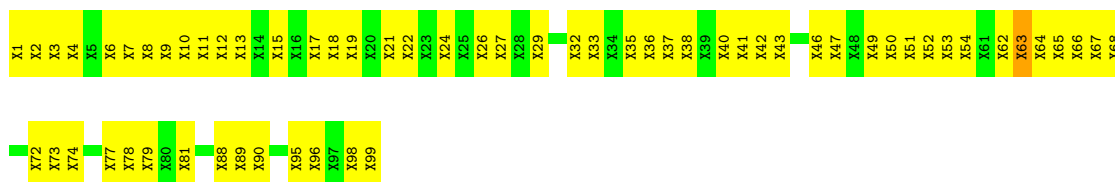
• Molecule 23: Unassigned secondary structure





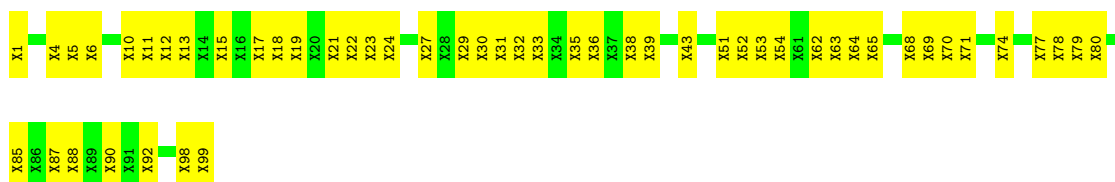
- Molecule 24: Unassigned secondary structure

Chain Ac: 34% 65%



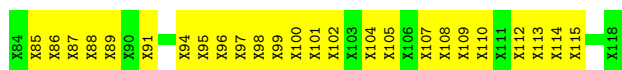
- Molecule 24: Unassigned secondary structure

Chain Cc: 45% 55%



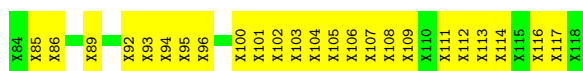
- Molecule 25: Unassigned secondary structure

Chain Ad: 29% 71%



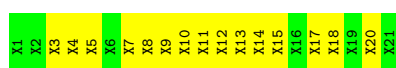
- Molecule 25: Unassigned secondary structure

Chain Cd: 31% 69%



- Molecule 26: Unassigned secondary structure

Chain Ae: 29% 71%



- Molecule 26: Unassigned secondary structure

Chain Bj: 52% 48%



- Molecule 26: Unassigned secondary structure

Chain Dj:  62% 38%

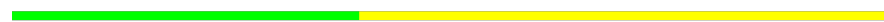


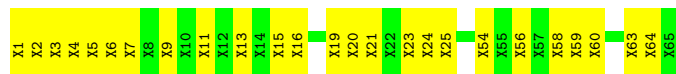
- Molecule 27: Unassigned secondary structure

Chain Af:  64% 36%

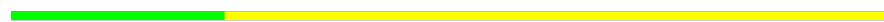


- Molecule 28: Unassigned secondary structure

Chain Ah:  39% 61%



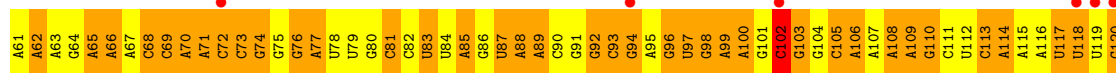
- Molecule 28: Unassigned secondary structure

Chain Ch:  24% 76%



- Molecule 29: 25S ribosomal RNA

Chain B1:  5% 41% 50% 6%



A1085	C1023	G963	G902	G842	U782	G722	U682	A602	G542	C301
C1086	G1024	A843	U903	G844	A784	U723	G663	G603	C543	U302
G1087	A1025	A965	G907	G845	A785	U724	U664	A604	C544	G303
U1088	A1026	U966	G908	A846	G786	G725	A665	U605	U545	A304
A1027	A1027	A967	G909	A847	G787	G726	A666	C606	C546	U305
U1028	U1028	G968	G908	A847	G787	G727	C667	A607	G547	A306
A1091	G1029	C969	G909	A848	C788	G728	G668	G608	U428	A307
C1092	A1030	A870	G910	C849	A789	C729	U669	G609	U549	A308
A1093	C1031	G971	G911	U850	U790	C730	C670	G610	U430	A309
U1094	C1032	A972	G912	C851	A791	U731	U671	A611	U431	U310
C1033	U1033	A973	A913	U852	G792	C732	A672	U612	G552	C311
U1096	U1034	G974	A914	G853	G793	G733	U673	G613	U553	G312
G1097	G1035	C975	A915	G854	U794	C734	G674	C614	A554	A313
A1098	A1036	U976	G916	C855	G795	A735	C675	U615	U555	U314
A1099	C1037	C977	A917	G856	U796	A736	G676	G616	U556	C315
U1100	U1038	G978	G918	G857	G797	G737	A677	G617	A557	U316
C1101	U1039	U979	U919	A858	U798	A738	G678	C618	U558	A317
A1102	A1040	A980	A920	C859	G799	G739	U679	A619	A559	A318
U1103	U1041	U981	A921	G860	G800	G740	G680	U620	C560	A319
G1104	U1042	C982	U922	C861	A801	U741	U681	A621	G561	G320
A1105	C1043	A983	G923	U862	C802	G742	U682	A622	C562	C321
G1106	C1043	C984	C924	C863	C803	C743	U683	U623	G563	U322
C1107	A1046	U985	A925	G864	C804	A744	G684	G624	G564	A323
U1108	A1047	U986	A926	U865	G805	C745	G685	G625	U565	A324
U1109	A1048	U987	C927	A866	A806	A746	G686	U626	G566	A325
C1049	C1049	U988	C928	G867	A807	A747	U687	A627	U567	A326
U1110	U1050	A989	A929	C968	A808	U748	G688	A628	G568	A327
A1111	U1051	G990	U930	G869	G809	C749	U689	U629	A569	A328
C1112	U1052	G991	C931	G870	A810	G750	A690	A630	U570	U329
G1113	U1053	A992	U932	U871	U811	A751	A691	U631	U571	C330
U1114	A1054	G993	A933	U872	G812	C752	A692	G632	A572	G331
C1115	A1055	G994	A934	C873	G813	C753	A693	C633	C573	C332
G1116	U1056	U995	U935	U874	U814	G754	C694	A634	U574	G333
C1117	A1057	A996	A936	G875	G815	A755	C695	G635	G575	A334
U1118	U1058	A997	G937	A876	A816	U756	C696	C636	C576	G335
C1119	U1058	A997	G937	A876	A816	U756	C696	C636	C576	G335
A1120	G1059	A998	C938	C877	A817	C757	A697	C637	C577	A336
U1121	U1060	G999	U939	C878	C818	C758	U698	C638	A578	A337
U1122	A1061	C1000	G940	U879	U819	U759	A699	G639	G579	A338
U1123	A1062	G1001	G941	G880	A820	C760	C700	U640	C580	C339
C1124	G1063	A1002	U942	C881	U821	A761	G701	C641	U581	G340
U1125	A1064	A1003	U943	A882	G822	U762	C702	U642	G582	C341
G1126	A1065	U1004	C944	A883	C823	G763	G703	U643	G583	A342
U1127	G1066	G1005	C945	A884	C824	C764	U704	G644	G584	U343
U1128	U1067	A1006	U946	U885	U825	C765	A705	A645	A585	A344
C1130	C1068	U1007	G947	C886	G826	U766	A706	A646	C586	G345
A1131	C1068	U1008	C948	G887	A827	U767	U707	A647	U587	C346
U1132	U1071	A1009	G949	A888	U828	C768	G708	C648	G588	A347
C1133	G1072	G1010	G950	U889	U829	G769	A709	A649	A589	A348
A1134	U1073	A1011	A951	C990	A830	G770	A710	C650	G590	A349
G1135	U1074	G1012	A952	G991	A711	C771	A711	G651	C591	C350
A1136	A1075	G1013	G953	U892	G832	U772	G712	G652	A592	A351
C1137	C1076	U1014	U954	C993	G833	U773	U713	A653	C593	A352
U1138	U1077	U1015	U955	G894	U834	G774	G714	C654	U594	G353
U1139	U1078	C1016	U956	A895	G835	A775	A715	C655	G595	U354
G1140	A1079	C1017	C957	A996	A836	U776	A716	A656	C596	U355
C1141	U1080	G1018	C958	U897	A837	U777	C717	A657	G597	A356
U1142	U1081	G1019	C959	U898	G838	U778	G718	G658	A598	C357
G1143	U1082	G1020	U960	U899	C839	G779	U719	C659	C599	U359
A1144	G1083	G1021	C961	G900	C840	A780	A720	A660	U600	G360
U1145	A1084	U1022	A962	C961	A841	G781	C721	C661	U601	A361

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A1945	U1884	G1703	U1523	A1461	A1401	C1339	C1279	C1219	A1159
A1946	U1885	A1704	A1524	A1462	A1402	G1340	C1280	U1220	C1160
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C1951	U1890	G1709	A1529	U1467	A1407	U1348	G1285	A1225	A1165
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G1953	G1892	G1711	G1531	A1469	A1409	U1350	A1287	C1227	U1167
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G	U1903	U1721	G1541	U1481	A1419	C1360	G1297	G1237	U1177
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C	G1905	A1723	G1543	U1483	G1421	G1362	U1299	C1239	A1179
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U	C1907	G1725	A1545	U1485	C1423	C1364	A1301	U1241	U1181
G	A1908	C1726	A1546	G1486	C1424	G1365	A1302	G1242	A1182
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C	U1911	A1729	U1549	A1489	U1427	G1368	U1305	A1245	C1185
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C	A1915	G1733	U1553	G1493	G1431	C1372	U1309	G1249	C1189
G	U1916	G1734	U1554	U1494	C1432	A1373	G1310	G1250	A1190
C	C1917	G1735	C1615	U1495	A1433	G1374	G1311	A1251	U1191
C	U1918	G1736	C1616	U1496	G1434	G1375	A1252	U1252	A1192
A	G1919	A1737	U1557	C1497	A1435	C1376	G1313	U1253	A1193
C	U1920	U1738	A1558	U1498	U1436	G1377	C1314	C1254	G1194
G	A1921	A1739	A1559	C1499	C1437	G1378	U1315	C1255	A1195
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C	U1924	U1742	C1562	C1502	G1440	A1381	A1318	U1258	C1198
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U2718	U2719	U2720	A2721	U2722	U2723	U2724	U2725	U2726	A2727	U2728	U2729	U2730	U2731	U2732	A2733	A2734	U2735	U2736	U2737	U2738	U2739	U2740	U2741	U2742	U2743	U2744	U2745	U2746	U2747	U2748	U2749	U2750	U2751	U2752	U2753	U2754	U2755	U2756	U2757	U2758	U2759	U2760	U2761	U2762	U2763	U2764	U2765	U2766	U2767	U2768	U2769	U2770	U2771	U2772	U2773	U2774	U2775	U2776	U2777																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
A2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	U2668	U2669	G2670	G2671	A2672	A2673	A2674	G2675	A2676	G2677	U2678	A2679	U2680	U2681	U2682	U2683	U2684	G2685	G2686	G2687	U2688	U2689	U2690	A2691	U2692	G2693	A2694	G2695	G2696	G2697	G2698	G2699	U2700	U2701	A2702	A2703	A2704	A2705	U2706	U2707	C2708	C2709	C2710	U2711	U2712	U2713	U2714	A2715	U2716	U2717																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U2597	U2598	U2599	G2600	A2601	G2602	G2603	U2604	G2605	G2606	G2607	G2608	A2609	G2610	U2611	U2612	U2613	G2614	G2615	U2616	G2617	U2618	U2619	U2620	U2621	G2622	G2623	G2624	G2625	G2626	U2627	U2628	A2629	U2630	U2631	G2632	U2633	U2634	U2635	U2636	U2637	U2638	G2639	U2640	U2641	U2642	U2643	U2644	G2645	U2646	U2647	U2648	U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U2537	U2538	C2539	A2540	U2541	U2542	U2543	U2544	U2545	U2546	U2547	U2548	A2549	U2550	U2551	U2552	U2553	A2554	U2555	U2556	U2557	U2558	U2559	U2560	A2561	A2562	U2563	U2564	U2565	U2566	U2567	U2568	U2569	U2570	U2571	U2572	U2573	U2574	U2575	U2576	U2577	U2578	U2579	U2580	U2581	U2582	U2583	U2584	U2585	U2586	U2587	U2588	U2589	U2590	U2591	U2592	U2593	U2594	U2595	U2596																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U2472	C2473	G2474	G2475	G2476	G2477	U2478	C2479	U2480	U2481	U2482	G2483	A2484	A2485	A2486	U2487	U2488	U2489	C2490	A2491	C2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	U2501	U2502	G2503	U2504	U2505	U2506	U2507	U2508	U2509	U2510	A2511	U2512	U2513	U2514	U2515	U2516	U2517	U2518	U2519	U2520	U2521	U2522	A2523	U2524	U2525	U2526	U2527	U2528	A2529	U2530	U2531	U2532																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U2411	G2412	A2413	G2414	G2415	U2416	U2417	U2418	A2419	U2420	U2421	U2422	U2423	A2424	U2425	U2426	U2427	U2428	U2429	A2430	U2431	U2432	U2433	U2434	U2435	U2436	U2437	U2438	U2439	U2440	U2441	U2442	A2443	U2444	U2445	U2446	U2447	U2448	U2449	G2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U2351	A2352	G2353	G2354	G2355	A2356	U2357	A2358	C2359	G2360	A2361	G2362	A2363	G2364	G2365	G2366	A2367	A2368	G2369	U2370	G2371	A2372	A2373	C2374	G2375	G2376	G2377	U2378	U2379	U2380	U2381	G2382	G2383	A2384	G2385	A2386	A2387	U2388	U2389	U2390	U2391	G2392	G2393	U2394	G2395	G2396	U2397	U2398	A2399	U2400	U2401	U2402	G2403	U2404	U2405	U2406	U2407	U2408	U2409	U2410																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
A2291	U2292	G2293	U2294	A2295	A2296	U2297	U2298	U2299	G2300	U2301	G2302	A2303	G2304	G2305	G2306	G2307	A2308	A2309	U2310	G2311	A2312	U2313	U2314	G2315	G2316	A2317	U2318	U2319	U2320	U2321	U2322	U2323	A2324	G2325	A2326	U2327	U2328	C2329	G2330	G2331	A2332	G2333	U2334	G2335	U2336	G2337	U2338	U2339	U2340	A2341	U2342	G2343	U2344	A2345	U2346	U2347	U2348	U2349	U2350																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
C2231	A2232	A2233	G2234	U2235	G2236	U2237	U2238	G2239	G2240	U2241	A2242	A2243	U2244	G2245	G2246	G2247	A2248	C2249	G2250	G2251	U2252	U2253	U2254	A2255	A2256	C2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	A2271	G2272	G2273	U2274	G2275	G2276	U2277	U2278	A2279	A2280	U2281	U2282	G2283	G2284	U2285	U2286	U2287	U2288	U2289	U2290																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G2171	U2172	U2173	U2174	U2175	U2176	U2177	A2178	U2179	U2180	U2181	A2182	U2183	U2184	U2185	U2186	U2187	A2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	C2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G2111	U2112	C2113	C2114	G2115	G2116	U2117	G2118	U2119	A2120	G2121	G2122	U2123	G2124	A2125	U2126	U2127	U2128	U2129	U2130	A2131	G2132	U2133	C2134	U2135	C2136	U2137	U2138	A2139	U2140	U2141	U2142	U2143	U2144	U2145	C2146	U2147	U2148	A2149	G2150	U2151	G2152	C2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	G2161	U2162	U2163	A2164	U2165	U2166	A2167	U2168	U2169	U2170																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G	U	C	U	C	U	U	G	U	U	G	U	U	C	U	C	U	U	G	C	A	C	C	C	C	U	U	U	C	A	U	G	C	C	A	C	C	A	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U

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G2840	G2841	G3200	G3140	G3200	G3260	U3380	A3320	G3260	G3200	G3140	U3020	C2960	A2900	G2840
U2842	U2843	C3201	C3141	C3201	C3261	U3381	C3321	C3261	C3201	C3141	A3021	C2961	G2901	U2841
C2844	U2845	G3202	G3142	G3202	U3262	U3382	A3322	U3262	G3202	G3142	U3022	C2962	A2902	U2842
U2846	U2847	U3203	C3143	U3203	G3263	U3383	A3323	G3263	U3203	C3143	U3023	C2963	A2903	U2843
C2848	C2849	C3204	G3144	C3204	G3264	U3384	A3324	G3264	C3204	G3144	A3024	C2964	U2904	C2844
U2850	U2851	G3205	C3145	G3205	C3265	U3385	G3325	C3265	G3205	C3145	C3025	U2965	U2905	C2845
U2852	U2853	G3206	G3266	G3206	G3266	U3386	G3326	G3266	G3206	G3266	C3026	U2966	C2906	U2846
U2854	U2855	U3207	G3146	U3207	A3267	U3387	G3327	A3267	U3207	G3146	A3027	A2967	G2907	U2847
U2856	U2857	G3208	U3148	G3208	A3268	U3388	G3328	A3268	G3208	U3148	U3028	G2968	G2908	U2848
C2858	U2859	U3209	G3149	A3209	A3269	U3389	G3329	A3269	U3209	G3149	A3029	A2969	U2909	C2849
U2860	U2861	A3330	U3270	A3210	U3270	U3390	A3330	U3270	A3210	U3270	G3030	C2970	U2910	U2850
U2862	U2863	G3271	G3271	C3211	G3271	A3391	U3331	G3271	C3211	U3151	G3031	A2971	A2911	U2851
U2864	U2865	C3212	C3212	C3212	C3212	U3392	G3332	C3212	C3212	U3152	A3032	G2972	G2912	C2852
U2866	U2867	A3273	A3273	A3273	A3273	U3393	G3333	A3273	A3273	U3153	A3033	G2973	C2913	U2853
C2868	U2869	A3274	A3274	A3274	A3274	U3394	G3334	A3274	A3274	C3154	A3034	U2974	G2914	U2854
U2870	U2871	U3281	U3281	U3281	U3281	U3395	A3335	U3281	U3281	U3155	A3035	U2975	U2915	U2855
U2872	U2873	G3276	G3276	G3276	G3276	U3396	A3336	G3276	G3276	U3156	A3036	A2976	U2916	C2856
U2874	U2875	U3277	U3277	U3277	U3277	U3397	G3337	U3277	U3277	U3157	U3037	C2977	G2917	C2857
C2876	C2877	C3278	C3278	C3278	C3278	U3398	G3338	C3278	C3278	U3158	U3038	U2978	G2918	U2858
U2878	U2879	A3279	A3279	A3279	A3279	U3399	G3339	A3279	A3279	U3159	C3039	U2979	U2919	U2859
U2880	U2881	U3280	U3280	U3280	U3280	U3400	G3340	U3280	U3280	U3160	A3040	U2980	U2920	U2860
C2882	C2883	U3281	U3281	U3281	U3281	U3401	G3341	U3281	U3281	G3161	U3041	U2981	U2921	U2861
U2884	U2885	G3282	G3282	G3282	G3282	U3402	G3342	G3282	G3282	C3162	U3042	A2982	G2922	U2862
U2886	U2887	A3283	A3283	A3283	A3283	U3403	G3343	A3283	A3283	A3163	C3043	C2983	U2923	G2863
U2888	U2889	G3284	G3284	G3284	G3284	U3404	G3344	G3284	G3284	C3164	C3044	C2984	U2924	U2864
C2890	C2891	C3285	C3285	C3285	C3285	U3405	G3345	C3285	C3285	A3165	G3045	C2985	U2925	U2865
U2890	U2891	A3286	A3286	A3286	A3286	U3406	G3346	A3286	A3286	C3166	A3046	U2986	A2926	U2866
U2892	U2893	U3287	U3287	U3287	U3287	U3407	G3347	U3287	U3287	A3167	U3047	A2987	C2927	C2867
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U2896	U2897	C3289	C3289	C3289	C3289	U3409	G3349	C3289	C3289	U3169	A3049	U2989	C2929	U2869
U2898	U2899	U3290	U3290	U3290	U3290	U3410	G3350	U3290	U3290	A3170	U3050	G2990	A2930	C2870
C2899	C2900	G3291	G3291	G3291	G3291	U3411	G3351	G3291	G3291	U3171	U3051	A2991	C2931	U2871
U2900	U2901	A3292	A3292	A3292	A3292	U3412	G3352	A3292	A3292	A3172	U3052	U2992	U2932	U2872
U2902	U2903	U3293	U3293	U3293	U3293	U3413	G3353	U3293	U3293	G3173	G3053	G2993	A2933	U2873
U2904	U2905	A3294	A3294	A3294	A3294	U3414	G3354	A3294	A3294	A3174	U3054	A2994	A2934	G2874
U2906	U2907	U3295	U3295	U3295	U3295	U3415	G3355	U3295	U3295	U3175	U3055	A2995	U2935	U2875
U2908	U2909	A3296	A3296	A3296	A3296	U3416	G3356	A3296	A3296	G3176	U3056	U2996	A2936	C2876
U2910	U2911	U3297	U3297	U3297	U3297	U3417	G3357	U3297	U3297	G3177	U3057	G2997	G2937	C2877
U2912	U2913	C3298	C3298	C3298	C3298	U3418	G3358	C3298	C3298	A3178	U3058	U2998	G2938	C2878
U2914	U2915	A3299	A3299	A3299	A3299	U3419	G3359	A3299	A3299	U3179	G3059	U2999	G2939	C2879
U2916	U2917	U3300	U3300	U3300	U3300	U3420	G3360	U3300	U3300	A3180	C3060	A3000	A2940	U2880
U2918	U2919	G3301	G3301	G3301	G3301	U3421	G3361	G3301	G3301	C3181	G3061	C3001	A2941	C2881
U2920	U2921	U3302	U3302	U3302	U3302	U3422	G3362	U3302	U3302	G3182	G3062	C3002	C2942	U2882
U2922	U2923	C3303	C3303	C3303	C3303	U3423	G3363	C3303	C3303	A3183	C3063	G3003	G2943	U2883
U2924	U2925	U3304	U3304	U3304	U3304	U3424	G3364	U3304	U3304	A3184	U3064	C3004	U2944	C2884
U2926	U2927	A3305	A3305	A3305	A3305	U3425	G3365	A3305	A3305	U3185	G3065	A3005	G2945	C2885
U2928	U2929	U3306	U3306	U3306	U3306	U3426	G3366	U3306	U3306	A3186	U3066	A3006	A2946	U2886
U2930	U2931	G3307	G3307	G3307	G3307	U3427	G3367	G3307	G3307	A3187	C3067	U3007	G2947	A2887
U2932	U2933	C3308	C3308	C3308	C3308	U3428	G3368	C3308	C3308	U3188	U3068	A3008	C2948	U2888
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U2936	U2937	A3310	A3310	A3310	A3310	U3430	G3370	A3310	A3310	C3190	A3070	U3010	G2950	U2890
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U2946	U2947	U3315	U3315	U3315	U3315	U3435	G3375	U3315	U3315	U3195	G3075	G3015	U2955	C2895
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U2950	U2951	U3317	U3317	U3317	U3317	U3437	G3377	U3317	U3317	G3197	A3077	A3017	G2957	A2897

• Molecule 29: 25S ribosomal RNA



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U1840	G1779	G1719	G1658	U1598	G1538	U1478	G1417	G1357	C1296	G1236	C1176	G1116	A1055
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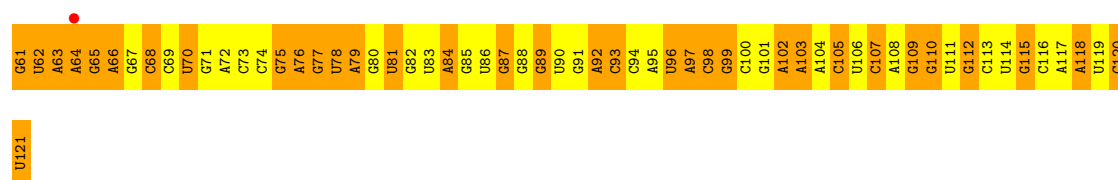
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G2594	G2594	A2535	U2472	G2412	A2352	U2292	A2232	A2172	U2112	G	U	A1932	C1871
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G2599	G2599	G2539	G2477	U2417	A2357	U2297	G2237	U2177	A2117	G	U	U1937	G1876
G2600	G2600	A2540	G2478	G2418	A2358	U2298	G2238	A2178	C2118	U	G	U1938	U1877
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G2602	G2602	U2543	G2480	C2420	C2360	G2300	G2240	G2180	A2120	A	U	G1940	A1879
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U3384	G3204	G3144	A3024	G2964	U2904	C2844	U2784	U2724
C3325	G3205	C3145	C3025	U2965	U2905	A2845	U2785	U2725
G3252	C3206	G3146	G3026	U2966	C2906	U2846	G2786	C2726
G3253	U3207	A3147	A3027	A2967	C2907	A2847	G2787	A2727
U3254	A3268	U3148	G3028	G2968	C2908	G2848	C2788	G2728
U3255	G3209	G3149	A3029	A2969	U2909	C2849	U2789	U2729
G3256	U3210	A3150	G3030	C2970	A2910	G2850	U2790	G2730
G3257	C3211	U3151	G3031	A2971	A2911	A2851	G2791	U2731
U3258	C3212	U3152	A3032	G2972	G2912	C2852	A2792	G2732
U3259	A3213	U3153	C3093	C2973	C2913	A2853	G2793	A2733
U3260	U3214	C3154	C3034	U2974	G2914	U2854	G2794	A2734
C3261	A3215	U3155	A3035	U2975	U2915	U2855	U2795	U2735
C3262	G3216	U3156	G3036	A2976	U2916	G2856	G2796	A2736
G3263	C3217	U3157	U3037	G2977	G2917	C2857	C2797	C2737
G3264	A3218	G3158	U3038	U2978	G2918	U2858	C2798	A2738
G3265	G3219	C3159	C3099	U2979	A2919	U2859	A2799	A2739
G3266	U3220	U3160	A3040	U2980	U2920	G2860	G2800	A2740
G3267	C3221	C3161	U3041	U2981	U2921	U2861	A2801	C2741
G3268	U3222	C3162	U3042	A2982	G2922	U2862	A2802	G2742
G3269	A3223	A3163	C3043	C2983	U2923	G2863	A2803	A2743
G3270	G3224	C3164	G3044	C2984	U2924	A2864	A2804	U2744
G3271	C3225	A3165	G3045	C2985	C2925	U2865	G2805	G2745
G3272	A3226	C3166	A3046	U2986	A2926	U2866	U2806	A2746
G3273	C3227	A3167	U3047	A2987	C2927	C2867	U2807	A2747
G3274	G3228	A3168	A3048	C2988	C2928	U2868	A2808	A2748
G3275	U3229	U3169	A3049	U2989	C2929	U2869	C2809	G2749
G3276	G3230	A3170	U3050	G2990	A2930	C2870	C2810	U2750
G3277	U3231	C3171	U3051	A2991	C2931	G2871	A2811	G2751
G3278	G3232	A3172	G3052	U2992	U2932	A2872	C2812	U2752
G3279	C3233	C3173	G3053	G2993	A2933	U2873	A2813	G2753
G3280	A3234	A3174	U3054	A2994	A2934	G2874	G2814	C2754
G3281	C3235	U3175	U3055	A2995	U2935	U2875	G2815	C2755
G3282	U3236	G3176	U3056	U2996	A2936	C2876	G2816	C2756
G3283	U3237	C3177	U3057	G2997	C2937	A2877	A2817	U2757
G3284	G3238	A3178	U3058	U2998	G2938	G2878	U2818	A2758
G3285	C3239	U3179	G3059	U2999	G2939	C2879	A2819	U2759
G3286	U3300	A3180	C3060	A3000	A2940	U2880	A2820	C2760
G3287	G3241	C3181	G3061	C3001	A2941	C2881	C2821	G2761
G3288	G3242	G3182	G3062	C3002	C2942	U2882	U2822	A2762
G3289	A3243	A3183	C3063	G3003	C2943	U2883	G2823	U2763
G3290	C3244	A3184	U3064	C3004	U2944	C2884	G2824	C2764
G3291	A3245	U3185	G3065	A3005	G2945	C2885	C2825	C2765
G3292	G3246	A3186	U3066	A3006	A2946	U2886	U2826	U2766
G3293	U3247	A3187	C3067	U3007	G2947	A2887	U2827	U2767
G3294	C3248	G3188	U3068	A3008	C2948	U2888	G2828	U2768
G3295	G3249	C3189	G3069	G3009	U2949	C2889	U2829	A2769
G3296	U3250	A3190	A3070	U3010	U2950	G2890	G2770	G2770
G3297	U3251	G3191	U3071	A3011	G2951	U2891	G2831	U2771

• Molecule 30: 5S ribosomal RNA

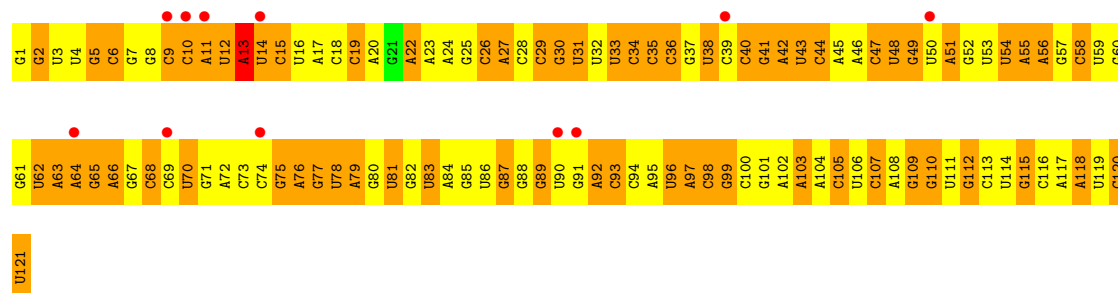


G1	G2	U3	U4	G5	G6	G7	G8	C9	C10	A11	U12	A13	U14	C15	U16	C17	C18	G19	A20	G21	A22	A23	A24	G25	C26	A27	C28	C29	G30	U31	U32	U33	C34	C35	C36	G37	U38	C39	G40	G41	A42	U43	C44	A45	A46	C47	U48	G49	U50	A51	G52	U53	U54	A55	A56	G57	C58	U59	A60
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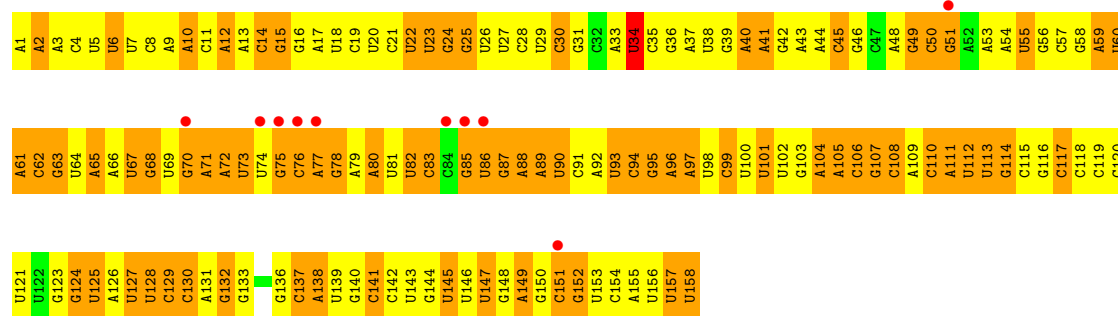
• Molecule 30: 5S ribosomal RNA

Chain D2: . 9% 44% 55% .



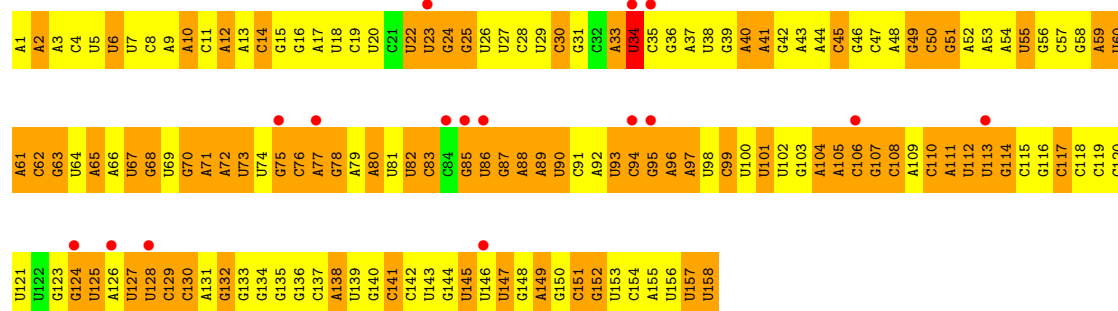
• Molecule 31: 5.8S ribosomal RNA

Chain B3: . 6% 46% 49% .



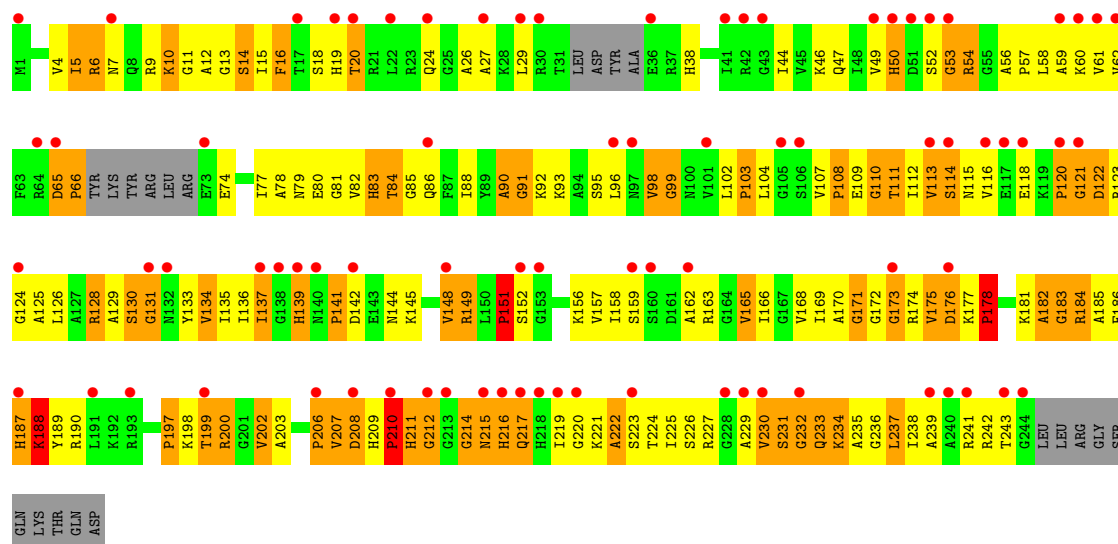
• Molecule 31: 5.8S ribosomal RNA

Chain D3: . 10% 48% 49% .

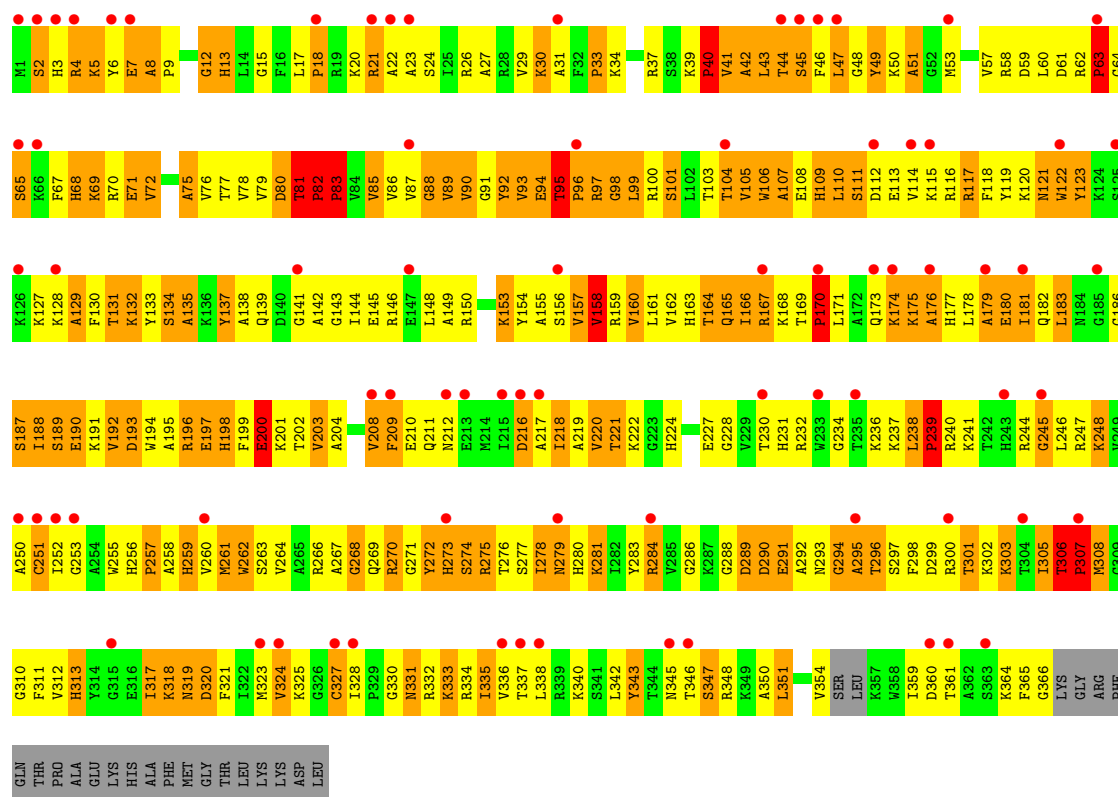
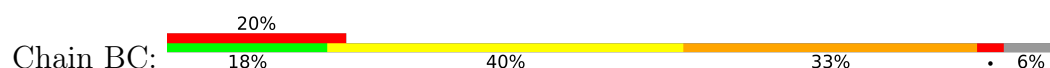


• Molecule 32: 60S ribosomal protein L1

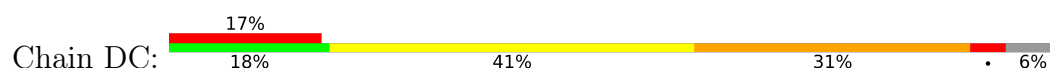


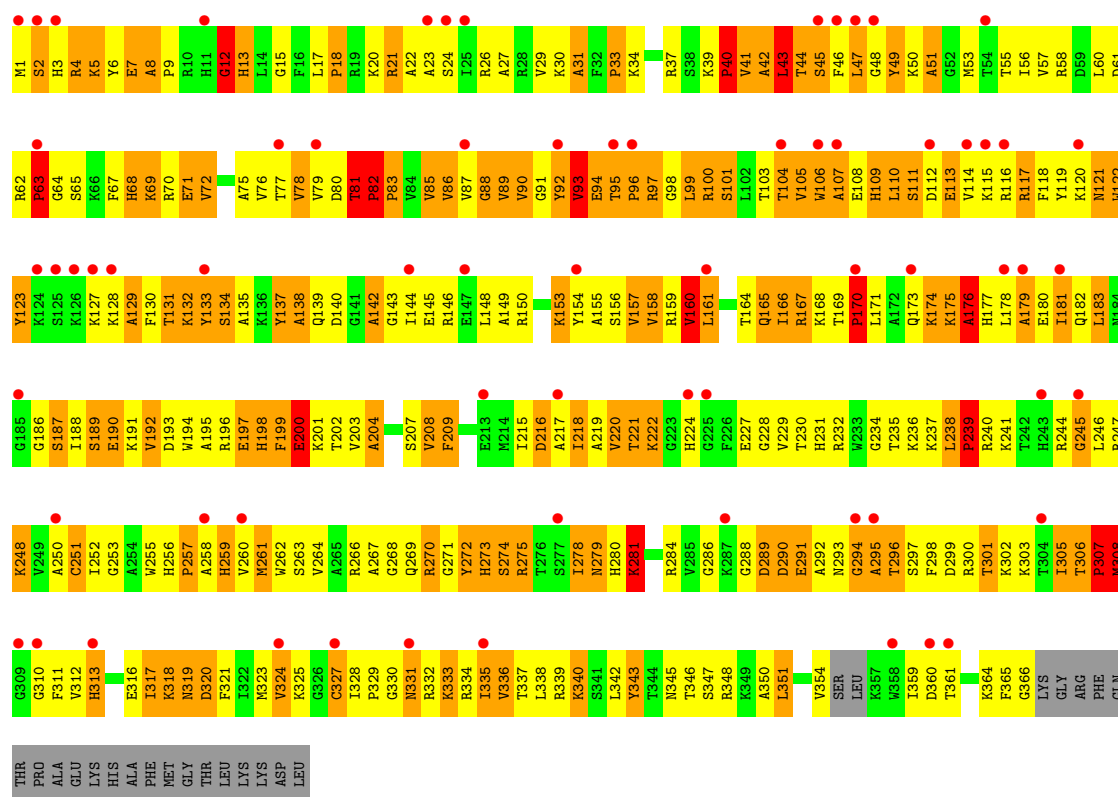


• Molecule 34: 60S ribosomal protein L3

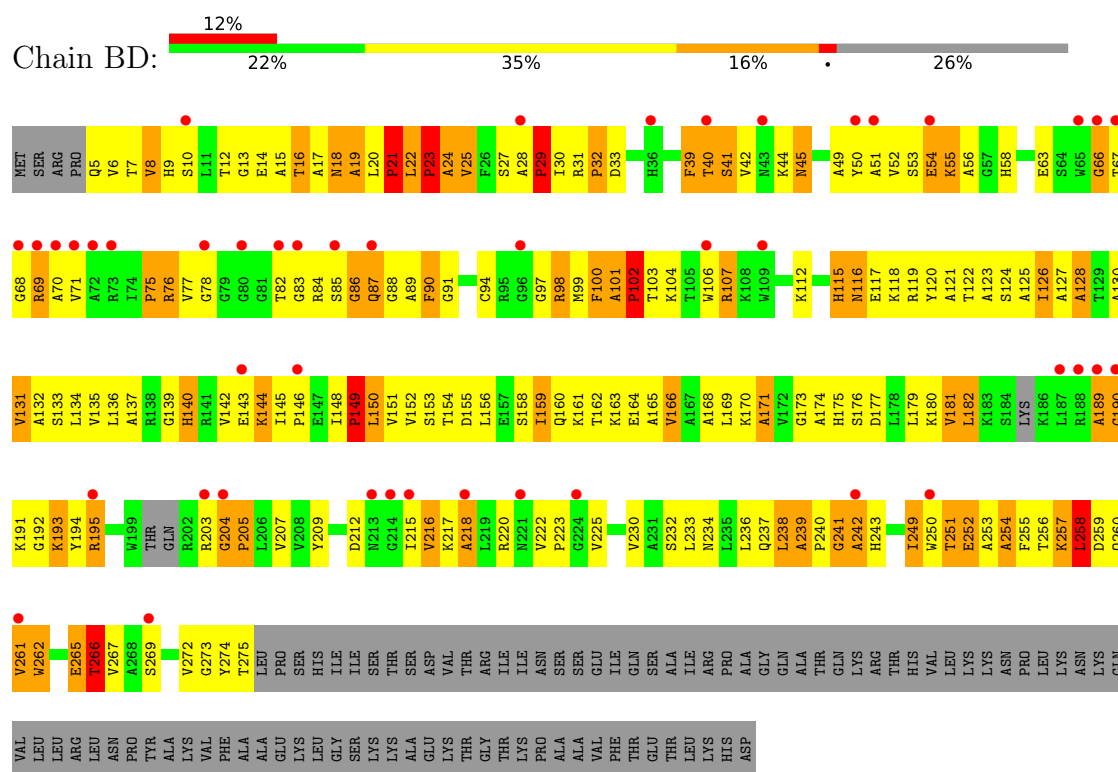


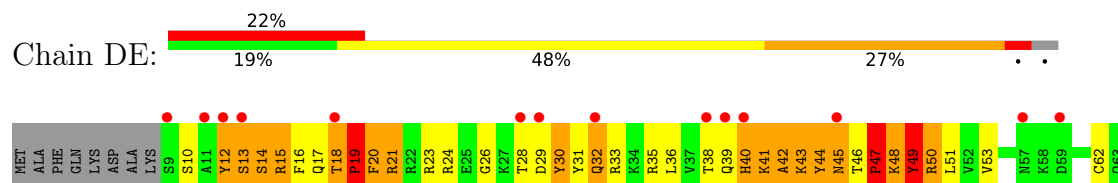
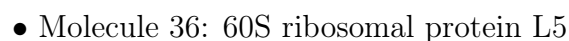
• Molecule 34: 60S ribosomal protein L3

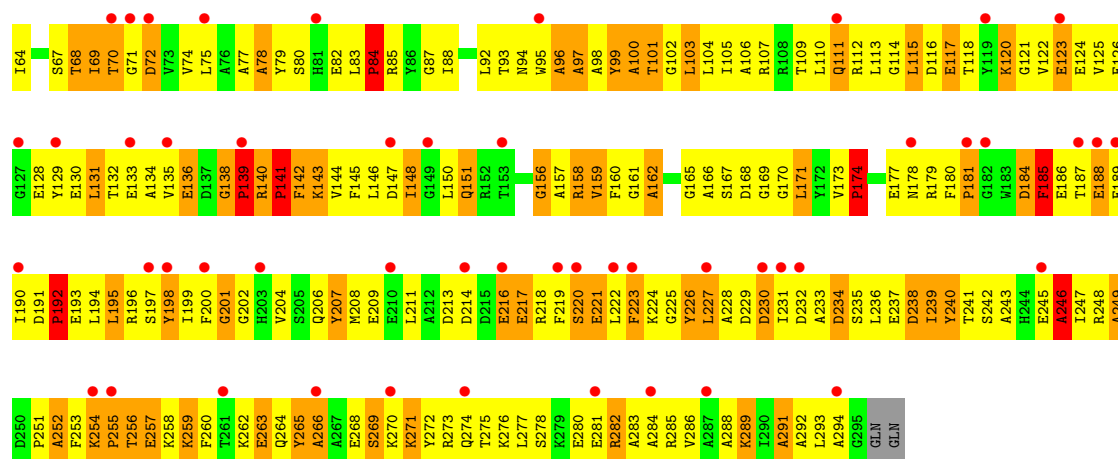




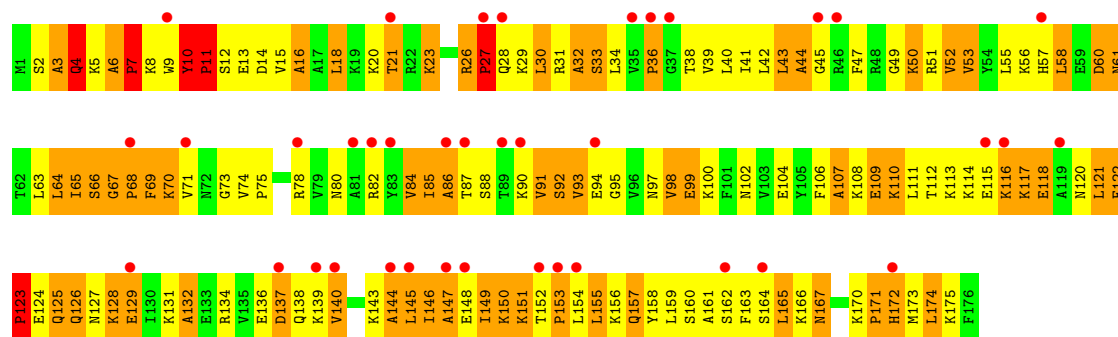
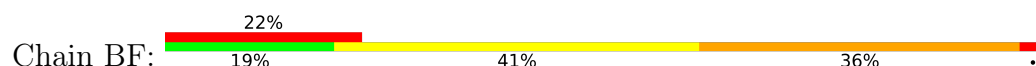
• Molecule 35: 60S ribosomal protein L4-A



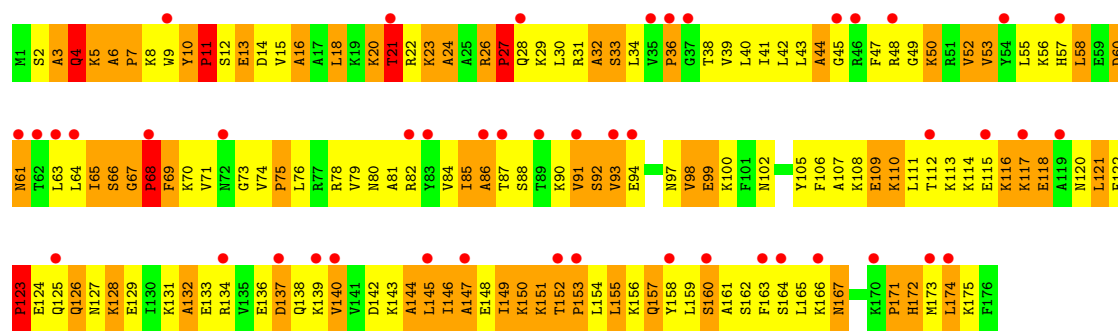
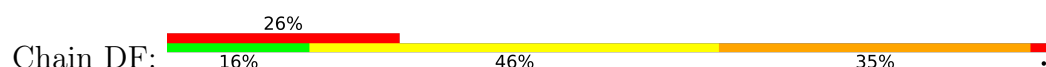


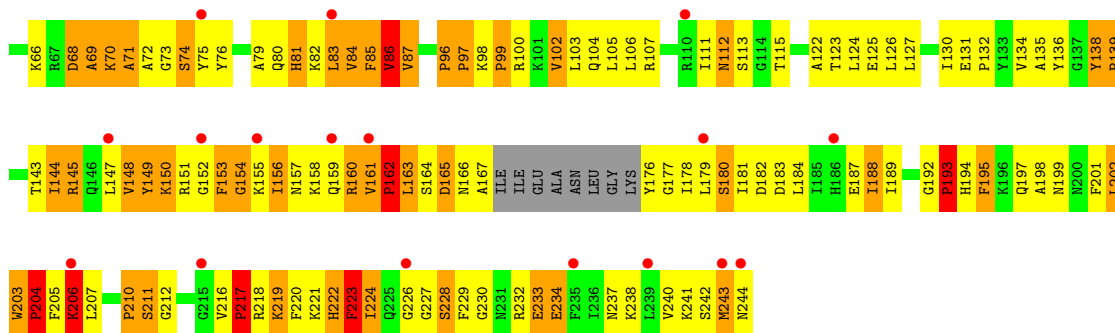


• Molecule 37: 60S ribosomal protein L6-A

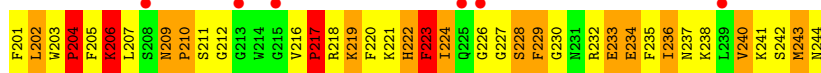
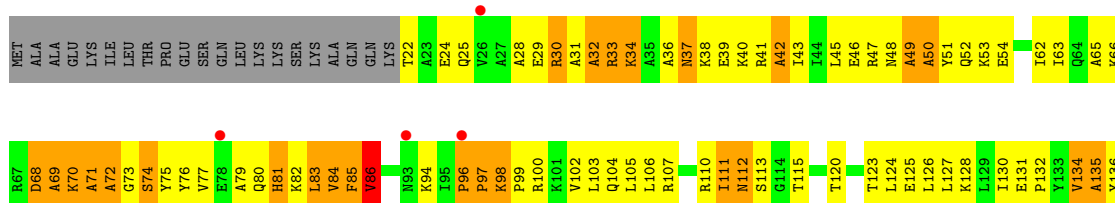
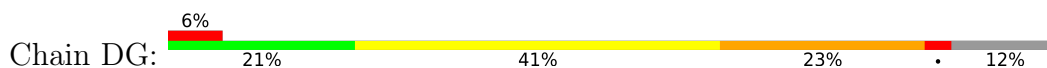


• Molecule 37: 60S ribosomal protein L6-A

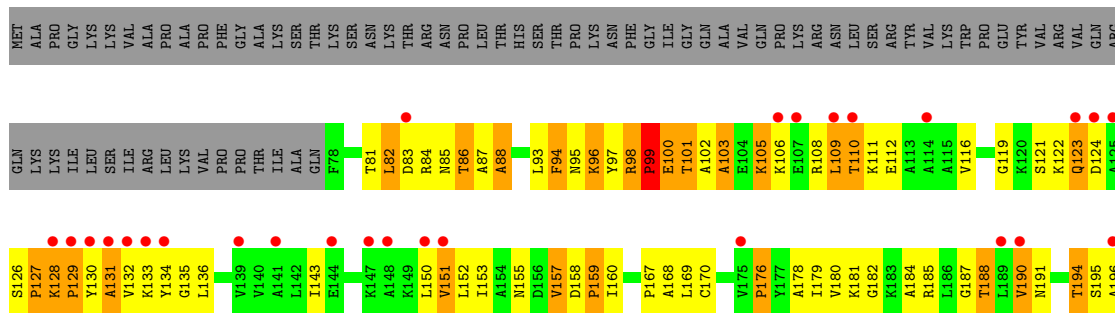
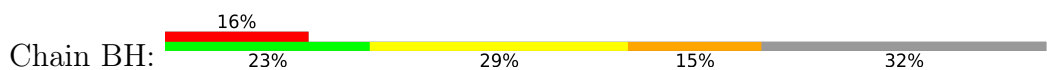




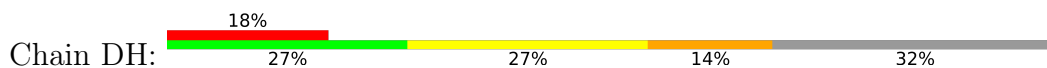
- Molecule 38: 60S ribosomal protein L7-A

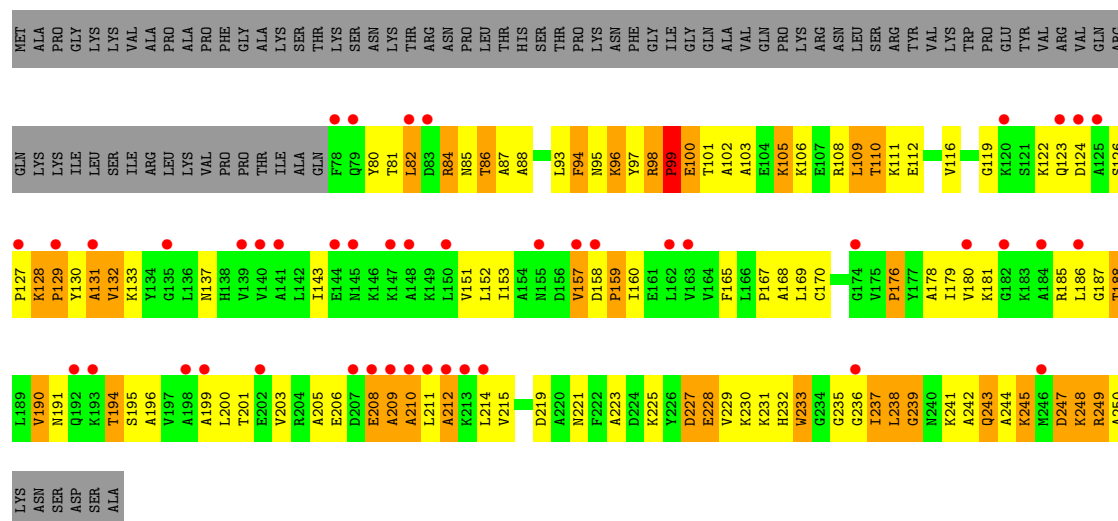


- Molecule 39: 60S ribosomal protein L8-A

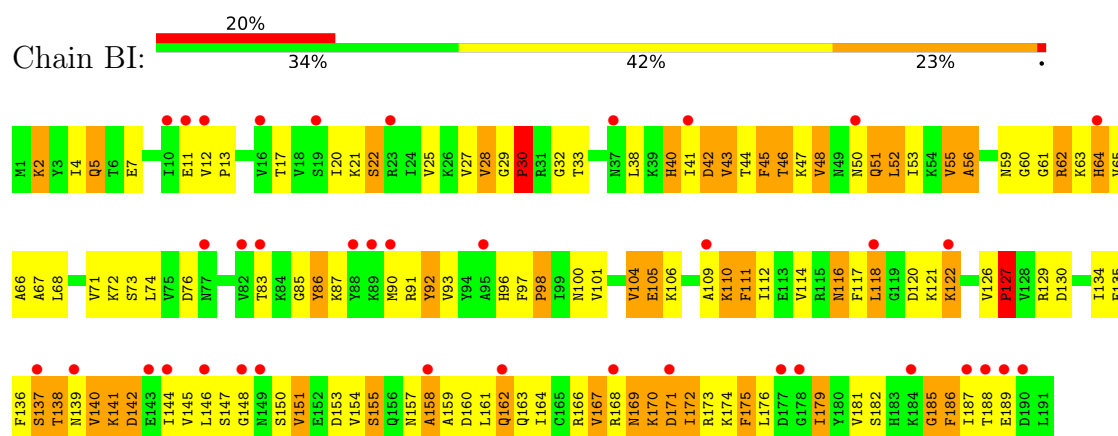


- Molecule 39: 60S ribosomal protein L8-A

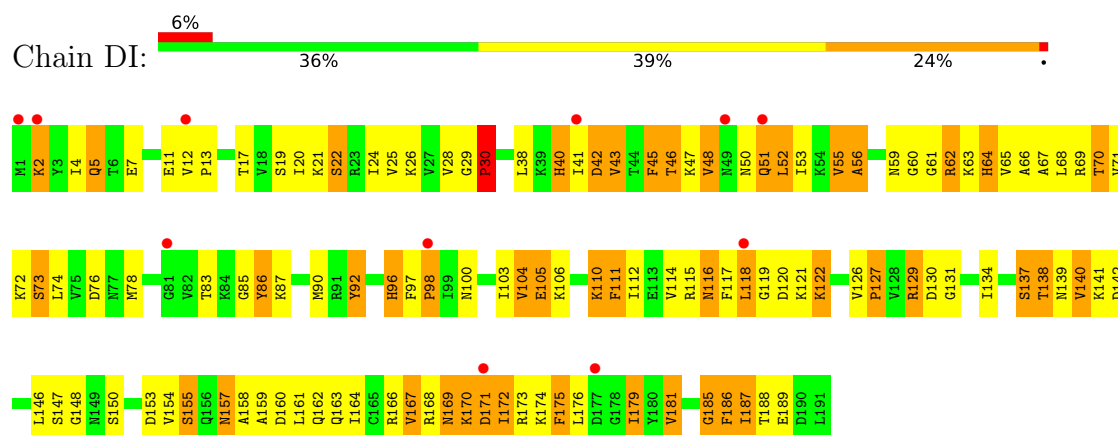




• Molecule 40: 60S ribosomal protein L9-A

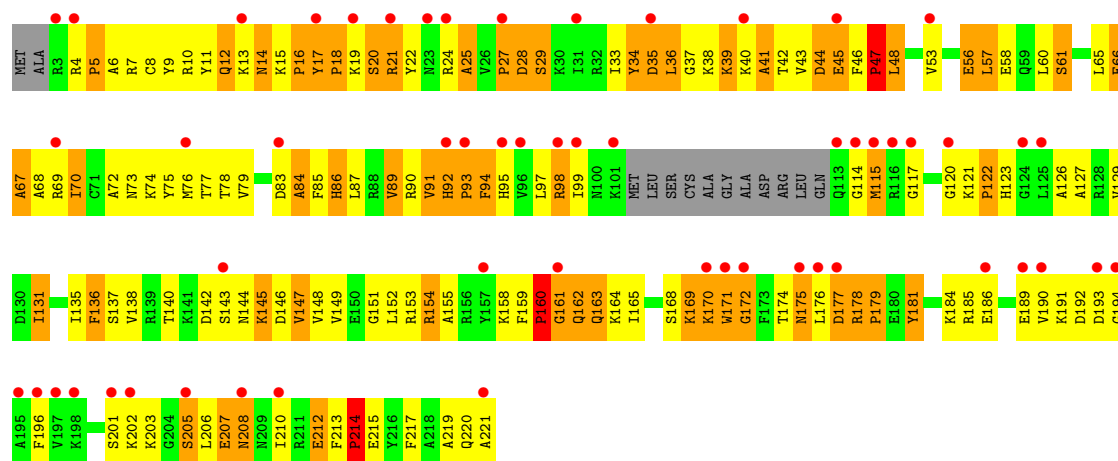


• Molecule 40: 60S ribosomal protein L9-A

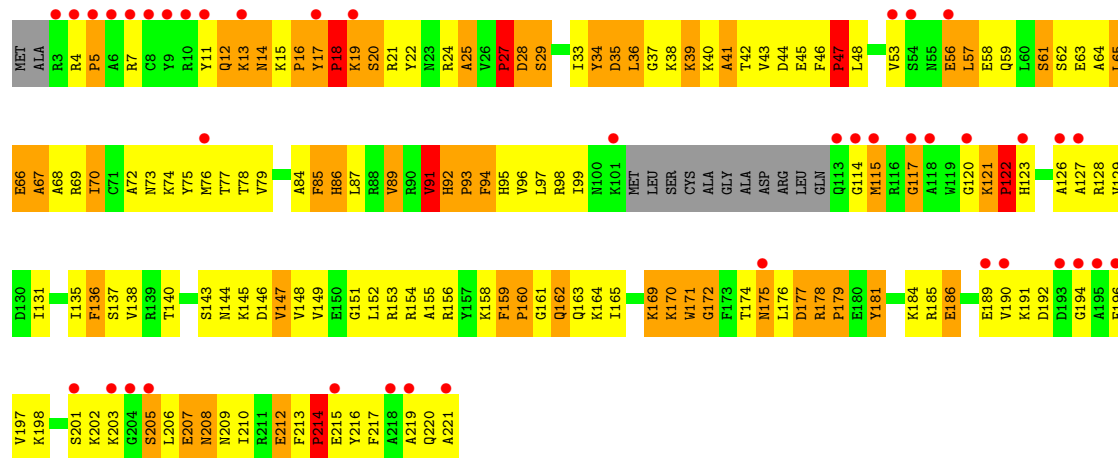


• Molecule 41: 60S ribosomal protein L10

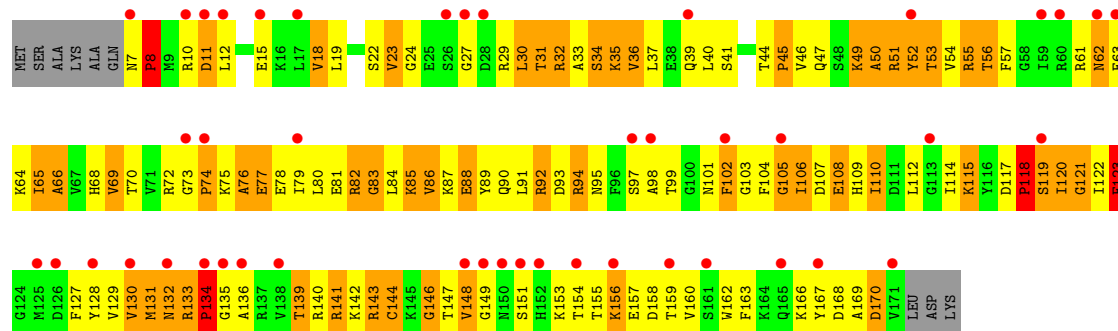
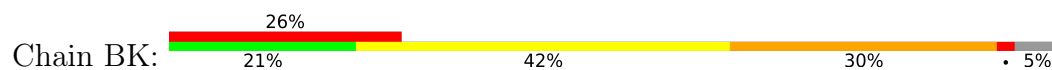




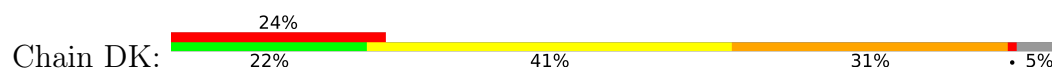
• Molecule 41: 60S ribosomal protein L10

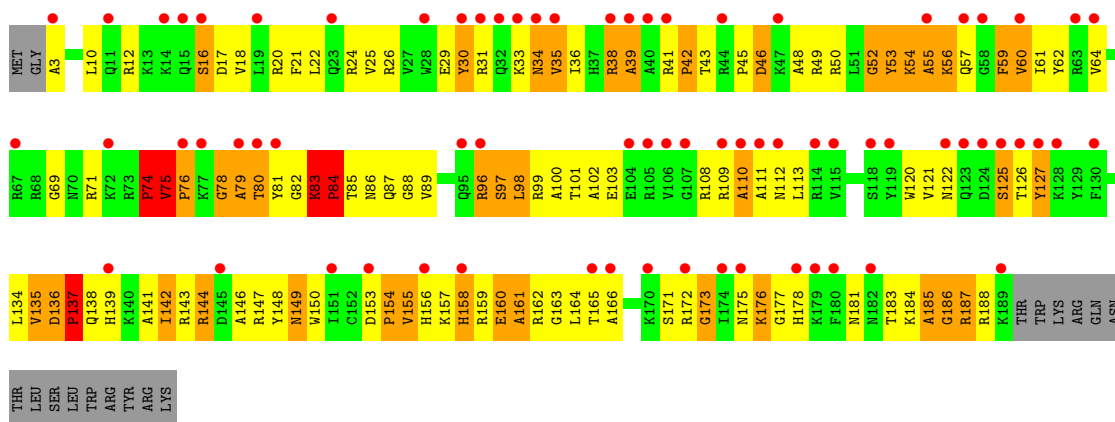
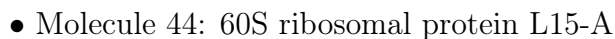


• Molecule 42: 60S ribosomal protein L11-A

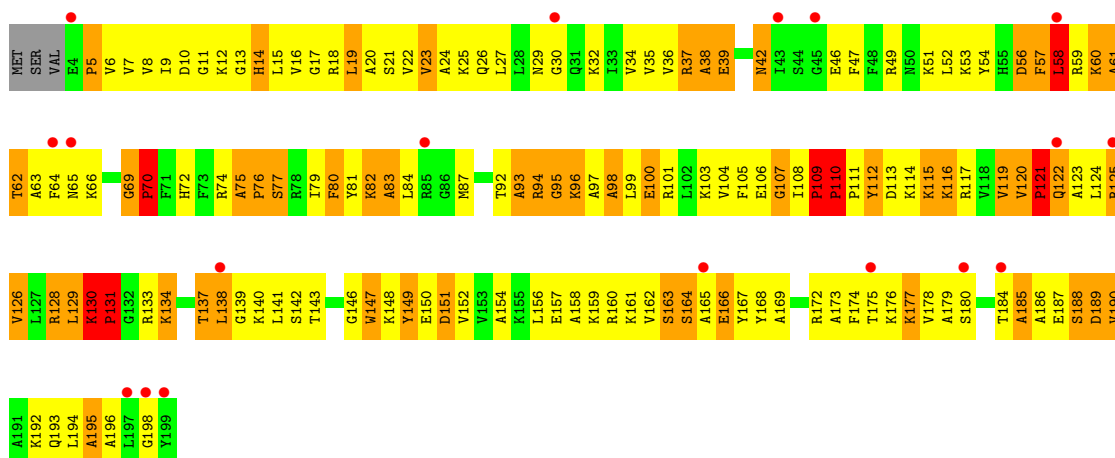


• Molecule 42: 60S ribosomal protein L11-A

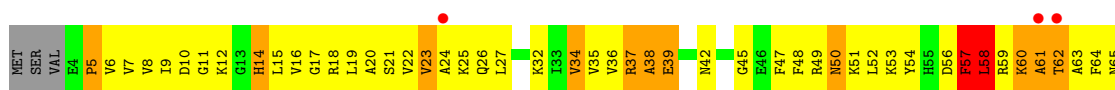


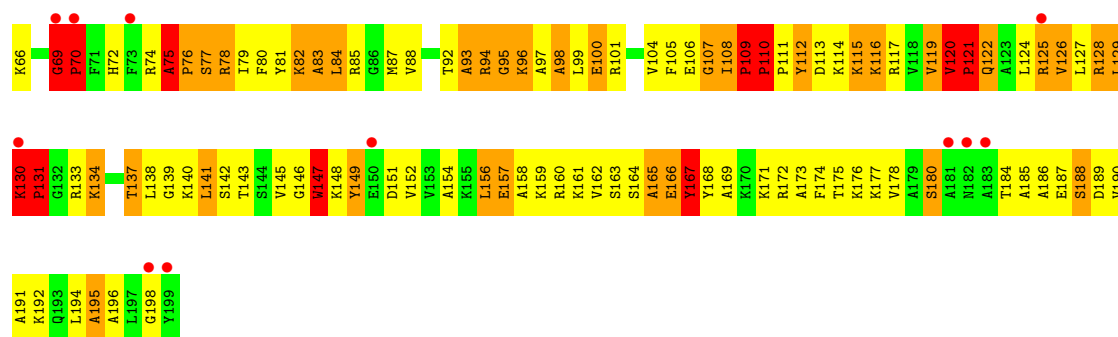


- Molecule 45: 60S ribosomal protein L16-A

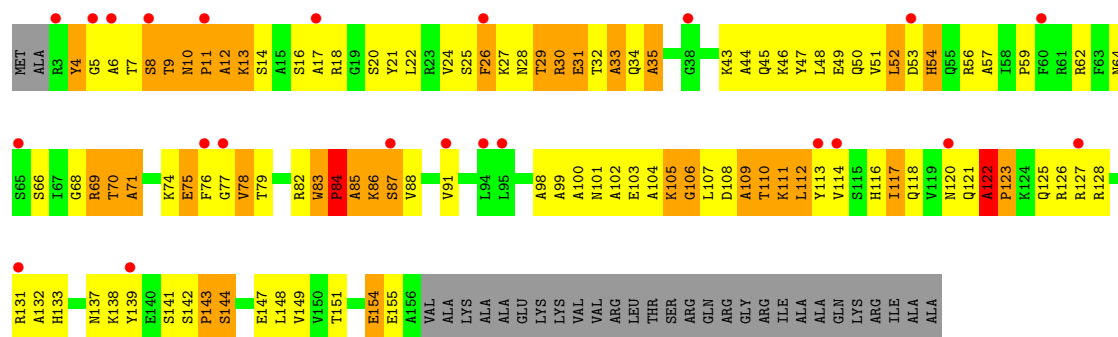
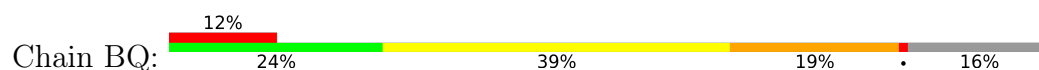


- Molecule 45: 60S ribosomal protein L16-A

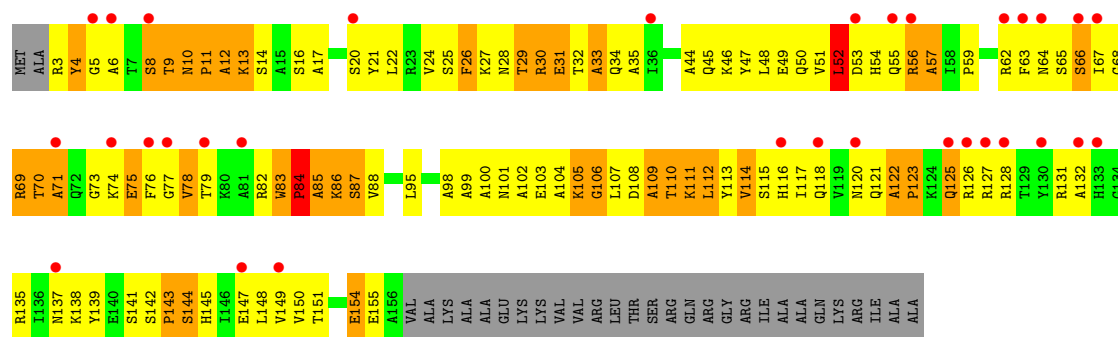
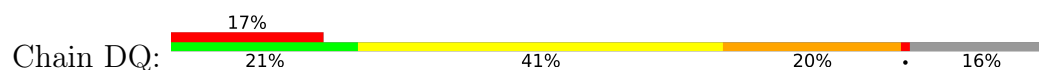




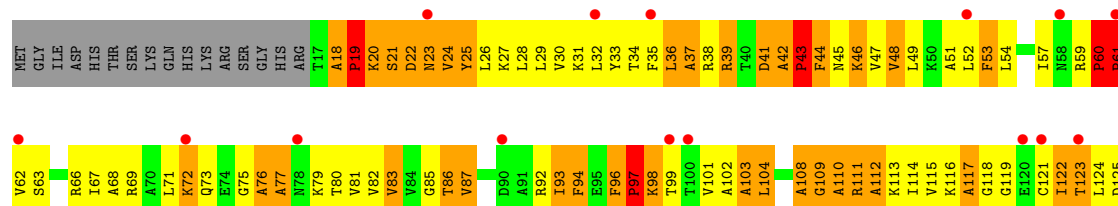
• Molecule 46: 60S ribosomal protein L17-A



• Molecule 46: 60S ribosomal protein L17-A

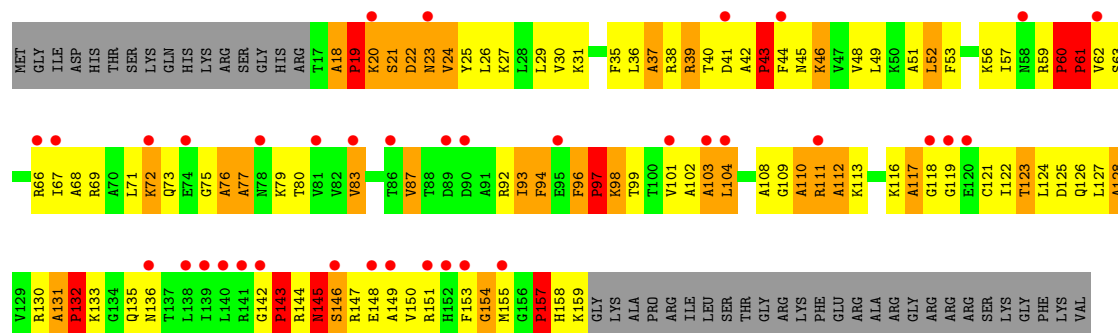
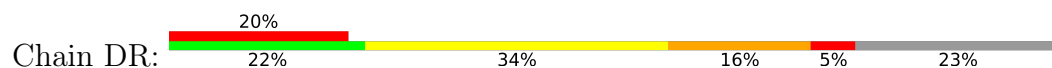


• Molecule 47: 60S ribosomal protein L18

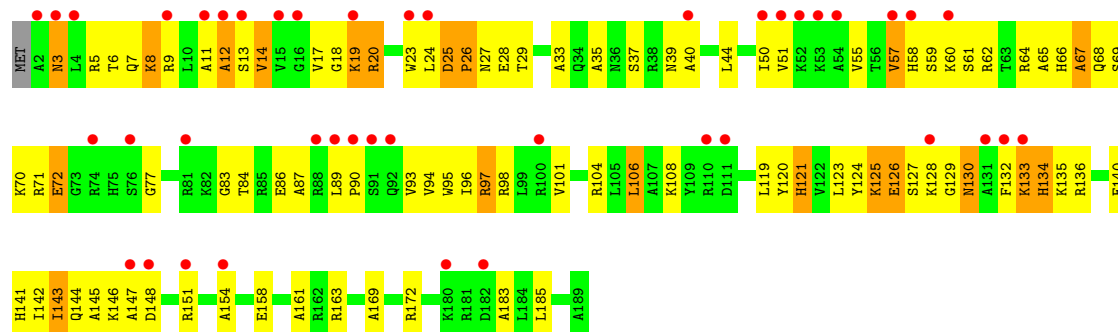




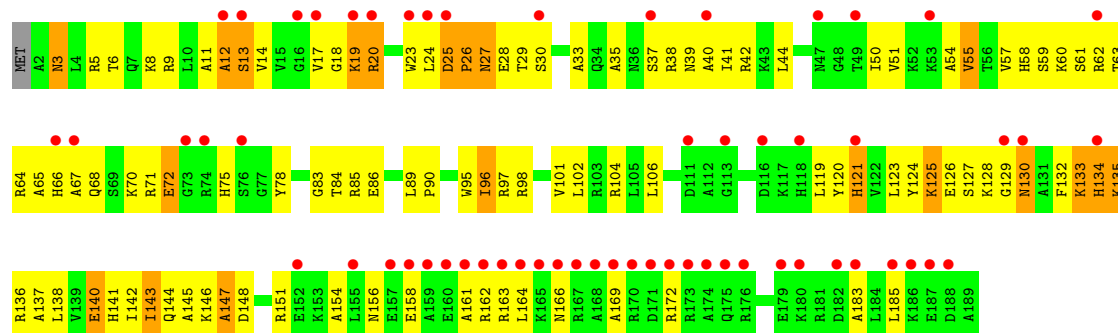
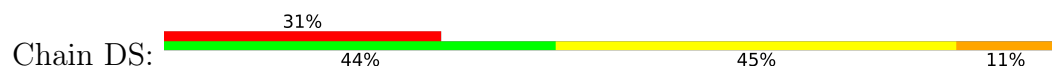
• Molecule 47: 60S ribosomal protein L18



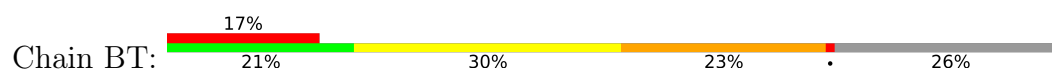
• Molecule 48: 60S ribosomal protein L19

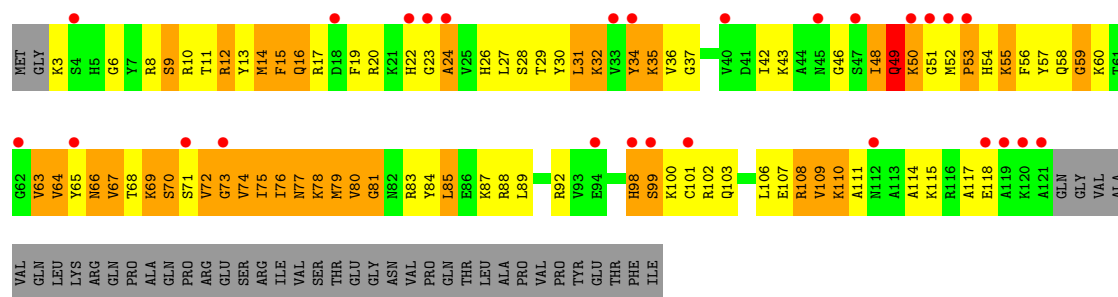


• Molecule 48: 60S ribosomal protein L19

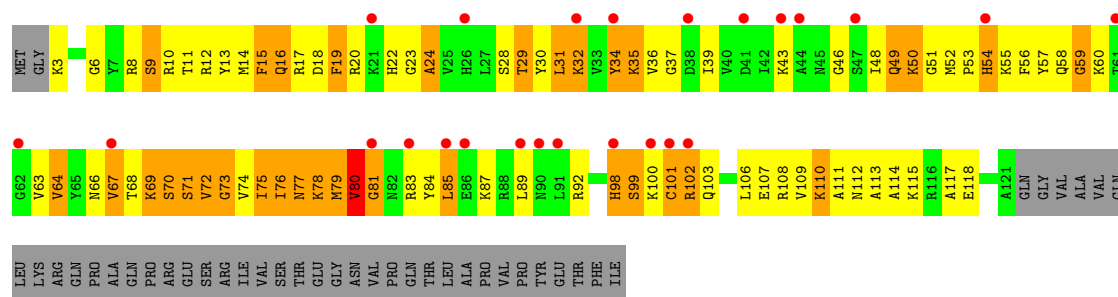
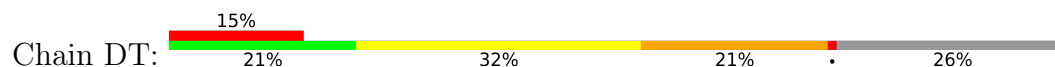


• Molecule 49: 60S ribosomal protein L21-A

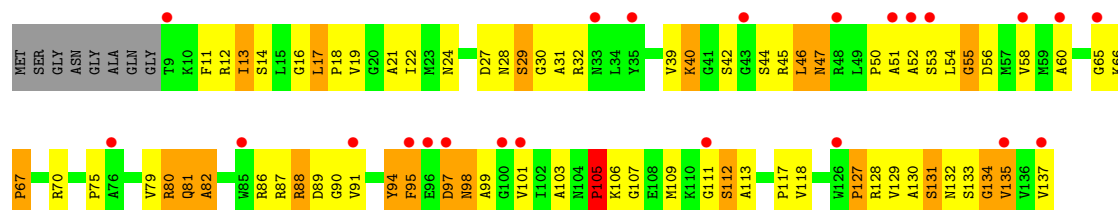




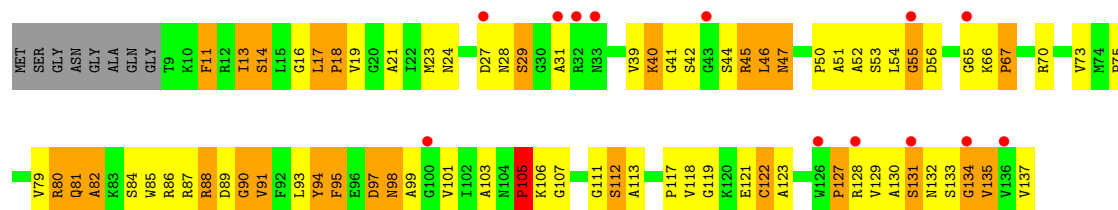
• Molecule 49: 60S ribosomal protein L21-A



• Molecule 50: 60S ribosomal protein L23



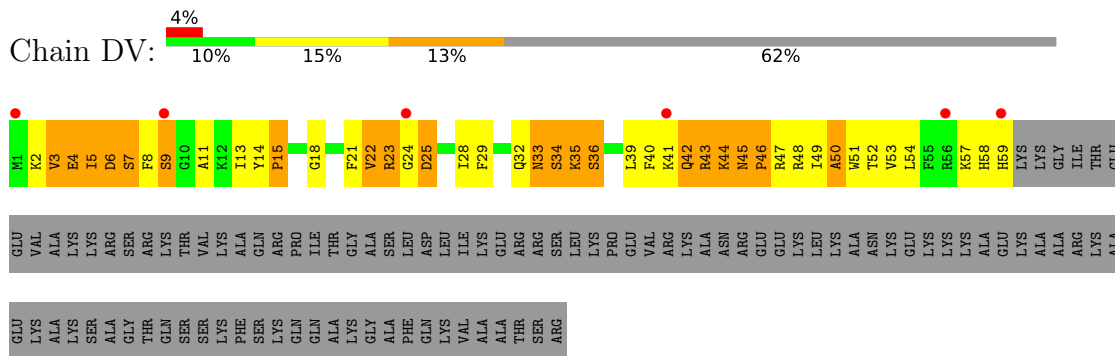
• Molecule 50: 60S ribosomal protein L23



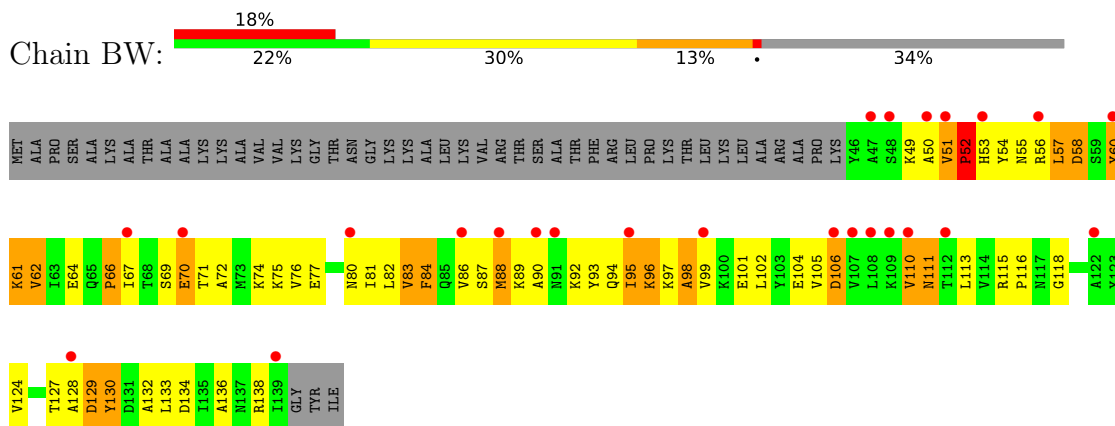
• Molecule 51: 60S ribosomal protein L24-A



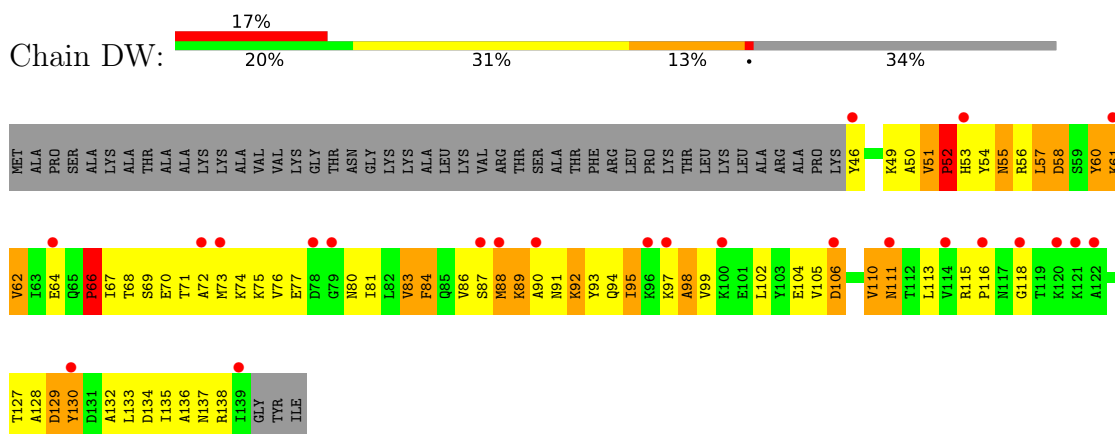
- Molecule 51: 60S ribosomal protein L24-A



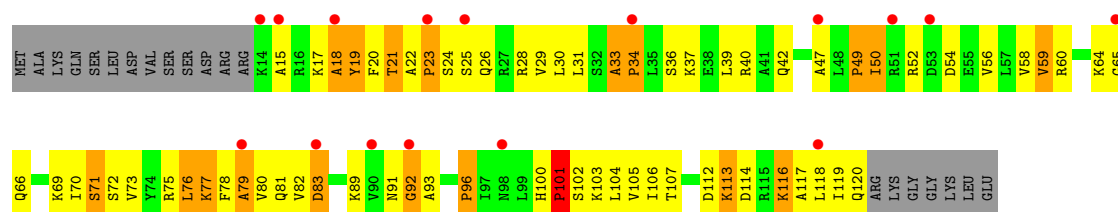
- Molecule 52: 60S ribosomal protein L25



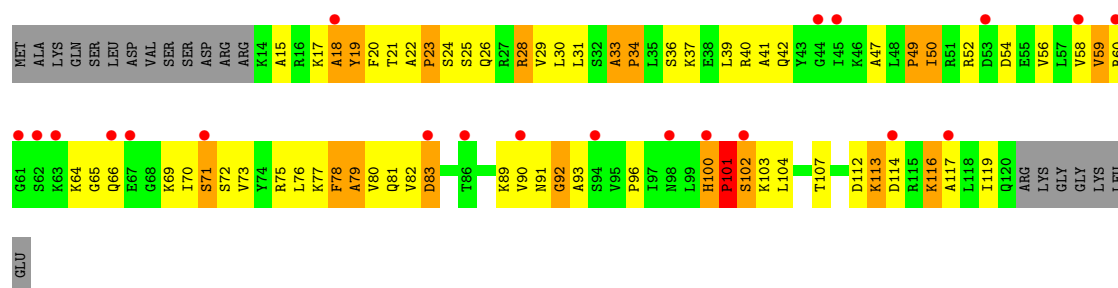
- Molecule 52: 60S ribosomal protein L25



