



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 07:48 AM BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

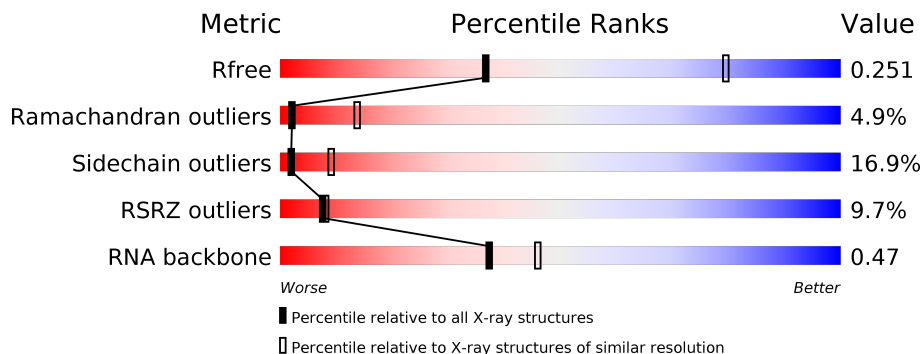
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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

Mol	Chain	Length	Quality of chain
1	2	1800	 6% 71% 25% ..
1	6	1800	 4% 72% 26% .
2	S0	206	 53% 78% 20% .
2	s0	206	 28% 78% 20% .
3	S1	216	 13% 71% 26% ..
3	s1	216	 17% 81% 16% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	S2	217	46% 81% 18%
4	s2	217	21% 78% 20%
5	S3	223	24% 83% 16%
5	s3	223	5% 83% 15%
6	S4	260	23% 82% 17%
6	s4	260	10% 85% 14%
7	S5	206	22% 79% 20%
7	s5	206	20% 78% 22%
8	S6	226	20% 83% 16%
8	s6	226	15% 77% 18%
9	S7	186	6% 75% 23%
9	s7	186	16% 81% 18%
10	S8	199	22% 79% 14% 6%
10	s8	199	13% 82% 11% 6%
11	S9	185	33% 81% 18%
11	s9	185	9% 84% 15%
12	C0	96	2% 82% 17%
13	C1	155	24% 85% 15%
13	c1	155	23% 73% 21% 6%
14	C2	124	10% 70% 27%
15	C3	150	4% 85% 13%
15	c3	150	5% 83% 15%
16	C4	128	16% 79% 18%
16	c4	128	44% 79% 20%
17	C5	131	11% 79% 14% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	C6	142	26% 80% 18%
18	c6	142	30% 84% 15%
19	C7	125	31% 74% 18%
19	c7	125	10% 77% 15% 6%
20	C8	145	17% 74% 21%
20	c8	145	18% 80% 19%
21	C9	143	19% 81% 18%
21	c9	143	25% 86% 13%
22	D0	110	22% 75% 22%
22	d0	110	30% 70% 28%
23	D1	87	54% 76% 24%
23	d1	87	32% 80% 18%
24	D2	129	30% 83% 15%
24	d2	129	30% 89% 10%
25	D3	144	8% 83% 15%
25	d3	144	8% 87% 13%
26	D4	134	4% 81% 16%
26	d4	134	5% 83% 16%
27	D5	70	7% 63% 34%
27	d5	70	13% 81% 16%
28	D6	97	43% 71% 21% 6%
28	d6	97	74% 81% 16%
29	D7	81	6% 88% 12%
29	d7	81	15% 80% 20%
30	D8	63	44% 78% 22%








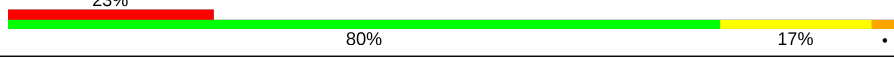

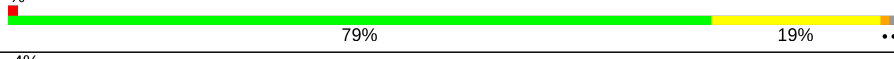



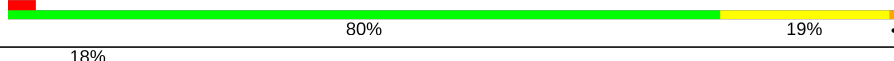

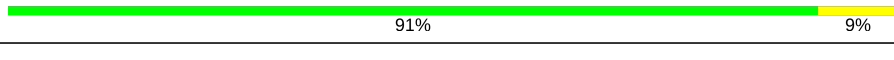
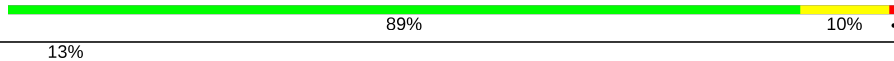






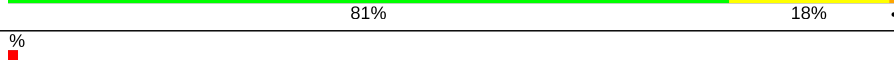

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	d8	63	75% 78% 21% .
31	D9	53	4% 75% 23% .
31	d9	53	8% 77% 23%
32	E0	62	19% 84% 10% . .
32	e0	62	2% 73% 23% 5%
33	E1	76	20% 59% 29% 5% 7%
33	e1	76	41% 61% 32% . .
34	SR	318	34% 90% 10%
35	SM	159	21% 84% 14% .
36	1	3394	2% 67% 23% . 7%
36	5	3394	% 66% 23% . 7%
37	3	121	83% 16% .
37	7	121	% 81% 17% .
38	4	158	% 68% 30% .
38	8	158	% 73% 25% .
39	L2	252	5% 86% 13% .
39	l2	252	2% 83% 15% .
40	L3	386	2% 82% 17% .
40	l3	386	2% 83% 16% .
41	L4	361	82% 17%
41	l4	361	3% 81% 17% .
42	L5	296	18% 81% 18% .
42	l5	296	2% 83% 15% . .
43	L6	175	% 78% 10% . 11%
43	l6	175	2% 78% 10% . 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
44	L7	223	 89% 10%
44	l7	223	 86% 13%
45	L8	233	 81% 18% 7%
46	L9	191	 81% 19% 7%
46	l9	191	 79% 20%
47	M0	220	 79% 16%
47	m0	220	 79% 16% 4%
48	M1	169	 80% 17% 23%
48	m1	169	 79% 19%
49	M3	194	 79% 19%
49	m3	194	 84% 16% 4%
50	M4	137	 82% 15%
50	m4	137	 86% 13% 3%
51	M5	203	 80% 19% 3%
51	m5	203	 86% 13% 18%
52	M6	197	 91% 9%
52	m6	197	 89% 10%
53	M7	183	 81% 18% 13%
53	m7	183	 69% 15% 15%
54	M8	185	 88% 12% 4%
54	m8	185	 84% 16% 3%
55	M9	188	 85% 15% 7%
55	m9	188	 85% 15% 3%
56	N0	172	 81% 18% 8%
56	n0	172	 83% 17%

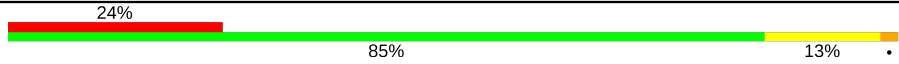



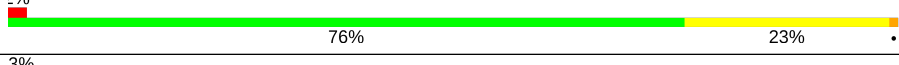
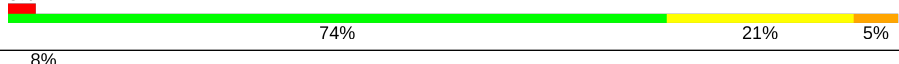
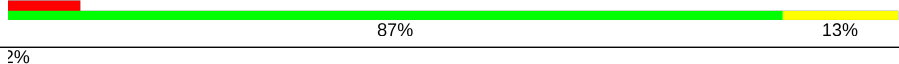

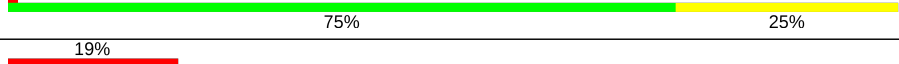


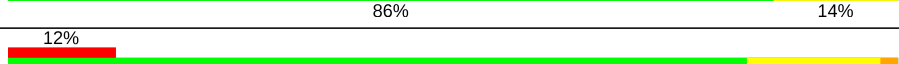

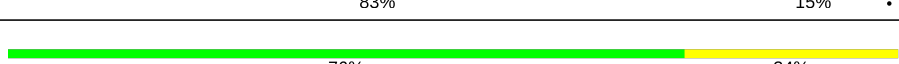

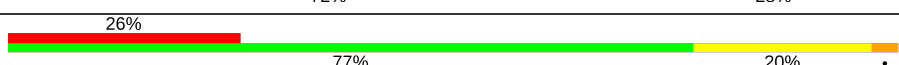
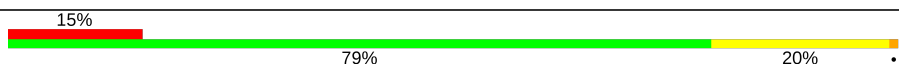
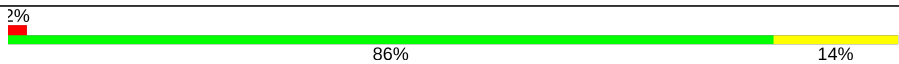
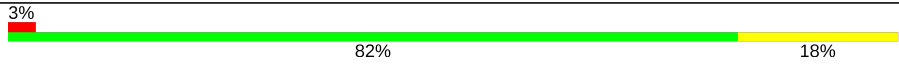


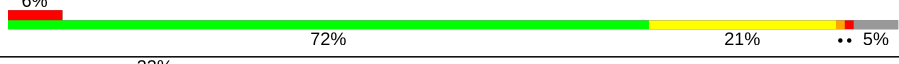
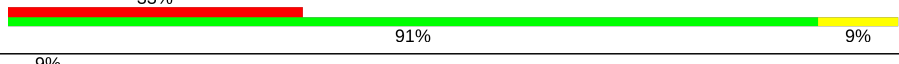


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
57	N1	159	4% 80% 19%
57	n1	159	4% 81% 18%
58	N2	100	12% 86% 14%
58	n2	100	7% 82% 16%
59	N3	136	2% 85% 15%
59	n3	136	2% 91% 8%
60	N4	98	35% 87% 13%
61	N5	121	10% 81% 18%
61	n5	121	12% 79% 18%
62	N6	126	3% 75% 24%
62	n6	126	75% 24%
63	N7	135	10% 81% 16%
63	n7	135	5% 76% 21%
64	N8	148	7% 81% 18%
64	n8	148	5% 84% 16%
65	N9	58	26% 81% 16%
65	n9	58	9% 72% 22% 5%
66	O0	100	2% 83% 14%
66	o0	100	5% 84% 16%
67	O1	109	13% 84% 14%
67	o1	109	7% 80% 20%
68	O2	127	2% 89% 11%
68	o2	127	84% 15%
69	O3	106	89% 10%
69	o3	106	% 86% 13%

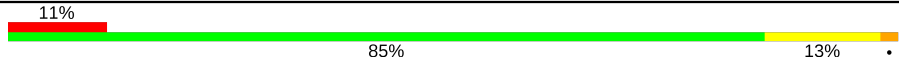
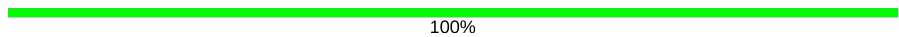