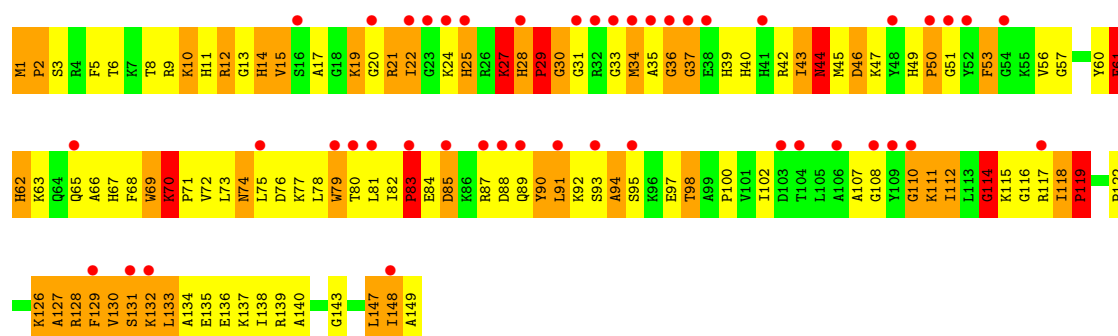
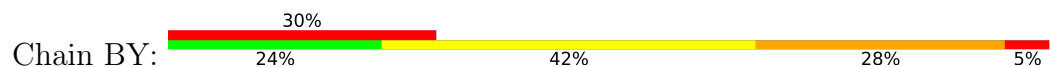
- Molecule 53: 60S ribosomal protein L26-A



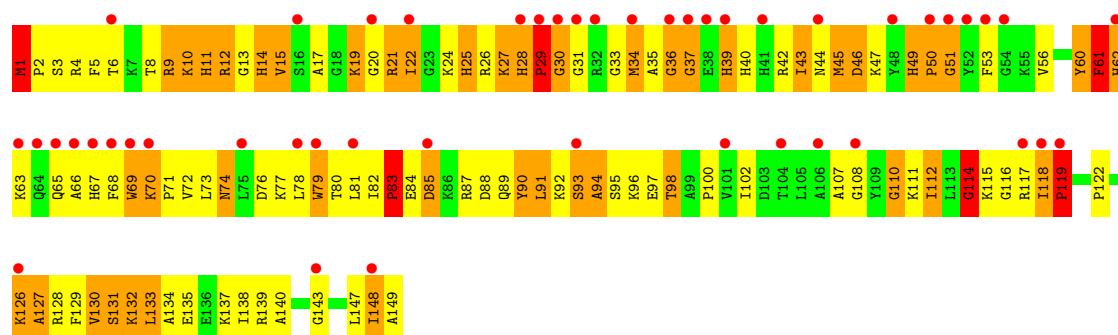
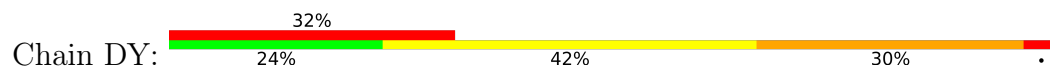
• Molecule 53: 60S ribosomal protein L26-A



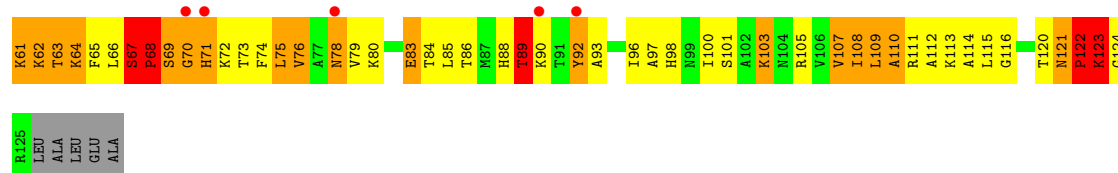
• Molecule 54: 60S ribosomal protein L28



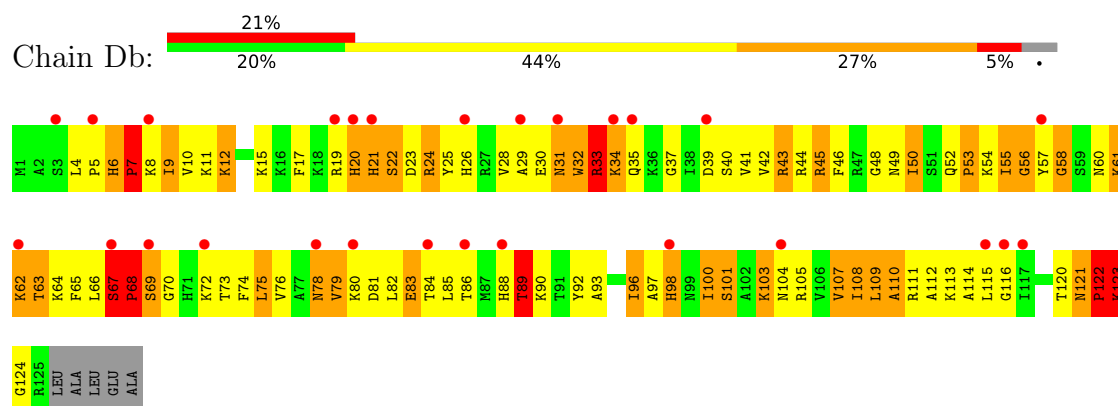
• Molecule 54: 60S ribosomal protein L28



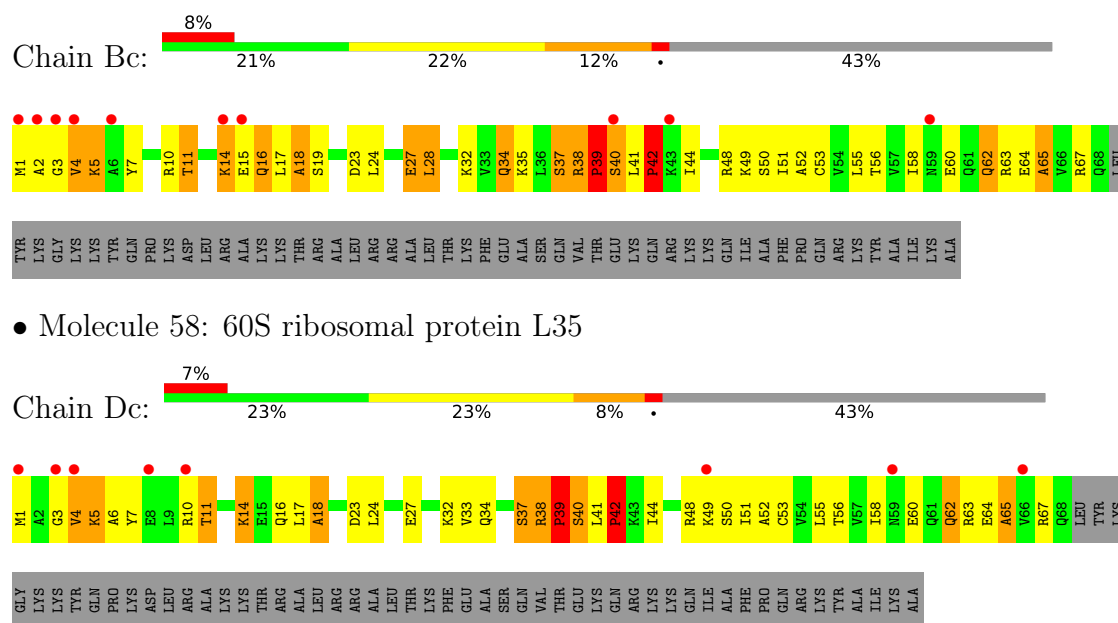
- | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|-----|
| H1 | A2 | S3 | L4 | P5 | H6 | P7 | K8 | T9 | V10 | K11 | K12 | H13 | T14 | K15 | F16 | F17 | K18 | R19 | H20 | H21 | S22 | D23 | R24 | Y25 | H26 | R27 | V28 | A29 | E30 | N31 | W32 | R33 | K34 | Q35 | Q36 | G37 | L38 | D39 | S40 | V41 | V42 | R43 | R44 | R45 | F46 | R47 | G48 | N49 | L50 | S51 | P52 | P53 | K54 | L55 | G56 | Y57 | G58 | S59 | H60 |
|----|----|----|----|----|----|----|----|----|-----|



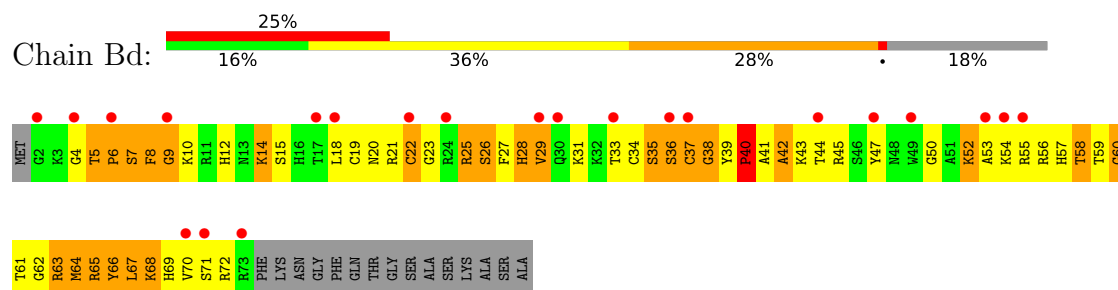
• Molecule 57: 60S ribosomal protein L32



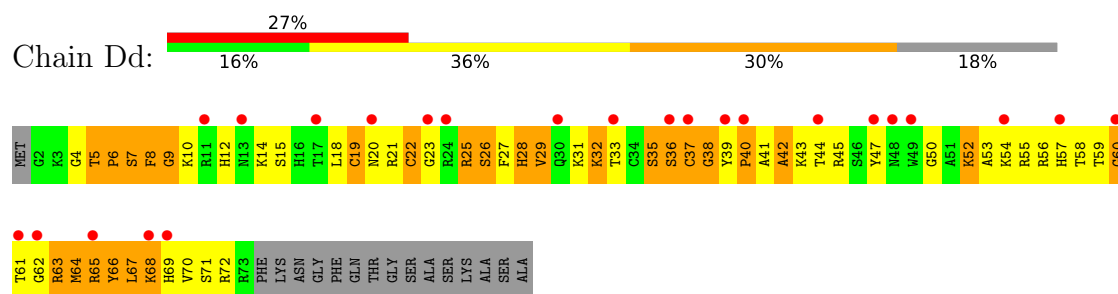
• Molecule 58: 60S ribosomal protein L35



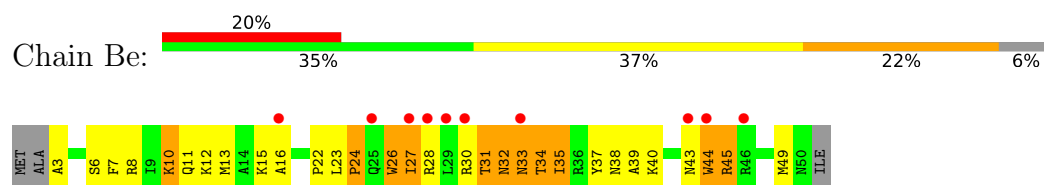
• Molecule 59: 60S ribosomal protein L37-A



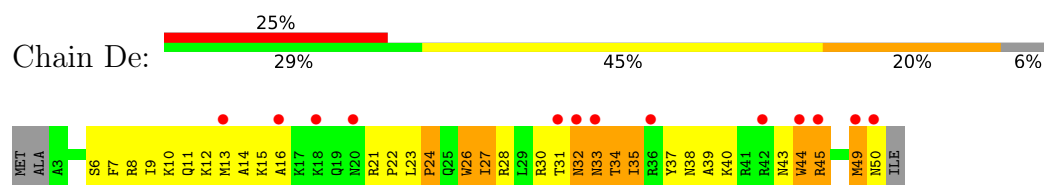
• Molecule 59: 60S ribosomal protein L37-A



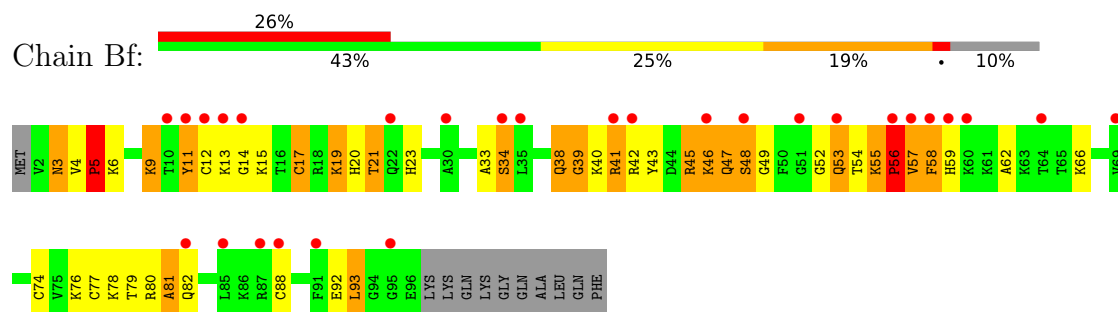
• Molecule 60: 60S ribosomal protein L39



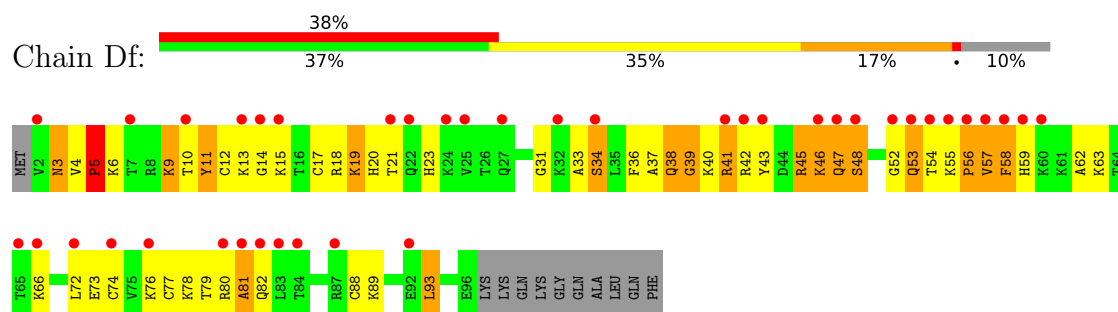
• Molecule 60: 60S ribosomal protein L39



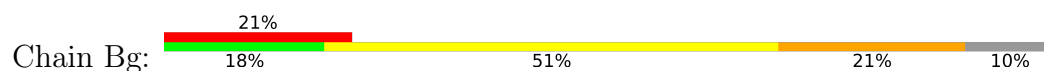
• Molecule 61: 60S ribosomal protein L42

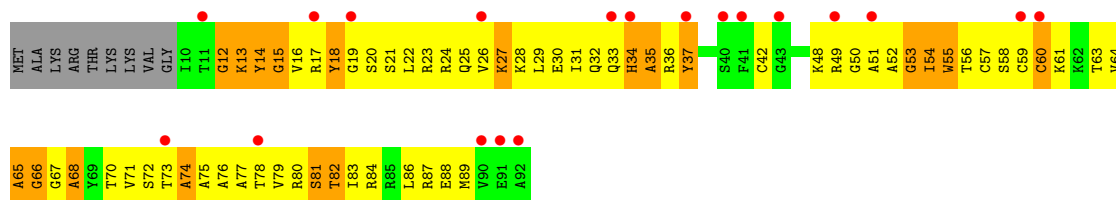


• Molecule 61: 60S ribosomal protein L42

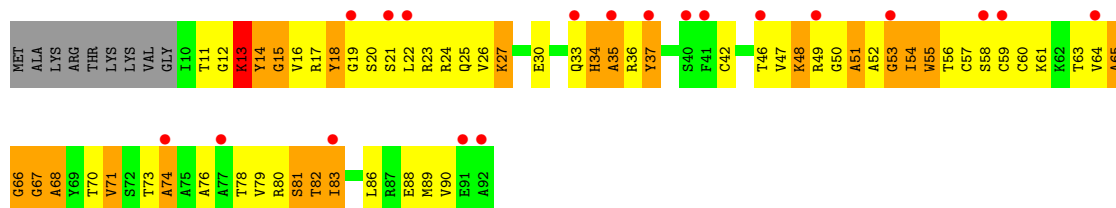
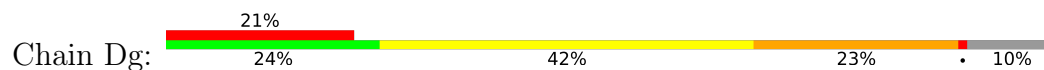


• Molecule 62: 60S ribosomal protein L43





• Molecule 62: 60S ribosomal protein L43



• Molecule 63: Unassigned secondary structure



• Molecule 63: Unassigned secondary structure



• Molecule 64: Unassigned secondary structure



• Molecule 64: Unassigned secondary structure

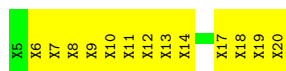


• Molecule 65: Unassigned secondary structure





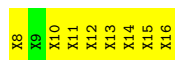
- Molecule 65: Unassigned secondary structure



- Molecule 66: Unassigned secondary structure



- Molecule 67: Unassigned secondary structure



- Molecule 68: Unassigned secondary structure



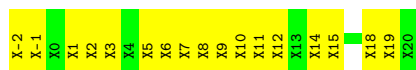
- Molecule 69: Unassigned secondary structure



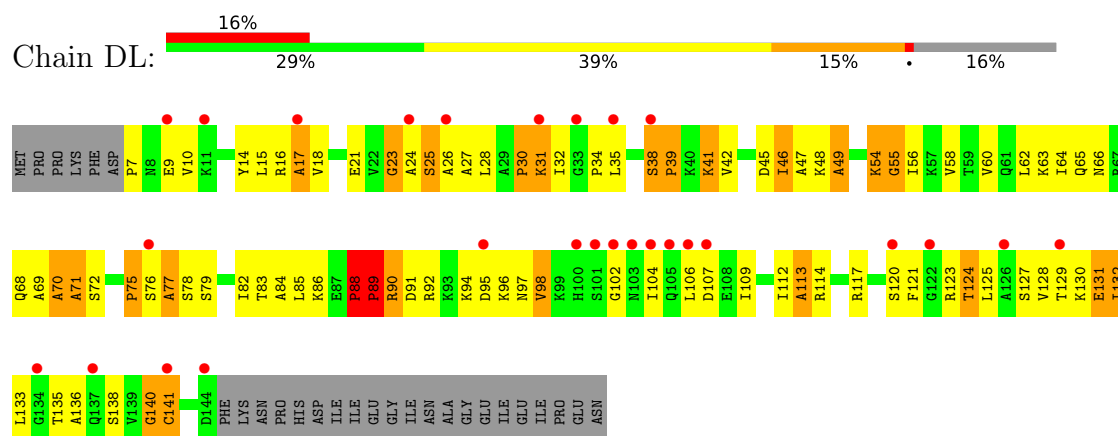
- Molecule 70: Unassigned secondary structure



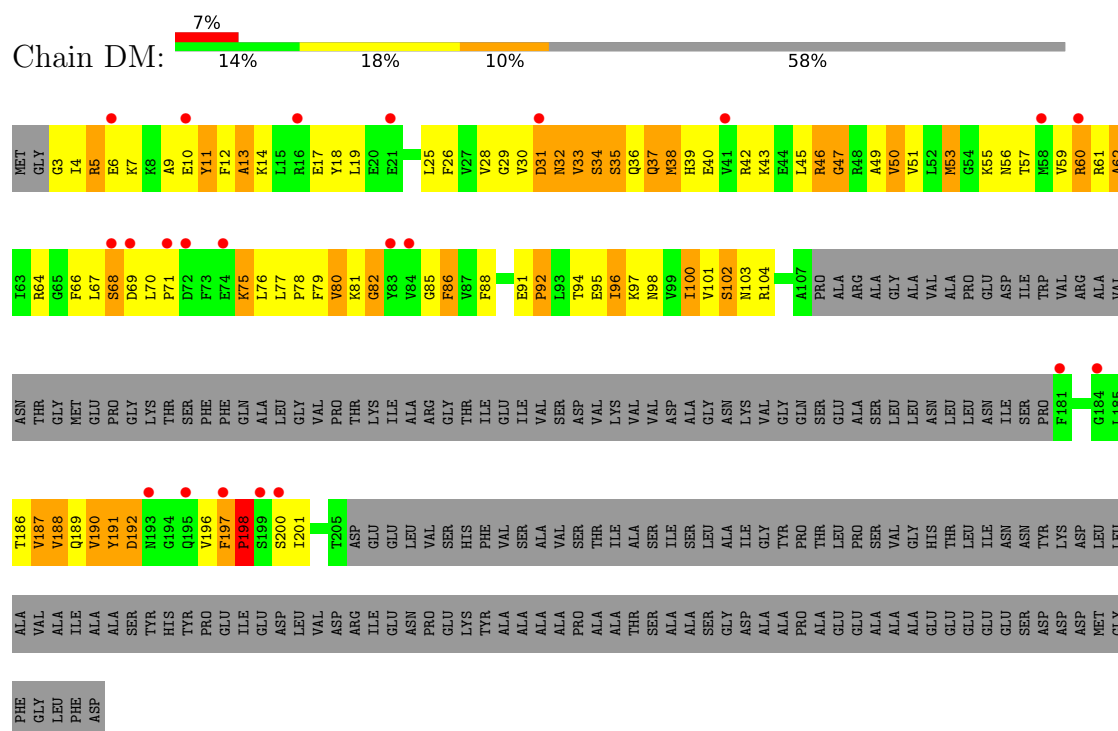
- Molecule 71: Unassigned secondary structure



- Molecule 72: 60S ribosomal protein L12



- Molecule 73: 60S acidic ribosomal protein P0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	437.11Å 288.38Å 306.56Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	268.00 – 4.00 268.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (268.00-4.00) 97.9 (268.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 4.02Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.278 , 0.341 0.284 , 0.343	Depositor DCC
R_{free} test set	12353 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	147.1	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 273.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	309610	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: OHX

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	A1	0.44	5/42619 (0.0%)	0.54	9/66408 (0.0%)
1	C1	0.48	2/42619 (0.0%)	0.55	7/66408 (0.0%)
2	AA	0.69	0/1089	1.33	27/1517 (1.8%)
2	CA	0.78	0/1089	1.35	29/1517 (1.9%)
3	AB	0.83	1/1073 (0.1%)	1.40	23/1488 (1.5%)
3	CB	0.85	0/1073	1.38	21/1488 (1.4%)
4	AC	0.77	0/927	1.10	9/1286 (0.7%)
4	CC	0.71	0/927	1.05	7/1286 (0.5%)
5	AD	0.69	0/834	1.10	9/1159 (0.8%)
5	CD	0.77	0/834	1.21	14/1159 (1.2%)
6	AE	0.72	0/775	1.14	7/1077 (0.6%)
6	CE	0.81	0/775	1.13	9/1077 (0.8%)
7	AF	0.99	0/381	1.48	10/530 (1.9%)
7	CF	0.95	0/381	1.48	10/530 (1.9%)
8	AG	0.76	0/579	1.28	11/806 (1.4%)
8	CG	0.81	0/579	1.32	9/806 (1.1%)
9	AH	0.64	0/626	1.14	7/867 (0.8%)
9	CH	0.68	0/626	1.12	6/867 (0.7%)
10	AI	0.66	0/595	1.29	9/826 (1.1%)
10	CI	0.77	0/595	1.32	11/826 (1.3%)
11	AJ	0.75	0/657	1.21	11/911 (1.2%)
11	CJ	0.83	0/657	1.25	8/911 (0.9%)
12	AK	0.65	0/331	1.22	5/460 (1.1%)
12	CK	0.60	0/331	1.19	5/460 (1.1%)
13	AL	0.70	0/589	1.18	9/816 (1.1%)
13	CL	0.76	0/589	1.24	7/816 (0.9%)
14	AM	0.81	0/518	1.39	10/715 (1.4%)
14	CM	0.98	0/518	1.45	11/715 (1.5%)
15	AN	0.76	0/550	1.26	11/766 (1.4%)
15	CN	0.78	0/550	1.33	9/766 (1.2%)
16	AO	0.82	0/621	1.36	10/860 (1.2%)
16	CO	0.89	0/621	1.40	11/860 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AP	0.99	2/565 (0.4%)	1.38	10/781 (1.3%)
17	CP	1.11	1/565 (0.2%)	1.43	10/781 (1.3%)
18	AQ	0.64	0/331	1.16	2/460 (0.4%)
18	CQ	0.66	0/311	1.27	2/432 (0.5%)
19	AR	0.59	0/229	1.05	2/316 (0.6%)
19	CR	0.65	0/229	1.12	2/316 (0.6%)
20	AS	0.86	1/189 (0.5%)	0.97	1/260 (0.4%)
20	CS	0.86	1/189 (0.5%)	0.99	1/260 (0.4%)
21	AT	0.64	1/1541 (0.1%)	1.02	9/2141 (0.4%)
21	CT	0.67	0/1541	1.06	11/2141 (0.5%)
29	B1	0.61	1/76764 (0.0%)	0.65	21/119684 (0.0%)
29	D1	0.59	3/76764 (0.0%)	0.64	18/119684 (0.0%)
30	B2	0.58	0/2883	0.68	1/4491 (0.0%)
30	D2	0.64	0/2883	0.70	2/4491 (0.0%)
31	B3	0.53	0/3746	0.57	1/5832 (0.0%)
31	D3	0.46	0/3746	0.54	1/5832 (0.0%)
32	BA	0.50	0/1054	1.05	12/1468 (0.8%)
32	DA	0.49	0/1054	1.00	11/1468 (0.7%)
33	BB	0.95	0/1103	1.42	25/1501 (1.7%)
33	DB	0.82	0/1103	1.35	23/1501 (1.5%)
34	BC	1.08	1/1790 (0.1%)	1.55	45/2487 (1.8%)
34	DC	1.20	6/1790 (0.3%)	1.60	44/2487 (1.8%)
35	BD	1.06	1/1311 (0.1%)	1.48	29/1817 (1.6%)
35	DD	0.87	0/1311	1.42	27/1817 (1.5%)
36	BE	0.81	0/1411	1.45	38/1960 (1.9%)
36	DE	0.92	0/1411	1.52	43/1960 (2.2%)
37	BF	1.19	2/872 (0.2%)	1.74	38/1215 (3.1%)
37	DF	1.34	3/872 (0.3%)	1.77	36/1215 (3.0%)
38	BG	1.15	2/1059 (0.2%)	1.64	29/1471 (2.0%)
38	DG	1.23	6/1059 (0.6%)	1.65	33/1471 (2.2%)
39	BH	0.72	0/855	1.26	13/1190 (1.1%)
39	DH	0.69	0/855	1.21	11/1190 (0.9%)
40	BI	1.02	1/941 (0.1%)	1.34	14/1308 (1.1%)
40	DI	1.18	0/941	1.45	14/1308 (1.1%)
41	BJ	1.00	0/1025	1.37	20/1424 (1.4%)
41	DJ	1.08	2/1025 (0.2%)	1.36	16/1424 (1.1%)
42	BK	0.85	0/809	1.34	18/1122 (1.6%)
42	DK	0.93	0/809	1.35	14/1122 (1.2%)
43	BN	1.04	0/592	1.56	15/823 (1.8%)
43	DN	1.23	0/592	1.67	18/823 (2.2%)
44	BO	0.92	0/922	1.35	16/1282 (1.2%)
44	DO	0.77	0/922	1.31	17/1282 (1.3%)
45	BP	1.25	1/966 (0.1%)	1.68	28/1343 (2.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
45	DP	1.32	6/966 (0.6%)	1.73	33/1343 (2.5%)
46	BQ	1.12	2/760 (0.3%)	1.38	10/1057 (0.9%)
46	DQ	1.05	1/760 (0.1%)	1.32	13/1057 (1.2%)
47	BR	1.09	1/705 (0.1%)	1.48	15/980 (1.5%)
47	DR	0.91	0/705	1.36	14/980 (1.4%)
48	BS	0.79	0/930	1.09	9/1295 (0.7%)
48	DS	0.74	0/930	1.03	9/1295 (0.7%)
49	BT	1.06	1/585 (0.2%)	1.35	7/812 (0.9%)
49	DT	1.08	0/585	1.41	10/812 (1.2%)
50	BU	1.00	0/630	1.34	10/872 (1.1%)
50	DU	1.21	2/630 (0.3%)	1.47	13/872 (1.5%)
51	BV	0.80	0/290	1.15	2/402 (0.5%)
51	DV	0.89	0/290	1.21	2/402 (0.5%)
52	BW	0.84	0/467	1.23	8/651 (1.2%)
52	DW	0.76	0/467	1.24	8/651 (1.2%)
53	BX	0.86	0/529	1.27	9/736 (1.2%)
53	DX	0.76	0/529	1.28	11/736 (1.5%)
54	BY	1.10	3/726 (0.4%)	1.66	20/1004 (2.0%)
54	DY	0.99	3/726 (0.4%)	1.56	19/1004 (1.9%)
55	BZ	0.72	0/480	1.15	5/665 (0.8%)
55	DZ	0.67	0/480	1.14	3/665 (0.5%)
56	Ba	0.98	0/424	1.40	6/589 (1.0%)
56	Da	0.96	0/424	1.42	6/589 (1.0%)
57	Bb	1.10	2/617 (0.3%)	1.64	16/858 (1.9%)
57	Db	0.94	0/617	1.57	18/858 (2.1%)
58	Bc	0.79	0/338	1.35	7/471 (1.5%)
58	Dc	0.65	0/338	1.23	6/471 (1.3%)
59	Bd	0.97	0/351	1.46	8/485 (1.6%)
59	Dd	0.77	0/351	1.41	8/485 (1.6%)
60	Be	0.89	0/239	1.31	3/333 (0.9%)
60	De	0.75	0/239	1.24	4/333 (1.2%)
61	Bf	0.65	0/466	1.04	3/646 (0.5%)
61	Df	0.54	0/466	1.00	3/646 (0.5%)
62	Bg	0.82	0/406	1.25	5/562 (0.9%)
62	Dg	0.73	0/406	1.07	4/562 (0.7%)
72	DL	0.62	0/678	1.18	12/941 (1.3%)
73	DM	0.70	0/639	1.16	9/886 (1.0%)
All	All	0.65	64/326627 (0.0%)	0.82	1440/496371 (0.3%)

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	AB	0	2
3	CB	0	2
17	AP	0	1
17	CP	0	1
18	AQ	0	1
18	CQ	0	1
22	Bo	0	1
23	Ab	0	1
23	Cb	0	1
24	Ac	0	1
29	B1	0	3
29	D1	0	3
34	BC	0	5
34	DC	0	6
35	BD	0	1
35	DD	0	2
36	BE	0	1
36	DE	0	1
37	BF	0	4
37	DF	0	4
38	BG	0	1
38	DG	0	1
42	BK	0	1
42	DK	0	1
44	DO	0	1
45	BP	0	4
45	DP	0	5
49	BT	0	1
49	DT	0	1
51	BV	0	1
51	DV	0	1
54	BY	0	2
54	DY	0	2
56	Ba	0	1
56	Da	0	1
57	Bb	0	1
57	Db	0	1
All	All	0	68

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	DF	88	SER	CA-C	6.88	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	243	G	C1'-N9	-6.85	1.37	1.48
35	BD	230	VAL	CA-CB	-6.81	1.47	1.55
54	BY	45	MET	CA-C	6.81	1.61	1.53
1	C1	129	U	C1'-N1	6.75	1.57	1.47

The worst 5 of 1440 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	DD	126	ILE	N-CA-C	-14.57	96.72	110.42
35	BD	126	ILE	N-CA-C	-13.80	97.56	110.53
14	CM	55	TYR	N-CA-C	-12.56	97.90	113.97
45	DP	65	ASN	N-CA-C	-12.17	97.71	111.71
62	Bg	12	GLY	N-CA-C	-12.00	98.65	114.25

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AB	224	PHE	Peptide
3	AB	225	LEU	Peptide
17	AP	28	ASN	Peptide
18	AQ	41	ILE	Peptide
23	Ab	14	UNK	Peptide

5.2 Too-close contacts [i](#)

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	A1	38107	0	19170	5871	0
1	C1	38107	0	19169	6031	0
2	AA	1090	0	508	139	0
2	CA	1090	0	508	140	0
3	AB	1074	0	502	150	0
3	CB	1074	0	502	158	0
4	AC	928	0	448	101	0
4	CC	928	0	448	105	0
5	AD	836	0	391	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	CD	836	0	391	126	0
6	AE	777	0	362	99	0
6	CE	777	0	362	102	0
7	AF	382	0	164	27	0
7	CF	382	0	164	25	0
8	AG	580	0	266	78	0
8	CG	580	0	266	70	0
9	AH	627	0	312	69	0
9	CH	627	0	312	79	0
10	AI	596	0	272	63	0
10	CI	596	0	272	79	0
11	AJ	658	0	307	88	0
11	CJ	658	0	307	96	0
12	AK	332	0	146	32	0
12	CK	332	0	146	27	0
13	AL	591	0	261	82	0
13	CL	591	0	261	84	0
14	AM	521	0	251	73	0
14	CM	521	0	251	74	0
15	AN	551	0	229	84	0
15	CN	551	0	229	80	0
16	AO	622	0	283	66	0
16	CO	622	0	283	60	0
17	AP	566	0	260	81	0
17	CP	566	0	260	78	0
18	AQ	332	0	149	19	0
18	CQ	312	0	135	17	0
19	AR	230	0	100	12	0
19	CR	230	0	100	13	0
20	AS	190	0	85	50	0
20	CS	190	0	85	48	0
21	AT	1543	0	743	105	0
21	CT	1543	0	743	111	0
22	Aa	100	0	25	6	0
22	Bo	100	0	23	7	0
22	Ca	100	0	23	10	0
23	Ab	525	0	141	44	0
23	Cb	525	0	138	58	0
24	Ac	465	0	122	59	0
24	Cc	465	0	120	48	0
25	Ad	175	0	39	25	0
25	Cd	175	0	41	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Ae	105	0	25	18	0
26	Bj	105	0	23	9	0
26	Dj	105	0	24	7	0
27	Af	55	0	15	3	0
28	Ah	205	0	51	29	0
28	Ch	205	0	50	33	0
29	B1	68577	0	34452	11544	0
29	D1	68577	0	34452	11469	0
30	B2	2579	0	1304	605	0
30	D2	2579	0	1304	616	0
31	B3	3353	0	1695	674	0
31	D3	3353	0	1695	623	0
32	BA	1055	0	453	36	0
32	DA	1055	0	453	40	0
33	BB	1106	0	512	108	0
33	DB	1106	0	512	128	0
34	BC	1791	0	839	282	0
34	DC	1791	0	839	282	0
35	BD	1312	0	651	182	0
35	DD	1312	0	651	173	0
36	BE	1412	0	670	238	0
36	DE	1412	0	670	237	0
37	BF	873	0	400	159	0
37	DF	873	0	400	156	0
38	BG	1061	0	492	157	0
38	DG	1061	0	492	161	0
39	BH	856	0	432	85	0
39	DH	856	0	432	77	0
40	BI	942	0	414	96	0
40	DI	942	0	414	97	0
41	BJ	1027	0	468	108	0
41	DJ	1027	0	468	112	0
42	BK	810	0	360	136	0
42	DK	810	0	360	130	0
43	BN	593	0	299	113	0
43	DN	593	0	299	121	0
44	BO	923	0	423	143	0
44	DO	923	0	423	128	0
45	BP	967	0	468	158	0
45	DP	967	0	468	169	0
46	BQ	761	0	371	106	0
46	DQ	761	0	371	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BR	706	0	340	106	0
47	DR	706	0	340	98	0
48	BS	931	0	460	80	0
48	DS	931	0	460	87	0
49	BT	586	0	269	92	0
49	DT	586	0	269	77	0
50	BU	631	0	306	39	0
50	DU	631	0	306	45	0
51	BV	291	0	131	43	0
51	DV	291	0	131	39	0
52	BW	468	0	213	42	0
52	DW	468	0	213	50	0
53	BX	530	0	240	52	0
53	DX	530	0	240	48	0
54	BY	727	0	346	109	0
54	DY	727	0	346	106	0
55	BZ	481	0	224	33	0
55	DZ	481	0	224	37	0
56	Ba	425	0	191	54	0
56	Da	425	0	191	60	0
57	Bb	618	0	284	81	0
57	Db	618	0	284	85	0
58	Bc	339	0	155	39	0
58	Dc	339	0	155	42	0
59	Bd	352	0	161	67	0
59	Dd	352	0	161	63	0
60	Be	240	0	105	24	0
60	De	240	0	105	25	0
61	Bf	467	0	210	41	0
61	Df	467	0	210	44	0
62	Bg	407	0	203	66	0
62	Dg	407	0	203	69	0
63	Bh	220	0	57	34	0
63	Dh	220	0	53	35	0
64	Bi	60	0	16	5	0
64	Di	60	0	14	4	0
65	Bk	80	0	20	21	0
65	Dk	80	0	21	23	0
66	Bl	95	0	21	6	0
67	Bm	45	0	12	7	0
68	Bn	135	0	34	7	0
69	Bp	40	0	11	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	Bq	85	0	25	20	0
71	Br	115	0	27	20	0
72	DL	679	0	325	52	0
73	DM	641	0	281	71	0
74	A1	714	0	0	93	0
74	AL	7	0	0	0	0
74	AS	7	0	0	18	0
74	AT	7	0	0	1	0
74	Ac	7	0	0	0	0
74	B1	1547	0	0	191	0
74	B2	70	0	0	12	0
74	B3	84	0	0	14	0
74	BC	7	0	0	1	0
74	BO	7	0	0	0	0
74	BT	7	0	0	2	0
74	Bd	14	0	0	10	0
74	Bg	7	0	0	10	0
74	C1	707	0	0	100	0
74	CI	7	0	0	0	0
74	CS	14	0	0	16	0
74	CT	7	0	0	0	0
74	D1	1575	0	0	185	0
74	D2	63	0	0	16	0
74	D3	84	0	0	22	0
74	DC	7	0	0	0	0
74	DE	7	0	0	0	0
74	DJ	7	0	0	0	0
74	DO	14	0	0	6	0
74	DT	7	0	0	0	0
74	Dd	14	0	0	11	0
74	Dg	7	0	0	11	0
All	All	309610	0	149262	46170	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 101.

The worst 5 of 46170 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)
63:Dh:14:UNK:CB	63:Dh:14:UNK:CA	1.77	1.60
23:Cb:23:UNK:CB	23:Cb:23:UNK:CA	1.79	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B1:592:A:H2'	29:B1:593:C:C4'	1.31	1.55
29:B1:606:C:H3'	29:B1:607:A:C8	1.39	1.54
29:D1:606:C:H3'	29:D1:607:A:C8	1.43	1.52

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	AA	218/252 (86%)	75 (34%)	68 (31%)	75 (34%)	0	0
2	CA	218/252 (86%)	78 (36%)	63 (29%)	77 (35%)	0	0
3	AB	217/254 (85%)	85 (39%)	54 (25%)	78 (36%)	0	0
3	CB	217/254 (85%)	81 (37%)	62 (29%)	74 (34%)	0	0
4	AC	187/240 (78%)	72 (38%)	56 (30%)	59 (32%)	0	0
4	CC	187/240 (78%)	69 (37%)	55 (29%)	63 (34%)	0	0
5	AD	165/225 (73%)	55 (33%)	46 (28%)	64 (39%)	0	0
5	CD	165/225 (73%)	58 (35%)	44 (27%)	63 (38%)	0	0
6	AE	153/197 (78%)	48 (31%)	54 (35%)	51 (33%)	0	0
6	CE	153/197 (78%)	48 (31%)	49 (32%)	56 (37%)	0	0
7	AF	75/156 (48%)	32 (43%)	18 (24%)	25 (33%)	0	0
7	CF	75/156 (48%)	31 (41%)	20 (27%)	24 (32%)	0	0
8	AG	115/151 (76%)	46 (40%)	38 (33%)	31 (27%)	0	0
8	CG	115/151 (76%)	49 (43%)	33 (29%)	33 (29%)	0	0
9	AH	126/137 (92%)	52 (41%)	38 (30%)	36 (29%)	0	0
9	CH	126/137 (92%)	51 (40%)	39 (31%)	36 (29%)	0	0
10	AI	119/142 (84%)	38 (32%)	40 (34%)	41 (34%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CI	119/142 (84%)	43 (36%)	35 (29%)	41 (34%)	0	0
11	AJ	132/143 (92%)	57 (43%)	33 (25%)	42 (32%)	0	0
11	CJ	132/143 (92%)	52 (39%)	37 (28%)	43 (33%)	0	0
12	AK	65/136 (48%)	27 (42%)	16 (25%)	22 (34%)	0	0
12	CK	65/136 (48%)	28 (43%)	16 (25%)	21 (32%)	0	0
13	AL	116/146 (80%)	48 (41%)	34 (29%)	34 (29%)	0	0
13	CL	116/146 (80%)	48 (41%)	33 (28%)	35 (30%)	0	0
14	AM	100/144 (69%)	38 (38%)	28 (28%)	34 (34%)	0	0
14	CM	100/144 (69%)	36 (36%)	27 (27%)	37 (37%)	0	0
15	AN	109/121 (90%)	49 (45%)	30 (28%)	30 (28%)	0	0
15	CN	109/121 (90%)	49 (45%)	29 (27%)	31 (28%)	0	0
16	AO	125/130 (96%)	48 (38%)	40 (32%)	37 (30%)	0	0
16	CO	125/130 (96%)	49 (39%)	36 (29%)	40 (32%)	0	0
17	AP	114/145 (79%)	48 (42%)	24 (21%)	42 (37%)	0	0
17	CP	114/145 (79%)	45 (40%)	28 (25%)	41 (36%)	0	0
18	AQ	65/108 (60%)	28 (43%)	21 (32%)	16 (25%)	0	1
18	CQ	61/108 (56%)	28 (46%)	18 (30%)	15 (25%)	0	1
19	AR	45/67 (67%)	17 (38%)	12 (27%)	16 (36%)	0	0
19	CR	45/67 (67%)	17 (38%)	11 (24%)	17 (38%)	0	0
20	AS	37/56 (66%)	8 (22%)	14 (38%)	15 (40%)	0	0
20	CS	37/56 (66%)	8 (22%)	13 (35%)	16 (43%)	0	0
21	AT	309/319 (97%)	180 (58%)	71 (23%)	58 (19%)	0	2
21	CT	309/319 (97%)	184 (60%)	66 (21%)	59 (19%)	0	2
32	BA	211/217 (97%)	76 (36%)	67 (32%)	68 (32%)	0	0
32	DA	211/217 (97%)	76 (36%)	79 (37%)	56 (26%)	0	0
33	BB	228/254 (90%)	80 (35%)	55 (24%)	93 (41%)	0	0
33	DB	228/254 (90%)	83 (36%)	55 (24%)	90 (40%)	0	0
34	BC	362/387 (94%)	112 (31%)	100 (28%)	150 (41%)	0	0
34	DC	362/387 (94%)	109 (30%)	102 (28%)	151 (42%)	0	0
35	BD	266/362 (74%)	111 (42%)	79 (30%)	76 (29%)	0	0
35	DD	266/362 (74%)	109 (41%)	78 (29%)	79 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BE	285/297 (96%)	108 (38%)	82 (29%)	95 (33%)	0	0
36	DE	285/297 (96%)	105 (37%)	79 (28%)	101 (35%)	0	0
37	BF	174/176 (99%)	44 (25%)	62 (36%)	68 (39%)	0	0
37	DF	174/176 (99%)	43 (25%)	61 (35%)	70 (40%)	0	0
38	BG	211/244 (86%)	85 (40%)	62 (29%)	64 (30%)	0	0
38	DG	211/244 (86%)	89 (42%)	60 (28%)	62 (29%)	0	0
39	BH	171/256 (67%)	59 (34%)	58 (34%)	54 (32%)	0	0
39	DH	171/256 (67%)	60 (35%)	62 (36%)	49 (29%)	0	0
40	BI	189/191 (99%)	76 (40%)	60 (32%)	53 (28%)	0	0
40	DI	189/191 (99%)	79 (42%)	57 (30%)	53 (28%)	0	0
41	BJ	204/221 (92%)	80 (39%)	52 (26%)	72 (35%)	0	0
41	DJ	204/221 (92%)	75 (37%)	55 (27%)	74 (36%)	0	0
42	BK	163/174 (94%)	57 (35%)	42 (26%)	64 (39%)	0	0
42	DK	163/174 (94%)	56 (34%)	46 (28%)	61 (37%)	0	0
43	BN	118/138 (86%)	27 (23%)	44 (37%)	47 (40%)	0	0
43	DN	118/138 (86%)	28 (24%)	39 (33%)	51 (43%)	0	0
44	BO	185/204 (91%)	77 (42%)	49 (26%)	59 (32%)	0	0
44	DO	185/204 (91%)	76 (41%)	53 (29%)	56 (30%)	0	0
45	BP	194/199 (98%)	81 (42%)	56 (29%)	57 (29%)	0	0
45	DP	194/199 (98%)	77 (40%)	62 (32%)	55 (28%)	0	0
46	BQ	152/184 (83%)	62 (41%)	44 (29%)	46 (30%)	0	0
46	DQ	152/184 (83%)	62 (41%)	45 (30%)	45 (30%)	0	0
47	BR	141/186 (76%)	63 (45%)	28 (20%)	50 (36%)	0	0
47	DR	141/186 (76%)	59 (42%)	32 (23%)	50 (36%)	0	0
48	BS	186/189 (98%)	104 (56%)	57 (31%)	25 (13%)	0	3
48	DS	186/189 (98%)	101 (54%)	60 (32%)	25 (13%)	0	3
49	BT	117/160 (73%)	53 (45%)	18 (15%)	46 (39%)	0	0
49	DT	117/160 (73%)	50 (43%)	23 (20%)	44 (38%)	0	0
50	BU	127/137 (93%)	64 (50%)	28 (22%)	35 (28%)	0	0
50	DU	127/137 (93%)	70 (55%)	21 (16%)	36 (28%)	0	0
51	BV	57/155 (37%)	14 (25%)	19 (33%)	24 (42%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DV	57/155 (37%)	15 (26%)	16 (28%)	26 (46%)	0	0
52	BW	92/142 (65%)	30 (33%)	30 (33%)	32 (35%)	0	0
52	DW	92/142 (65%)	32 (35%)	28 (30%)	32 (35%)	0	0
53	BX	105/127 (83%)	53 (50%)	28 (27%)	24 (23%)	0	1
53	DX	105/127 (83%)	55 (52%)	30 (29%)	20 (19%)	0	2
54	BY	147/149 (99%)	37 (25%)	47 (32%)	63 (43%)	0	0
54	DY	147/149 (99%)	36 (24%)	51 (35%)	60 (41%)	0	0
55	BZ	96/105 (91%)	48 (50%)	28 (29%)	20 (21%)	0	1
55	DZ	96/105 (91%)	51 (53%)	28 (29%)	17 (18%)	0	2
56	Ba	84/113 (74%)	27 (32%)	27 (32%)	30 (36%)	0	0
56	Da	84/113 (74%)	25 (30%)	28 (33%)	31 (37%)	0	0
57	Bb	123/130 (95%)	39 (32%)	28 (23%)	56 (46%)	0	0
57	Db	123/130 (95%)	41 (33%)	31 (25%)	51 (42%)	0	0
58	Bc	66/120 (55%)	28 (42%)	23 (35%)	15 (23%)	0	1
58	Dc	66/120 (55%)	28 (42%)	26 (39%)	12 (18%)	0	2
59	Bd	70/88 (80%)	19 (27%)	20 (29%)	31 (44%)	0	0
59	Dd	70/88 (80%)	17 (24%)	24 (34%)	29 (41%)	0	0
60	Be	46/51 (90%)	25 (54%)	8 (17%)	13 (28%)	0	0
60	De	46/51 (90%)	22 (48%)	12 (26%)	12 (26%)	0	1
61	Bf	93/106 (88%)	37 (40%)	28 (30%)	28 (30%)	0	0
61	Df	93/106 (88%)	37 (40%)	28 (30%)	28 (30%)	0	0
62	Bg	81/92 (88%)	31 (38%)	27 (33%)	23 (28%)	0	0
62	Dg	81/92 (88%)	32 (40%)	24 (30%)	25 (31%)	0	0
72	DL	136/165 (82%)	42 (31%)	42 (31%)	52 (38%)	0	0
73	DM	126/312 (40%)	48 (38%)	31 (25%)	47 (37%)	0	0
All	All	14930/18123 (82%)	5798 (39%)	4273 (29%)	4859 (32%)	0	0

5 of 4859 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	11	PRO
2	AA	13	ASP
2	AA	14	ALA

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Mol	Chain	Res	Type
2	AA	21	ASN
2	AA	24	LEU

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1787/1800 (99%)	1004 (56%)	148 (8%)
1	C1	1787/1800 (99%)	993 (55%)	150 (8%)
29	B1	3203/3396 (94%)	1734 (54%)	259 (8%)
29	D1	3203/3396 (94%)	1726 (53%)	257 (8%)
30	B2	120/121 (99%)	70 (58%)	12 (10%)
30	D2	120/121 (99%)	66 (55%)	12 (10%)
31	B3	157/158 (99%)	80 (50%)	9 (5%)
31	D3	157/158 (99%)	79 (50%)	9 (5%)
All	All	10534/10950 (96%)	5752 (54%)	856 (8%)

5 of 5752 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	U
1	A1	4	C
1	A1	7	G
1	A1	8	U

5 of 856 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	262	U
1	C1	1761	U
29	D1	3093	C
1	C1	380	U
1	C1	254	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

715 ligands 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	$\# Z > 2$
74	OHX	C1	1978	-	0,6,6	-	-	-		
74	OHX	B1	3561	-	0,6,6	-	-	-		
74	OHX	C1	1986	-	0,6,6	-	-	-		
74	OHX	A1	1953	-	0,6,6	-	-	-		
74	OHX	D1	3567	-	0,6,6	-	-	-		
74	OHX	D1	3484	-	0,6,6	-	-	-		
74	OHX	D1	3442	-	0,6,6	-	-	-		
74	OHX	B1	3569	-	0,6,6	-	-	-		
74	OHX	Bd	101	-	0,6,6	-	-	-		
74	OHX	B1	3590	-	0,6,6	-	-	-		
74	OHX	B2	203	-	0,6,6	-	-	-		
74	OHX	C1	1901	-	0,6,6	-	-	-		
74	OHX	C1	1938	-	0,6,6	-	-	-		
74	OHX	B1	3603	-	0,6,6	-	-	-		
74	OHX	C1	1925	-	0,6,6	-	-	-		
74	OHX	A1	1960	-	0,6,6	-	-	-		
74	OHX	C1	1949	-	0,6,6	-	-	-		
74	OHX	D1	3508	-	0,6,6	-	-	-		
74	OHX	D1	3514	-	0,6,6	-	-	-		
74	OHX	B1	3493	-	0,6,6	-	-	-		
74	OHX	D1	3515	-	0,6,6	-	-	-		
74	OHX	C1	1911	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	C1	1952	-	0,6,6	-	-	-		
74	OHX	B3	202	-	0,6,6	-	-	-		
74	OHX	D1	3414	-	0,6,6	-	-	-		
74	OHX	B1	3565	-	0,6,6	-	-	-		
74	OHX	C1	2000	-	0,6,6	-	-	-		
74	OHX	D1	3558	-	0,6,6	-	-	-		
74	OHX	B1	3509	-	0,6,6	-	-	-		
74	OHX	A1	1986	-	0,6,6	-	-	-		
74	OHX	B1	3457	-	0,6,6	-	-	-		
74	OHX	B1	3417	-	0,6,6	-	-	-		
74	OHX	A1	1914	-	0,6,6	-	-	-		
74	OHX	B1	3431	-	0,6,6	-	-	-		
74	OHX	D1	3543	-	0,6,6	-	-	-		
74	OHX	D3	209	-	0,6,6	-	-	-		
74	OHX	B3	209	-	0,6,6	-	-	-		
74	OHX	D1	3546	-	0,6,6	-	-	-		
74	OHX	D1	3583	-	0,6,6	-	-	-		
74	OHX	A1	1941	-	0,6,6	-	-	-		
74	OHX	B1	3408	-	0,6,6	-	-	-		
74	OHX	B1	3507	-	0,6,6	-	-	-		
74	OHX	A1	1911	-	0,6,6	-	-	-		
74	OHX	B1	3550	-	0,6,6	-	-	-		
74	OHX	C1	1921	-	0,6,6	-	-	-		
74	OHX	D1	3544	-	0,6,6	-	-	-		
74	OHX	B1	3560	-	0,6,6	-	-	-		
74	OHX	A1	1944	-	0,6,6	-	-	-		
74	OHX	Bg	101	-	0,6,6	-	-	-		
74	OHX	D1	3577	-	0,6,6	-	-	-		
74	OHX	A1	1955	-	0,6,6	-	-	-		
74	OHX	B1	3606	-	0,6,6	-	-	-		
74	OHX	A1	1957	-	0,6,6	-	-	-		
74	OHX	D1	3576	-	0,6,6	-	-	-		
74	OHX	B1	3519	-	0,6,6	-	-	-		
74	OHX	D1	3464	-	0,6,6	-	-	-		
74	OHX	A1	1982	-	0,6,6	-	-	-		
74	OHX	B1	3458	-	0,6,6	-	-	-		
74	OHX	B1	3528	-	0,6,6	-	-	-		
74	OHX	B3	207	-	0,6,6	-	-	-		
74	OHX	D1	3513	-	0,6,6	-	-	-		
74	OHX	A1	1907	-	0,6,6	-	-	-		
74	OHX	B1	3540	-	0,6,6	-	-	-		
74	OHX	D1	3415	-	0,6,6	-	-	-		
74	OHX	D1	3521	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	D1	3465	-	0,6,6	-	-	-		
74	OHX	C1	1905	-	0,6,6	-	-	-		
74	OHX	D1	3571	-	0,6,6	-	-	-		
74	OHX	B1	3506	-	0,6,6	-	-	-		
74	OHX	A1	1997	-	0,6,6	-	-	-		
74	OHX	B3	206	-	0,6,6	-	-	-		
74	OHX	B1	3470	-	0,6,6	-	-	-		
74	OHX	D3	207	-	0,6,6	-	-	-		
74	OHX	D1	3453	-	0,6,6	-	-	-		
74	OHX	D1	3474	-	0,6,6	-	-	-		
74	OHX	D1	3561	-	0,6,6	-	-	-		
74	OHX	C1	1956	-	0,6,6	-	-	-		
74	OHX	B1	3535	-	0,6,6	-	-	-		
74	OHX	B2	205	-	0,6,6	-	-	-		
74	OHX	D1	3569	-	0,6,6	-	-	-		
74	OHX	D1	3606	-	0,6,6	-	-	-		
74	OHX	B1	3429	-	0,6,6	-	-	-		
74	OHX	D1	3458	-	0,6,6	-	-	-		
74	OHX	D1	3528	-	0,6,6	-	-	-		
74	OHX	C1	1920	-	0,6,6	-	-	-		
74	OHX	C1	1918	-	0,6,6	-	-	-		
74	OHX	C1	1908	-	0,6,6	-	-	-		
74	OHX	A1	1951	-	0,6,6	-	-	-		
74	OHX	C1	1982	-	0,6,6	-	-	-		
74	OHX	B1	3486	-	0,6,6	-	-	-		
74	OHX	D1	3613	-	0,6,6	-	-	-		
74	OHX	C1	1953	-	0,6,6	-	-	-		
74	OHX	C1	1957	-	0,6,6	-	-	-		
74	OHX	B1	3491	-	0,6,6	-	-	-		
74	OHX	C1	1939	-	0,6,6	-	-	-		
74	OHX	D1	3585	-	0,6,6	-	-	-		
74	OHX	A1	1942	-	0,6,6	-	-	-		
74	OHX	C1	1932	-	0,6,6	-	-	-		
74	OHX	D1	3509	-	0,6,6	-	-	-		
74	OHX	BO	301	-	0,6,6	-	-	-		
74	OHX	C1	1972	-	0,6,6	-	-	-		
74	OHX	D1	3548	-	0,6,6	-	-	-		
74	OHX	B1	3502	-	0,6,6	-	-	-		
74	OHX	D1	3560	-	0,6,6	-	-	-		
74	OHX	D3	210	-	0,6,6	-	-	-		
74	OHX	B1	3451	-	0,6,6	-	-	-		
74	OHX	D1	3536	-	0,6,6	-	-	-		
74	OHX	C1	1903	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	B1	3460	-	0,6,6	-	-	-		
74	OHX	AL	201	-	0,6,6	-	-	-		
74	OHX	D1	3432	-	0,6,6	-	-	-		
74	OHX	D1	3501	-	0,6,6	-	-	-		
74	OHX	D1	3594	-	0,6,6	-	-	-		
74	OHX	B1	3597	-	0,6,6	-	-	-		
74	OHX	A1	1948	-	0,6,6	-	-	-		
74	OHX	A1	1959	-	0,6,6	-	-	-		
74	OHX	D1	3614	-	0,6,6	-	-	-		
74	OHX	DO	302	-	0,6,6	-	-	-		
74	OHX	A1	1954	-	0,6,6	-	-	-		
74	OHX	D1	3550	-	0,6,6	-	-	-		
74	OHX	B1	3441	-	0,6,6	-	-	-		
74	OHX	C1	1943	-	0,6,6	-	-	-		
74	OHX	B1	3544	-	0,6,6	-	-	-		
74	OHX	A1	1912	-	0,6,6	-	-	-		
74	OHX	D1	3598	-	0,6,6	-	-	-		
74	OHX	D3	205	-	0,6,6	-	-	-		
74	OHX	B1	3424	-	0,6,6	-	-	-		
74	OHX	C1	1941	-	0,6,6	-	-	-		
74	OHX	C1	1948	-	0,6,6	-	-	-		
74	OHX	D1	3461	-	0,6,6	-	-	-		
74	OHX	D1	3519	-	0,6,6	-	-	-		
74	OHX	C1	1923	-	0,6,6	-	-	-		
74	OHX	A1	1945	-	0,6,6	-	-	-		
74	OHX	D1	3462	-	0,6,6	-	-	-		
74	OHX	Ac	100	-	0,6,6	-	-	-		
74	OHX	C1	1974	-	0,6,6	-	-	-		
74	OHX	D3	206	-	0,6,6	-	-	-		
74	OHX	B1	3445	-	0,6,6	-	-	-		
74	OHX	A1	1928	-	0,6,6	-	-	-		
74	OHX	D1	3468	-	0,6,6	-	-	-		
74	OHX	B1	3403	-	0,6,6	-	-	-		
74	OHX	C1	1910	-	0,6,6	-	-	-		
74	OHX	C1	1967	-	0,6,6	-	-	-		
74	OHX	A1	1905	-	0,6,6	-	-	-		
74	OHX	B1	3410	-	0,6,6	-	-	-		
74	OHX	B1	3435	-	0,6,6	-	-	-		
74	OHX	D1	3511	-	0,6,6	-	-	-		
74	OHX	D3	201	-	0,6,6	-	-	-		
74	OHX	B1	3554	-	0,6,6	-	-	-		
74	OHX	D1	3424	-	0,6,6	-	-	-		
74	OHX	D1	3436	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	D1	3615	-	0,6,6	-	-	-		
74	OHX	C1	1933	-	0,6,6	-	-	-		
74	OHX	B1	3599	-	0,6,6	-	-	-		
74	OHX	A1	2000	-	0,6,6	-	-	-		
74	OHX	D1	3428	-	0,6,6	-	-	-		
74	OHX	A1	1978	-	0,6,6	-	-	-		
74	OHX	B1	3593	-	0,6,6	-	-	-		
74	OHX	B1	3612	-	0,6,6	-	-	-		
74	OHX	D1	3499	-	0,6,6	-	-	-		
74	OHX	A1	1927	-	0,6,6	-	-	-		
74	OHX	CS	102	-	0,6,6	-	-	-		
74	OHX	A1	1931	1	0,6,6	-	-	-		
74	OHX	C1	1934	-	0,6,6	-	-	-		
74	OHX	D1	3557	-	0,6,6	-	-	-		
74	OHX	B1	3453	-	0,6,6	-	-	-		
74	OHX	C1	1999	-	0,6,6	-	-	-		
74	OHX	B1	3433	-	0,6,6	-	-	-		
74	OHX	D1	3502	-	0,6,6	-	-	-		
74	OHX	A1	2001	-	0,6,6	-	-	-		
74	OHX	C1	1913	-	0,6,6	-	-	-		
74	OHX	A1	1989	-	0,6,6	-	-	-		
74	OHX	D1	3564	-	0,6,6	-	-	-		
74	OHX	B1	3418	-	0,6,6	-	-	-		
74	OHX	D1	3504	-	0,6,6	-	-	-		
74	OHX	D1	3410	-	0,6,6	-	-	-		
74	OHX	D1	3435	-	0,6,6	-	-	-		
74	OHX	C1	1909	-	0,6,6	-	-	-		
74	OHX	B1	3501	-	0,6,6	-	-	-		
74	OHX	C1	1990	-	0,6,6	-	-	-		
74	OHX	B1	3525	-	0,6,6	-	-	-		
74	OHX	CT	401	-	0,6,6	-	-	-		
74	OHX	D1	3517	-	0,6,6	-	-	-		
74	OHX	D1	3506	-	0,6,6	-	-	-		
74	OHX	B1	3568	-	0,6,6	-	-	-		
74	OHX	B1	3402	-	0,6,6	-	-	-		
74	OHX	C1	1997	-	0,6,6	-	-	-		
74	OHX	B1	3547	-	0,6,6	-	-	-		
74	OHX	D2	206	-	0,6,6	-	-	-		
74	OHX	D1	3587	-	0,6,6	-	-	-		
74	OHX	D1	3426	-	0,6,6	-	-	-		
74	OHX	C1	1987	-	0,6,6	-	-	-		
74	OHX	D1	3565	-	0,6,6	-	-	-		
74	OHX	B1	3530	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	D1	3608	-	0,6,6	-	-	-		
74	OHX	D1	3510	-	0,6,6	-	-	-		
74	OHX	B1	3595	-	0,6,6	-	-	-		
74	OHX	A1	1939	-	0,6,6	-	-	-		
74	OHX	A1	1936	-	0,6,6	-	-	-		
74	OHX	A1	1975	-	0,6,6	-	-	-		
74	OHX	D1	3403	-	0,6,6	-	-	-		
74	OHX	A1	1940	-	0,6,6	-	-	-		
74	OHX	A1	1903	-	0,6,6	-	-	-		
74	OHX	B1	3542	-	0,6,6	-	-	-		
74	OHX	D1	3411	-	0,6,6	-	-	-		
74	OHX	B1	3589	-	0,6,6	-	-	-		
74	OHX	B3	205	-	0,6,6	-	-	-		
74	OHX	B1	3446	-	0,6,6	-	-	-		
74	OHX	DE	301	-	0,6,6	-	-	-		
74	OHX	B1	3437	-	0,6,6	-	-	-		
74	OHX	D1	3568	-	0,6,6	-	-	-		
74	OHX	B1	3485	-	0,6,6	-	-	-		
74	OHX	C1	1924	-	0,6,6	-	-	-		
74	OHX	A1	1979	-	0,6,6	-	-	-		
74	OHX	B3	203	-	0,6,6	-	-	-		
74	OHX	D1	3450	-	0,6,6	-	-	-		
74	OHX	D3	211	-	0,6,6	-	-	-		
74	OHX	D2	208	-	0,6,6	-	-	-		
74	OHX	B1	3484	-	0,6,6	-	-	-		
74	OHX	D1	3526	-	0,6,6	-	-	-		
74	OHX	D1	3547	-	0,6,6	-	-	-		
74	OHX	B1	3492	-	0,6,6	-	-	-		
74	OHX	D1	3593	-	0,6,6	-	-	-		
74	OHX	B1	3564	-	0,6,6	-	-	-		
74	OHX	A1	1972	-	0,6,6	-	-	-		
74	OHX	B1	3483	-	0,6,6	-	-	-		
74	OHX	B1	3536	-	0,6,6	-	-	-		
74	OHX	B1	3462	-	0,6,6	-	-	-		
74	OHX	D1	3500	-	0,6,6	-	-	-		
74	OHX	D1	3572	-	0,6,6	-	-	-		
74	OHX	D1	3579	-	0,6,6	-	-	-		
74	OHX	C1	1959	-	0,6,6	-	-	-		
74	OHX	C1	1992	-	0,6,6	-	-	-		
74	OHX	D1	3595	-	0,6,6	-	-	-		
74	OHX	A1	1985	-	0,6,6	-	-	-		
74	OHX	B1	3552	-	0,6,6	-	-	-		
74	OHX	A1	1919	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	B1	3577	-	0,6,6	-	-	-		
74	OHX	C1	1915	-	0,6,6	-	-	-		
74	OHX	B1	3548	-	0,6,6	-	-	-		
74	OHX	D1	3418	-	0,6,6	-	-	-		
74	OHX	D1	3545	-	0,6,6	-	-	-		
74	OHX	A1	1929	-	0,6,6	-	-	-		
74	OHX	C1	1984	-	0,6,6	-	-	-		
74	OHX	A1	1970	-	0,6,6	-	-	-		
74	OHX	C1	1935	-	0,6,6	-	-	-		
74	OHX	B1	3404	-	0,6,6	-	-	-		
74	OHX	B1	3533	-	0,6,6	-	-	-		
74	OHX	B1	3549	-	0,6,6	-	-	-		
74	OHX	D1	3446	-	0,6,6	-	-	-		
74	OHX	B1	3490	-	0,6,6	-	-	-		
74	OHX	B1	3521	-	0,6,6	-	-	-		
74	OHX	B1	3515	-	0,6,6	-	-	-		
74	OHX	A1	1974	-	0,6,6	-	-	-		
74	OHX	C1	1993	-	0,6,6	-	-	-		
74	OHX	B1	3574	-	0,6,6	-	-	-		
74	OHX	B1	3498	-	0,6,6	-	-	-		
74	OHX	BC	401	-	0,6,6	-	-	-		
74	OHX	Dd	102	-	0,6,6	-	-	-		
74	OHX	C1	1966	-	0,6,6	-	-	-		
74	OHX	B1	3578	-	0,6,6	-	-	-		
74	OHX	C1	1996	-	0,6,6	-	-	-		
74	OHX	C1	1989	-	0,6,6	-	-	-		
74	OHX	D1	3492	-	0,6,6	-	-	-		
74	OHX	D1	3540	-	0,6,6	-	-	-		
74	OHX	B1	3467	-	0,6,6	-	-	-		
74	OHX	B1	3555	-	0,6,6	-	-	-		
74	OHX	B1	3472	-	0,6,6	-	-	-		
74	OHX	B1	3571	-	0,6,6	-	-	-		
74	OHX	DT	201	-	0,6,6	-	-	-		
74	OHX	D1	3402	-	0,6,6	-	-	-		
74	OHX	D1	3467	-	0,6,6	-	-	-		
74	OHX	D1	3552	-	0,6,6	-	-	-		
74	OHX	B1	3601	-	0,6,6	-	-	-		
74	OHX	C1	1965	-	0,6,6	-	-	-		
74	OHX	C1	1931	-	0,6,6	-	-	-		
74	OHX	C1	1930	1	0,6,6	-	-	-		
74	OHX	B1	3422	-	0,6,6	-	-	-		
74	OHX	B1	3452	-	0,6,6	-	-	-		
74	OHX	B1	3432	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	A1	1935	-	0,6,6	-	-	-		
74	OHX	D1	3401	-	0,6,6	-	-	-		
74	OHX	D1	3440	-	0,6,6	-	-	-		
74	OHX	A1	1917	-	0,6,6	-	-	-		
74	OHX	A1	1910	-	0,6,6	-	-	-		
74	OHX	B1	3523	-	0,6,6	-	-	-		
74	OHX	D1	3429	-	0,6,6	-	-	-		
74	OHX	D2	205	-	0,6,6	-	-	-		
74	OHX	D1	3404	-	0,6,6	-	-	-		
74	OHX	D1	3448	-	0,6,6	-	-	-		
74	OHX	B1	3488	-	0,6,6	-	-	-		
74	OHX	B1	3510	-	0,6,6	-	-	-		
74	OHX	A1	1926	-	0,6,6	-	-	-		
74	OHX	A1	1964	-	0,6,6	-	-	-		
74	OHX	D1	3603	-	0,6,6	-	-	-		
74	OHX	A1	1913	-	0,6,6	-	-	-		
74	OHX	D1	3460	-	0,6,6	-	-	-		
74	OHX	D1	3578	-	0,6,6	-	-	-		
74	OHX	B1	3497	-	0,6,6	-	-	-		
74	OHX	B1	3465	-	0,6,6	-	-	-		
74	OHX	B1	3576	-	0,6,6	-	-	-		
74	OHX	B1	3434	-	0,6,6	-	-	-		
74	OHX	D1	3589	-	0,6,6	-	-	-		
74	OHX	D1	3472	-	0,6,6	-	-	-		
74	OHX	D1	3437	-	0,6,6	-	-	-		
74	OHX	D1	3438	-	0,6,6	-	-	-		
74	OHX	B1	3430	-	0,6,6	-	-	-		
74	OHX	D1	3476	-	0,6,6	-	-	-		
74	OHX	D1	3601	-	0,6,6	-	-	-		
74	OHX	B1	3588	-	0,6,6	-	-	-		
74	OHX	B1	3620	-	0,6,6	-	-	-		
74	OHX	B3	210	-	0,6,6	-	-	-		
74	OHX	D1	3422	-	0,6,6	-	-	-		
74	OHX	B3	212	-	0,6,6	-	-	-		
74	OHX	B1	3585	-	0,6,6	-	-	-		
74	OHX	A1	1950	-	0,6,6	-	-	-		
74	OHX	D1	3523	-	0,6,6	-	-	-		
74	OHX	B1	3487	-	0,6,6	-	-	-		
74	OHX	D1	3604	-	0,6,6	-	-	-		
74	OHX	B1	3455	-	0,6,6	-	-	-		
74	OHX	B1	3600	-	0,6,6	-	-	-		
74	OHX	C1	1927	-	0,6,6	-	-	-		
74	OHX	B1	3570	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	A1	1966	-	0,6,6	-	-	-		
74	OHX	B1	3618	-	0,6,6	-	-	-		
74	OHX	D1	3427	-	0,6,6	-	-	-		
74	OHX	D1	3434	-	0,6,6	-	-	-		
74	OHX	D1	3533	-	0,6,6	-	-	-		
74	OHX	D2	204	-	0,6,6	-	-	-		
74	OHX	A1	1969	-	0,6,6	-	-	-		
74	OHX	A1	1973	-	0,6,6	-	-	-		
74	OHX	D3	202	-	0,6,6	-	-	-		
74	OHX	C1	1919	-	0,6,6	-	-	-		
74	OHX	B1	3413	-	0,6,6	-	-	-		
74	OHX	D1	3496	-	0,6,6	-	-	-		
74	OHX	A1	1938	-	0,6,6	-	-	-		
74	OHX	B1	3405	-	0,6,6	-	-	-		
74	OHX	D1	3620	-	0,6,6	-	-	-		
74	OHX	D1	3495	-	0,6,6	-	-	-		
74	OHX	B1	3406	-	0,6,6	-	-	-		
74	OHX	B1	3401	-	0,6,6	-	-	-		
74	OHX	D2	202	-	0,6,6	-	-	-		
74	OHX	B2	202	-	0,6,6	-	-	-		
74	OHX	B1	3466	-	0,6,6	-	-	-		
74	OHX	B1	3582	-	0,6,6	-	-	-		
74	OHX	C1	1945	-	0,6,6	-	-	-		
74	OHX	C1	1983	1	0,6,6	-	-	-		
74	OHX	B1	3594	-	0,6,6	-	-	-		
74	OHX	C1	1975	-	0,6,6	-	-	-		
74	OHX	D1	3452	-	0,6,6	-	-	-		
74	OHX	D1	3473	-	0,6,6	-	-	-		
74	OHX	A1	1962	-	0,6,6	-	-	-		
74	OHX	C1	1994	-	0,6,6	-	-	-		
74	OHX	D1	3485	-	0,6,6	-	-	-		
74	OHX	D1	3405	-	0,6,6	-	-	-		
74	OHX	A1	1992	-	0,6,6	-	-	-		
74	OHX	B2	209	-	0,6,6	-	-	-		
74	OHX	D1	3591	-	0,6,6	-	-	-		
74	OHX	B1	3423	-	0,6,6	-	-	-		
74	OHX	B1	3421	-	0,6,6	-	-	-		
74	OHX	B1	3443	-	0,6,6	-	-	-		
74	OHX	C1	1980	-	0,6,6	-	-	-		
74	OHX	D1	3494	-	0,6,6	-	-	-		
74	OHX	B1	3478	-	0,6,6	-	-	-		
74	OHX	A1	1993	-	0,6,6	-	-	-		
74	OHX	D1	3597	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	D1	3477	-	0,6,6	-	-	-		
74	OHX	D1	3622	-	0,6,6	-	-	-		
74	OHX	DJ	301	-	0,6,6	-	-	-		
74	OHX	D1	3549	-	0,6,6	-	-	-		
74	OHX	C1	2001	-	0,6,6	-	-	-		
74	OHX	B1	3409	-	0,6,6	-	-	-		
74	OHX	B1	3615	-	0,6,6	-	-	-		
74	OHX	B1	3520	-	0,6,6	-	-	-		
74	OHX	B1	3580	-	0,6,6	-	-	-		
74	OHX	C1	1902	-	0,6,6	-	-	-		
74	OHX	A1	1901	-	0,6,6	-	-	-		
74	OHX	D1	3455	-	0,6,6	-	-	-		
74	OHX	D1	3441	-	0,6,6	-	-	-		
74	OHX	C1	1904	-	0,6,6	-	-	-		
74	OHX	B1	3412	-	0,6,6	-	-	-		
74	OHX	D1	3554	-	0,6,6	-	-	-		
74	OHX	A1	1952	-	0,6,6	-	-	-		
74	OHX	B1	3420	-	0,6,6	-	-	-		
74	OHX	B1	3436	-	0,6,6	-	-	-		
74	OHX	D1	3443	-	0,6,6	-	-	-		
74	OHX	A1	1980	-	0,6,6	-	-	-		
74	OHX	B1	3534	-	0,6,6	-	-	-		
74	OHX	D1	3408	-	0,6,6	-	-	-		
74	OHX	D1	3625	-	0,6,6	-	-	-		
74	OHX	B1	3482	-	0,6,6	-	-	-		
74	OHX	A1	1965	-	0,6,6	-	-	-		
74	OHX	D1	3520	-	0,6,6	-	-	-		
74	OHX	DO	301	-	0,6,6	-	-	-		
74	OHX	C1	1916	-	0,6,6	-	-	-		
74	OHX	D1	3406	-	0,6,6	-	-	-		
74	OHX	D1	3566	-	0,6,6	-	-	-		
74	OHX	A1	1984	-	0,6,6	-	-	-		
74	OHX	B1	3495	-	0,6,6	-	-	-		
74	OHX	B1	3454	-	0,6,6	-	-	-		
74	OHX	D1	3431	-	0,6,6	-	-	-		
74	OHX	D1	3471	-	0,6,6	-	-	-		
74	OHX	D2	209	-	0,6,6	-	-	-		
74	OHX	A1	1906	-	0,6,6	-	-	-		
74	OHX	B1	3447	-	0,6,6	-	-	-		
74	OHX	B1	3449	-	0,6,6	-	-	-		
74	OHX	D1	3582	-	0,6,6	-	-	-		
74	OHX	D3	208	-	0,6,6	-	-	-		
74	OHX	D1	3580	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	A1	1958	-	0,6,6	-	-	-		
74	OHX	D1	3534	-	0,6,6	-	-	-		
74	OHX	B1	3553	-	0,6,6	-	-	-		
74	OHX	B1	3610	-	0,6,6	-	-	-		
74	OHX	B1	3619	-	0,6,6	-	-	-		
74	OHX	D1	3524	-	0,6,6	-	-	-		
74	OHX	B1	3527	-	0,6,6	-	-	-		
74	OHX	B1	3481	-	0,6,6	-	-	-		
74	OHX	D1	3420	-	0,6,6	-	-	-		
74	OHX	D1	3623	-	0,6,6	-	-	-		
74	OHX	B2	201	-	0,6,6	-	-	-		
74	OHX	C1	1917	-	0,6,6	-	-	-		
74	OHX	D1	3423	-	0,6,6	-	-	-		
74	OHX	D1	3507	-	0,6,6	-	-	-		
74	OHX	A1	1930	-	0,6,6	-	-	-		
74	OHX	D1	3512	-	0,6,6	-	-	-		
74	OHX	C1	1937	-	0,6,6	-	-	-		
74	OHX	B1	3489	-	0,6,6	-	-	-		
74	OHX	B2	210	-	0,6,6	-	-	-		
74	OHX	C1	1964	-	0,6,6	-	-	-		
74	OHX	C1	1922	-	0,6,6	-	-	-		
74	OHX	D1	3609	-	0,6,6	-	-	-		
74	OHX	D1	3454	-	0,6,6	-	-	-		
74	OHX	AT	401	-	0,6,6	-	-	-		
74	OHX	A1	1963	-	0,6,6	-	-	-		
74	OHX	B1	3503	-	0,6,6	-	-	-		
74	OHX	B1	3609	-	0,6,6	-	-	-		
74	OHX	B1	3584	-	0,6,6	-	-	-		
74	OHX	D1	3553	-	0,6,6	-	-	-		
74	OHX	B1	3579	-	0,6,6	-	-	-		
74	OHX	B1	3531	-	0,6,6	-	-	-		
74	OHX	B1	3598	-	0,6,6	-	-	-		
74	OHX	B1	3496	-	0,6,6	-	-	-		
74	OHX	D1	3527	-	0,6,6	-	-	-		
74	OHX	B1	3537	-	0,6,6	-	-	-		
74	OHX	C1	1942	-	0,6,6	-	-	-		
74	OHX	D1	3481	-	0,6,6	-	-	-		
74	OHX	D1	3532	-	0,6,6	-	-	-		
74	OHX	B1	3463	-	0,6,6	-	-	-		
74	OHX	B1	3551	-	0,6,6	-	-	-		
74	OHX	D1	3586	-	0,6,6	-	-	-		
74	OHX	A1	1998	-	0,6,6	-	-	-		
74	OHX	B1	3469	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	D1	3621	-	0,6,6	-	-	-		
74	OHX	B1	3411	-	0,6,6	-	-	-		
74	OHX	B1	3513	-	0,6,6	-	-	-		
74	OHX	B2	206	-	0,6,6	-	-	-		
74	OHX	B1	3596	-	0,6,6	-	-	-		
74	OHX	D1	3538	-	0,6,6	-	-	-		
74	OHX	BT	201	-	0,6,6	-	-	-		
74	OHX	A1	1934	-	0,6,6	-	-	-		
74	OHX	B1	3475	-	0,6,6	-	-	-		
74	OHX	A1	1920	-	0,6,6	-	-	-		
74	OHX	D1	3417	-	0,6,6	-	-	-		
74	OHX	D1	3489	-	0,6,6	-	-	-		
74	OHX	Dg	101	-	0,6,6	-	-	-		
74	OHX	B3	211	-	0,6,6	-	-	-		
74	OHX	B1	3617	-	0,6,6	-	-	-		
74	OHX	A1	1994	-	0,6,6	-	-	-		
74	OHX	A1	1904	-	0,6,6	-	-	-		
74	OHX	B1	3444	-	0,6,6	-	-	-		
74	OHX	D1	3482	-	0,6,6	-	-	-		
74	OHX	B1	3559	-	0,6,6	-	-	-		
74	OHX	C1	1969	-	0,6,6	-	-	-		
74	OHX	D3	204	-	0,6,6	-	-	-		
74	OHX	B1	3563	-	0,6,6	-	-	-		
74	OHX	D1	3537	-	0,6,6	-	-	-		
74	OHX	Bd	102	-	0,6,6	-	-	-		
74	OHX	D1	3491	-	0,6,6	-	-	-		
74	OHX	B1	3546	-	0,6,6	-	-	-		
74	OHX	D1	3449	-	0,6,6	-	-	-		
74	OHX	D1	3529	-	0,6,6	-	-	-		
74	OHX	B1	3428	-	0,6,6	-	-	-		
74	OHX	D1	3605	-	0,6,6	-	-	-		
74	OHX	B1	3545	-	0,6,6	-	-	-		
74	OHX	A1	1987	-	0,6,6	-	-	-		
74	OHX	A1	1946	-	0,6,6	-	-	-		
74	OHX	D1	3596	-	0,6,6	-	-	-		
74	OHX	D1	3619	-	0,6,6	-	-	-		
74	OHX	A1	2002	-	0,6,6	-	-	-		
74	OHX	B1	3557	-	0,6,6	-	-	-		
74	OHX	B1	3476	-	0,6,6	-	-	-		
74	OHX	B1	3566	-	0,6,6	-	-	-		
74	OHX	C1	1906	-	0,6,6	-	-	-		
74	OHX	B3	201	-	0,6,6	-	-	-		
74	OHX	C1	1962	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	C1	1940	-	0,6,6	-	-	-		
74	OHX	B1	3607	-	0,6,6	-	-	-		
74	OHX	B1	3567	-	0,6,6	-	-	-		
74	OHX	D1	3409	-	0,6,6	-	-	-		
74	OHX	C1	1954	-	0,6,6	-	-	-		
74	OHX	B1	3587	-	0,6,6	-	-	-		
74	OHX	D1	3530	-	0,6,6	-	-	-		
74	OHX	C1	1979	-	0,6,6	-	-	-		
74	OHX	D1	3456	-	0,6,6	-	-	-		
74	OHX	D1	3503	-	0,6,6	-	-	-		
74	OHX	D1	3584	-	0,6,6	-	-	-		
74	OHX	C1	1977	-	0,6,6	-	-	-		
74	OHX	C1	1981	-	0,6,6	-	-	-		
74	OHX	B1	3504	-	0,6,6	-	-	-		
74	OHX	B1	3505	-	0,6,6	-	-	-		
74	OHX	A1	1916	-	0,6,6	-	-	-		
74	OHX	C1	1926	-	0,6,6	-	-	-		
74	OHX	D2	203	-	0,6,6	-	-	-		
74	OHX	D1	3480	-	0,6,6	-	-	-		
74	OHX	D1	3551	-	0,6,6	-	-	-		
74	OHX	D1	3413	-	0,6,6	-	-	-		
74	OHX	A1	1968	-	0,6,6	-	-	-		
74	OHX	B1	3471	-	0,6,6	-	-	-		
74	OHX	C1	1929	-	0,6,6	-	-	-		
74	OHX	A1	1933	-	0,6,6	-	-	-		
74	OHX	B1	3583	-	0,6,6	-	-	-		
74	OHX	D1	3430	-	0,6,6	-	-	-		
74	OHX	B2	208	-	0,6,6	-	-	-		
74	OHX	B1	3573	-	0,6,6	-	-	-		
74	OHX	A1	1995	-	0,6,6	-	-	-		
74	OHX	A1	1947	-	0,6,6	-	-	-		
74	OHX	D1	3516	-	0,6,6	-	-	-		
74	OHX	A1	1981	-	0,6,6	-	-	-		
74	OHX	A1	1999	-	0,6,6	-	-	-		
74	OHX	D1	3444	-	0,6,6	-	-	-		
74	OHX	D2	207	-	0,6,6	-	-	-		
74	OHX	B1	3604	-	0,6,6	-	-	-		
74	OHX	C1	1928	-	0,6,6	-	-	-		
74	OHX	D1	3563	-	0,6,6	-	-	-		
74	OHX	A1	1922	-	0,6,6	-	-	-		
74	OHX	D1	3497	-	0,6,6	-	-	-		
74	OHX	B1	3581	-	0,6,6	-	-	-		
74	OHX	B1	3468	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	C1	1958	-	0,6,6	-	-	-		
74	OHX	B1	3526	-	0,6,6	-	-	-		
74	OHX	B1	3477	-	0,6,6	-	-	-		
74	OHX	AS	101	-	0,6,6	-	-	-		
74	OHX	A1	1923	-	0,6,6	-	-	-		
74	OHX	C1	1971	-	0,6,6	-	-	-		
74	OHX	D3	212	-	0,6,6	-	-	-		
74	OHX	A1	1937	-	0,6,6	-	-	-		
74	OHX	B1	3494	-	0,6,6	-	-	-		
74	OHX	B3	204	-	0,6,6	-	-	-		
74	OHX	A1	1915	-	0,6,6	-	-	-		
74	OHX	B2	204	-	0,6,6	-	-	-		
74	OHX	D1	3457	-	0,6,6	-	-	-		
74	OHX	C1	1968	-	0,6,6	-	-	-		
74	OHX	D1	3451	-	0,6,6	-	-	-		
74	OHX	A1	1902	-	0,6,6	-	-	-		
74	OHX	B1	3518	-	0,6,6	-	-	-		
74	OHX	B1	3592	-	0,6,6	-	-	-		
74	OHX	D1	3607	-	0,6,6	-	-	-		
74	OHX	D1	3493	-	0,6,6	-	-	-		
74	OHX	D1	3574	-	0,6,6	-	-	-		
74	OHX	B1	3556	-	0,6,6	-	-	-		
74	OHX	A1	1949	-	0,6,6	-	-	-		
74	OHX	D1	3466	-	0,6,6	-	-	-		
74	OHX	D1	3518	-	0,6,6	-	-	-		
74	OHX	B1	3440	-	0,6,6	-	-	-		
74	OHX	B1	3621	-	0,6,6	-	-	-		
74	OHX	B1	3524	-	0,6,6	-	-	-		
74	OHX	A1	1971	-	0,6,6	-	-	-		
74	OHX	D1	3412	-	0,6,6	-	-	-		
74	OHX	B1	3439	-	0,6,6	-	-	-		
74	OHX	D1	3505	-	0,6,6	-	-	-		
74	OHX	B1	3611	-	0,6,6	-	-	-		
74	OHX	D1	3570	-	0,6,6	-	-	-		
74	OHX	C1	1963	-	0,6,6	-	-	-		
74	OHX	D1	3483	-	0,6,6	-	-	-		
74	OHX	B1	3591	-	0,6,6	-	-	-		
74	OHX	A1	1925	-	0,6,6	-	-	-		
74	OHX	B1	3613	-	0,6,6	-	-	-		
74	OHX	CI	201	-	0,6,6	-	-	-		
74	OHX	A1	1924	-	0,6,6	-	-	-		
74	OHX	C1	1988	-	0,6,6	-	-	-		
74	OHX	D1	3624	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	C1	1973	-	0,6,6	-	-	-		
74	OHX	B1	3614	-	0,6,6	-	-	-		
74	OHX	C1	1936	-	0,6,6	-	-	-		
74	OHX	D1	3535	-	0,6,6	-	-	-		
74	OHX	D1	3618	-	0,6,6	-	-	-		
74	OHX	D1	3498	-	0,6,6	-	-	-		
74	OHX	Dd	101	-	0,6,6	-	-	-		
74	OHX	B1	3416	-	0,6,6	-	-	-		
74	OHX	B1	3459	-	0,6,6	-	-	-		
74	OHX	C1	1976	-	0,6,6	-	-	-		
74	OHX	B1	3419	-	0,6,6	-	-	-		
74	OHX	B1	3414	-	0,6,6	-	-	-		
74	OHX	B1	3438	-	0,6,6	-	-	-		
74	OHX	D1	3470	-	0,6,6	-	-	-		
74	OHX	D1	3486	-	0,6,6	-	-	-		
74	OHX	B1	3407	-	0,6,6	-	-	-		
74	OHX	A1	1932	-	0,6,6	-	-	-		
74	OHX	D1	3581	-	0,6,6	-	-	-		
74	OHX	C1	1947	-	0,6,6	-	-	-		
74	OHX	B1	3538	-	0,6,6	-	-	-		
74	OHX	D1	3447	-	0,6,6	-	-	-		
74	OHX	D1	3590	-	0,6,6	-	-	-		
74	OHX	C1	1985	-	0,6,6	-	-	-		
74	OHX	B1	3461	-	0,6,6	-	-	-		
74	OHX	D1	3425	-	0,6,6	-	-	-		
74	OHX	C1	1946	-	0,6,6	-	-	-		
74	OHX	D1	3592	-	0,6,6	-	-	-		
74	OHX	D1	3478	-	0,6,6	-	-	-		
74	OHX	B1	3562	-	0,6,6	-	-	-		
74	OHX	C1	1970	-	0,6,6	-	-	-		
74	OHX	D1	3556	-	0,6,6	-	-	-		
74	OHX	B2	207	-	0,6,6	-	-	-		
74	OHX	B1	3511	-	0,6,6	-	-	-		
74	OHX	B1	3474	-	0,6,6	-	-	-		
74	OHX	B1	3500	-	0,6,6	-	-	-		
74	OHX	D1	3419	-	0,6,6	-	-	-		
74	OHX	D3	203	-	0,6,6	-	-	-		
74	OHX	D1	3463	-	0,6,6	-	-	-		
74	OHX	A1	1918	-	0,6,6	-	-	-		
74	OHX	CS	101	-	0,6,6	-	-	-		
74	OHX	B1	3514	-	0,6,6	-	-	-		
74	OHX	D1	3407	-	0,6,6	-	-	-		
74	OHX	B1	3448	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	B1	3522	-	0,6,6	-	-	-		
74	OHX	D1	3611	-	0,6,6	-	-	-		
74	OHX	B1	3541	-	0,6,6	-	-	-		
74	OHX	A1	1983	-	0,6,6	-	-	-		
74	OHX	B1	3517	-	0,6,6	-	-	-		
74	OHX	B1	3575	-	0,6,6	-	-	-		
74	OHX	B1	3558	-	0,6,6	-	-	-		
74	OHX	D1	3575	-	0,6,6	-	-	-		
74	OHX	A1	1977	-	0,6,6	-	-	-		
74	OHX	A1	1996	-	0,6,6	-	-	-		
74	OHX	C1	1991	-	0,6,6	-	-	-		
74	OHX	B1	3539	-	0,6,6	-	-	-		
74	OHX	D1	3421	-	0,6,6	-	-	-		
74	OHX	B1	3450	-	0,6,6	-	-	-		
74	OHX	B1	3516	-	0,6,6	-	-	-		
74	OHX	D1	3439	-	0,6,6	-	-	-		
74	OHX	B1	3616	-	0,6,6	-	-	-		
74	OHX	D1	3490	-	0,6,6	-	-	-		
74	OHX	D1	3416	-	0,6,6	-	-	-		
74	OHX	C1	1944	-	0,6,6	-	-	-		
74	OHX	C1	1914	-	0,6,6	-	-	-		
74	OHX	D1	3610	-	0,6,6	-	-	-		
74	OHX	D1	3612	-	0,6,6	-	-	-		
74	OHX	C1	1995	-	0,6,6	-	-	-		
74	OHX	D1	3599	-	0,6,6	-	-	-		
74	OHX	D1	3469	-	0,6,6	-	-	-		
74	OHX	D1	3555	-	0,6,6	-	-	-		
74	OHX	D1	3588	-	0,6,6	-	-	-		
74	OHX	A1	1956	-	0,6,6	-	-	-		
74	OHX	B1	3586	-	0,6,6	-	-	-		
74	OHX	B1	3427	-	0,6,6	-	-	-		
74	OHX	D1	3445	-	0,6,6	-	-	-		
74	OHX	B1	3532	-	0,6,6	-	-	-		
74	OHX	A1	1921	-	0,6,6	-	-	-		
74	OHX	A1	1991	-	0,6,6	-	-	-		
74	OHX	C1	1907	-	0,6,6	-	-	-		
74	OHX	B1	3608	-	0,6,6	-	-	-		
74	OHX	C1	1955	-	0,6,6	-	-	-		
74	OHX	D1	3433	-	0,6,6	-	-	-		
74	OHX	D1	3600	-	0,6,6	-	-	-		
74	OHX	D1	3475	-	0,6,6	-	-	-		
74	OHX	D1	3539	-	0,6,6	-	-	-		
74	OHX	DC	401	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	B1	3425	-	0,6,6	-	-	-		
74	OHX	D1	3488	-	0,6,6	-	-	-		
74	OHX	A1	1990	-	0,6,6	-	-	-		
74	OHX	D1	3616	-	0,6,6	-	-	-		
74	OHX	D1	3525	-	0,6,6	-	-	-		
74	OHX	D1	3522	-	0,6,6	-	-	-		
74	OHX	C1	1950	-	0,6,6	-	-	-		
74	OHX	A1	1988	-	0,6,6	-	-	-		
74	OHX	B1	3480	-	0,6,6	-	-	-		
74	OHX	B1	3529	-	0,6,6	-	-	-		
74	OHX	B1	3605	-	0,6,6	-	-	-		
74	OHX	B1	3602	-	0,6,6	-	-	-		
74	OHX	B1	3479	-	0,6,6	-	-	-		
74	OHX	C1	1961	-	0,6,6	-	-	-		
74	OHX	B1	3473	-	0,6,6	-	-	-		
74	OHX	C1	1951	-	0,6,6	-	-	-		
74	OHX	A1	1908	-	0,6,6	-	-	-		
74	OHX	D1	3541	-	0,6,6	-	-	-		
74	OHX	A1	1976	-	0,6,6	-	-	-		
74	OHX	B1	3543	-	0,6,6	-	-	-		
74	OHX	A1	1943	-	0,6,6	-	-	-		
74	OHX	B1	3572	-	0,6,6	-	-	-		
74	OHX	C1	1912	-	0,6,6	-	-	-		
74	OHX	A1	1967	-	0,6,6	-	-	-		
74	OHX	C1	1998	-	0,6,6	-	-	-		
74	OHX	B1	3512	-	0,6,6	-	-	-		
74	OHX	D1	3617	-	0,6,6	-	-	-		
74	OHX	D1	3487	-	0,6,6	-	-	-		
74	OHX	D2	201	-	0,6,6	-	-	-		
74	OHX	D1	3459	-	0,6,6	-	-	-		
74	OHX	A1	1909	-	0,6,6	-	-	-		
74	OHX	B1	3456	-	0,6,6	-	-	-		
74	OHX	B1	3442	-	0,6,6	-	-	-		
74	OHX	B1	3499	-	0,6,6	-	-	-		
74	OHX	B1	3508	-	0,6,6	-	-	-		
74	OHX	B1	3426	-	0,6,6	-	-	-		
74	OHX	D1	3542	-	0,6,6	-	-	-		
74	OHX	D1	3602	-	0,6,6	-	-	-		
74	OHX	A1	1961	-	0,6,6	-	-	-		
74	OHX	D1	3479	-	0,6,6	-	-	-		
74	OHX	B1	3464	-	0,6,6	-	-	-		
74	OHX	C1	1960	-	0,6,6	-	-	-		
74	OHX	B3	208	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OHX	D1	3573	-	0,6,6	-	-	-		
74	OHX	D1	3559	-	0,6,6	-	-	-		
74	OHX	B1	3415	-	0,6,6	-	-	-		
74	OHX	D1	3531	-	0,6,6	-	-	-		
74	OHX	D1	3562	-	0,6,6	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

220 monomers are involved in 719 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	B1	3561	OHX	1	0
74	D1	3567	OHX	5	0
74	Bd	101	OHX	10	0
74	C1	1901	OHX	3	0
74	D1	3514	OHX	3	0
74	C1	1952	OHX	1	0
74	B3	202	OHX	1	0
74	A1	1986	OHX	6	0
74	B1	3417	OHX	3	0
74	D1	3543	OHX	7	0
74	D3	209	OHX	1	0
74	D1	3583	OHX	6	0
74	A1	1941	OHX	1	0
74	Bg	101	OHX	10	0
74	D1	3577	OHX	1	0
74	D1	3576	OHX	2	0
74	D1	3464	OHX	2	0
74	B1	3540	OHX	1	0
74	D1	3415	OHX	13	0
74	D1	3465	OHX	1	0
74	C1	1905	OHX	1	0
74	B1	3506	OHX	1	0
74	B3	206	OHX	8	0
74	B1	3429	OHX	2	0
74	C1	1918	OHX	2	0
74	C1	1908	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	C1	1953	OHX	3	0
74	C1	1939	OHX	1	0
74	D1	3585	OHX	2	0
74	C1	1903	OHX	2	0
74	B1	3460	OHX	1	0
74	A1	1959	OHX	3	0
74	B1	3544	OHX	1	0
74	D1	3598	OHX	1	0
74	D3	205	OHX	4	0
74	D1	3462	OHX	1	0
74	C1	1910	OHX	1	0
74	A1	1905	OHX	1	0
74	D3	201	OHX	3	0
74	C1	1933	OHX	7	0
74	B1	3599	OHX	4	0
74	D1	3428	OHX	2	0
74	A1	1978	OHX	1	0
74	B1	3593	OHX	1	0
74	A1	1931	OHX	7	0
74	D1	3557	OHX	3	0
74	C1	1999	OHX	3	0
74	B1	3433	OHX	1	0
74	D1	3502	OHX	5	0
74	A1	1989	OHX	2	0
74	B1	3568	OHX	2	0
74	C1	1997	OHX	1	0
74	D1	3608	OHX	1	0
74	B1	3595	OHX	1	0
74	A1	1939	OHX	1	0
74	A1	1936	OHX	3	0
74	A1	1975	OHX	4	0
74	A1	1903	OHX	1	0
74	B3	205	OHX	2	0
74	D1	3568	OHX	4	0
74	B1	3485	OHX	1	0
74	C1	1924	OHX	8	0
74	D1	3526	OHX	1	0
74	D1	3547	OHX	1	0
74	B1	3492	OHX	10	0
74	A1	1972	OHX	1	0
74	B1	3483	OHX	3	0
74	B1	3536	OHX	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	C1	1915	OHX	1	0
74	A1	1929	OHX	1	0
74	A1	1970	OHX	1	0
74	B1	3404	OHX	2	0
74	D1	3446	OHX	1	0
74	B1	3490	OHX	1	0
74	C1	1993	OHX	3	0
74	B1	3574	OHX	1	0
74	BC	401	OHX	1	0
74	D1	3492	OHX	3	0
74	D1	3402	OHX	3	0
74	C1	1930	OHX	10	0
74	A1	1935	OHX	2	0
74	A1	1917	OHX	4	0
74	A1	1910	OHX	5	0
74	B1	3523	OHX	1	0
74	D2	205	OHX	1	0
74	D1	3448	OHX	2	0
74	A1	1913	OHX	6	0
74	D1	3578	OHX	1	0
74	B1	3434	OHX	2	0
74	D1	3589	OHX	1	0
74	B1	3620	OHX	4	0
74	B3	212	OHX	2	0
74	A1	1950	OHX	2	0
74	D1	3523	OHX	3	0
74	C1	1927	OHX	3	0
74	D1	3434	OHX	1	0
74	D2	204	OHX	1	0
74	A1	1969	OHX	2	0
74	D3	202	OHX	7	0
74	B1	3413	OHX	1	0
74	B1	3405	OHX	2	0
74	D1	3495	OHX	2	0
74	B1	3406	OHX	2	0
74	C1	1983	OHX	4	0
74	D1	3452	OHX	12	0
74	D1	3473	OHX	5	0
74	C1	1994	OHX	1	0
74	B2	209	OHX	3	0
74	D1	3591	OHX	3	0
74	B1	3478	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	D1	3597	OHX	3	0
74	C1	2001	OHX	2	0
74	C1	1902	OHX	1	0
74	A1	1901	OHX	6	0
74	D1	3455	OHX	1	0
74	A1	1952	OHX	2	0
74	B1	3420	OHX	2	0
74	D1	3408	OHX	8	0
74	D1	3625	OHX	3	0
74	DO	301	OHX	6	0
74	C1	1916	OHX	4	0
74	D1	3406	OHX	1	0
74	D1	3431	OHX	7	0
74	B1	3447	OHX	1	0
74	B1	3449	OHX	7	0
74	D1	3582	OHX	10	0
74	A1	1958	OHX	3	0
74	B1	3553	OHX	1	0
74	D1	3524	OHX	2	0
74	B1	3527	OHX	1	0
74	B1	3481	OHX	1	0
74	B2	201	OHX	7	0
74	C1	1917	OHX	6	0
74	B1	3489	OHX	3	0
74	C1	1964	OHX	6	0
74	D1	3454	OHX	1	0
74	AT	401	OHX	1	0
74	B1	3503	OHX	1	0
74	B1	3496	OHX	3	0
74	B1	3537	OHX	8	0
74	B1	3469	OHX	2	0
74	B1	3513	OHX	3	0
74	BT	201	OHX	2	0
74	D1	3489	OHX	2	0
74	Dg	101	OHX	11	0
74	B3	211	OHX	1	0
74	B1	3559	OHX	1	0
74	D3	204	OHX	1	0
74	B1	3563	OHX	5	0
74	D1	3537	OHX	3	0
74	B1	3428	OHX	8	0
74	D1	3619	OHX	1	0

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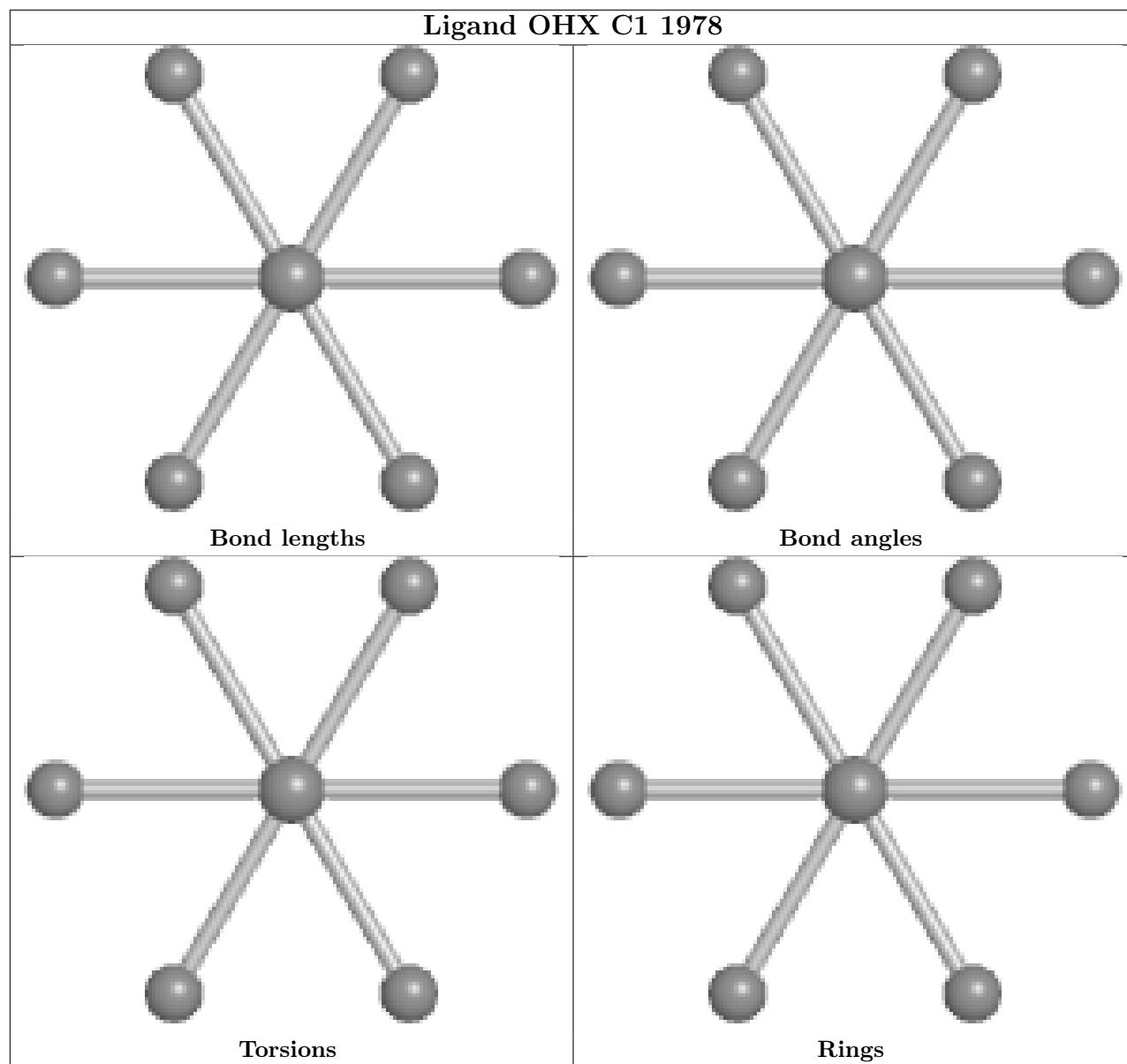
Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	B1	3567	OHX	7	0
74	B1	3587	OHX	7	0
74	D1	3530	OHX	2	0
74	D1	3456	OHX	1	0
74	B1	3505	OHX	4	0
74	A1	1916	OHX	5	0
74	D1	3480	OHX	4	0
74	D1	3551	OHX	1	0
74	D1	3413	OHX	3	0
74	B1	3471	OHX	1	0
74	C1	1929	OHX	1	0
74	D1	3430	OHX	4	0
74	D2	207	OHX	6	0
74	C1	1928	OHX	5	0
74	B1	3581	OHX	7	0
74	AS	101	OHX	18	0
74	A1	1923	OHX	2	0
74	D3	212	OHX	12	0
74	A1	1937	OHX	2	0
74	A1	1915	OHX	5	0
74	B2	204	OHX	2	0
74	A1	1902	OHX	1	0
74	B1	3592	OHX	1	0
74	D1	3574	OHX	7	0
74	A1	1949	OHX	4	0
74	B1	3440	OHX	1	0
74	D1	3570	OHX	1	0
74	Dd	101	OHX	11	0
74	B1	3438	OHX	12	0
74	D1	3470	OHX	2	0
74	A1	1932	OHX	2	0
74	D1	3447	OHX	3	0
74	C1	1985	OHX	1	0
74	C1	1970	OHX	6	0
74	D1	3556	OHX	3	0
74	D1	3419	OHX	1	0
74	D1	3463	OHX	6	0
74	CS	101	OHX	16	0
74	D1	3407	OHX	1	0
74	B1	3558	OHX	6	0
74	C1	1991	OHX	1	0
74	B1	3539	OHX	2	0

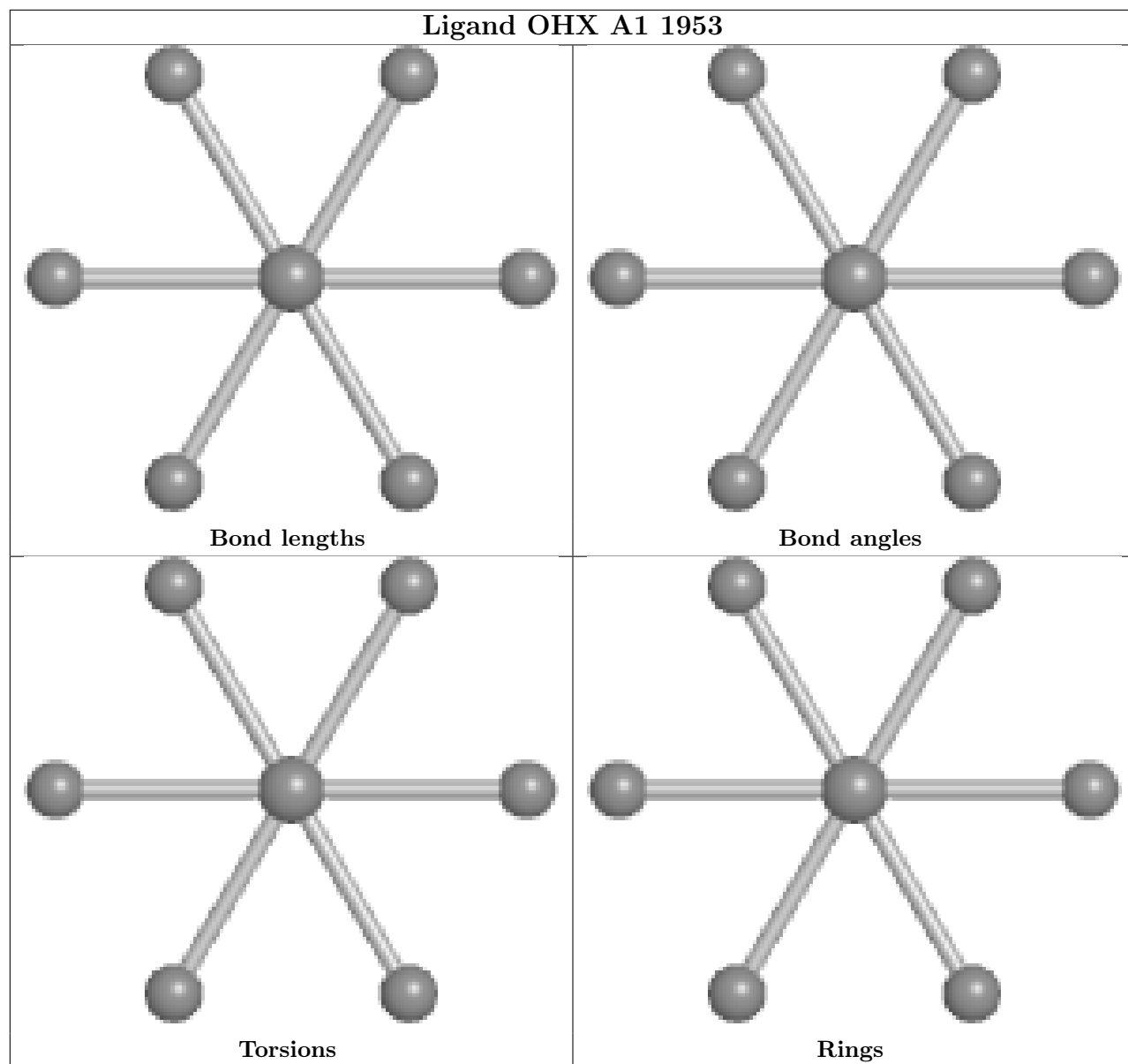
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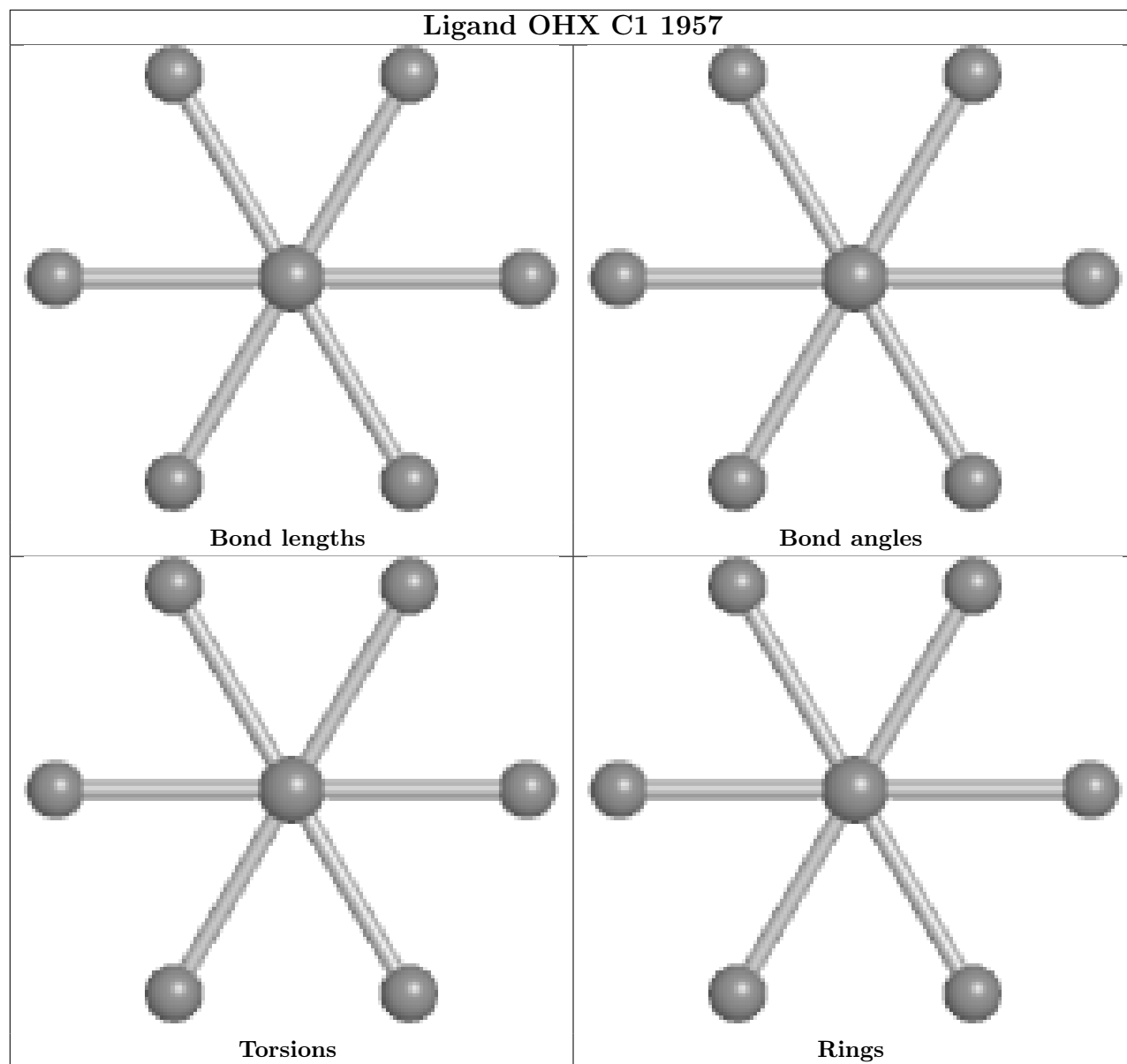
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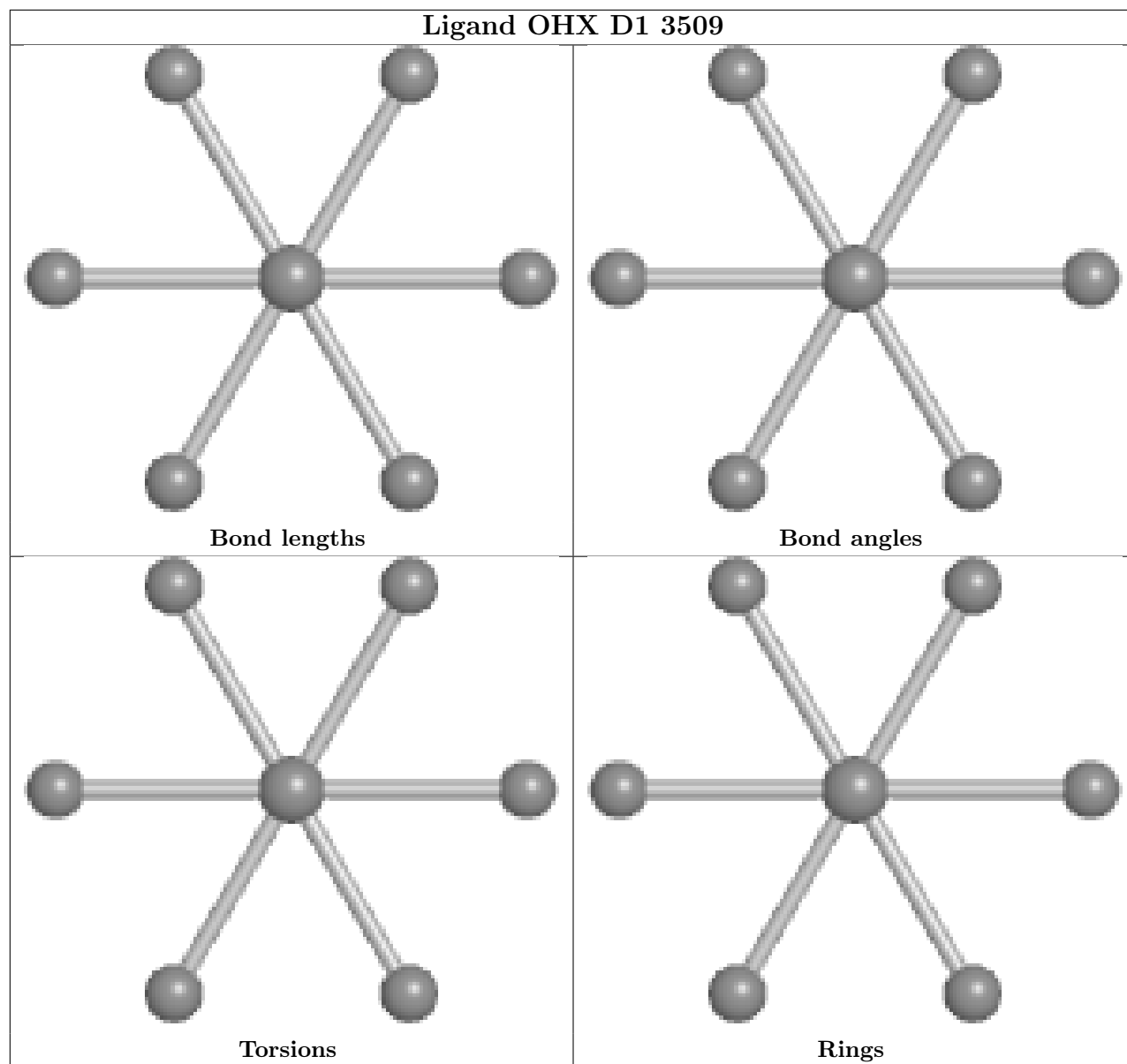
Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	B1	3450	OHX	17	0
74	D1	3416	OHX	1	0
74	C1	1944	OHX	1	0
74	C1	1914	OHX	1	0
74	C1	1995	OHX	3	0
74	D1	3599	OHX	3	0
74	D1	3588	OHX	5	0
74	C1	1907	OHX	1	0
74	C1	1955	OHX	5	0
74	D1	3539	OHX	1	0
74	A1	1990	OHX	3	0
74	B1	3529	OHX	4	0
74	B1	3479	OHX	10	0
74	C1	1961	OHX	2	0
74	C1	1951	OHX	2	0
74	A1	1908	OHX	1	0
74	A1	1976	OHX	5	0
74	A1	1943	OHX	5	0
74	C1	1912	OHX	1	0
74	D2	201	OHX	8	0
74	A1	1909	OHX	3	0
74	B1	3456	OHX	2	0
74	B1	3442	OHX	1	0
74	B1	3464	OHX	1	0
74	D1	3559	OHX	3	0
74	B1	3415	OHX	2	0

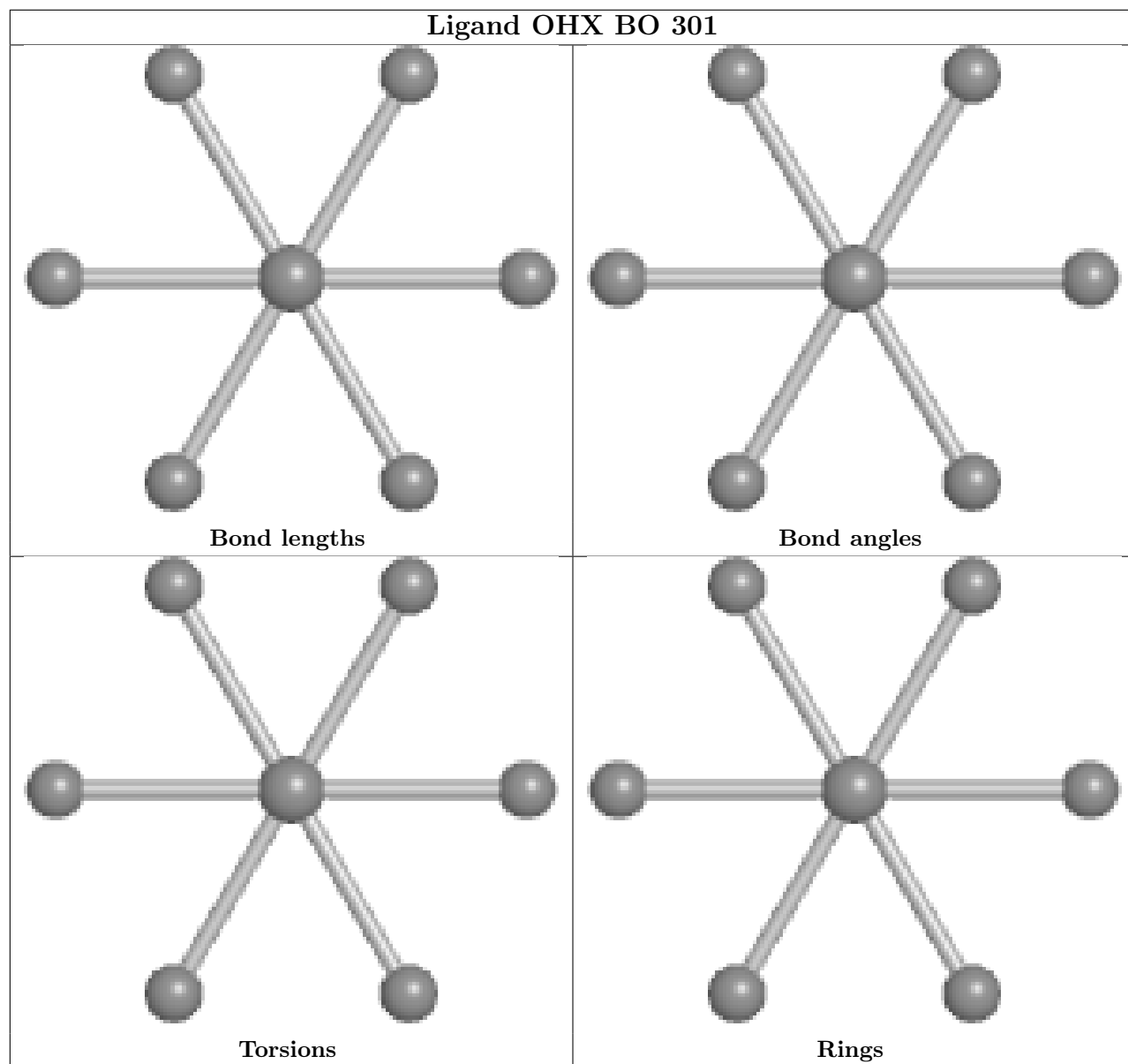
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