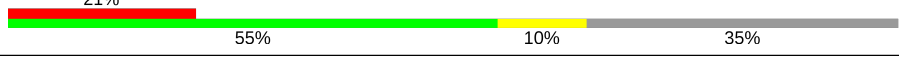
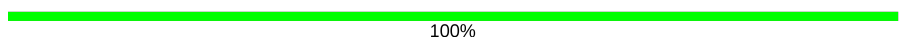
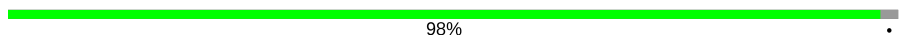
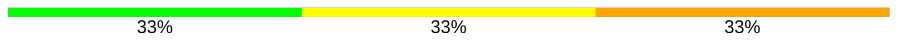
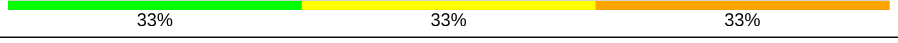
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
70	O4	112	
70	o4	112	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	c0	96	
81	c2	124	
82	c5	142	
83	sR	318	
84	sM	104	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	1	3421	-	-	-	X
91	MG	1	3472	-	-	-	X
91	MG	1	3480	-	-	-	X
91	MG	1	3484	-	-	-	X
91	MG	1	3503	-	-	-	X
91	MG	1	3510	-	-	-	X
91	MG	1	3512	-	-	-	X
91	MG	1	3557	-	-	-	X
91	MG	1	3569	-	-	-	X
91	MG	1	3575	-	-	-	X
91	MG	1	3602	-	-	-	X
91	MG	1	3637	-	-	-	X
91	MG	1	3640	-	-	-	X
91	MG	1	3641	-	-	-	X
91	MG	1	3644	-	-	-	X
91	MG	1	3648	-	-	-	X
91	MG	1	3665	-	-	-	X
91	MG	1	3668	-	-	-	X
91	MG	1	3671	-	-	-	X
91	MG	1	3680	-	-	-	X
91	MG	1	3685	-	-	-	X
91	MG	1	3693	-	-	-	X
91	MG	1	3697	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	1	3710	-	-	-	X
91	MG	1	3712	-	-	-	X
91	MG	1	3714	-	-	-	X
91	MG	1	3715	-	-	-	X
91	MG	1	3719	-	-	-	X
91	MG	1	3721	-	-	-	X
91	MG	1	3723	-	-	-	X
91	MG	1	3734	-	-	-	X
91	MG	1	3741	-	-	-	X
91	MG	1	3748	-	-	-	X
91	MG	1	3749	-	-	-	X
91	MG	1	3760	-	-	-	X
91	MG	1	3766	-	-	-	X
91	MG	1	3768	-	-	-	X
91	MG	1	3772	-	-	-	X
91	MG	1	3776	-	-	-	X
91	MG	1	3779	-	-	-	X
91	MG	1	3785	-	-	-	X
91	MG	1	3788	-	-	-	X
91	MG	1	3791	-	-	-	X
91	MG	1	3808	-	-	-	X
91	MG	1	3822	-	-	-	X
91	MG	1	3838	-	-	-	X
91	MG	1	3844	-	-	-	X
91	MG	1	3850	-	-	-	X
91	MG	1	3857	-	-	-	X
91	MG	1	3860	-	-	-	X
91	MG	1	3868	-	-	-	X
91	MG	1	3869	-	-	-	X
91	MG	1	3872	-	-	-	X
91	MG	1	3875	-	-	-	X
91	MG	1	3876	-	-	-	X
91	MG	1	3882	-	-	-	X
91	MG	1	3889	-	-	-	X
91	MG	1	3895	-	-	-	X
91	MG	1	3903	-	-	-	X
91	MG	1	3922	-	-	-	X
91	MG	1	3930	-	-	-	X
91	MG	1	3939	-	-	-	X
91	MG	1	3943	-	-	-	X
91	MG	1	3947	-	-	-	X
91	MG	1	3949	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	1	3953	-	-	-	X
91	MG	1	3954	-	-	-	X
91	MG	1	3955	-	-	-	X
91	MG	1	3960	-	-	-	X
91	MG	1	3962	-	-	-	X
91	MG	1	3966	-	-	-	X
91	MG	1	3975	-	-	-	X
91	MG	1	3978	-	-	-	X
91	MG	1	3981	-	-	-	X
91	MG	1	3993	-	-	-	X
91	MG	1	3998	-	-	-	X
91	MG	1	4008	-	-	-	X
91	MG	1	4012	-	-	-	X
91	MG	1	4019	-	-	-	X
91	MG	1	4021	-	-	-	X
91	MG	1	4026	-	-	-	X
91	MG	1	4029	-	-	-	X
91	MG	1	4044	-	-	-	X
91	MG	1	4051	-	-	-	X
91	MG	1	4055	-	-	-	X
91	MG	1	4063	-	-	-	X
91	MG	1	4069	-	-	-	X
91	MG	1	4076	-	-	-	X
91	MG	1	4077	-	-	-	X
91	MG	1	4082	-	-	-	X
91	MG	1	4083	-	-	-	X
91	MG	1	4084	-	-	-	X
91	MG	1	4088	-	-	-	X
91	MG	1	4094	-	-	-	X
91	MG	1	4098	-	-	-	X
91	MG	2	1912	-	-	-	X
91	MG	2	1918	-	-	-	X
91	MG	2	1920	-	-	-	X
91	MG	2	1927	-	-	-	X
91	MG	2	1945	-	-	-	X
91	MG	2	1946	-	-	-	X
91	MG	2	1947	-	-	-	X
91	MG	2	1955	-	-	-	X
91	MG	2	1958	-	-	-	X
91	MG	2	1964	-	-	-	X
91	MG	2	1966	-	-	-	X
91	MG	2	1972	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	2	1981	-	-	-	X
91	MG	2	1992	-	-	-	X
91	MG	2	1993	-	-	-	X
91	MG	2	1999	-	-	-	X
91	MG	2	2002	-	-	-	X
91	MG	2	2005	-	-	-	X
91	MG	2	2007	-	-	-	X
91	MG	2	2009	-	-	-	X
91	MG	2	2013	-	-	-	X
91	MG	2	2014	-	-	-	X
91	MG	2	2016	-	-	-	X
91	MG	2	2023	-	-	-	X
91	MG	2	2024	-	-	-	X
91	MG	2	2025	-	-	-	X
91	MG	2	2026	-	-	-	X
91	MG	2	2029	-	-	-	X
91	MG	2	2035	-	-	-	X
91	MG	2	2038	-	-	-	X
91	MG	2	2047	-	-	-	X
91	MG	2	2053	-	-	-	X
91	MG	2	2055	-	-	-	X
91	MG	2	2057	-	-	-	X
91	MG	2	2059	-	-	-	X
91	MG	3	217	-	-	-	X
91	MG	4	227	-	-	-	X
91	MG	4	229	-	-	-	X
91	MG	5	3418	-	-	-	X
91	MG	5	3440	-	-	-	X
91	MG	5	3452	-	-	-	X
91	MG	5	3476	-	-	-	X
91	MG	5	3532	-	-	-	X
91	MG	5	3567	-	-	-	X
91	MG	5	3621	-	-	-	X
91	MG	5	3635	-	-	-	X
91	MG	5	3650	-	-	-	X
91	MG	5	3653	-	-	-	X
91	MG	5	3664	-	-	-	X
91	MG	5	3668	-	-	-	X
91	MG	5	3669	-	-	-	X
91	MG	5	3676	-	-	-	X
91	MG	5	3678	-	-	-	X
91	MG	5	3681	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	5	3688	-	-	-	X
91	MG	5	3690	-	-	-	X
91	MG	5	3703	-	-	-	X
91	MG	5	3715	-	-	-	X
91	MG	5	3718	-	-	-	X
91	MG	5	3719	-	-	-	X
91	MG	5	3730	-	-	-	X
91	MG	5	3744	-	-	-	X
91	MG	5	3747	-	-	-	X
91	MG	5	3752	-	-	-	X
91	MG	5	3760	-	-	-	X
91	MG	5	3767	-	-	-	X
91	MG	5	3768	-	-	-	X
91	MG	5	3779	-	-	-	X
91	MG	5	3784	-	-	-	X
91	MG	5	3788	-	-	-	X
91	MG	5	3798	-	-	-	X
91	MG	5	3803	-	-	-	X
91	MG	5	3804	-	-	-	X
91	MG	5	3806	-	-	-	X
91	MG	5	3809	-	-	-	X
91	MG	5	3819	-	-	-	X
91	MG	5	3823	-	-	-	X
91	MG	5	3832	-	-	-	X
91	MG	5	3834	-	-	-	X
91	MG	5	3840	-	-	-	X
91	MG	5	3842	-	-	-	X
91	MG	5	3846	-	-	-	X
91	MG	5	3861	-	-	-	X
91	MG	5	3863	-	-	-	X
91	MG	5	3870	-	-	-	X
91	MG	5	3875	-	-	-	X
91	MG	5	3881	-	-	-	X
91	MG	5	3891	-	-	-	X
91	MG	5	3898	-	-	-	X
91	MG	5	3904	-	-	-	X
91	MG	5	3909	-	-	-	X
91	MG	5	3917	-	-	-	X
91	MG	5	3920	-	-	-	X
91	MG	5	3927	-	-	-	X
91	MG	5	3931	-	-	-	X
91	MG	5	3932	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	5	3936	-	-	-	X
91	MG	5	3944	-	-	-	X
91	MG	5	3948	-	-	-	X
91	MG	5	3964	-	-	-	X
91	MG	5	3965	-	-	-	X
91	MG	5	3966	-	-	-	X
91	MG	5	3969	-	-	-	X
91	MG	5	3970	-	-	-	X
91	MG	5	3971	-	-	-	X
91	MG	5	3977	-	-	-	X
91	MG	5	3982	-	-	-	X
91	MG	5	3983	-	-	-	X
91	MG	5	3989	-	-	-	X
91	MG	5	3992	-	-	-	X
91	MG	5	4003	-	-	-	X
91	MG	5	4004	-	-	-	X
91	MG	5	4007	-	-	-	X
91	MG	5	4014	-	-	-	X
91	MG	5	4029	-	-	-	X
91	MG	5	4030	-	-	-	X
91	MG	5	4033	-	-	-	X
91	MG	5	4047	-	-	-	X
91	MG	5	4051	-	-	-	X
91	MG	5	4054	-	-	-	X
91	MG	5	4061	-	-	-	X
91	MG	5	4062	-	-	-	X
91	MG	5	4063	-	-	-	X
91	MG	5	4064	-	-	-	X
91	MG	5	4068	-	-	-	X
91	MG	5	4086	-	-	-	X
91	MG	5	4088	-	-	-	X
91	MG	5	4093	-	-	-	X
91	MG	5	4097	-	-	-	X
91	MG	5	4100	-	-	-	X
91	MG	5	4102	-	-	-	X
91	MG	5	4103	-	-	-	X
91	MG	5	4105	-	-	-	X
91	MG	5	4106	-	-	-	X
91	MG	5	4120	-	-	-	X
91	MG	5	4135	-	-	-	X
91	MG	5	4138	-	-	-	X
91	MG	5	4140	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	5	4142	-	-	-	X
91	MG	5	4150	-	-	-	X
91	MG	5	4151	-	-	-	X
91	MG	5	4154	-	-	-	X
91	MG	5	4155	-	-	-	X
91	MG	6	1909	-	-	-	X
91	MG	6	1915	-	-	-	X
91	MG	6	1917	-	-	-	X
91	MG	6	1926	-	-	-	X
91	MG	6	1934	-	-	-	X
91	MG	6	1970	-	-	-	X
91	MG	6	1972	-	-	-	X
91	MG	6	1974	-	-	-	X
91	MG	6	1984	-	-	-	X
91	MG	6	1995	-	-	-	X
91	MG	6	1997	-	-	-	X
91	MG	6	2001	-	-	-	X
91	MG	6	2003	-	-	-	X
91	MG	6	2020	-	-	-	X
91	MG	6	2026	-	-	-	X
91	MG	6	2027	-	-	-	X
91	MG	6	2036	-	-	-	X
91	MG	6	2043	-	-	-	X
91	MG	6	2044	-	-	-	X
91	MG	6	2057	-	-	-	X
91	MG	6	2058	-	-	-	X
91	MG	6	2065	-	-	-	X
91	MG	6	2068	-	-	-	X
91	MG	6	2069	-	-	-	X
91	MG	6	2079	-	-	-	X
91	MG	6	2083	-	-	-	X
91	MG	6	2086	-	-	-	X
91	MG	6	2087	-	-	-	X
91	MG	6	2088	-	-	-	X
91	MG	6	2096	-	-	-	X
91	MG	6	2099	-	-	-	X
91	MG	6	2107	-	-	-	X
91	MG	6	2110	-	-	-	X
91	MG	6	2111	-	-	-	X
91	MG	6	2114	-	-	-	X
91	MG	6	2119	-	-	-	X
91	MG	6	2131	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	6	2132	-	-	-	X
91	MG	6	2137	-	-	-	X
91	MG	6	2139	-	-	-	X
91	MG	6	2140	-	-	-	X
91	MG	6	2341	-	-	-	X
91	MG	7	209	-	-	-	X
91	MG	7	222	-	-	-	X
91	MG	7	225	-	-	-	X
91	MG	8	216	-	-	-	X
91	MG	C5	201	-	-	-	X
91	MG	D0	201	-	-	-	X
91	MG	D3	201	-	-	-	X
91	MG	L3	401	-	-	-	X
91	MG	L4	406	-	-	-	X
91	MG	M5	306	-	-	-	X
91	MG	M5	308	-	-	-	X
91	MG	M7	205	-	-	-	X
91	MG	N3	204	-	-	-	X
91	MG	O2	201	-	-	-	X
91	MG	O2	202	-	-	-	X
91	MG	O3	202	-	-	-	X
91	MG	S4	301	-	-	-	X
91	MG	c6	201	-	-	-	X
91	MG	c6	202	-	-	-	X
91	MG	c6	203	-	-	-	X
91	MG	d2	201	-	-	-	X
91	MG	l2	304	-	-	-	X
91	MG	l3	404	-	-	-	X
91	MG	l4	401	-	-	-	X
91	MG	l4	402	-	-	-	X
91	MG	l5	306	-	-	-	X
91	MG	l7	304	-	-	-	X
91	MG	l8	301	-	-	-	X
91	MG	l9	202	-	-	-	X
91	MG	l9	203	-	-	-	X
91	MG	m6	204	-	-	-	X
91	MG	m7	206	-	-	-	X
91	MG	n3	203	-	-	-	X
91	MG	o3	203	-	-	-	X
91	MG	o3	204	-	-	-	X
91	MG	o3	205	-	-	-	X
91	MG	q1	101	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
91	MG	s8	303	-	-	-	X
92	OHX	1	4423	-	-	-	X
92	OHX	1	4429	-	-	-	X
92	OHX	1	4434	-	-	-	X
92	OHX	1	4450	-	-	-	X
92	OHX	1	4463	-	-	-	X
92	OHX	1	4477	-	-	-	X
92	OHX	1	4485	-	-	-	X
92	OHX	2	2197	-	-	-	X
92	OHX	2	2231	-	-	-	X
92	OHX	2	2246	-	-	-	X
92	OHX	5	4495	-	-	-	X
92	OHX	5	4513	-	-	-	X
92	OHX	5	4520	-	-	-	X
92	OHX	5	4528	-	-	-	X
92	OHX	5	4534	-	-	-	X
92	OHX	5	4536	-	-	-	X
92	OHX	5	4541	-	-	-	X
92	OHX	5	4549	-	-	-	X
92	OHX	5	4562	-	-	-	X
92	OHX	6	2305	-	-	-	X
92	OHX	6	2314	-	-	-	X
92	OHX	6	2322	-	-	-	X
92	OHX	6	2328	-	-	-	X
92	OHX	6	2336	-	-	-	X
92	OHX	7	239	-	-	-	X

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	12	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	13	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	14	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	15	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	16	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	19	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	n8	4	Total Mg 4 4	0	0
91	c6	3	Total Mg 3 3	0	0
91	Q0	2	Total Mg 2 2	0	0
91	sM	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	O3	3	Total Mg 3 3	0	0
91	D3	1	Total Mg 1 1	0	0
91	M9	3	Total Mg 3 3	0	0
91	q0	1	Total Mg 1 1	0	0
91	O2	2	Total Mg 2 2	0	0
91	D9	2	Total Mg 2 2	0	0
91	m9	1	Total Mg 1 1	0	0
91	M3	4	Total Mg 4 4	0	0
91	S4	1	Total Mg 1 1	0	0
91	l5	7	Total Mg 7 7	0	0
91	L6	1	Total Mg 1 1	0	0
91	m6	6	Total Mg 6 6	0	0
91	o2	3	Total Mg 3 3	0	0
91	d5	1	Total Mg 1 1	0	0
91	d9	2	Total Mg 2 2	0	0
91	m3	2	Total Mg 2 2	0	0
91	s4	1	Total Mg 1 1	0	0
91	M6	4	Total Mg 4 4	0	0
91	N9	1	Total Mg 1 1	0	0
91	p0	1	Total Mg 1 1	0	0
91	n0	5	Total Mg 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	C8	1	Total Mg 1 1	0	0
91	n9	2	Total Mg 2 2	0	0
91	M5	8	Total Mg 8 8	0	0
91	S2	2	Total Mg 2 2	0	0
91	N6	1	Total Mg 1 1	0	0
91	n6	1	Total Mg 1 1	0	0
91	m5	2	Total Mg 2 2	0	0
91	D0	1	Total Mg 1 1	0	0
91	S8	2	Total Mg 2 2	0	0
91	M8	3	Total Mg 3 3	0	0
91	q3	2	Total Mg 2 2	0	0
91	N3	4	Total Mg 4 4	0	0
91	4	32	Total Mg 32 32	0	0
91	L2	4	Total Mg 4 4	0	0
91	E1	1	Total Mg 1 1	0	0
91	O1	1	Total Mg 1 1	0	0
91	s8	4	Total Mg 4 4	0	0
91	m8	2	Total Mg 2 2	0	0
91	n3	3	Total Mg 3 3	0	0
91	l2	5	Total Mg 5 5	0	0
91	N0	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	L7	1	Total Mg 1 1	0	0
91	6	242	Total Mg 242 242	0	0
91	O4	1	Total Mg 1 1	0	0
91	C1	2	Total Mg 2 2	0	0
91	M1	1	Total Mg 1 1	0	0
91	D6	1	Total Mg 1 1	0	0
91	S6	1	Total Mg 1 1	0	0
91	c9	1	Total Mg 1 1	0	0
91	l7	4	Total Mg 4 4	0	0
91	L8	1	Total Mg 1 1	0	0
91	o4	3	Total Mg 3 3	0	0
91	m1	2	Total Mg 2 2	0	0
91	d6	1	Total Mg 1 1	0	0
91	M4	1	Total Mg 1 1	0	0
91	1	700	Total Mg 700 700	1	0
91	S1	1	Total Mg 1 1	0	0
91	l8	1	Total Mg 1 1	0	0
91	Q2	3	Total Mg 3 3	0	0
91	o7	3	Total Mg 3 3	0	0
91	m4	1	Total Mg 1 1	0	0
91	O7	5	Total Mg 5 5	0	0

Continued on next page...

Continued from previous page...

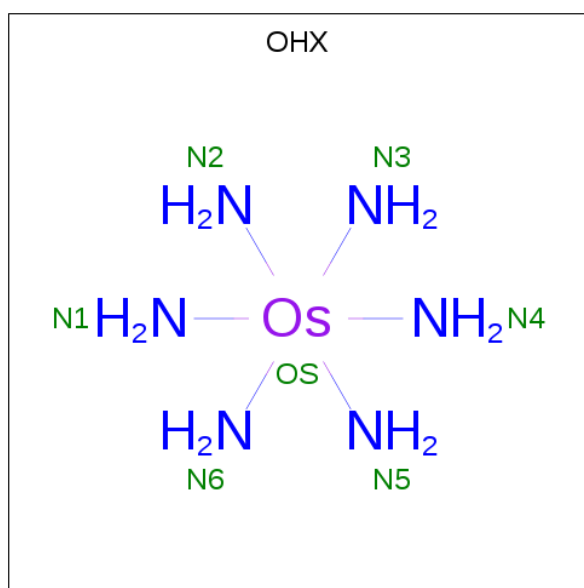
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
91	s1	1	Total Mg 1 1	0	0
91	q2	1	Total Mg 1 1	0	0
91	L3	6	Total Mg 6 6	0	0
91	8	21	Total Mg 21 21	0	0
91	3	18	Total Mg 18 18	0	0
91	C5	1	Total Mg 1 1	0	0
91	q1	1	Total Mg 1 1	0	0
91	l3	11	Total Mg 11 11	0	0
91	N1	1	Total Mg 1 1	0	0
91	2	169	Total Mg 169 169	0	0
91	o9	1	Total Mg 1 1	0	0
91	L4	7	Total Mg 7 7	0	0
91	M0	4	Total Mg 4 4	0	0
91	5	758	Total Mg 758 758	0	0
91	n1	3	Total Mg 3 3	0	0
91	c8	3	Total Mg 3 3	0	0
91	l4	3	Total Mg 3 3	0	0
91	d2	1	Total Mg 1 1	0	0
91	d3	1	Total Mg 1 1	0	0
91	o3	5	Total Mg 5 5	0	0
91	O9	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
91	m0	1	Total	Mg	0	0
			1	1		
91	M7	8	Total	Mg	0	0
			8	8		
91	N8	7	Total	Mg	0	0
			7	7		
91	l9	3	Total	Mg	0	0
			3	3		
91	7	27	Total	Mg	0	0
			27	27		
91	o6	1	Total	Mg	0	0
			1	1		
91	m7	7	Total	Mg	0	0
			7	7		

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
92	d9	1	7	6	1	0	0
92	sR	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0
92	5	1	7	6	1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	q0	1	Total	Zn	0	0
			1	1		

Continued on next page...

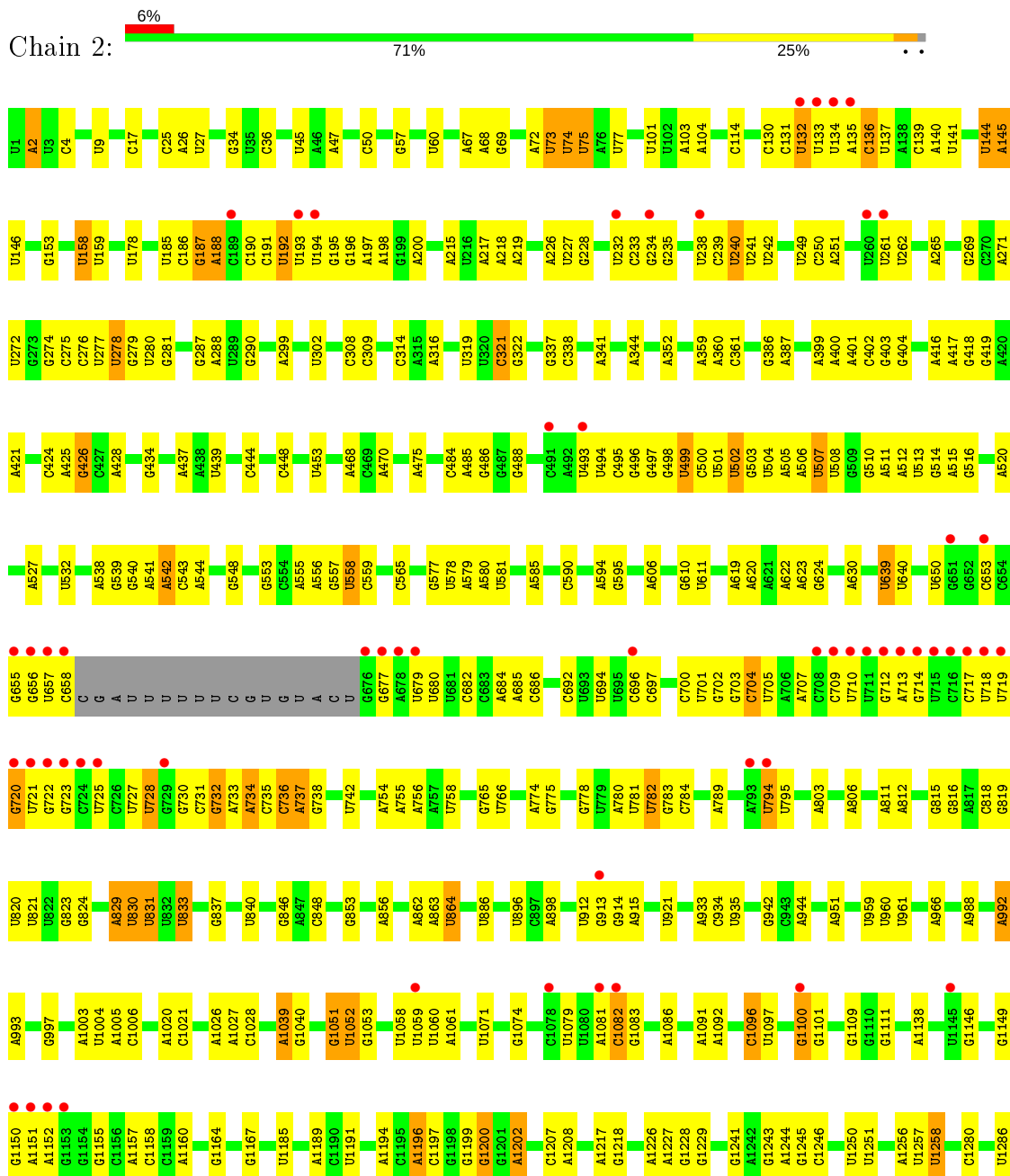
Continued from previous page...

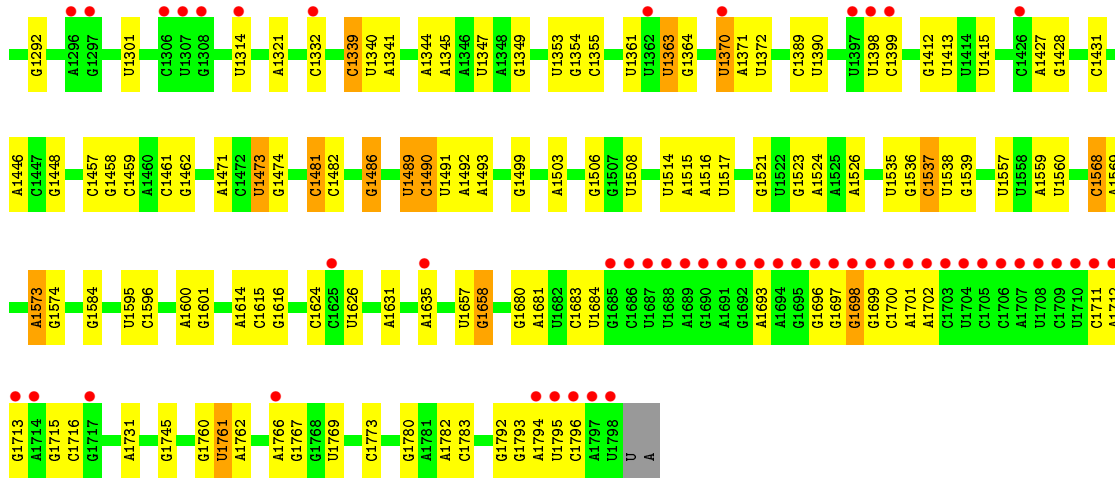
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
93	D6	1	Total 1	Zn 1	0	0
93	Q2	1	Total 1	Zn 1	0	0
93	e1	1	Total 1	Zn 1	0	0
93	Q3	1	Total 1	Zn 1	0	0
93	D9	1	Total 1	Zn 1	0	0
93	E1	1	Total 1	Zn 1	0	0
93	Q0	1	Total 1	Zn 1	0	0
93	d7	1	Total 1	Zn 1	0	0
93	q3	1	Total 1	Zn 1	0	0
93	d9	1	Total 1	Zn 1	0	0
93	D7	1	Total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

3 Residue-property plots

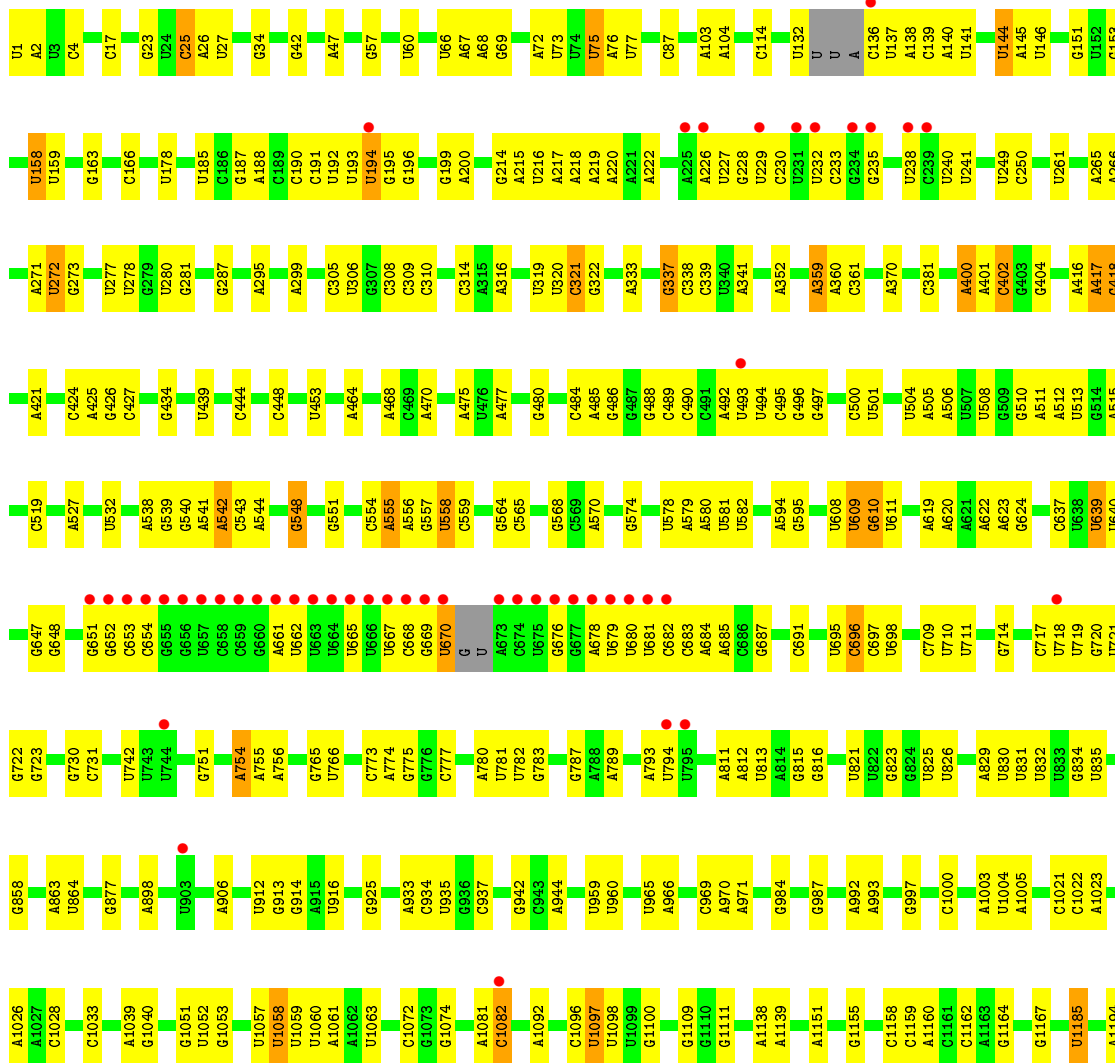
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

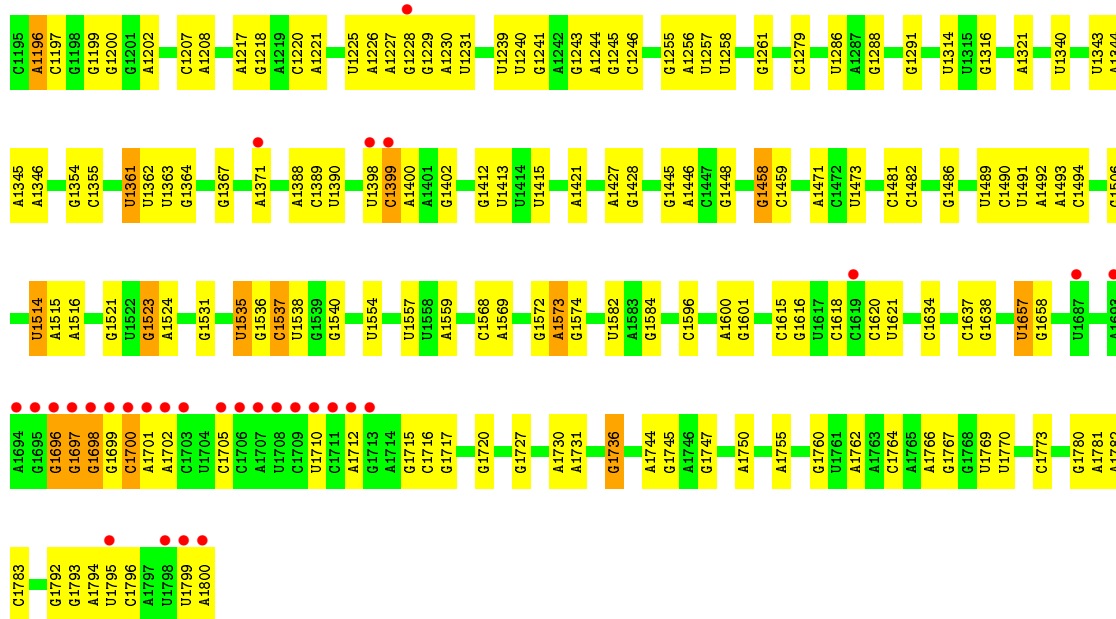
• Molecule 1: 18S rRNA



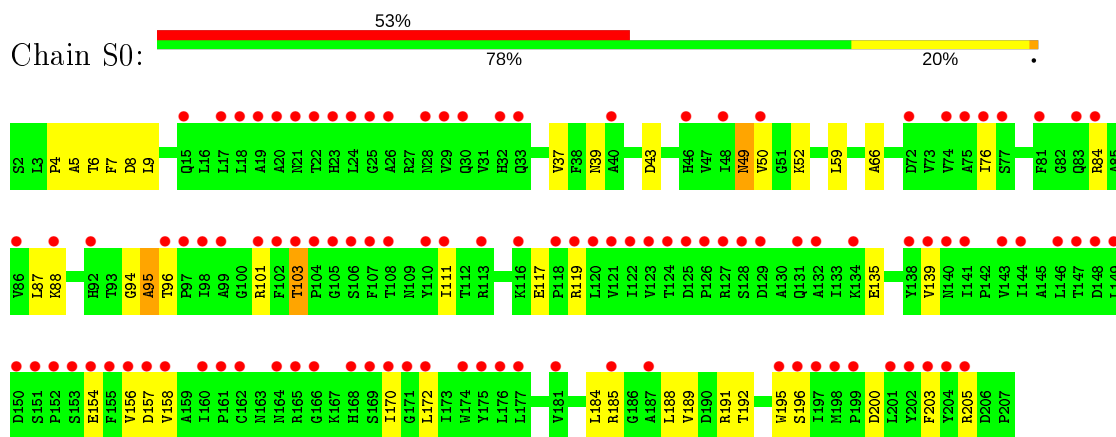


• Molecule 1: 18S rRNA

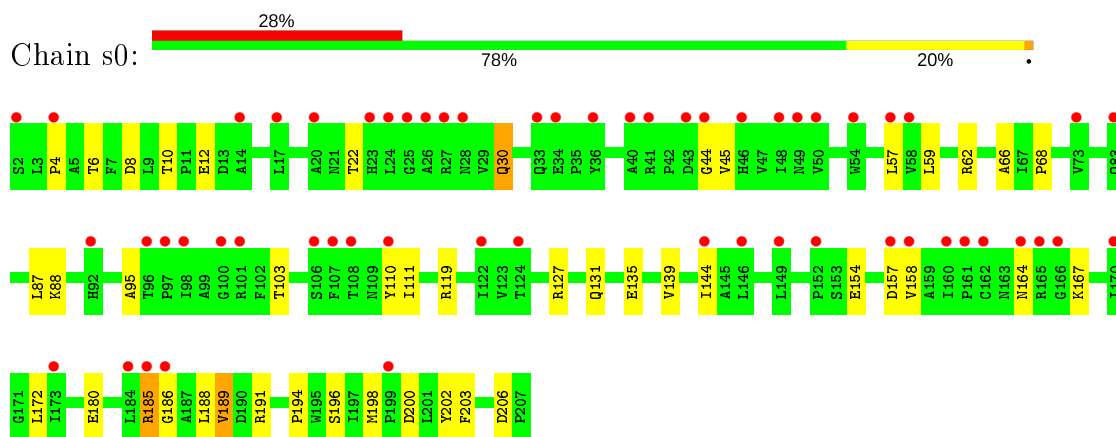




• Molecule 2: 40S ribosomal protein S0-A

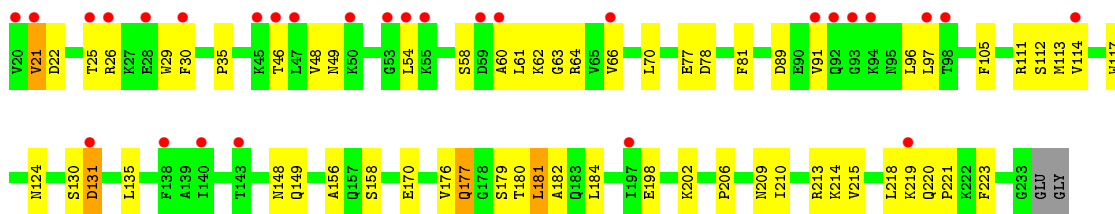


• Molecule 2: 40S ribosomal protein S0-A




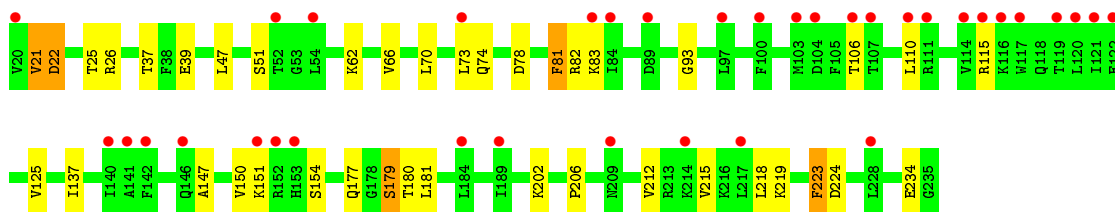
• Molecule 3: 40S ribosomal protein S1-A

Chain S1: 

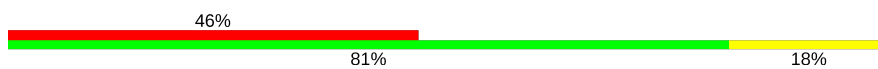


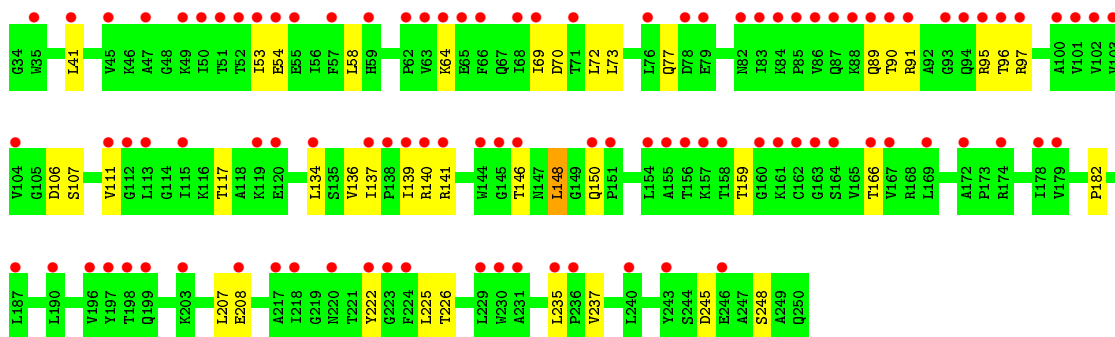
- Molecule 3: 40S ribosomal protein S1-A

Chain s1: 




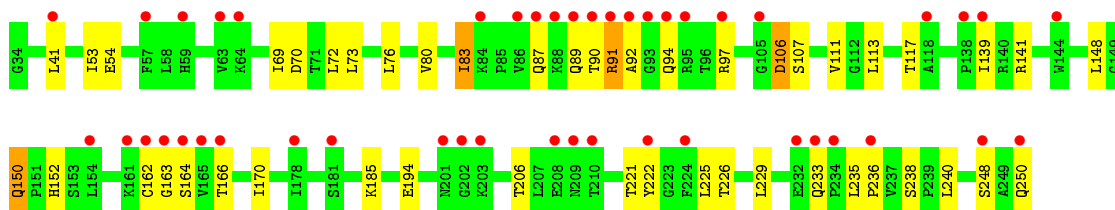
- Molecule 4: 40S ribosomal protein S2

Chain S2: 




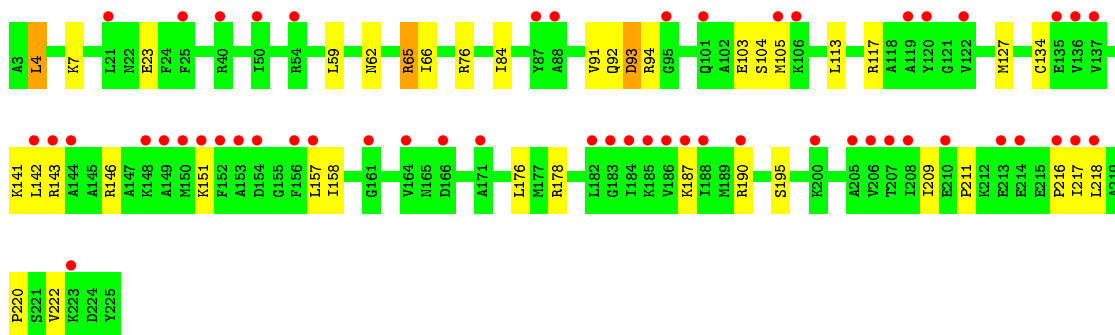
- Molecule 4: 40S ribosomal protein S2

Chain s2: 