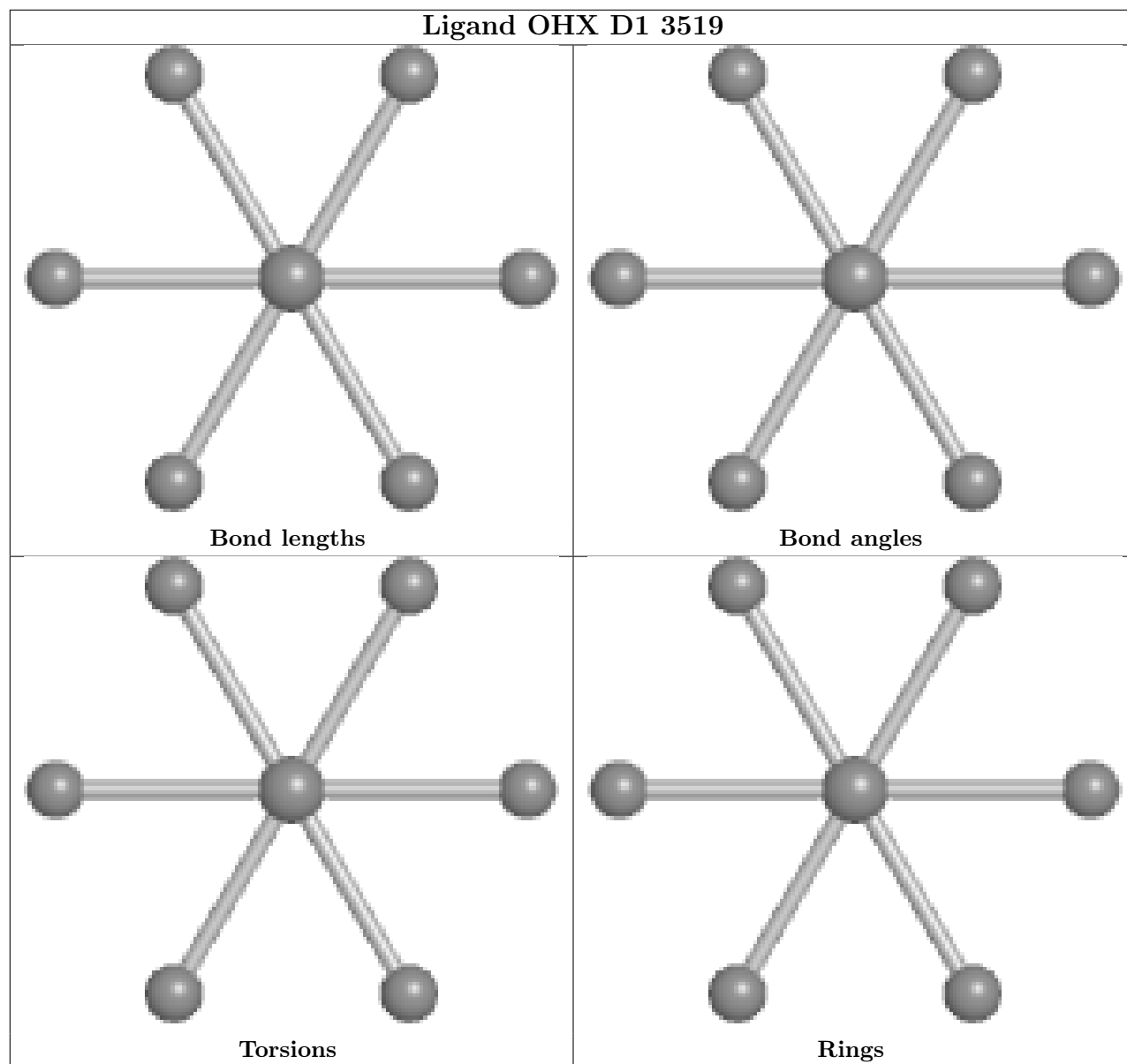


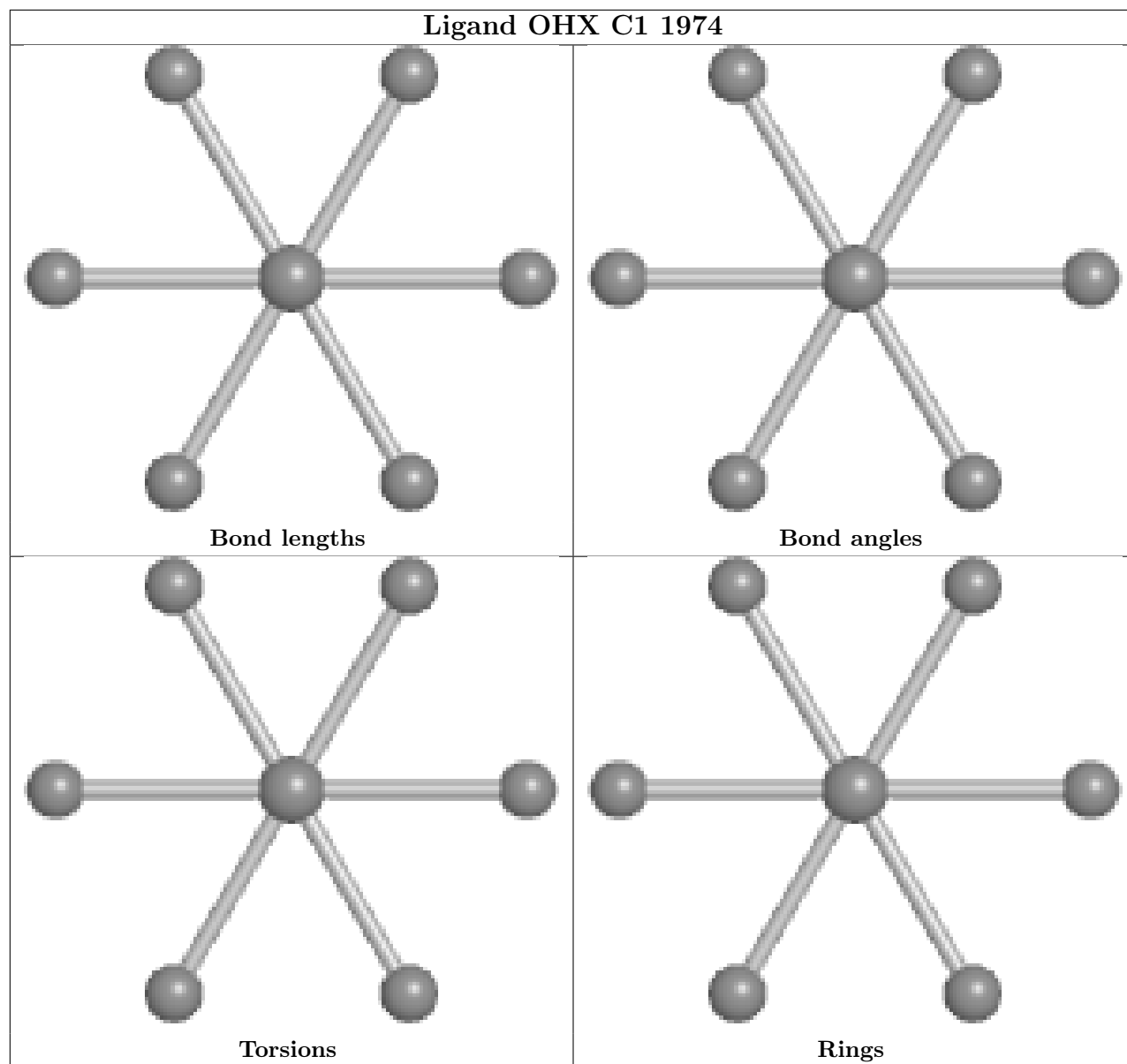


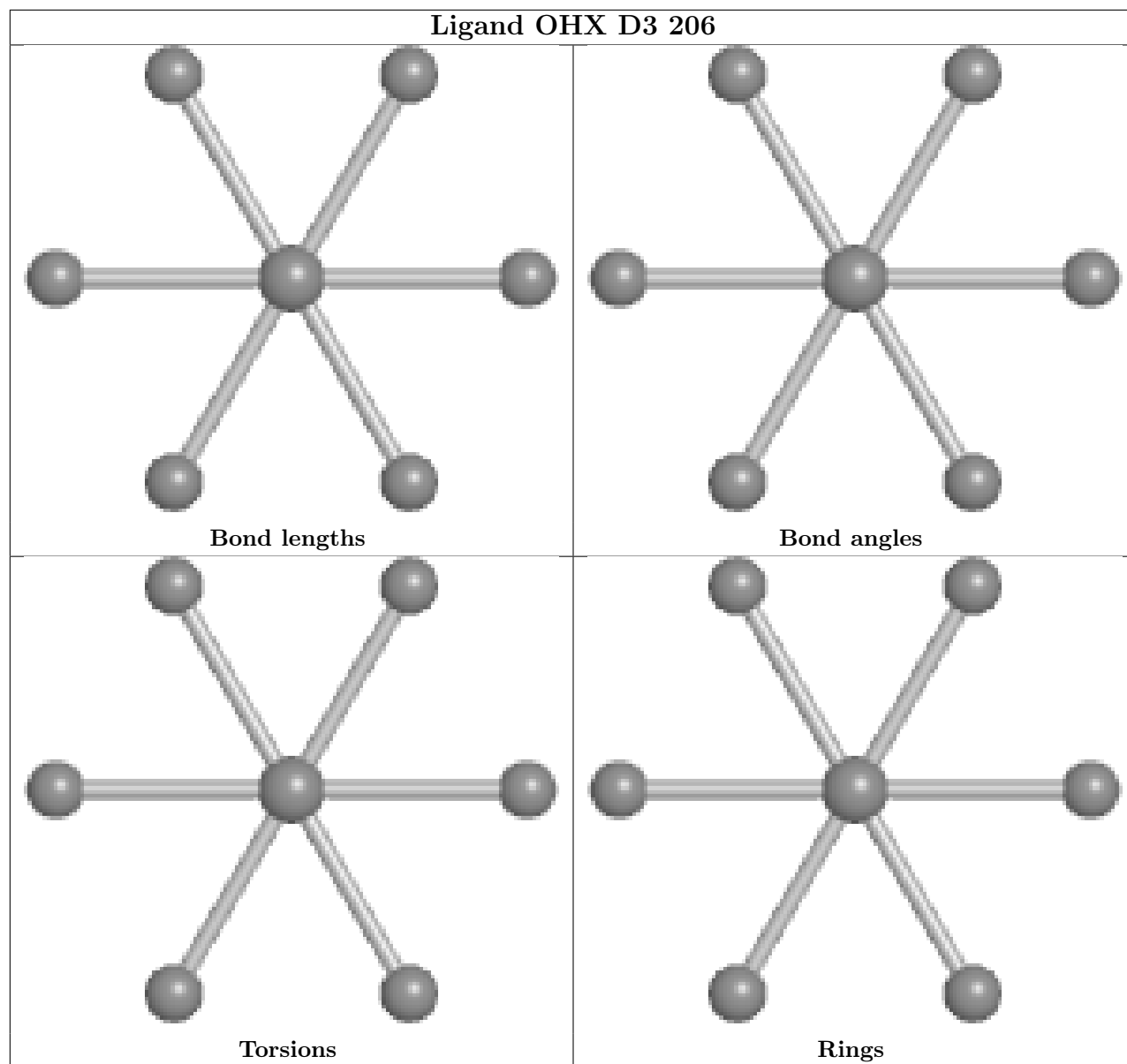


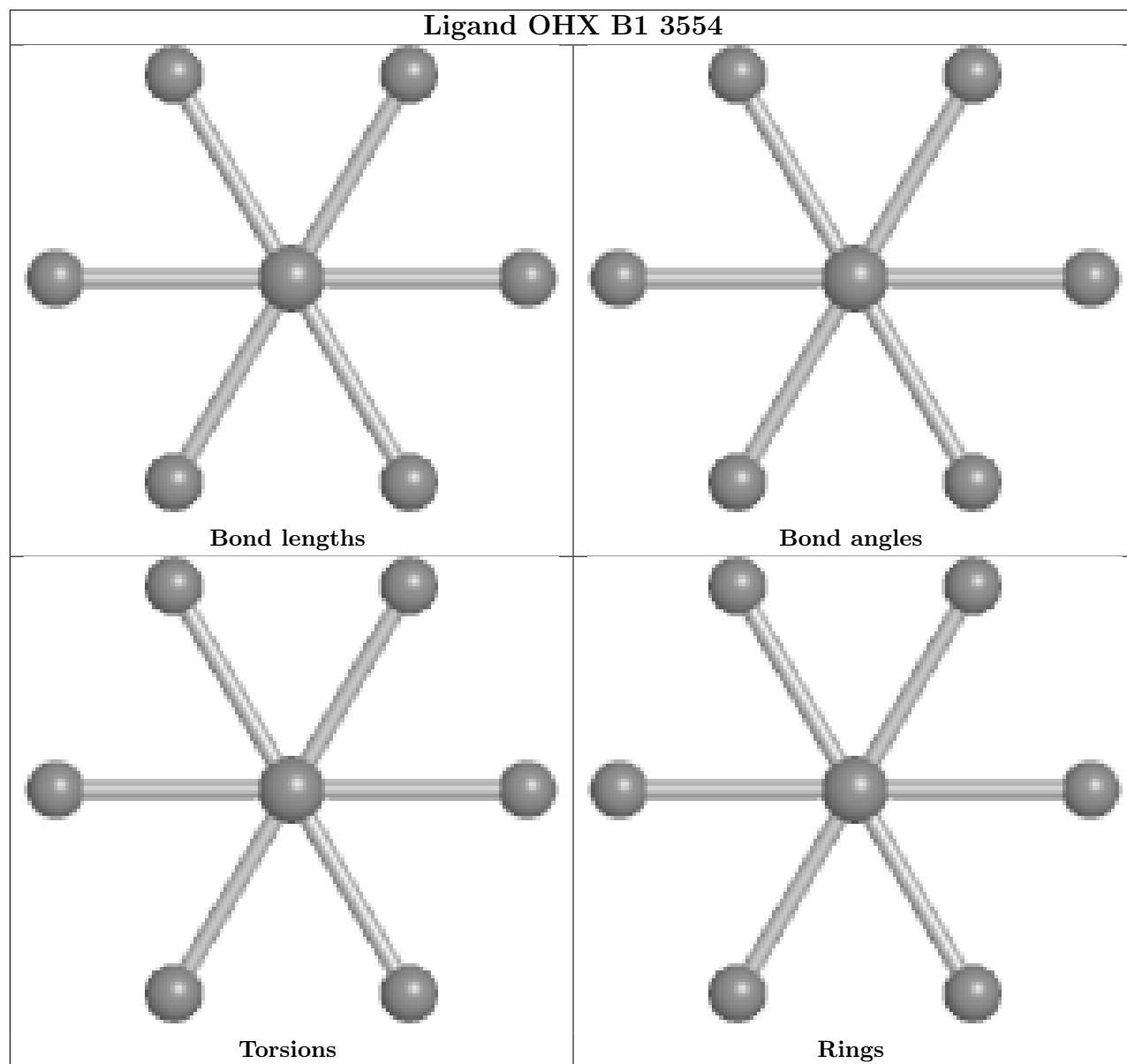


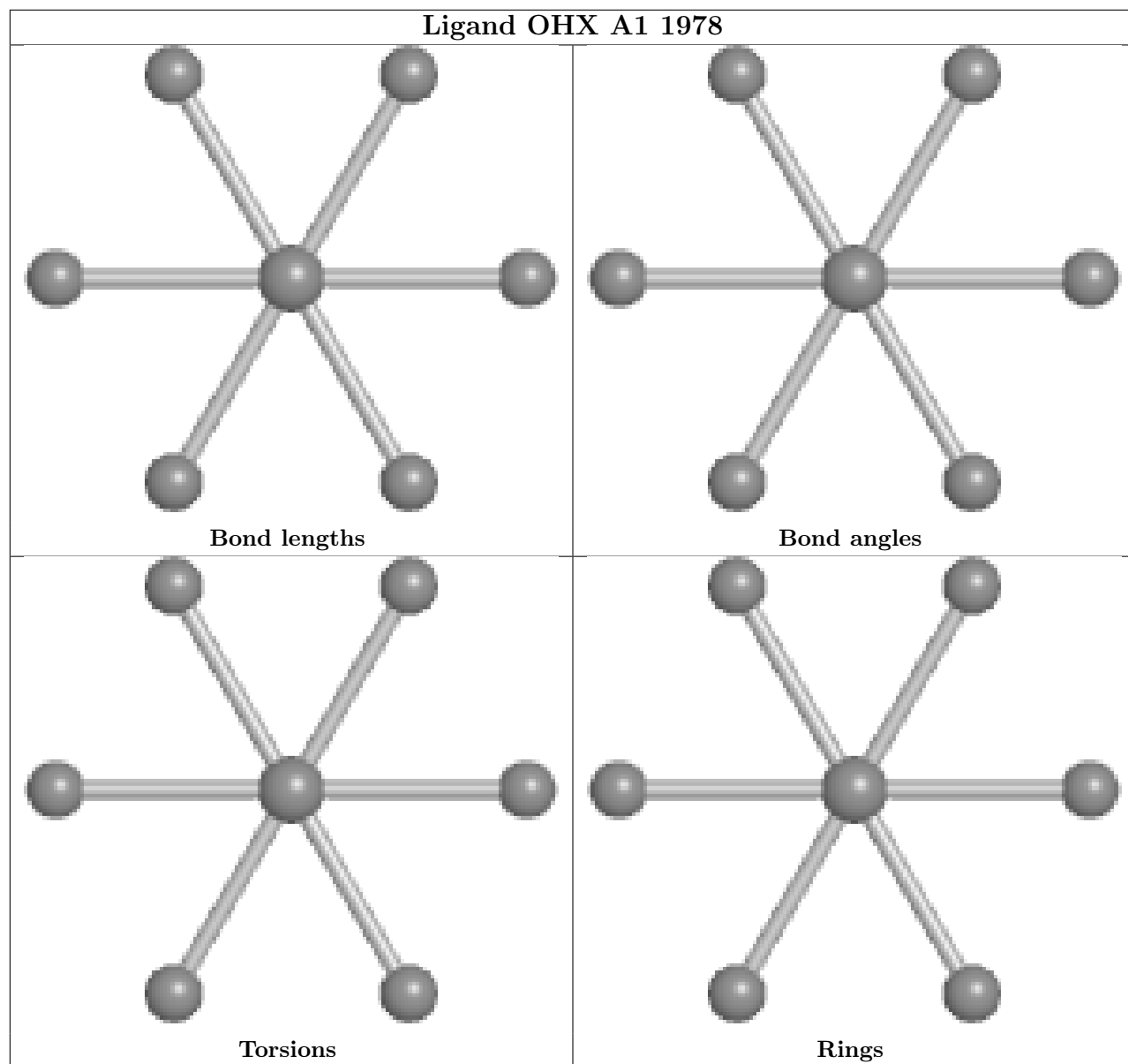


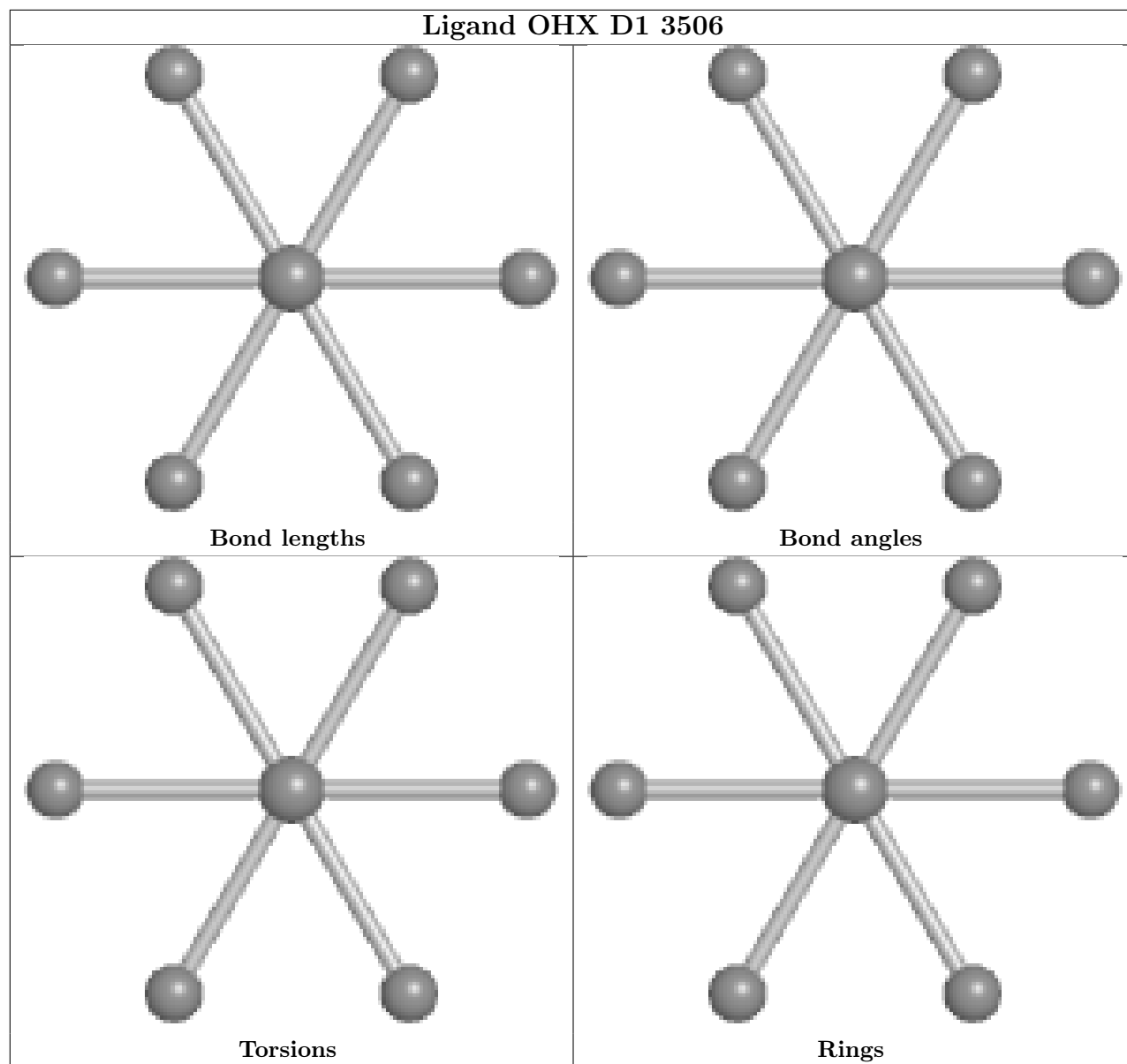


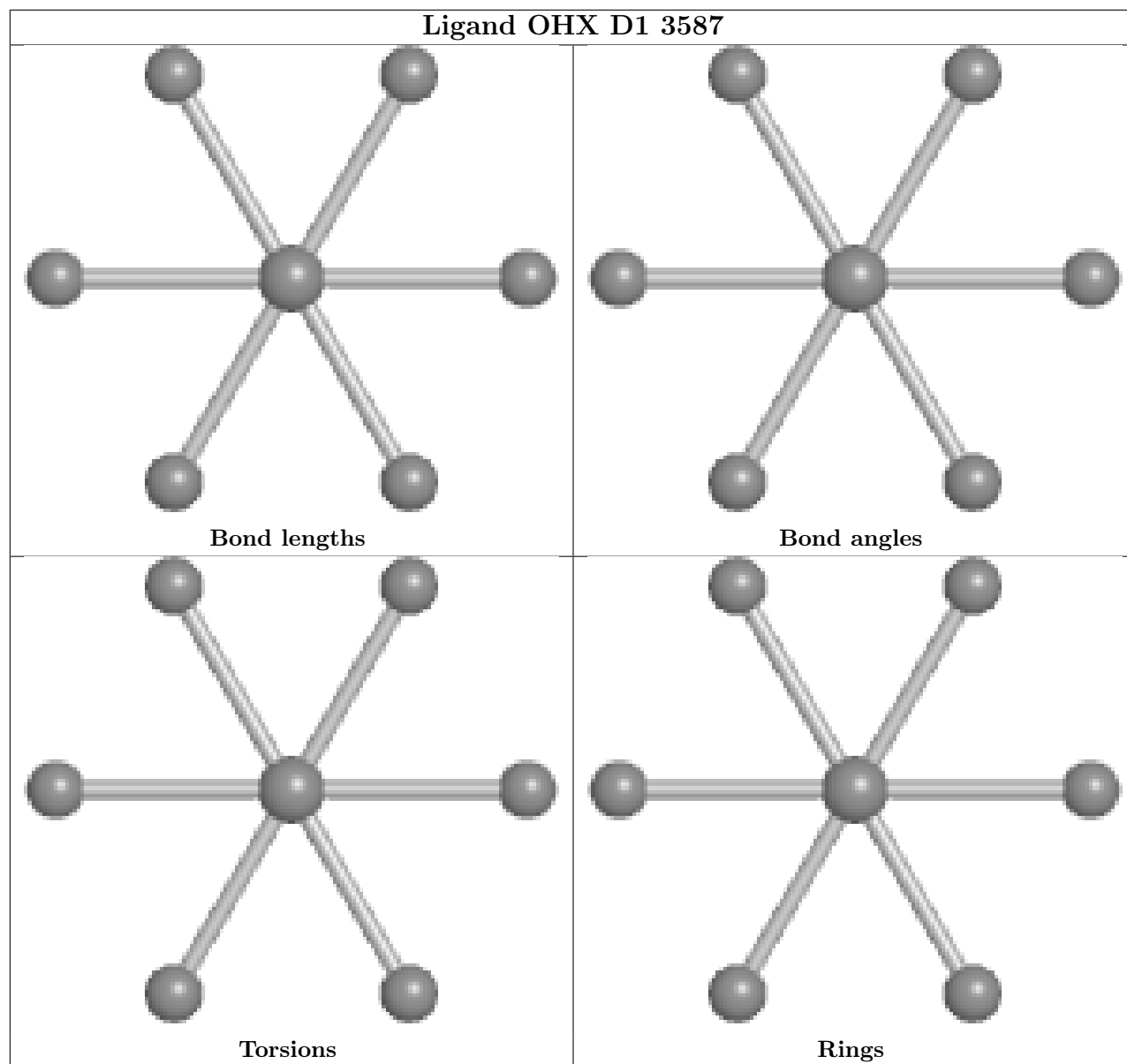


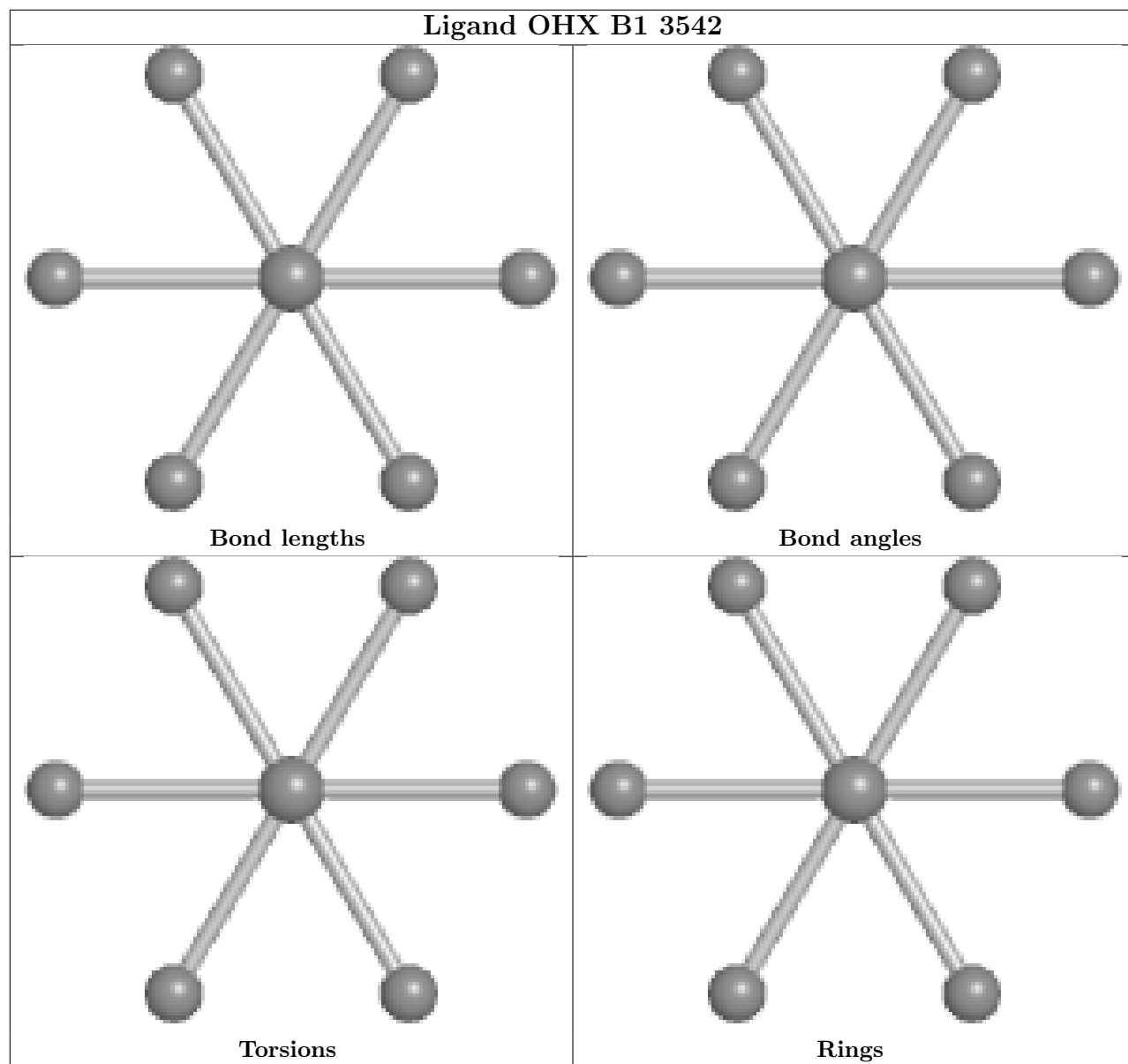


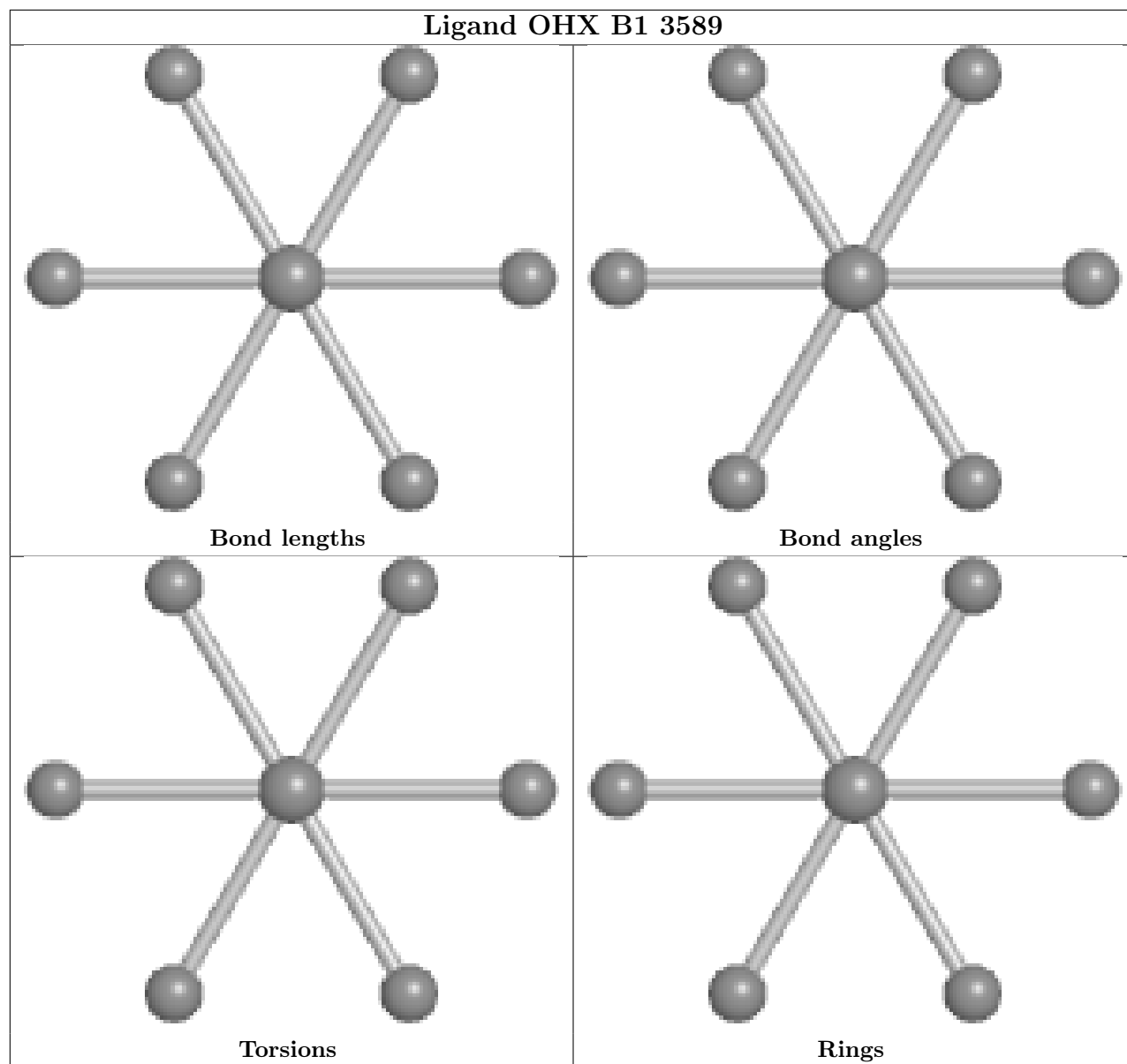


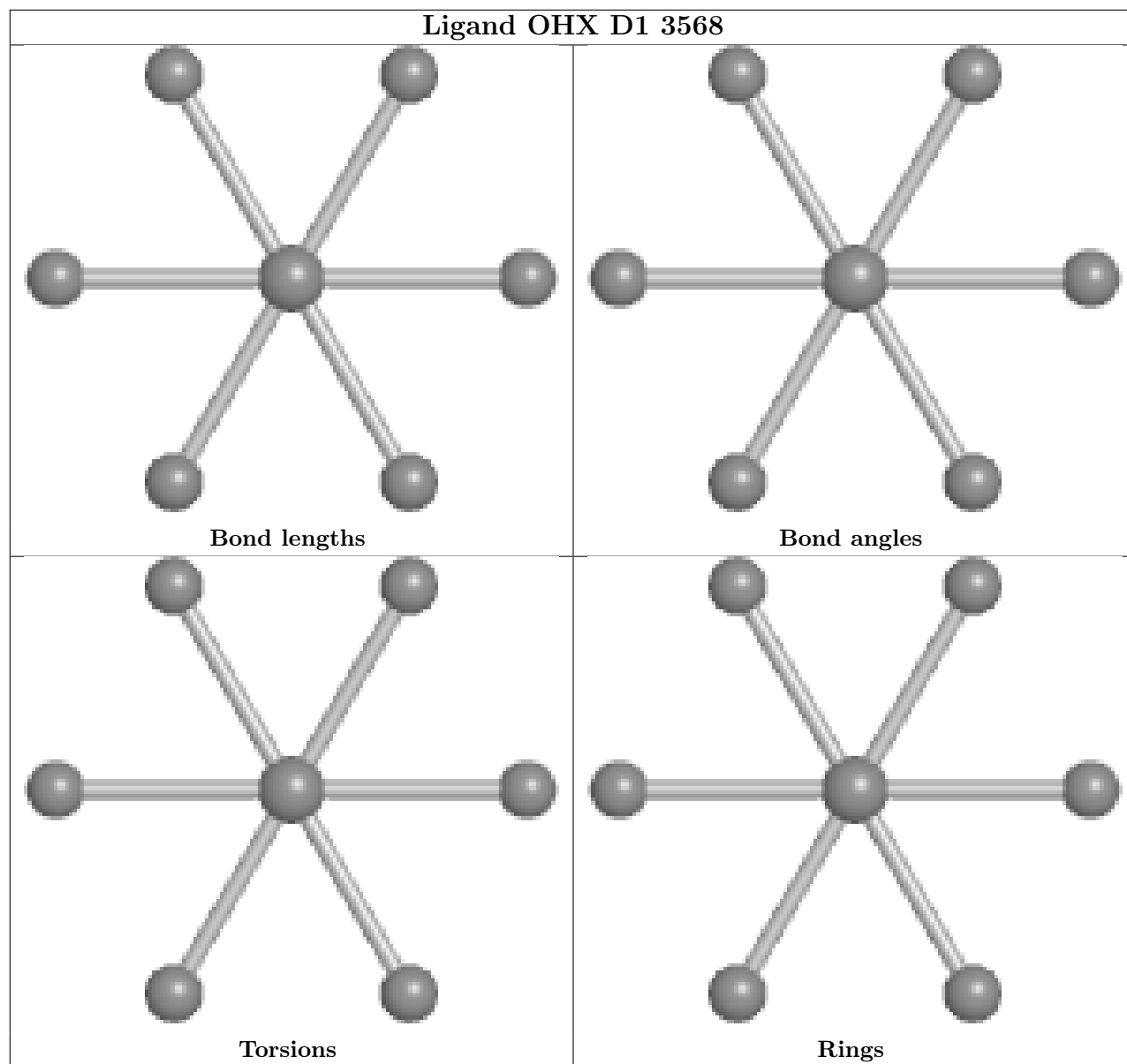


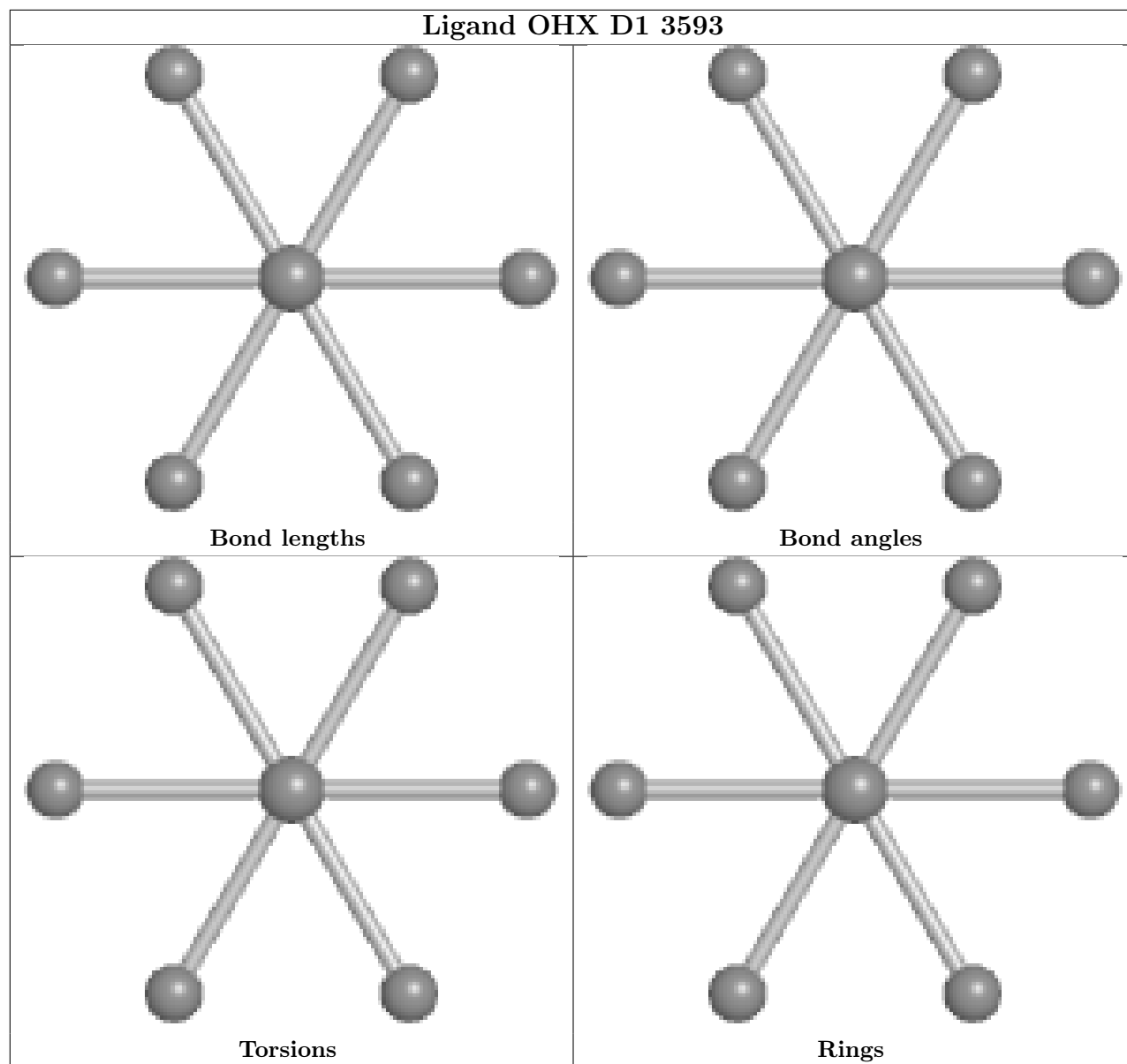


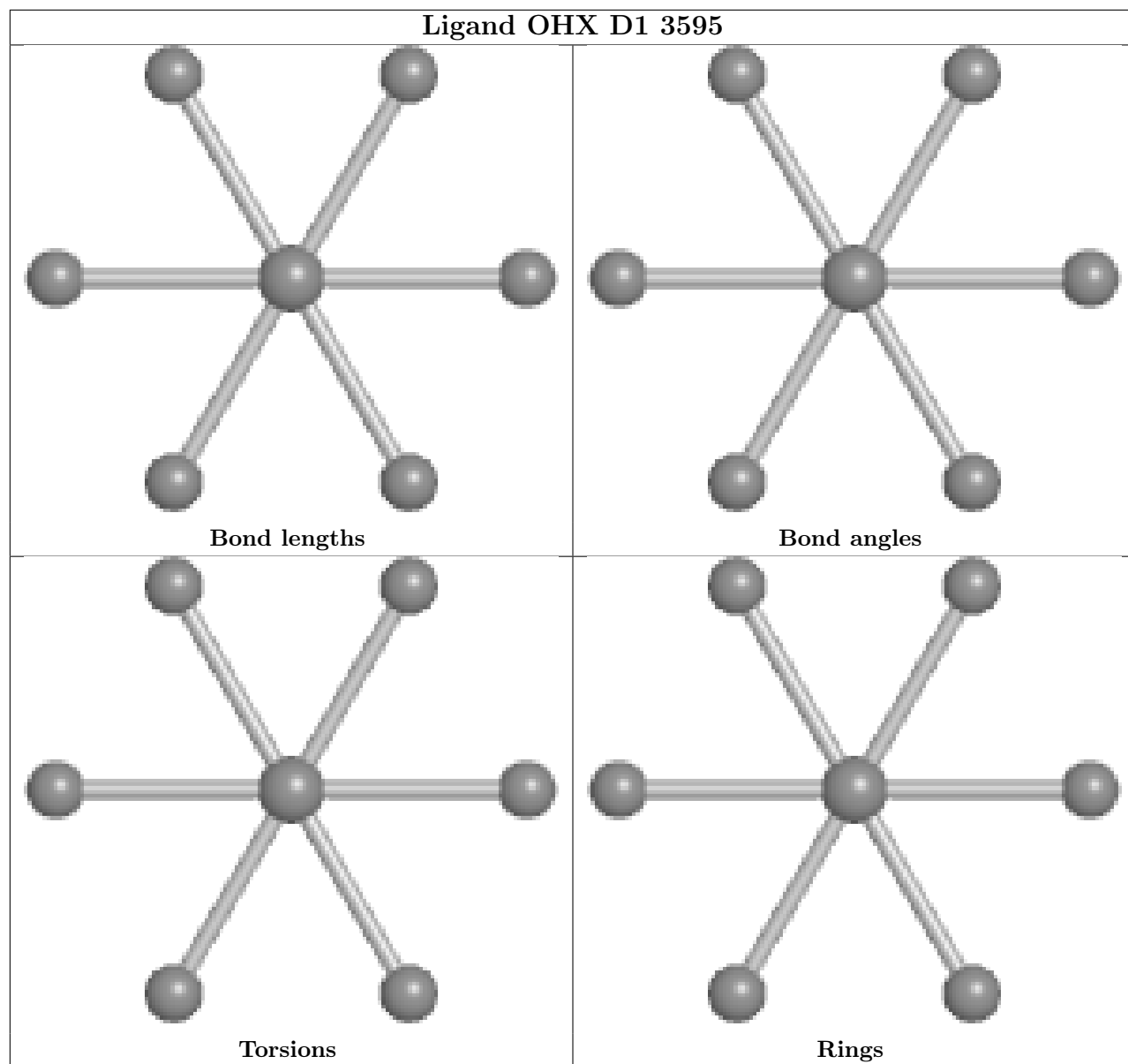


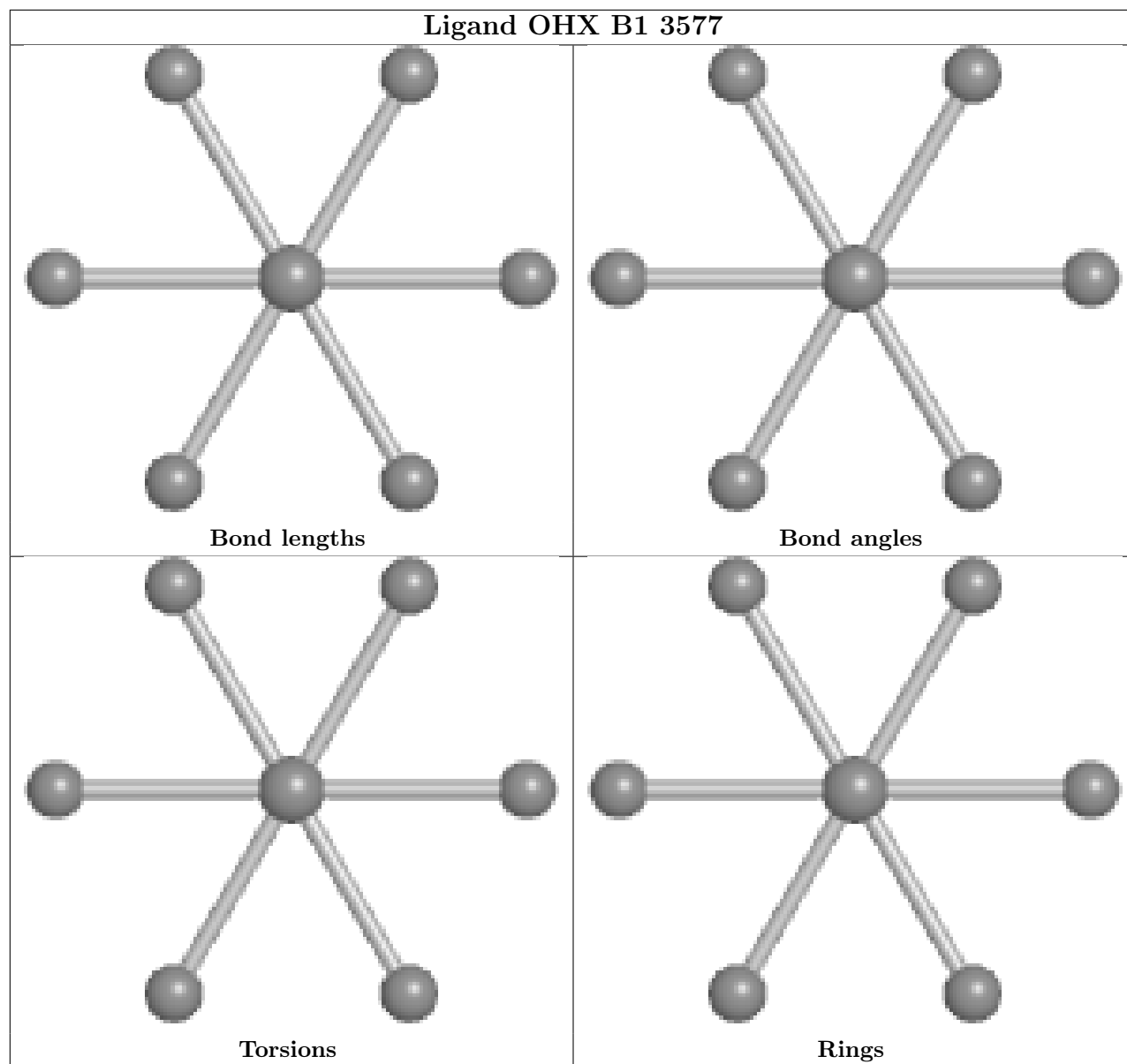


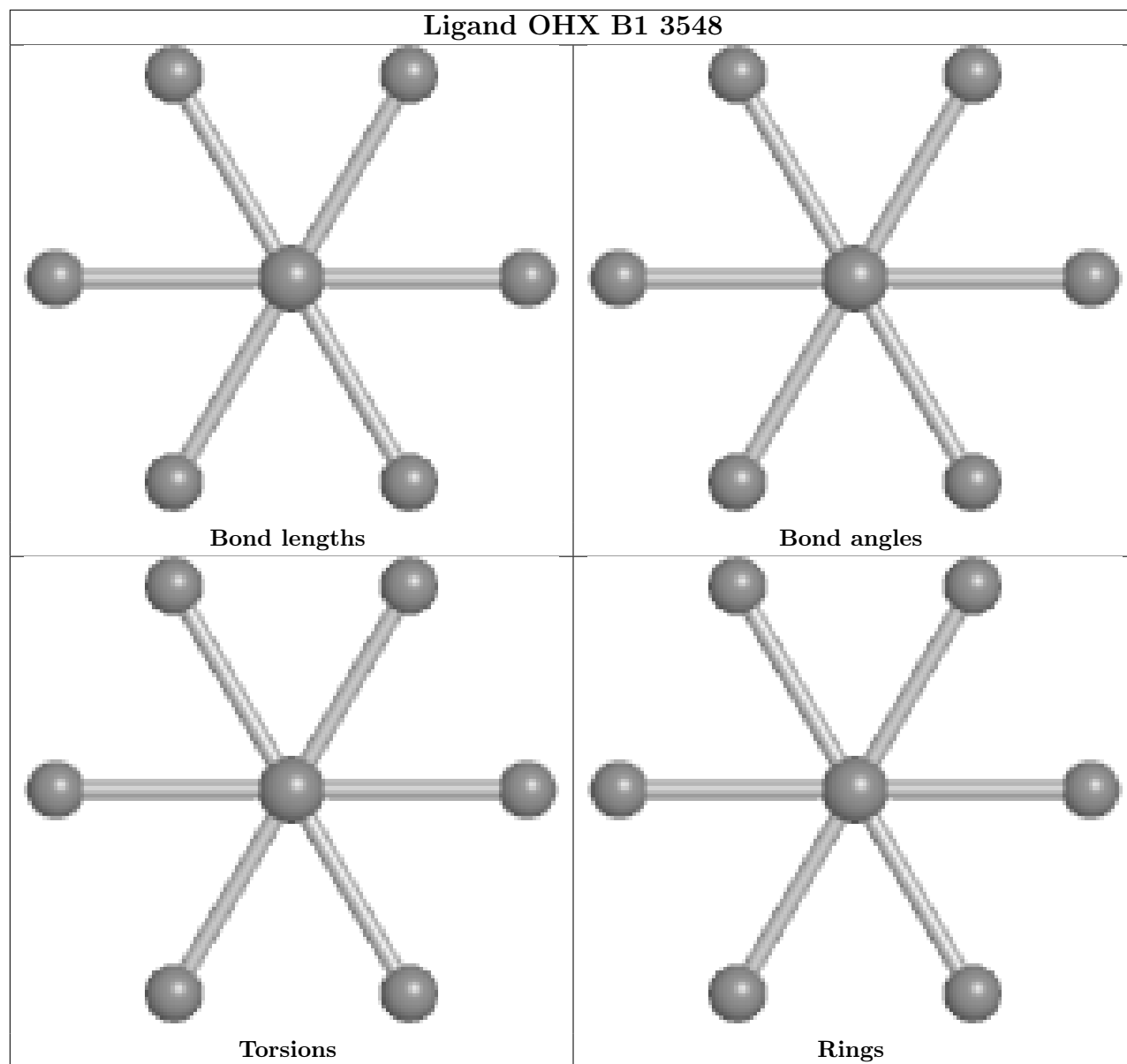


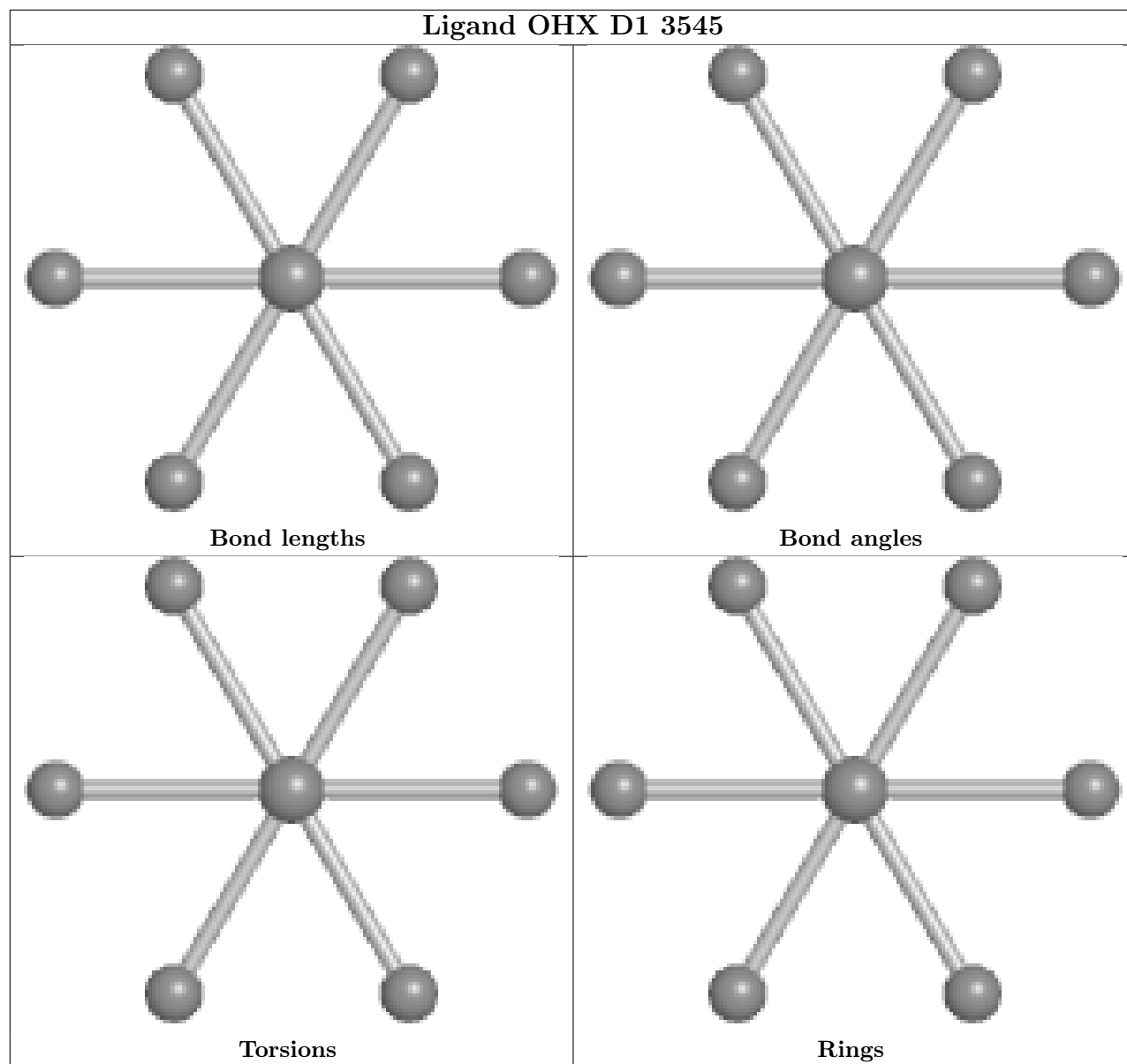


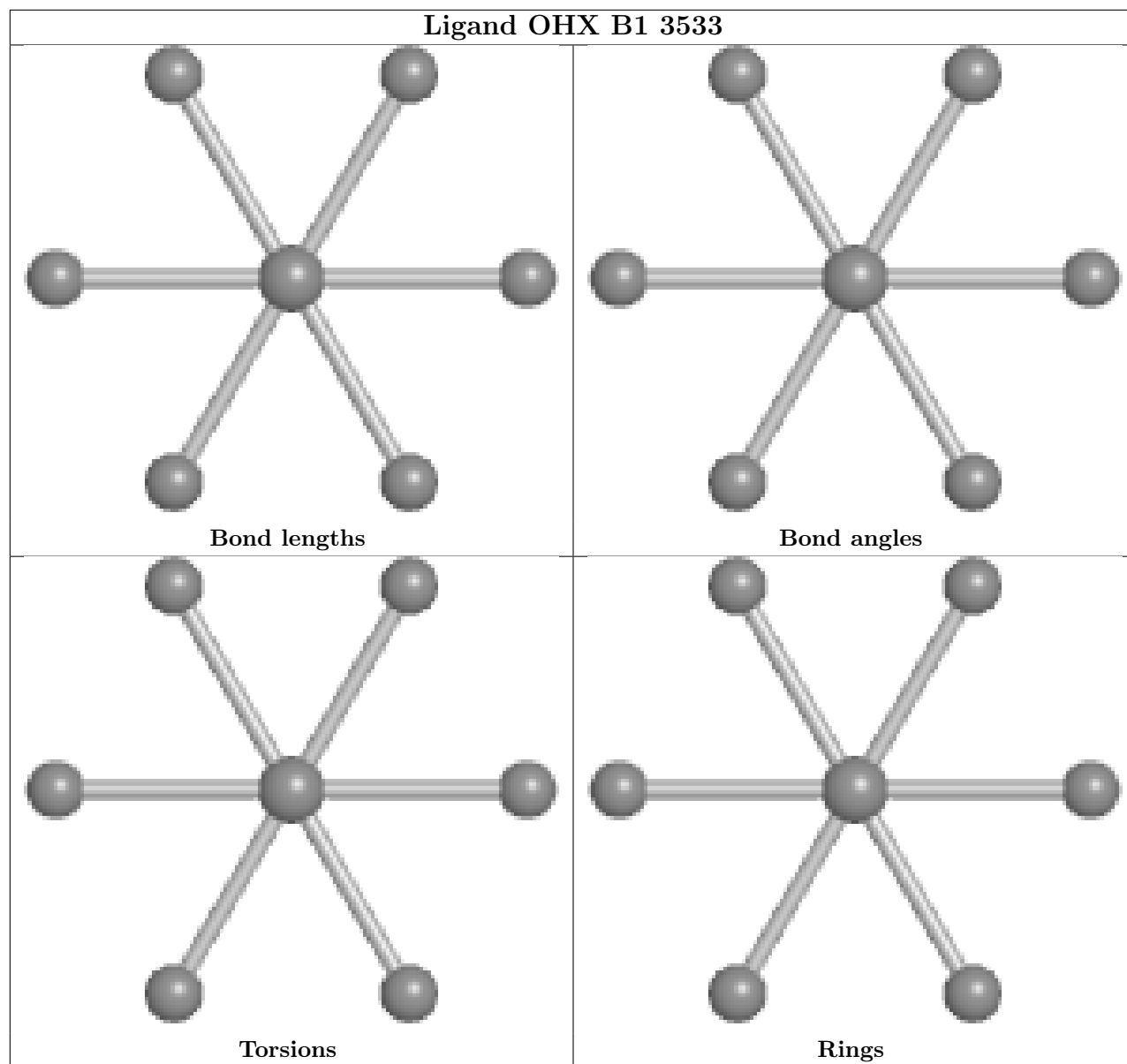


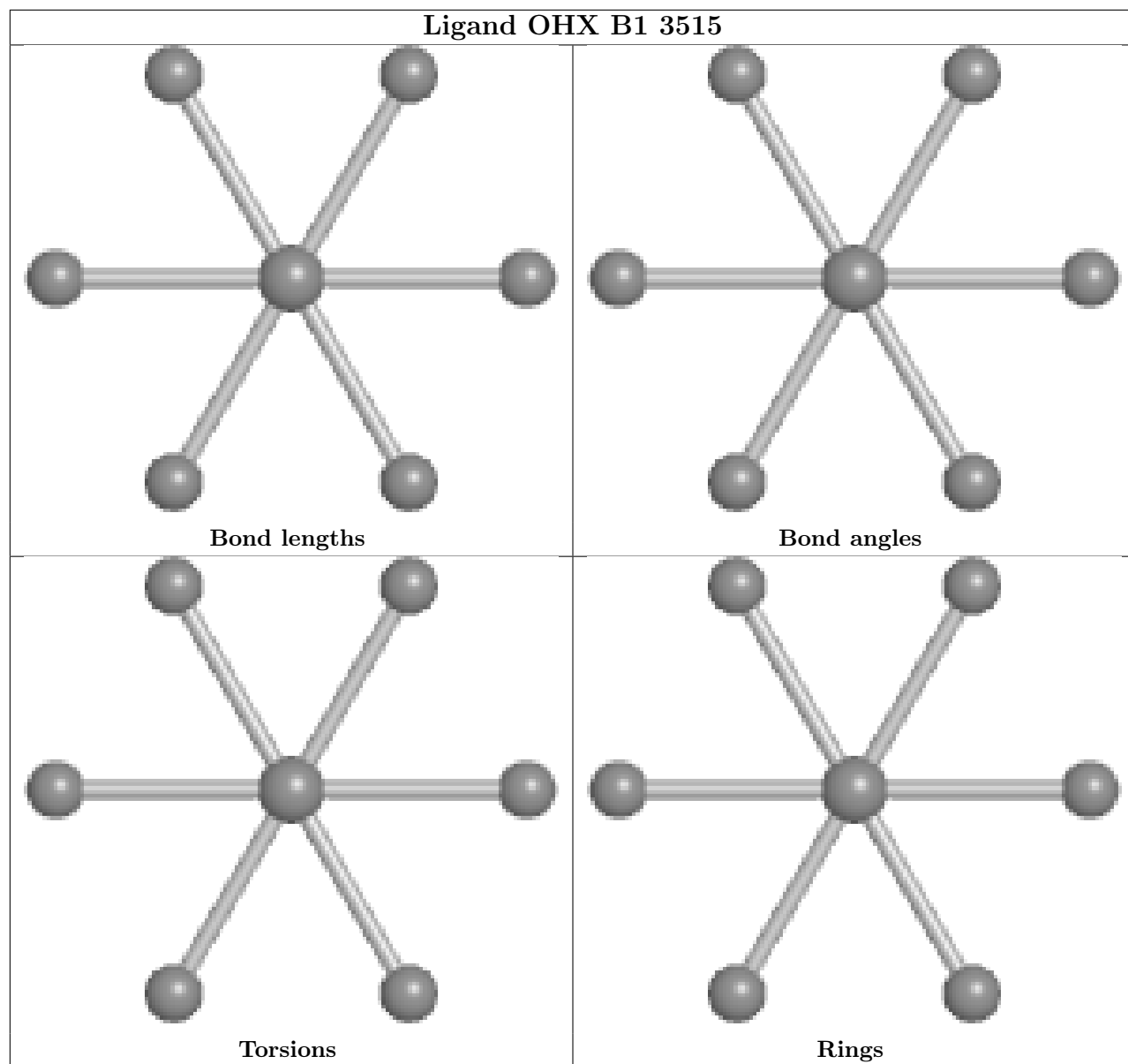


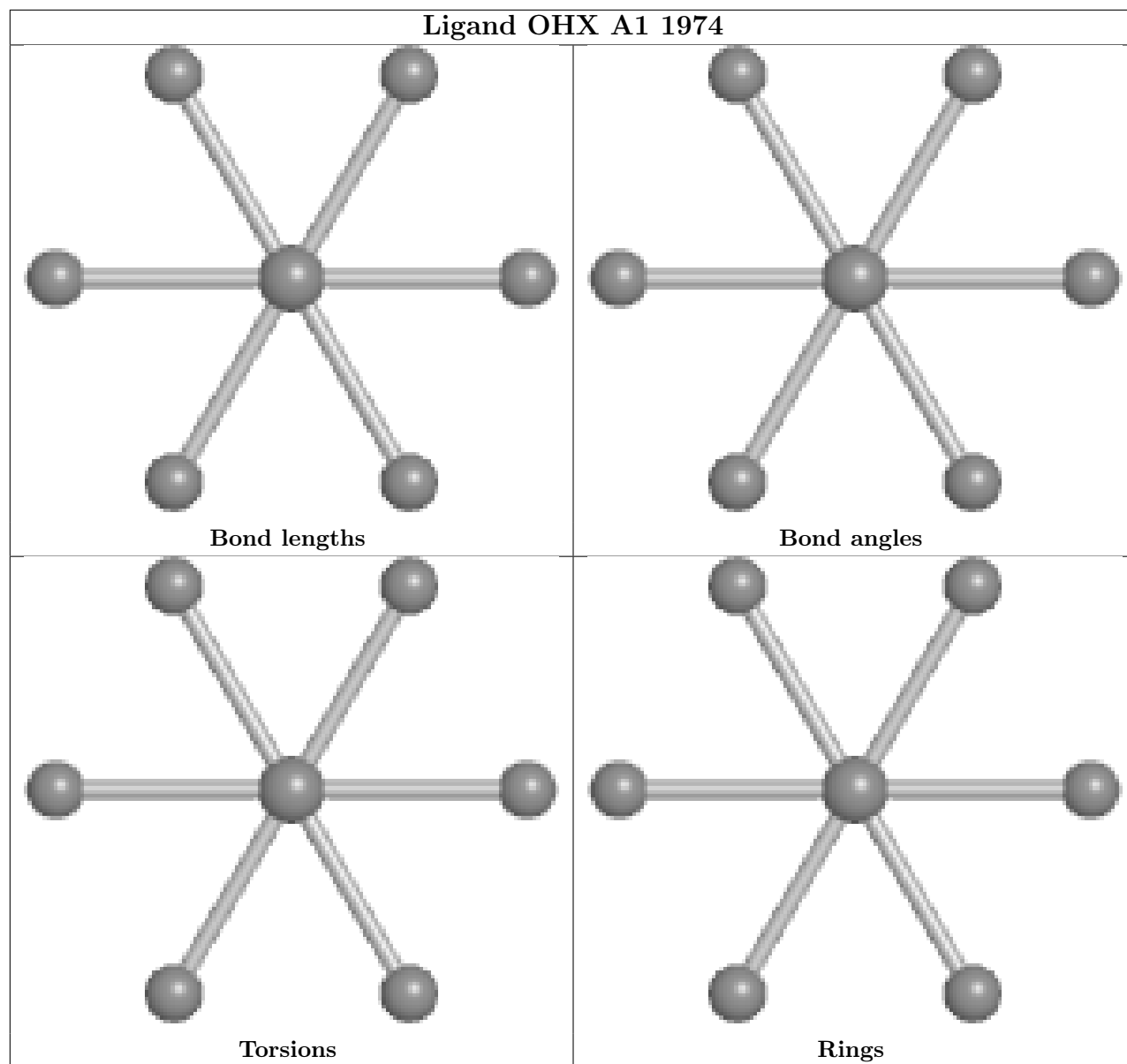


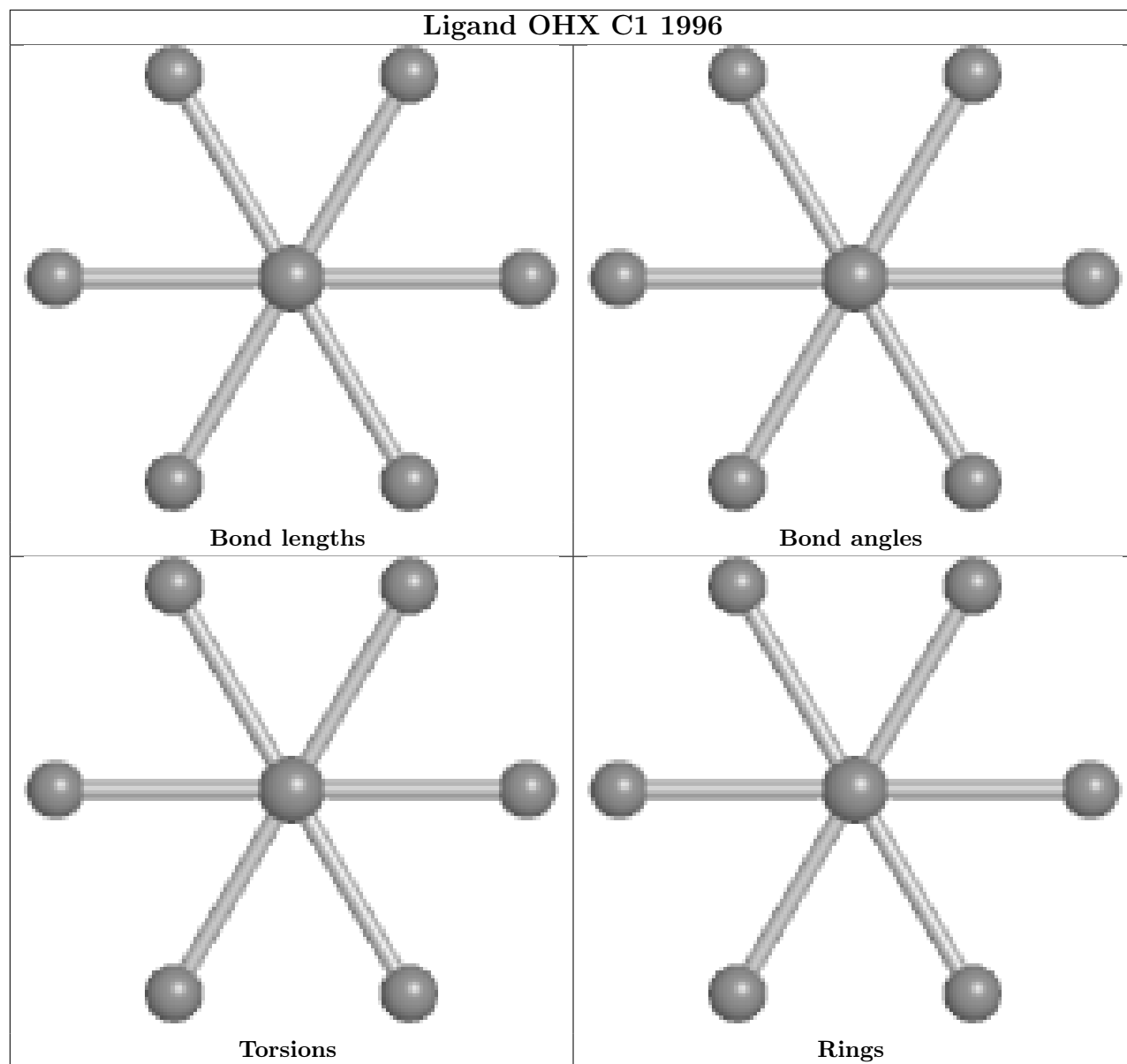


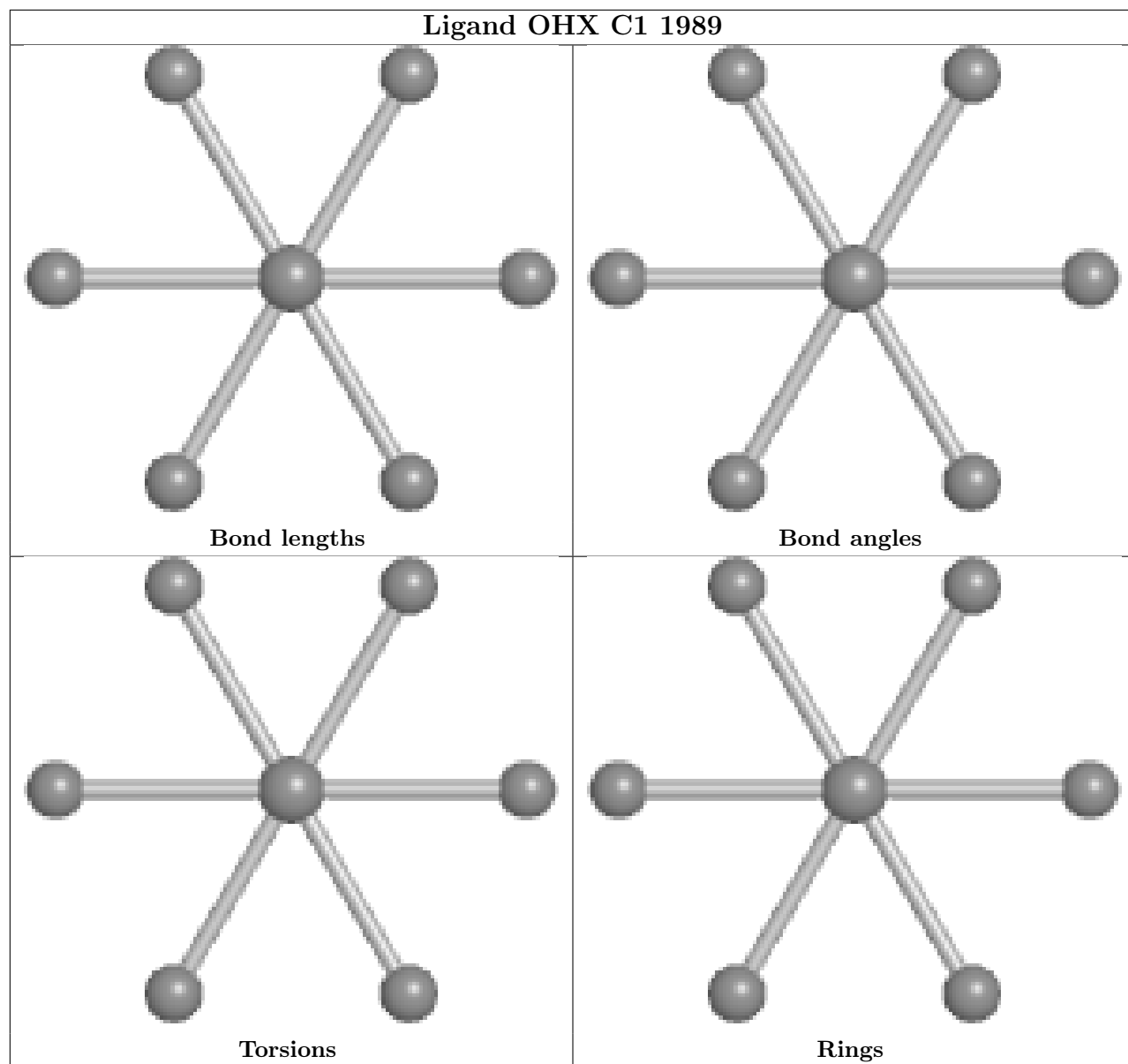


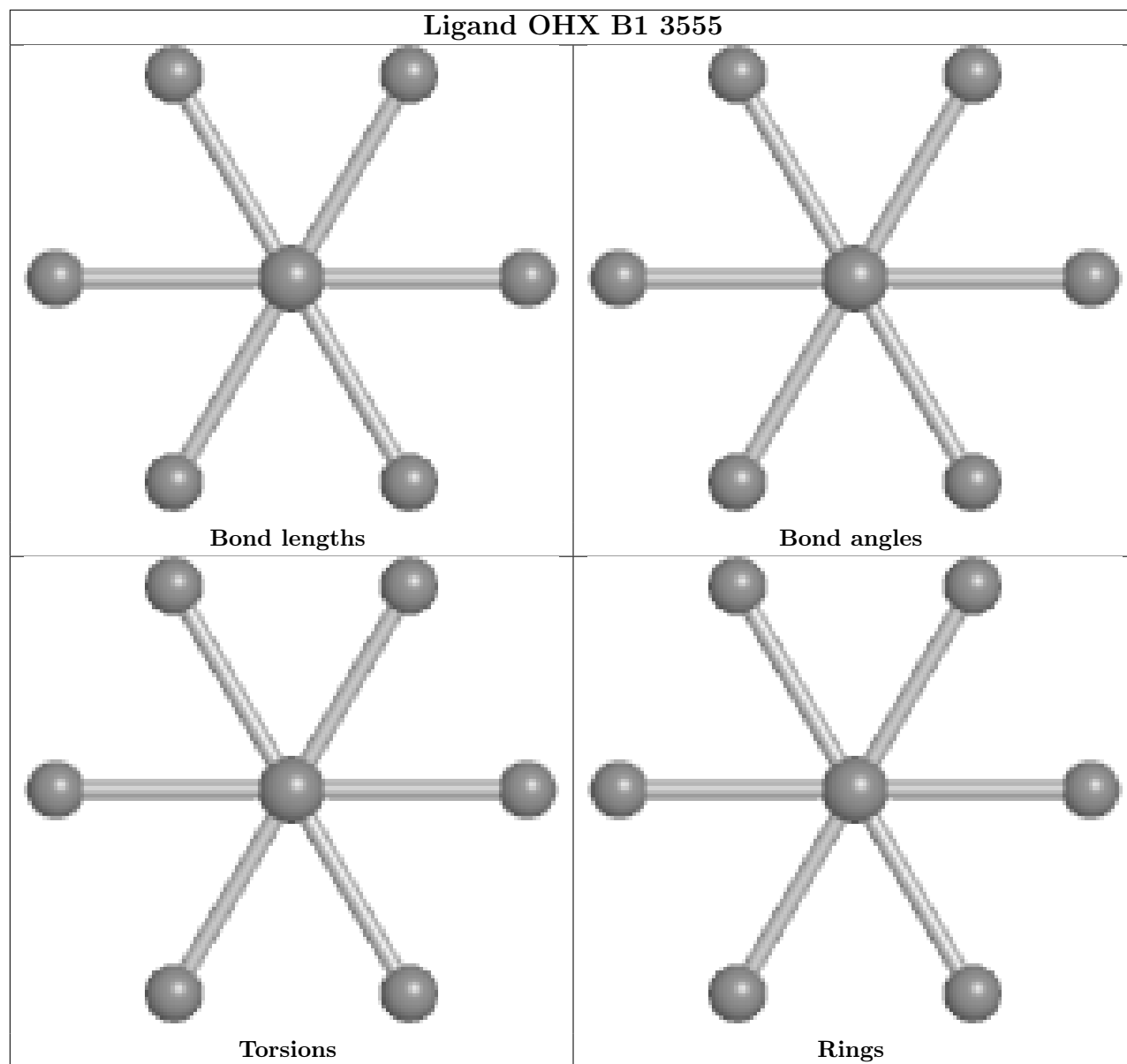


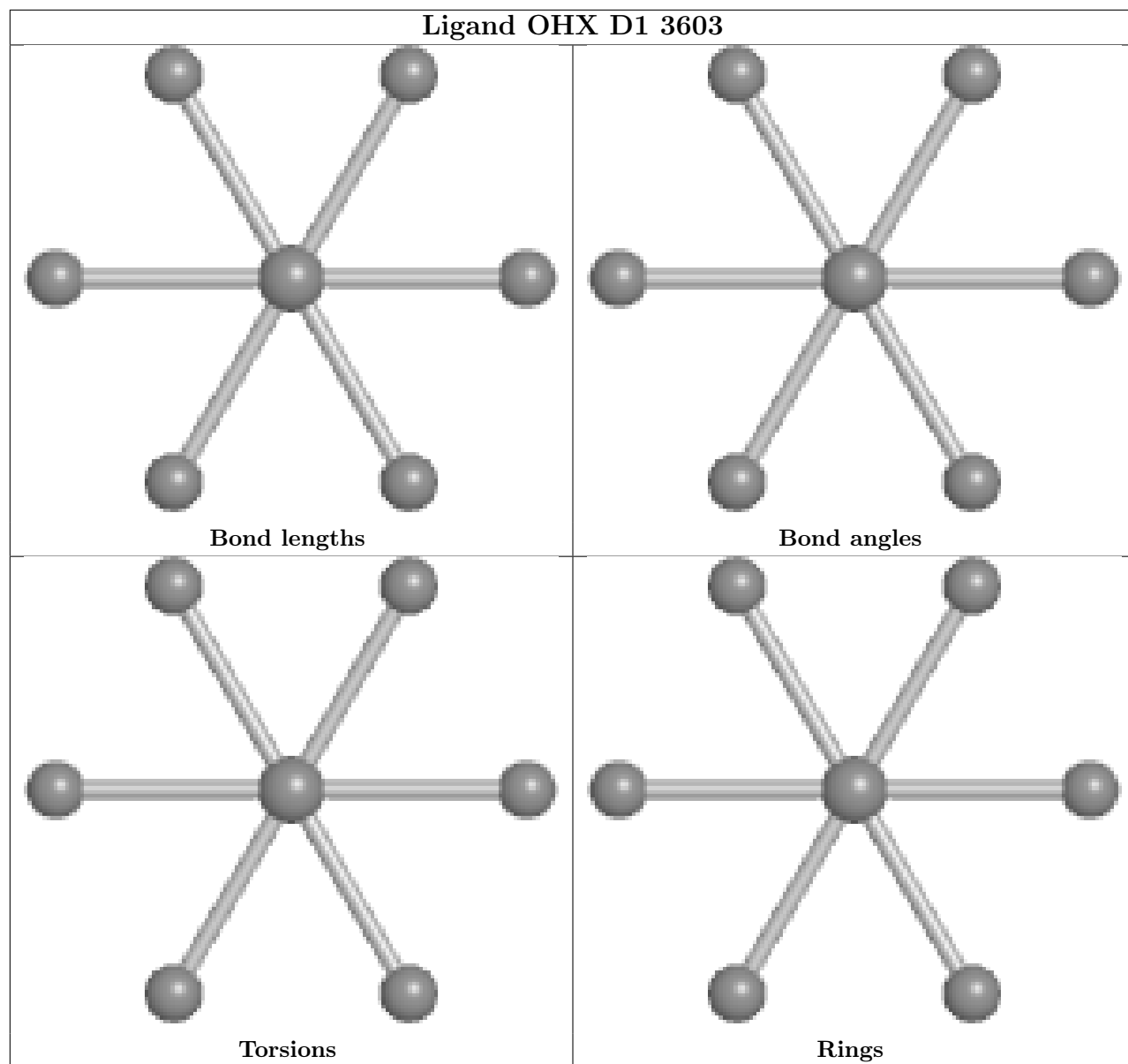


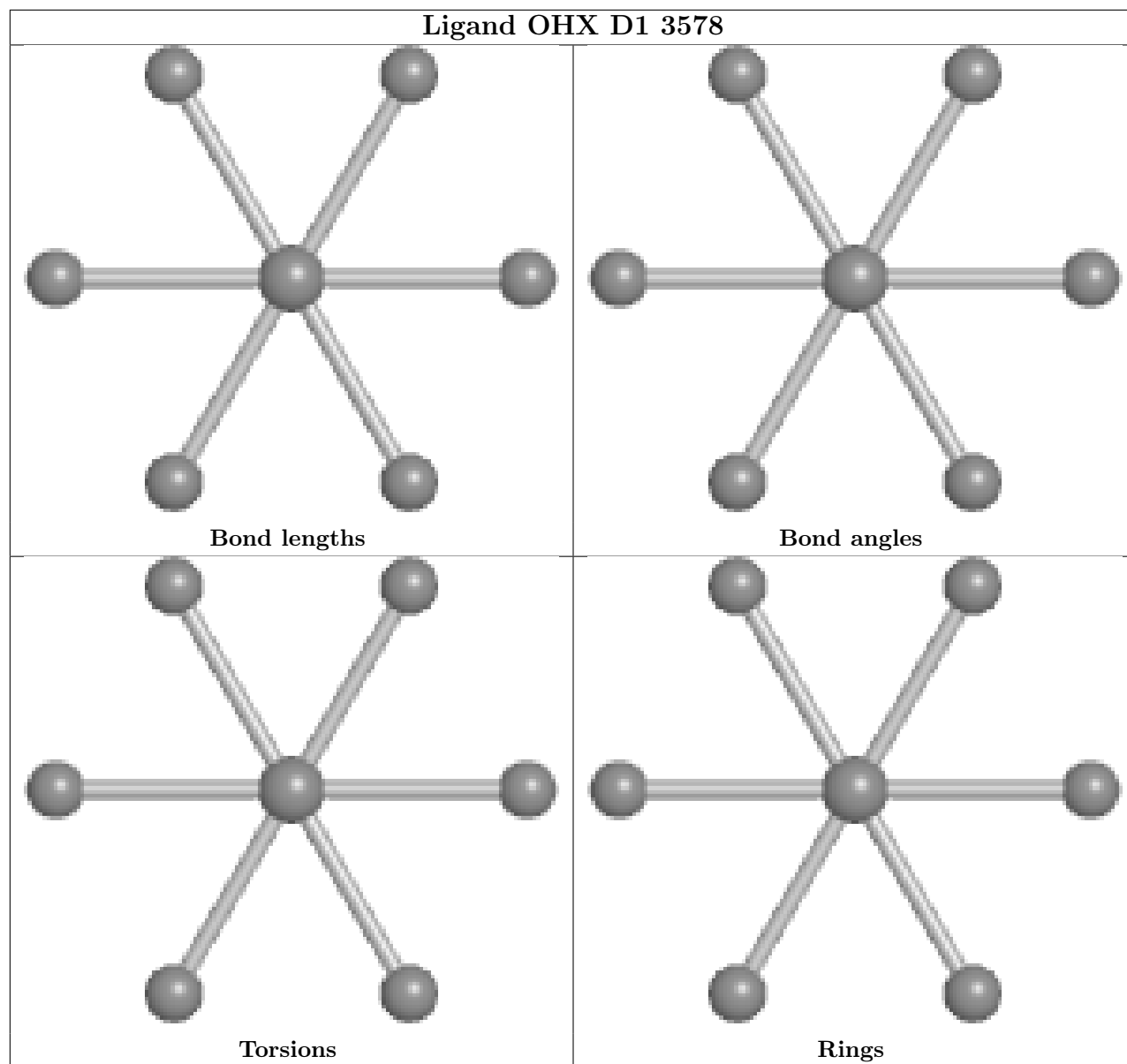


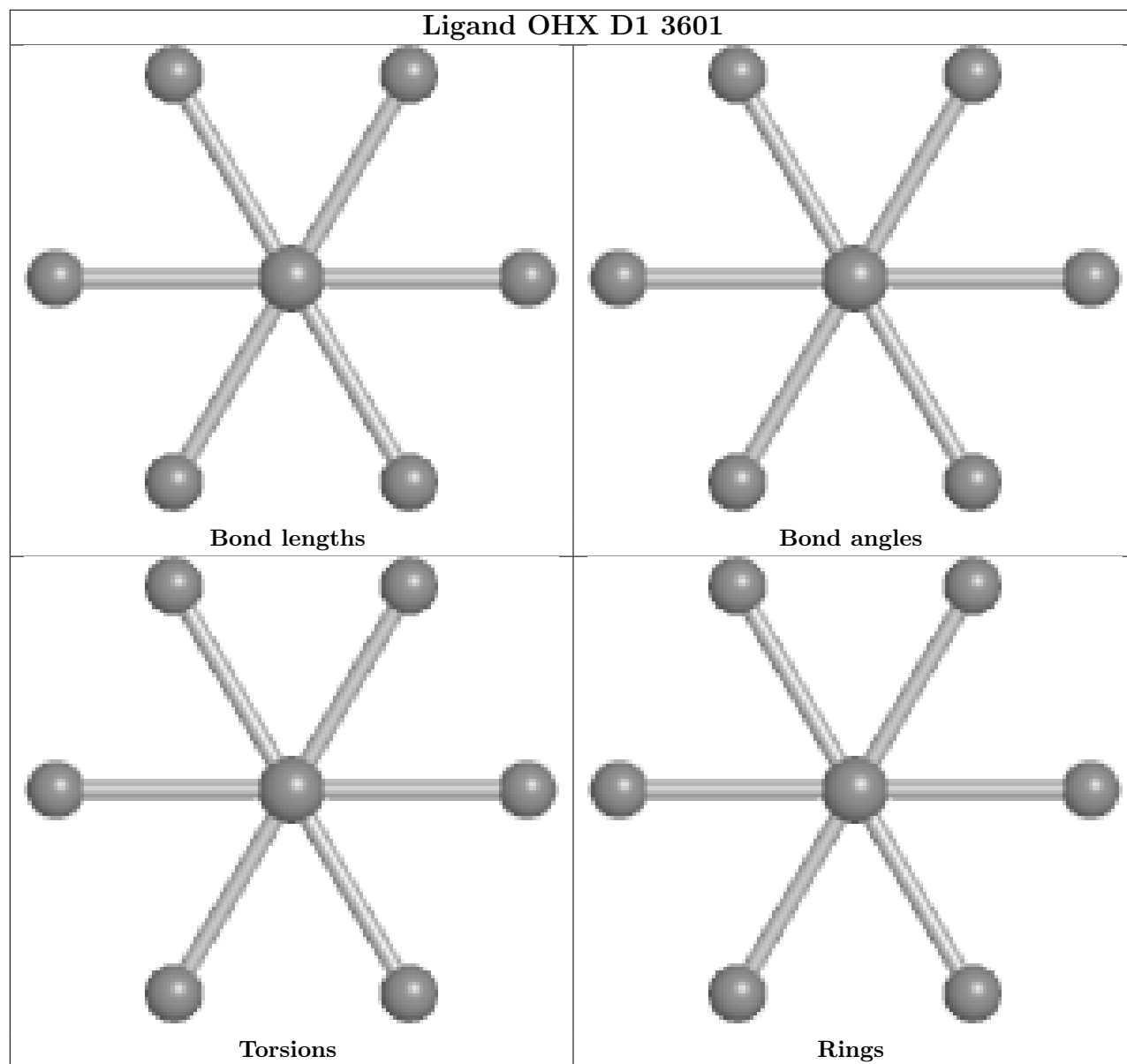


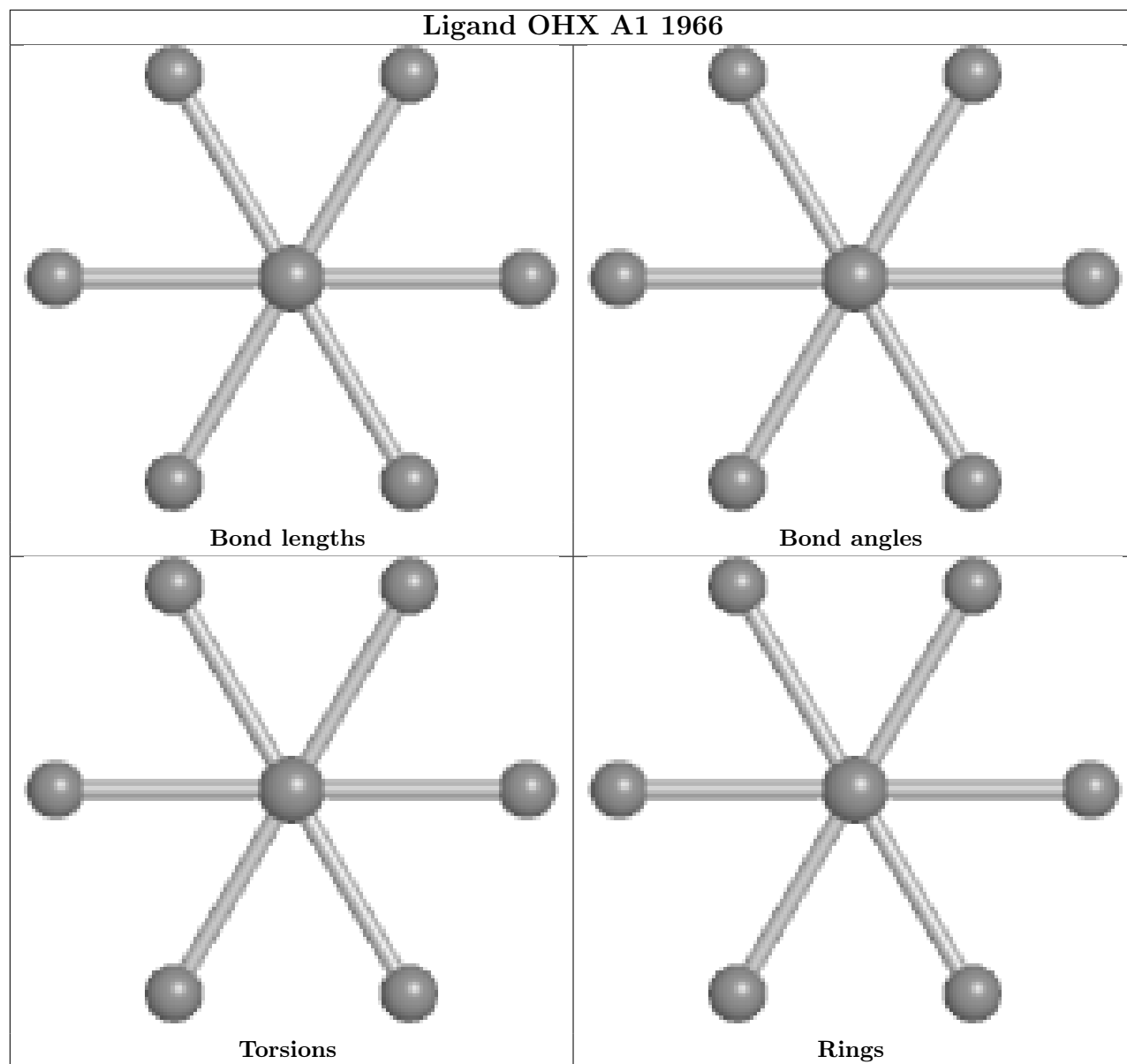


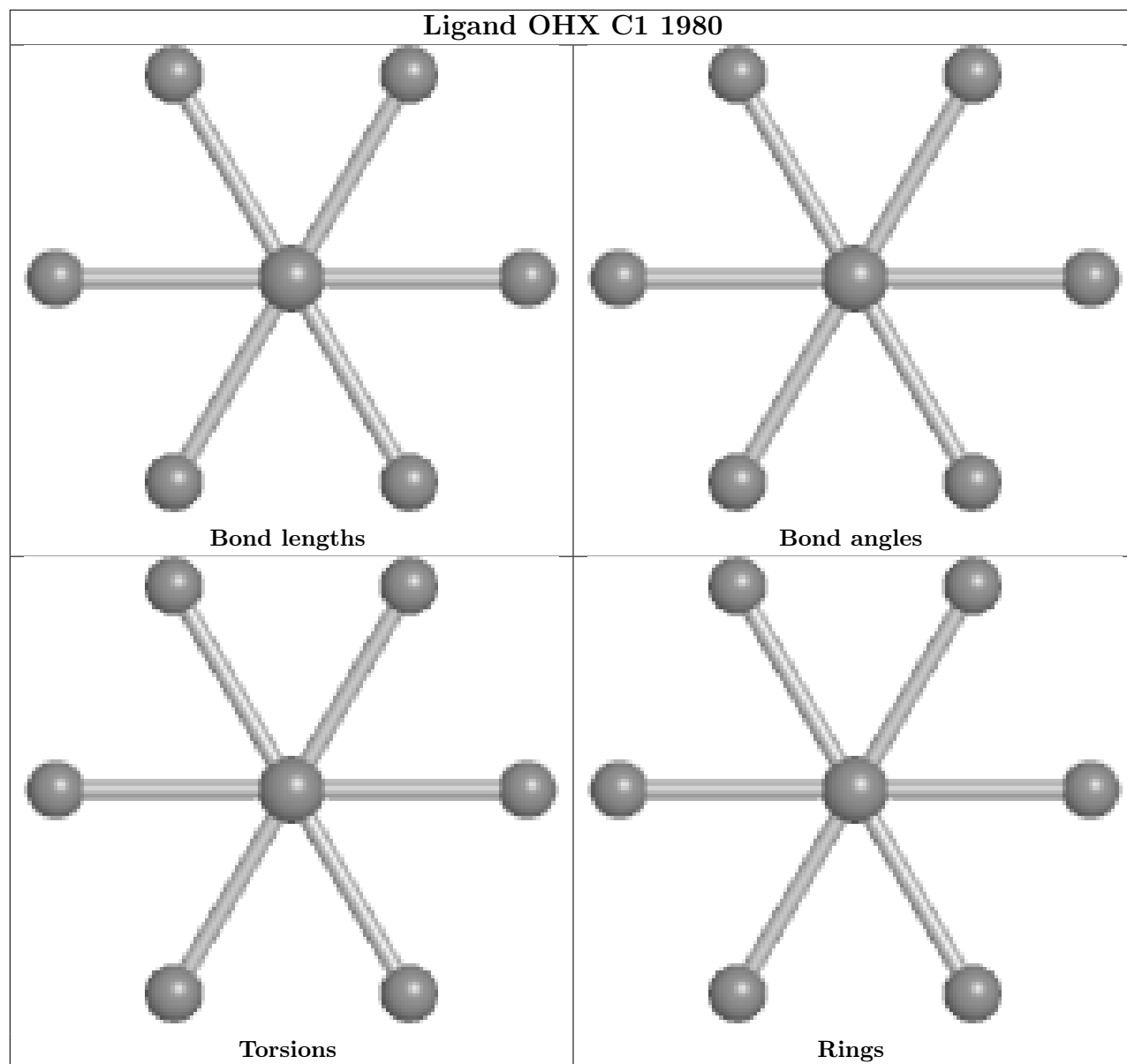


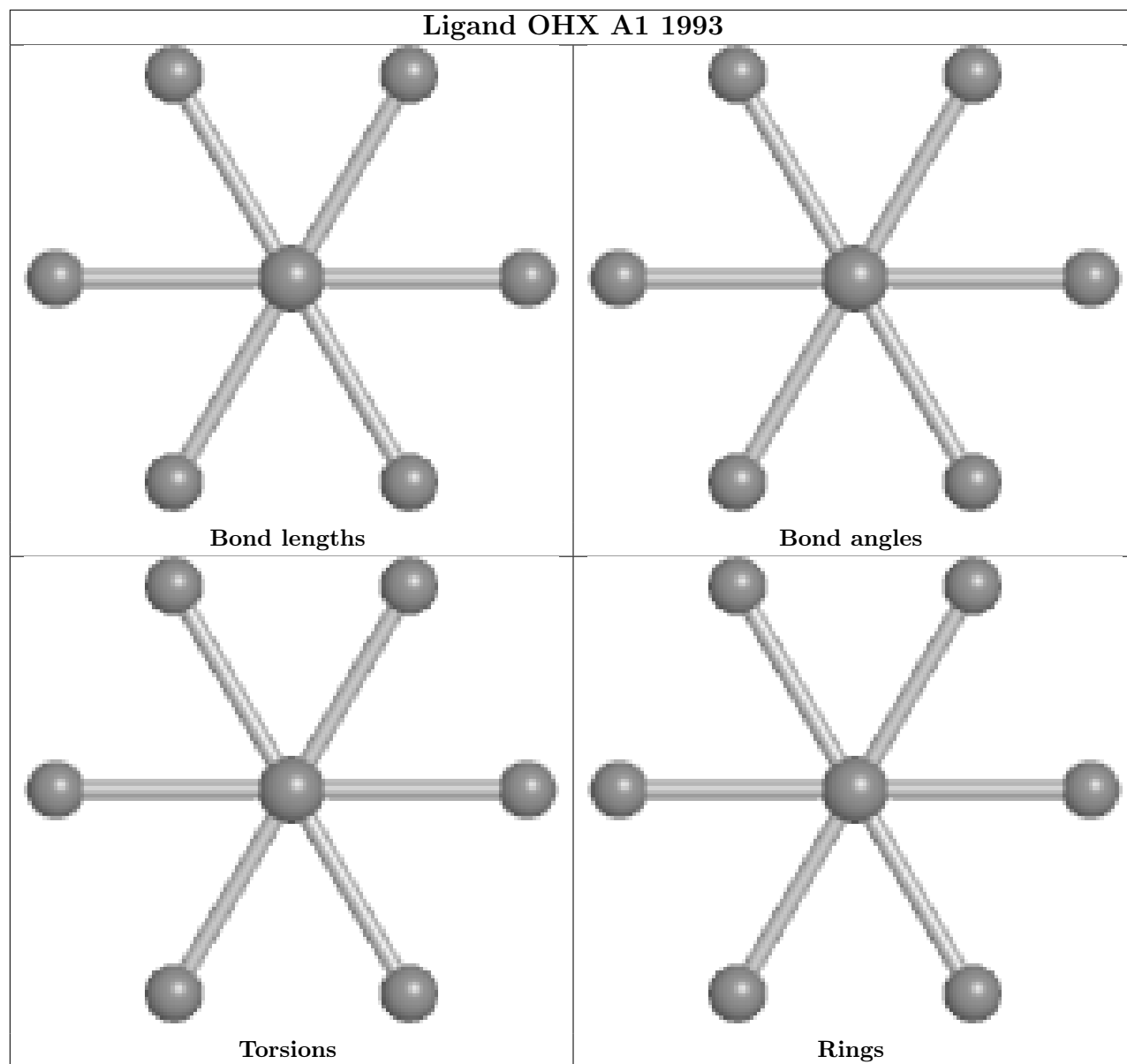


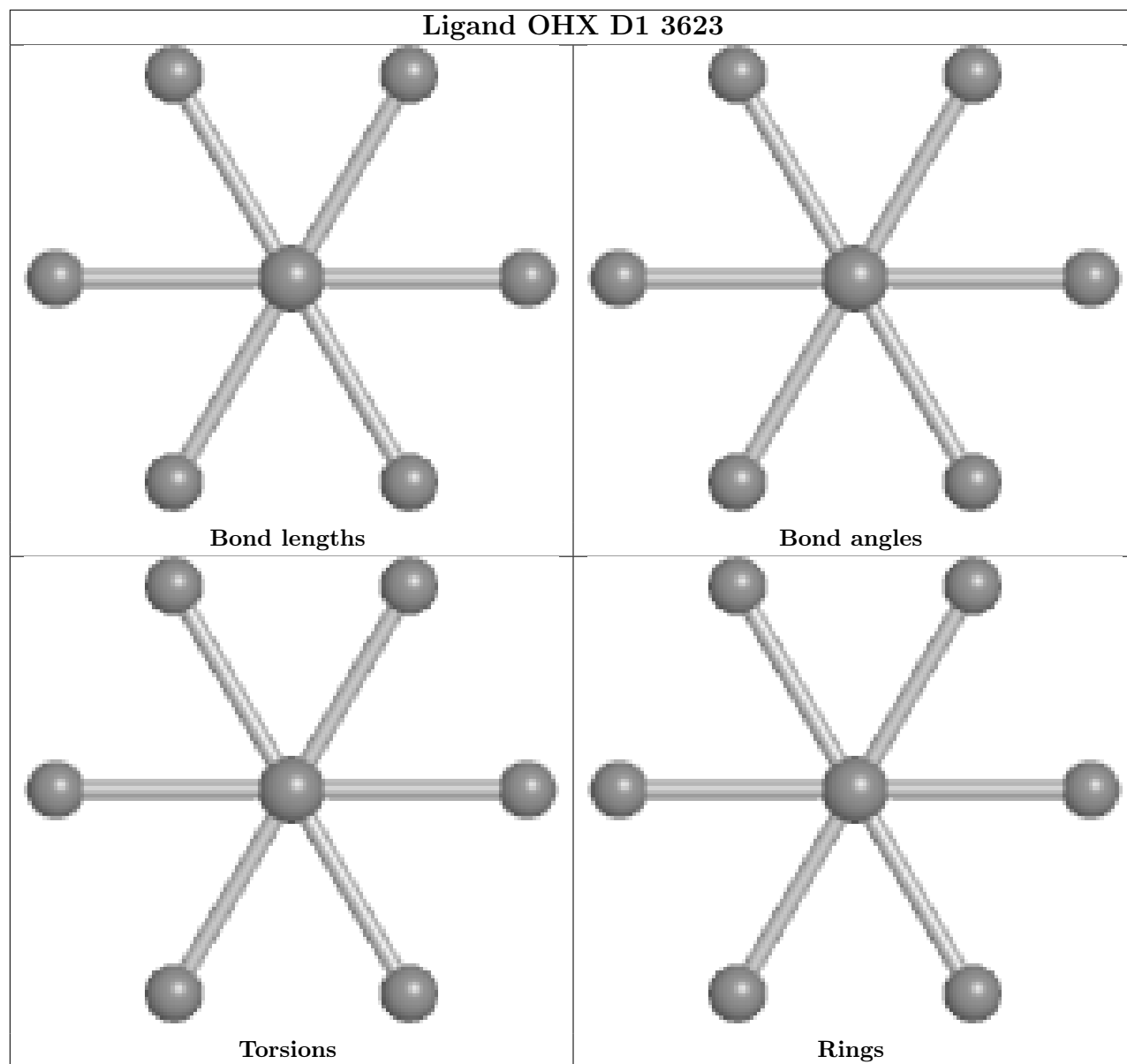


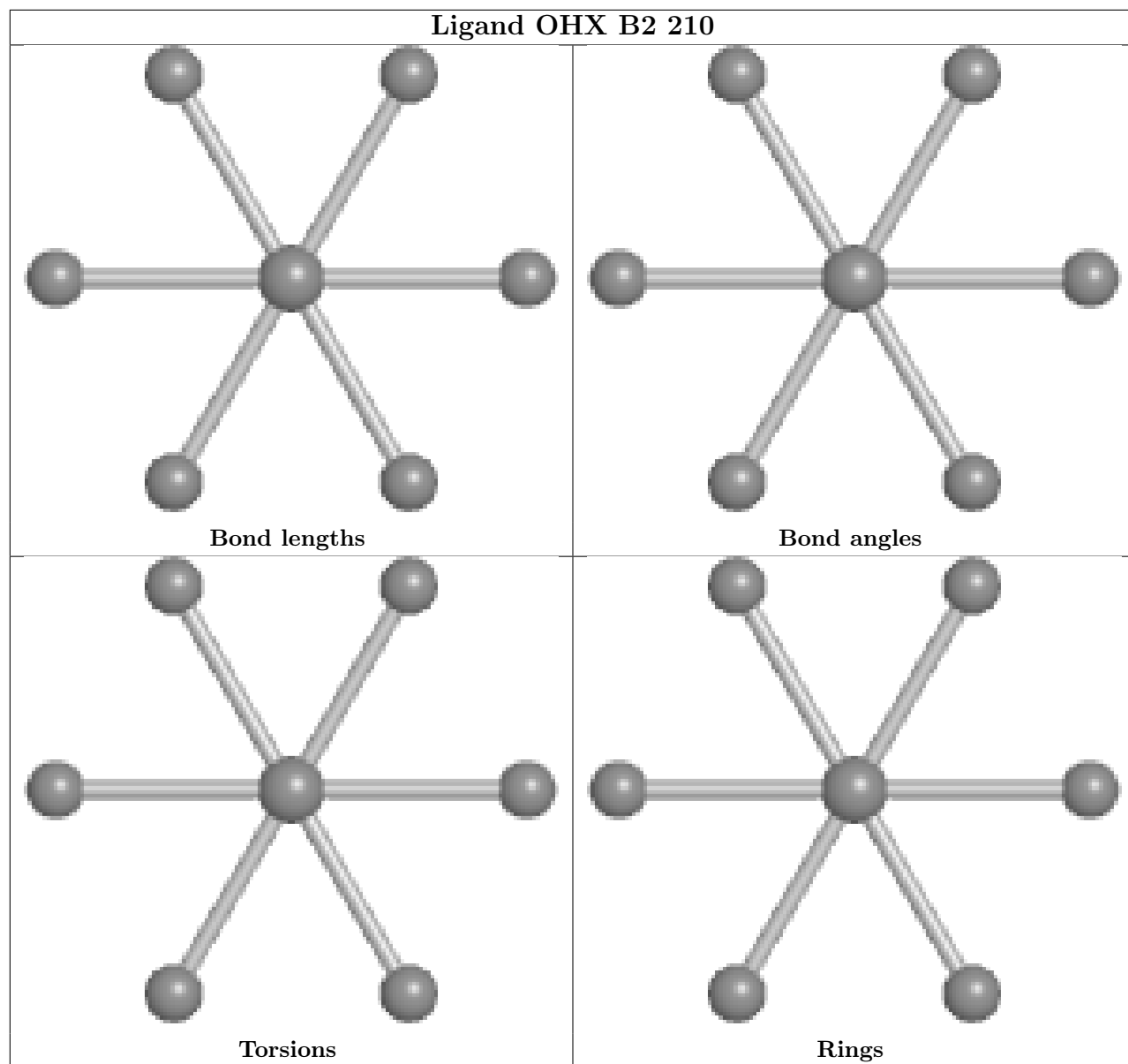


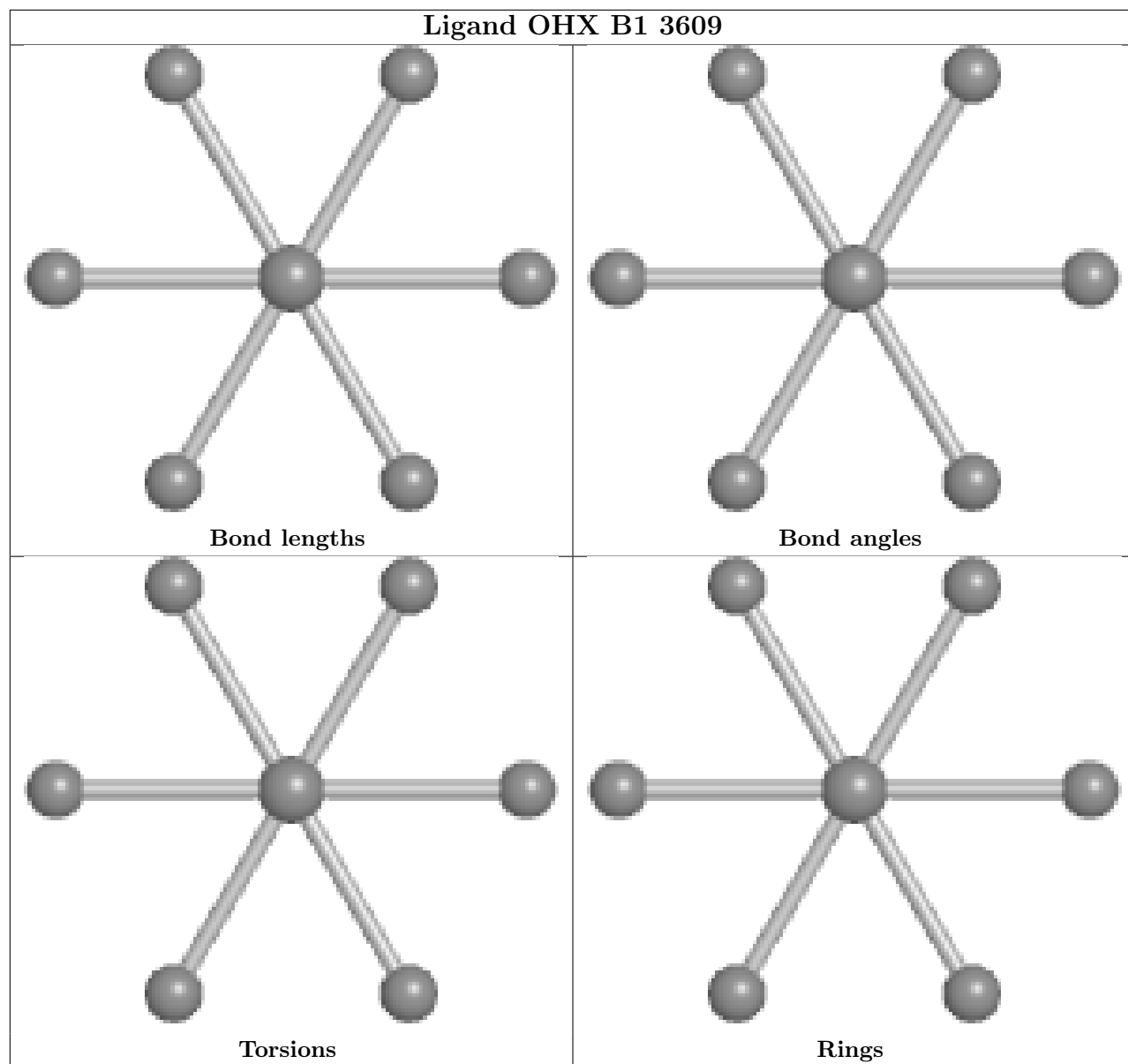


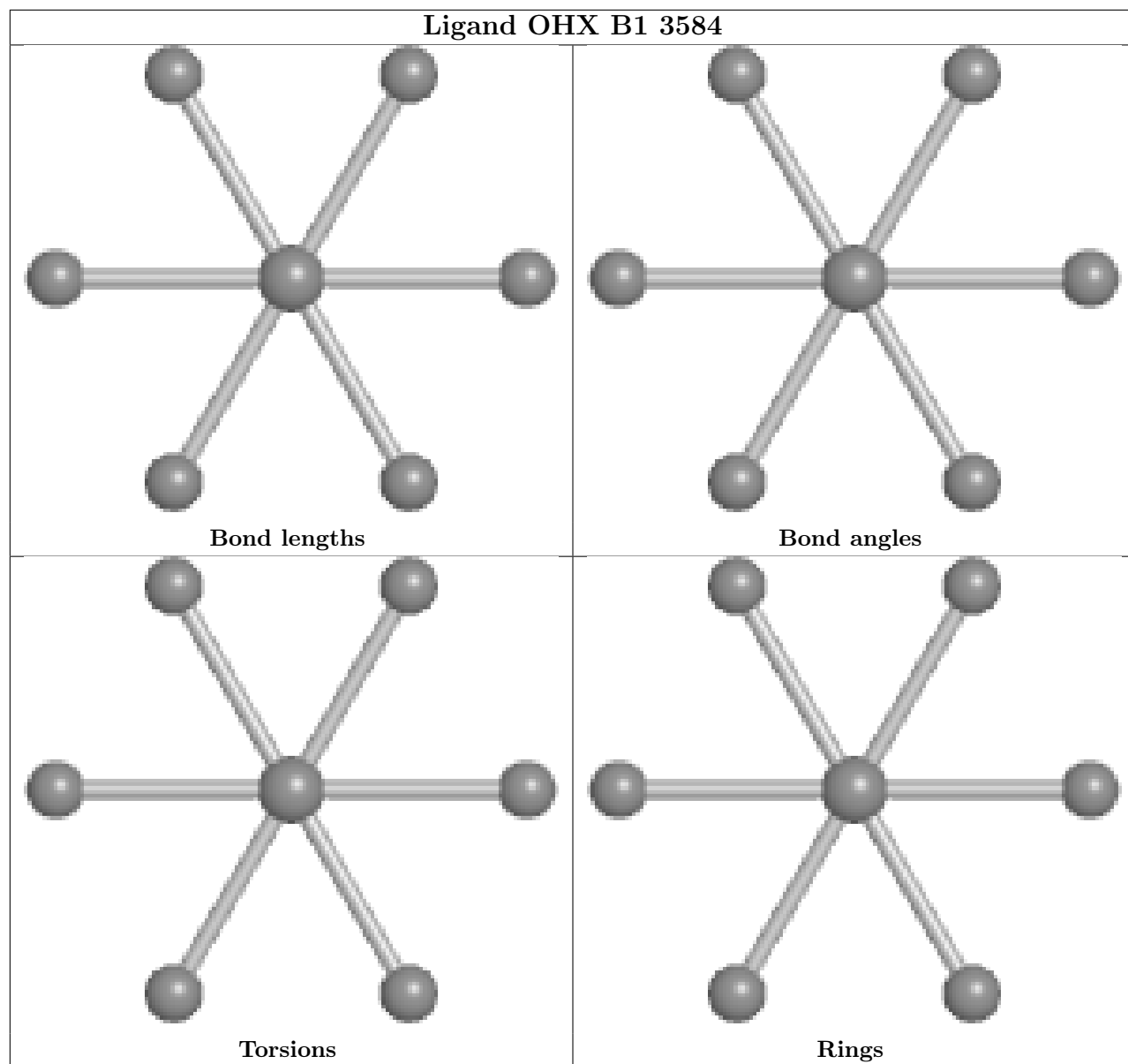


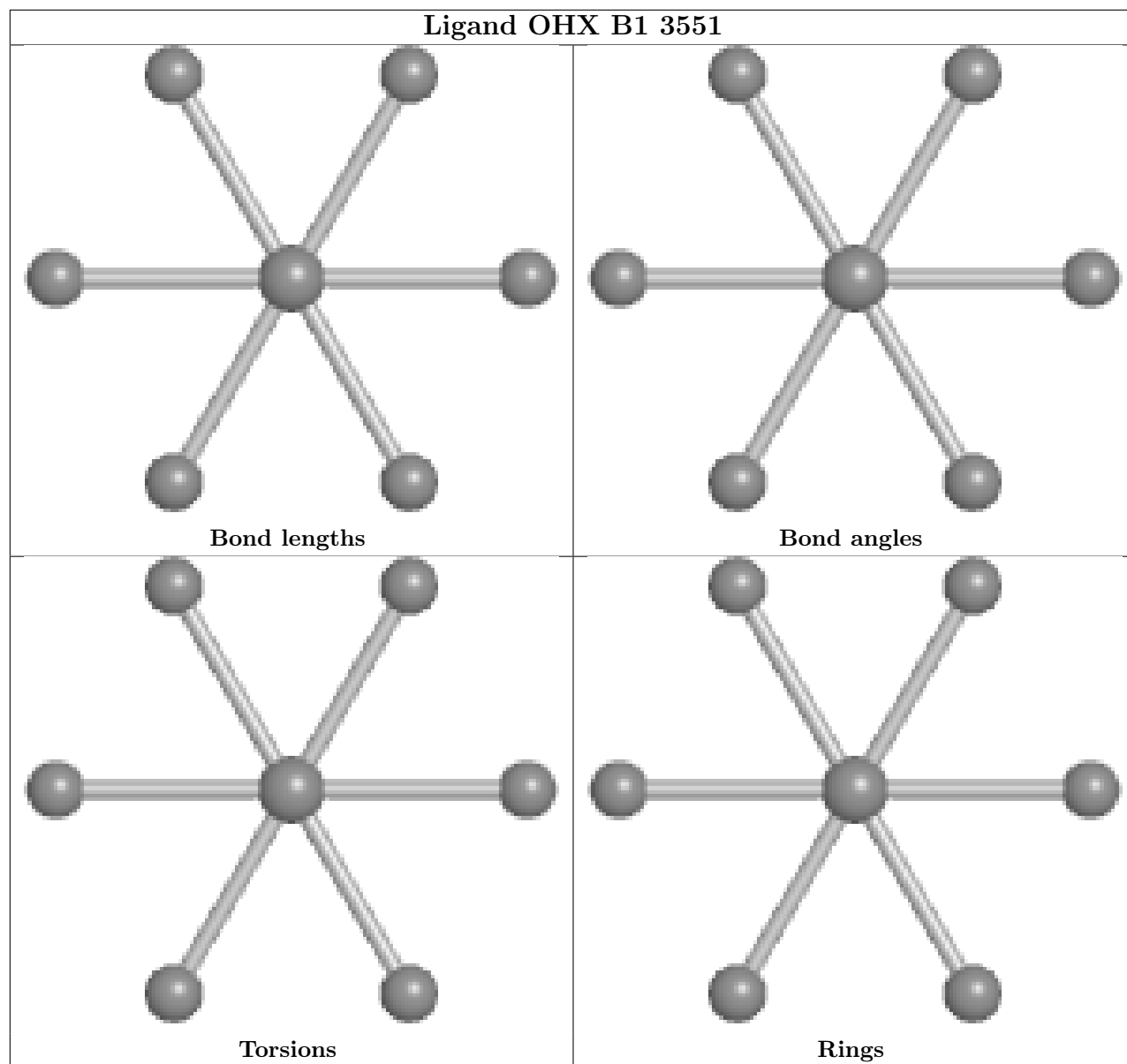


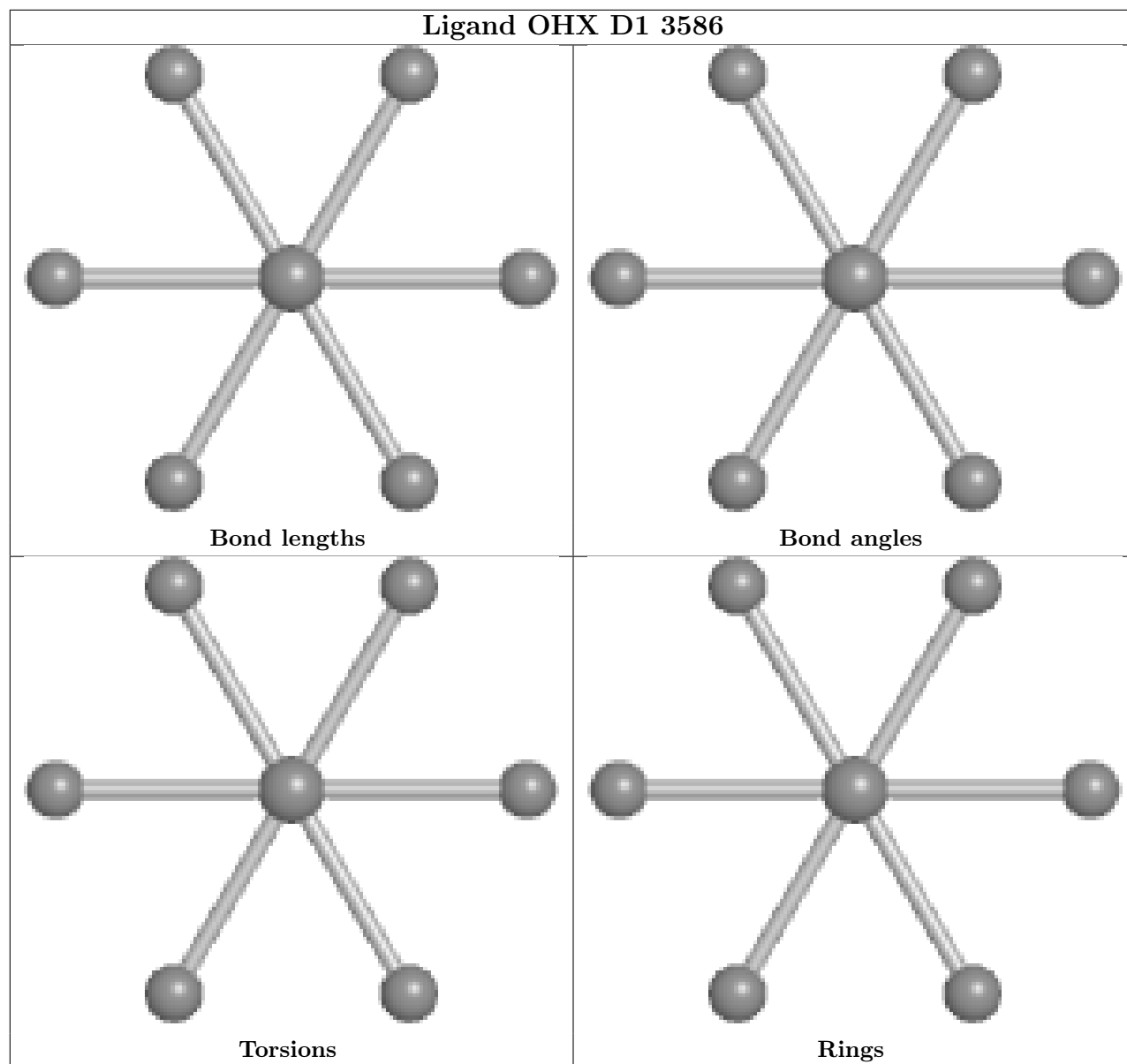


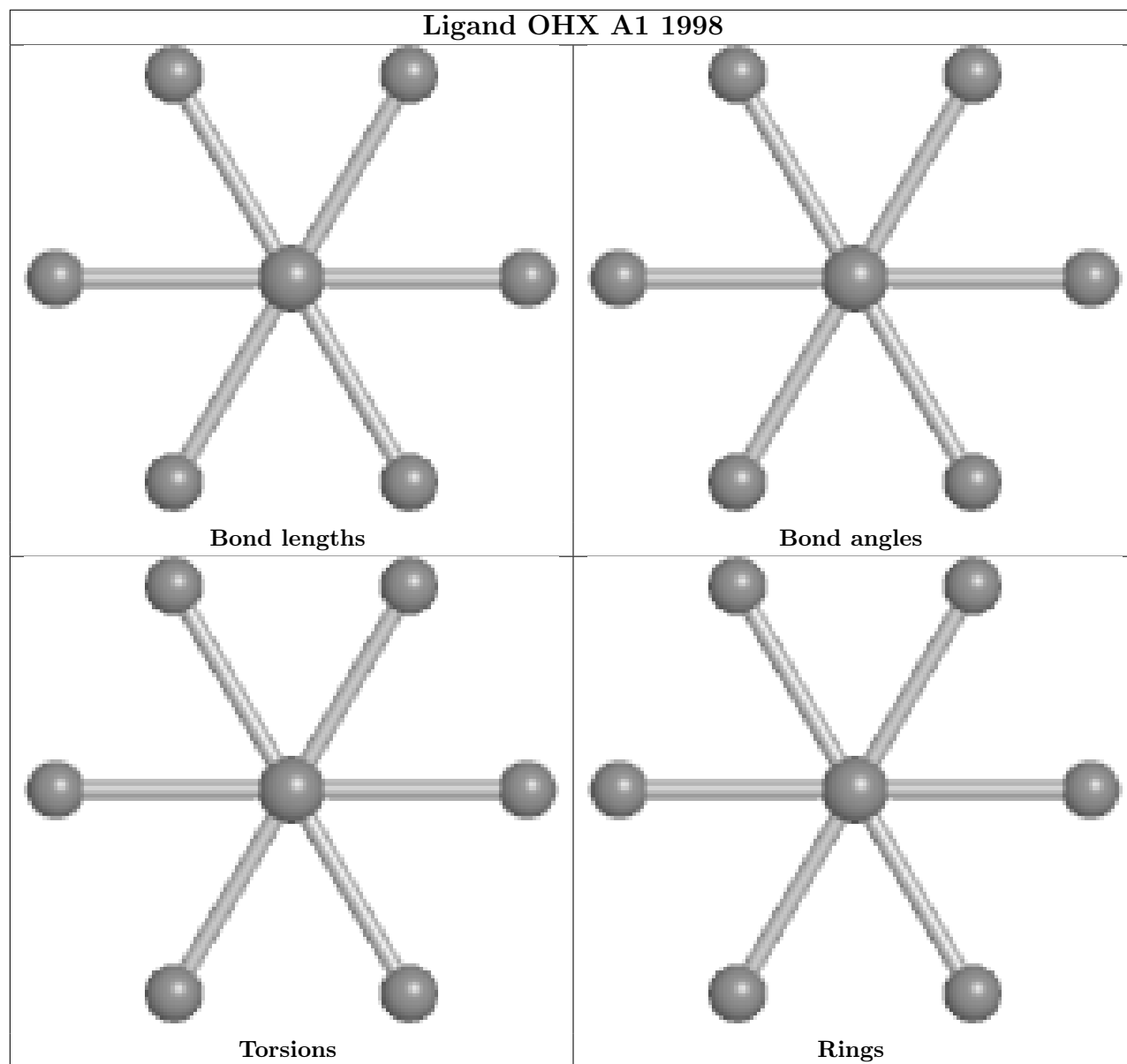


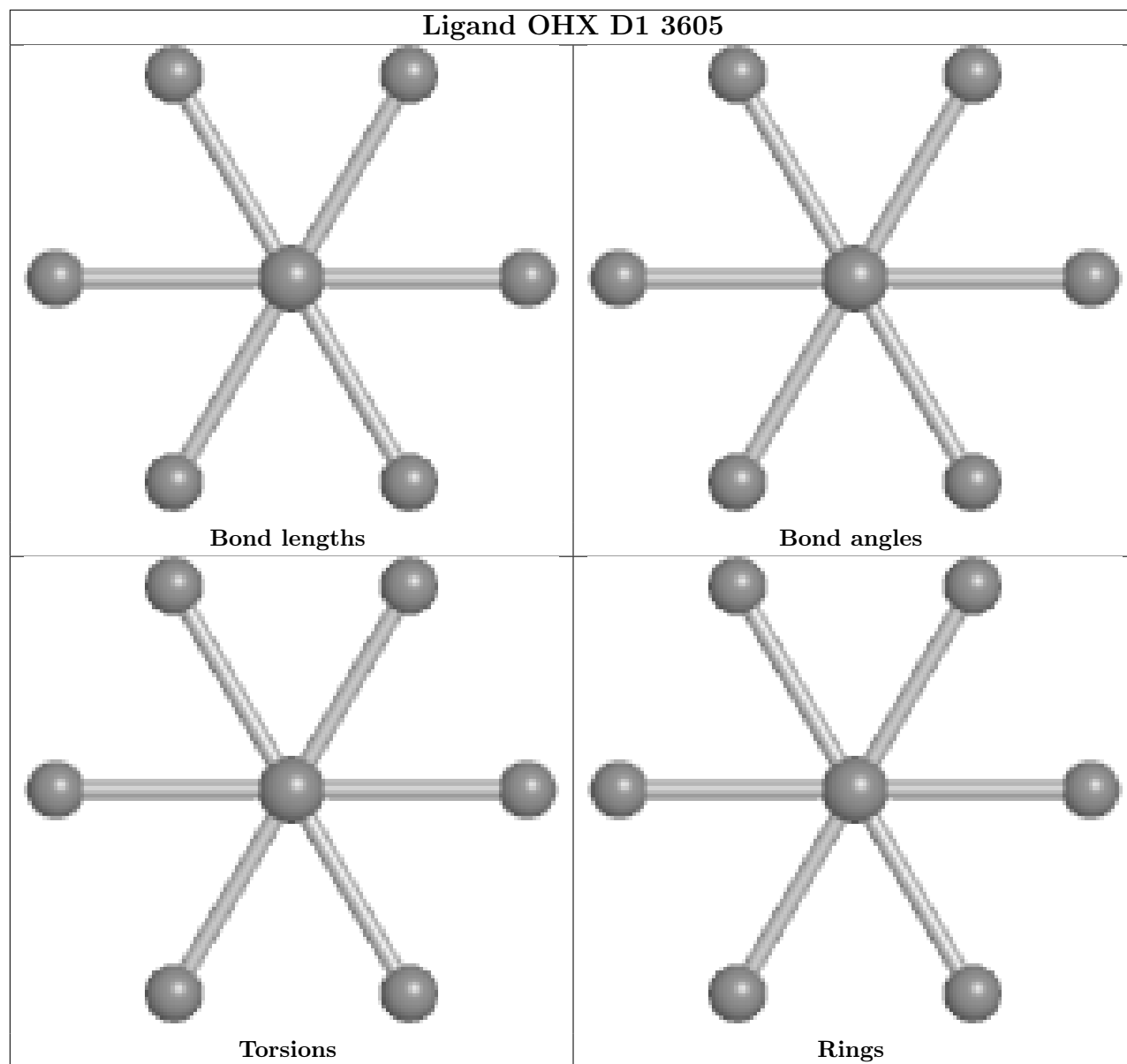