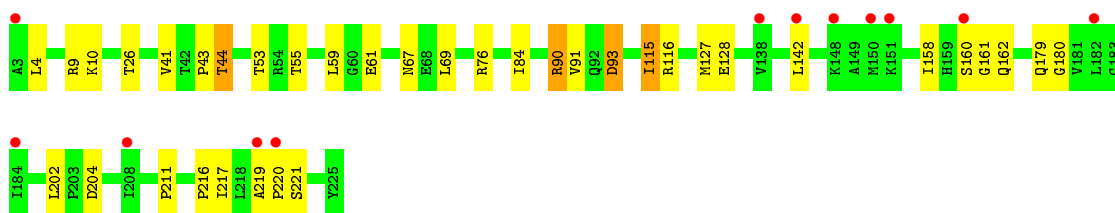
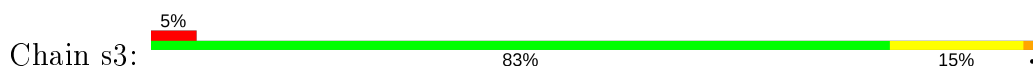


- Molecule 5: 40S ribosomal protein S3

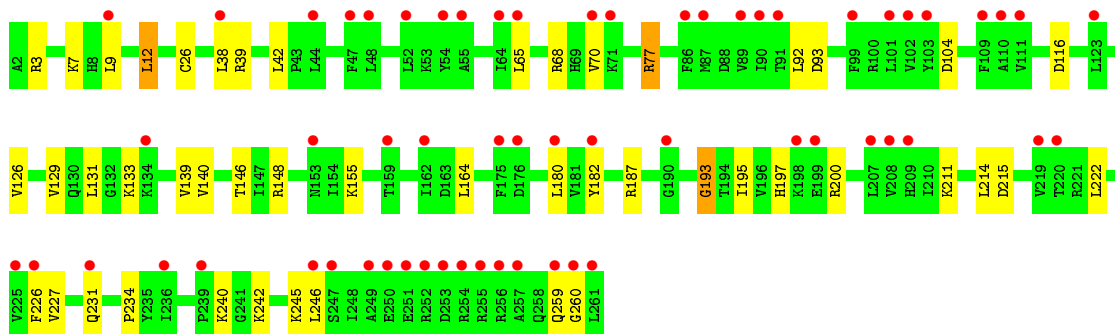
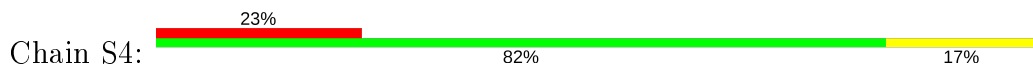
Chain S3: 



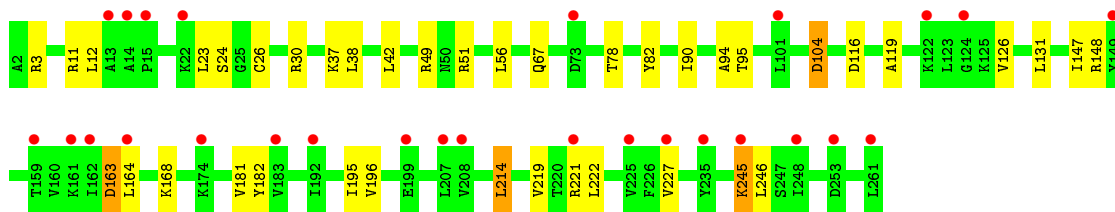
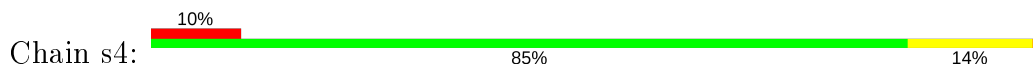
- Molecule 5: 40S ribosomal protein S3



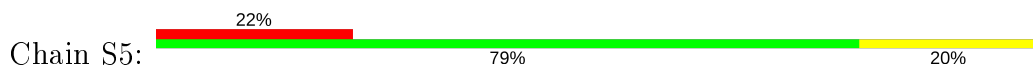
- Molecule 6: 40S ribosomal protein S4-A

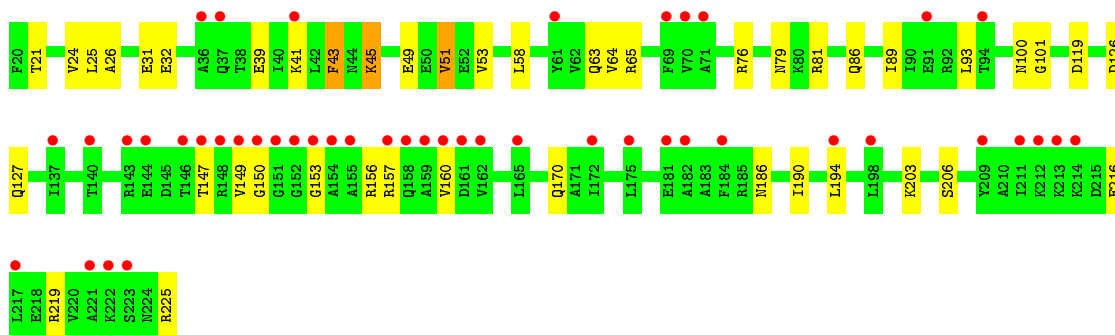


- Molecule 6: 40S ribosomal protein S4-A

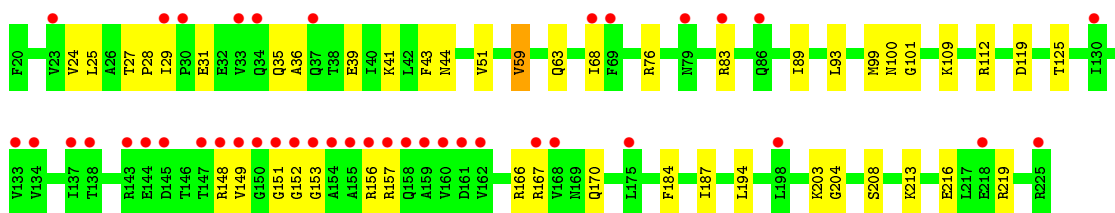
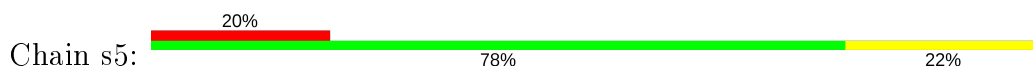


- Molecule 7: 40S ribosomal protein S5

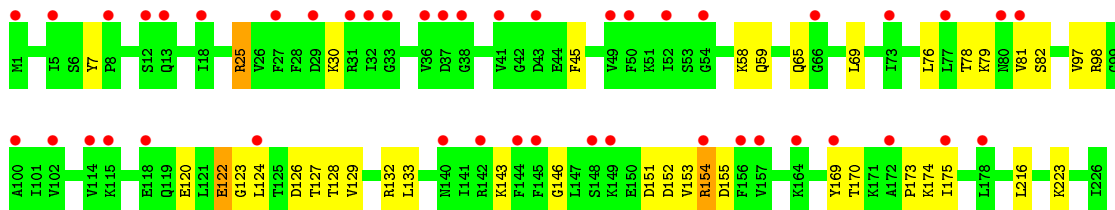
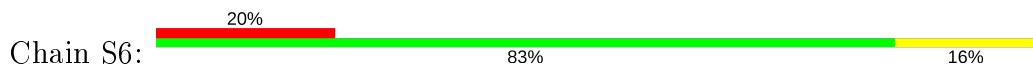




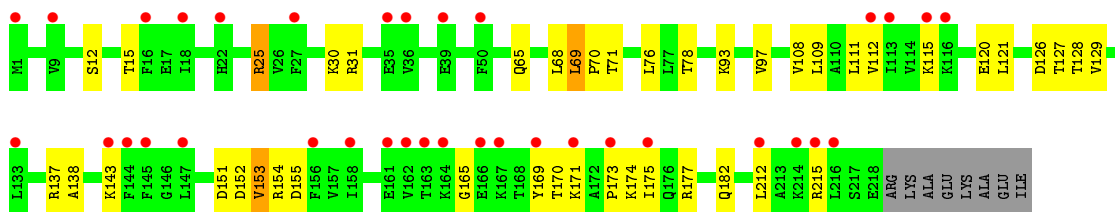
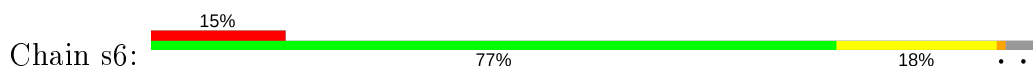
- Molecule 7: 40S ribosomal protein S5



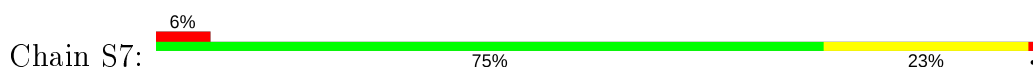
- Molecule 8: 40S ribosomal protein S6-A

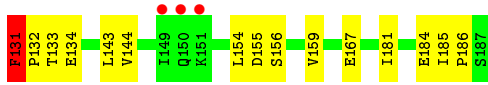


- Molecule 8: 40S ribosomal protein S6-A

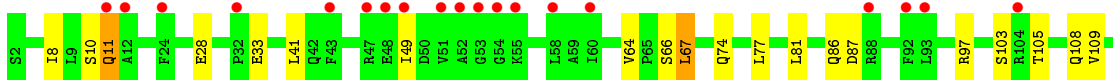
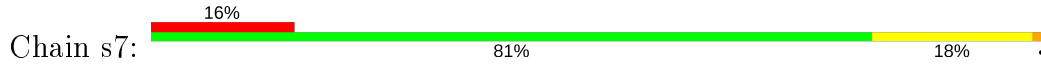


- Molecule 9: 40S ribosomal protein S7-A

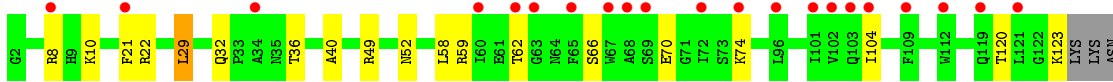
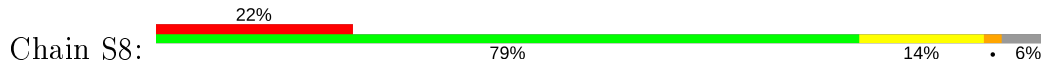




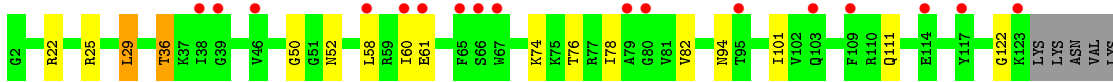
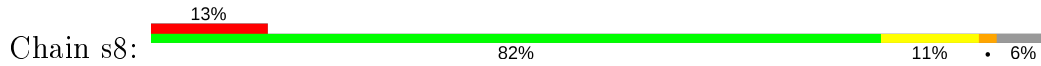
- Molecule 9: 40S ribosomal protein S7-A



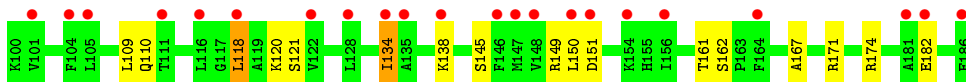
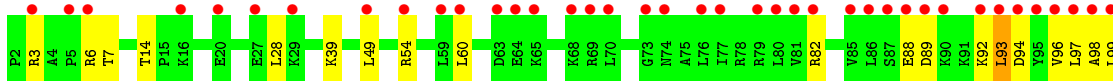
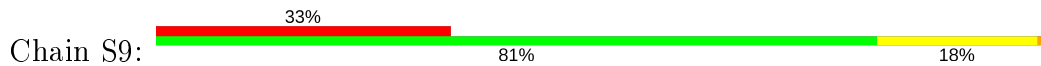
- Molecule 10: 40S ribosomal protein S8-A



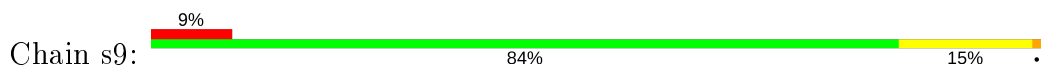
- Molecule 10: 40S ribosomal protein S8-A

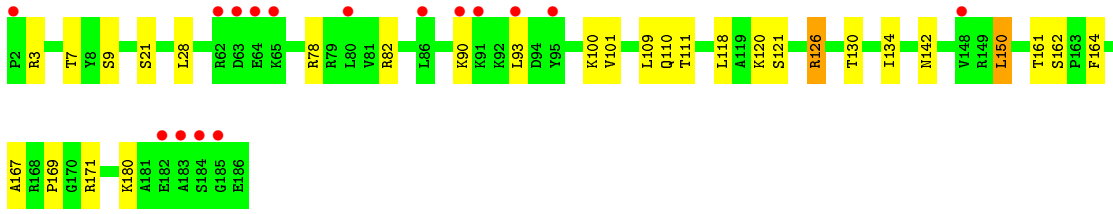


- Molecule 11: 40S ribosomal protein S9-A

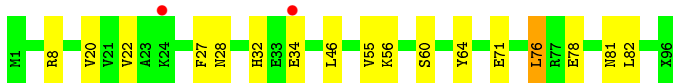
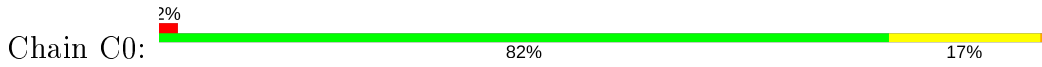


- Molecule 11: 40S ribosomal protein S9-A

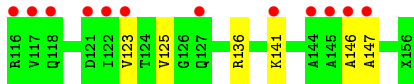
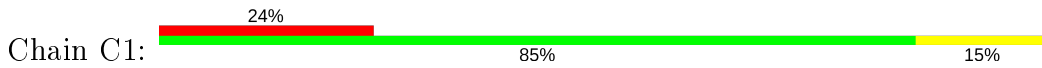




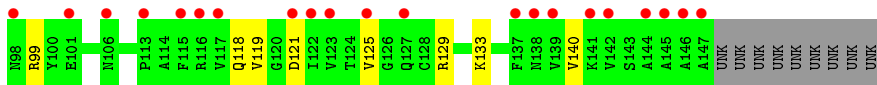
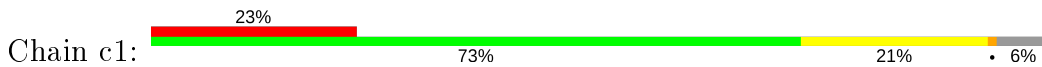
- Molecule 12: 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10-A



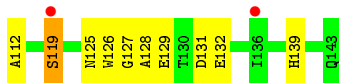
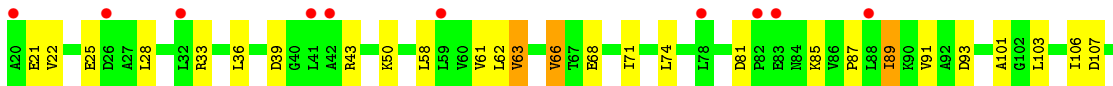
- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S Ribosomal Protein S11-A



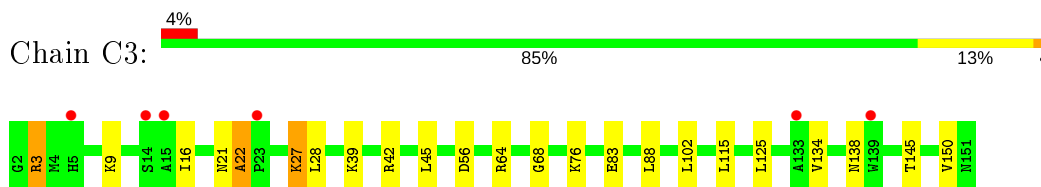
- Molecule 13: 40S ribosomal protein S11-A,40S ribosomal protein S11-A,40S Ribosomal Protein S11-A



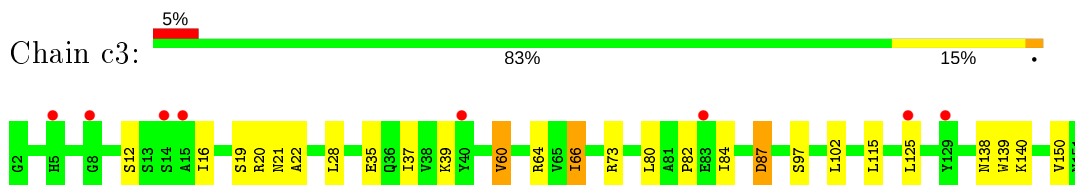
- Molecule 14: 40S Ribosomal Protein S12



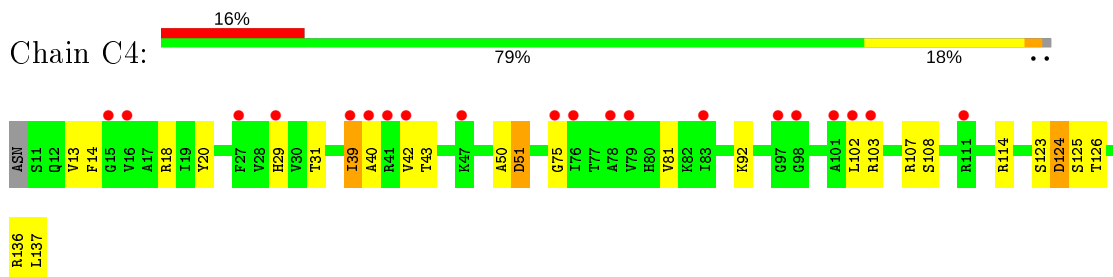
- Molecule 15: 40S ribosomal protein S13



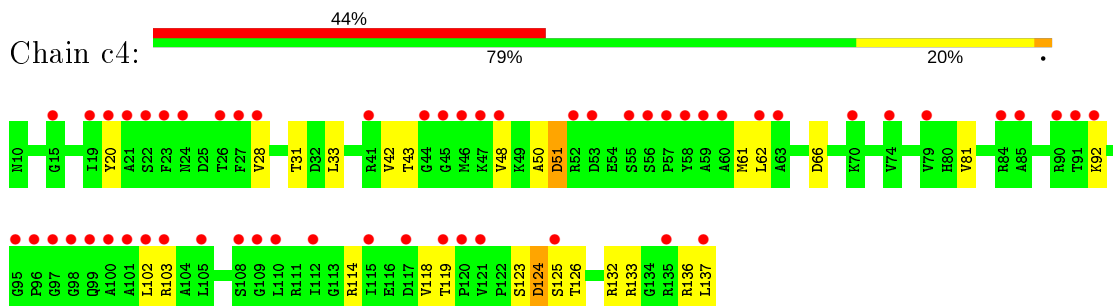
- Molecule 15: 40S ribosomal protein S13



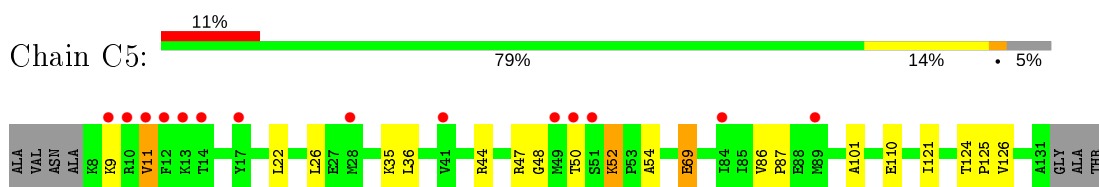
- Molecule 16: 40S Ribosomal Protein S14



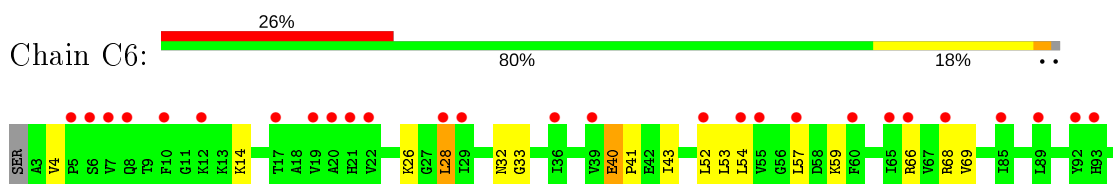
- Molecule 16: 40S Ribosomal Protein S14

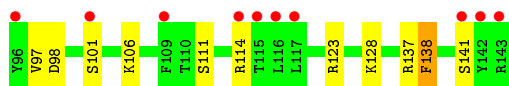


- Molecule 17: 40S ribosomal protein S15

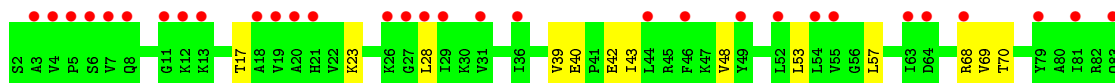
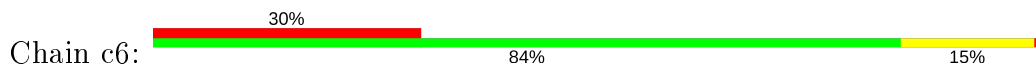


- Molecule 18: 40S ribosomal protein S16-A

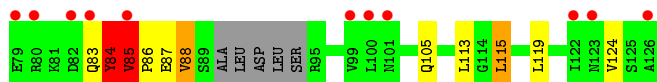
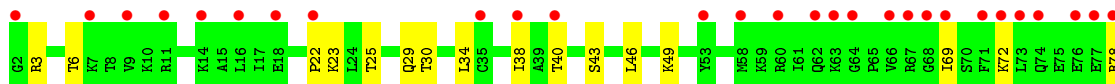
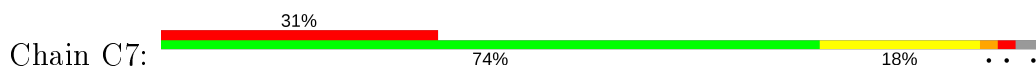




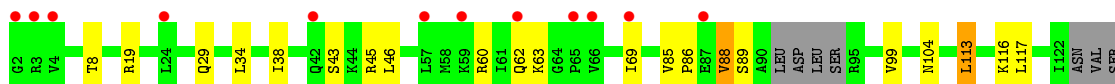
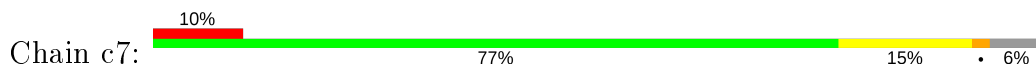
- Molecule 18: 40S ribosomal protein S16-A



- Molecule 19: 40S ribosomal protein S17-A

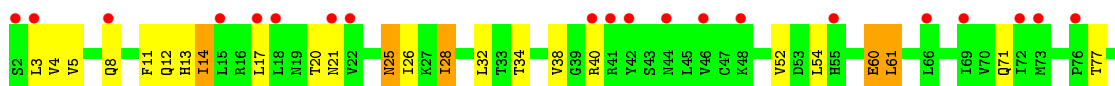
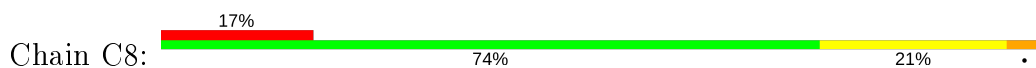


- Molecule 19: 40S ribosomal protein S17-A

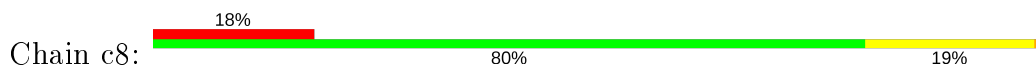


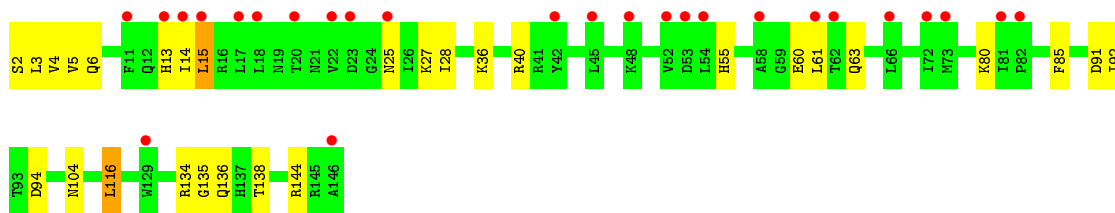
ALA

- Molecule 20: 40S ribosomal protein S18-A

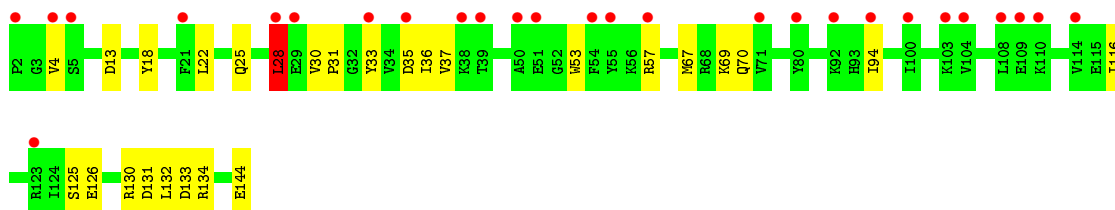
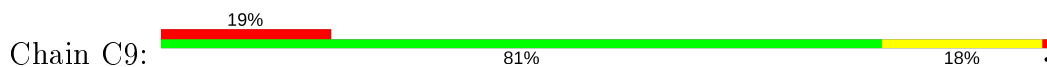


- Molecule 20: 40S ribosomal protein S18-A

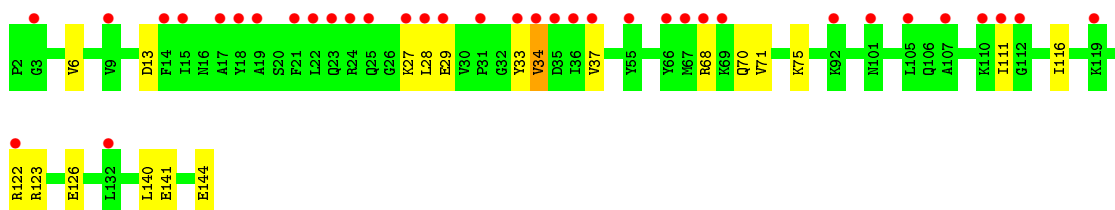
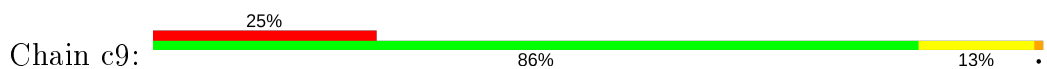




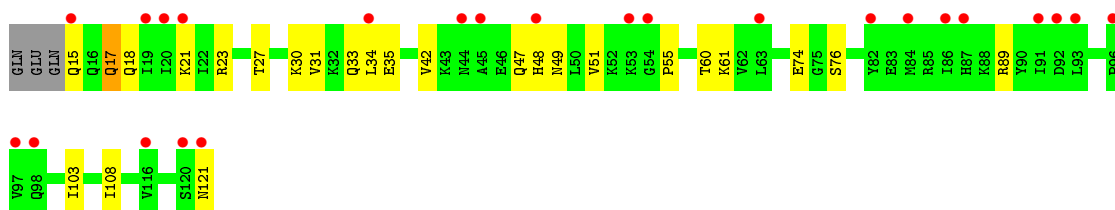
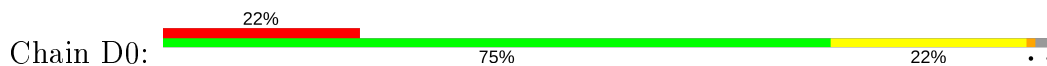
- Molecule 21: 40S ribosomal protein S19-A



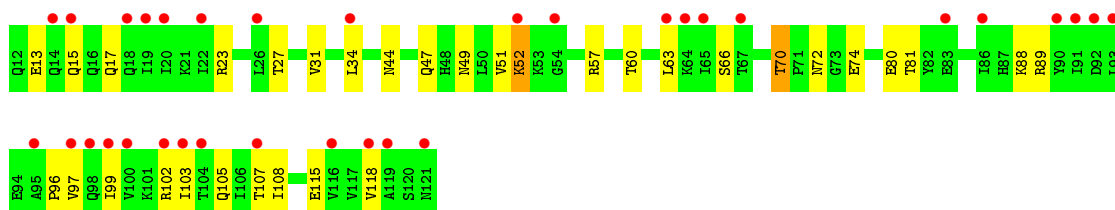
- Molecule 21: 40S ribosomal protein S19-A



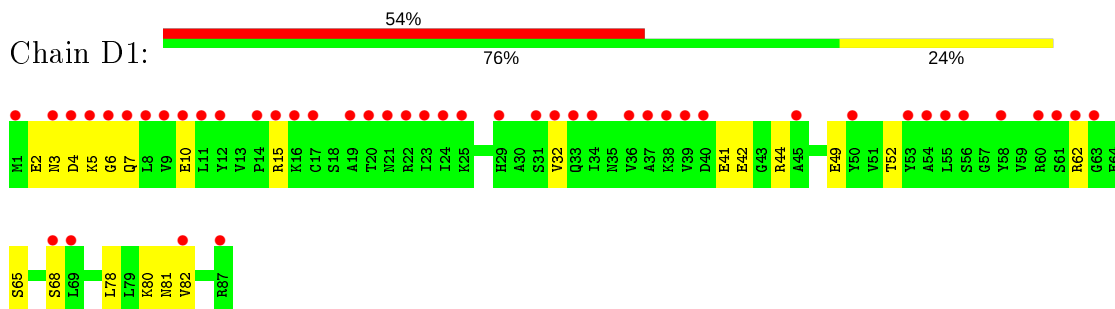
- Molecule 22: 40S ribosomal protein S20



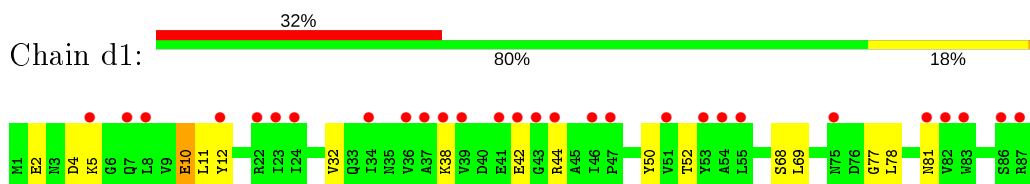
- Molecule 22: 40S ribosomal protein S20



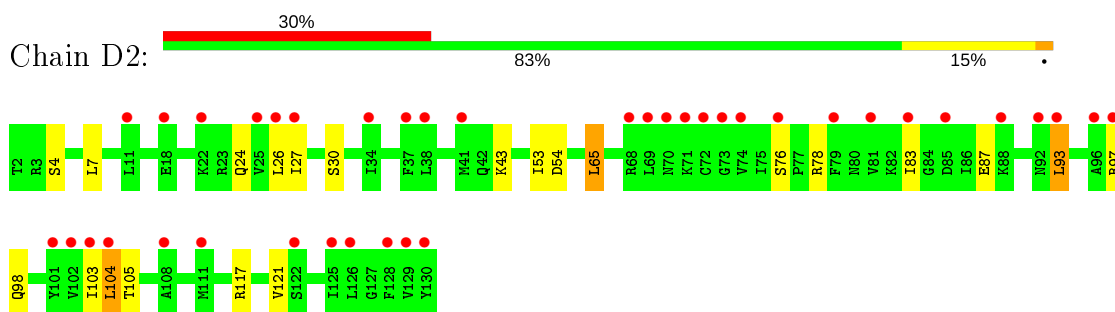
- Molecule 23: 40S ribosomal protein S21-A



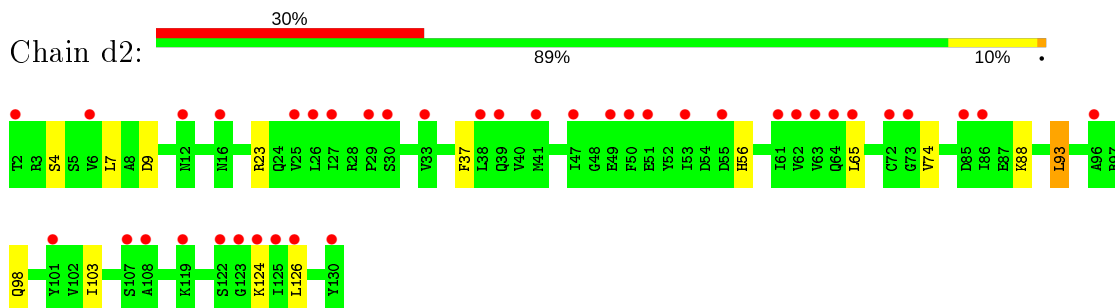
- Molecule 23: 40S ribosomal protein S21-A



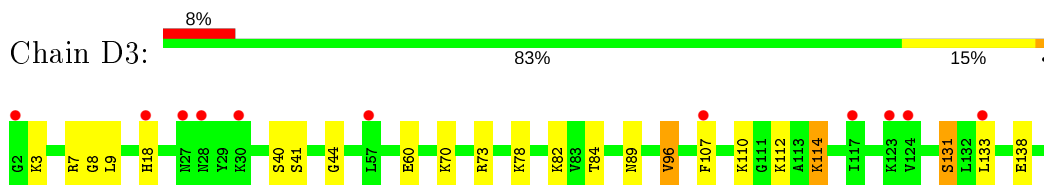
- Molecule 24: 40S ribosomal protein S22-A



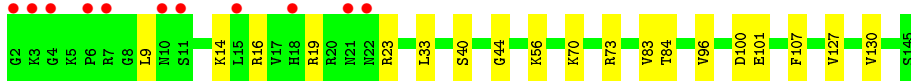
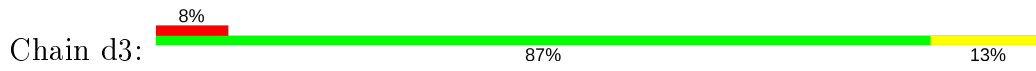
- Molecule 24: 40S ribosomal protein S22-A



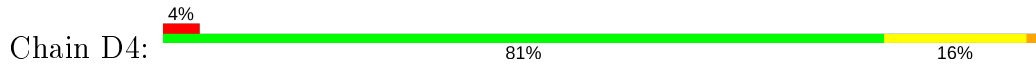
- Molecule 25: 40S ribosomal protein S23-A



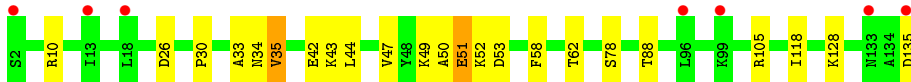
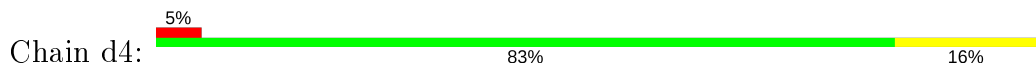
- Molecule 25: 40S ribosomal protein S23-A



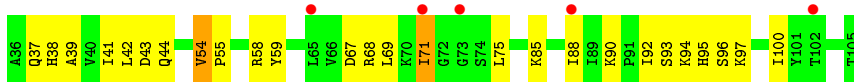
- Molecule 26: 40S ribosomal protein S24-A



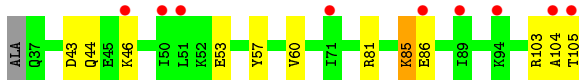
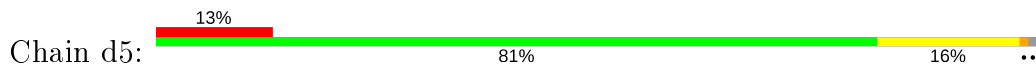
- Molecule 26: 40S ribosomal protein S24-A



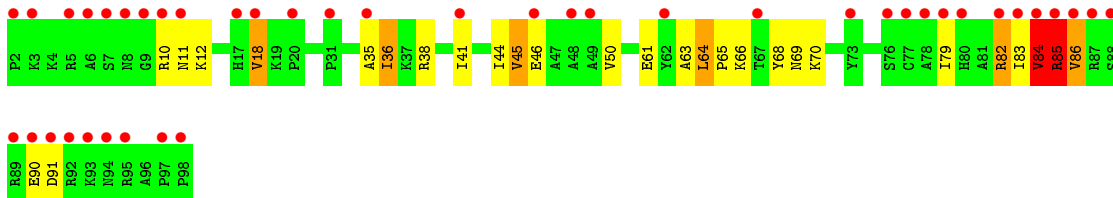
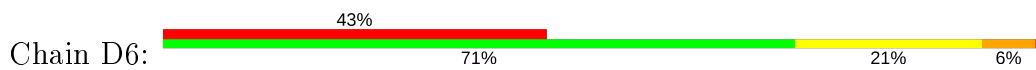
- Molecule 27: 40S ribosomal protein S25-A