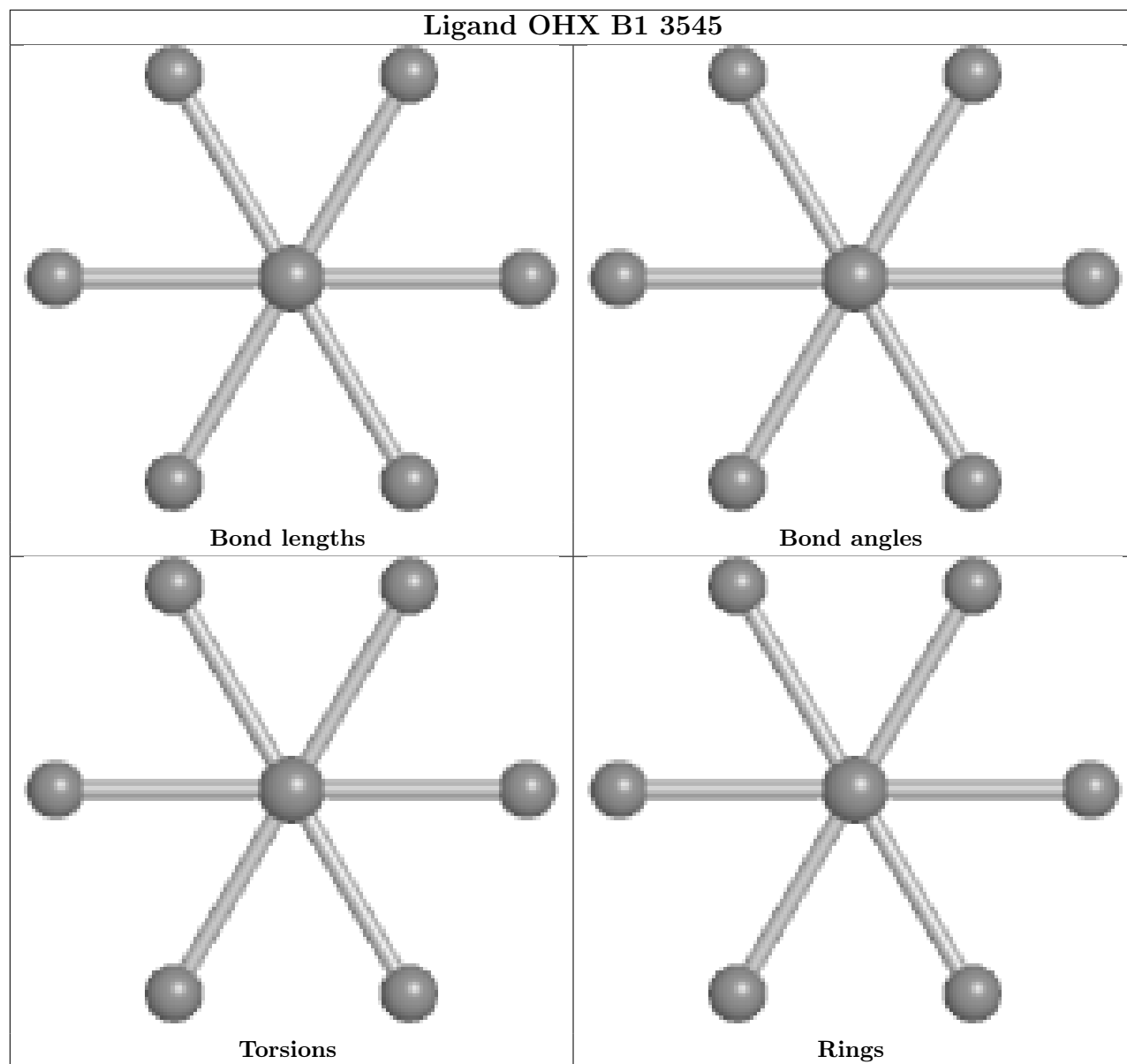


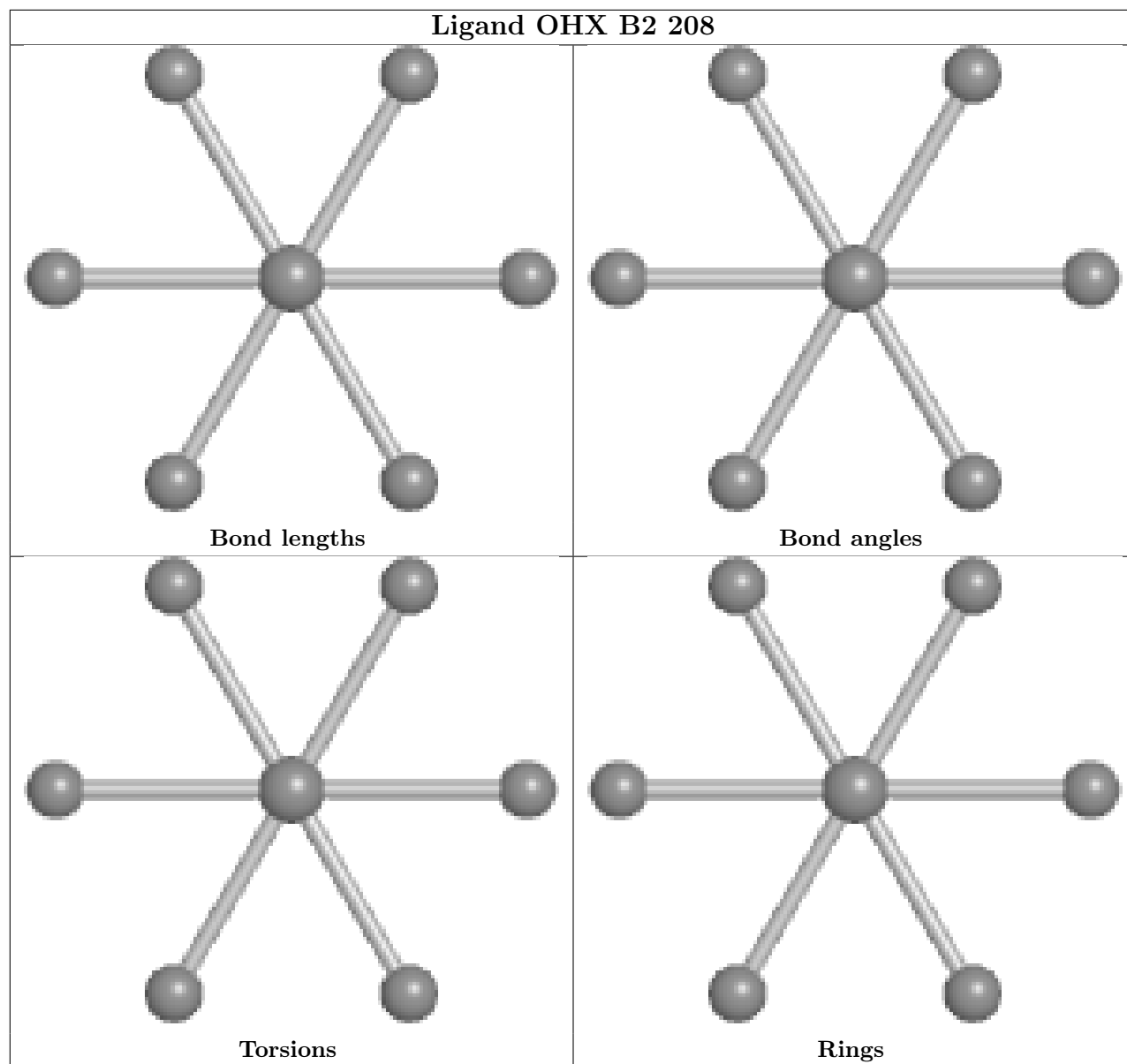


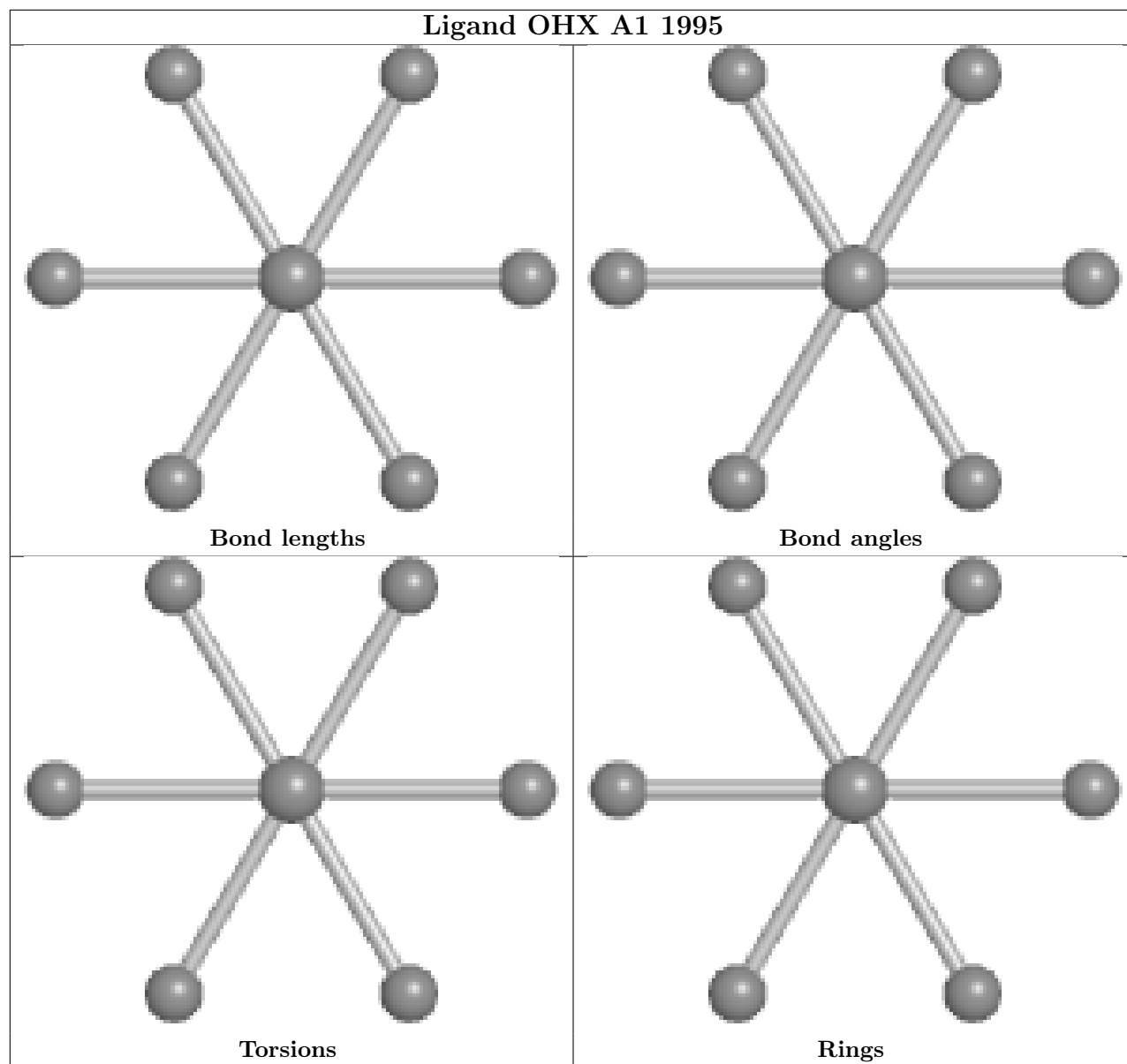


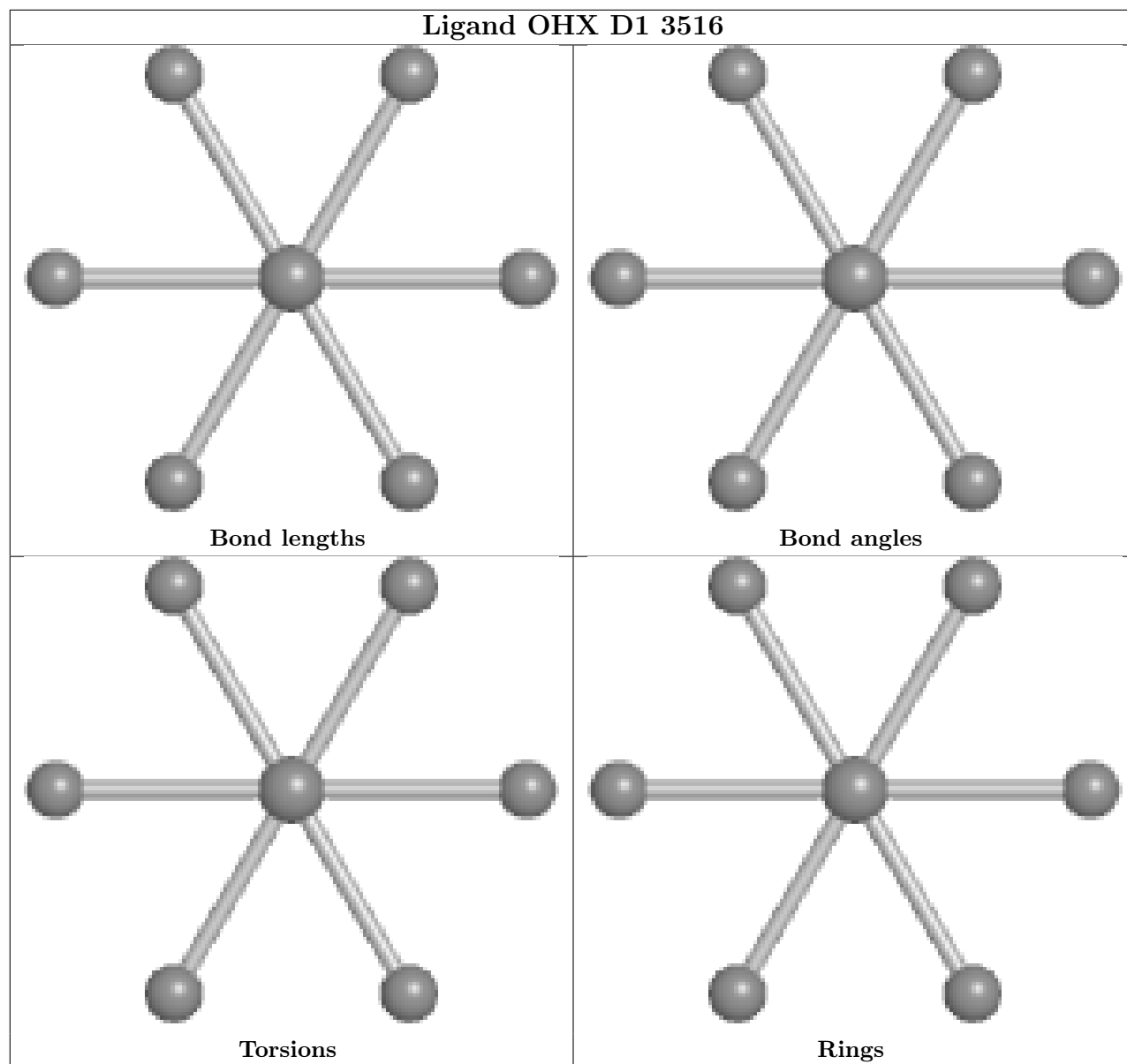


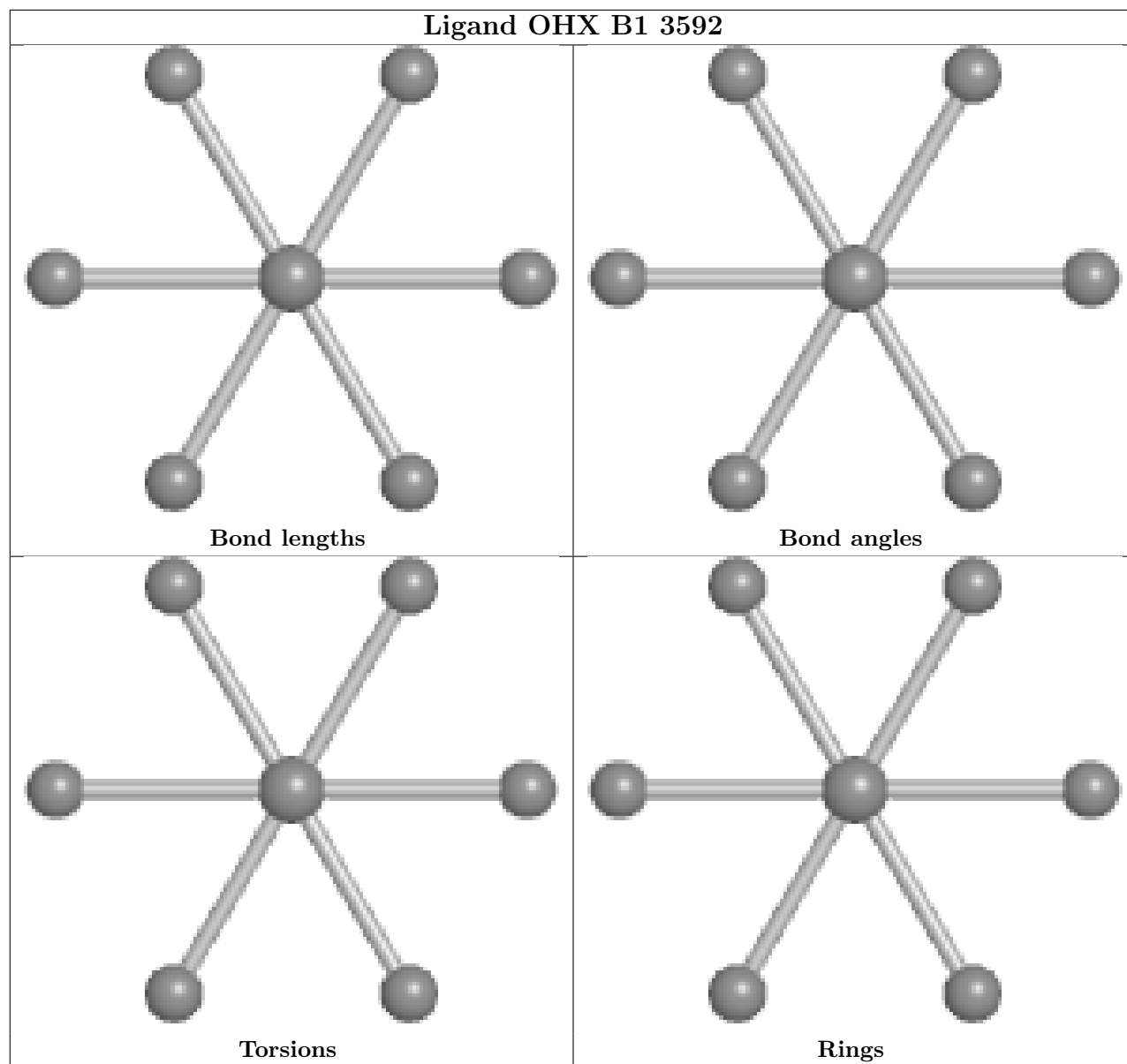


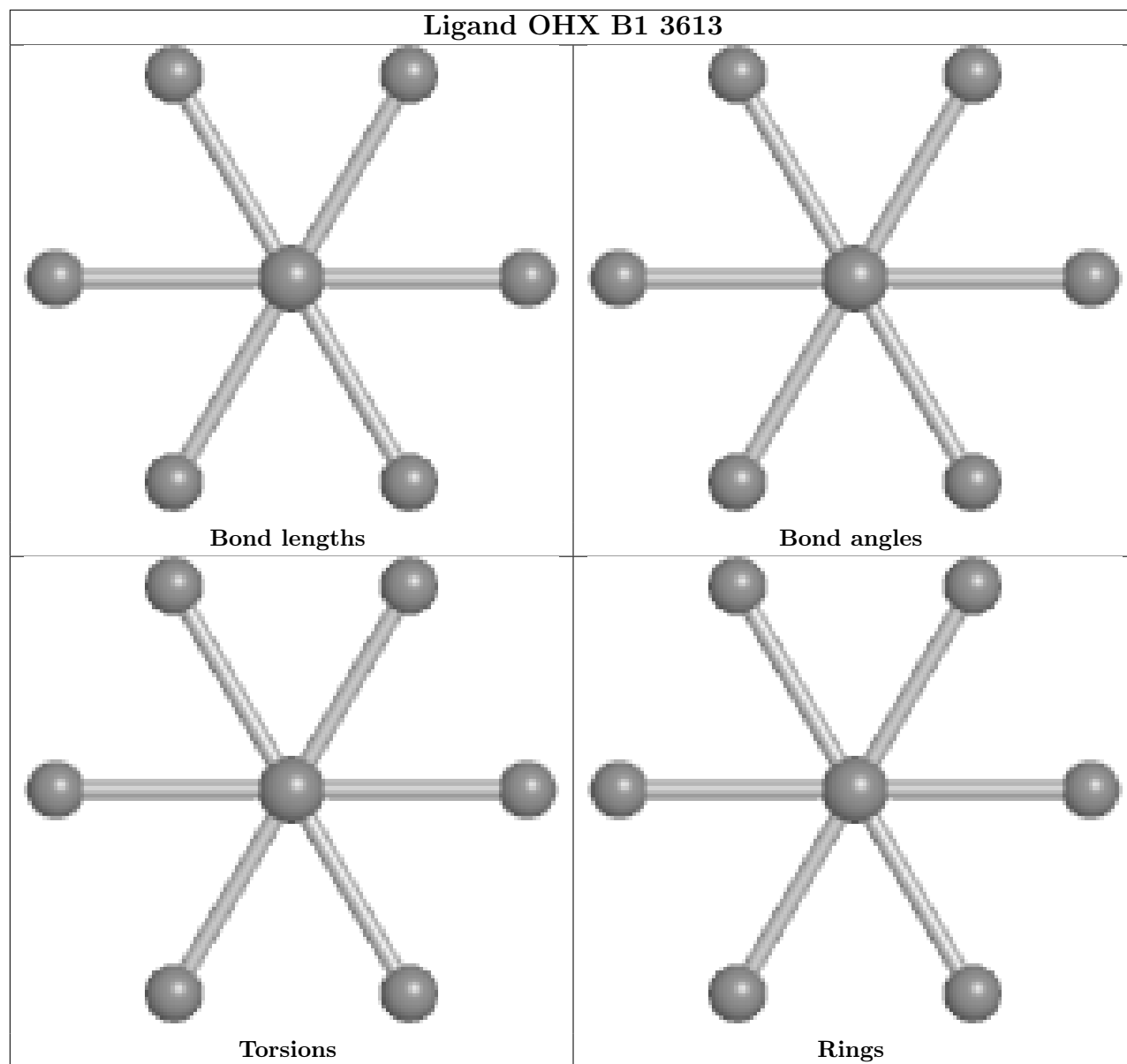


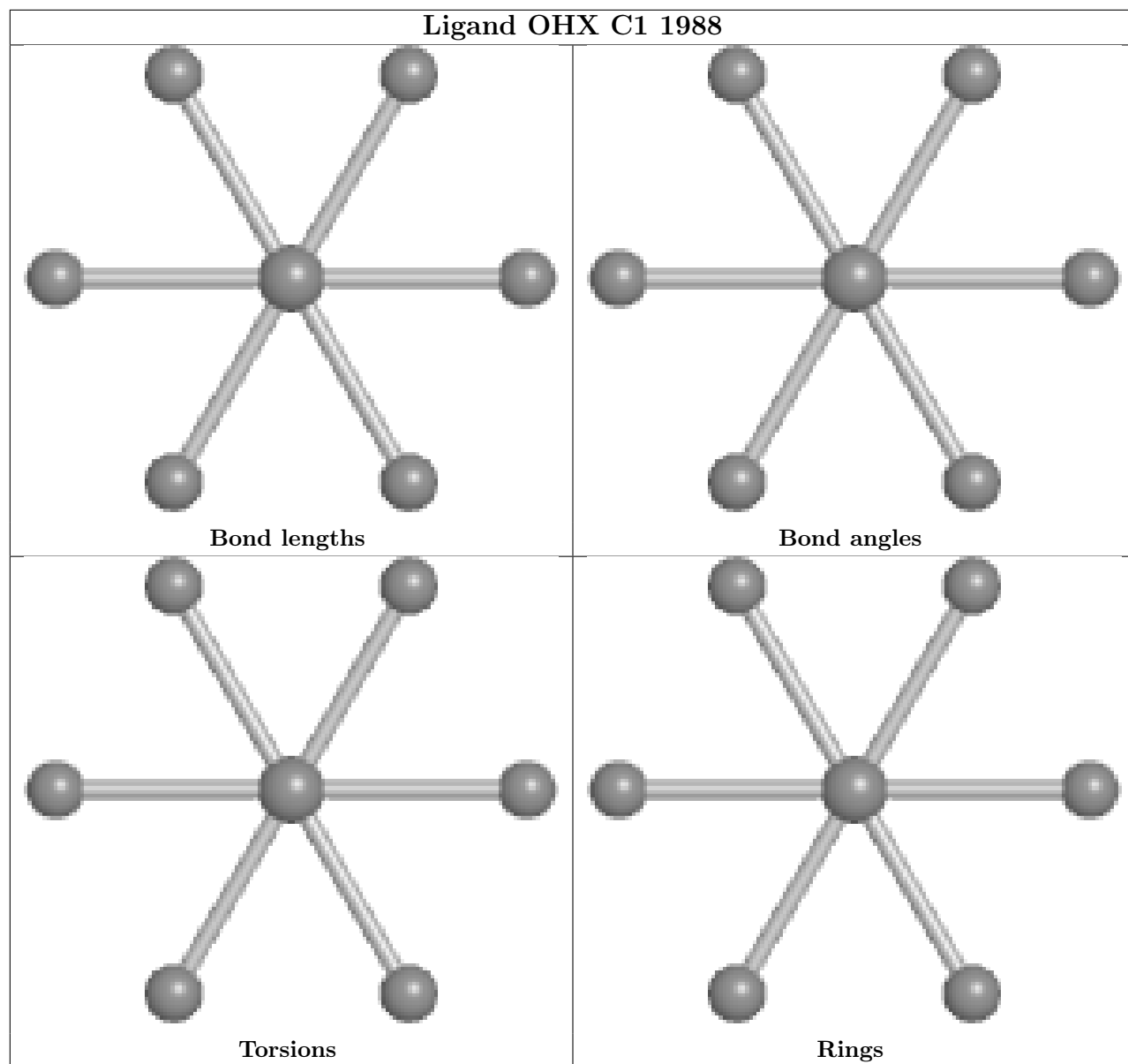


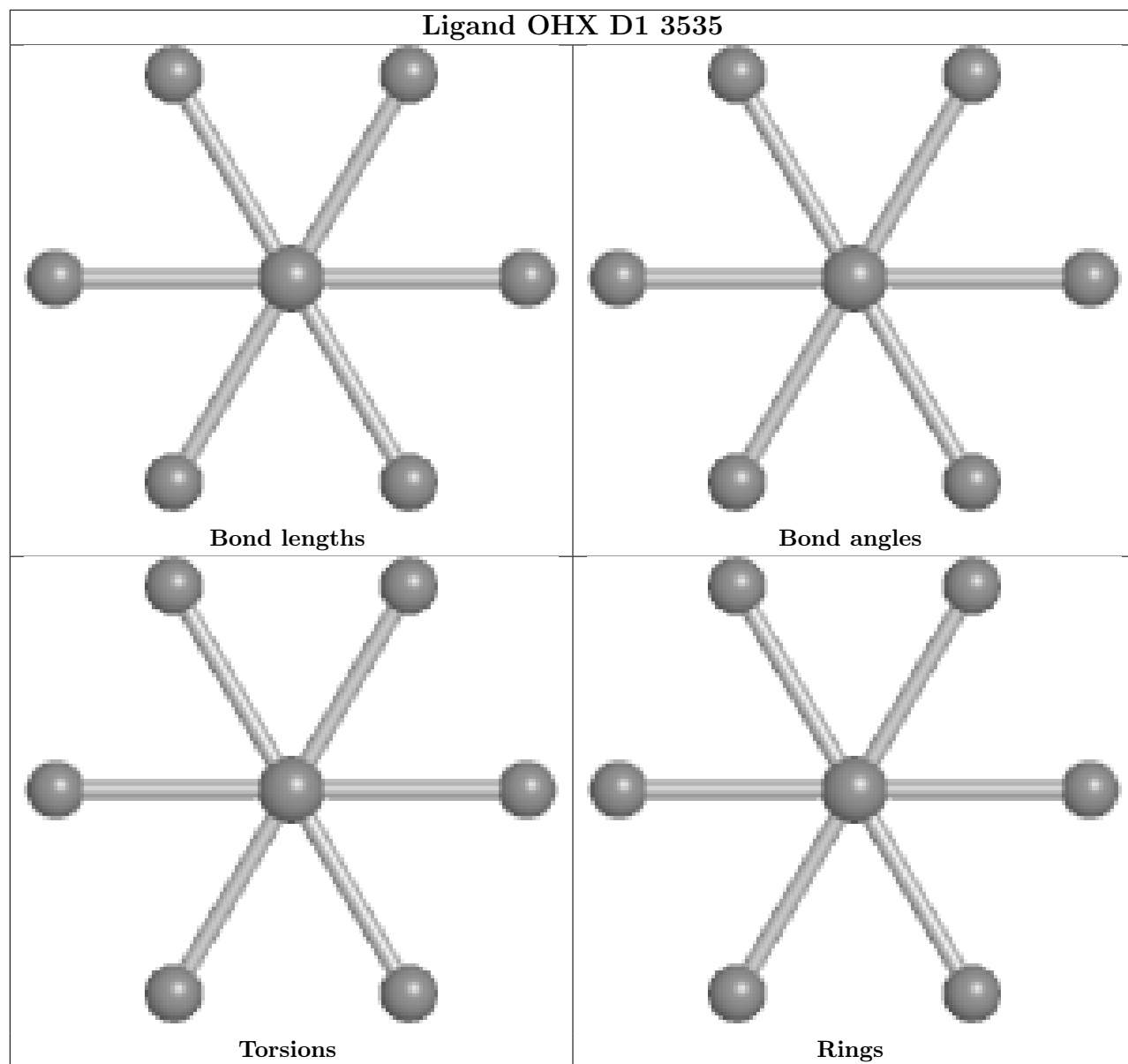


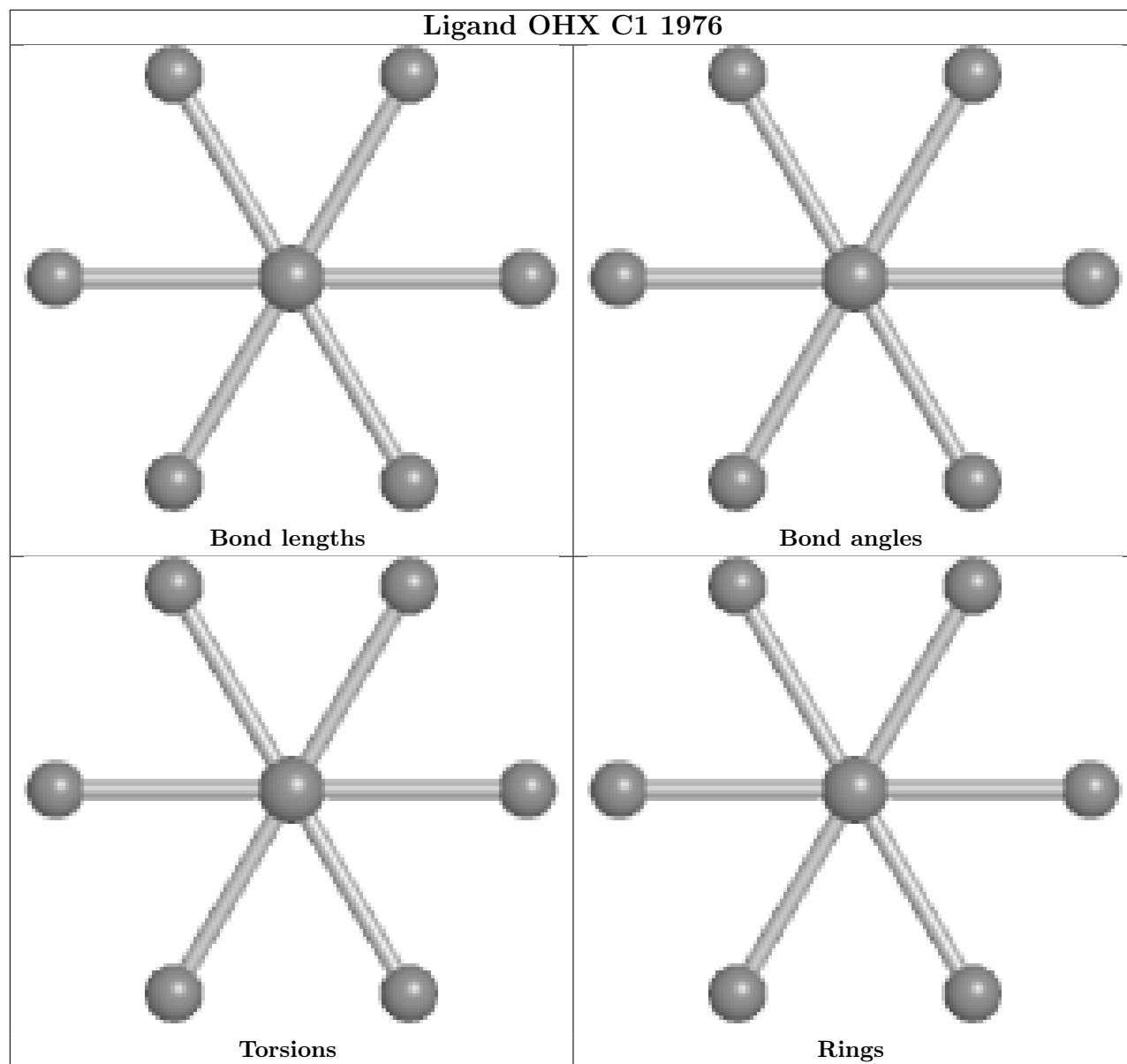


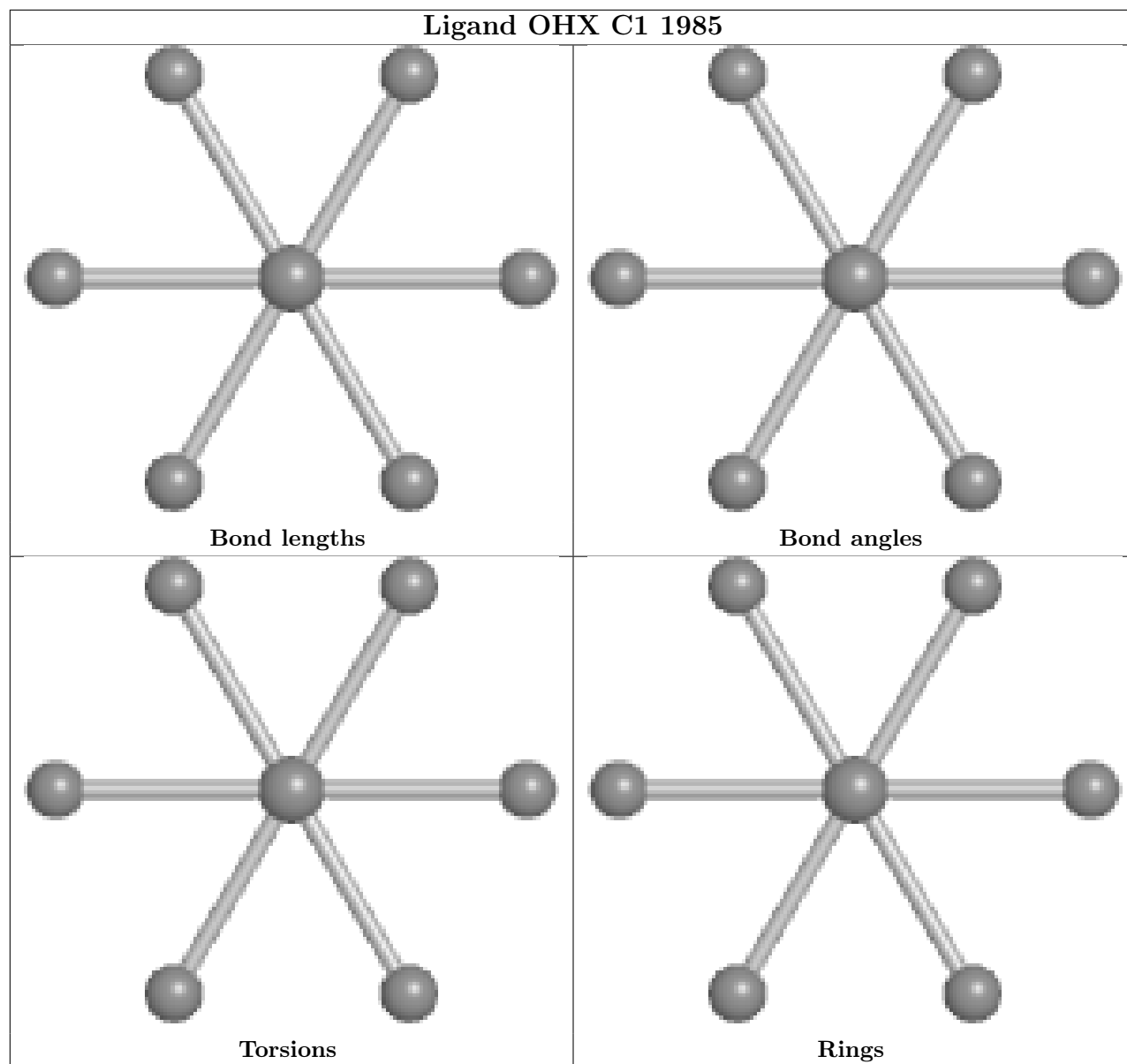


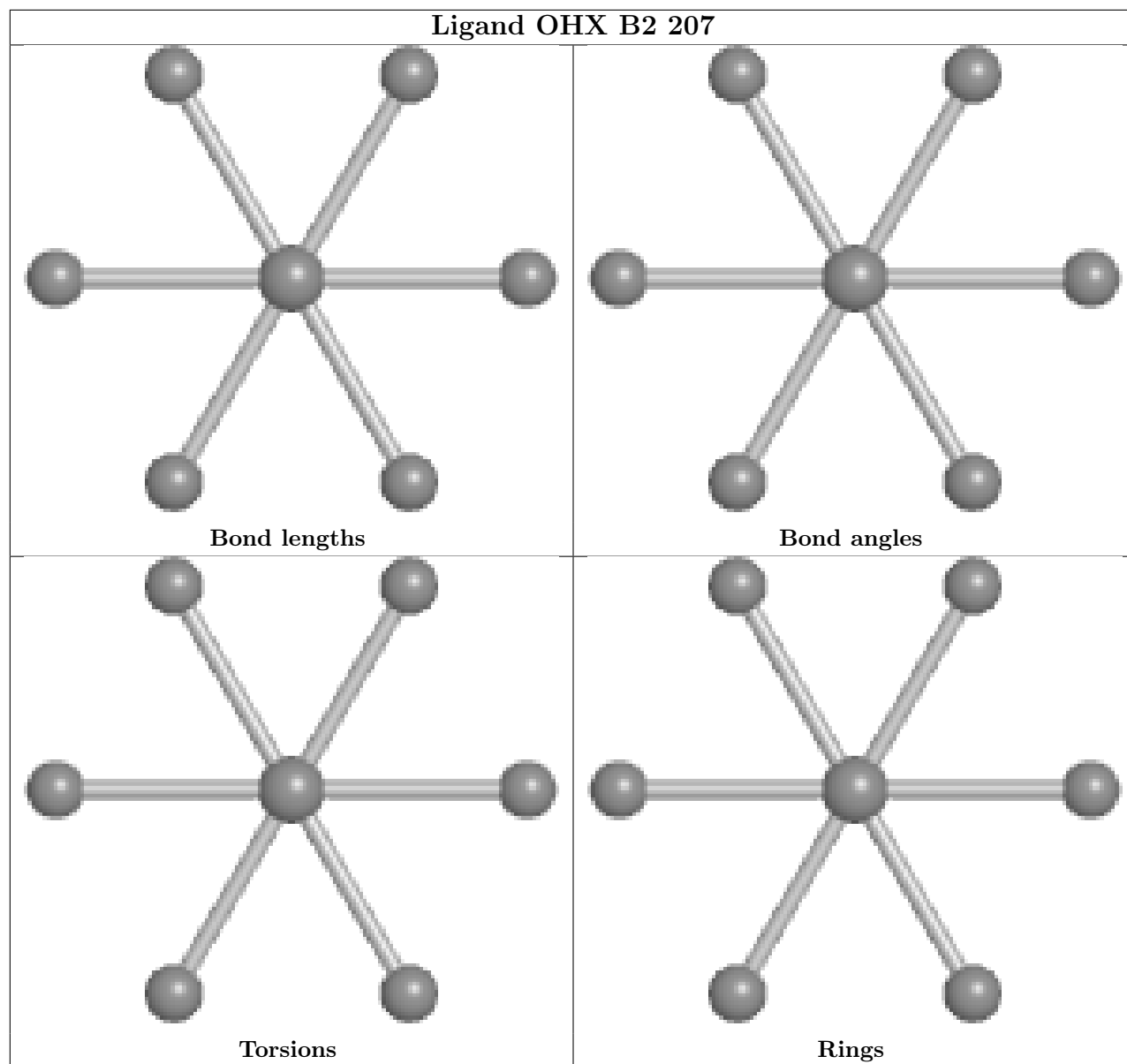


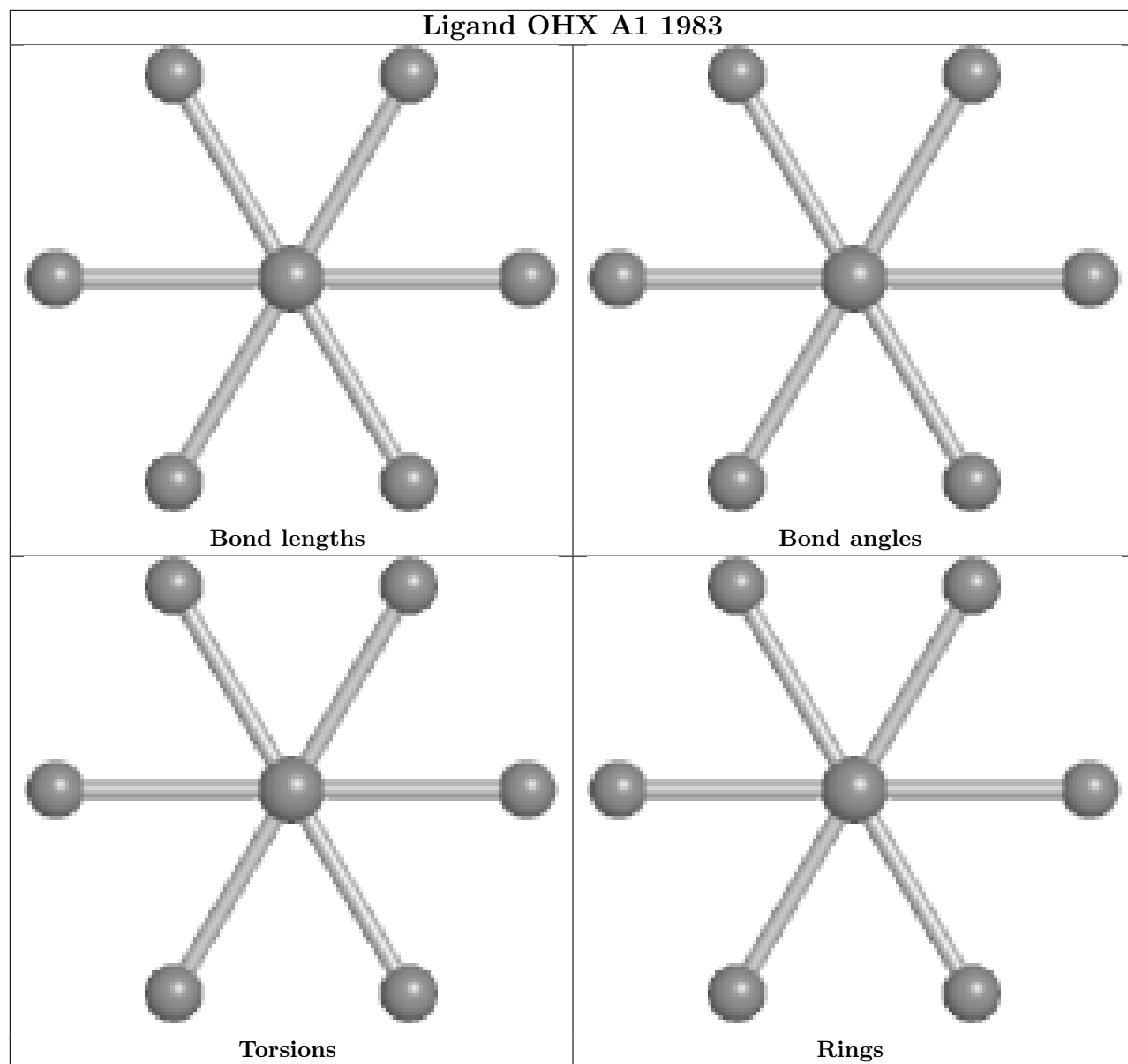


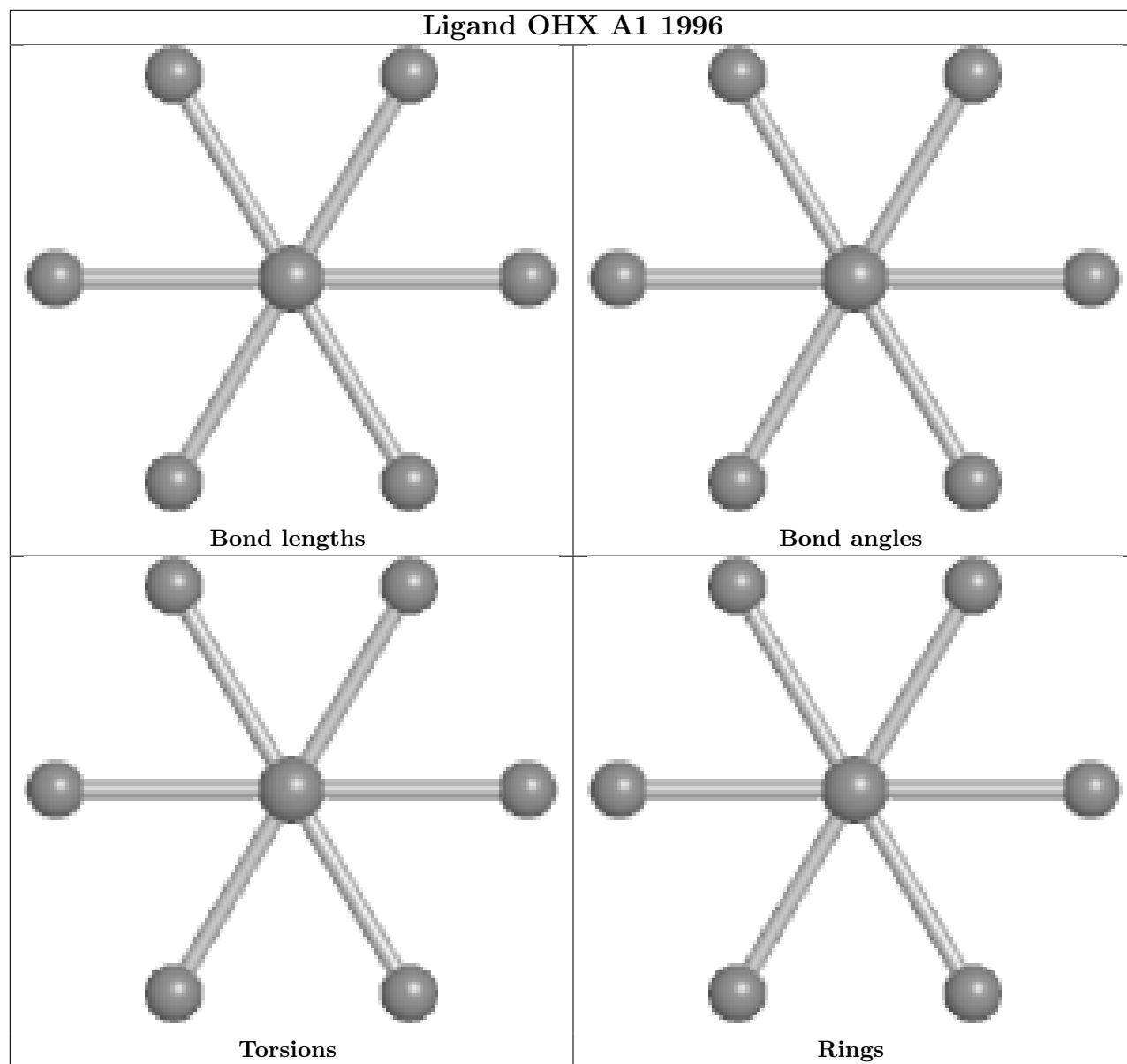


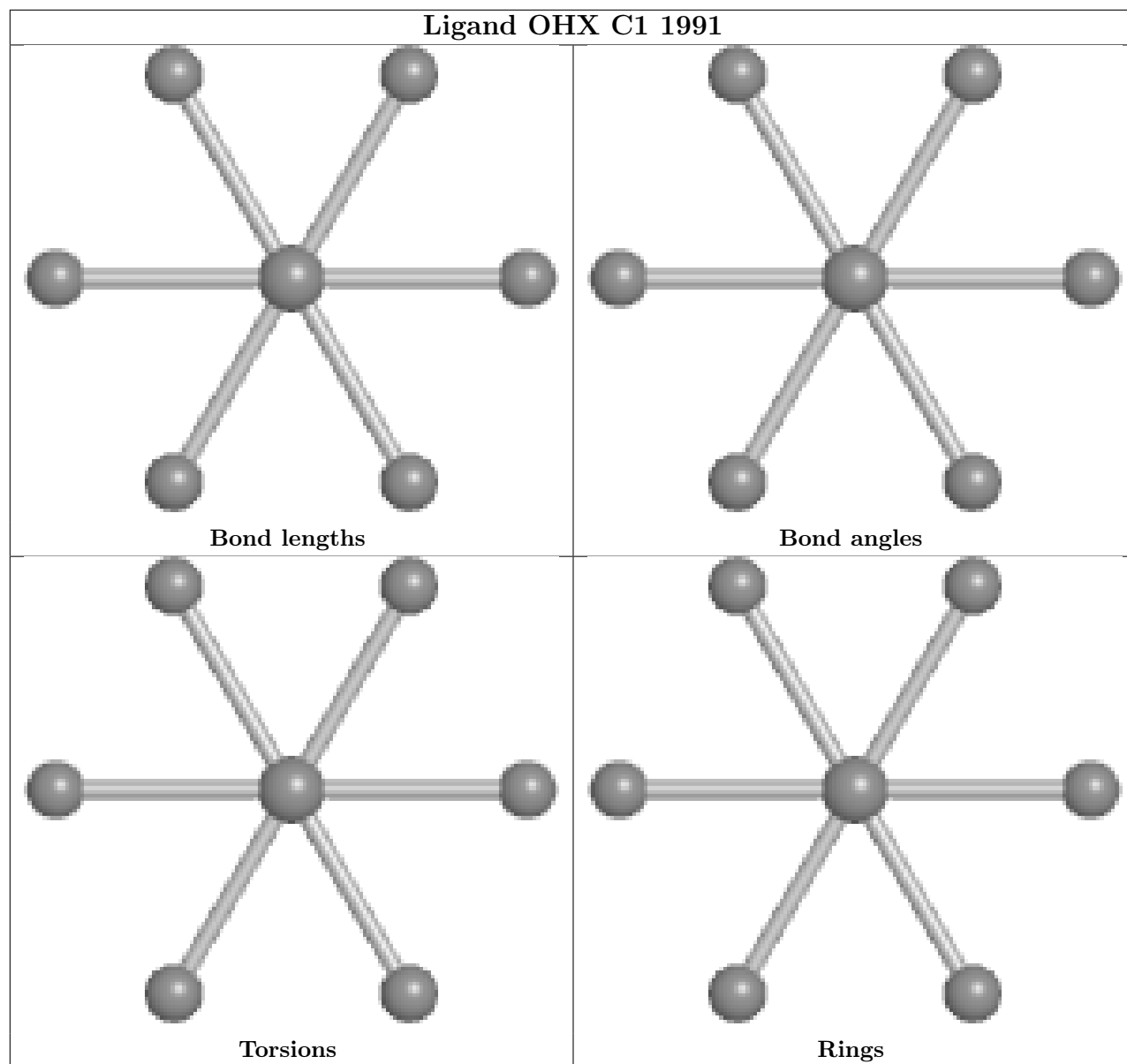


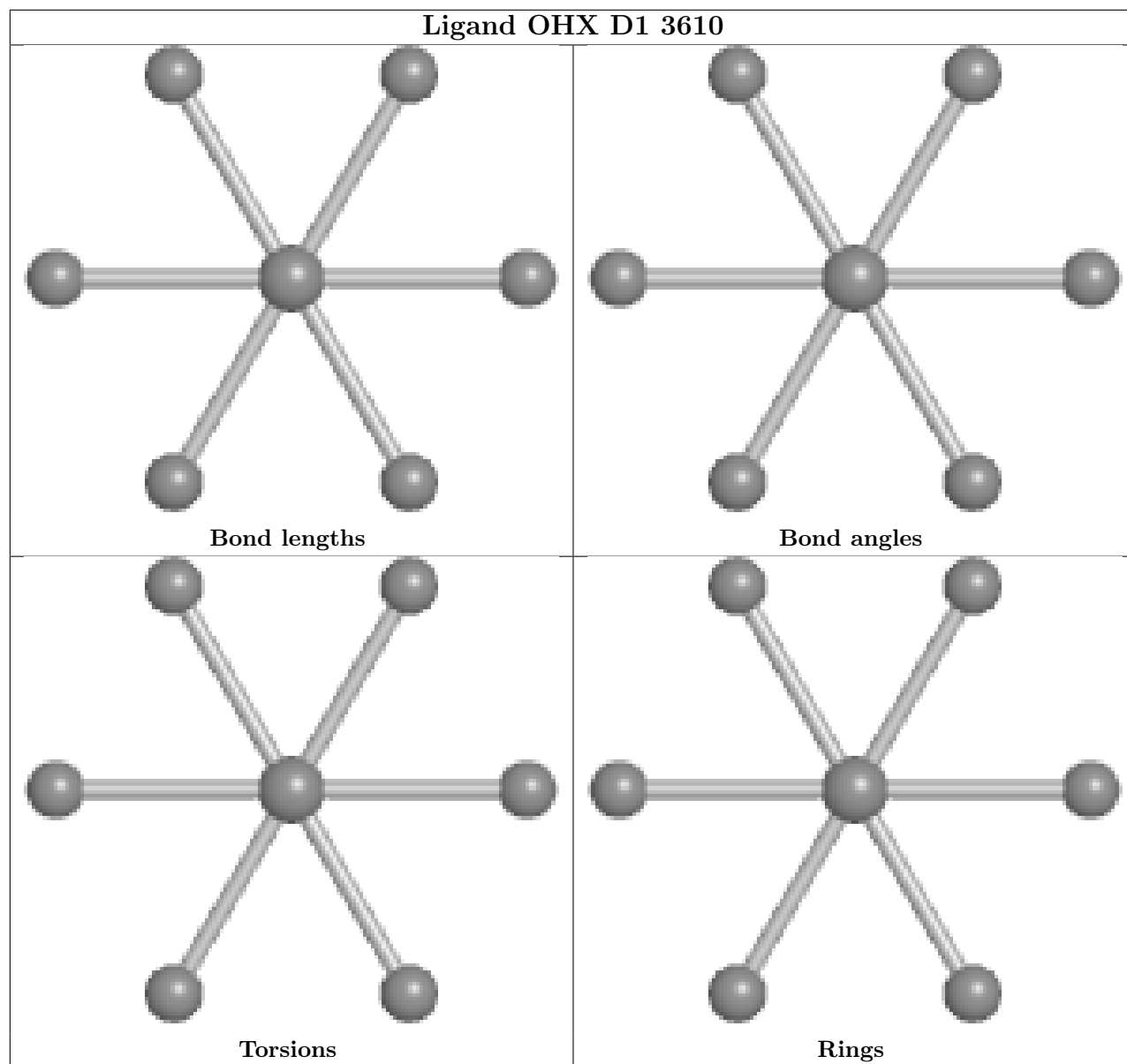


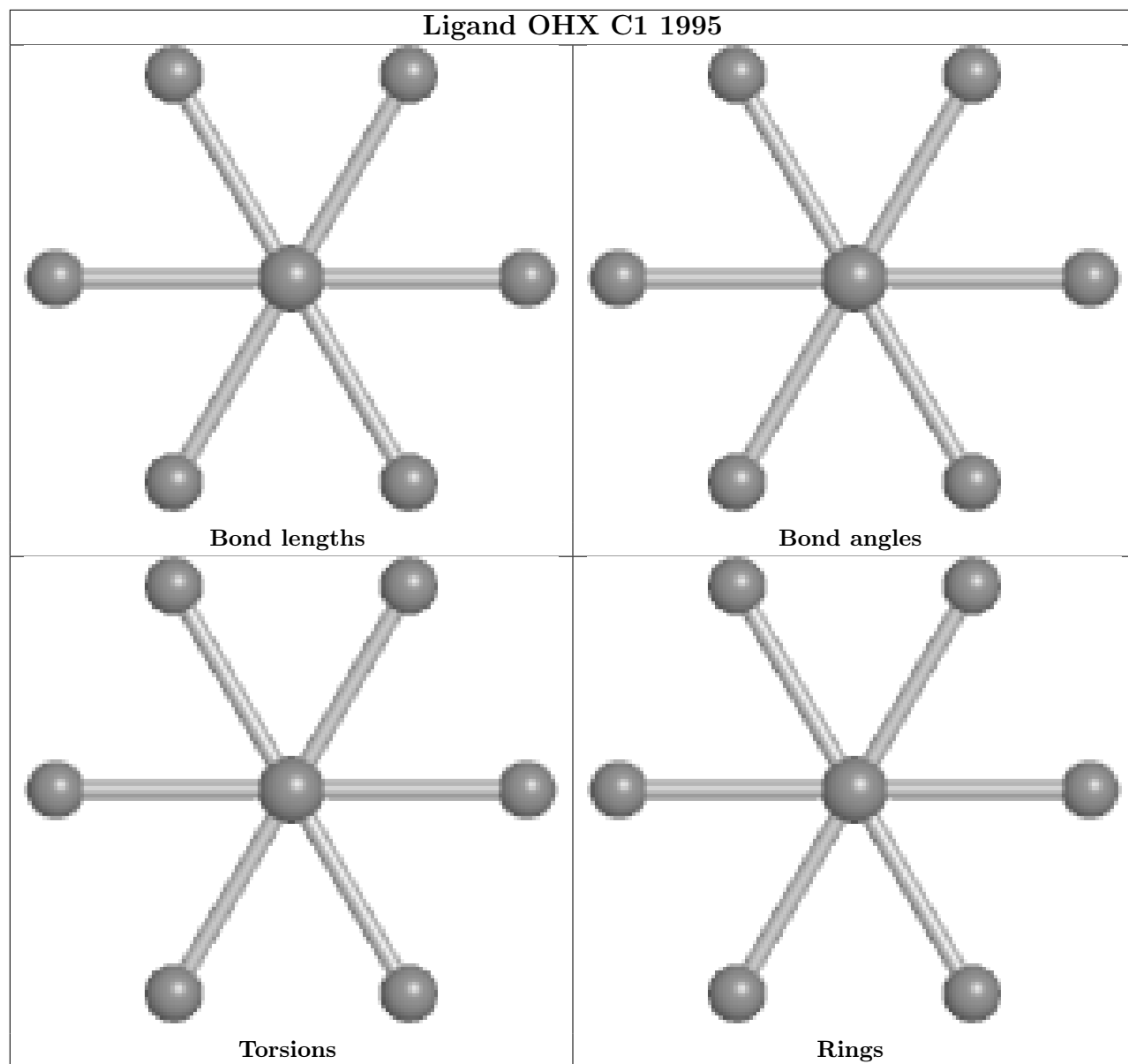


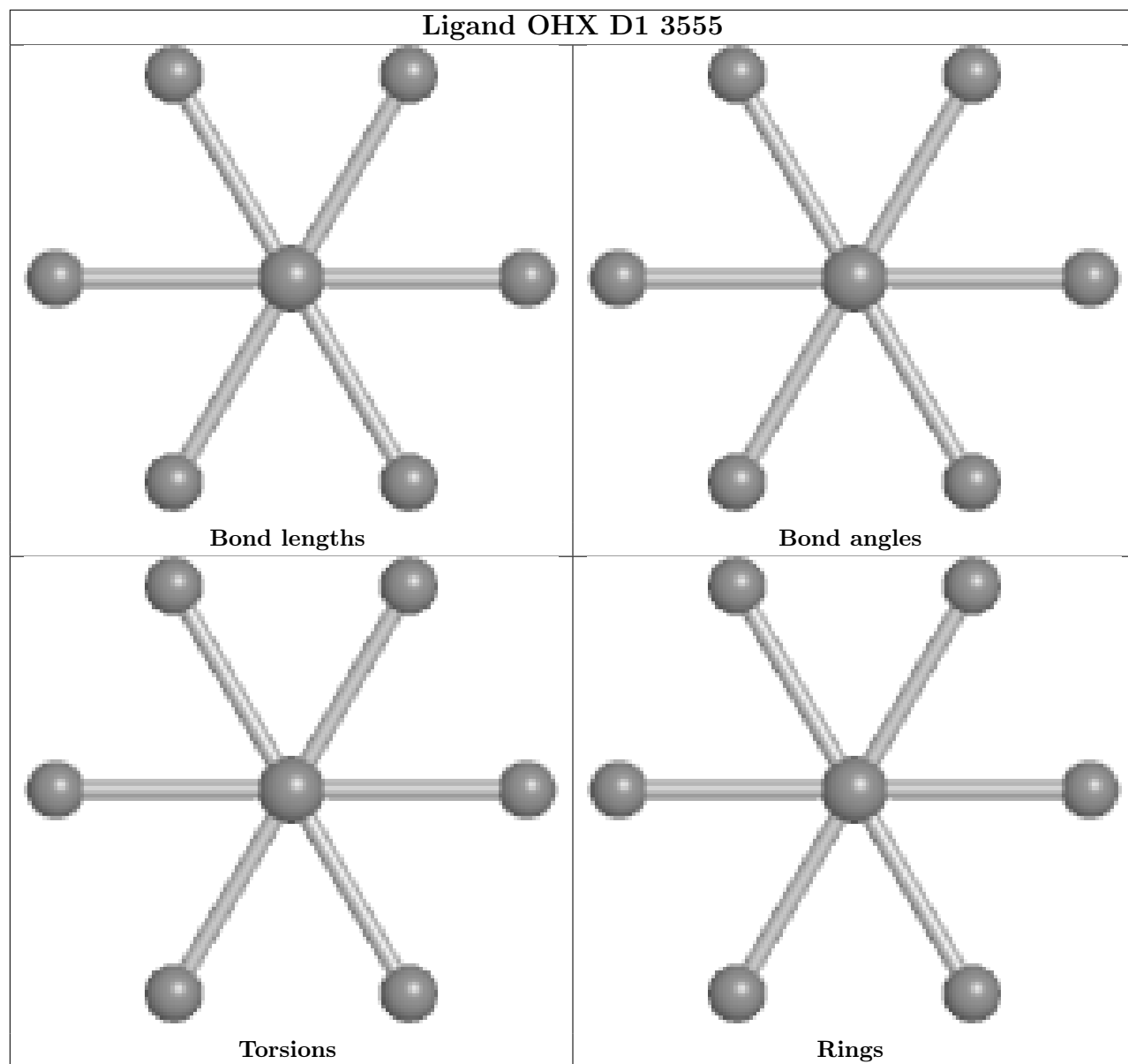


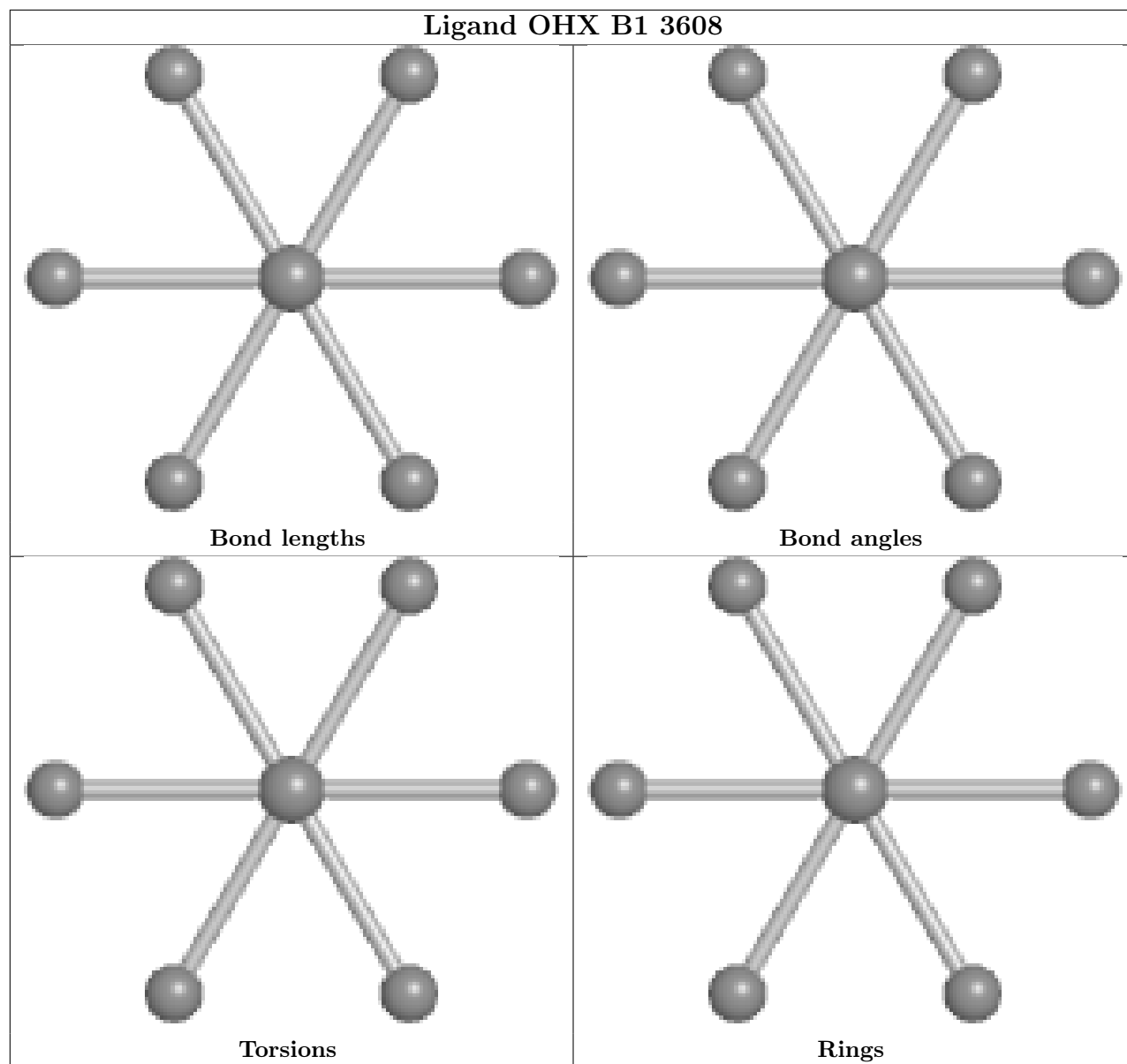


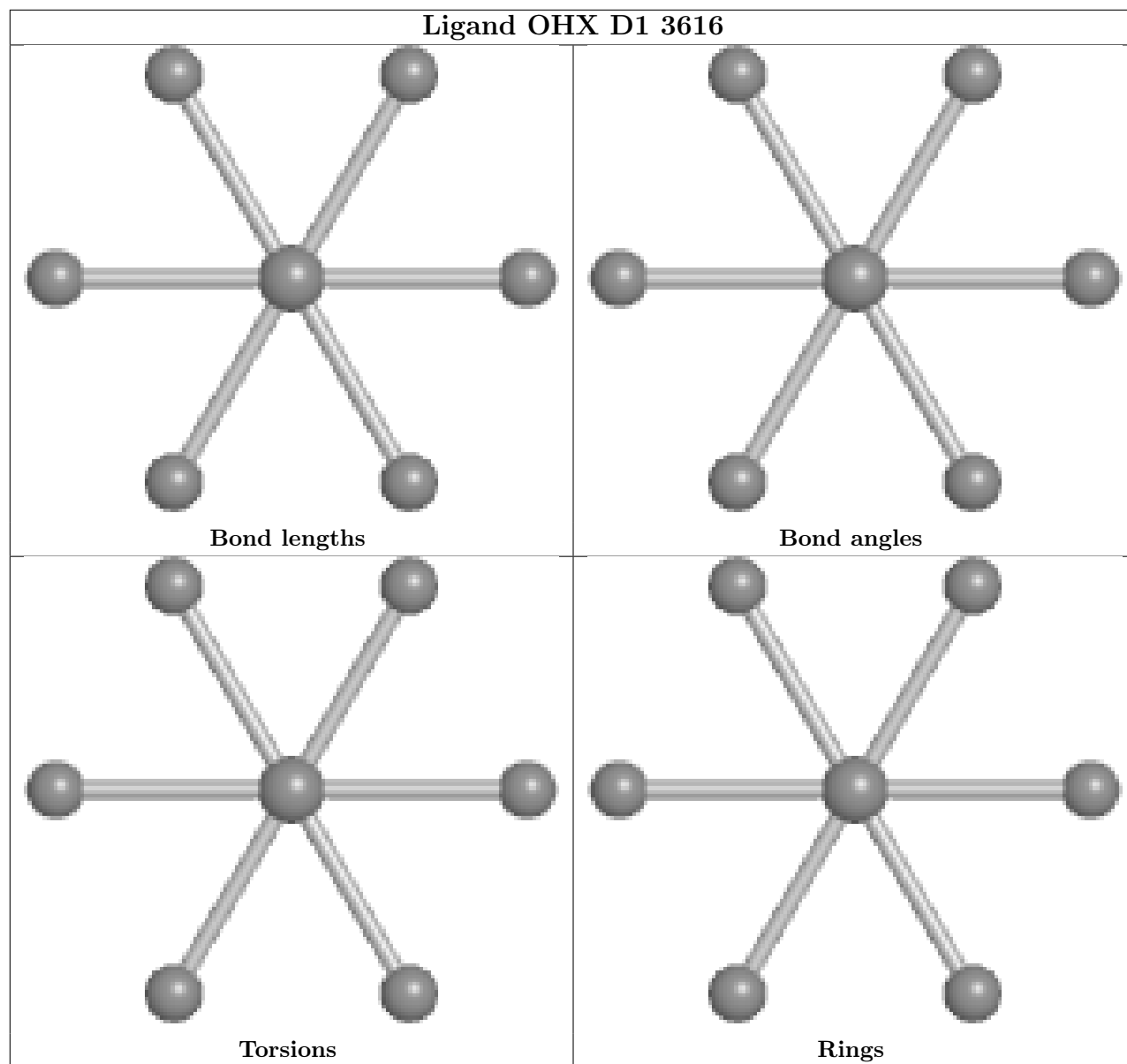


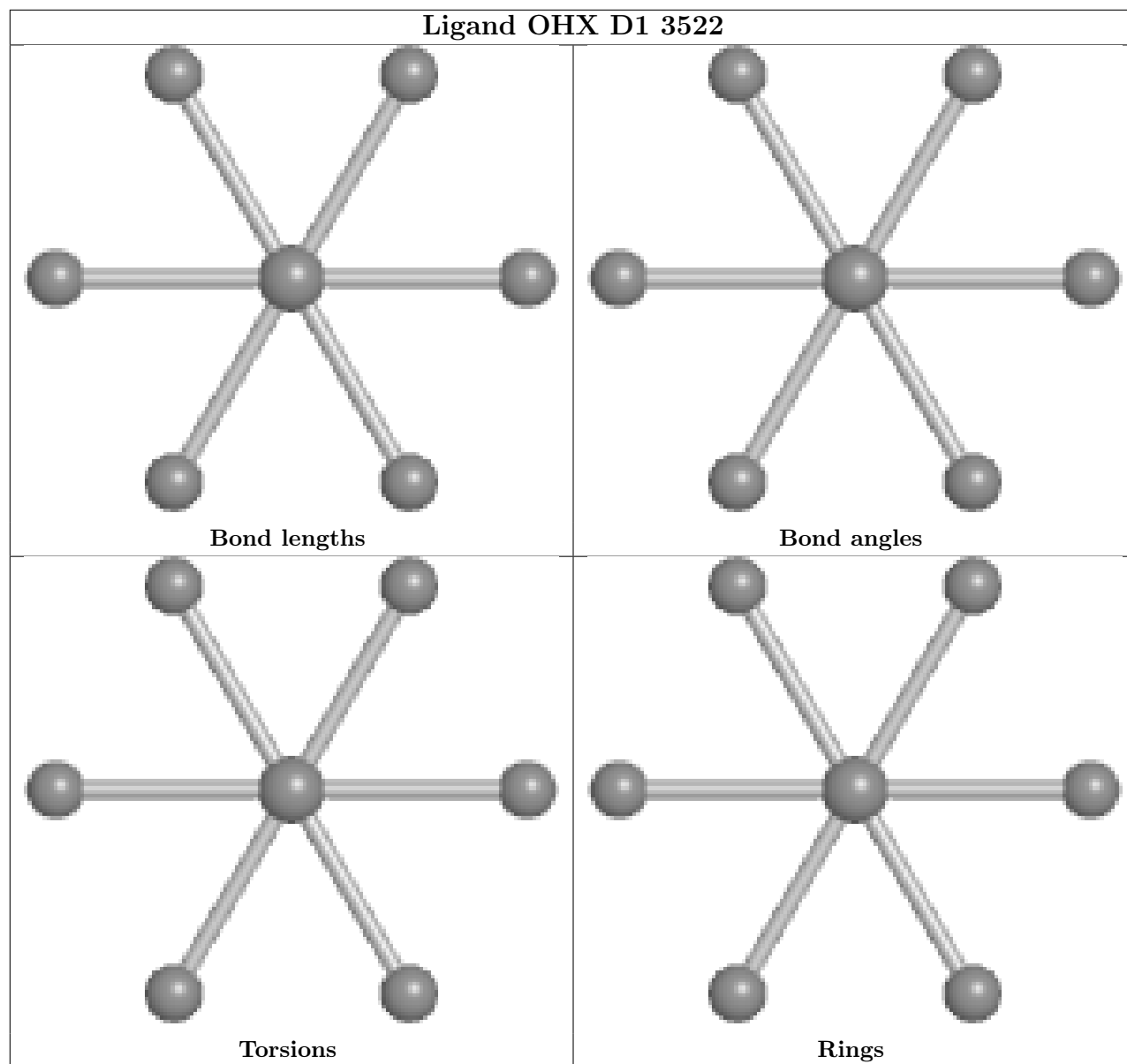


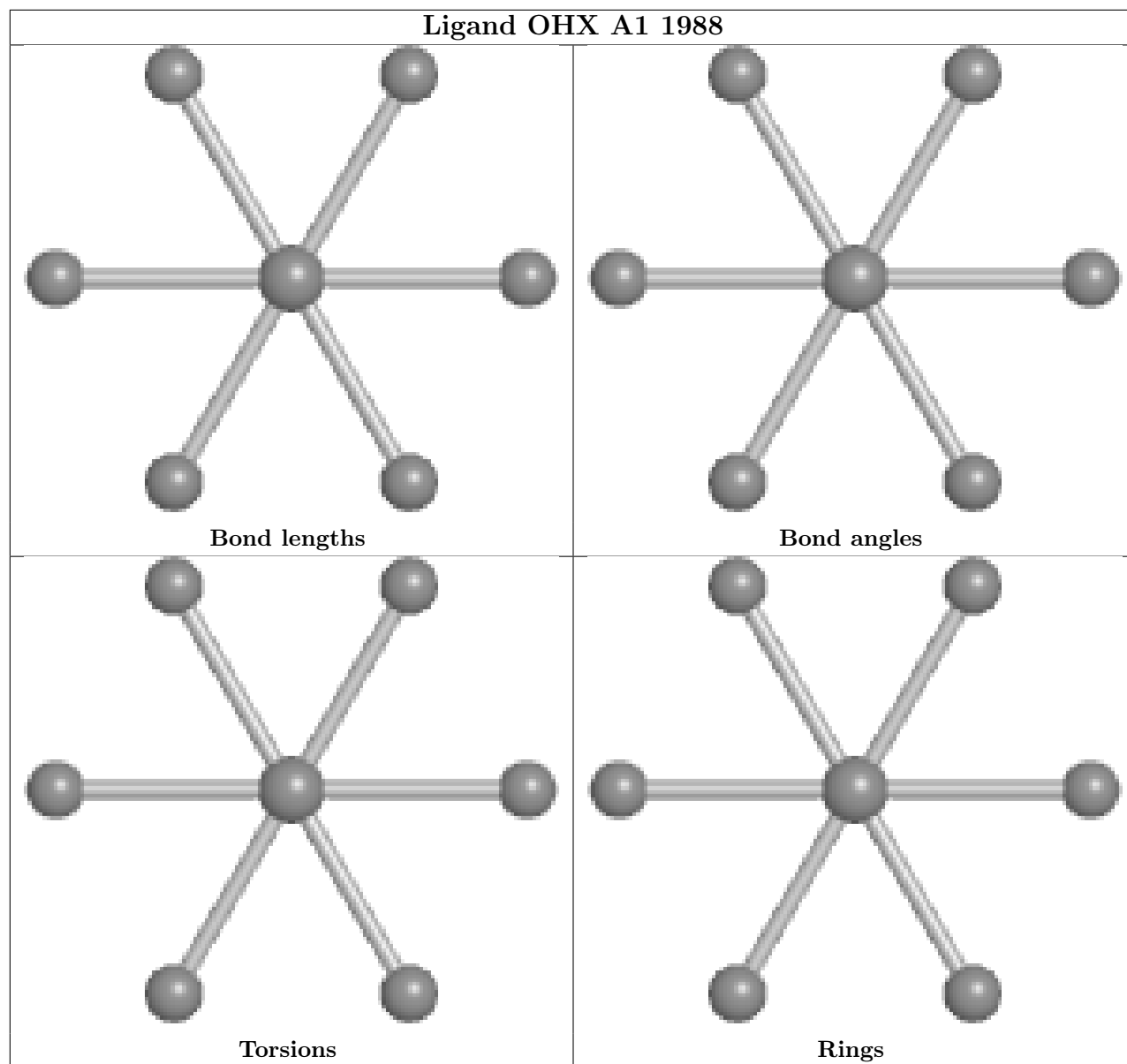


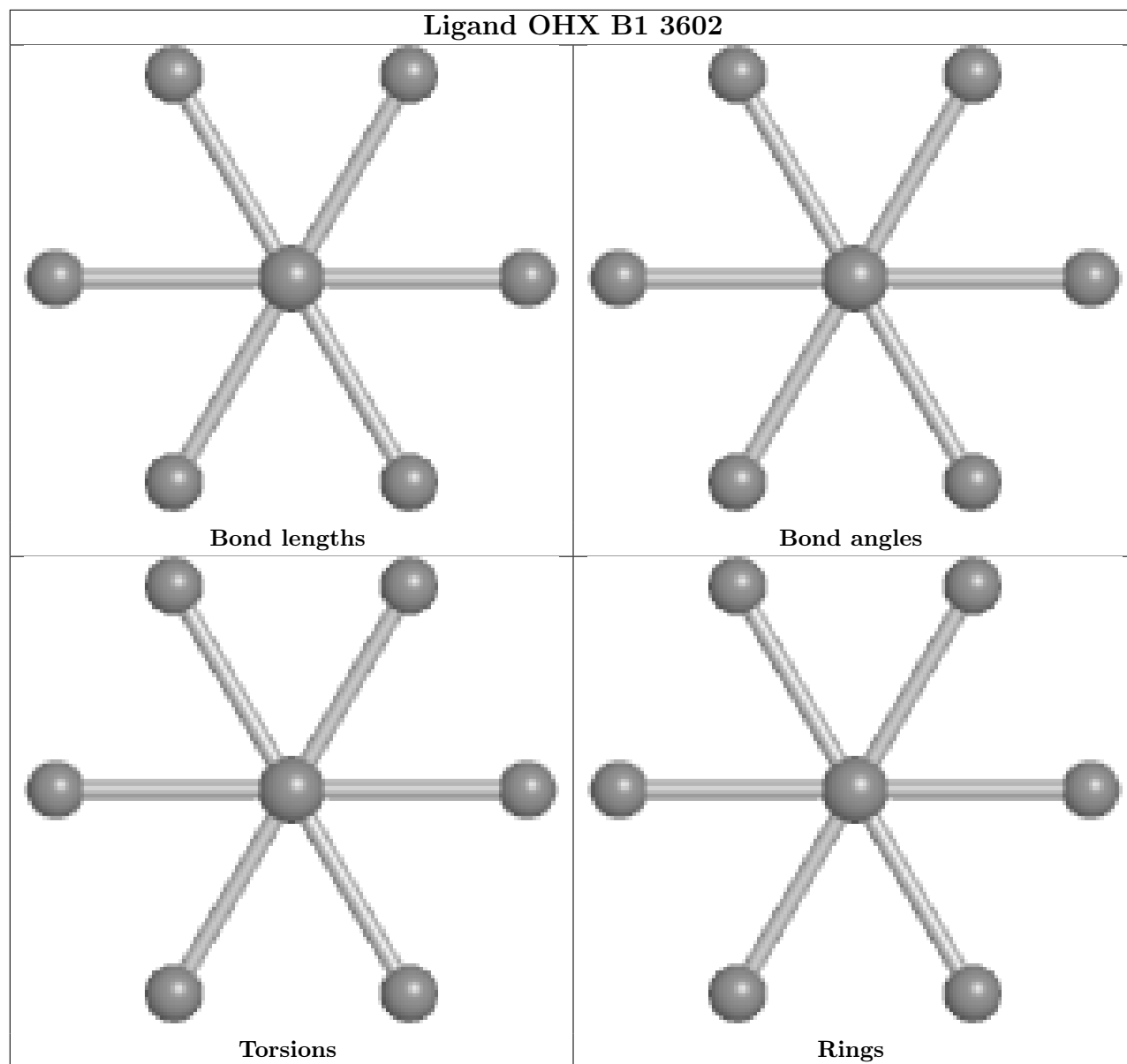


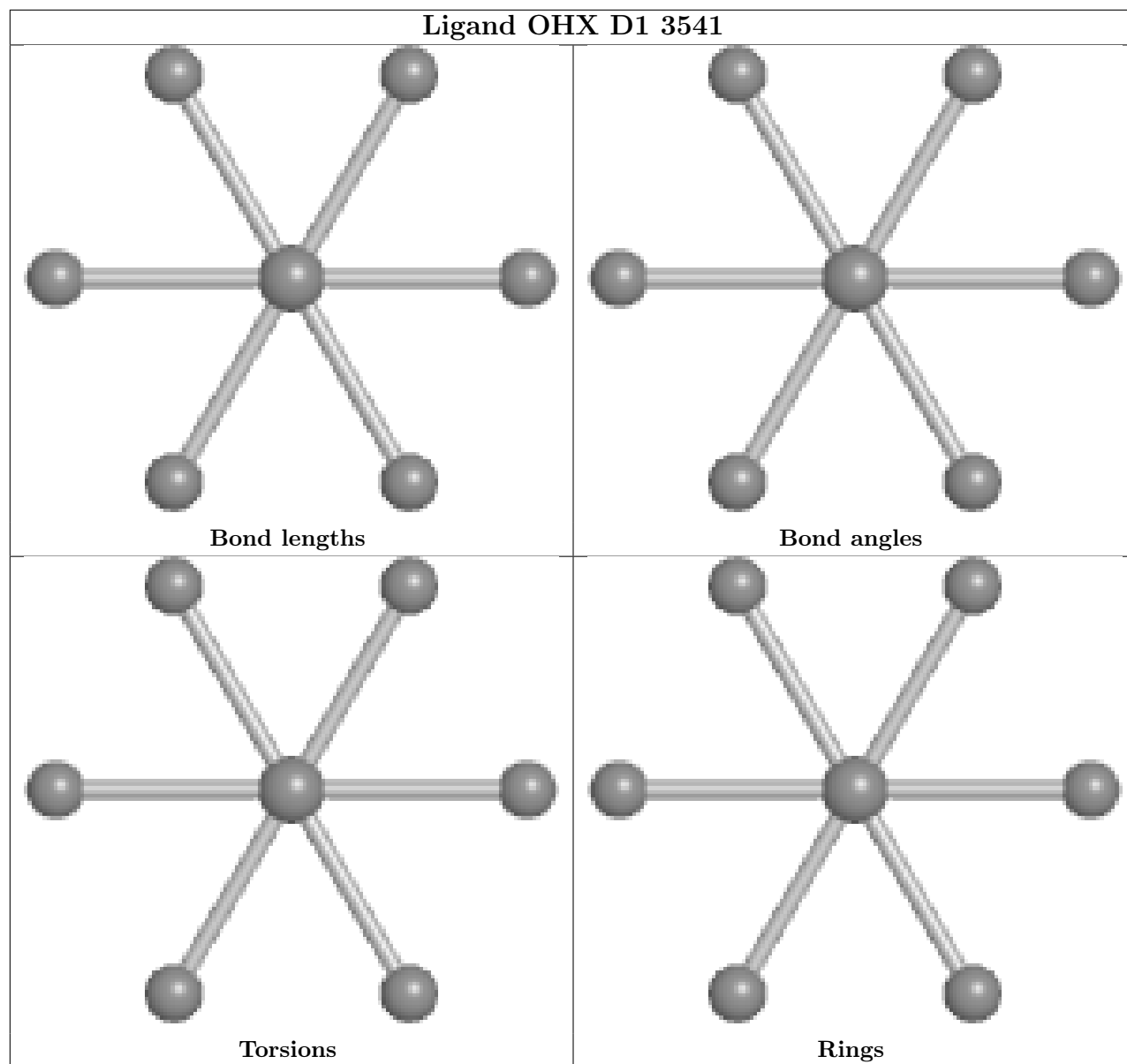


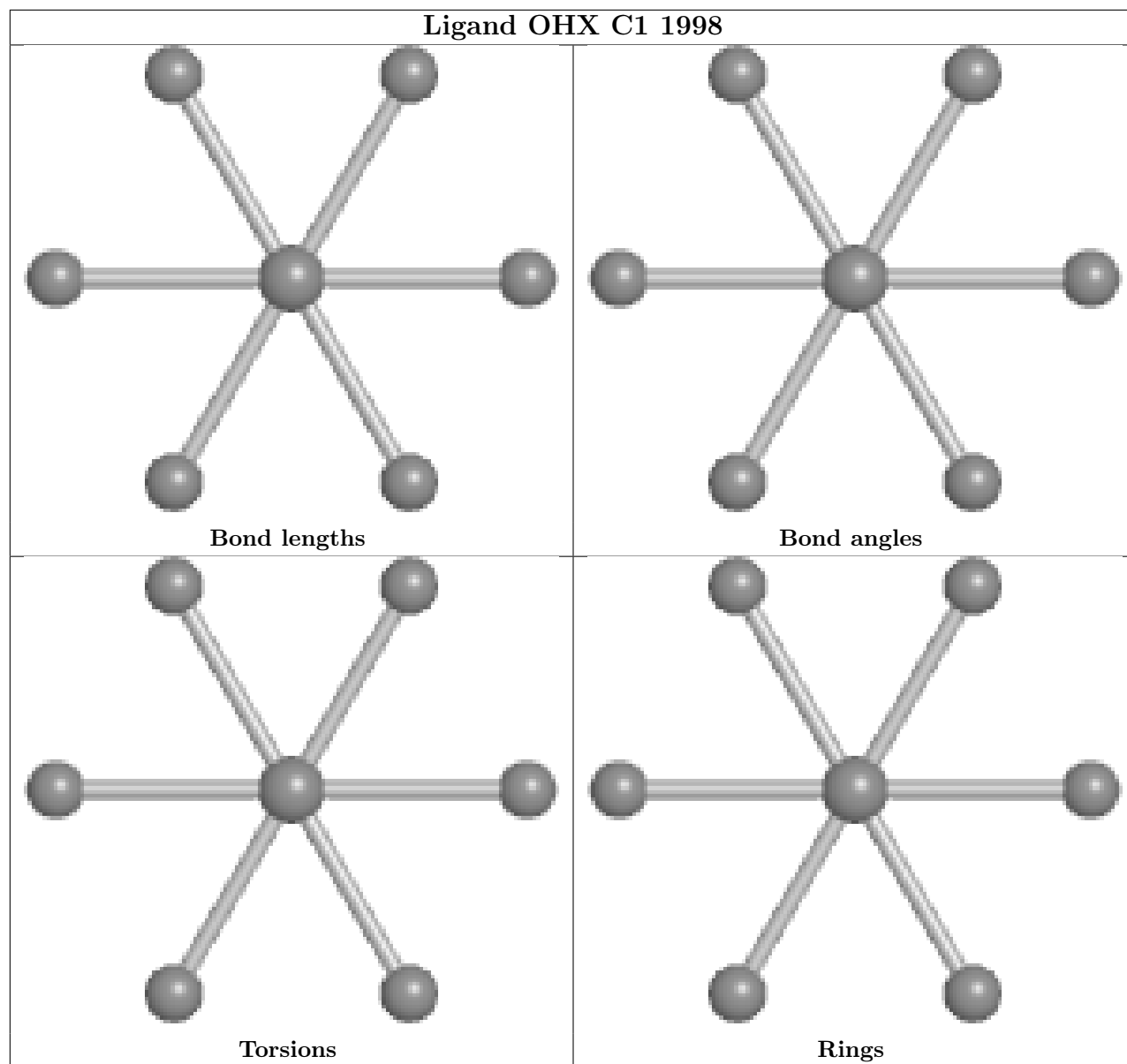


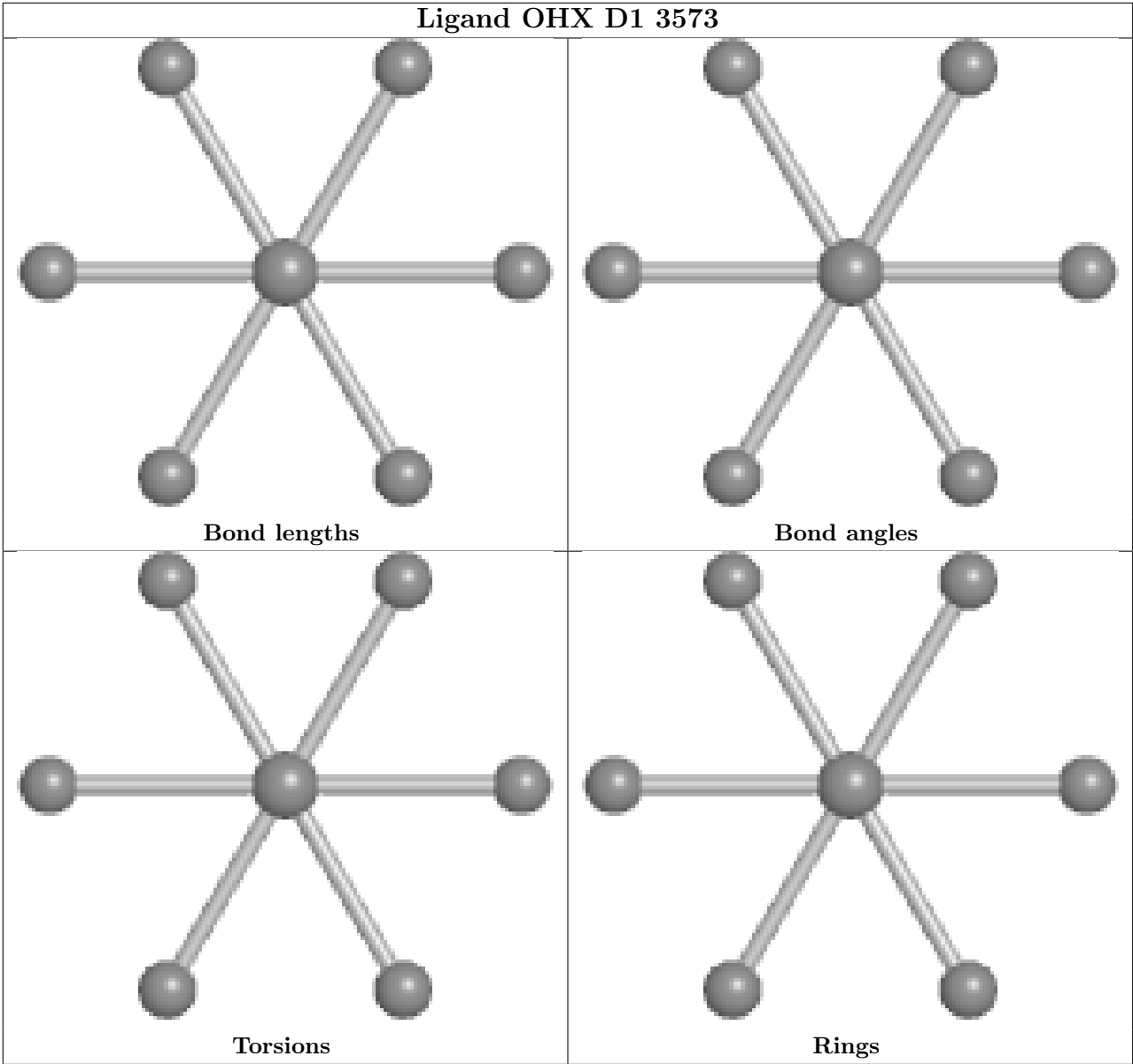












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	Ab	4
23	Cb	4
63	Bh	1

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Mol	Chain	Number of breaks
63	Dh	1
28	Ch	1
68	Bn	1
28	Ah	1
24	Cc	1
24	Ac	1

The worst 5 of 15 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bh	23:UNK	C	34:UNK	N	29.25
1	Dh	23:UNK	C	34:UNK	N	28.80
1	Ch	25:UNK	C	50:UNK	N	22.77
1	Ab	19:UNK	C	21:UNK	N	20.41
1	Bn	19:UNK	C	27:UNK	N	20.28