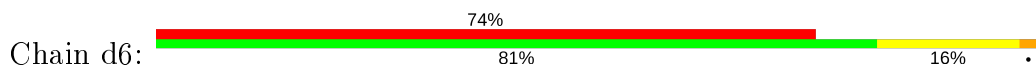
- Molecule 27: 40S ribosomal protein S25-A

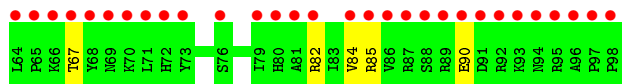
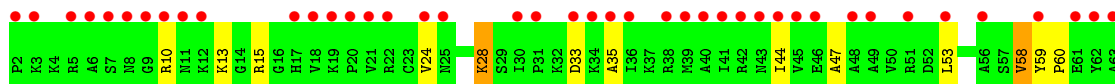


- Molecule 28: 40S ribosomal protein S26-B

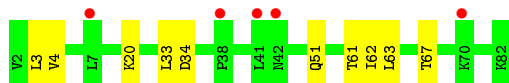
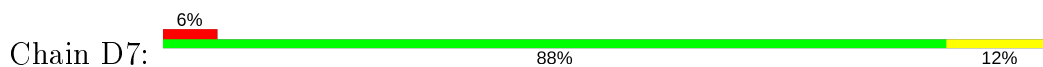


- Molecule 28: 40S ribosomal protein S26-B

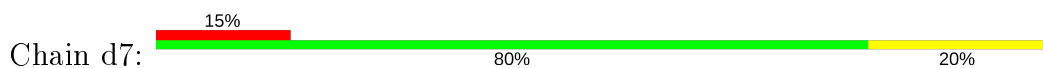




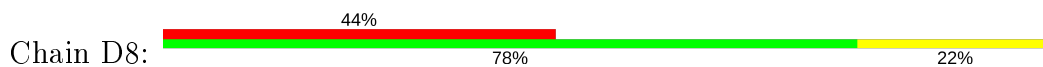
- Molecule 29: 40S ribosomal protein S27-A



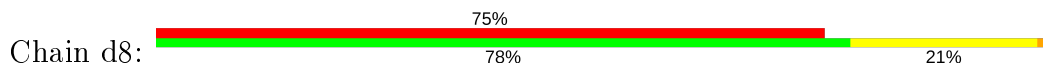
- Molecule 29: 40S ribosomal protein S27-A



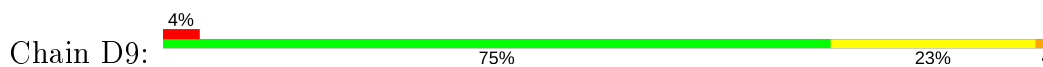
- Molecule 30: 40S ribosomal protein S28-A



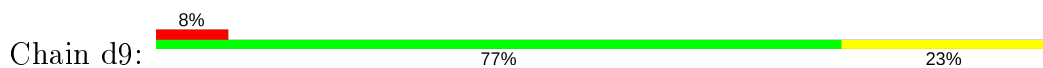
- Molecule 30: 40S ribosomal protein S28-A

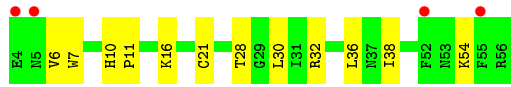


- Molecule 31: 40S ribosomal protein S29-A

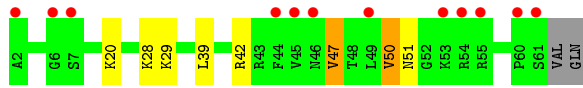
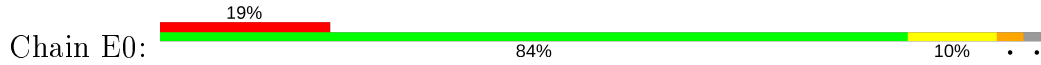


- Molecule 31: 40S ribosomal protein S29-A

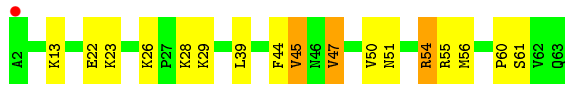
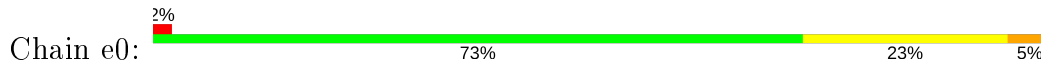




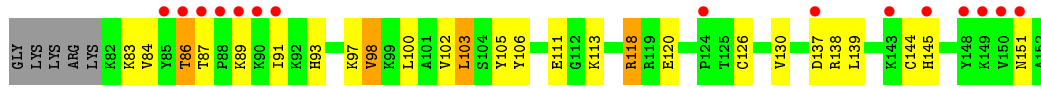
• Molecule 32: 40S ribosomal protein S30-A



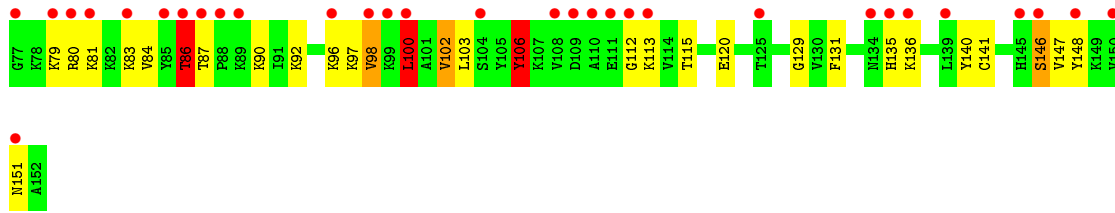
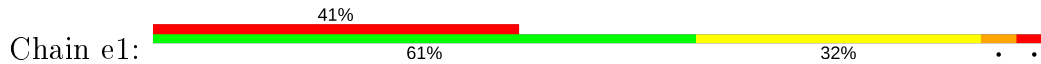
• Molecule 32: 40S ribosomal protein S30-A



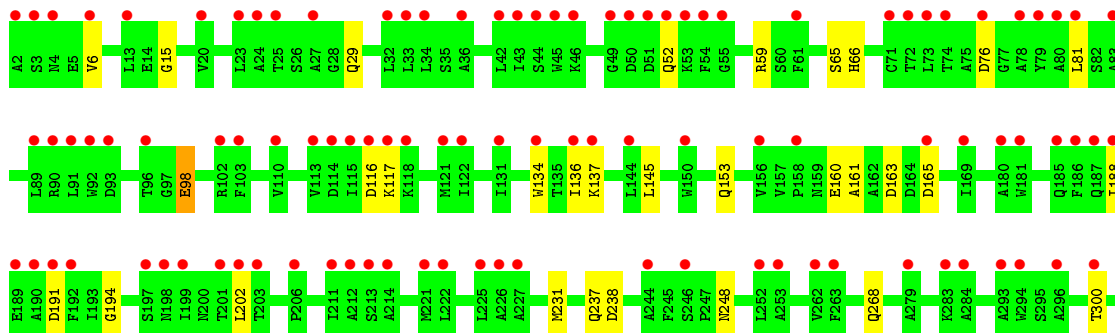
• Molecule 33: Ubiquitin-40S ribosomal protein S31

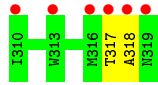


• Molecule 33: Ubiquitin-40S ribosomal protein S31

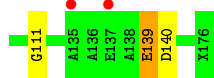
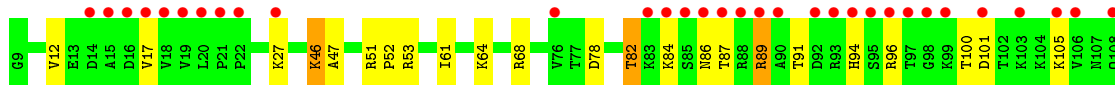
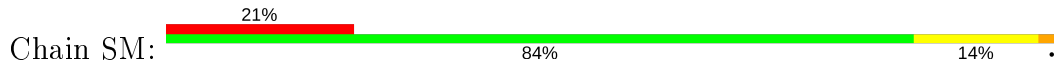


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

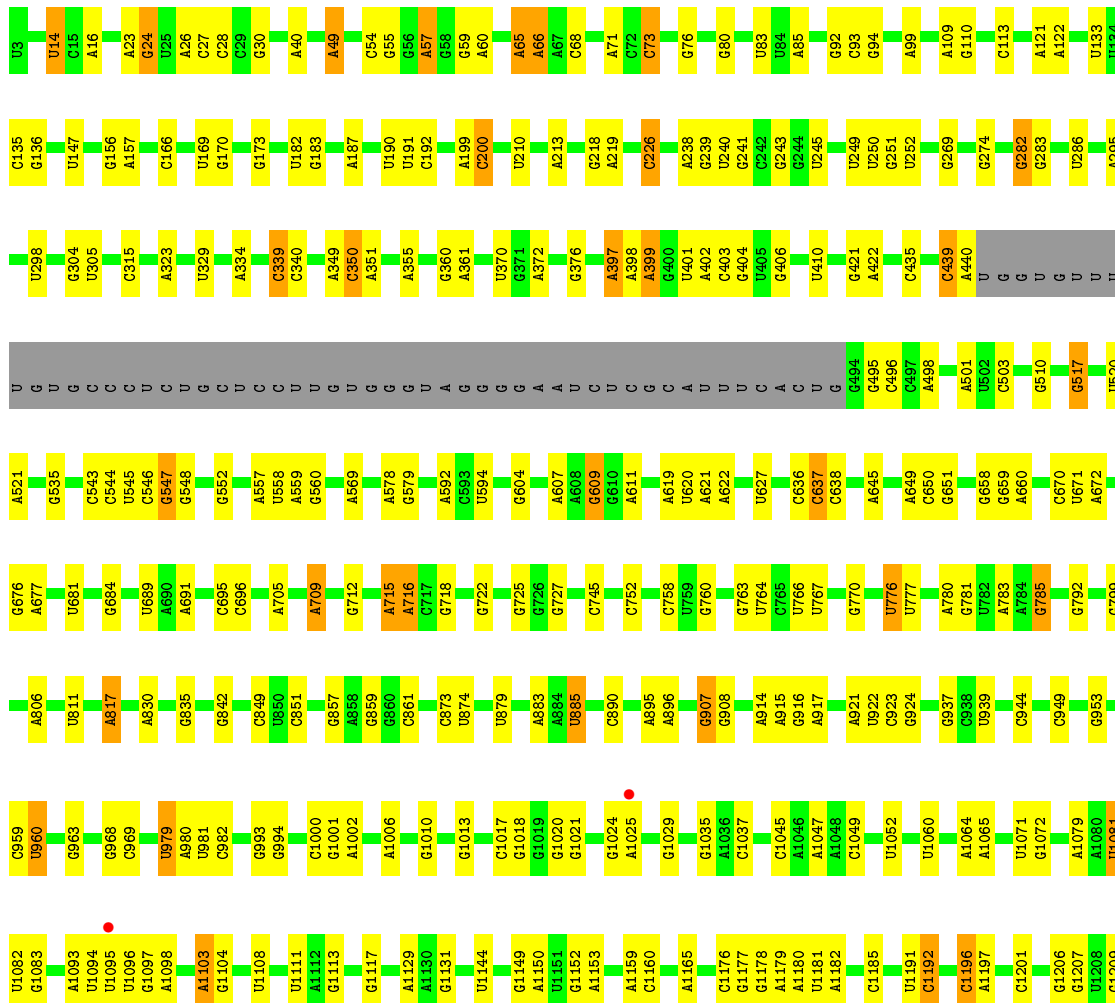


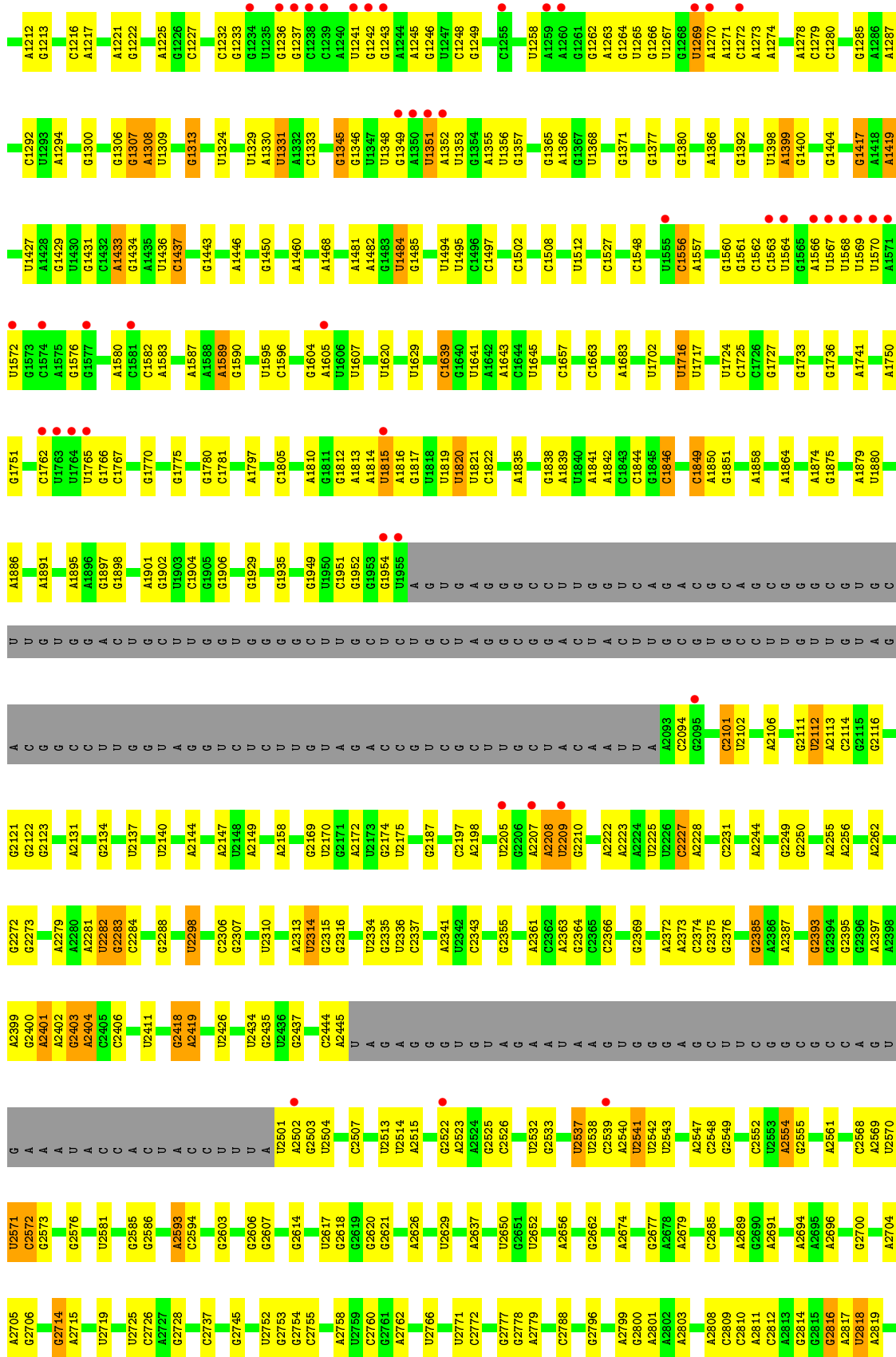


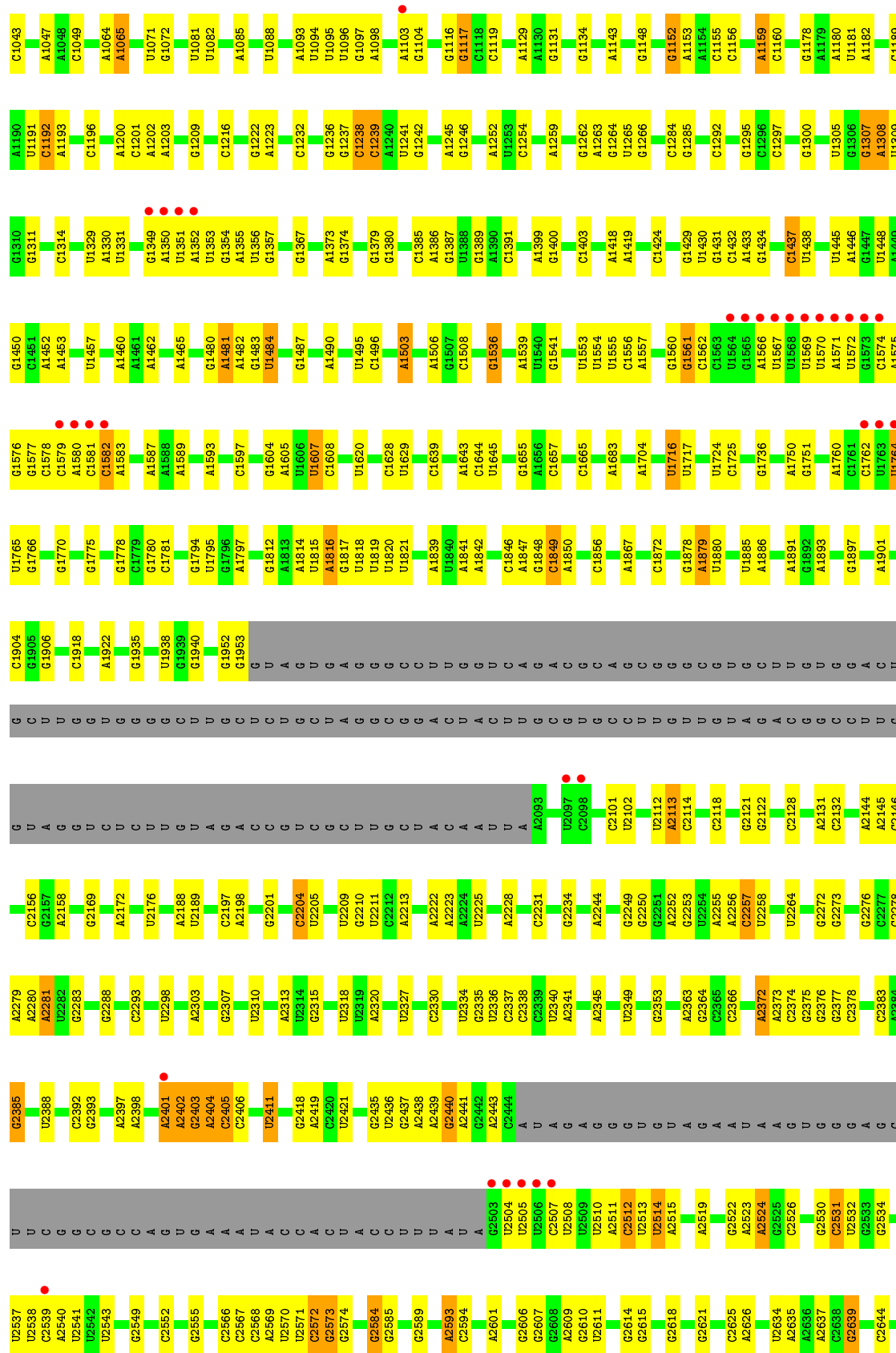
- Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1

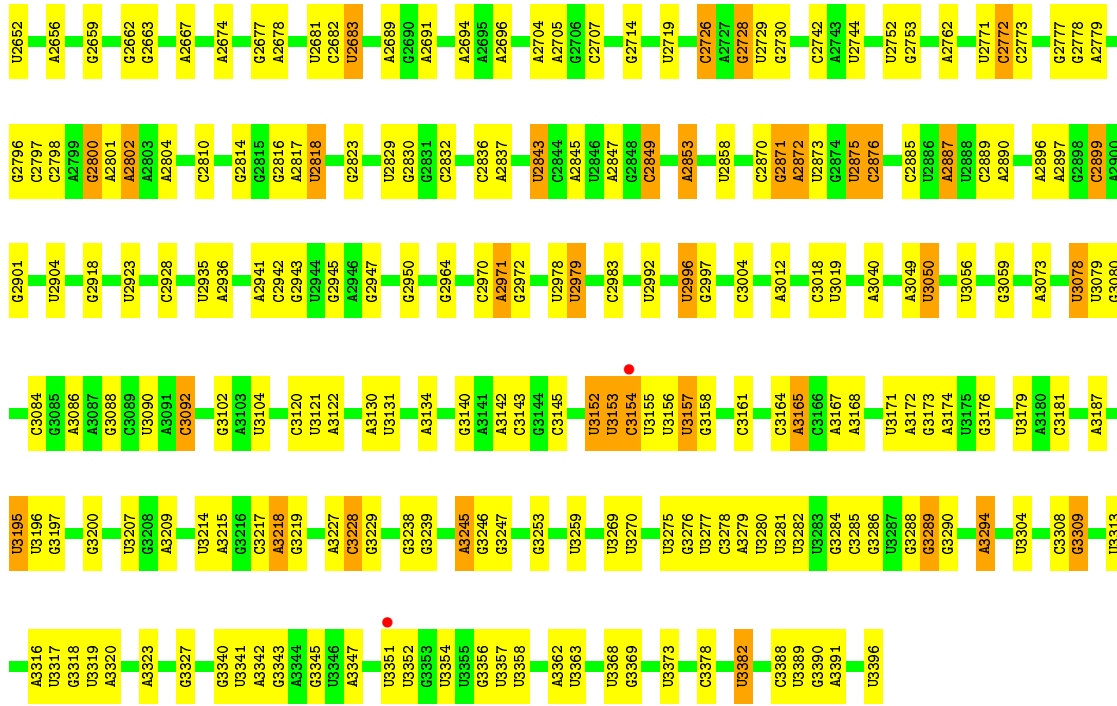


- Molecule 36: 25S rRNA

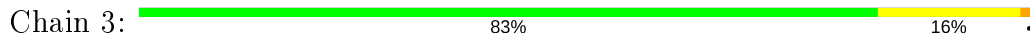




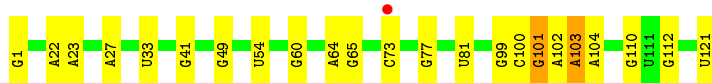
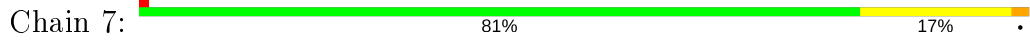




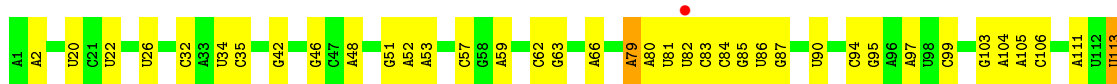
● Molecule 37: 5S rRNA



● Molecule 37: 5S rRNA



● Molecule 38: 5.8S rRNA

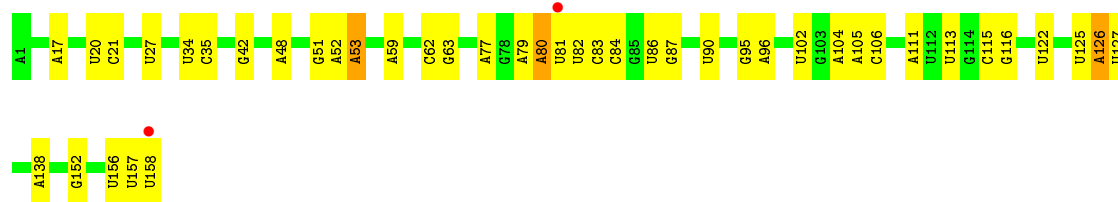


● Molecule 38: 5.8S rRNA

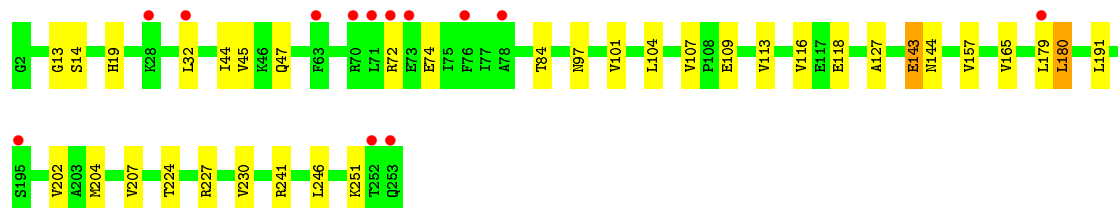
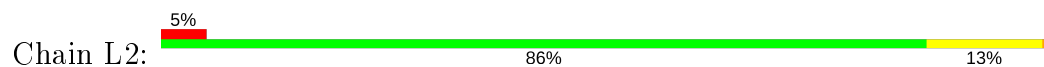


● Molecule 38: 5.8S rRNA

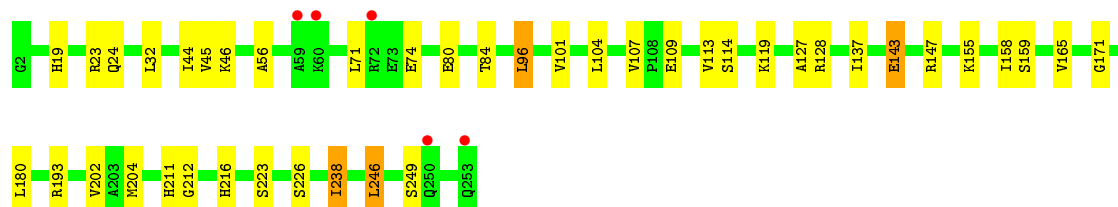
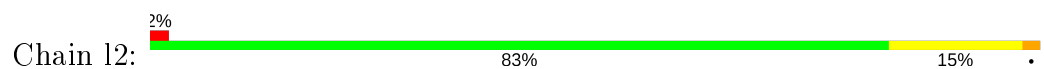




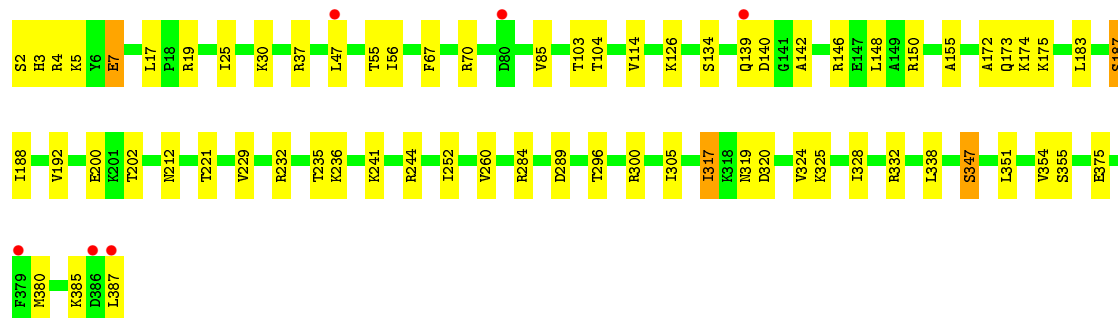
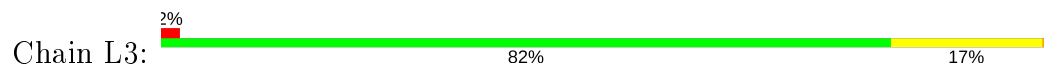
- Molecule 39: 60S ribosomal protein L2-A



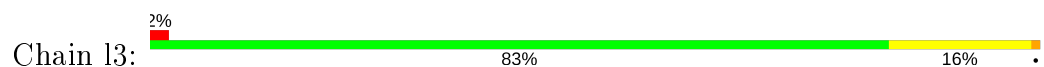
- Molecule 39: 60S ribosomal protein L2-A

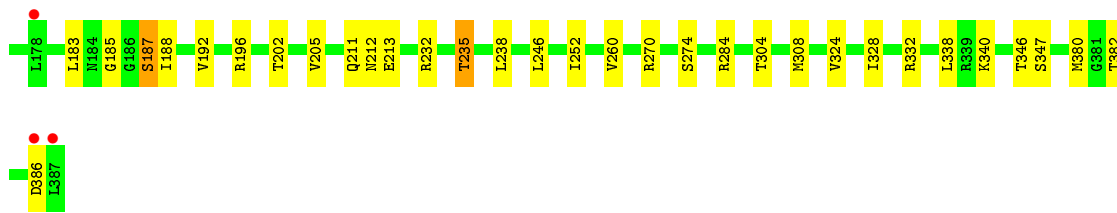


- Molecule 40: 60S ribosomal protein L3

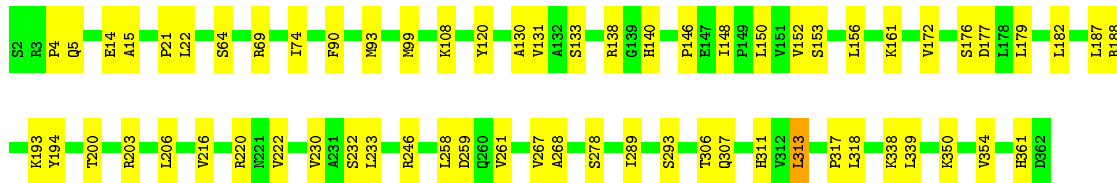
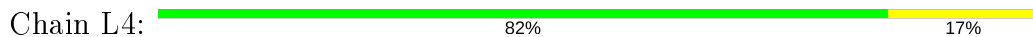


- Molecule 40: 60S ribosomal protein L3

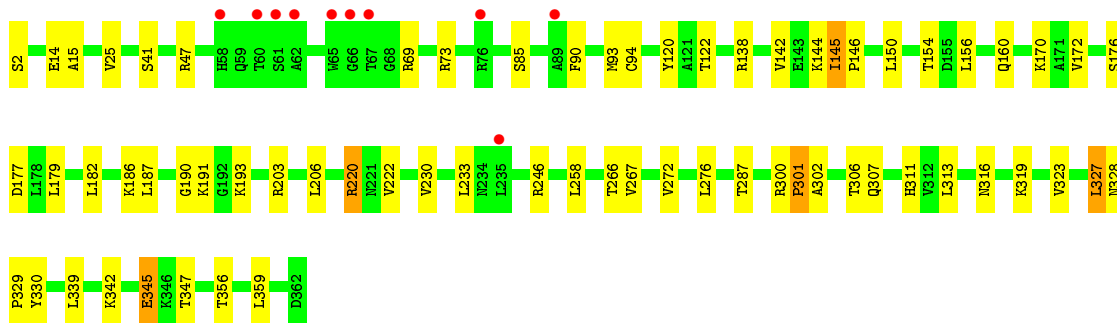
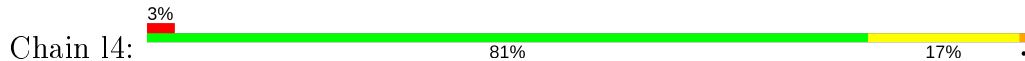




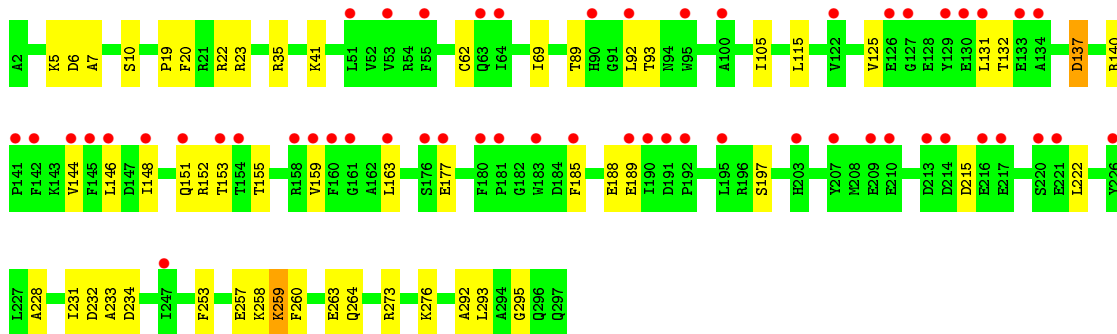
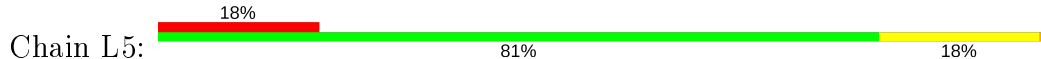
• Molecule 41: 60S ribosomal protein L4-A



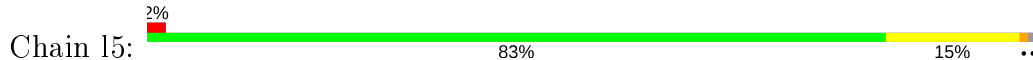
• Molecule 41: 60S ribosomal protein L4-A

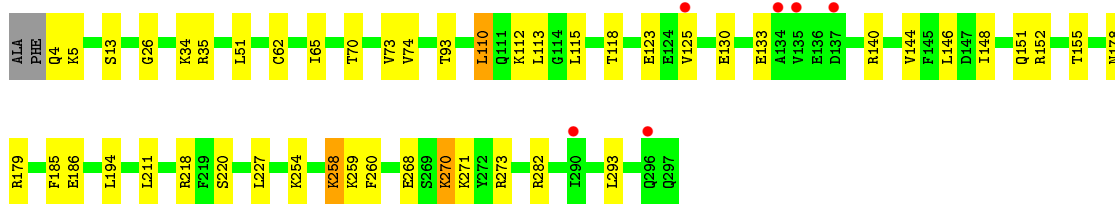


• Molecule 42: 60S ribosomal protein L5

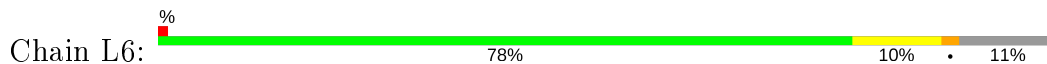


• Molecule 42: 60S ribosomal protein L5

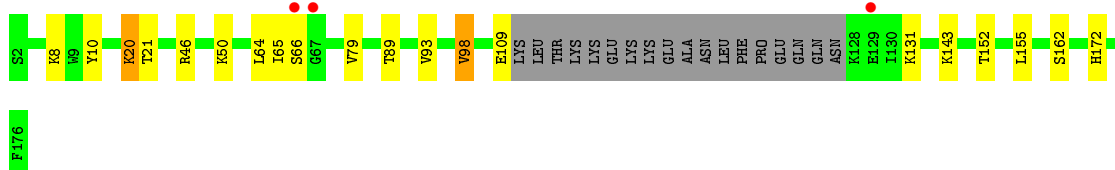
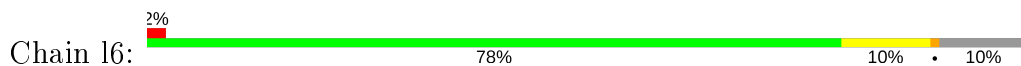




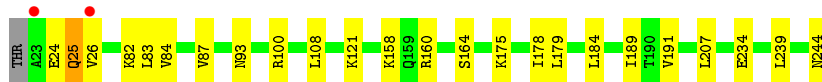
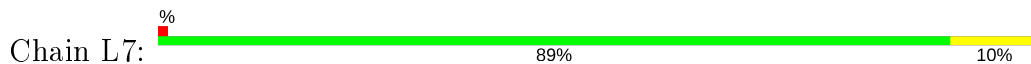
- Molecule 43: 60S ribosomal protein L6-A



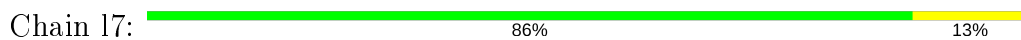
- Molecule 43: 60S ribosomal protein L6-A



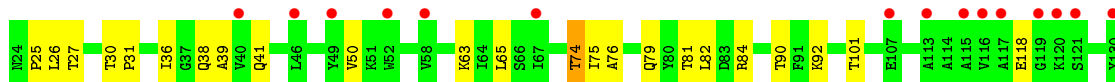
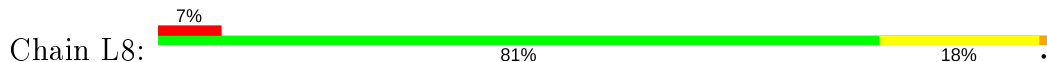
- Molecule 44: 60S ribosomal protein L7-A