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	A1	1789/1800 (99%)	0.64	135 (7%) 20 20	45, 138, 429, 753	0
1	C1	1789/1800 (99%)	0.68	135 (7%) 20 20	42, 120, 419, 674	0
2	AA	220/252 (87%)	1.20	51 (23%) 2 4	64, 150, 323, 474	0
2	CA	220/252 (87%)	1.04	42 (19%) 3 6	66, 119, 336, 538	0
3	AB	219/254 (86%)	0.90	35 (15%) 5 8	42, 117, 298, 500	0
3	CB	219/254 (86%)	0.93	41 (18%) 3 6	50, 108, 288, 386	0
4	AC	189/240 (78%)	0.96	35 (18%) 3 6	52, 120, 278, 403	0
4	CC	189/240 (78%)	0.74	26 (13%) 6 10	41, 120, 262, 460	0
5	AD	169/225 (75%)	0.95	33 (19%) 3 6	58, 150, 355, 516	0
5	CD	169/225 (75%)	1.27	46 (27%) 1 3	33, 108, 269, 383	0
6	AE	157/197 (79%)	1.11	30 (19%) 3 6	44, 140, 362, 438	0
6	CE	157/197 (79%)	0.95	30 (19%) 3 6	31, 99, 330, 482	0
7	AF	77/156 (49%)	1.17	19 (24%) 2 4	45, 95, 205, 412	0
7	CF	77/156 (49%)	1.96	30 (38%) 1 2	56, 91, 267, 342	0
8	AG	117/151 (77%)	0.68	23 (19%) 3 5	35, 108, 284, 362	0
8	CG	117/151 (77%)	1.01	25 (21%) 2 5	46, 97, 263, 458	0
9	AH	128/137 (93%)	1.35	38 (29%) 1 3	53, 186, 349, 436	0
9	CH	128/137 (93%)	1.18	36 (28%) 1 3	39, 132, 354, 482	0
10	AI	121/142 (85%)	1.07	30 (24%) 2 4	55, 140, 329, 419	0
10	CI	121/142 (85%)	1.61	43 (35%) 1 2	46, 116, 273, 447	0
11	AJ	134/143 (93%)	1.08	32 (23%) 2 4	74, 144, 302, 340	0
11	CJ	134/143 (93%)	1.37	36 (26%) 1 3	44, 99, 288, 381	0
12	AK	67/136 (49%)	0.96	11 (16%) 4 8	52, 142, 319, 407	0
12	CK	67/136 (49%)	1.97	28 (41%) 0 1	64, 199, 350, 401	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AL	120/146 (82%)	1.07	28 (23%)	2	4	55, 146, 298, 514	0
13	CL	120/146 (82%)	0.94	24 (20%)	3	5	52, 96, 293, 519	0
14	AM	106/144 (73%)	0.75	16 (15%)	5	9	71, 138, 348, 425	0
14	CM	106/144 (73%)	0.97	21 (19%)	3	5	42, 81, 260, 338	0
15	AN	111/121 (91%)	1.75	39 (35%)	1	2	68, 129, 336, 412	0
15	CN	111/121 (91%)	1.19	30 (27%)	1	3	32, 111, 286, 424	0
16	AO	127/130 (97%)	0.75	20 (15%)	5	9	53, 95, 256, 411	0
16	CO	127/130 (97%)	0.90	20 (15%)	5	9	54, 91, 229, 441	0
17	AP	116/145 (80%)	1.10	26 (22%)	2	4	29, 95, 247, 384	0
17	CP	116/145 (80%)	1.08	23 (19%)	3	5	29, 71, 190, 418	0
18	AQ	67/108 (62%)	1.13	11 (16%)	4	8	94, 210, 332, 355	0
18	CQ	63/108 (58%)	1.74	25 (39%)	1	1	68, 150, 282, 307	0
19	AR	47/67 (70%)	1.27	11 (23%)	2	4	107, 245, 393, 457	0
19	CR	47/67 (70%)	1.75	14 (29%)	1	3	51, 221, 381, 425	0
20	AS	39/56 (69%)	1.45	11 (28%)	1	3	58, 108, 181, 260	0
20	CS	39/56 (69%)	0.99	4 (10%)	12	14	37, 95, 140, 292	0
21	AT	313/319 (98%)	1.33	76 (24%)	2	4	106, 195, 286, 348	0
21	CT	313/319 (98%)	1.53	90 (28%)	1	3	67, 158, 257, 328	0
22	Aa	0/20	-	-			-	-
22	Bo	0/20	-	-			-	-
22	Ca	0/20	-	-			-	-
23	Ab	0/105	-	-			-	-
23	Cb	0/105	-	-			-	-
24	Ac	0/93	-	-			-	-
24	Cc	0/93	-	-			-	-
25	Ad	0/35	-	-			-	-
25	Cd	0/35	-	-			-	-
26	Ae	0/21	-	-			-	-
26	Bj	0/21	-	-			-	-
26	Dj	0/21	-	-			-	-
27	Af	0/11	-	-			-	-
28	Ah	0/41	-	-			-	-
28	Ch	0/41	-	-			-	-
29	B1	3206/3396 (94%)	0.48	178 (5%)	30	26	33, 86, 395, 634	0
29	D1	3206/3396 (94%)	0.53	224 (6%)	22	21	30, 94, 427, 674	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	B2	121/121 (100%)	0.56	8 (6%) 24 22	46, 118, 189, 323	0
30	D2	121/121 (100%)	0.61	11 (9%) 15 17	36, 95, 180, 349	0
31	B3	158/158 (100%)	0.46	10 (6%) 26 23	46, 108, 258, 619	0
31	D3	158/158 (100%)	0.71	16 (10%) 12 14	59, 136, 358, 586	0
32	BA	213/217 (98%)	1.14	40 (18%) 3 6	137, 327, 441, 483	0
32	DA	213/217 (98%)	1.14	43 (20%) 3 5	159, 354, 442, 484	0
33	BB	234/254 (92%)	1.45	70 (29%) 1 3	25, 83, 246, 419	0
33	DB	234/254 (92%)	1.52	80 (34%) 1 2	54, 108, 254, 417	0
34	BC	364/387 (94%)	1.03	77 (21%) 2 5	20, 66, 216, 560	0
34	DC	364/387 (94%)	0.95	67 (18%) 3 6	29, 58, 208, 543	0
35	BD	268/362 (74%)	0.90	45 (16%) 4 7	34, 70, 207, 500	0
35	DD	268/362 (74%)	1.30	64 (23%) 2 4	50, 102, 274, 463	0
36	BE	287/297 (96%)	1.39	82 (28%) 1 3	58, 119, 355, 497	0
36	DE	287/297 (96%)	1.09	64 (22%) 2 4	38, 91, 302, 478	0
37	BF	176/176 (100%)	1.02	38 (21%) 2 4	25, 81, 305, 519	0
37	DF	176/176 (100%)	1.29	46 (26%) 1 4	31, 69, 342, 518	0
38	BG	215/244 (88%)	0.39	20 (9%) 14 16	21, 59, 226, 486	0
38	DG	215/244 (88%)	0.45	15 (6%) 22 21	25, 49, 167, 330	0
39	BH	173/256 (67%)	1.07	41 (23%) 2 4	45, 110, 297, 429	0
39	DH	173/256 (67%)	1.30	45 (26%) 1 4	70, 146, 316, 422	0
40	BI	191/191 (100%)	1.08	38 (19%) 3 5	27, 83, 237, 347	0
40	DI	191/191 (100%)	0.18	11 (5%) 29 25	22, 49, 164, 286	0
41	BJ	208/221 (94%)	1.34	56 (26%) 1 3	39, 93, 251, 452	0
41	DJ	208/221 (94%)	0.96	41 (19%) 3 5	25, 64, 257, 456	0
42	BK	165/174 (94%)	1.50	45 (27%) 1 3	56, 125, 348, 497	0
42	DK	165/174 (94%)	1.32	41 (24%) 2 4	45, 97, 330, 532	0
43	BN	120/138 (86%)	1.07	29 (24%) 2 4	34, 77, 260, 387	0
43	DN	120/138 (86%)	0.96	21 (17%) 4 7	33, 60, 262, 325	0
44	BO	187/204 (91%)	1.26	48 (25%) 1 4	38, 86, 178, 383	0
44	DO	187/204 (91%)	1.72	72 (38%) 1 2	57, 119, 255, 327	0
45	BP	196/199 (98%)	0.37	18 (9%) 14 17	23, 48, 152, 409	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DP	196/199 (98%)	0.51	14 (7%) 22 21	23, 45, 111, 424	0
46	BQ	154/184 (83%)	0.81	23 (14%) 5 9	30, 55, 144, 337	0
46	DQ	154/184 (83%)	0.90	32 (20%) 2 5	37, 77, 243, 373	0
47	BR	143/186 (76%)	0.75	20 (13%) 6 10	38, 70, 200, 421	0
47	DR	143/186 (76%)	1.36	37 (25%) 1 4	60, 87, 244, 378	0
48	BS	188/189 (99%)	1.02	42 (22%) 2 4	52, 101, 419, 569	0
48	DS	188/189 (99%)	1.49	59 (31%) 1 3	59, 109, 589, 657	0
49	BT	119/160 (74%)	1.12	27 (22%) 2 4	42, 73, 221, 310	0
49	DT	119/160 (74%)	1.12	24 (20%) 3 5	36, 72, 184, 282	0
50	BU	129/137 (94%)	1.02	23 (17%) 4 6	27, 70, 208, 391	0
50	DU	129/137 (94%)	0.60	13 (10%) 12 14	20, 48, 151, 235	0
51	BV	59/155 (38%)	1.08	14 (23%) 2 4	29, 84, 259, 363	0
51	DV	59/155 (38%)	0.85	6 (10%) 12 14	53, 73, 197, 320	0
52	BW	94/142 (66%)	1.33	25 (26%) 1 4	53, 91, 211, 312	0
52	DW	94/142 (66%)	1.36	24 (25%) 1 4	64, 124, 247, 337	0
53	BX	107/127 (84%)	0.69	16 (14%) 5 9	58, 91, 182, 233	0
53	DX	107/127 (84%)	1.19	21 (19%) 3 5	56, 106, 248, 361	0
54	BY	149/149 (100%)	1.57	45 (30%) 1 3	30, 76, 331, 456	0
54	DY	149/149 (100%)	1.56	47 (31%) 1 3	49, 95, 277, 409	0
55	BZ	98/105 (93%)	0.96	16 (16%) 4 8	52, 128, 269, 360	0
55	DZ	98/105 (93%)	0.93	18 (18%) 3 6	56, 134, 272, 365	0
56	Ba	86/113 (76%)	0.95	19 (22%) 2 4	38, 83, 232, 396	0
56	Da	86/113 (76%)	1.19	25 (29%) 1 3	51, 82, 274, 430	0
57	Bb	125/130 (96%)	0.82	22 (17%) 4 7	26, 54, 138, 435	0
57	Db	125/130 (96%)	1.12	27 (21%) 2 4	39, 77, 168, 380	0
58	Bc	68/120 (56%)	0.70	10 (14%) 6 9	46, 89, 202, 381	0
58	Dc	68/120 (56%)	0.66	8 (11%) 9 12	50, 123, 270, 348	0
59	Bd	72/88 (81%)	1.53	22 (30%) 1 3	36, 79, 322, 434	0
59	Dd	72/88 (81%)	1.51	24 (33%) 1 2	30, 103, 268, 336	0
60	Be	48/51 (94%)	0.93	10 (20%) 2 5	30, 72, 159, 290	0
60	De	48/51 (94%)	1.44	13 (27%) 1 3	40, 118, 222, 333	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	Bf	95/106 (89%)	1.63	28 (29%) 1 3	57, 145, 363, 475	0
61	Df	95/106 (89%)	2.15	40 (42%) 0 1	62, 195, 389, 486	0
62	Bg	83/92 (90%)	1.13	19 (22%) 2 4	35, 98, 311, 431	0
62	Dg	83/92 (90%)	1.06	19 (22%) 2 4	42, 103, 241, 369	0
63	Bh	0/44	-	-	-	-
63	Dh	0/44	-	-	-	-
64	Bi	0/12	-	-	-	-
64	Di	0/12	-	-	-	-
65	Bk	0/16	-	-	-	-
65	Dk	0/16	-	-	-	-
66	Bl	0/19	-	-	-	-
67	Bm	0/9	-	-	-	-
68	Bn	0/27	-	-	-	-
69	Bp	0/8	-	-	-	-
70	Bq	0/17	-	-	-	-
71	Br	0/23	-	-	-	-
72	DL	138/165 (83%)	1.00	27 (19%) 3 5	84, 172, 387, 465	0
73	DM	130/312 (41%)	1.02	22 (16%) 4 7	47, 121, 305, 409	0
All	All	25728/30002 (85%)	0.88	4064 (15%) 5 9	20, 105, 353, 753	0

The worst 5 of 4064 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	B1	136	G	15.9
14	CM	31	PRO	11.8
42	BK	154	THR	11.4
21	CT	212	ALA	11.2
42	DK	152	HIS	10.8

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

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

6.3 Carbohydrates ⓘ

There are no 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
74	OHX	C1	1998	7/7	0.26	0.63	129,129,129,129	7
74	OHX	A1	1983	7/7	0.30	0.69	122,122,122,122	7
74	OHX	B1	3554	7/7	0.44	0.50	156,156,156,156	7
74	OHX	B1	3548	7/7	0.46	0.47	153,153,153,153	7
74	OHX	D1	3586	7/7	0.46	0.64	115,115,115,115	7
74	OHX	C1	1989	7/7	0.48	0.53	114,114,114,114	7
74	OHX	B1	3613	7/7	0.51	0.55	93,93,93,93	7
74	OHX	B1	3608	7/7	0.56	0.53	75,75,75,75	7
74	OHX	B1	3599	7/7	0.58	0.40	87,87,87,87	7
74	OHX	D1	3535	7/7	0.59	0.58	142,142,142,142	7
74	OHX	B1	3592	7/7	0.60	0.66	106,106,106,106	7
74	OHX	A1	1993	7/7	0.60	0.43	108,108,108,108	7
74	OHX	B1	3577	7/7	0.62	0.57	148,148,148,148	7
74	OHX	D1	3564	7/7	0.62	0.40	85,85,85,85	7
74	OHX	D1	3490	7/7	0.62	0.39	167,167,167,167	7
74	OHX	D1	3616	7/7	0.62	0.43	150,150,150,150	7
74	OHX	D1	3601	7/7	0.63	0.67	99,99,99,99	7
74	OHX	A1	1964	7/7	0.63	0.40	85,85,85,85	7
74	OHX	B1	3552	7/7	0.64	0.39	138,138,138,138	7
74	OHX	D1	3605	7/7	0.64	0.52	93,93,93,93	7
74	OHX	B1	3600	7/7	0.64	0.36	135,135,135,135	7
74	OHX	C1	1974	7/7	0.65	0.45	118,118,118,118	7
74	OHX	A1	1966	7/7	0.65	0.43	120,120,120,120	7
74	OHX	D1	3541	7/7	0.66	0.47	141,141,141,141	7
74	OHX	A1	1925	7/7	0.66	0.38	165,165,165,165	7
74	OHX	C1	1991	7/7	0.66	0.49	77,77,77,77	7
74	OHX	B1	3535	7/7	0.66	0.38	170,170,170,170	7
74	OHX	C1	1956	7/7	0.66	0.37	170,170,170,170	7
74	OHX	B1	3589	7/7	0.66	0.71	85,85,85,85	7
74	OHX	C1	1950	7/7	0.67	0.28	215,215,215,215	7
74	OHX	D1	3609	7/7	0.67	0.36	73,73,73,73	7
74	OHX	A1	1954	7/7	0.67	0.30	153,153,153,153	7
74	OHX	D3	206	7/7	0.67	0.42	77,77,77,77	7
74	OHX	B2	208	7/7	0.68	0.59	152,152,152,152	7
74	OHX	C1	1978	7/7	0.68	0.41	145,145,145,145	7
74	OHX	B2	210	7/7	0.68	0.56	131,131,131,131	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	B1	3574	7/7	0.69	0.34	136,136,136,136	7
74	OHX	C1	1985	7/7	0.70	0.42	153,153,153,153	7
74	OHX	D1	3550	7/7	0.70	0.39	100,100,100,100	7
74	OHX	C1	1988	7/7	0.70	0.42	146,146,146,146	7
74	OHX	B1	3502	7/7	0.70	0.39	166,166,166,166	7
74	OHX	D1	3599	7/7	0.70	0.32	93,93,93,93	7
74	OHX	B2	207	7/7	0.70	0.46	104,104,104,104	7
74	OHX	A1	1953	7/7	0.70	0.49	122,122,122,122	7
74	OHX	C1	1976	7/7	0.70	0.44	118,118,118,118	7
74	OHX	D1	3610	7/7	0.70	0.63	94,94,94,94	7
74	OHX	D1	3519	7/7	0.70	0.45	111,111,111,111	7
74	OHX	A1	1974	7/7	0.70	0.54	136,136,136,136	7
74	OHX	D1	3544	7/7	0.71	0.36	127,127,127,127	7
74	OHX	B1	3544	7/7	0.71	0.35	130,130,130,130	7
74	OHX	D1	3525	7/7	0.71	0.31	106,106,106,106	7
74	OHX	D1	3622	7/7	0.71	0.32	142,142,142,142	7
74	OHX	D1	3568	7/7	0.71	0.55	92,92,92,92	7
74	OHX	C1	1965	7/7	0.72	0.37	101,101,101,101	7
74	OHX	C1	1966	7/7	0.72	0.38	127,127,127,127	7
74	OHX	B1	3534	7/7	0.72	0.32	128,128,128,128	7
74	OHX	D1	3623	7/7	0.72	0.57	23,23,23,23	7
74	OHX	D1	3524	7/7	0.72	0.38	162,162,162,162	7
74	OHX	A1	1995	7/7	0.73	0.40	80,80,80,80	7
74	OHX	B1	3581	7/7	0.73	0.35	106,106,106,106	7
74	OHX	D1	3603	7/7	0.73	0.41	114,114,114,114	7
74	OHX	D1	3542	7/7	0.73	0.28	198,198,198,198	7
74	OHX	D1	3507	7/7	0.73	0.39	133,133,133,133	7
74	OHX	A1	1997	7/7	0.74	0.35	100,100,100,100	7
74	OHX	B3	206	7/7	0.74	0.22	201,201,201,201	7
74	OHX	D1	3522	7/7	0.74	0.41	133,133,133,133	7
74	OHX	D1	3555	7/7	0.74	0.46	150,150,150,150	7
74	OHX	A1	1978	7/7	0.74	0.49	139,139,139,139	7
74	OHX	A1	1958	7/7	0.74	0.31	116,116,116,116	7
74	OHX	D1	3578	7/7	0.74	0.46	222,222,222,222	7
74	OHX	B1	3603	7/7	0.74	0.23	63,63,63,63	7
74	OHX	D1	3506	7/7	0.74	0.47	131,131,131,131	7
74	OHX	D3	211	7/7	0.74	0.34	137,137,137,137	7
74	OHX	D1	3593	7/7	0.75	0.48	99,99,99,99	7
74	OHX	B1	3523	7/7	0.75	0.31	150,150,150,150	7
74	OHX	B1	3557	7/7	0.75	0.37	46,46,46,46	7
74	OHX	B1	3545	7/7	0.75	0.42	82,82,82,82	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	D1	3587	7/7	0.76	0.62	111,111,111,111	7
74	OHX	B1	3533	7/7	0.76	0.45	149,149,149,149	7
74	OHX	BO	301	7/7	0.76	0.47	110,110,110,110	7
74	OHX	D1	3505	7/7	0.76	0.35	160,160,160,160	7
74	OHX	A1	1996	7/7	0.76	0.45	100,100,100,100	7
74	OHX	B1	3515	7/7	0.76	0.43	119,119,119,119	7
74	OHX	C1	1957	7/7	0.76	0.41	226,226,226,226	7
74	OHX	D1	3559	7/7	0.76	0.29	116,116,116,116	7
74	OHX	A1	1998	7/7	0.76	0.58	125,125,125,125	7
74	OHX	D1	3566	7/7	0.76	0.32	88,88,88,88	7
74	OHX	B1	3584	7/7	0.76	0.44	99,99,99,99	7
74	OHX	C1	1996	7/7	0.76	0.45	86,86,86,86	7
74	OHX	D1	3529	7/7	0.76	0.35	130,130,130,130	7
74	OHX	DJ	301	7/7	0.76	0.26	138,138,138,138	7
74	OHX	A1	1988	7/7	0.77	0.47	25,25,25,25	7
74	OHX	A1	1970	7/7	0.77	0.29	66,66,66,66	7
74	OHX	B1	3546	7/7	0.77	0.32	148,148,148,148	7
74	OHX	B1	3602	7/7	0.77	0.40	75,75,75,75	7
74	OHX	A1	1963	7/7	0.77	0.38	137,137,137,137	7
74	OHX	D1	3595	7/7	0.77	0.41	90,90,90,90	7
74	OHX	D2	208	7/7	0.77	0.39	105,105,105,105	7
74	OHX	D3	205	7/7	0.77	0.23	199,199,199,199	7
74	OHX	D1	3475	7/7	0.77	0.37	142,142,142,142	7
74	OHX	B1	3539	7/7	0.77	0.32	137,137,137,137	7
74	OHX	B1	3542	7/7	0.77	0.47	64,64,64,64	7
74	OHX	D1	3611	7/7	0.78	0.30	82,82,82,82	7
74	OHX	D1	3556	7/7	0.78	0.37	146,146,146,146	7
74	OHX	D1	3618	7/7	0.78	0.26	62,62,62,62	7
74	OHX	C1	1980	7/7	0.78	0.47	162,162,162,162	7
74	OHX	B1	3609	7/7	0.78	0.49	80,80,80,80	7
74	OHX	B1	3510	7/7	0.78	0.36	153,153,153,153	7
74	OHX	B2	203	7/7	0.78	0.40	174,174,174,174	7
74	OHX	D1	3545	7/7	0.78	0.47	77,77,77,77	7
74	OHX	A1	2002	7/7	0.78	0.39	185,185,185,185	7
74	OHX	C1	1995	7/7	0.78	0.43	51,51,51,51	7
74	OHX	B1	3568	7/7	0.79	0.26	94,94,94,94	7
74	OHX	B1	3555	7/7	0.79	0.41	103,103,103,103	7
74	OHX	B2	209	7/7	0.79	0.34	148,148,148,148	7
74	OHX	B1	3551	7/7	0.79	0.54	84,84,84,84	7
74	OHX	C1	1962	7/7	0.79	0.31	180,180,180,180	7
74	OHX	D1	3509	7/7	0.79	0.44	120,120,120,120	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
74	OHX	B2	205	7/7	0.79	0.30	159,159,159,159	7
74	OHX	D1	3573	7/7	0.79	0.46	135,135,135,135	7
74	OHX	D3	208	7/7	0.79	0.33	135,135,135,135	7
74	OHX	C1	2000	7/7	0.79	0.40	82,82,82,82	7
74	OHX	D1	3585	7/7	0.79	0.28	102,102,102,102	7
74	OHX	A1	1991	7/7	0.80	0.40	98,98,98,98	7
74	OHX	B1	3511	7/7	0.80	0.31	160,160,160,160	7
74	OHX	D1	3516	7/7	0.80	0.43	138,138,138,138	7
74	OHX	B1	3611	7/7	0.80	0.34	68,68,68,68	7
74	OHX	A1	1999	7/7	0.80	0.27	99,99,99,99	7
74	OHX	D2	207	7/7	0.80	0.30	111,111,111,111	7
74	OHX	C1	1975	7/7	0.80	0.35	119,119,119,119	7
74	OHX	B3	209	7/7	0.80	0.34	99,99,99,99	7
74	OHX	B1	3621	7/7	0.80	0.29	83,83,83,83	7
74	OHX	B1	3504	7/7	0.80	0.35	140,140,140,140	7
74	OHX	D3	210	7/7	0.80	0.28	74,74,74,74	7
74	OHX	B1	3528	7/7	0.80	0.35	158,158,158,158	7
74	OHX	B1	3506	7/7	0.80	0.41	53,53,53,53	7
74	OHX	D1	3569	7/7	0.81	0.35	88,88,88,88	7
74	OHX	A1	1930	7/7	0.81	0.38	228,228,228,228	7
74	OHX	B3	210	7/7	0.81	0.38	64,64,64,64	7
74	OHX	B1	3570	7/7	0.81	0.37	91,91,91,91	7
74	OHX	B1	3594	7/7	0.81	0.36	100,100,100,100	7
74	OHX	B1	3532	7/7	0.81	0.31	172,172,172,172	7
74	OHX	D1	3590	7/7	0.81	0.47	55,55,55,55	7
74	OHX	B1	3575	7/7	0.81	0.36	123,123,123,123	7
74	OHX	B1	3601	7/7	0.81	0.69	158,158,158,158	7
74	OHX	B1	3520	7/7	0.81	0.39	109,109,109,109	7
74	OHX	A1	1947	7/7	0.81	0.34	143,143,143,143	7
74	OHX	B1	3582	7/7	0.81	0.40	83,83,83,83	7
74	OHX	B1	3560	7/7	0.81	0.40	105,105,105,105	7
74	OHX	D1	3471	7/7	0.81	0.31	260,260,260,260	7
74	OHX	B1	3617	7/7	0.82	0.32	90,90,90,90	7
74	OHX	C1	1981	7/7	0.82	0.25	87,87,87,87	7
74	OHX	A1	1940	7/7	0.82	0.34	166,166,166,166	7
74	OHX	C1	1987	7/7	0.82	0.24	108,108,108,108	7
74	OHX	B1	3514	7/7	0.82	0.26	123,123,123,123	7
74	OHX	D1	3614	7/7	0.82	0.48	83,83,83,83	7
74	OHX	D1	3574	7/7	0.82	0.37	114,114,114,114	7
74	OHX	A1	1989	7/7	0.82	0.43	70,70,70,70	7
74	OHX	D1	3580	7/7	0.82	0.36	114,114,114,114	7
74	OHX	B1	3610	7/7	0.82	0.32	68,68,68,68	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	D2	204	7/7	0.82	0.30	116,116,116,116	7
74	OHX	B1	3530	7/7	0.82	0.34	138,138,138,138	7
74	OHX	D1	3549	7/7	0.82	0.25	127,127,127,127	7
74	OHX	D1	3513	7/7	0.82	0.35	160,160,160,160	7
74	OHX	D1	3552	7/7	0.82	0.41	115,115,115,115	7
74	OHX	C1	1952	7/7	0.82	0.28	239,239,239,239	7
74	OHX	B1	3565	7/7	0.82	0.30	120,120,120,120	7
74	OHX	D1	3600	7/7	0.82	0.25	96,96,96,96	7
74	OHX	C1	1999	7/7	0.82	0.32	41,41,41,41	7
74	OHX	A1	1977	7/7	0.83	0.34	119,119,119,119	7
74	OHX	CT	401	7/7	0.83	0.27	117,117,117,117	7
74	OHX	D1	3548	7/7	0.83	0.36	77,77,77,77	7
74	OHX	D2	209	7/7	0.83	0.38	74,74,74,74	7
74	OHX	D1	3457	7/7	0.83	0.31	130,130,130,130	7
74	OHX	C1	1959	7/7	0.83	0.32	166,166,166,166	7
74	OHX	A1	1965	7/7	0.83	0.30	114,114,114,114	7
74	OHX	D1	3538	7/7	0.83	0.37	87,87,87,87	7
74	OHX	B1	3616	7/7	0.83	0.41	103,103,103,103	7
74	OHX	D1	3498	7/7	0.83	0.35	103,103,103,103	7
74	OHX	Dd	102	7/7	0.83	0.29	118,118,118,118	7
74	OHX	B1	3580	7/7	0.84	0.34	84,84,84,84	7
74	OHX	B1	3619	7/7	0.84	0.34	85,85,85,85	7
74	OHX	A1	1973	7/7	0.84	0.29	101,101,101,101	7
74	OHX	D1	3558	7/7	0.84	0.34	127,127,127,127	7
74	OHX	C1	1919	7/7	0.84	0.34	159,159,159,159	7
74	OHX	D1	3521	7/7	0.84	0.20	163,163,163,163	7
74	OHX	C1	1940	7/7	0.84	0.31	139,139,139,139	7
74	OHX	B1	3481	7/7	0.84	0.34	133,133,133,133	7
74	OHX	D1	3466	7/7	0.84	0.27	103,103,103,103	7
74	OHX	B1	3490	7/7	0.84	0.31	109,109,109,109	7
74	OHX	D1	3534	7/7	0.84	0.32	142,142,142,142	7
74	OHX	B1	3493	7/7	0.84	0.25	135,135,135,135	7
74	OHX	D1	3579	7/7	0.84	0.41	44,44,44,44	7
74	OHX	D1	3481	7/7	0.84	0.27	137,137,137,137	7
74	OHX	A1	1967	7/7	0.84	0.42	96,96,96,96	7
74	OHX	D1	3497	7/7	0.84	0.36	99,99,99,99	7
74	OHX	C1	1958	7/7	0.84	0.30	153,153,153,153	7
74	OHX	D1	3500	7/7	0.84	0.36	139,139,139,139	7
74	OHX	D1	3546	7/7	0.84	0.30	105,105,105,105	7
74	OHX	B1	3538	7/7	0.84	0.36	93,93,93,93	7
74	OHX	A1	1984	7/7	0.84	0.20	65,65,65,65	7
74	OHX	A1	1952	7/7	0.84	0.36	110,110,110,110	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	D1	3613	7/7	0.85	0.38	57,57,57,57	7
74	OHX	B1	3472	7/7	0.85	0.34	132,132,132,132	7
74	OHX	D1	3526	7/7	0.85	0.26	158,158,158,158	7
74	OHX	B1	3556	7/7	0.85	0.43	104,104,104,104	7
74	OHX	B1	3571	7/7	0.85	0.37	176,176,176,176	7
74	OHX	D1	3592	7/7	0.85	0.36	118,118,118,118	7
74	OHX	D1	3625	7/7	0.85	0.40	100,100,100,100	7
74	OHX	C1	2001	7/7	0.85	0.29	130,130,130,130	7
74	OHX	C1	1986	7/7	0.85	0.23	169,169,169,169	7
74	OHX	D1	3596	7/7	0.85	0.32	114,114,114,114	7
74	OHX	A1	2000	7/7	0.85	0.35	75,75,75,75	7
74	OHX	C1	1972	7/7	0.85	0.41	216,216,216,216	7
74	OHX	D1	3515	7/7	0.85	0.20	173,173,173,173	7
74	OHX	B1	3558	7/7	0.85	0.27	130,130,130,130	7
74	OHX	B1	3620	7/7	0.85	0.27	58,58,58,58	7
74	OHX	A1	1946	7/7	0.85	0.30	153,153,153,153	7
74	OHX	B1	3541	7/7	0.85	0.39	117,117,117,117	7
74	OHX	C1	1997	7/7	0.85	0.26	36,36,36,36	7
74	OHX	A1	1982	7/7	0.86	0.34	148,148,148,148	7
74	OHX	B3	212	7/7	0.86	0.27	98,98,98,98	7
74	OHX	B1	3618	7/7	0.86	0.36	109,109,109,109	7
74	OHX	D1	3602	7/7	0.86	0.45	109,109,109,109	7
74	OHX	D1	3517	7/7	0.86	0.31	126,126,126,126	7
74	OHX	D1	3557	7/7	0.86	0.22	148,148,148,148	7
74	OHX	A1	1935	7/7	0.86	0.24	156,156,156,156	7
74	OHX	B1	3579	7/7	0.86	0.31	47,47,47,47	7
74	OHX	D1	3563	7/7	0.86	0.36	99,99,99,99	7
74	OHX	C1	1979	7/7	0.86	0.19	190,190,190,190	7
74	OHX	C1	1945	7/7	0.86	0.27	122,122,122,122	7
74	OHX	D1	3615	7/7	0.86	0.35	73,73,73,73	7
74	OHX	C1	1947	7/7	0.86	0.33	70,70,70,70	7
74	OHX	B1	3495	7/7	0.86	0.39	108,108,108,108	7
74	OHX	D1	3528	7/7	0.86	0.39	96,96,96,96	7
74	OHX	B1	3566	7/7	0.86	0.35	107,107,107,107	7
74	OHX	D1	3532	7/7	0.86	0.24	102,102,102,102	7
74	OHX	D1	3485	7/7	0.86	0.29	90,90,90,90	7
74	OHX	B1	3501	7/7	0.86	0.40	99,99,99,99	7
74	OHX	D1	3494	7/7	0.86	0.34	105,105,105,105	7
74	OHX	A1	1921	7/7	0.86	0.27	148,148,148,148	7
74	OHX	B1	3588	7/7	0.86	0.27	78,78,78,78	7
74	OHX	B1	3517	7/7	0.86	0.22	111,111,111,111	7
74	OHX	C1	1992	7/7	0.86	0.34	76,76,76,76	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	B1	3573	7/7	0.86	0.33	111,111,111,111	7
74	OHX	D1	3594	7/7	0.86	0.19	30,30,30,30	7
74	OHX	DE	301	7/7	0.86	0.17	302,302,302,302	7
74	OHX	B1	3614	7/7	0.86	0.52	163,163,163,163	7
74	OHX	A1	1934	7/7	0.86	0.41	122,122,122,122	7
74	OHX	B1	3469	7/7	0.87	0.27	169,169,169,169	7
74	OHX	C1	1982	7/7	0.87	0.31	106,106,106,106	7
74	OHX	D1	3476	7/7	0.87	0.31	100,100,100,100	7
74	OHX	B1	3586	7/7	0.87	0.36	116,116,116,116	7
74	OHX	A1	1992	7/7	0.87	0.34	45,45,45,45	7
74	OHX	D1	3489	7/7	0.87	0.28	75,75,75,75	7
74	OHX	B1	3612	7/7	0.87	0.33	45,45,45,45	7
74	OHX	D1	3493	7/7	0.87	0.26	126,126,126,126	7
74	OHX	B1	3547	7/7	0.87	0.37	117,117,117,117	7
74	OHX	C1	1960	7/7	0.87	0.29	111,111,111,111	7
74	OHX	D1	3606	7/7	0.87	0.24	63,63,63,63	7
74	OHX	D1	3551	7/7	0.87	0.25	120,120,120,120	7
74	OHX	C1	1990	7/7	0.87	0.27	105,105,105,105	7
74	OHX	A1	1922	7/7	0.87	0.31	133,133,133,133	7
74	OHX	A1	1942	7/7	0.87	0.22	97,97,97,97	7
74	OHX	D1	3467	7/7	0.87	0.26	129,129,129,129	7
74	OHX	D1	3469	7/7	0.87	0.32	152,152,152,152	7
74	OHX	B1	3519	7/7	0.88	0.31	115,115,115,115	7
74	OHX	D1	3518	7/7	0.88	0.36	108,108,108,108	7
74	OHX	D1	3474	7/7	0.88	0.31	118,118,118,118	7
74	OHX	CI	201	7/7	0.88	0.22	143,143,143,143	7
74	OHX	D1	3499	7/7	0.88	0.21	114,114,114,114	7
74	OHX	A1	1985	7/7	0.88	0.44	86,86,86,86	7
74	OHX	D1	3480	7/7	0.88	0.26	127,127,127,127	7
74	OHX	B1	3564	7/7	0.88	0.32	126,126,126,126	7
74	OHX	D1	3527	7/7	0.88	0.26	146,146,146,146	7
74	OHX	D1	3460	7/7	0.88	0.23	138,138,138,138	7
74	OHX	D1	3584	7/7	0.88	0.40	47,47,47,47	7
74	OHX	D1	3487	7/7	0.88	0.33	103,103,103,103	7
74	OHX	D1	3511	7/7	0.88	0.36	85,85,85,85	7
74	OHX	A1	1944	7/7	0.88	0.33	108,108,108,108	7
74	OHX	D1	3589	7/7	0.88	0.34	56,56,56,56	7
74	OHX	B1	3604	7/7	0.88	0.28	53,53,53,53	7
74	OHX	B1	3572	7/7	0.88	0.24	56,56,56,56	7
74	OHX	CS	102	7/7	0.89	0.35	184,184,184,184	7
74	OHX	D1	3533	7/7	0.89	0.23	92,92,92,92	7
74	OHX	A1	1981	7/7	0.89	0.36	128,128,128,128	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	B1	3531	7/7	0.89	0.30	65,65,65,65	7
74	OHX	D1	3575	7/7	0.89	0.34	84,84,84,84	7
74	OHX	D1	3577	7/7	0.89	0.23	198,198,198,198	7
74	OHX	B1	3583	7/7	0.89	0.36	126,126,126,126	7
74	OHX	C1	1984	7/7	0.89	0.29	78,78,78,78	7
74	OHX	B2	206	7/7	0.89	0.24	128,128,128,128	7
74	OHX	B1	3491	7/7	0.89	0.32	99,99,99,99	7
74	OHX	B1	3437	7/7	0.89	0.29	156,156,156,156	7
74	OHX	A1	1919	7/7	0.89	0.31	141,141,141,141	7
74	OHX	B1	3516	7/7	0.89	0.31	136,136,136,136	7
74	OHX	D2	203	7/7	0.89	0.28	94,94,94,94	7
74	OHX	B1	3497	7/7	0.89	0.21	103,103,103,103	7
74	OHX	A1	1962	7/7	0.89	0.32	193,193,193,193	7
74	OHX	B1	3597	7/7	0.89	0.41	137,137,137,137	7
74	OHX	B1	3479	7/7	0.89	0.33	145,145,145,145	7
74	OHX	C1	1971	7/7	0.89	0.28	131,131,131,131	7
74	OHX	A1	1933	7/7	0.89	0.20	152,152,152,152	7
74	OHX	B1	3525	7/7	0.89	0.33	54,54,54,54	7
74	OHX	C1	1931	7/7	0.89	0.29	130,130,130,130	7
74	OHX	C1	1933	7/7	0.89	0.23	111,111,111,111	7
74	OHX	DC	401	7/7	0.89	0.25	93,93,93,93	7
74	OHX	C1	1938	7/7	0.89	0.34	191,191,191,191	7
74	OHX	B1	3487	7/7	0.89	0.28	116,116,116,116	7
74	OHX	D1	3531	7/7	0.89	0.24	136,136,136,136	7
74	OHX	D1	3488	7/7	0.90	0.23	141,141,141,141	7
74	OHX	C1	1954	7/7	0.90	0.25	116,116,116,116	7
74	OHX	B1	3513	7/7	0.90	0.23	171,171,171,171	7
74	OHX	B1	3595	7/7	0.90	0.25	73,73,73,73	7
74	OHX	A1	1990	7/7	0.90	0.37	117,117,117,117	7
74	OHX	A1	1968	7/7	0.90	0.36	180,180,180,180	7
74	OHX	A1	1969	7/7	0.90	0.23	87,87,87,87	7
74	OHX	AT	401	7/7	0.90	0.30	207,207,207,207	7
74	OHX	B1	3518	7/7	0.90	0.31	105,105,105,105	7
74	OHX	B1	3435	7/7	0.90	0.30	130,130,130,130	7
74	OHX	C1	1968	7/7	0.90	0.26	103,103,103,103	7
74	OHX	A1	1941	7/7	0.90	0.22	124,124,124,124	7
74	OHX	D1	3554	7/7	0.90	0.23	122,122,122,122	7
74	OHX	B1	3606	7/7	0.90	0.24	74,74,74,74	7
74	OHX	D1	3510	7/7	0.90	0.25	108,108,108,108	7
74	OHX	B1	3521	7/7	0.90	0.29	107,107,107,107	7
74	OHX	D1	3433	7/7	0.90	0.25	128,128,128,128	7
74	OHX	D1	3514	7/7	0.90	0.26	173,173,173,173	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	D1	3453	7/7	0.90	0.25	124,124,124,124	7
74	OHX	B1	3549	7/7	0.90	0.33	86,86,86,86	7
74	OHX	D1	3565	7/7	0.90	0.23	60,60,60,60	7
74	OHX	D1	3620	7/7	0.90	0.32	78,78,78,78	7
74	OHX	D1	3621	7/7	0.90	0.25	67,67,67,67	7
74	OHX	B1	3498	7/7	0.90	0.30	83,83,83,83	7
74	OHX	B1	3454	7/7	0.90	0.29	123,123,123,123	7
74	OHX	A1	1939	7/7	0.90	0.20	100,100,100,100	7
74	OHX	D2	202	7/7	0.90	0.23	106,106,106,106	7
74	OHX	D1	3570	7/7	0.90	0.32	49,49,49,49	7
74	OHX	D1	3572	7/7	0.90	0.23	91,91,91,91	7
74	OHX	B1	3503	7/7	0.90	0.29	86,86,86,86	7
74	OHX	C1	1936	7/7	0.90	0.30	126,126,126,126	7
74	OHX	A1	1948	7/7	0.90	0.27	106,106,106,106	7
74	OHX	A1	1960	7/7	0.90	0.29	70,70,70,70	7
74	OHX	C1	1943	7/7	0.90	0.25	141,141,141,141	7
74	OHX	B1	3509	7/7	0.90	0.26	124,124,124,124	7
74	OHX	A1	1936	7/7	0.90	0.26	129,129,129,129	7
74	OHX	D1	3482	7/7	0.90	0.24	107,107,107,107	7
74	OHX	D3	212	7/7	0.90	0.31	71,71,71,71	7
74	OHX	D1	3483	7/7	0.90	0.27	98,98,98,98	7
74	OHX	B1	3562	7/7	0.90	0.40	130,130,130,130	7
74	OHX	D1	3486	7/7	0.90	0.28	143,143,143,143	7
74	OHX	DO	301	7/7	0.90	0.33	285,285,285,285	7
74	OHX	B1	3483	7/7	0.90	0.29	71,71,71,71	7
74	OHX	B1	3596	7/7	0.91	0.32	56,56,56,56	7
74	OHX	B1	3550	7/7	0.91	0.22	137,137,137,137	7
74	OHX	B1	3482	7/7	0.91	0.27	111,111,111,111	7
74	OHX	Ac	100	7/7	0.91	0.32	131,131,131,131	7
74	OHX	B1	3553	7/7	0.91	0.26	66,66,66,66	7
74	OHX	A1	1927	7/7	0.91	0.26	139,139,139,139	7
74	OHX	D1	3503	7/7	0.91	0.31	120,120,120,120	7
74	OHX	D1	3461	7/7	0.91	0.28	128,128,128,128	7
74	OHX	D1	3536	7/7	0.91	0.29	140,140,140,140	7
74	OHX	B1	3578	7/7	0.91	0.28	112,112,112,112	7
74	OHX	D1	3619	7/7	0.91	0.26	86,86,86,86	7
74	OHX	D1	3576	7/7	0.91	0.20	76,76,76,76	7
74	OHX	D1	3539	7/7	0.91	0.23	69,69,69,69	7
74	OHX	A1	1955	7/7	0.91	0.27	110,110,110,110	7
74	OHX	B1	3605	7/7	0.91	0.28	52,52,52,52	7
74	OHX	B1	3536	7/7	0.91	0.30	324,324,324,324	7
74	OHX	A1	1957	7/7	0.91	0.27	129,129,129,129	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	B1	3459	7/7	0.91	0.23	160,160,160,160	7
74	OHX	D1	3547	7/7	0.91	0.22	64,64,64,64	7
74	OHX	B1	3522	7/7	0.91	0.24	129,129,129,129	7
74	OHX	A1	1949	7/7	0.91	0.23	101,101,101,101	7
74	OHX	C1	1994	7/7	0.91	0.20	47,47,47,47	7
74	OHX	B1	3512	7/7	0.91	0.31	113,113,113,113	7
74	OHX	C1	1910	7/7	0.91	0.22	138,138,138,138	7
74	OHX	D1	3553	7/7	0.91	0.33	145,145,145,145	7
74	OHX	D3	209	7/7	0.91	0.20	127,127,127,127	7
74	OHX	C1	1970	7/7	0.91	0.13	176,176,176,176	7
74	OHX	B1	3527	7/7	0.91	0.27	84,84,84,84	7
74	OHX	D1	3597	7/7	0.91	0.37	222,222,222,222	7
74	OHX	A1	1938	7/7	0.91	0.24	155,155,155,155	7
74	OHX	D1	3523	7/7	0.91	0.21	106,106,106,106	7
74	OHX	B1	3529	7/7	0.91	0.17	171,171,171,171	7
74	OHX	A1	1994	7/7	0.91	0.34	123,123,123,123	7
74	OHX	A1	1929	7/7	0.91	0.18	114,114,114,114	7
74	OHX	B1	3470	7/7	0.92	0.21	122,122,122,122	7
74	OHX	D1	3449	7/7	0.92	0.25	124,124,124,124	7
74	OHX	B1	3524	7/7	0.92	0.23	97,97,97,97	7
74	OHX	D1	3454	7/7	0.92	0.23	117,117,117,117	7
74	OHX	A1	1923	7/7	0.92	0.25	98,98,98,98	7
74	OHX	B1	3476	7/7	0.92	0.22	102,102,102,102	7
74	OHX	B1	3477	7/7	0.92	0.21	101,101,101,101	7
74	OHX	A1	1950	7/7	0.92	0.17	127,127,127,127	7
74	OHX	D1	3508	7/7	0.92	0.21	88,88,88,88	7
74	OHX	B1	3448	7/7	0.92	0.21	124,124,124,124	7
74	OHX	D1	3468	7/7	0.92	0.23	130,130,130,130	7
74	OHX	B1	3453	7/7	0.92	0.24	127,127,127,127	7
74	OHX	D1	3581	7/7	0.92	0.27	60,60,60,60	7
74	OHX	C1	1913	7/7	0.92	0.23	149,149,149,149	7
74	OHX	A1	1926	7/7	0.92	0.29	87,87,87,87	7
74	OHX	C1	1923	7/7	0.92	0.25	123,123,123,123	7
74	OHX	C1	1926	7/7	0.92	0.22	96,96,96,96	7
74	OHX	D1	3477	7/7	0.92	0.19	142,142,142,142	7
74	OHX	C1	1993	7/7	0.92	0.26	93,93,93,93	7
74	OHX	D1	3591	7/7	0.92	0.23	43,43,43,43	7
74	OHX	C1	1967	7/7	0.92	0.21	100,100,100,100	7
74	OHX	C1	1927	7/7	0.92	0.19	149,149,149,149	7
74	OHX	C1	1969	7/7	0.92	0.26	133,133,133,133	7
74	OHX	B1	3456	7/7	0.92	0.28	106,106,106,106	7
74	OHX	B1	3508	7/7	0.92	0.23	113,113,113,113	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	B2	204	7/7	0.92	0.20	132,132,132,132	7
74	OHX	D1	3598	7/7	0.92	0.25	65,65,65,65	7
74	OHX	B1	3569	7/7	0.92	0.17	95,95,95,95	7
74	OHX	D1	3562	7/7	0.92	0.28	121,121,121,121	7
74	OHX	C1	1939	7/7	0.92	0.20	103,103,103,103	7
74	OHX	A1	1971	7/7	0.92	0.20	94,94,94,94	7
74	OHX	A1	1972	7/7	0.92	0.23	87,87,87,87	7
74	OHX	DO	302	7/7	0.92	0.24	77,77,77,77	7
74	OHX	B1	3537	7/7	0.92	0.27	56,56,56,56	7
74	OHX	B1	3591	7/7	0.93	0.31	55,55,55,55	7
74	OHX	D1	3537	7/7	0.93	0.21	74,74,74,74	7
74	OHX	B1	3499	7/7	0.93	0.22	123,123,123,123	7
74	OHX	B2	202	7/7	0.93	0.19	106,106,106,106	7
74	OHX	D1	3540	7/7	0.93	0.25	85,85,85,85	7
74	OHX	B1	3425	7/7	0.93	0.21	108,108,108,108	7
74	OHX	C1	1951	7/7	0.93	0.16	152,152,152,152	7
74	OHX	A1	1951	7/7	0.93	0.28	259,259,259,259	7
74	OHX	A1	1979	7/7	0.93	0.17	81,81,81,81	7
74	OHX	B1	3438	7/7	0.93	0.18	168,168,168,168	7
74	OHX	B1	3443	7/7	0.93	0.24	134,134,134,134	7
74	OHX	D1	3495	7/7	0.93	0.18	160,160,160,160	7
74	OHX	B1	3446	7/7	0.93	0.20	113,113,113,113	7
74	OHX	A1	1914	7/7	0.93	0.24	145,145,145,145	7
74	OHX	A1	1943	7/7	0.93	0.18	176,176,176,176	7
74	OHX	B1	3484	7/7	0.93	0.22	143,143,143,143	7
74	OHX	D1	3501	7/7	0.93	0.17	102,102,102,102	7
74	OHX	B3	207	7/7	0.93	0.23	68,68,68,68	7
74	OHX	B1	3576	7/7	0.93	0.26	86,86,86,86	7
74	OHX	B1	3485	7/7	0.93	0.25	110,110,110,110	7
74	OHX	B1	3486	7/7	0.93	0.24	104,104,104,104	7
74	OHX	D1	3405	7/7	0.93	0.25	110,110,110,110	0
74	OHX	D1	3617	7/7	0.93	0.22	50,50,50,50	7
74	OHX	D1	3413	7/7	0.93	0.25	114,114,114,114	7
74	OHX	B1	3607	7/7	0.93	0.26	44,44,44,44	7
74	OHX	D1	3439	7/7	0.93	0.24	107,107,107,107	7
74	OHX	A1	1961	7/7	0.93	0.16	105,105,105,105	7
74	OHX	B1	3455	7/7	0.93	0.20	134,134,134,134	7
74	OHX	C1	1915	7/7	0.93	0.24	120,120,120,120	7
74	OHX	C1	1973	7/7	0.93	0.17	95,95,95,95	7
74	OHX	A1	1908	7/7	0.93	0.25	96,96,96,96	7
74	OHX	C1	1920	7/7	0.93	0.23	103,103,103,103	7
74	OHX	D1	3462	7/7	0.93	0.21	114,114,114,114	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	D2	205	7/7	0.93	0.20	84,84,84,84	7
74	OHX	D2	206	7/7	0.93	0.23	85,85,85,85	7
74	OHX	B1	3457	7/7	0.93	0.20	147,147,147,147	7
74	OHX	C1	1977	7/7	0.93	0.21	102,102,102,102	7
74	OHX	B1	3559	7/7	0.93	0.20	68,68,68,68	7
74	OHX	A1	1911	7/7	0.93	0.22	112,112,112,112	7
74	OHX	B1	3585	7/7	0.93	0.33	197,197,197,197	7
74	OHX	D3	207	7/7	0.93	0.22	123,123,123,123	7
74	OHX	D1	3473	7/7	0.93	0.18	123,123,123,123	7
74	OHX	B1	3615	7/7	0.93	0.22	49,49,49,49	7
74	OHX	B1	3561	7/7	0.93	0.42	280,280,280,280	7
74	OHX	C1	1983	7/7	0.93	0.25	59,59,59,59	7
74	OHX	D1	3583	7/7	0.93	0.20	88,88,88,88	7
74	OHX	D1	3530	7/7	0.93	0.22	51,51,51,51	7
74	OHX	B1	3587	7/7	0.93	0.28	154,154,154,154	7
74	OHX	D1	3479	7/7	0.93	0.26	99,99,99,99	7
74	OHX	B1	3466	7/7	0.93	0.17	120,120,120,120	7
74	OHX	A1	1987	7/7	0.93	0.24	72,72,72,72	7
74	OHX	C1	1942	7/7	0.93	0.20	112,112,112,112	7
74	OHX	B1	3431	7/7	0.94	0.16	125,125,125,125	7
74	OHX	D1	3520	7/7	0.94	0.21	109,109,109,109	7
74	OHX	C1	1961	7/7	0.94	0.20	101,101,101,101	7
74	OHX	D1	3607	7/7	0.94	0.23	78,78,78,78	7
74	OHX	D1	3608	7/7	0.94	0.26	14,14,14,14	7
74	OHX	B1	3526	7/7	0.94	0.22	174,174,174,174	7
74	OHX	C1	1963	7/7	0.94	0.20	94,94,94,94	7
74	OHX	C1	1964	7/7	0.94	0.23	88,88,88,88	7
74	OHX	C1	1916	7/7	0.94	0.25	169,169,169,169	7
74	OHX	B1	3507	7/7	0.94	0.26	104,104,104,104	7
74	OHX	D1	3484	7/7	0.94	0.19	116,116,116,116	7
74	OHX	A1	1915	7/7	0.94	0.21	129,129,129,129	7
74	OHX	C1	1922	7/7	0.94	0.23	142,142,142,142	7
74	OHX	A1	1959	7/7	0.94	0.28	110,110,110,110	7
74	OHX	B1	3460	7/7	0.94	0.20	137,137,137,137	7
74	OHX	B1	3461	7/7	0.94	0.21	101,101,101,101	7
74	OHX	B1	3462	7/7	0.94	0.20	90,90,90,90	7
74	OHX	D1	3492	7/7	0.94	0.23	112,112,112,112	7
74	OHX	B1	3488	7/7	0.94	0.16	104,104,104,104	7
74	OHX	D1	3624	7/7	0.94	0.24	95,95,95,95	7
74	OHX	B1	3465	7/7	0.94	0.20	142,142,142,142	7
74	OHX	C1	1937	7/7	0.94	0.18	124,124,124,124	7
74	OHX	A1	1932	7/7	0.94	0.20	142,142,142,142	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	D1	3441	7/7	0.94	0.20	124,124,124,124	7
74	OHX	B1	3468	7/7	0.94	0.25	89,89,89,89	7
74	OHX	B1	3441	7/7	0.94	0.23	129,129,129,129	7
74	OHX	AL	201	7/7	0.94	0.15	122,122,122,122	7
74	OHX	D1	3543	7/7	0.94	0.20	45,45,45,45	7
74	OHX	D1	3588	7/7	0.94	0.28	336,336,336,336	7
74	OHX	A1	1928	7/7	0.94	0.15	99,99,99,99	7
74	OHX	D1	3459	7/7	0.94	0.23	96,96,96,96	7
74	OHX	B3	203	7/7	0.94	0.20	140,140,140,140	7
74	OHX	B1	3474	7/7	0.94	0.19	179,179,179,179	7
74	OHX	C1	1949	7/7	0.94	0.17	97,97,97,97	7
74	OHX	D1	3463	7/7	0.94	0.19	140,140,140,140	7
74	OHX	A1	1924	7/7	0.94	0.21	150,150,150,150	7
74	OHX	B3	208	7/7	0.94	0.18	79,79,79,79	7
74	OHX	B1	3543	7/7	0.94	0.15	102,102,102,102	7
74	OHX	B1	3421	7/7	0.94	0.27	141,141,141,141	0
74	OHX	A1	1986	7/7	0.94	0.19	98,98,98,98	7
74	OHX	BC	401	7/7	0.94	0.16	66,66,66,66	7
74	OHX	B1	3590	7/7	0.94	0.18	69,69,69,69	7
74	OHX	B1	3426	7/7	0.94	0.20	111,111,111,111	7
74	OHX	D1	3491	7/7	0.95	0.17	37,37,37,37	7
74	OHX	A1	1980	7/7	0.95	0.14	136,136,136,136	7
74	OHX	B1	3494	7/7	0.95	0.19	118,118,118,118	7
74	OHX	B1	3429	7/7	0.95	0.17	93,93,93,93	7
74	OHX	D1	3458	7/7	0.95	0.17	103,103,103,103	7
74	OHX	B1	3496	7/7	0.95	0.19	122,122,122,122	7
74	OHX	B1	3447	7/7	0.95	0.22	126,126,126,126	7
74	OHX	C1	1941	7/7	0.95	0.18	109,109,109,109	7
74	OHX	B1	3430	7/7	0.95	0.20	99,99,99,99	7
74	OHX	C1	1914	7/7	0.95	0.15	128,128,128,128	7
74	OHX	D1	3502	7/7	0.95	0.16	79,79,79,79	7
74	OHX	D1	3464	7/7	0.95	0.16	92,92,92,92	7
74	OHX	D1	3465	7/7	0.95	0.19	101,101,101,101	7
74	OHX	B1	3403	7/7	0.95	0.26	126,126,126,126	0
74	OHX	B1	3500	7/7	0.95	0.21	116,116,116,116	7
74	OHX	C1	1948	7/7	0.95	0.20	117,117,117,117	7
74	OHX	B1	3409	7/7	0.95	0.22	122,122,122,122	0
74	OHX	B1	3416	7/7	0.95	0.25	113,113,113,113	0
74	OHX	B1	3598	7/7	0.95	0.20	100,100,100,100	7
74	OHX	A1	1976	7/7	0.95	0.24	51,51,51,51	7
74	OHX	B1	3440	7/7	0.95	0.24	105,105,105,105	7
74	OHX	C1	1955	7/7	0.95	0.20	106,106,106,106	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	B1	3473	7/7	0.95	0.17	91,91,91,91	7
74	OHX	D1	3478	7/7	0.95	0.17	117,117,117,117	7
74	OHX	C1	1928	7/7	0.95	0.22	165,165,165,165	7
74	OHX	C1	1930	7/7	0.95	0.18	112,112,112,112	7
74	OHX	B1	3458	7/7	0.95	0.25	114,114,114,114	7
74	OHX	D1	3436	7/7	0.95	0.24	125,125,125,125	7
74	OHX	D1	3437	7/7	0.95	0.22	103,103,103,103	7
74	OHX	A1	1945	7/7	0.95	0.16	108,108,108,108	7
74	OHX	D1	3440	7/7	0.95	0.25	137,137,137,137	7
74	OHX	C1	1934	7/7	0.95	0.18	141,141,141,141	7
74	OHX	D1	3448	7/7	0.95	0.22	107,107,107,107	7
74	OHX	D1	3604	7/7	0.95	0.18	44,44,44,44	7
74	OHX	C1	1935	7/7	0.95	0.15	93,93,93,93	7
74	OHX	D1	3450	7/7	0.95	0.22	112,112,112,112	7
74	OHX	D1	3567	7/7	0.95	0.16	106,106,106,106	7
74	OHX	D1	3451	7/7	0.95	0.22	112,112,112,112	7
74	OHX	C1	1932	7/7	0.96	0.18	115,115,115,115	7
74	OHX	A1	1904	7/7	0.96	0.18	137,137,137,137	7
74	OHX	A1	1937	7/7	0.96	0.16	158,158,158,158	7
74	OHX	D1	3512	7/7	0.96	0.16	108,108,108,108	7
74	OHX	A1	1920	7/7	0.96	0.15	126,126,126,126	7
74	OHX	B1	3433	7/7	0.96	0.21	98,98,98,98	7
74	OHX	A1	1910	7/7	0.96	0.19	146,146,146,146	7
74	OHX	D1	3561	7/7	0.96	0.17	65,65,65,65	7
74	OHX	D1	3470	7/7	0.96	0.13	84,84,84,84	7
74	OHX	B1	3436	7/7	0.96	0.15	104,104,104,104	7
74	OHX	A1	1905	7/7	0.96	0.19	118,118,118,118	0
74	OHX	D1	3612	7/7	0.96	0.18	36,36,36,36	7
74	OHX	CS	101	7/7	0.96	0.27	46,46,46,46	7
74	OHX	A1	1912	7/7	0.96	0.18	125,125,125,125	7
74	OHX	B1	3439	7/7	0.96	0.19	90,90,90,90	7
74	OHX	B1	3463	7/7	0.96	0.16	137,137,137,137	7
74	OHX	Bd	102	7/7	0.96	0.15	73,73,73,73	7
74	OHX	D1	3416	7/7	0.96	0.12	108,108,108,108	7
74	OHX	D1	3571	7/7	0.96	0.17	77,77,77,77	7
74	OHX	D1	3417	7/7	0.96	0.19	91,91,91,91	7
74	OHX	D1	3418	7/7	0.96	0.22	103,103,103,103	0
74	OHX	D1	3425	7/7	0.96	0.16	126,126,126,126	7
74	OHX	D1	3429	7/7	0.96	0.21	82,82,82,82	7
74	OHX	D1	3432	7/7	0.96	0.20	100,100,100,100	7
74	OHX	C1	1944	7/7	0.96	0.12	134,134,134,134	7
74	OHX	Bg	101	7/7	0.96	0.24	79,79,79,79	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	C1	1946	7/7	0.96	0.15	63,63,63,63	7
74	OHX	B1	3464	7/7	0.96	0.20	89,89,89,89	7
74	OHX	B1	3410	7/7	0.96	0.17	111,111,111,111	0
74	OHX	A1	1906	7/7	0.96	0.15	97,97,97,97	7
74	OHX	D1	3444	7/7	0.96	0.20	72,72,72,72	7
74	OHX	D1	3445	7/7	0.96	0.19	101,101,101,101	7
74	OHX	D1	3447	7/7	0.96	0.20	142,142,142,142	7
74	OHX	D3	203	7/7	0.96	0.14	86,86,86,86	7
74	OHX	D3	204	7/7	0.96	0.19	120,120,120,120	7
74	OHX	B1	3442	7/7	0.96	0.21	89,89,89,89	7
74	OHX	B1	3419	7/7	0.96	0.17	109,109,109,109	7
74	OHX	B1	3444	7/7	0.96	0.15	111,111,111,111	7
74	OHX	A1	1907	7/7	0.96	0.18	111,111,111,111	7
74	OHX	A1	1916	7/7	0.96	0.16	91,91,91,91	7
74	OHX	A1	2001	7/7	0.96	0.17	26,26,26,26	7
74	OHX	C1	1925	7/7	0.96	0.14	116,116,116,116	7
74	OHX	B1	3475	7/7	0.96	0.20	84,84,84,84	7
74	OHX	B1	3452	7/7	0.96	0.17	134,134,134,134	7
74	OHX	D1	3504	7/7	0.96	0.16	101,101,101,101	7
74	OHX	B1	3427	7/7	0.96	0.23	95,95,95,95	7
74	OHX	C1	1929	7/7	0.96	0.21	90,90,90,90	7
74	OHX	B1	3478	7/7	0.96	0.14	110,110,110,110	7
74	OHX	Dd	101	7/7	0.96	0.23	32,32,32,32	7
74	OHX	B1	3505	7/7	0.96	0.15	134,134,134,134	7
74	OHX	B1	3540	7/7	0.97	0.14	58,58,58,58	7
74	OHX	A1	1918	7/7	0.97	0.18	94,94,94,94	7
74	OHX	C1	1902	7/7	0.97	0.22	108,108,108,108	0
74	OHX	C1	1905	7/7	0.97	0.11	114,114,114,114	7
74	OHX	C1	1909	7/7	0.97	0.14	130,130,130,130	7
74	OHX	D1	3442	7/7	0.97	0.16	126,126,126,126	7
74	OHX	D1	3443	7/7	0.97	0.14	96,96,96,96	7
74	OHX	A1	1903	7/7	0.97	0.15	122,122,122,122	7
74	OHX	C1	1912	7/7	0.97	0.12	117,117,117,117	7
74	OHX	D1	3446	7/7	0.97	0.17	83,83,83,83	7
74	OHX	AS	101	7/7	0.97	0.19	29,29,29,29	7
74	OHX	B1	3418	7/7	0.97	0.14	106,106,106,106	0
74	OHX	B1	3593	7/7	0.97	0.15	46,46,46,46	7
74	OHX	B1	3432	7/7	0.97	0.17	79,79,79,79	7
74	OHX	A1	1909	7/7	0.97	0.12	115,115,115,115	7
74	OHX	A1	1975	7/7	0.97	0.17	67,67,67,67	7
74	OHX	C1	1921	7/7	0.97	0.12	145,145,145,145	7
74	OHX	D1	3496	7/7	0.97	0.18	155,155,155,155	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	D1	3455	7/7	0.97	0.16	110,110,110,110	7
74	OHX	D1	3456	7/7	0.97	0.19	131,131,131,131	7
74	OHX	B1	3423	7/7	0.97	0.21	91,91,91,91	7
74	OHX	B1	3492	7/7	0.97	0.20	70,70,70,70	7
74	OHX	C1	1924	7/7	0.97	0.12	82,82,82,82	7
74	OHX	B1	3451	7/7	0.97	0.15	86,86,86,86	7
74	OHX	D1	3401	7/7	0.97	0.20	96,96,96,96	0
74	OHX	D1	3403	7/7	0.97	0.19	96,96,96,96	0
74	OHX	B1	3567	7/7	0.97	0.11	126,126,126,126	7
74	OHX	D1	3406	7/7	0.97	0.12	107,107,107,107	0
74	OHX	D1	3409	7/7	0.97	0.14	114,114,114,114	0
74	OHX	D1	3410	7/7	0.97	0.22	96,96,96,96	0
74	OHX	C1	1953	7/7	0.97	0.16	56,56,56,56	7
74	OHX	B1	3424	7/7	0.97	0.19	105,105,105,105	7
74	OHX	A1	1917	7/7	0.97	0.15	130,130,130,130	7
74	OHX	B3	211	7/7	0.97	0.14	67,67,67,67	7
74	OHX	D1	3422	7/7	0.97	0.15	114,114,114,114	7
74	OHX	D1	3472	7/7	0.97	0.15	185,185,185,185	7
74	OHX	B1	3406	7/7	0.97	0.23	106,106,106,106	0
74	OHX	B1	3467	7/7	0.97	0.14	119,119,119,119	7
74	OHX	D1	3430	7/7	0.97	0.15	101,101,101,101	7
74	OHX	D1	3560	7/7	0.97	0.19	82,82,82,82	7
74	OHX	B2	201	7/7	0.97	0.10	141,141,141,141	7
74	OHX	DT	201	7/7	0.97	0.22	100,100,100,100	0
74	OHX	Bd	101	7/7	0.97	0.22	32,32,32,32	7
74	OHX	D1	3435	7/7	0.97	0.12	92,92,92,92	7
74	OHX	B1	3405	7/7	0.98	0.18	101,101,101,101	0
74	OHX	D1	3434	7/7	0.98	0.13	77,77,77,77	7
74	OHX	BT	201	7/7	0.98	0.17	91,91,91,91	7
74	OHX	B1	3422	7/7	0.98	0.12	93,93,93,93	7
74	OHX	A1	1901	7/7	0.98	0.14	100,100,100,100	0
74	OHX	B1	3480	7/7	0.98	0.10	85,85,85,85	7
74	OHX	B1	3407	7/7	0.98	0.12	105,105,105,105	0
74	OHX	C1	1903	7/7	0.98	0.16	115,115,115,115	0
74	OHX	C1	1904	7/7	0.98	0.18	113,113,113,113	0
74	OHX	B1	3408	7/7	0.98	0.17	98,98,98,98	0
74	OHX	C1	1907	7/7	0.98	0.18	123,123,123,123	7
74	OHX	B1	3563	7/7	0.98	0.17	152,152,152,152	7
74	OHX	A1	1902	7/7	0.98	0.14	112,112,112,112	0
74	OHX	C1	1911	7/7	0.98	0.11	96,96,96,96	7
74	OHX	A1	1931	7/7	0.98	0.14	96,96,96,96	7
74	OHX	B1	3428	7/7	0.98	0.15	109,109,109,109	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	B1	3411	7/7	0.98	0.14	105,105,105,105	0
74	OHX	D1	3402	7/7	0.98	0.20	100,100,100,100	0
74	OHX	D1	3582	7/7	0.98	0.13	71,71,71,71	7
74	OHX	B1	3413	7/7	0.98	0.13	106,106,106,106	7
74	OHX	D1	3404	7/7	0.98	0.21	99,99,99,99	0
74	OHX	B3	201	7/7	0.98	0.20	117,117,117,117	0
74	OHX	B3	202	7/7	0.98	0.11	116,116,116,116	0
74	OHX	D1	3407	7/7	0.98	0.15	113,113,113,113	0
74	OHX	D1	3408	7/7	0.98	0.13	143,143,143,143	0
74	OHX	B1	3449	7/7	0.98	0.14	105,105,105,105	7
74	OHX	B3	204	7/7	0.98	0.13	84,84,84,84	7
74	OHX	D1	3411	7/7	0.98	0.15	117,117,117,117	0
74	OHX	D1	3412	7/7	0.98	0.17	126,126,126,126	0
74	OHX	B3	205	7/7	0.98	0.11	123,123,123,123	7
74	OHX	B1	3489	7/7	0.98	0.13	129,129,129,129	7
74	OHX	B1	3414	7/7	0.98	0.13	106,106,106,106	0
74	OHX	A1	1956	7/7	0.98	0.11	159,159,159,159	7
74	OHX	D1	3419	7/7	0.98	0.14	92,92,92,92	0
74	OHX	D1	3421	7/7	0.98	0.12	98,98,98,98	7
74	OHX	B1	3417	7/7	0.98	0.12	102,102,102,102	0
74	OHX	D1	3423	7/7	0.98	0.09	88,88,88,88	7
74	OHX	D1	3424	7/7	0.98	0.09	125,125,125,125	7
74	OHX	B1	3434	7/7	0.98	0.17	102,102,102,102	7
74	OHX	D1	3426	7/7	0.98	0.15	112,112,112,112	7
74	OHX	D1	3427	7/7	0.98	0.12	90,90,90,90	7
74	OHX	A1	1913	7/7	0.98	0.11	135,135,135,135	7
74	OHX	B1	3404	7/7	0.98	0.15	114,114,114,114	0
74	OHX	B1	3420	7/7	0.98	0.15	93,93,93,93	7
74	OHX	Dg	101	7/7	0.98	0.19	69,69,69,69	7
74	OHX	B1	3401	7/7	0.99	0.18	90,90,90,90	0
74	OHX	D3	201	7/7	0.99	0.14	93,93,93,93	0
74	OHX	D3	202	7/7	0.99	0.14	116,116,116,116	0
74	OHX	C1	1908	7/7	0.99	0.11	104,104,104,104	7
74	OHX	B1	3415	7/7	0.99	0.14	93,93,93,93	7
74	OHX	D1	3428	7/7	0.99	0.11	80,80,80,80	7
74	OHX	B1	3412	7/7	0.99	0.13	121,121,121,121	0
74	OHX	D1	3414	7/7	0.99	0.11	114,114,114,114	0
74	OHX	D1	3431	7/7	0.99	0.12	109,109,109,109	7
74	OHX	D1	3415	7/7	0.99	0.10	139,139,139,139	0
74	OHX	C1	1901	7/7	0.99	0.14	100,100,100,100	0
74	OHX	D1	3452	7/7	0.99	0.10	94,94,94,94	7
74	OHX	B1	3450	7/7	0.99	0.14	91,91,91,91	7

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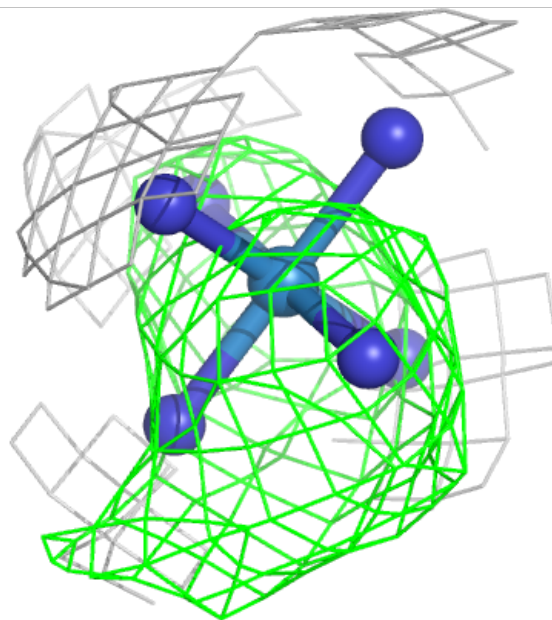
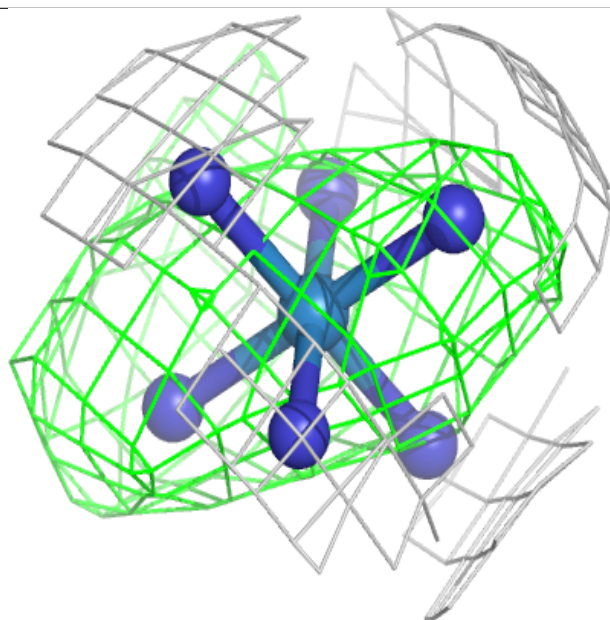
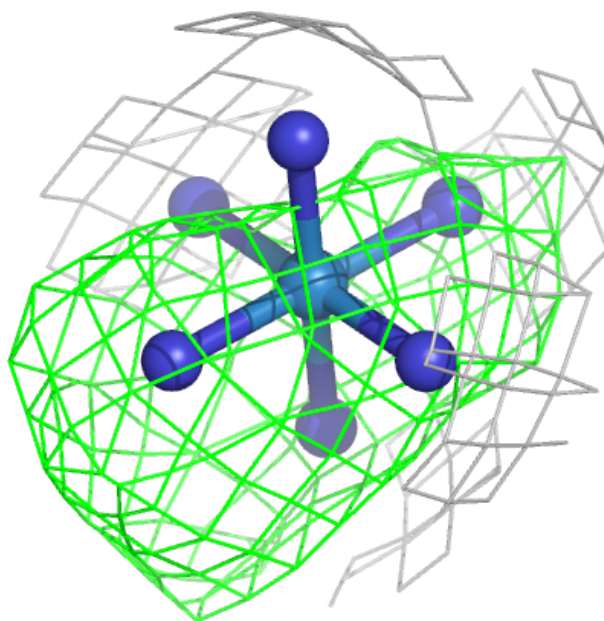
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
74	OHX	B1	3445	7/7	0.99	0.09	113,113,113,113	7
74	OHX	D2	201	7/7	0.99	0.09	94,94,94,94	7
74	OHX	B1	3402	7/7	0.99	0.15	99,99,99,99	0
74	OHX	D1	3420	7/7	0.99	0.10	112,112,112,112	0
74	OHX	D1	3438	7/7	0.99	0.11	98,98,98,98	7
74	OHX	B1	3471	7/7	0.99	0.11	130,130,130,130	7
74	OHX	C1	1906	7/7	0.99	0.13	101,101,101,101	7
74	OHX	C1	1917	7/7	0.99	0.15	130,130,130,130	7
74	OHX	C1	1918	7/7	0.99	0.14	123,123,123,123	7

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

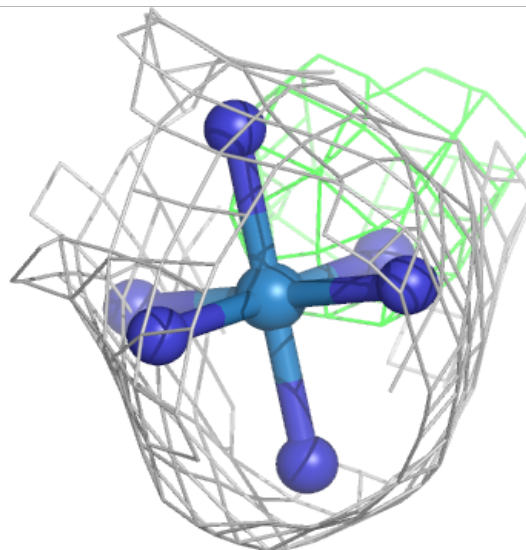
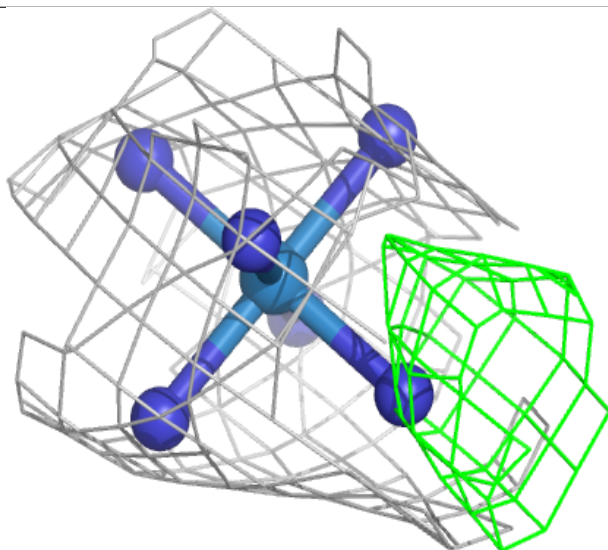
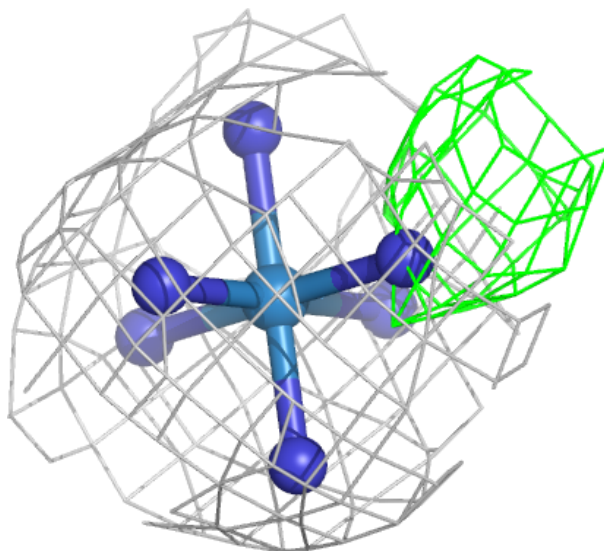
Electron density around OHX C1 1998:

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



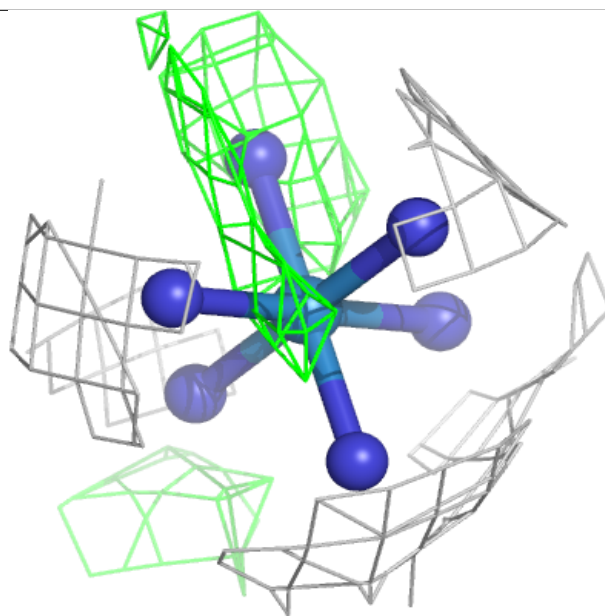
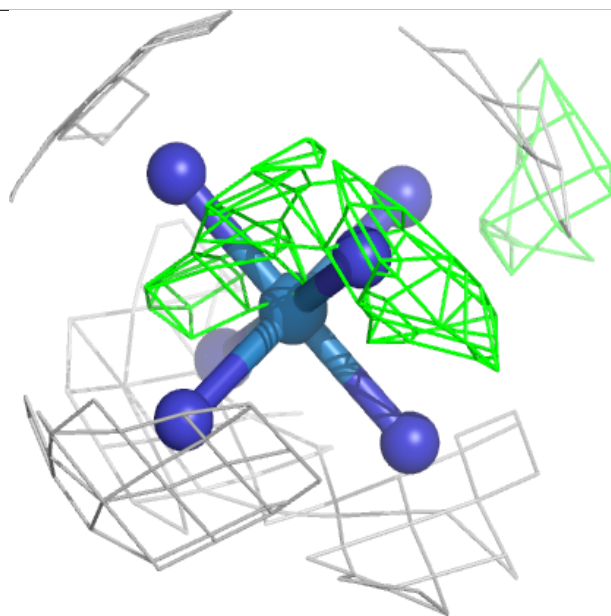
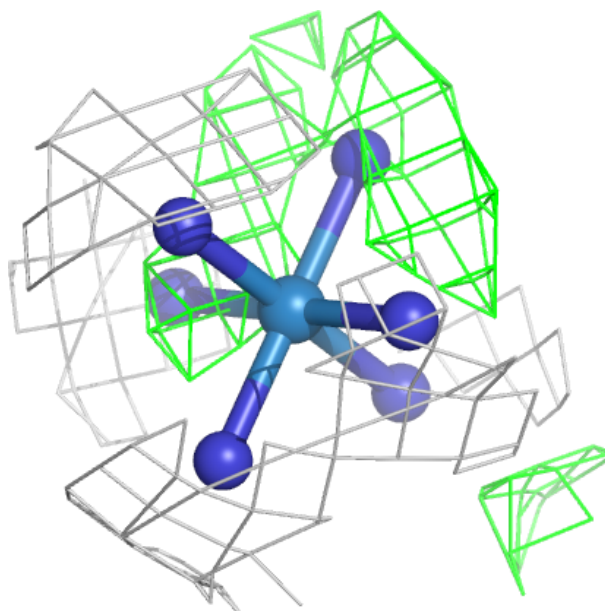
Electron density around OHX A1 1983:

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



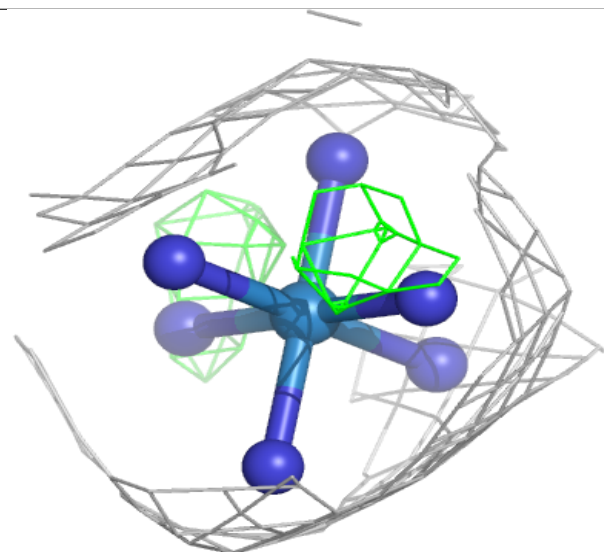
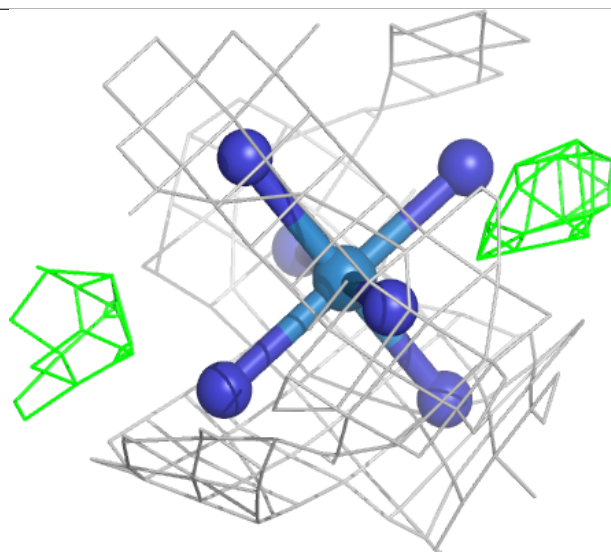
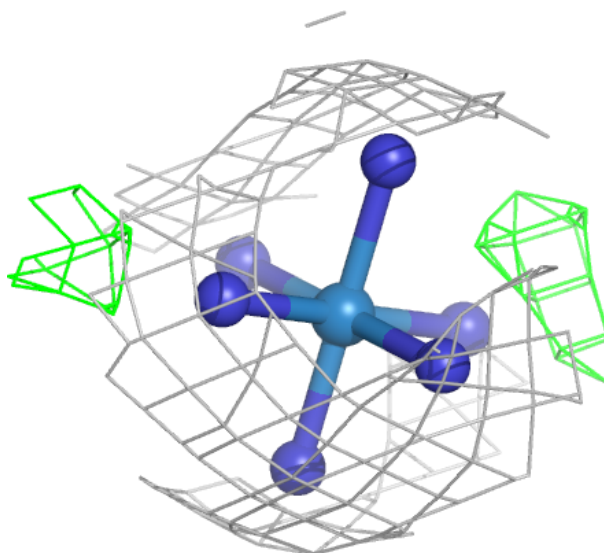
Electron density around OHX B1 3554:

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



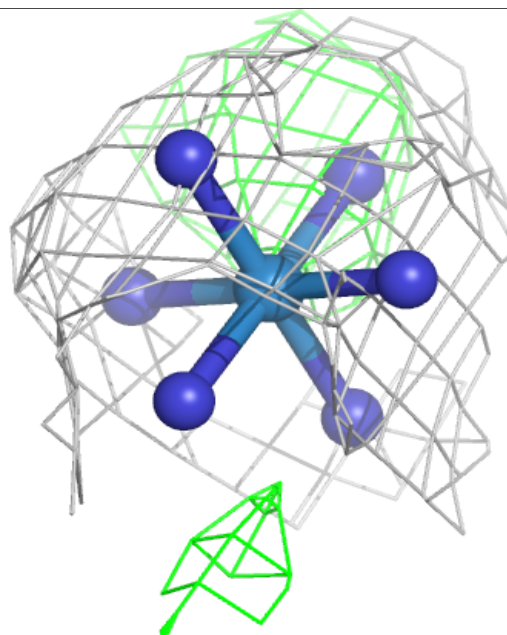
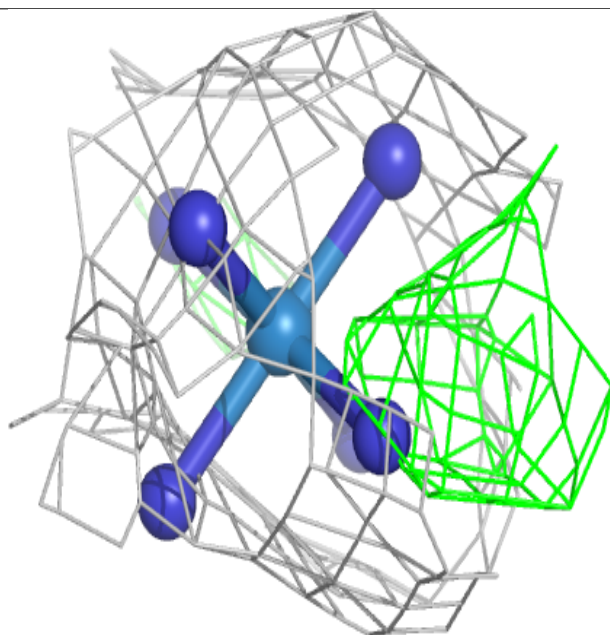
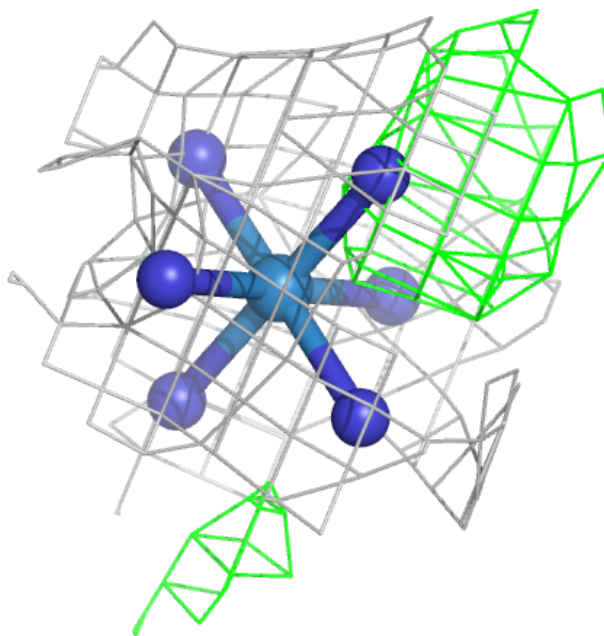
Electron density around OHX B1 3548:

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



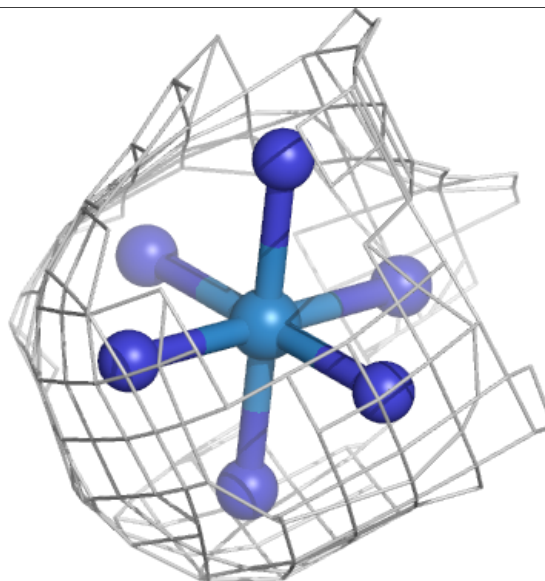
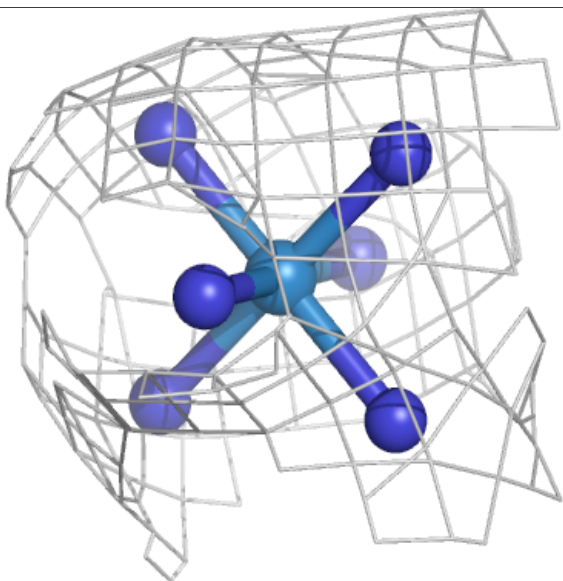
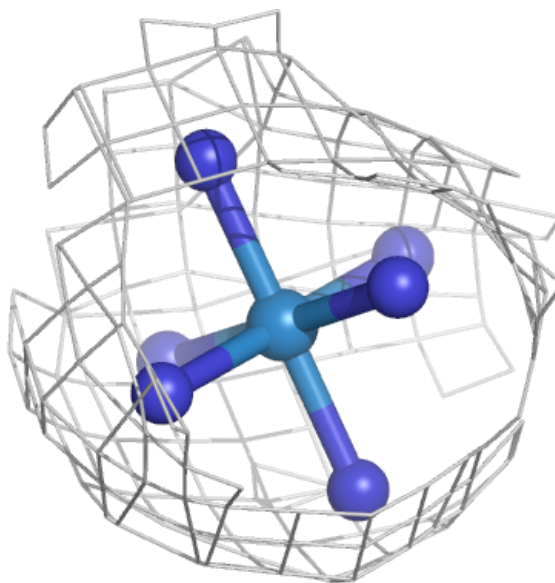
Electron density around OHX D1 3586:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



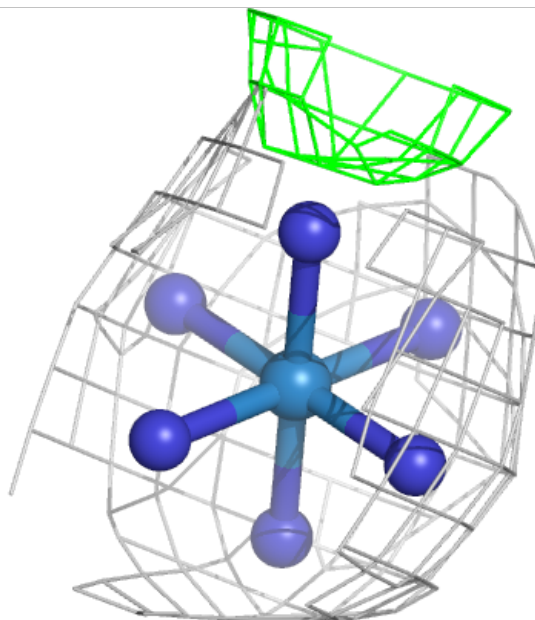
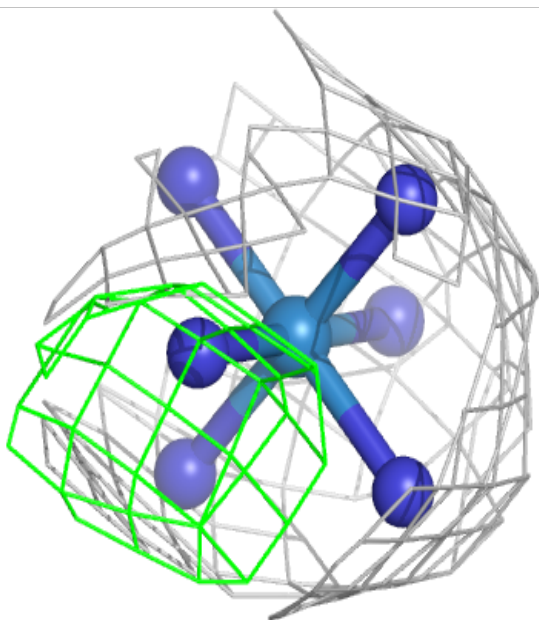
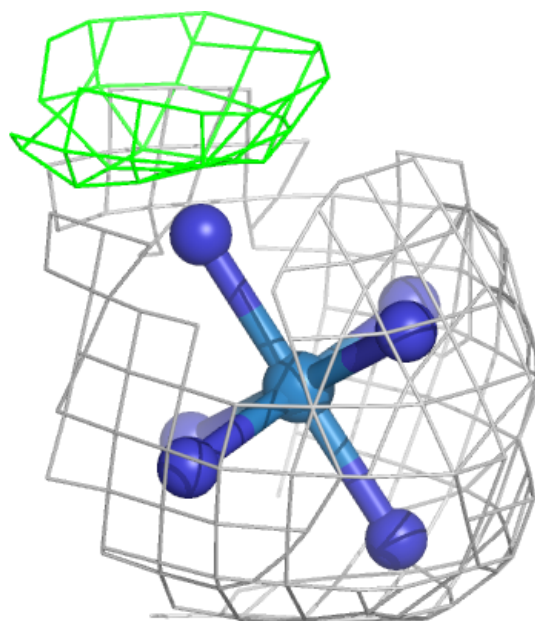
Electron density around OHX C1 1989:

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



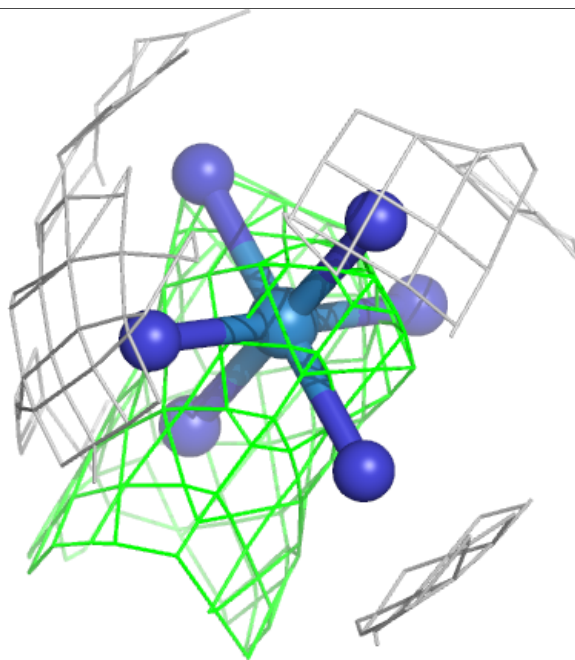
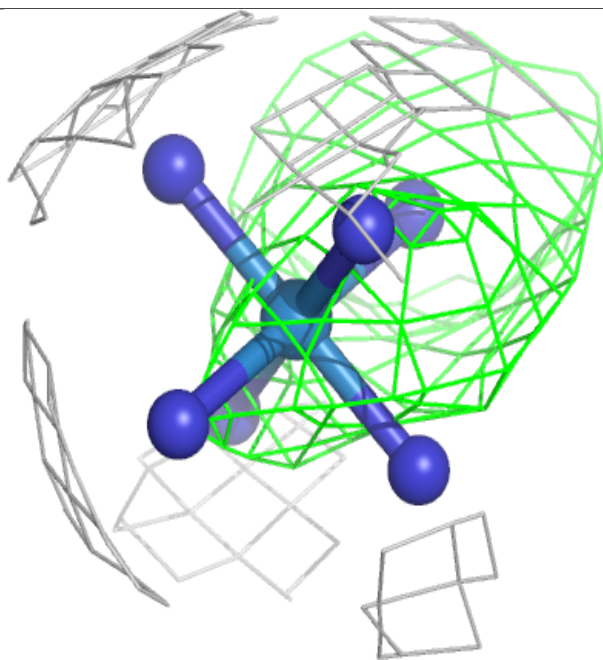
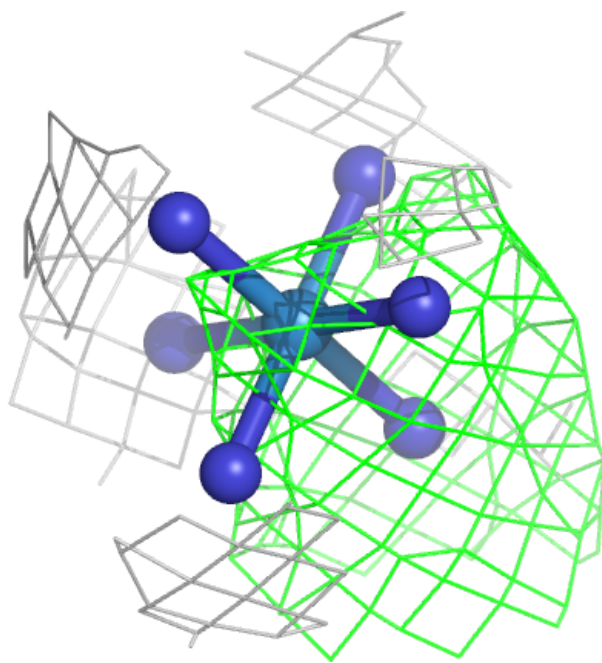
Electron density around OHX B1 3613:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



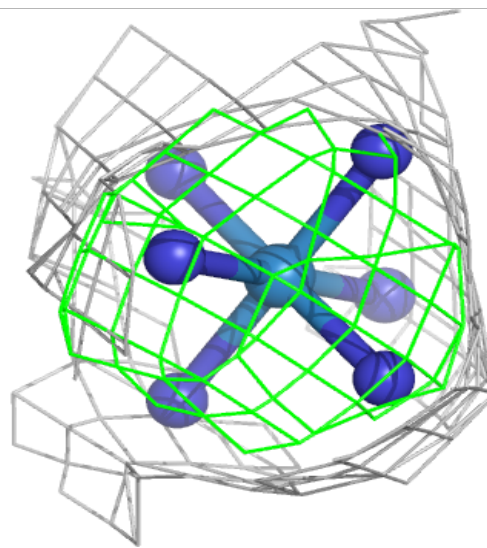
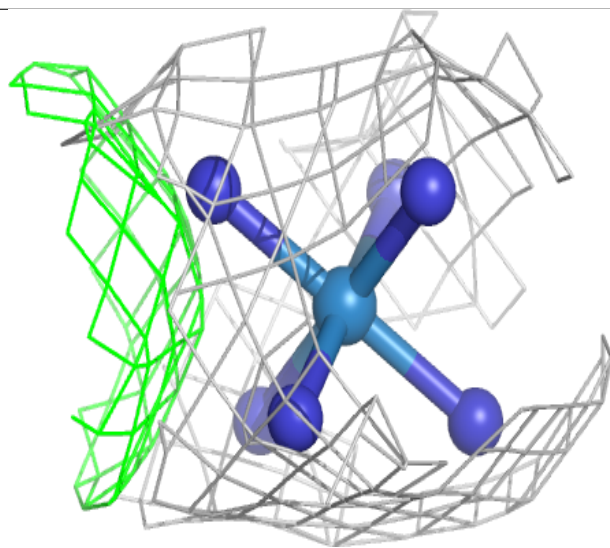
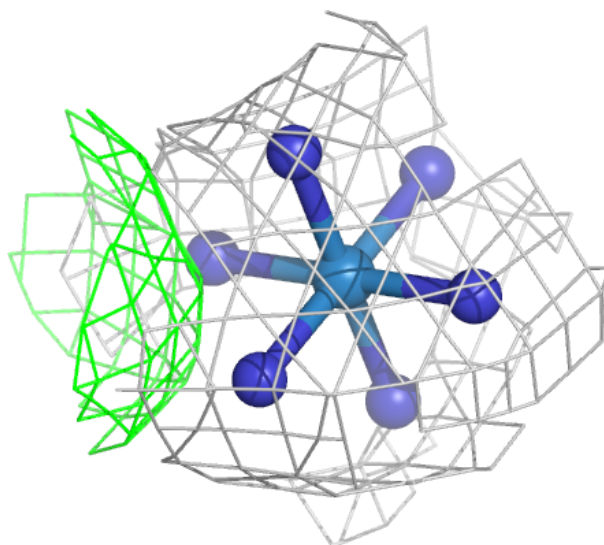
Electron density around OHX B1 3608:

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



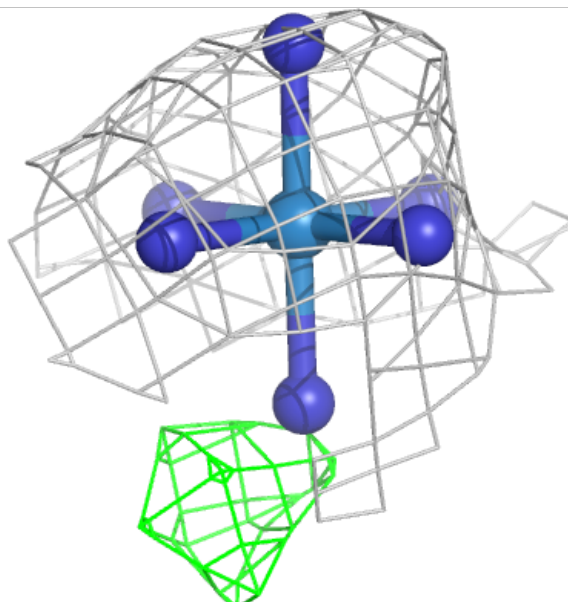
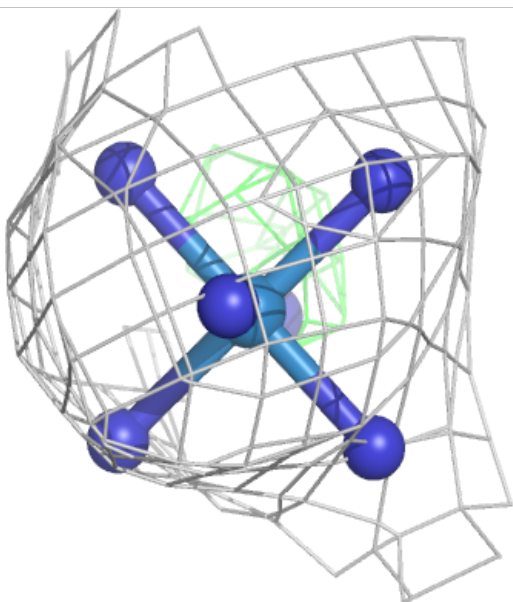
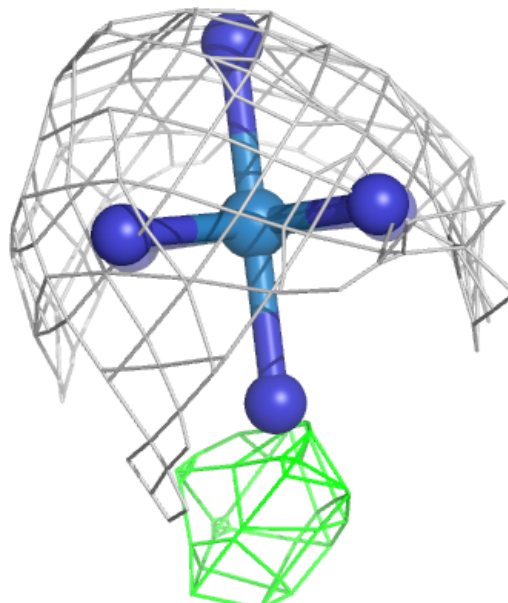
Electron density around OHX D1 3535:

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and green (positive)



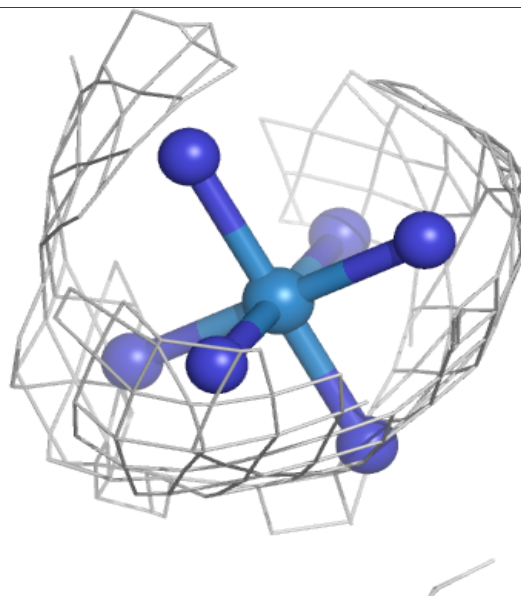
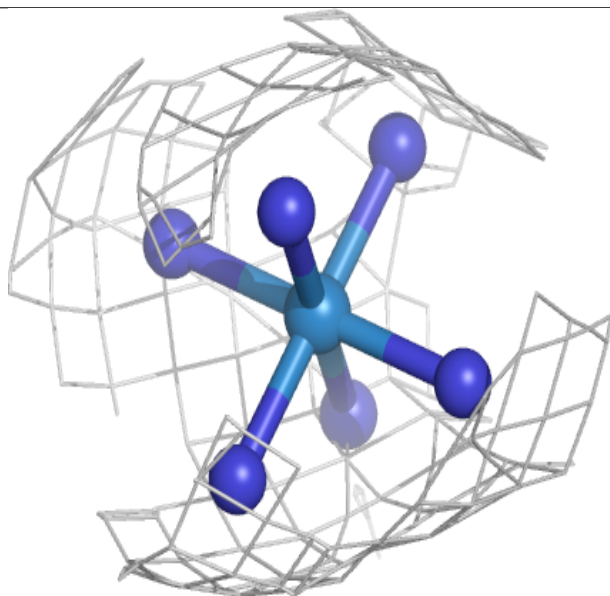
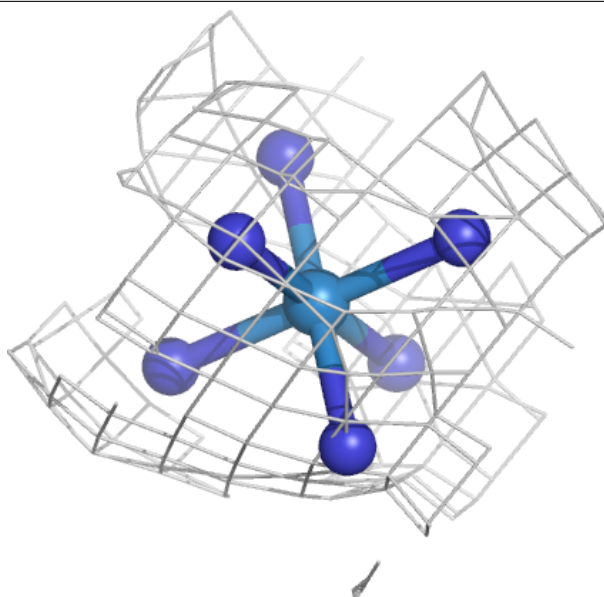
Electron density around OHX B1 3592:

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and green (positive)



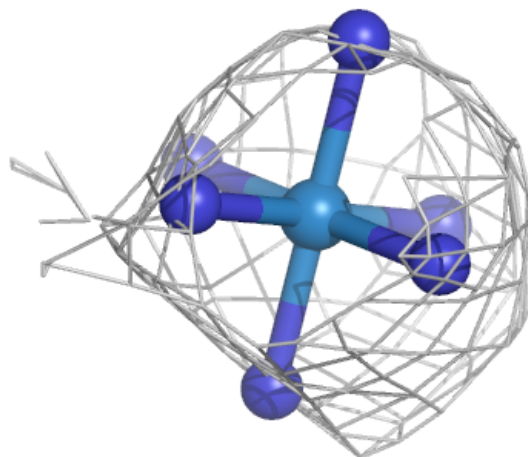
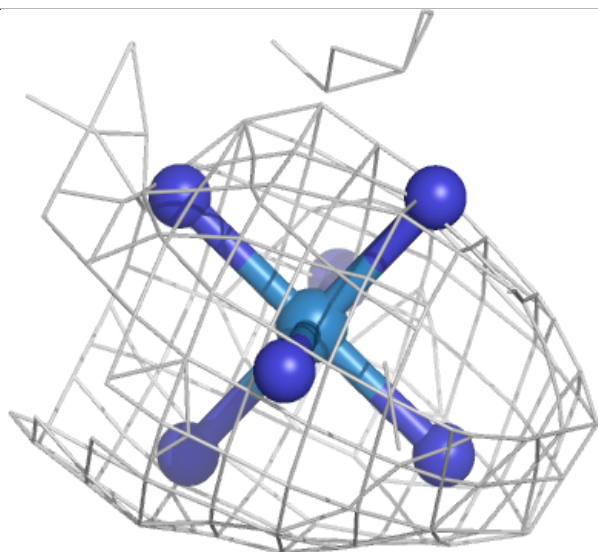
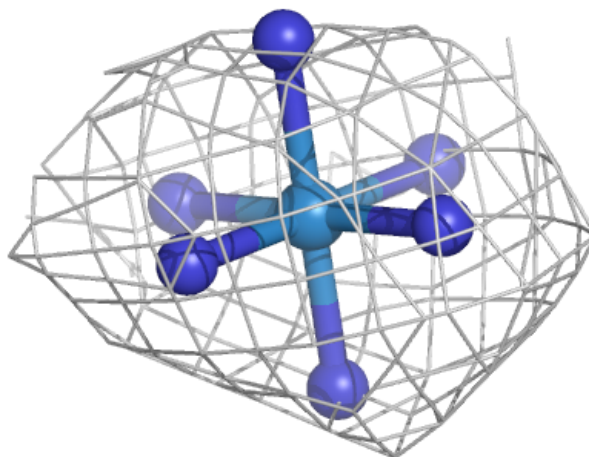
Electron density around OHX A1 1993:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



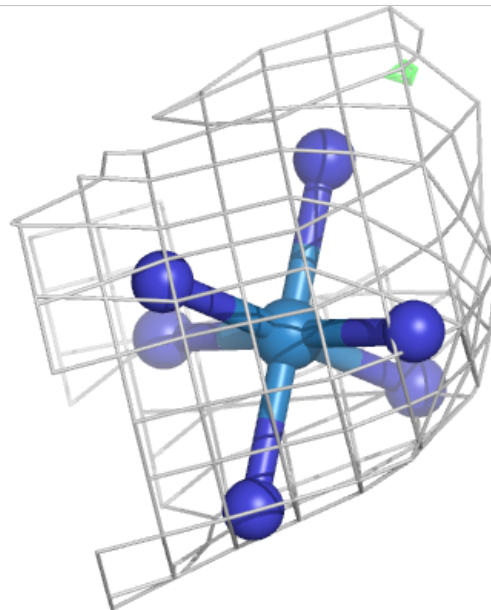
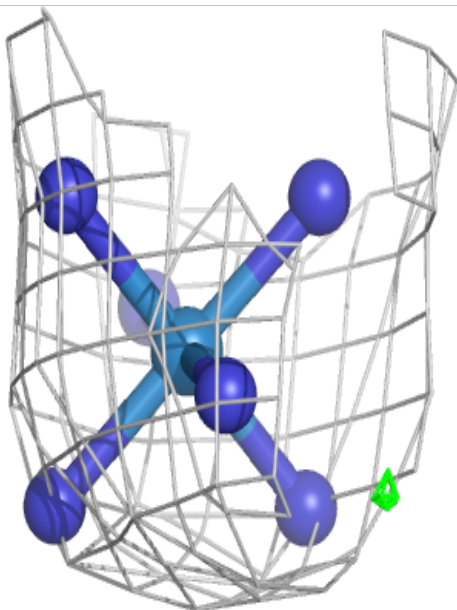
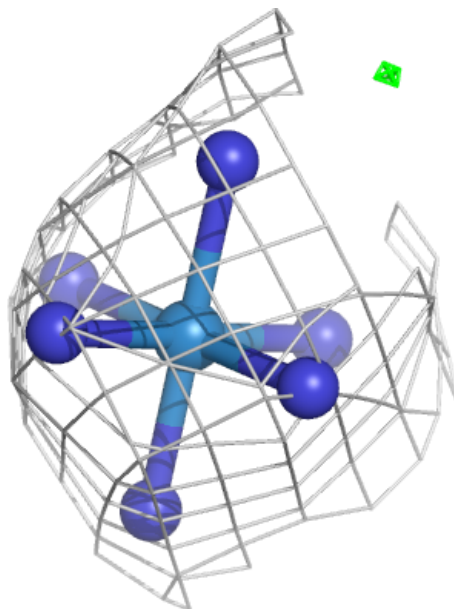
Electron density around OHX B1 3577:

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and green (positive)



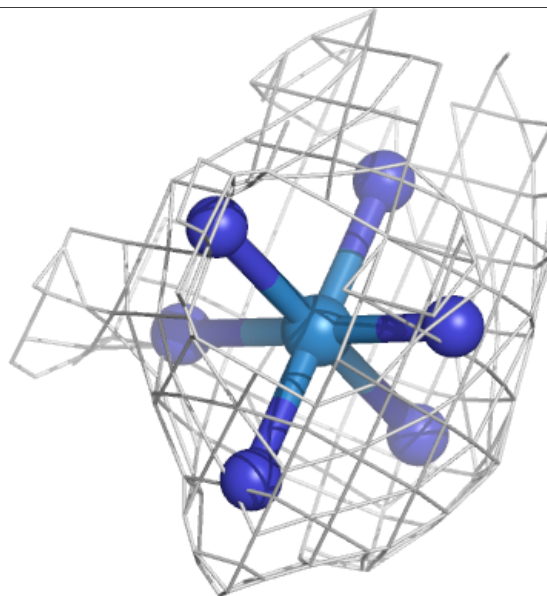
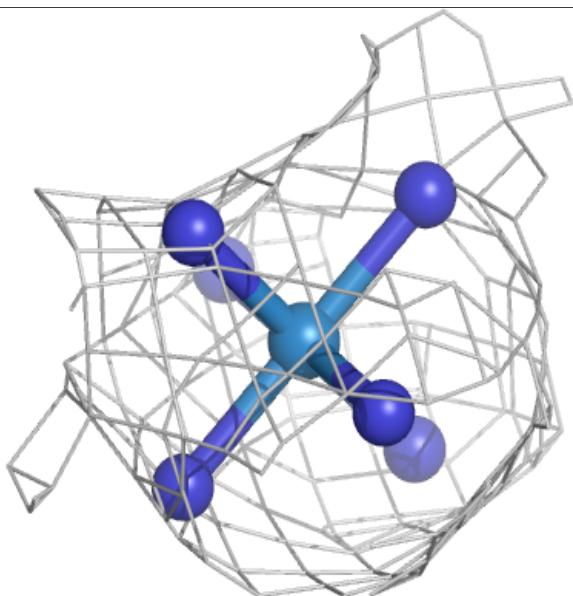
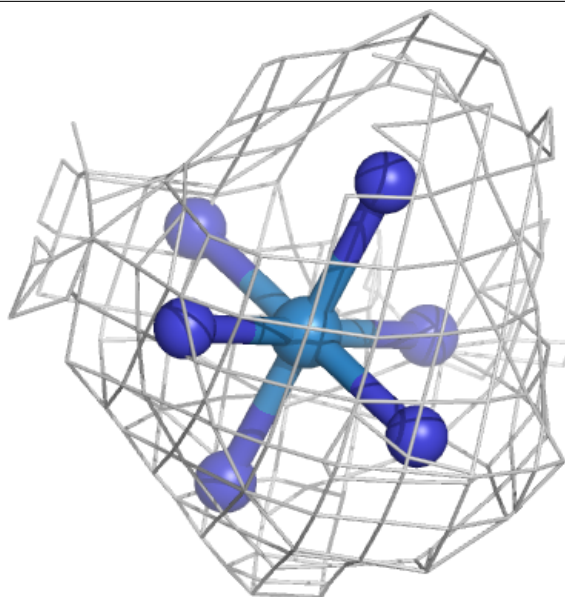
Electron density around OHX D1 3616:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



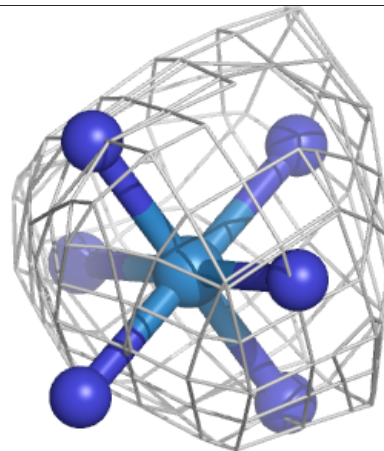
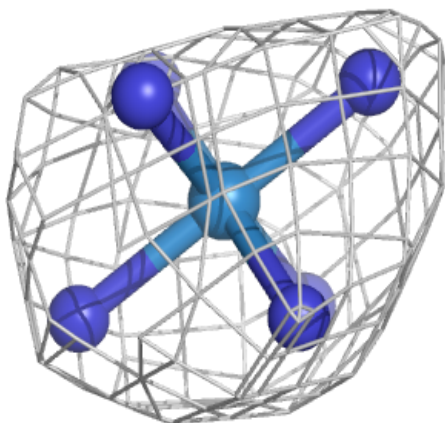
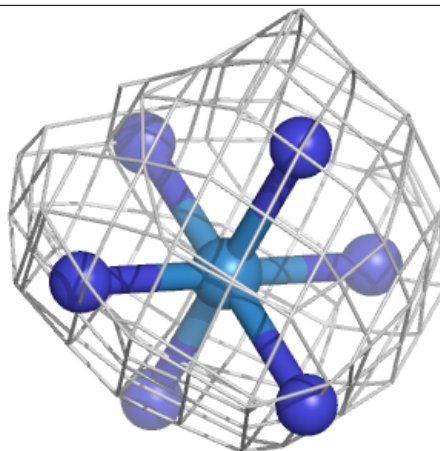
Electron density around OHX D1 3601:

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and green (positive)



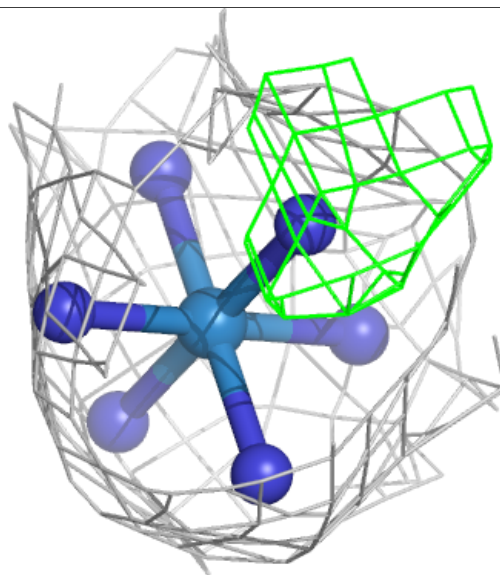
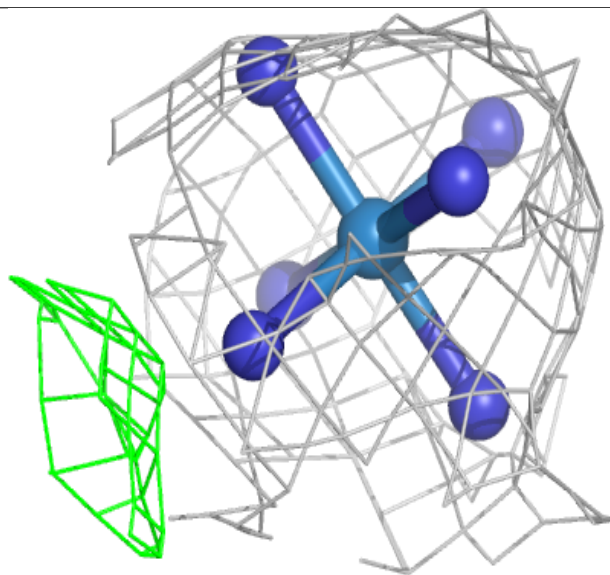
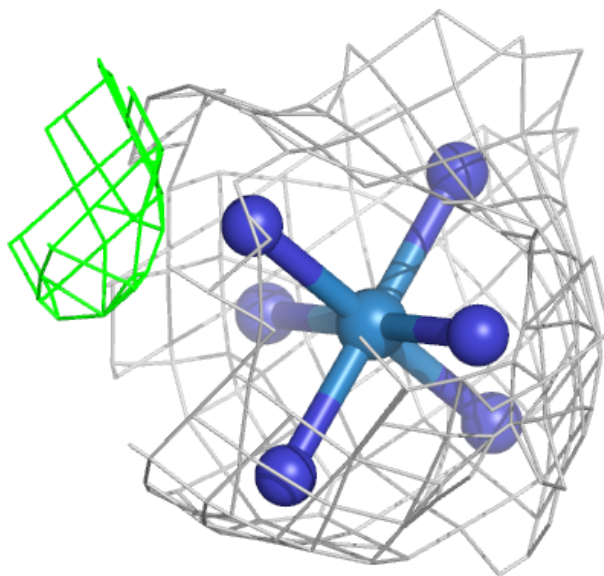
Electron density around OHX D1 3605:

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and green (positive)



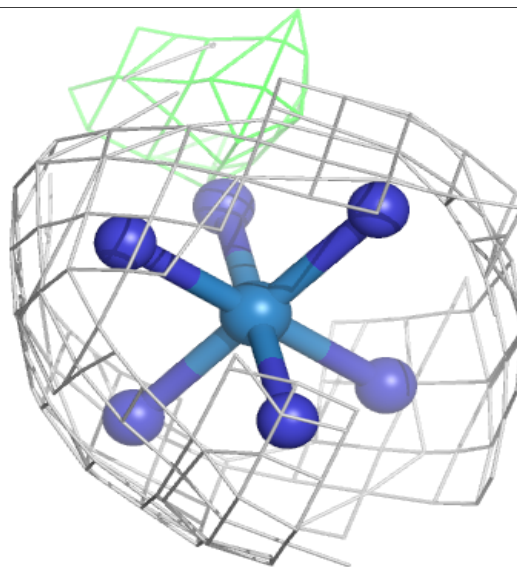
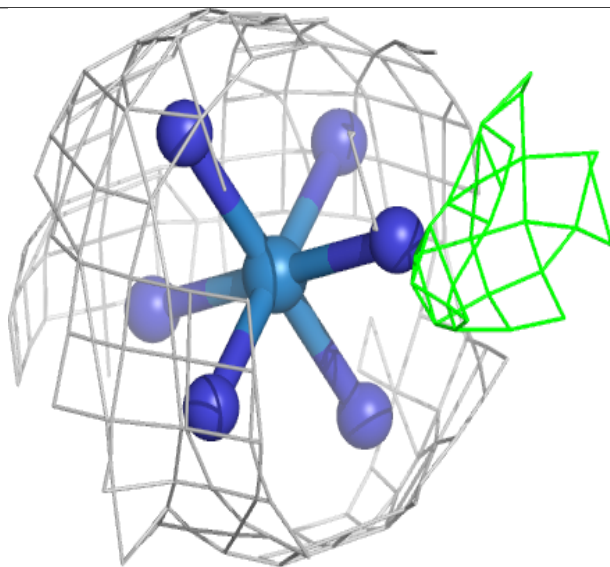
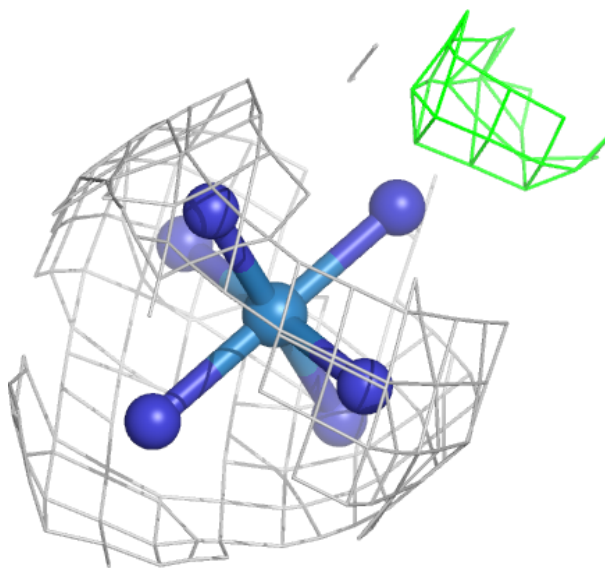
Electron density around OHX C1 1974:

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and green (positive)



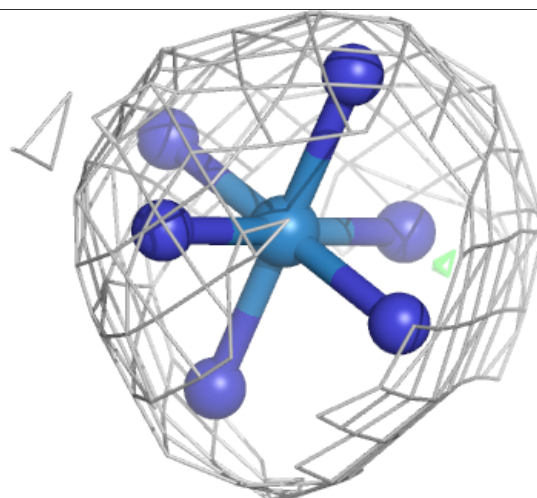
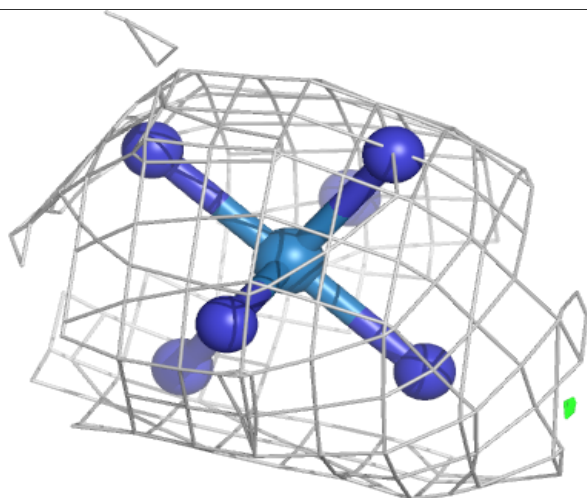
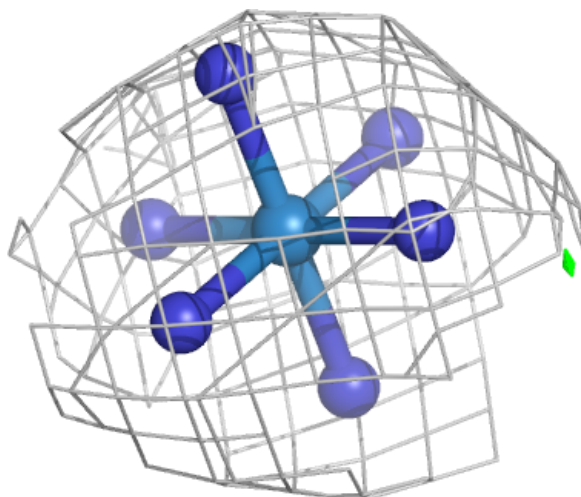
Electron density around OHX A1 1966:

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and green (positive)



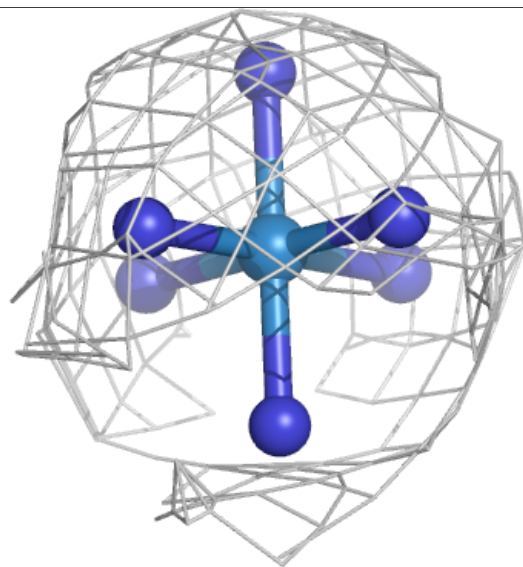
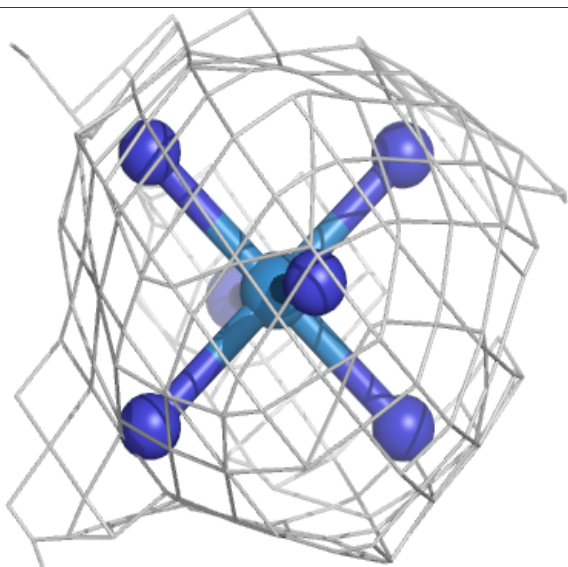
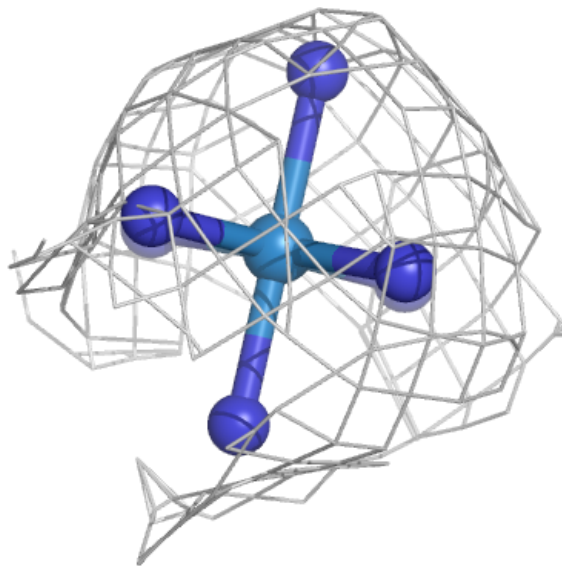
Electron density around OHX D1 3541:

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



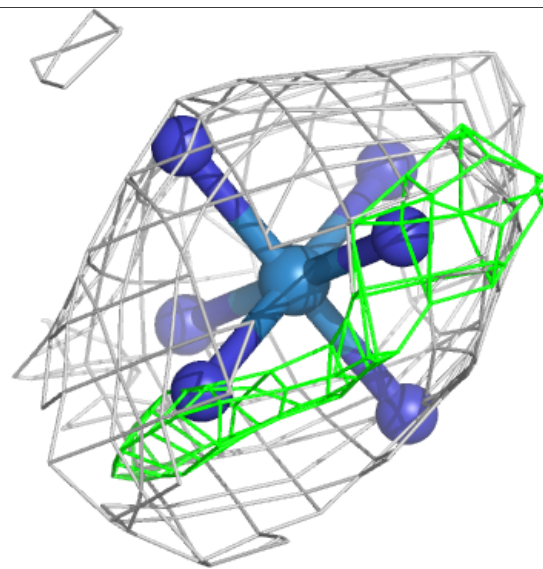
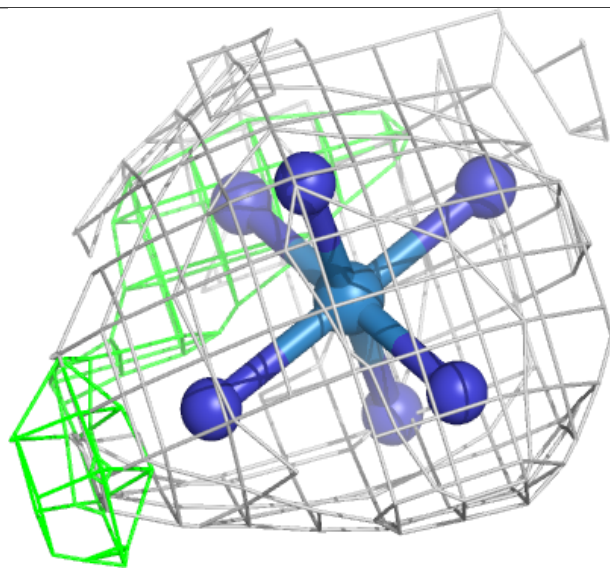
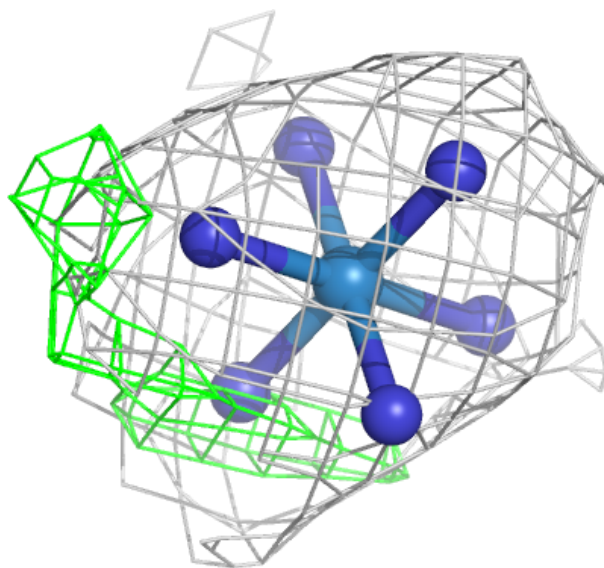
Electron density around OHX C1 1991:

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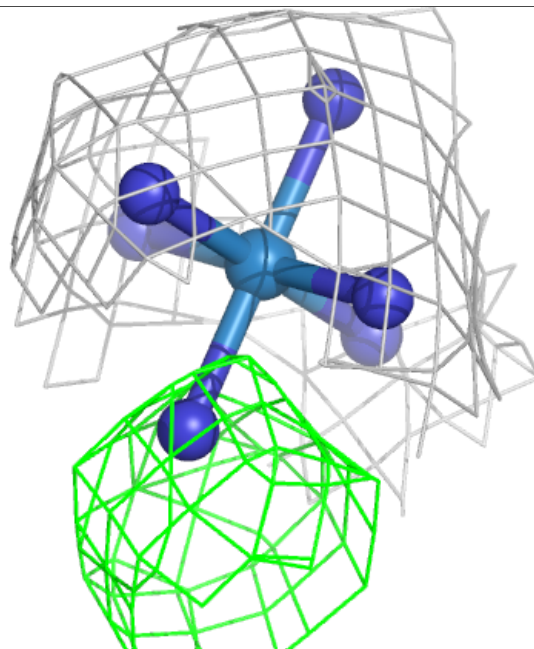
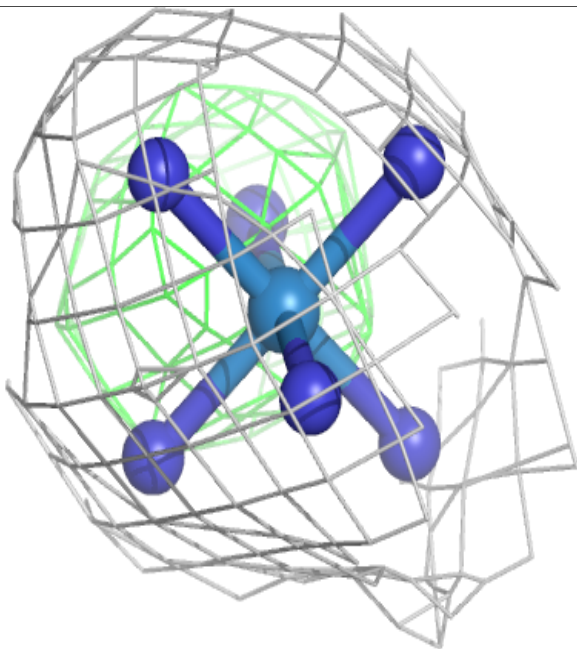
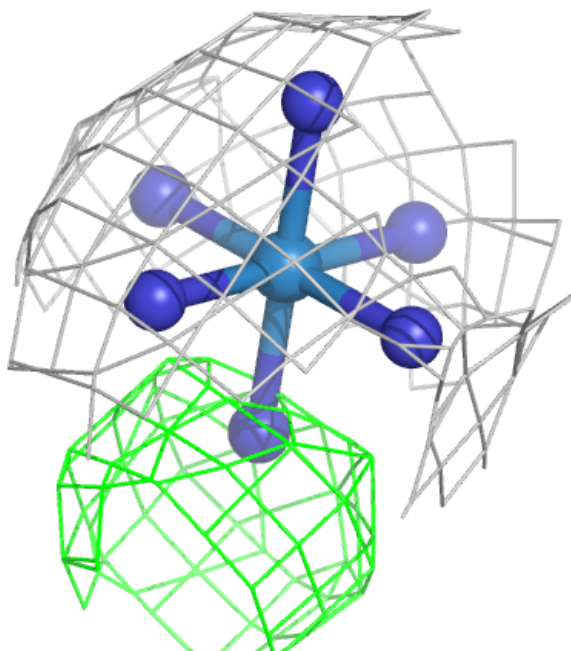
Electron density around OHX B1 3589:

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and green (positive)



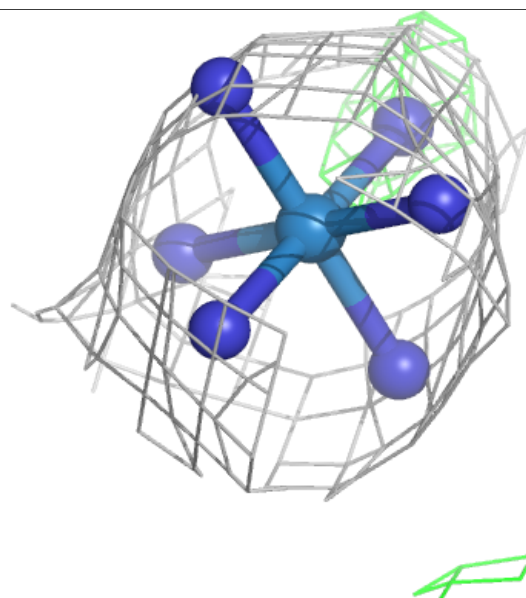
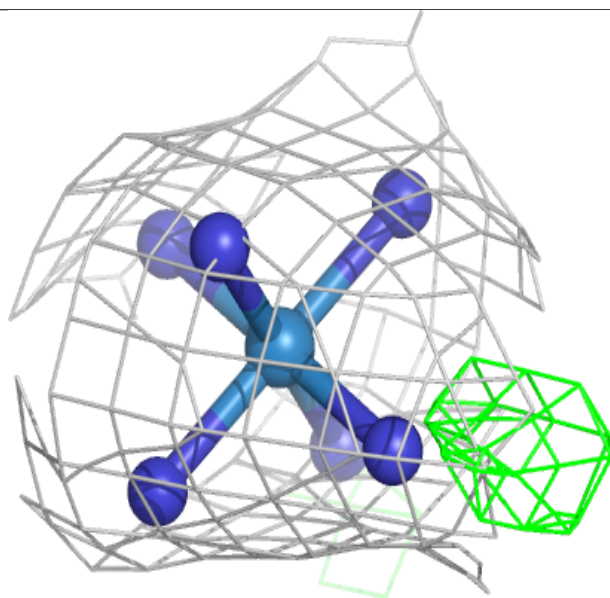
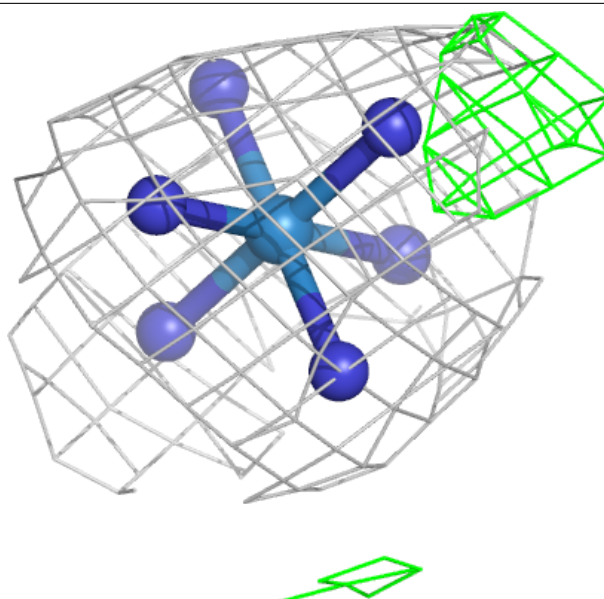
Electron density around OHX D3 206:

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



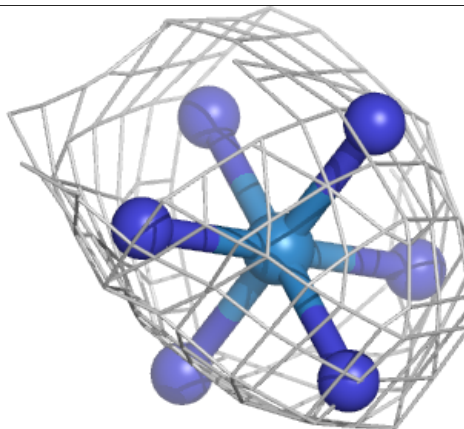
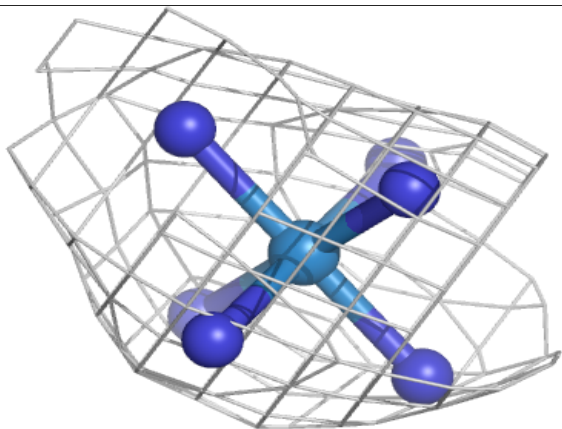
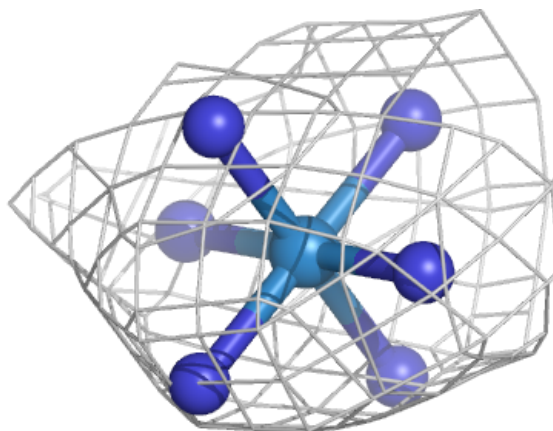
Electron density around OHX B2 208:

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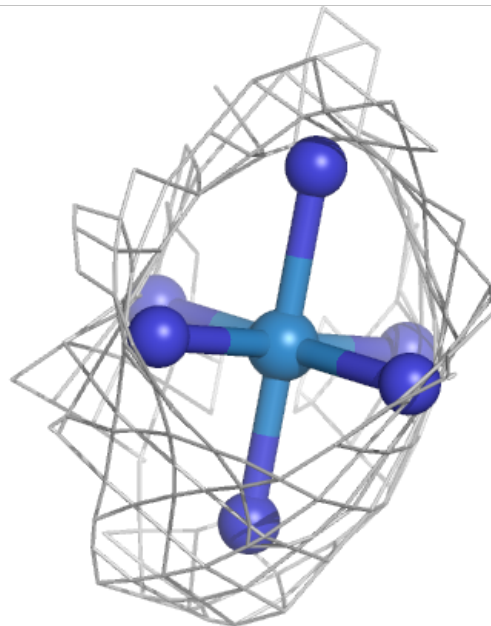
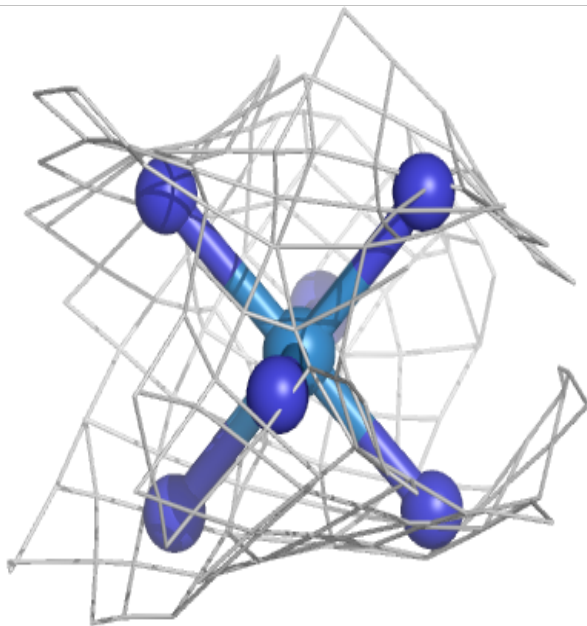
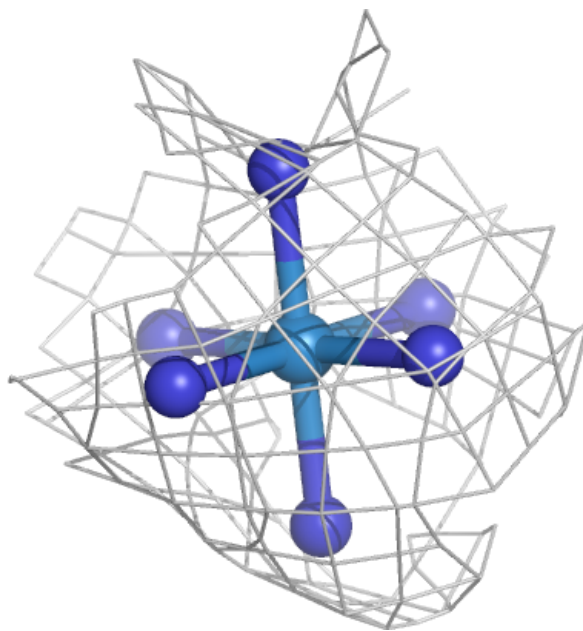
Electron density around OHX C1 1978:

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



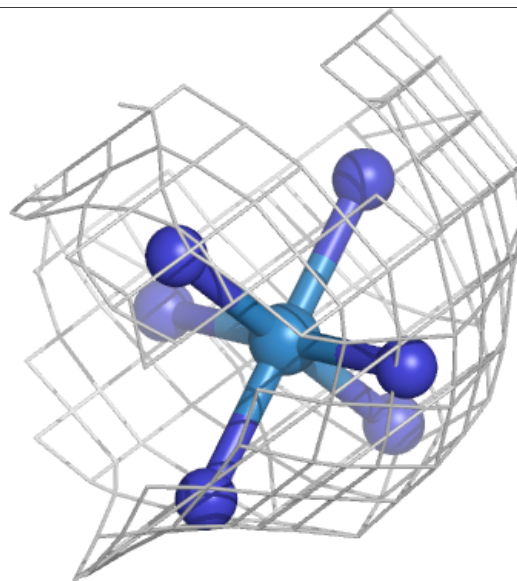
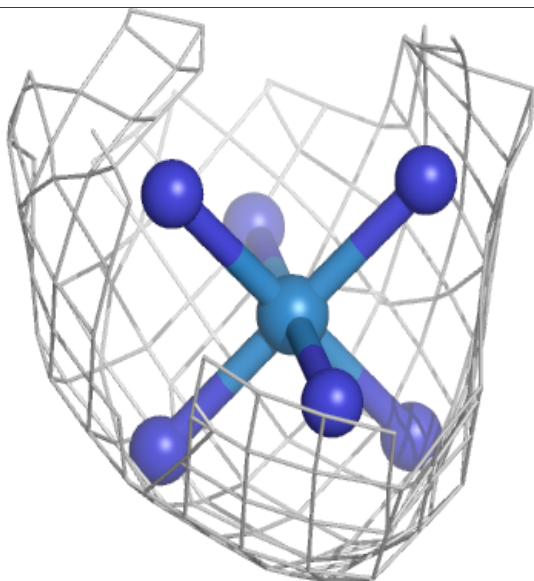
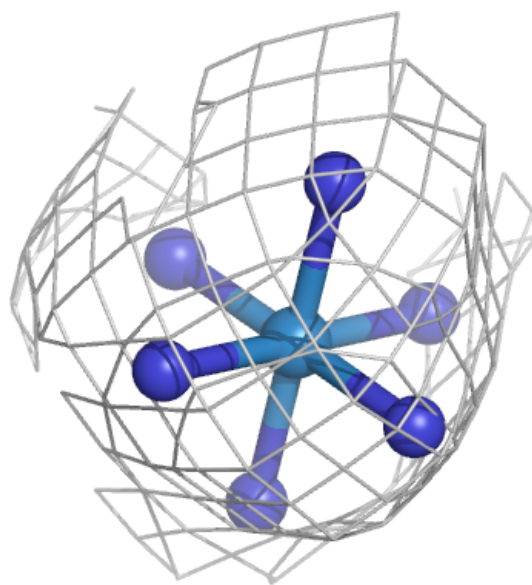
Electron density around OHX B2 210:

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



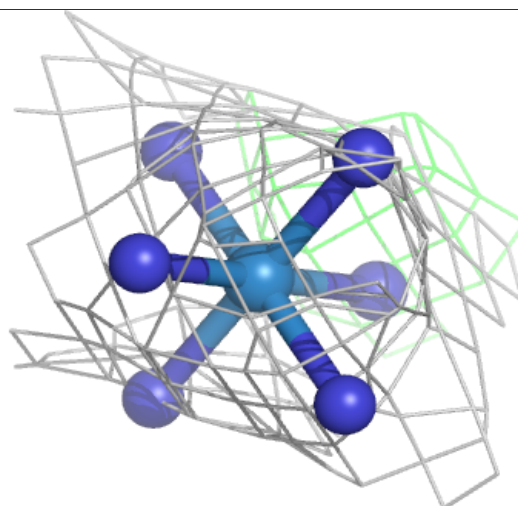
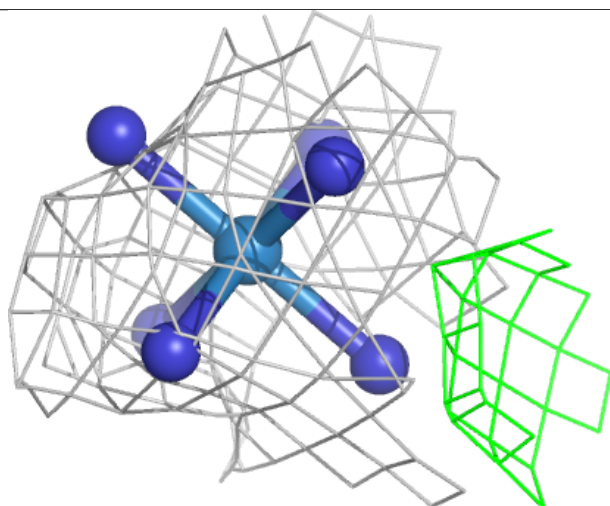
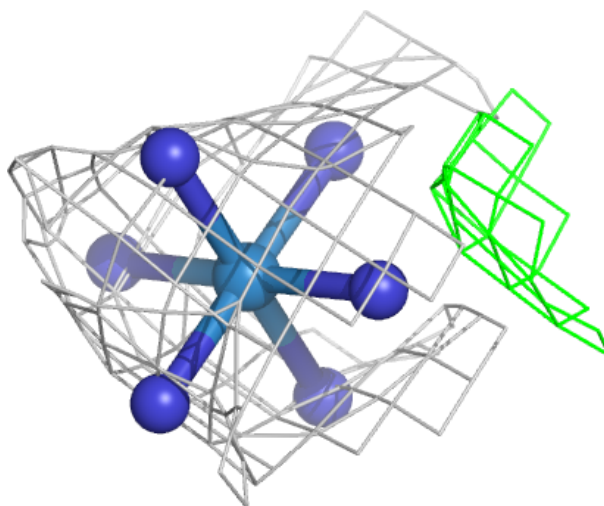
Electron density around OHX C1 1985:

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



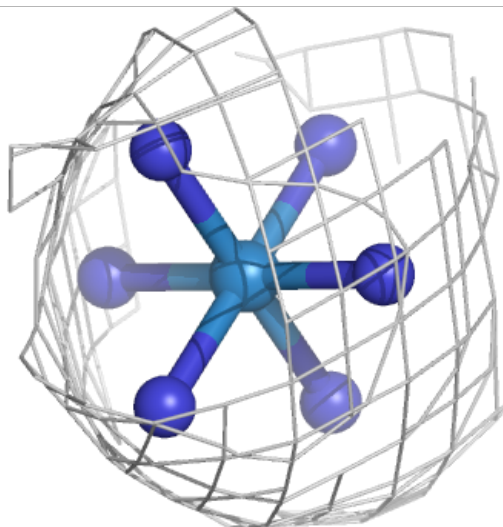
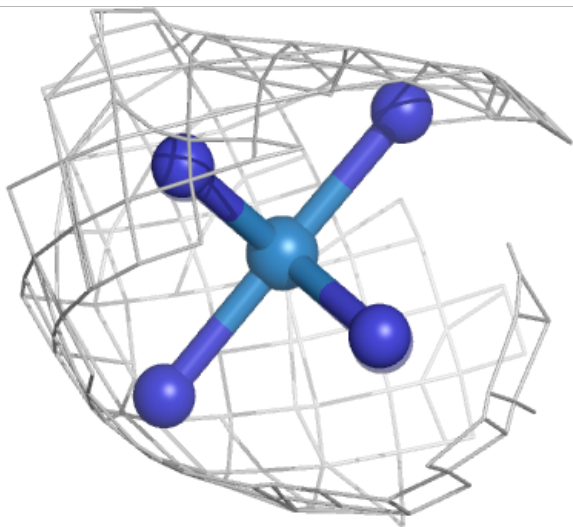
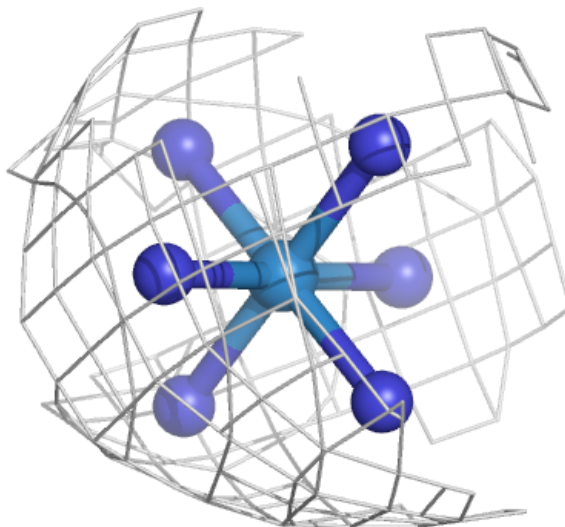
Electron density around OHX C1 1988:

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



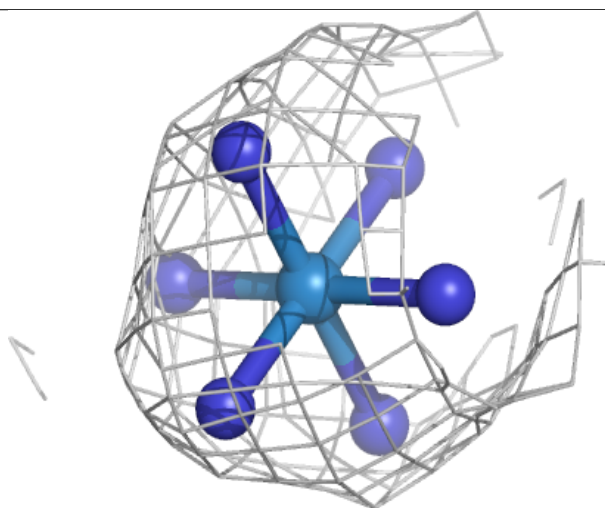
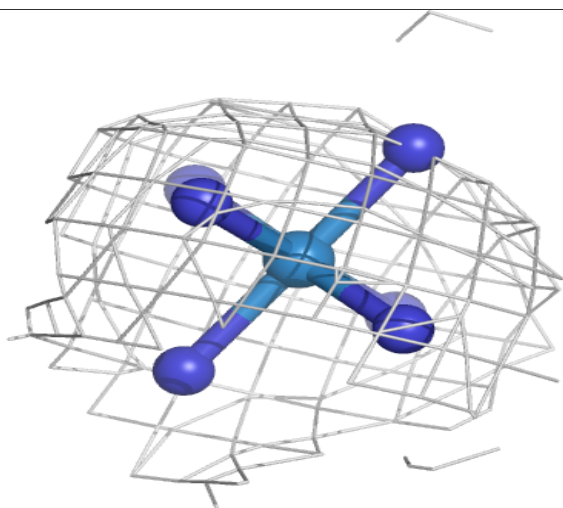
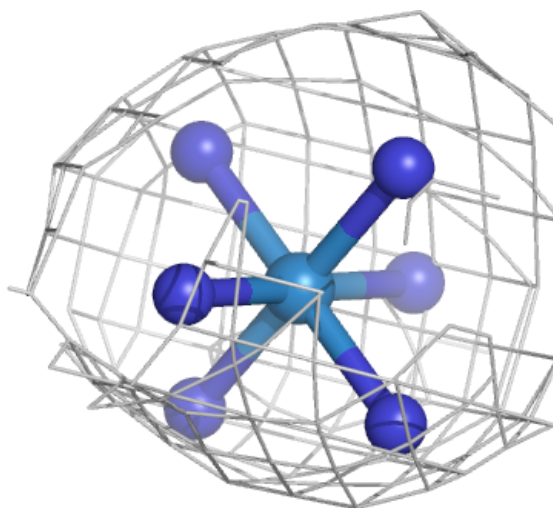
Electron density around OHX B2 207:

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



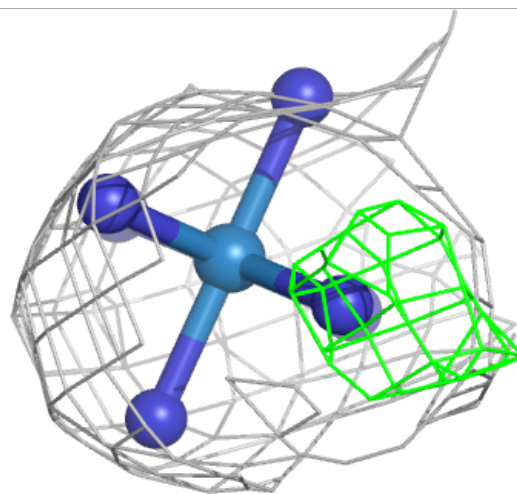
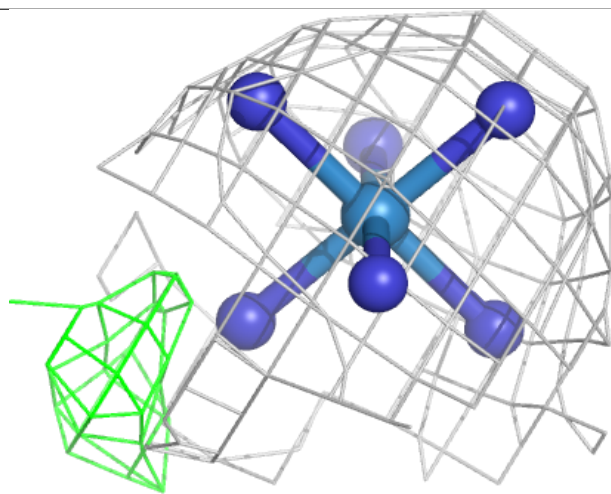
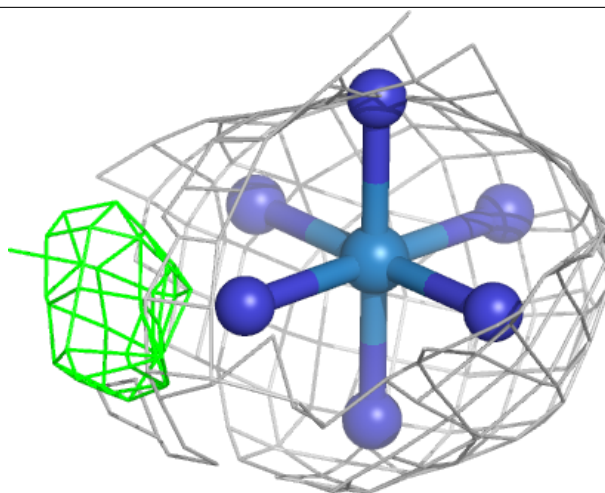
Electron density around OHX A1 1953:

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



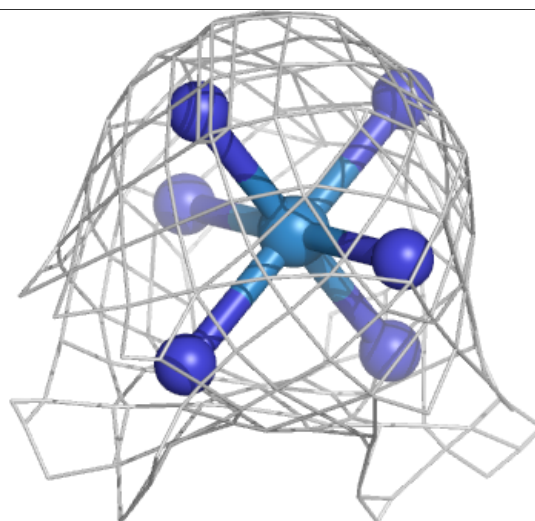
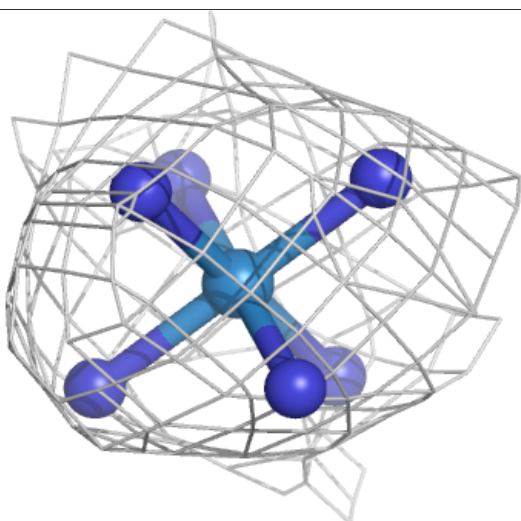
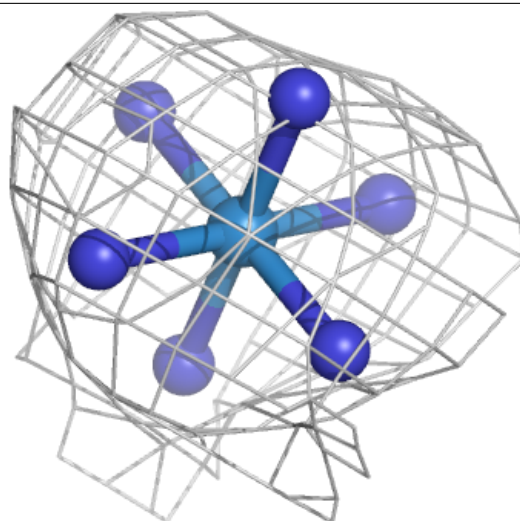
Electron density around OHX C1 1976:

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



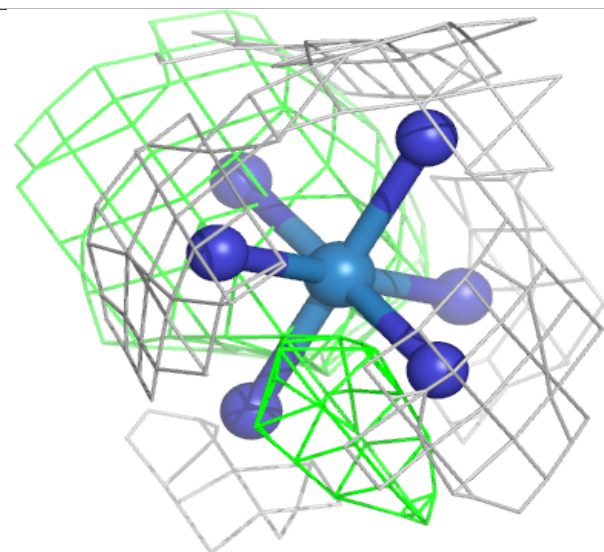
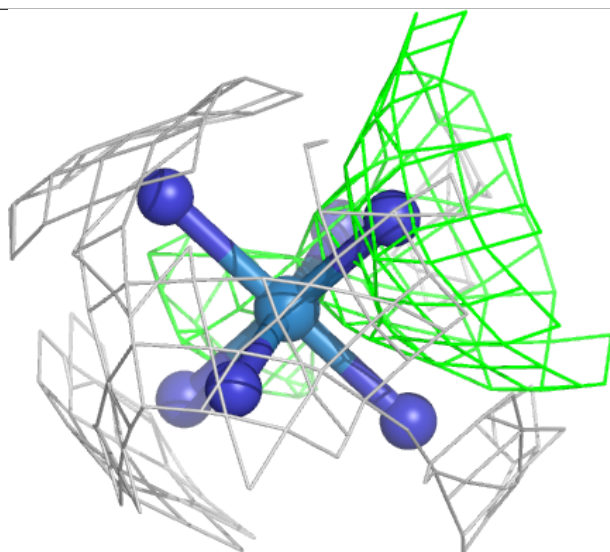
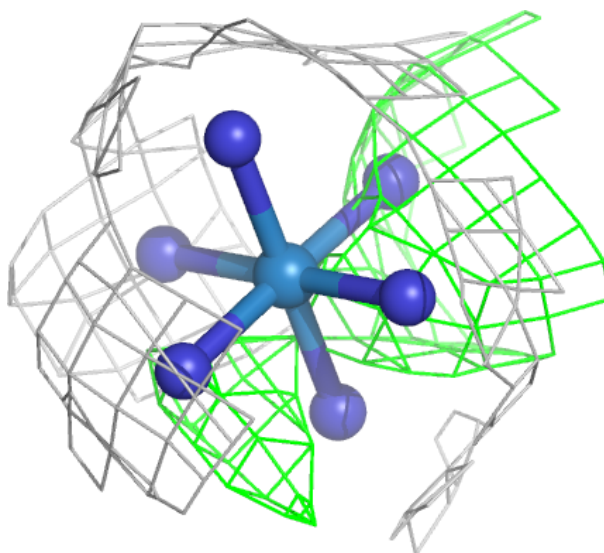
Electron density around OHX D1 3610:

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



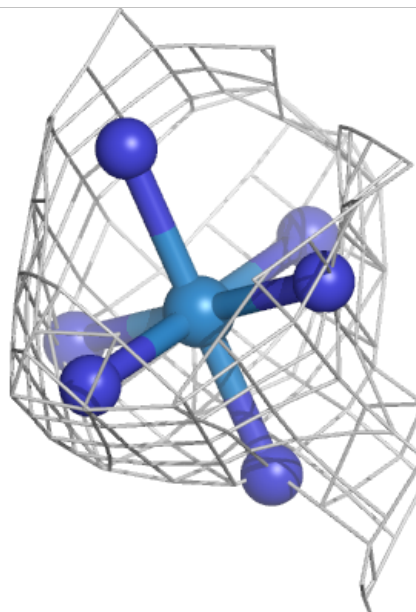
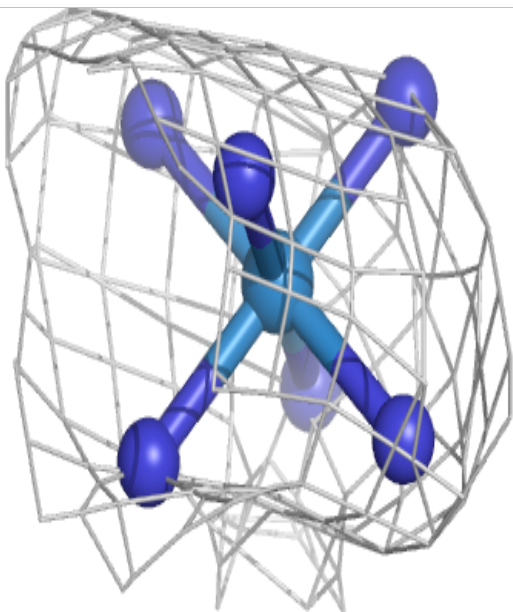
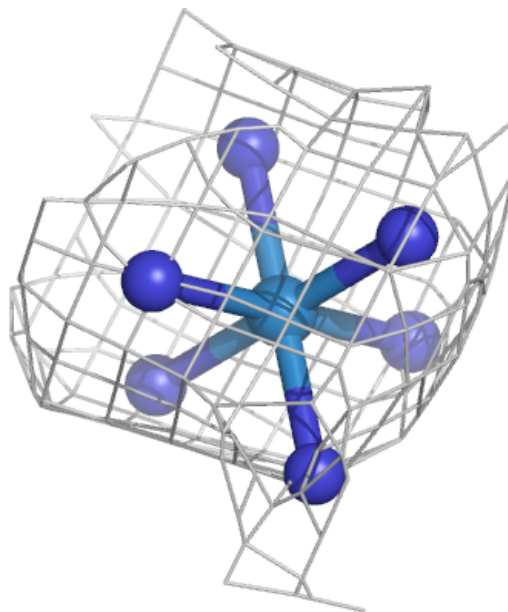
Electron density around OHX D1 3519:

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



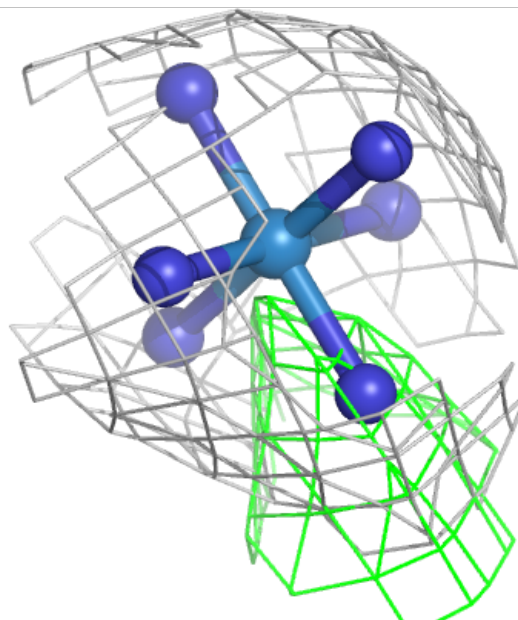
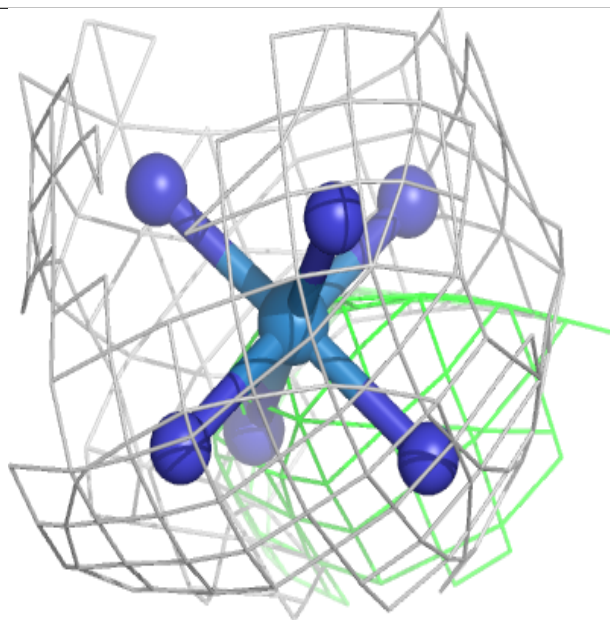
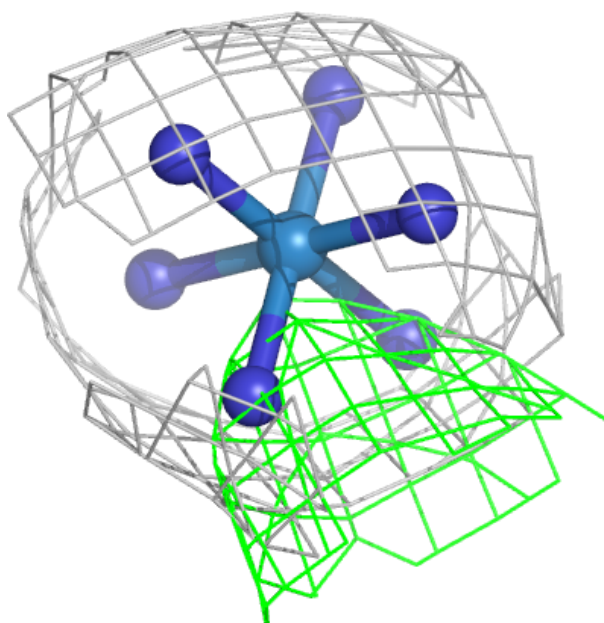
Electron density around OHX A1 1974:

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



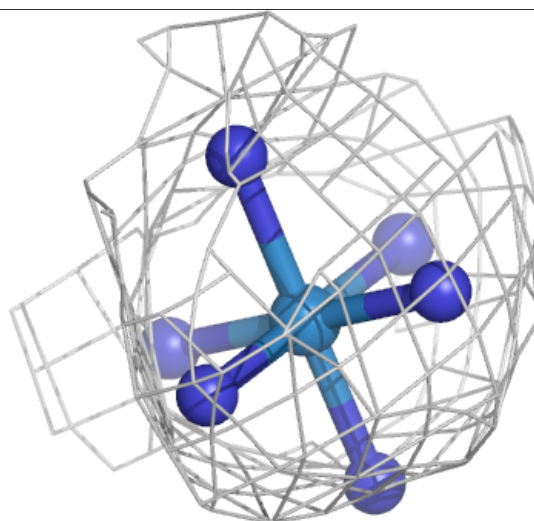
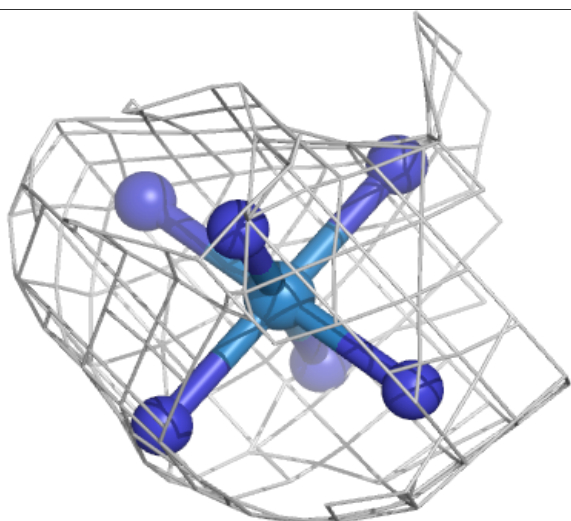
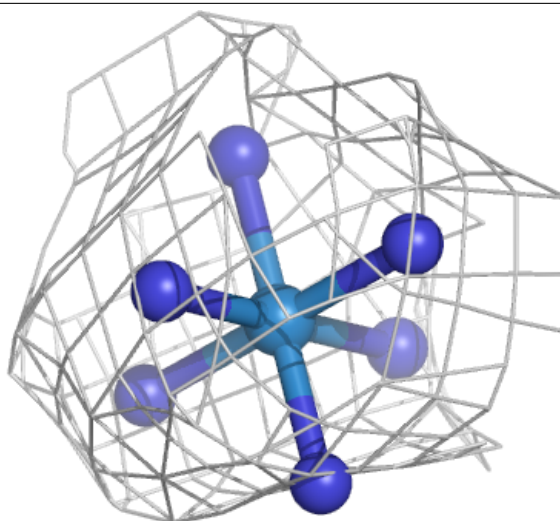
Electron density around OHX D1 3568:

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



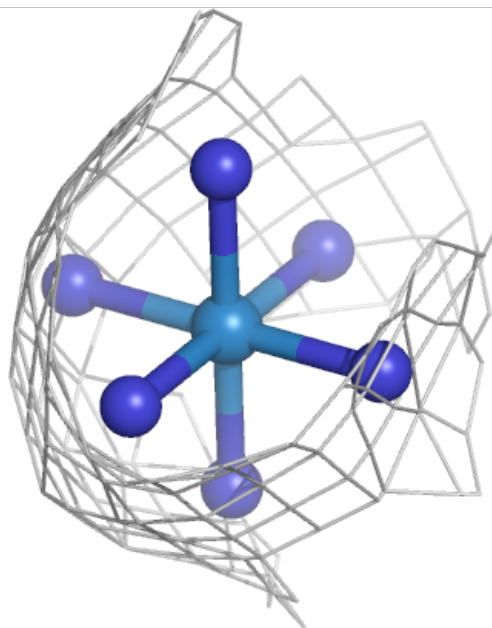
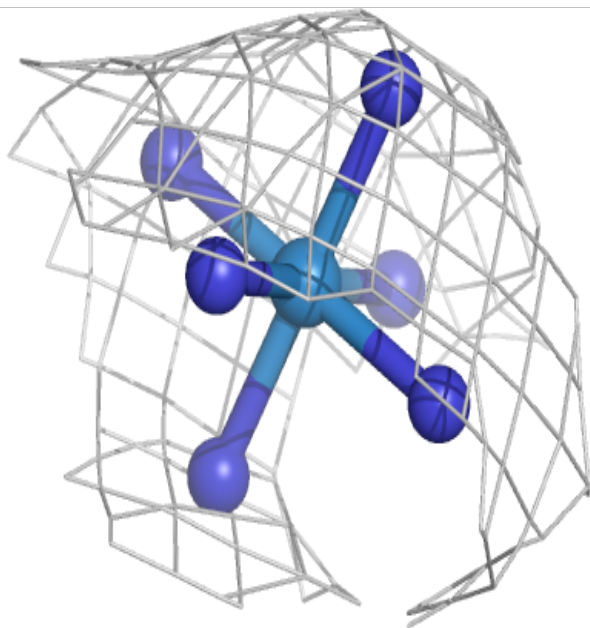
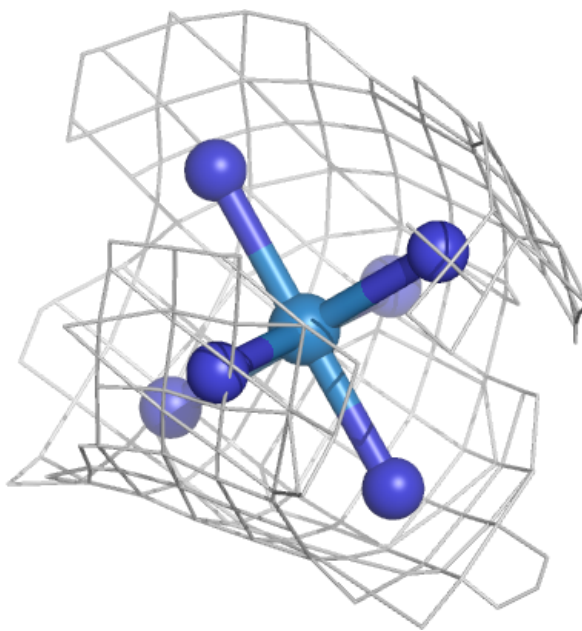
Electron density around OHX D1 3623:

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



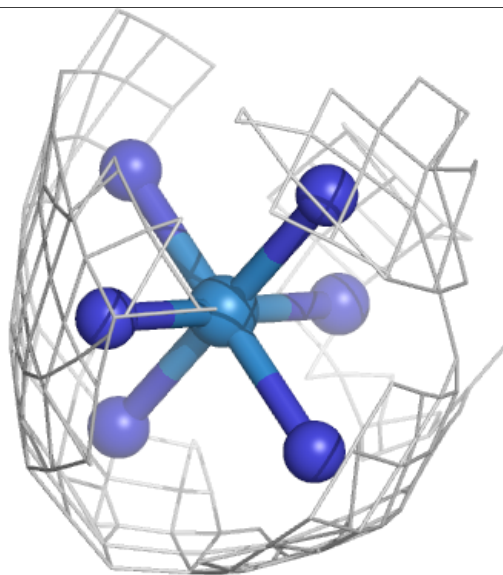
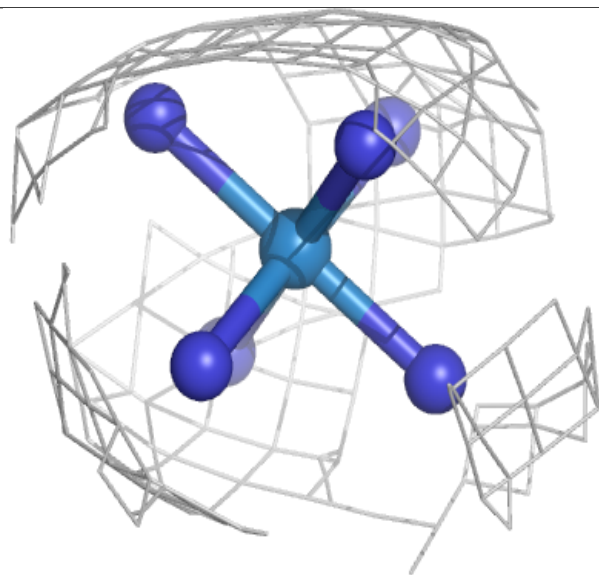
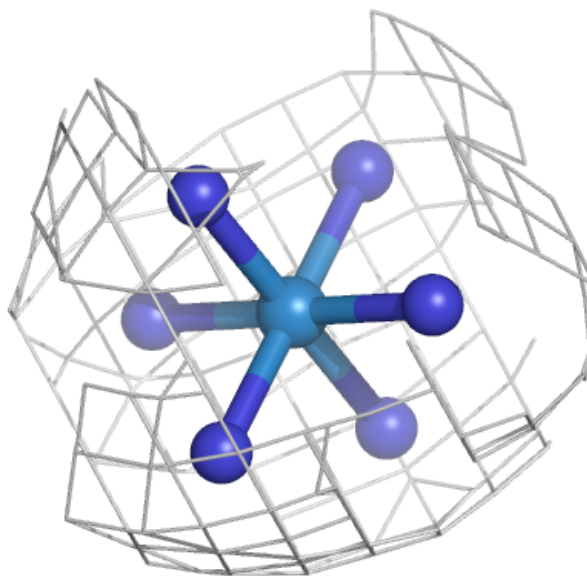
Electron density around OHX A1 1995:

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



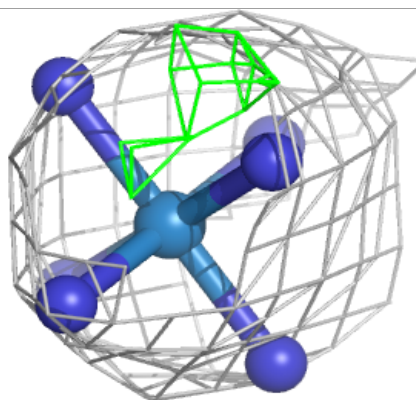
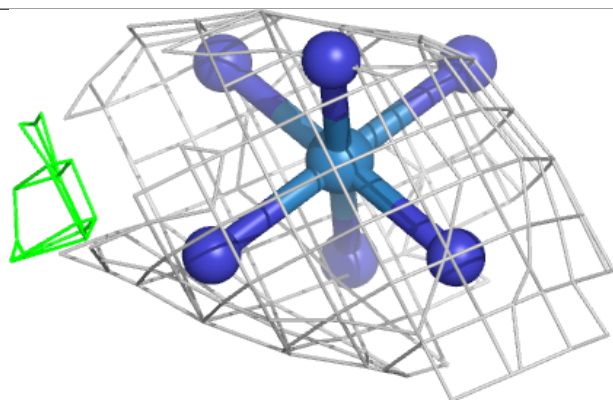
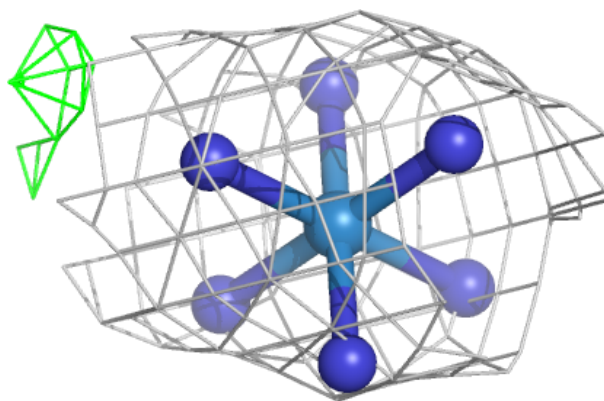
Electron density around OHX D1 3603:

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



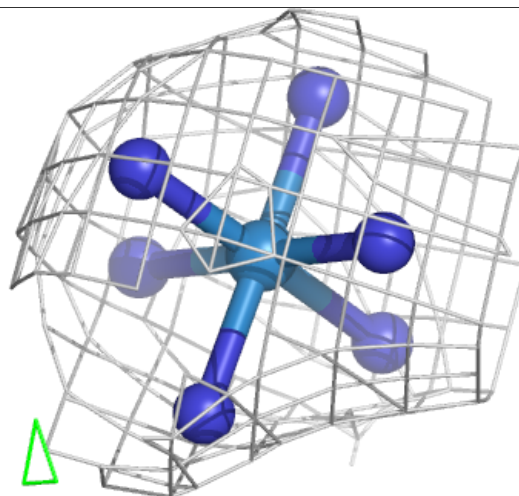
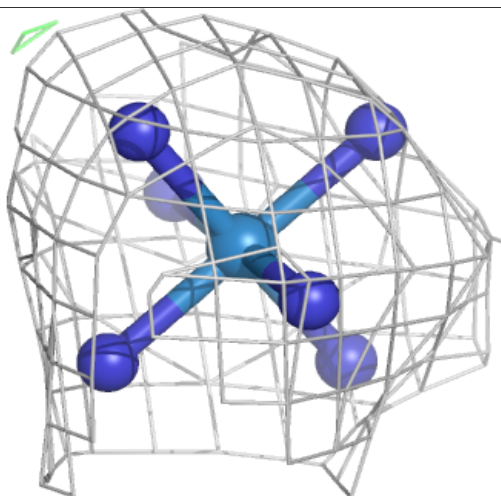
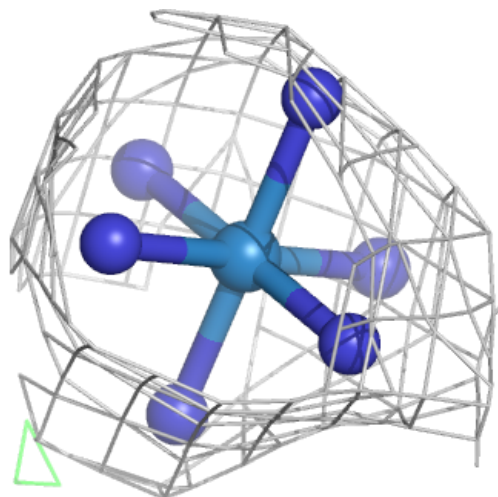
Electron density around OHX D1 3522:

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



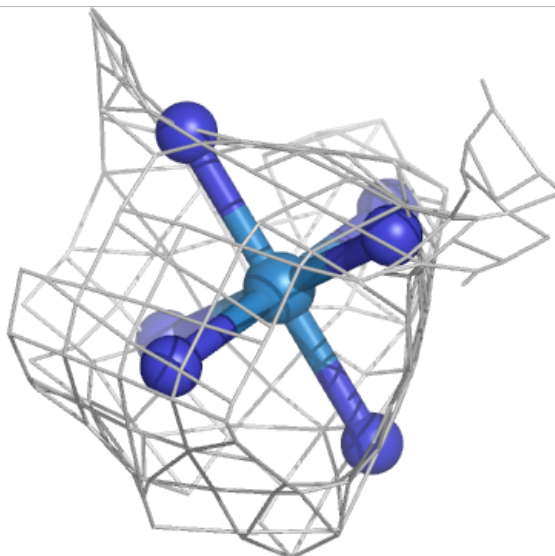
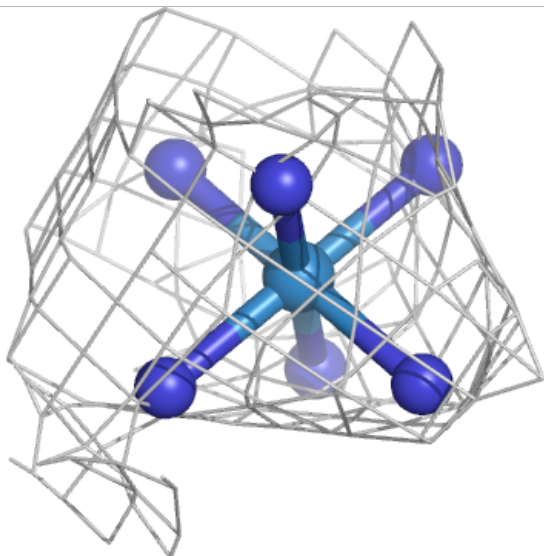
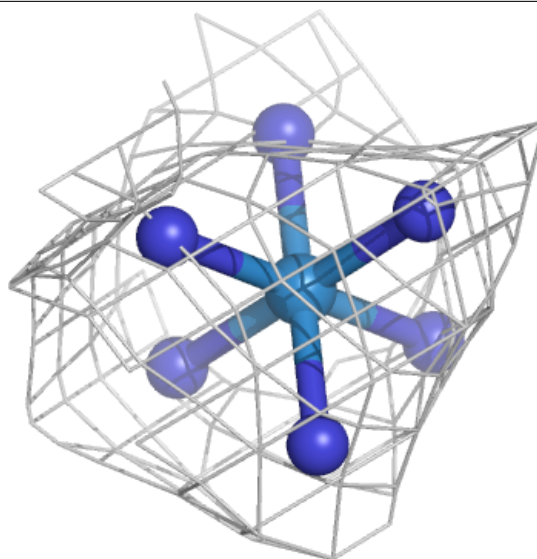
Electron density around OHX D1 3555:

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



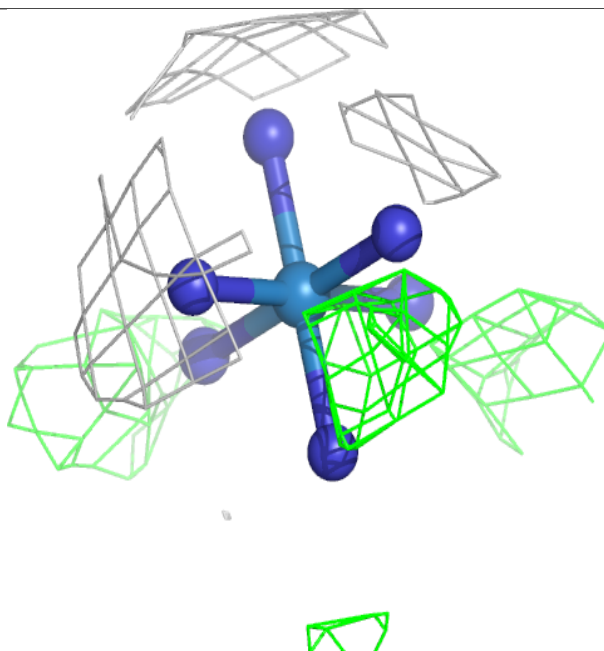
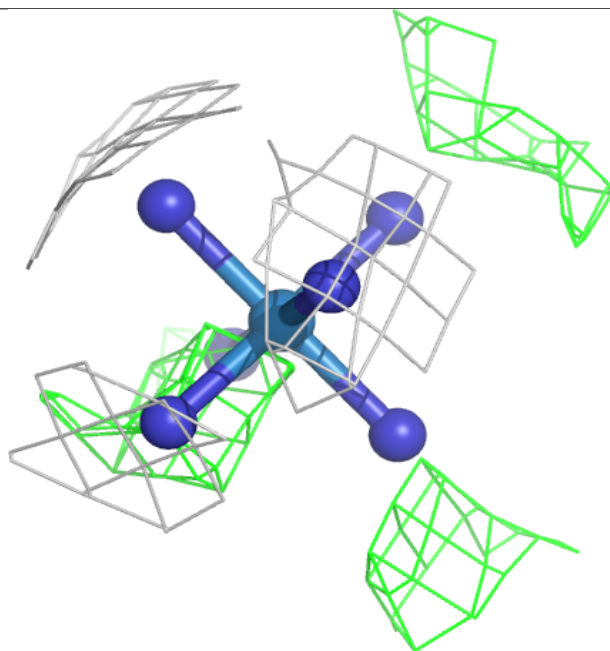
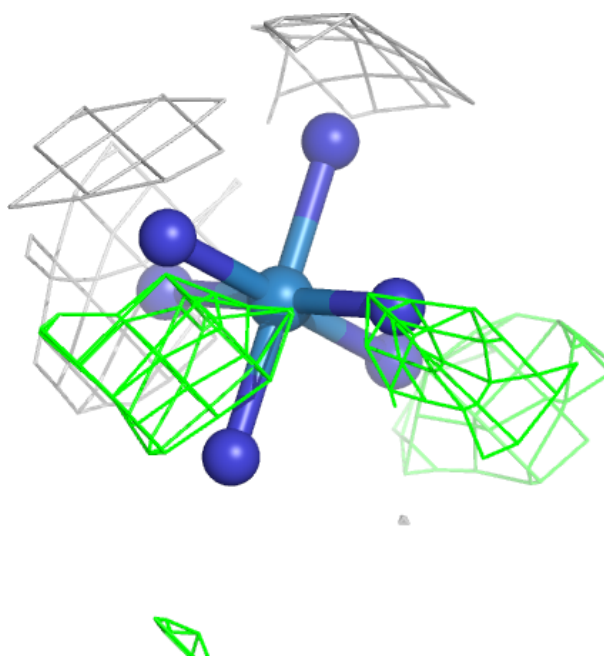
Electron density around OHX A1 1978:

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



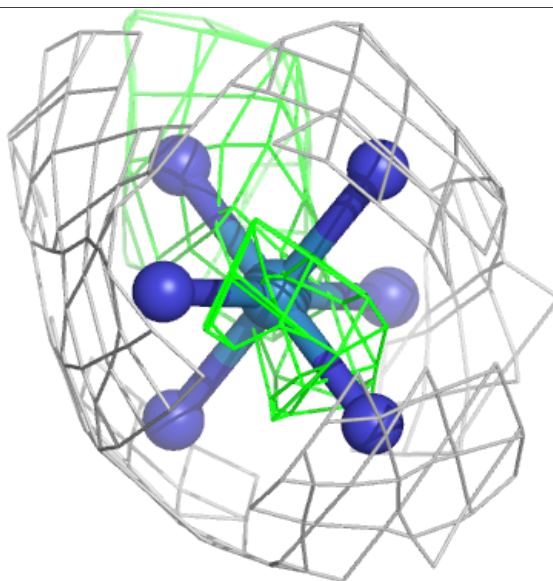
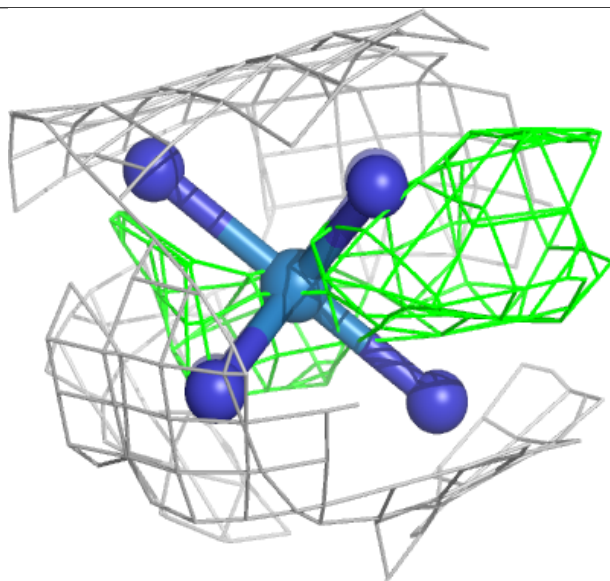
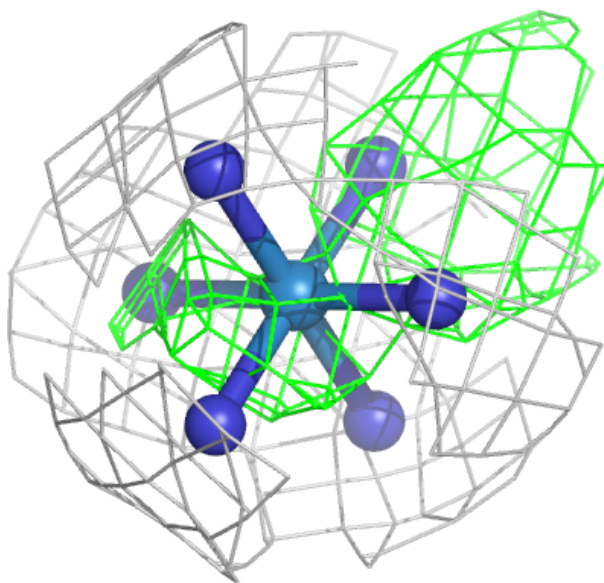
Electron density around OHX D1 3578:

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



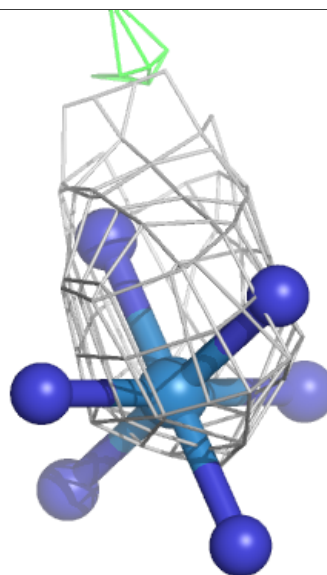
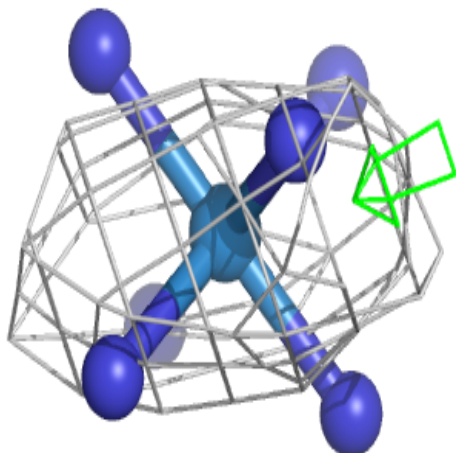
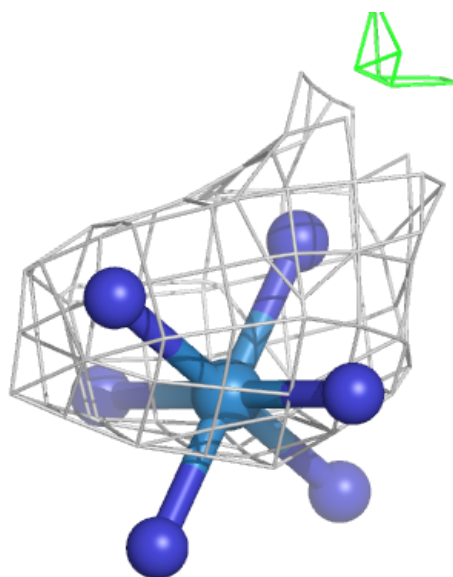
Electron density around OHX D1 3506:

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



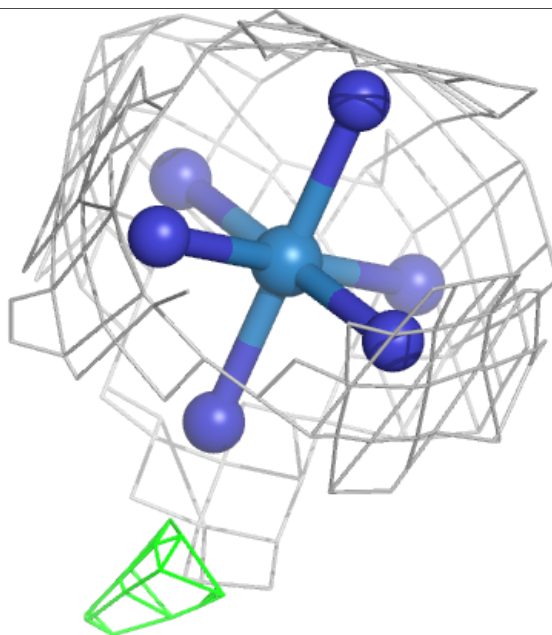
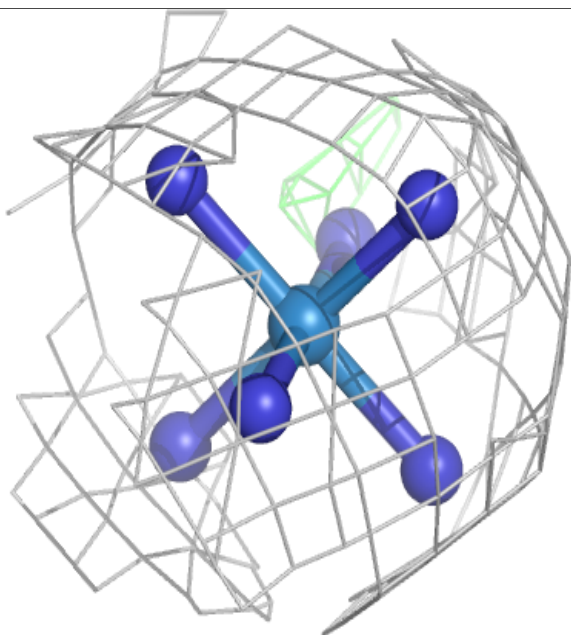
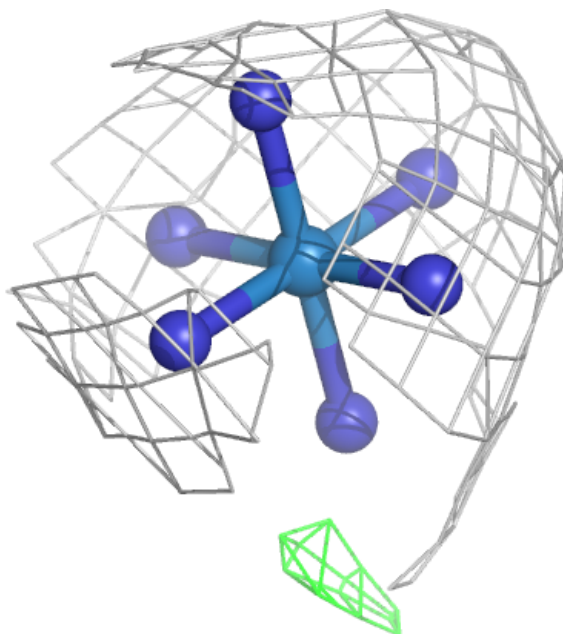
Electron density around OHX D1 3593:

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



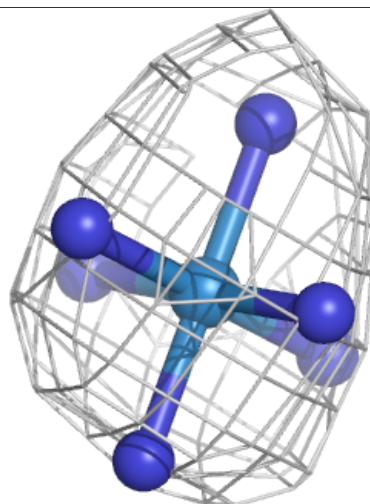
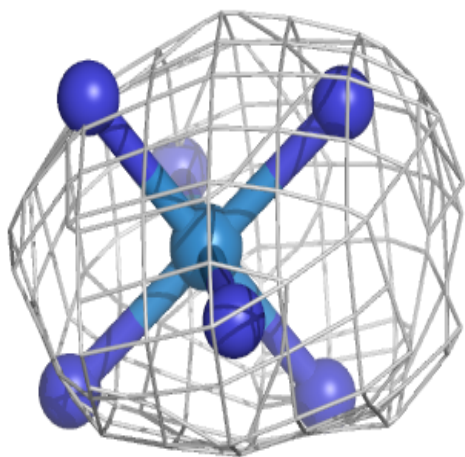
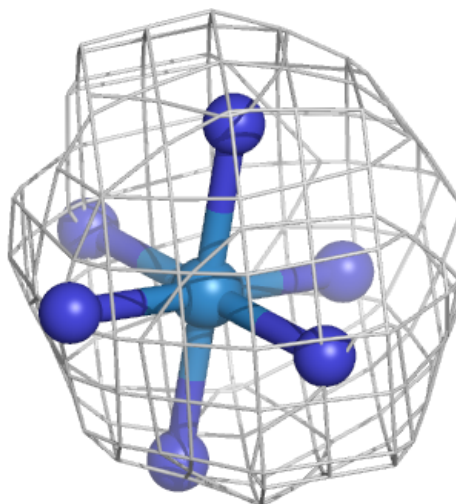
Electron density around OHX B1 3545:

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



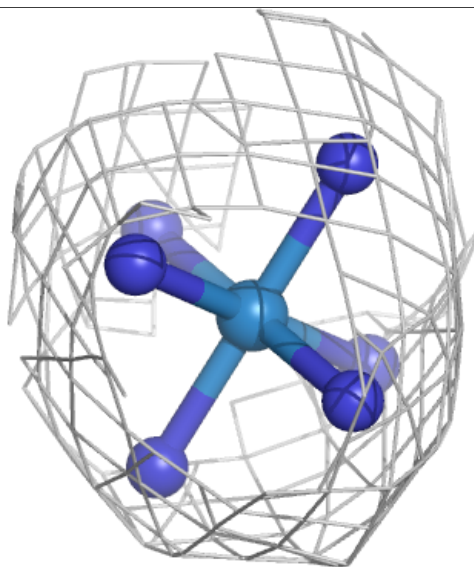
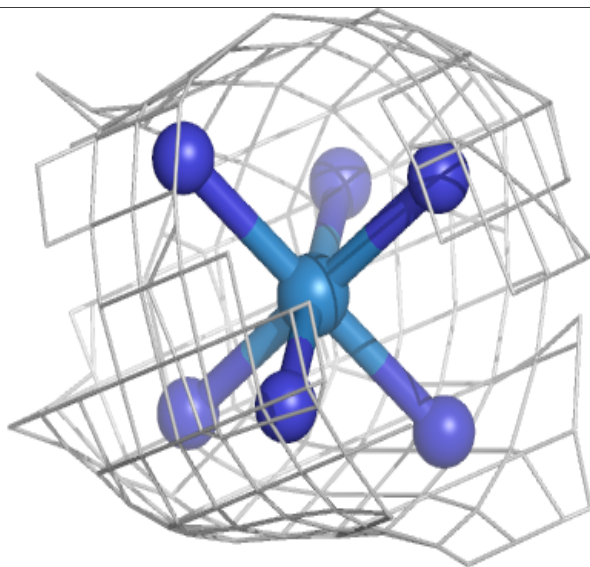
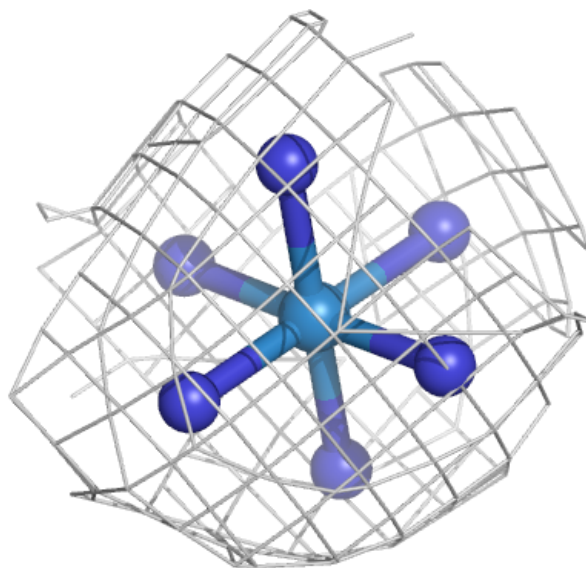
Electron density around OHX D1 3587:

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



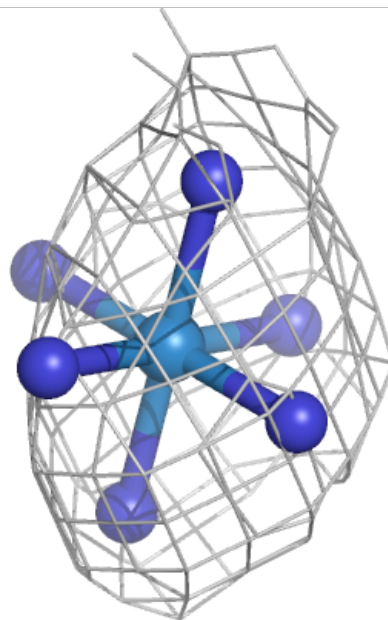
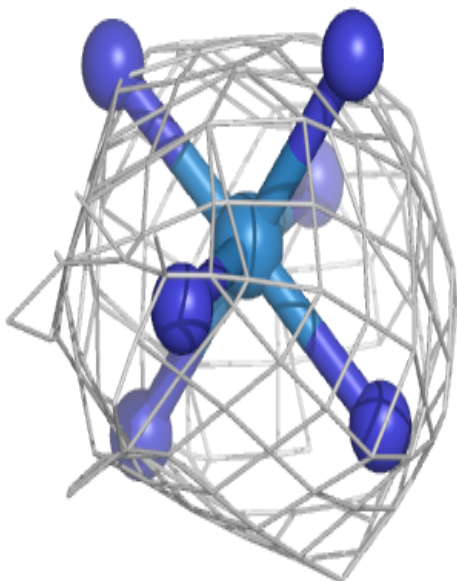
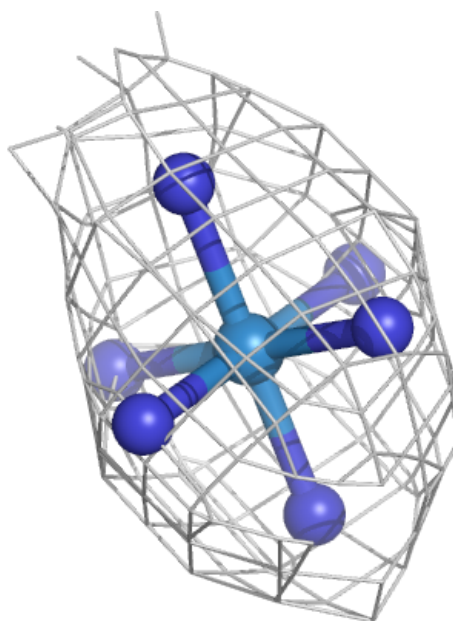
Electron density around OHX B1 3533:

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



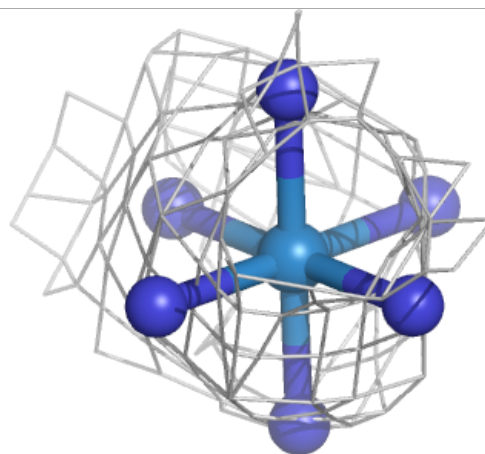
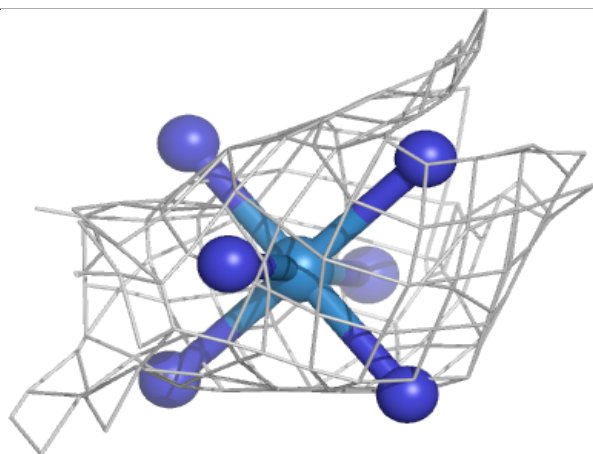
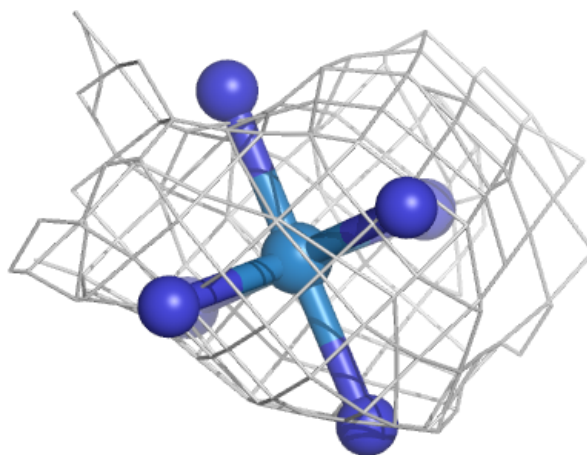
Electron density around OHX BO 301:

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



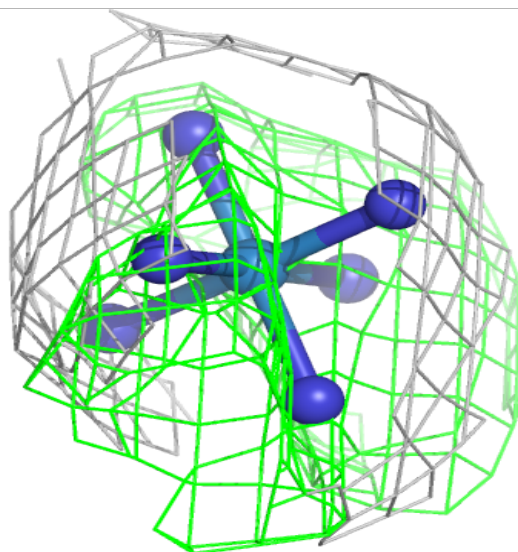
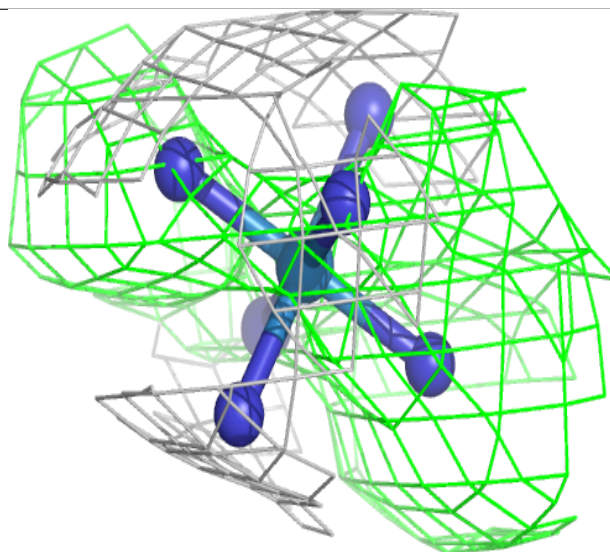
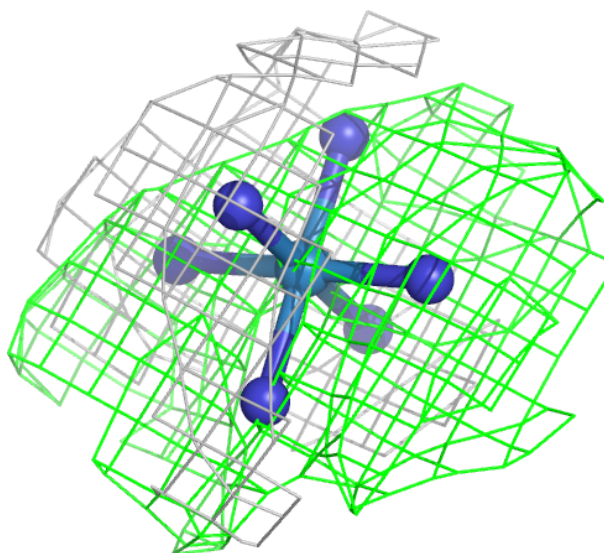
Electron density around OHX A1 1996:

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



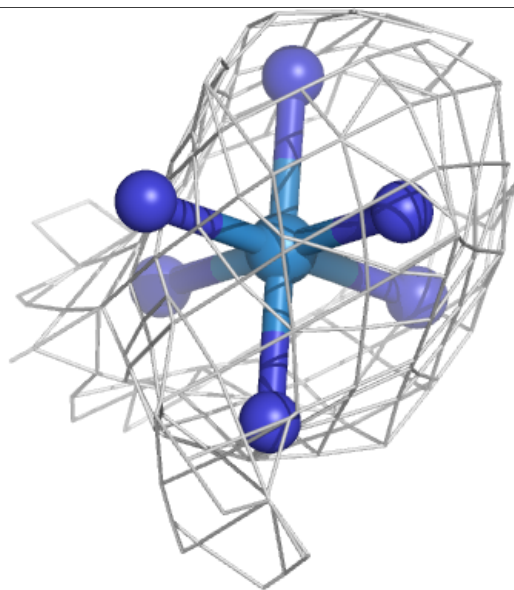
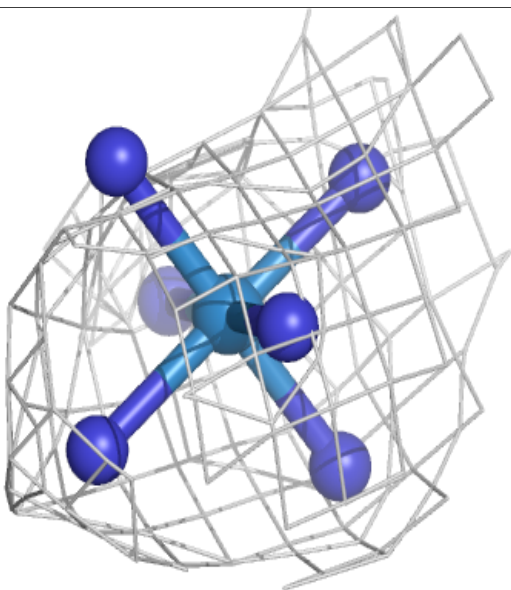
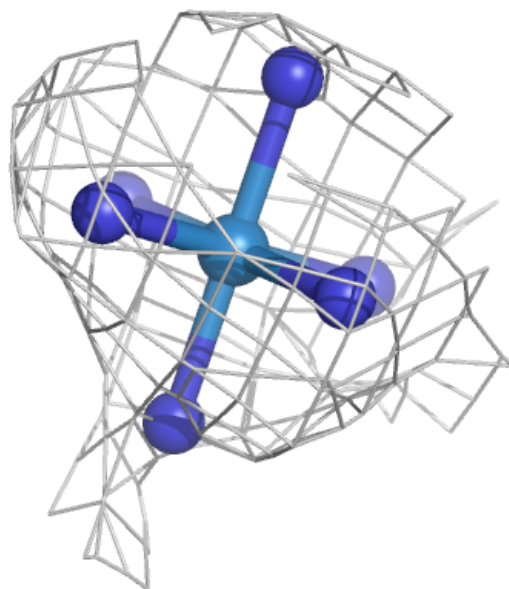
Electron density around OHX B1 3515:

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



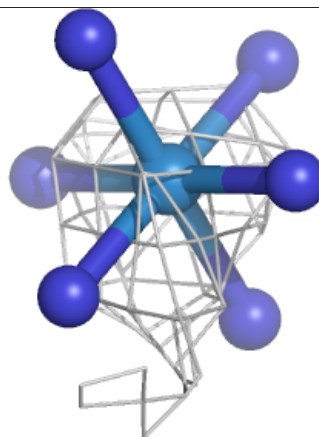
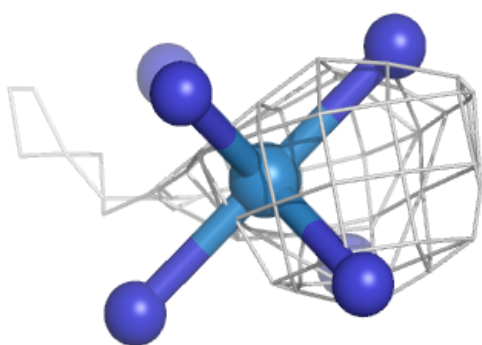
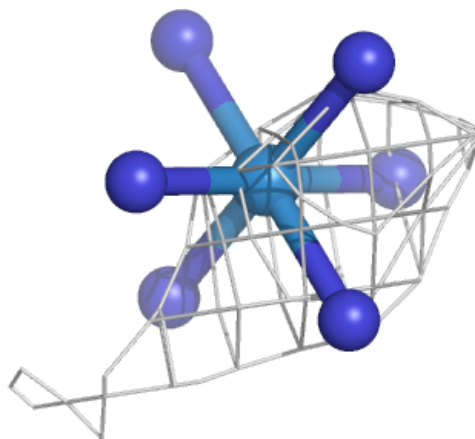
Electron density around OHX C1 1957:

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



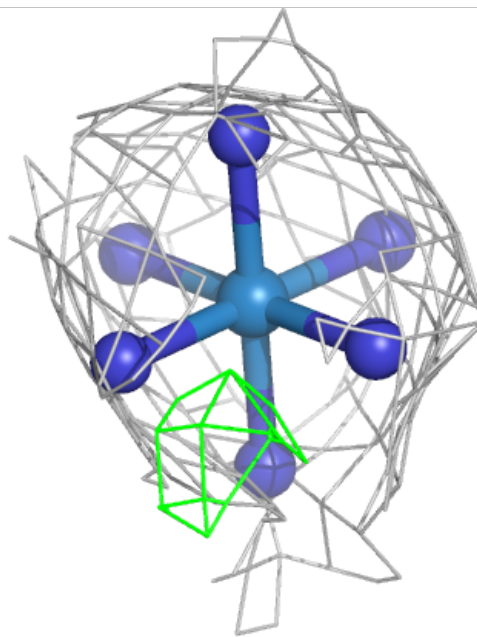
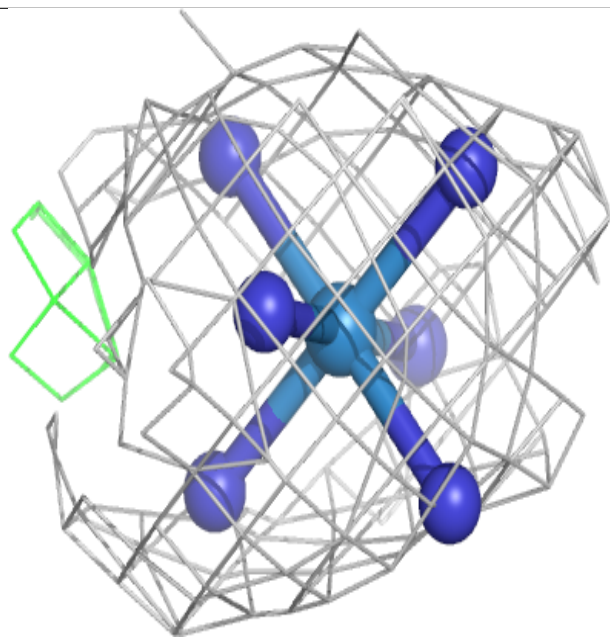
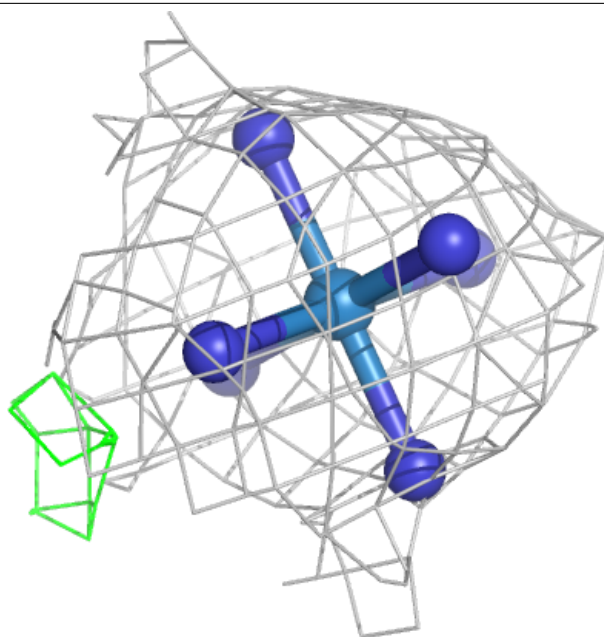
Electron density around OHX A1 1998:

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



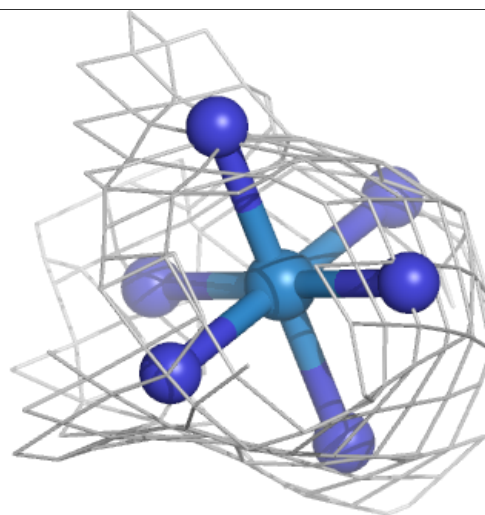
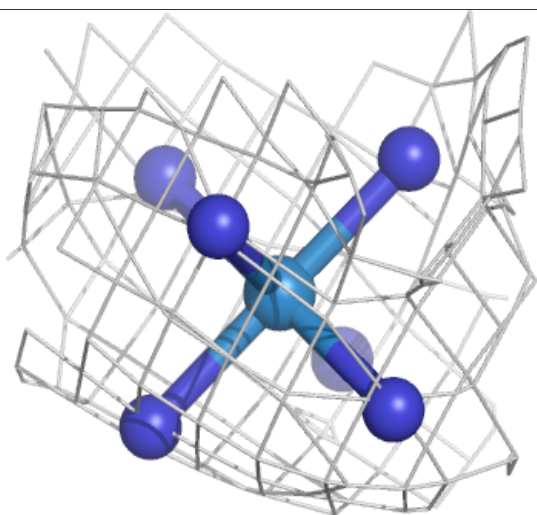
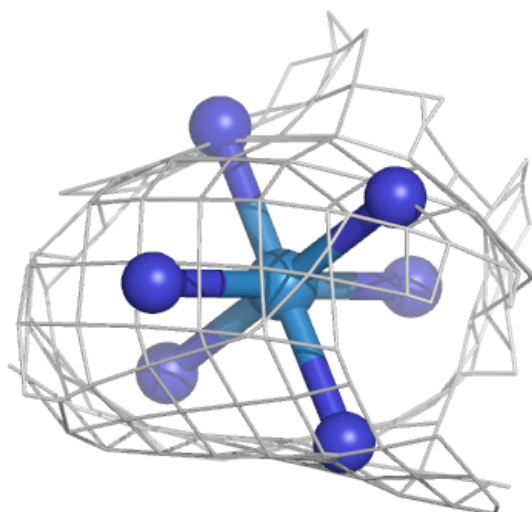
Electron density around OHX B1 3584:

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



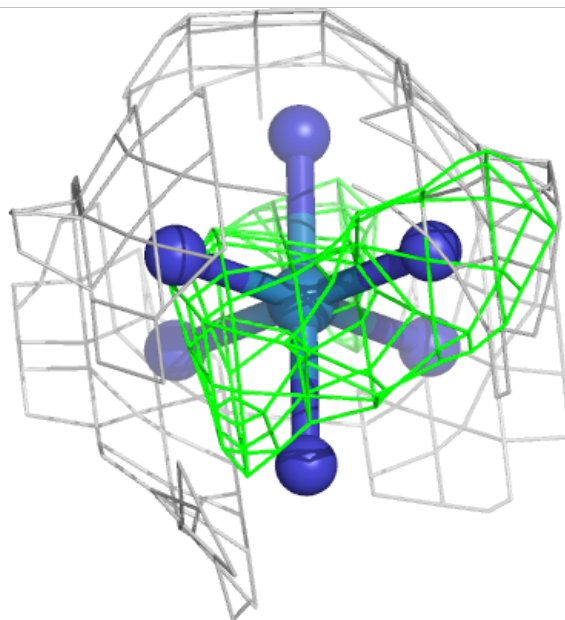
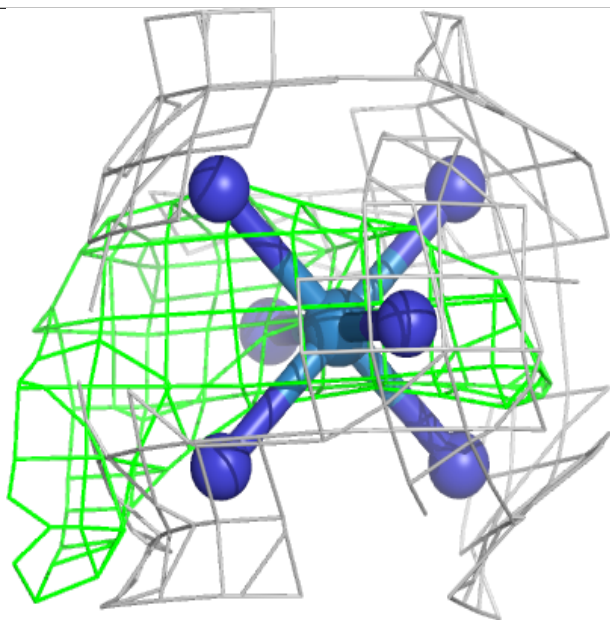
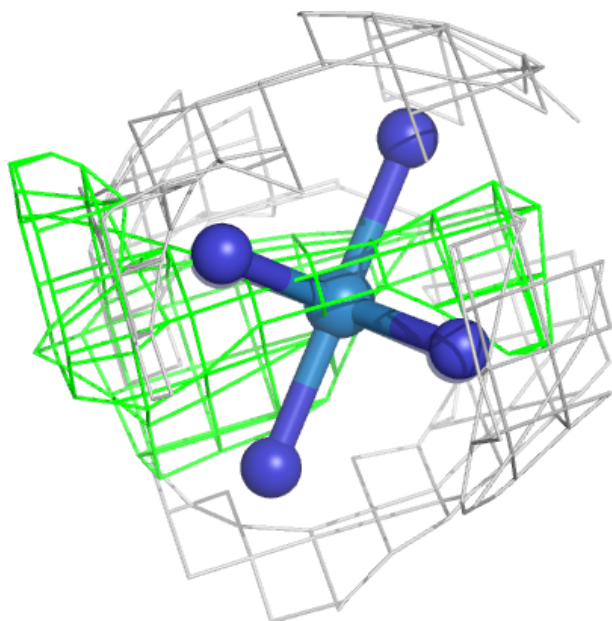
Electron density around OHX C1 1996:

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



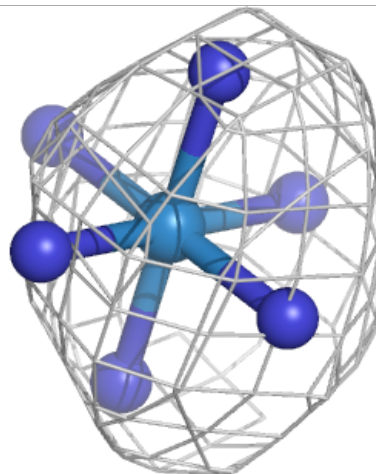
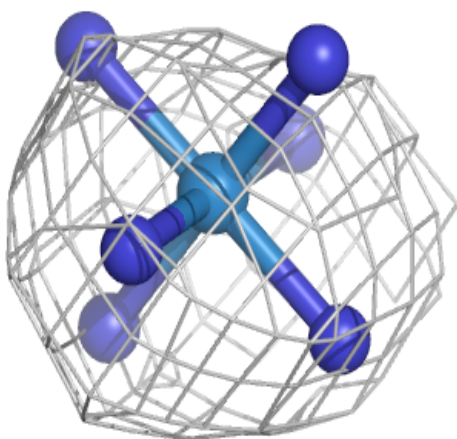
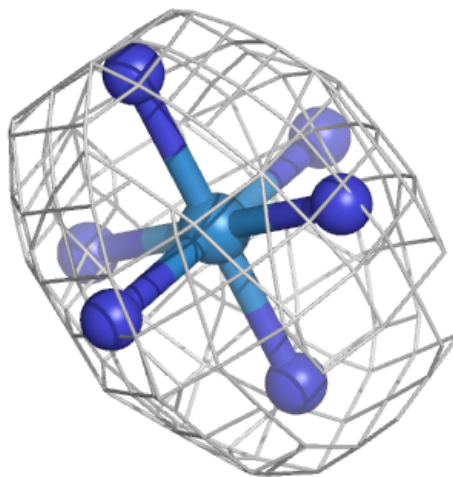
Electron density around OHX A1 1988:

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



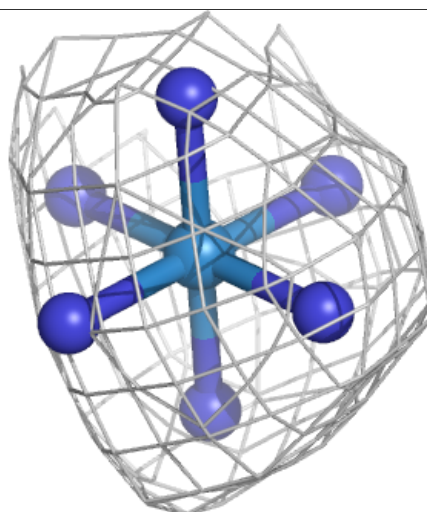
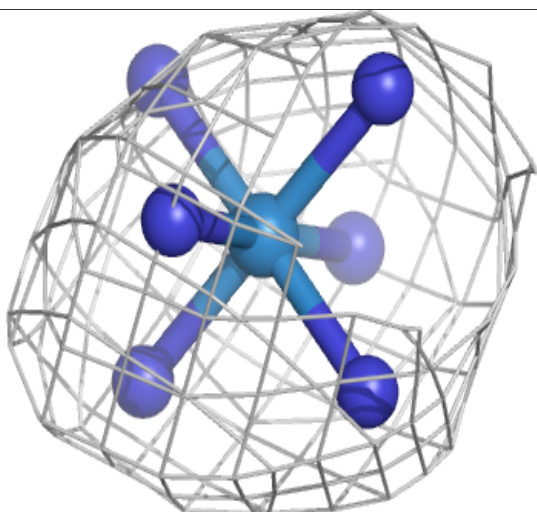
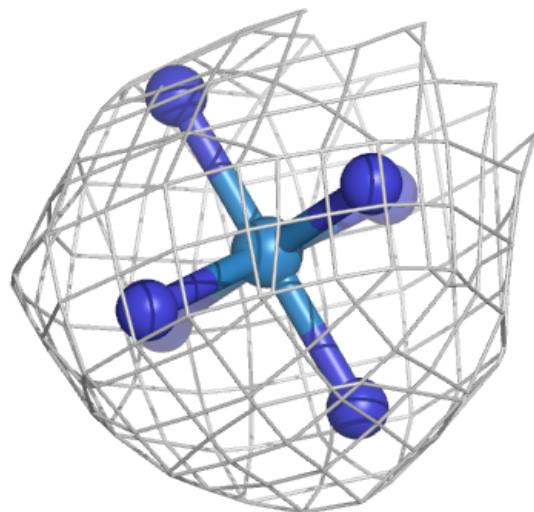
Electron density around OHX B1 3602:

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



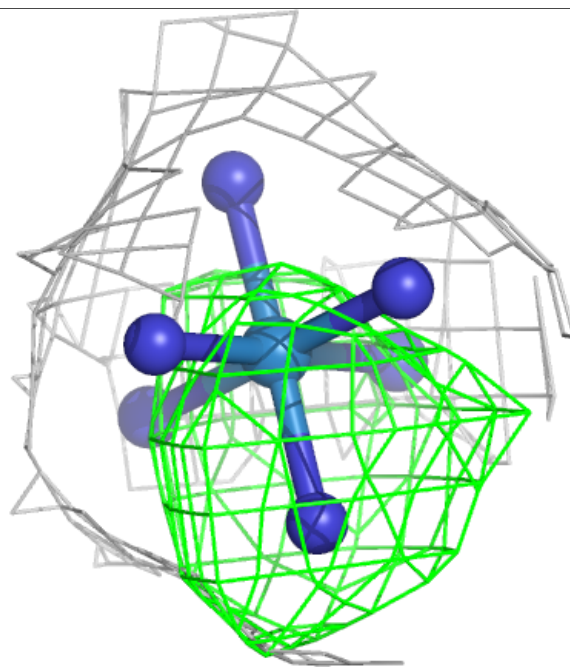
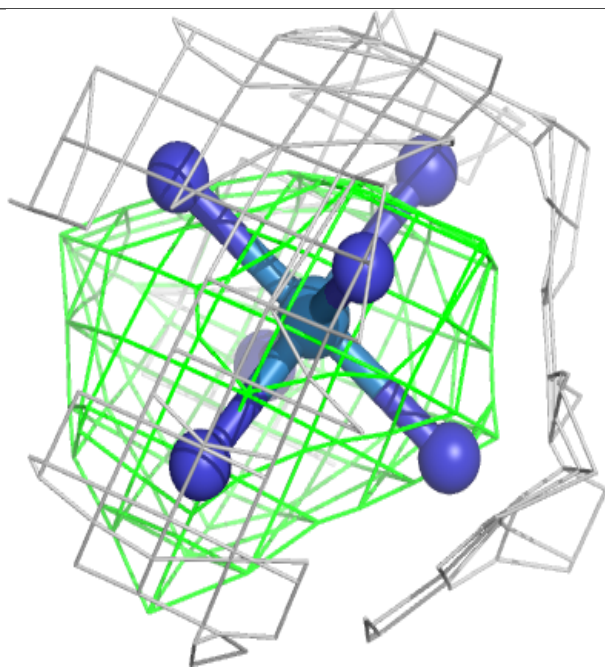
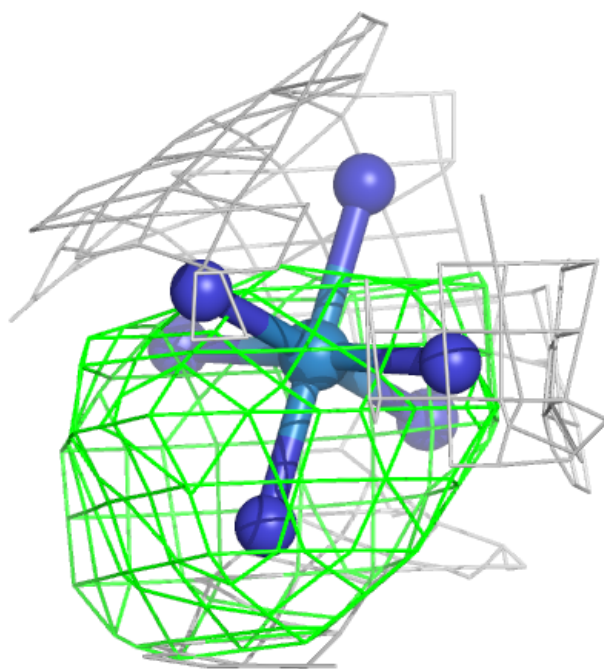
Electron density around OHX D1 3595:

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



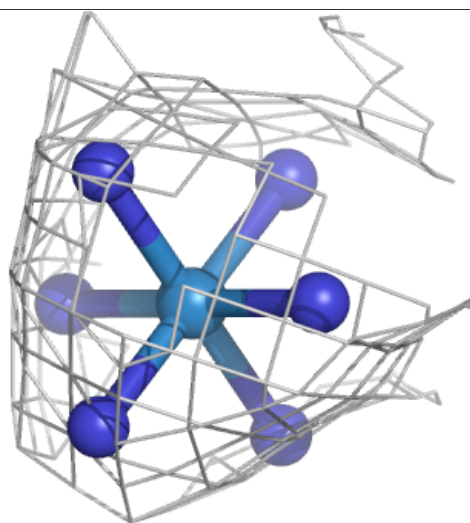
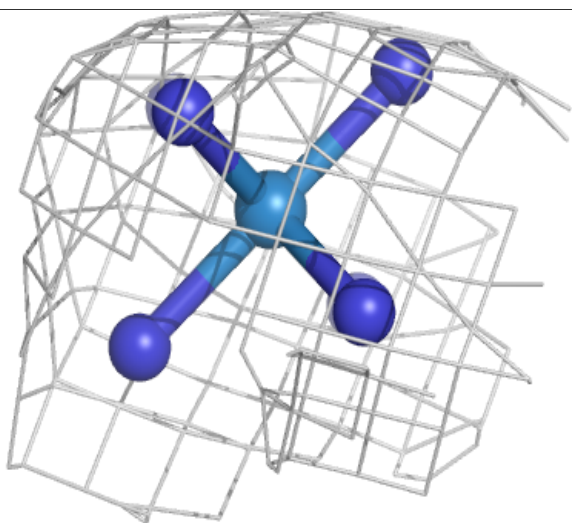
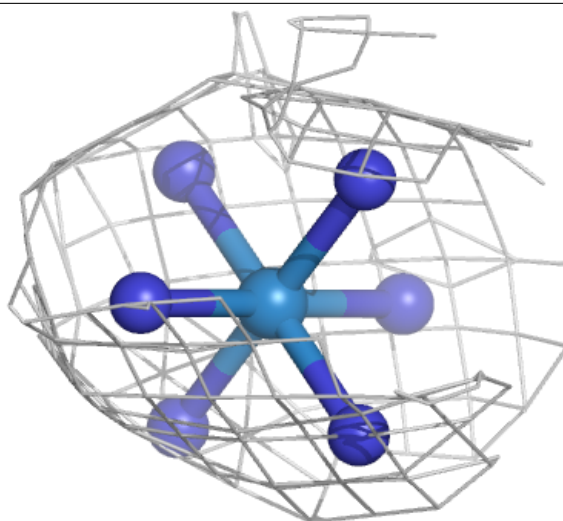
Electron density around OHX B1 3542:

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



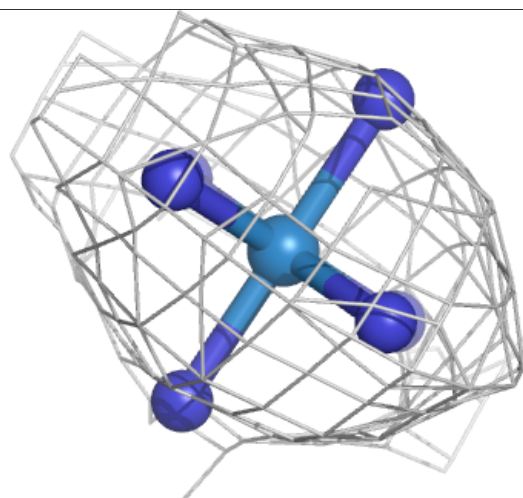
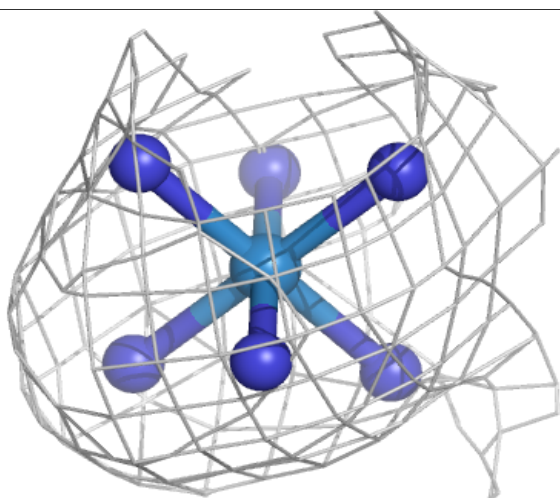
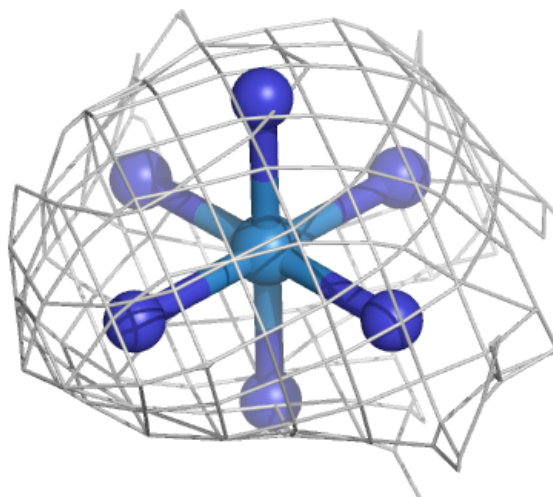
Electron density around OHX C1 1980:

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



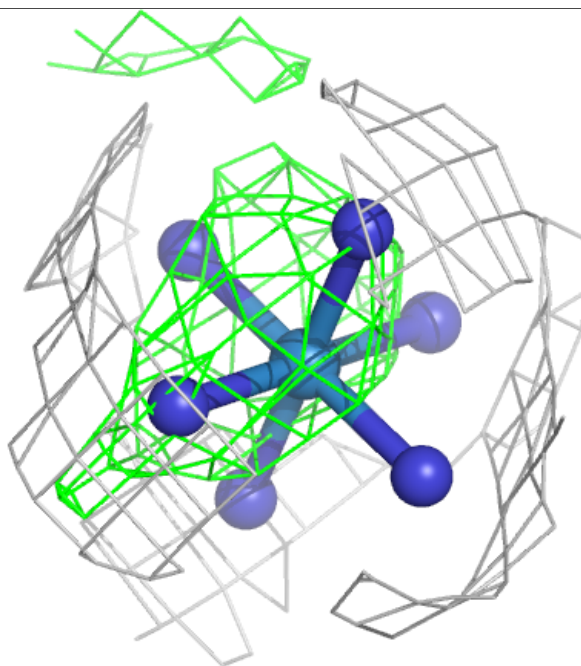
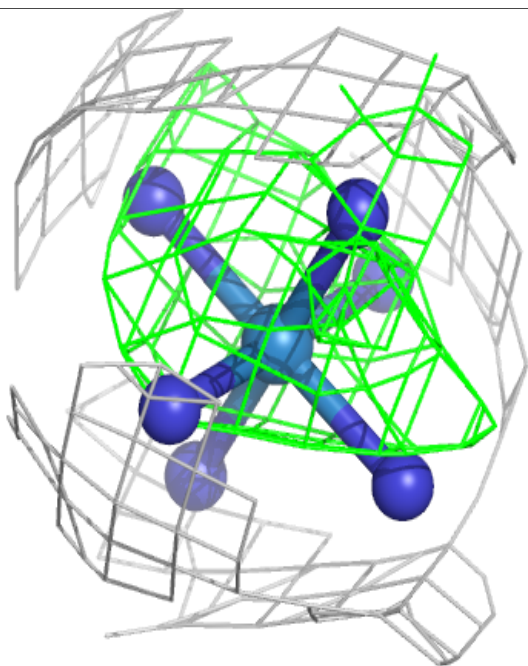
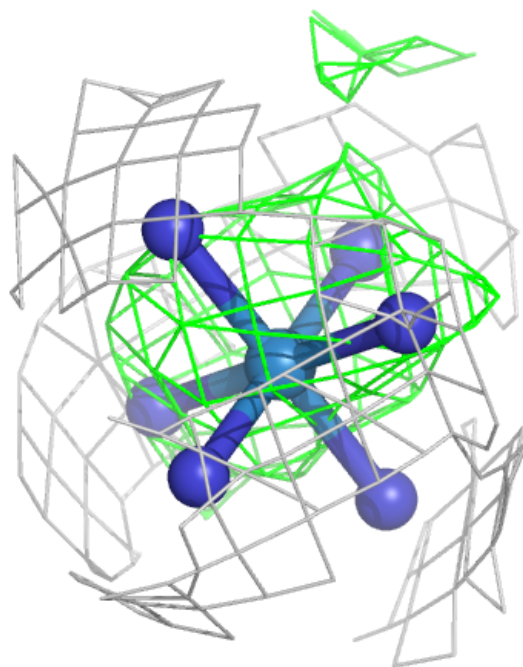
Electron density around OHX B1 3609:

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



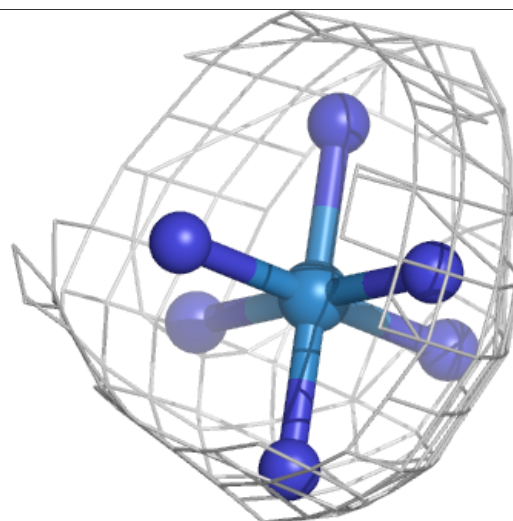
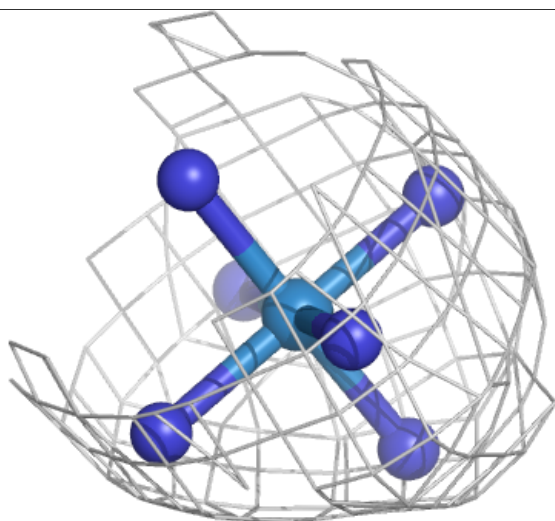
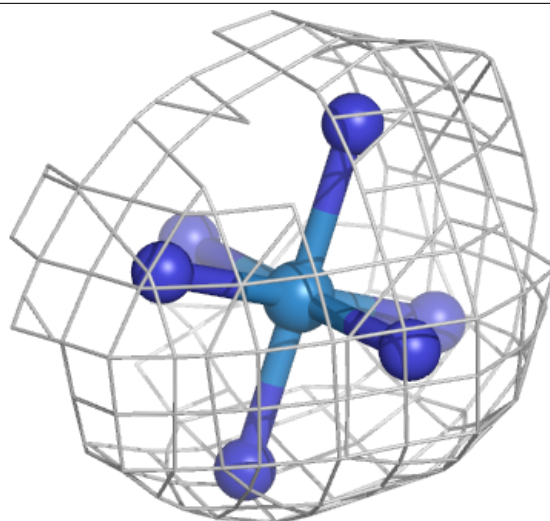
Electron density around OHX D1 3545:

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



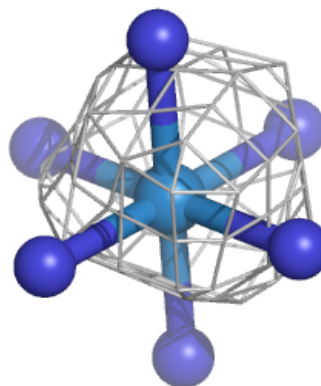
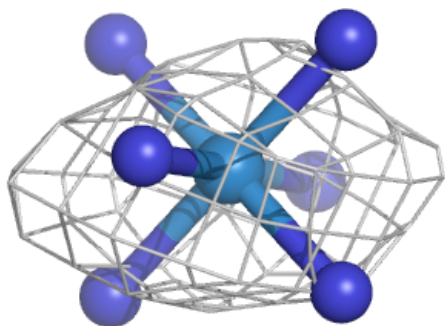
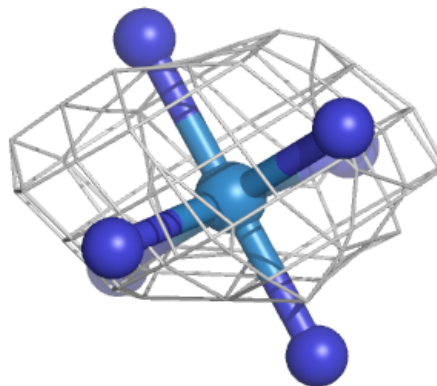
Electron density around OHX C1 1995:

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



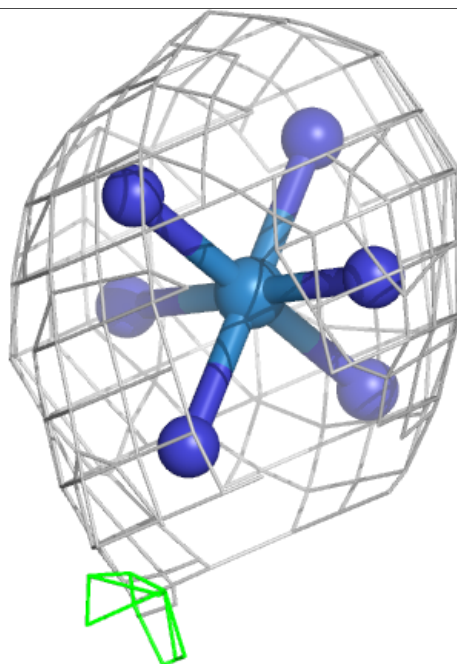
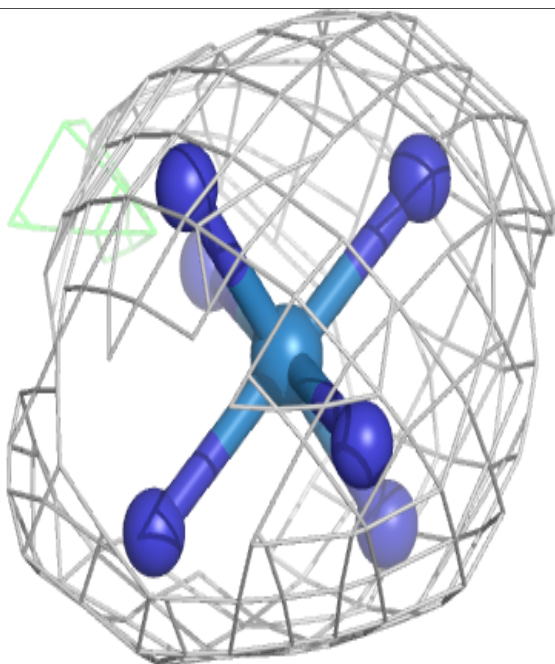
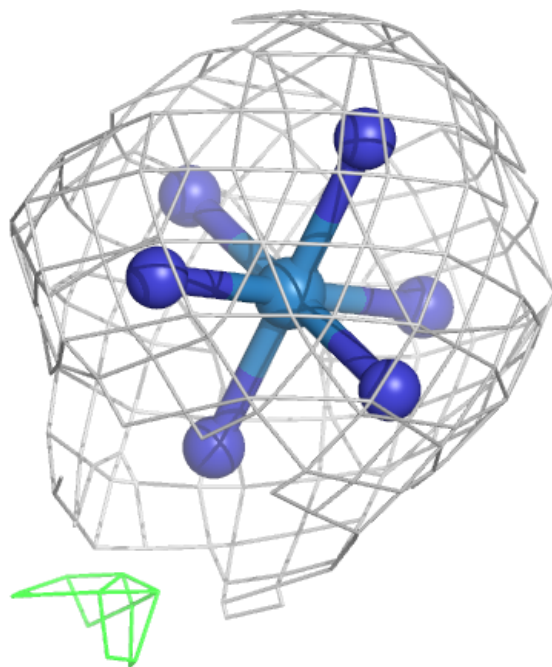
Electron density around OHX B1 3555:

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



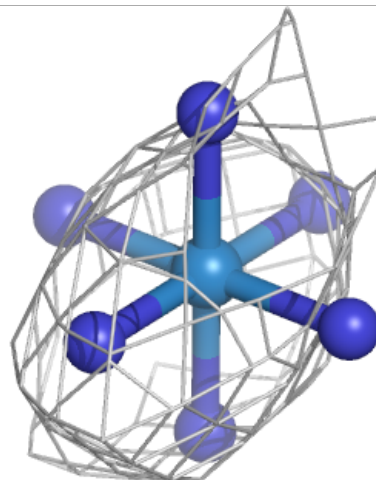
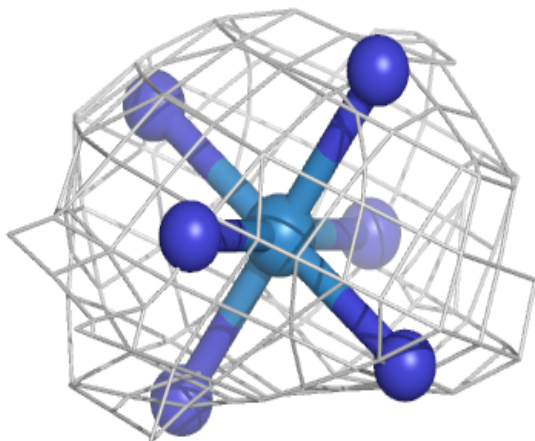
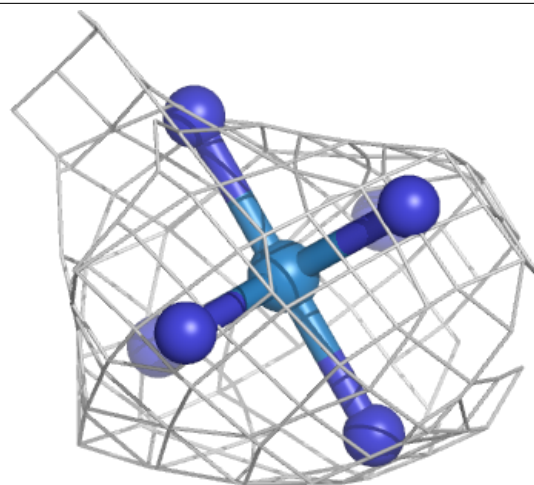
Electron density around OHX B1 3551:

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



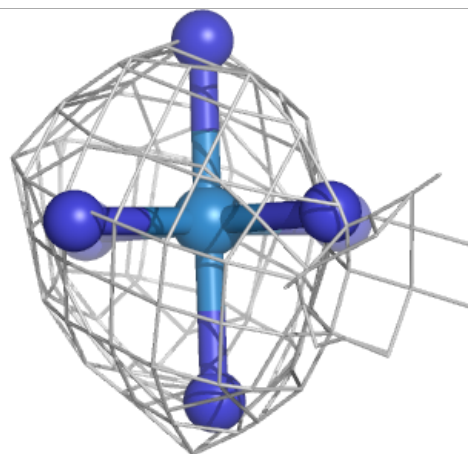
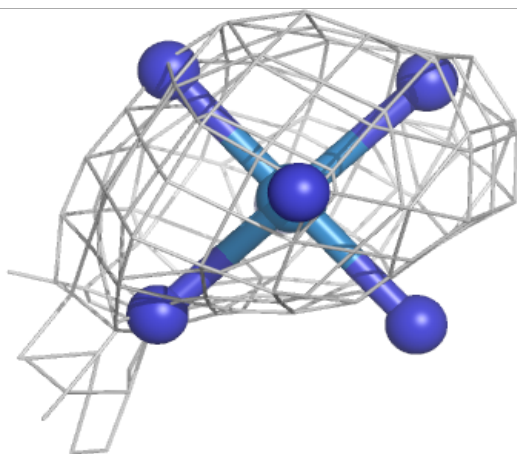
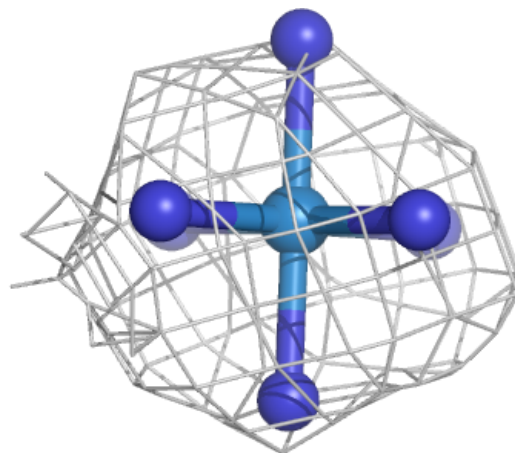
Electron density around OHX D1 3509:

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



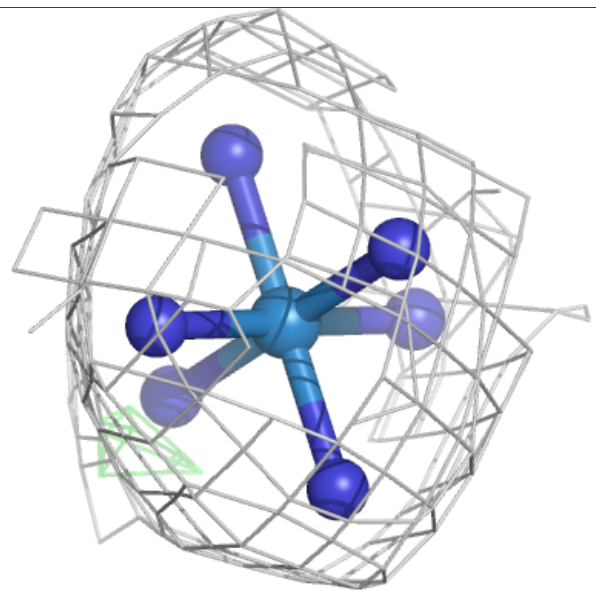
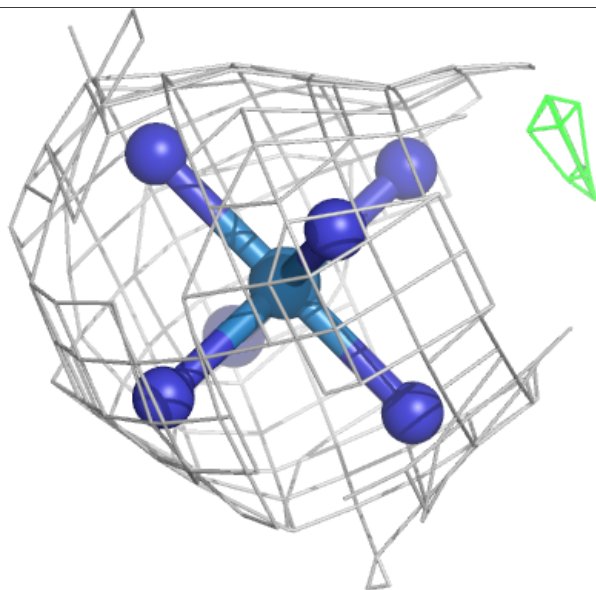
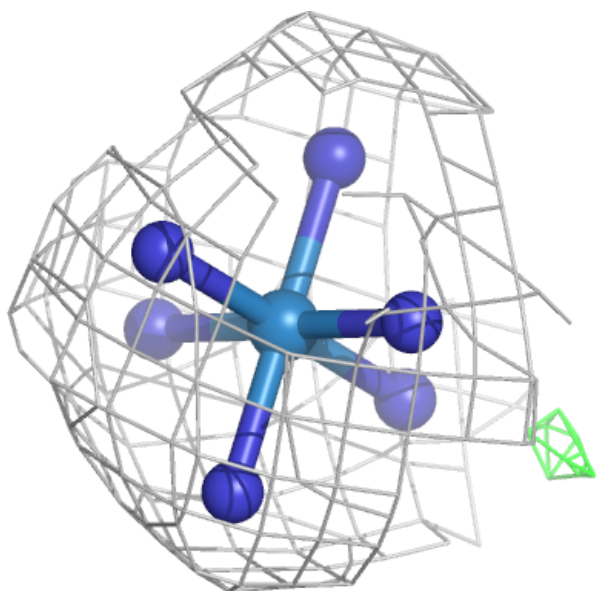
Electron density around OHX D1 3573:

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



Electron density around OHX D1 3516:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.