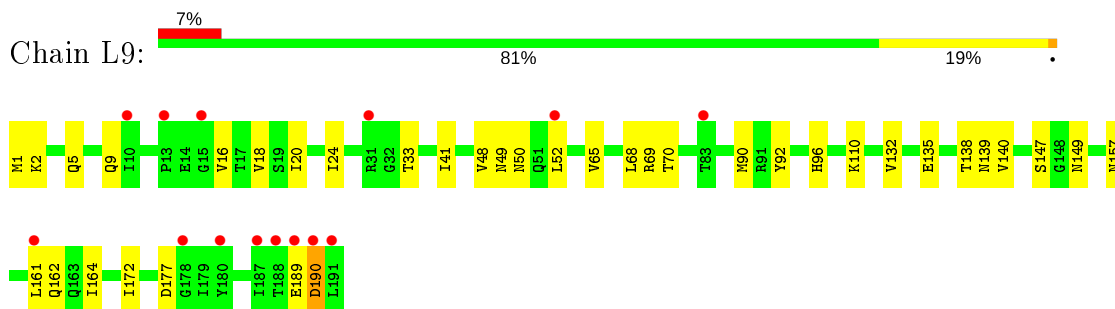
- Molecule 44: 60S ribosomal protein L7-A



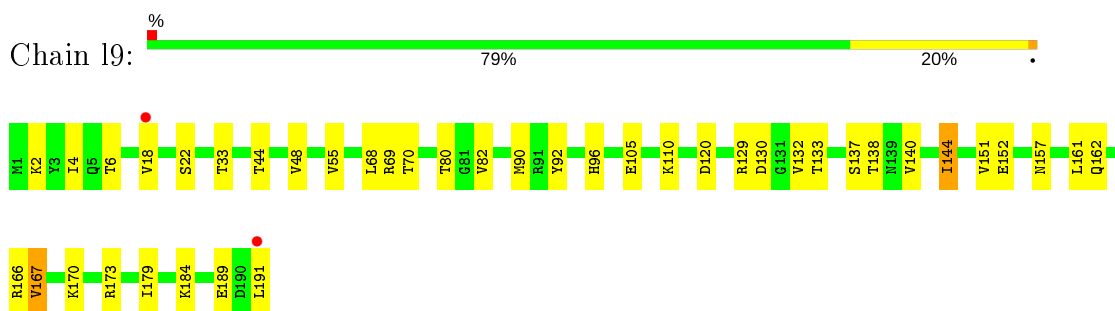
- Molecule 45: 60S ribosomal protein L8-A



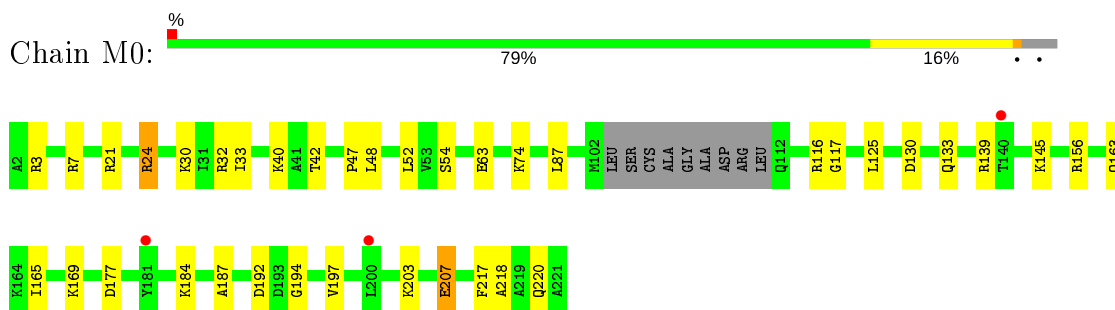
- Molecule 46: 60S ribosomal protein L9-A



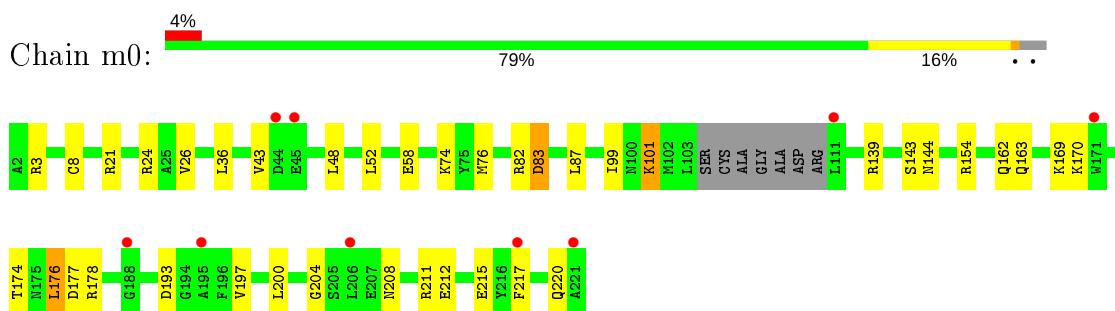
- Molecule 46: 60S ribosomal protein L9-A



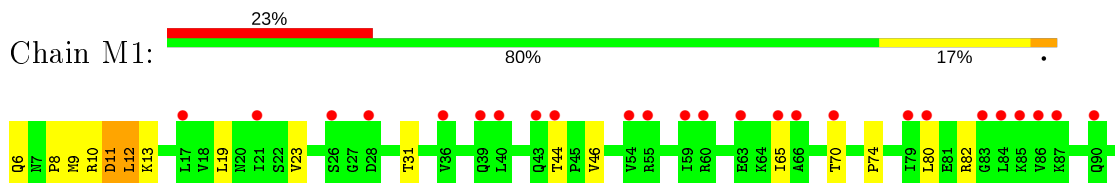
- Molecule 47: 60S ribosomal protein L10

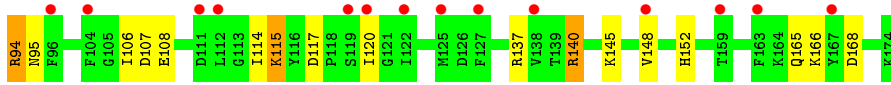


- Molecule 47: 60S ribosomal protein L10



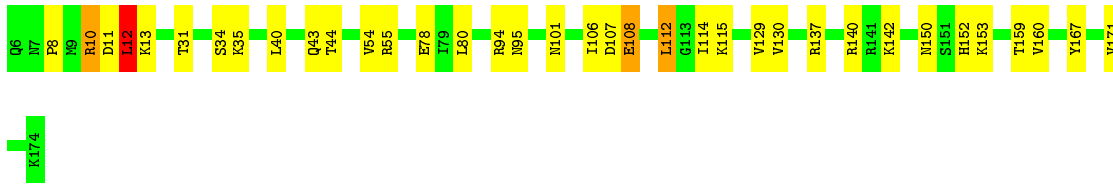
- Molecule 48: 60S ribosomal protein L11-B





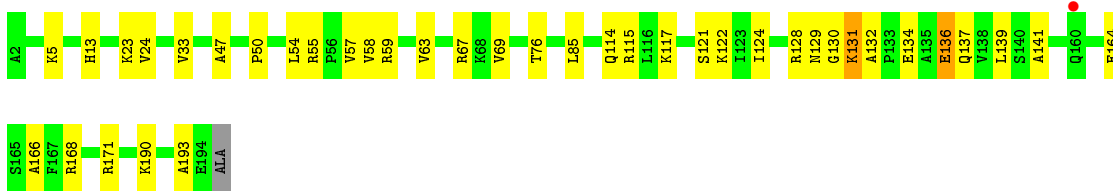
- Molecule 48: 60S ribosomal protein L11-B

Chain m1: 79% 19% ..



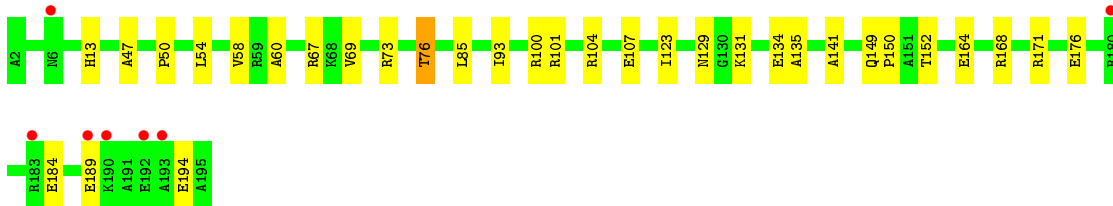
- Molecule 49: 60S ribosomal protein L13-A

Chain M3: 79% 19% ..



- Molecule 49: 60S ribosomal protein L13-A

Chain m3: 4% 84% 16% .



- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 82% 15% ..

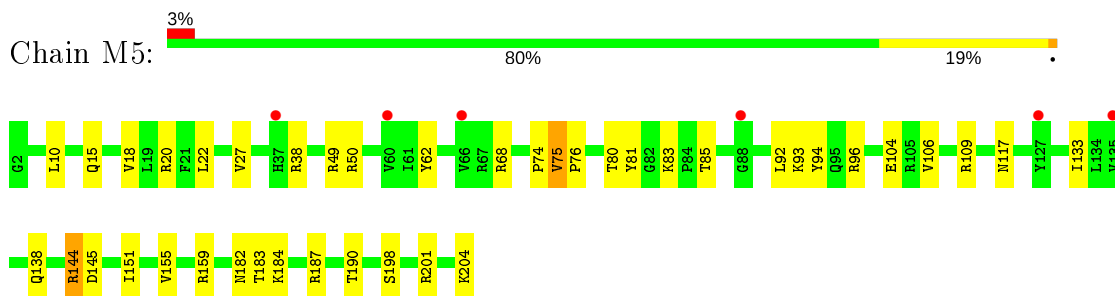


- Molecule 50: 60S ribosomal protein L14-A

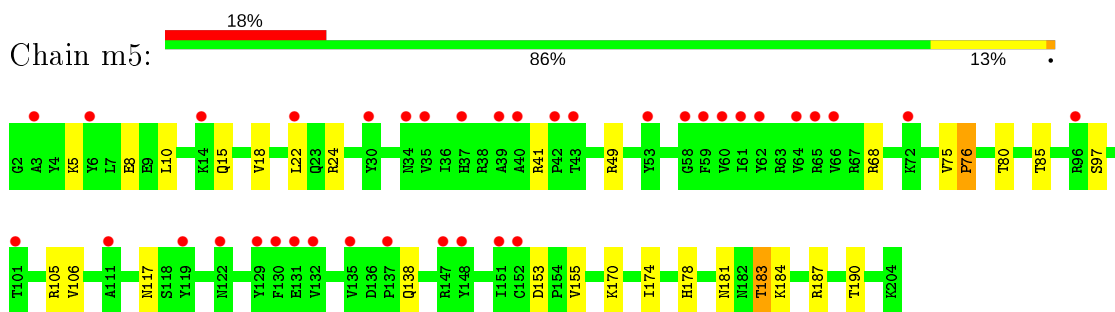
Chain m4: 3% 86% 13% .



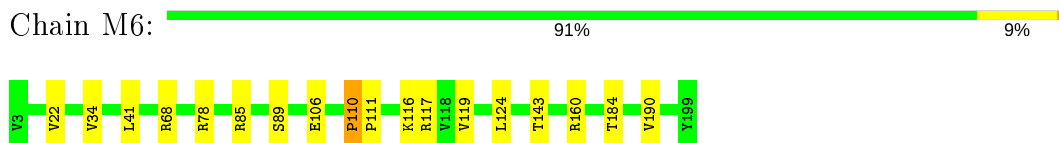
- Molecule 51: 60S ribosomal protein L15-A



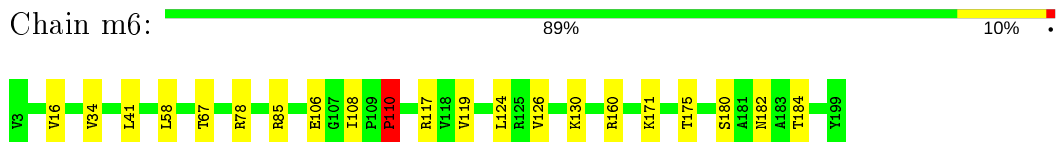
- Molecule 51: 60S ribosomal protein L15-A



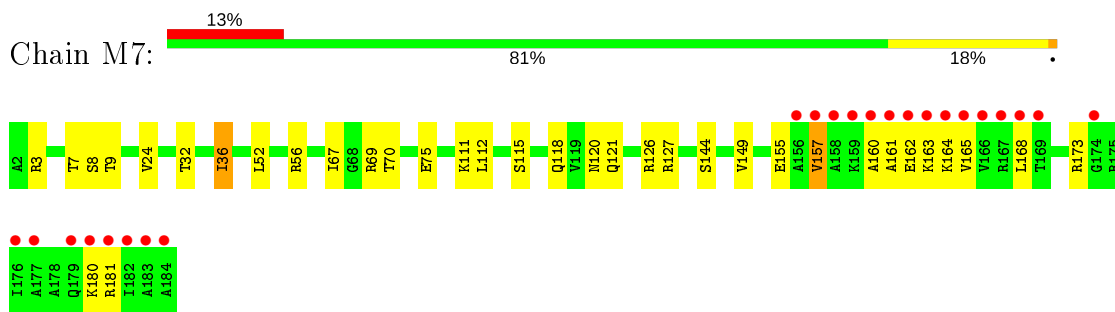
- Molecule 52: 60S ribosomal protein L16-A



- Molecule 52: 60S ribosomal protein L16-A

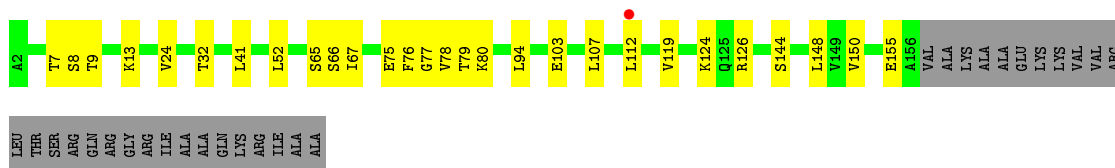


- Molecule 53: 60S ribosomal protein L17-A

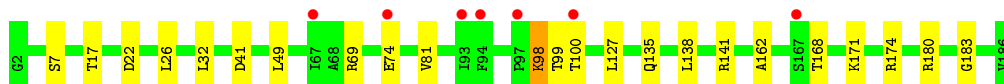
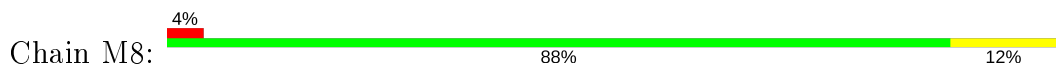


- Molecule 53: 60S ribosomal protein L17-A

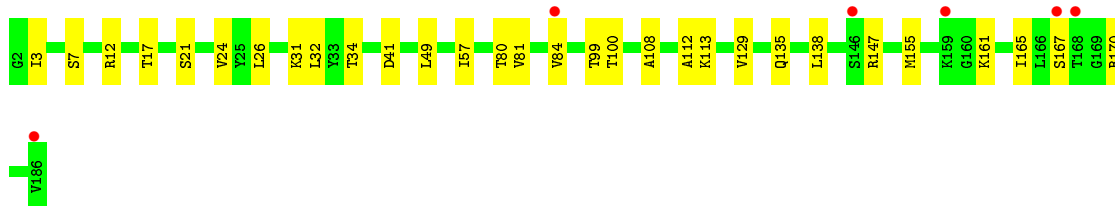
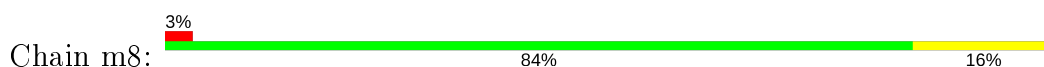




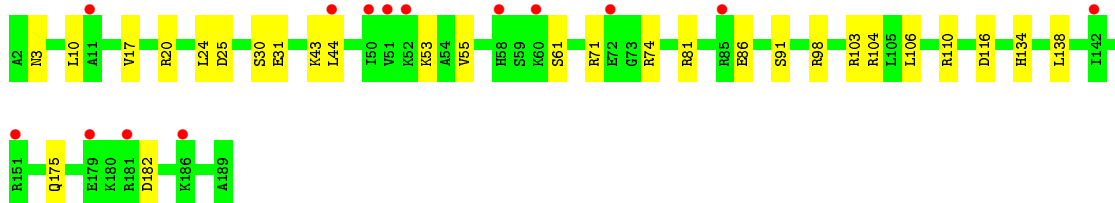
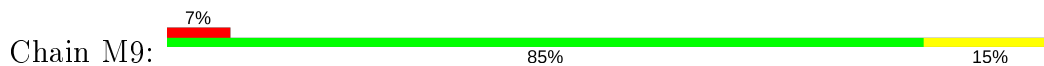
- Molecule 54: 60S ribosomal protein L18-A



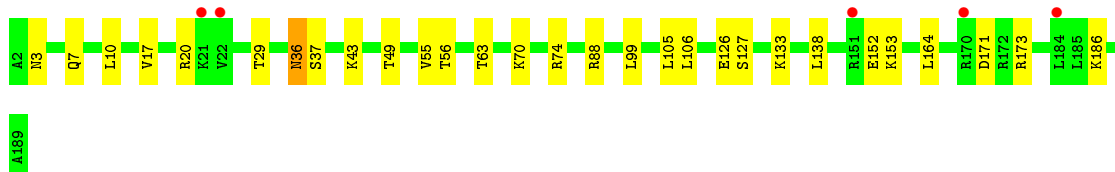
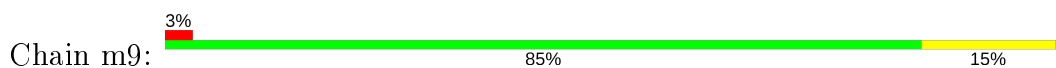
- Molecule 54: 60S ribosomal protein L18-A



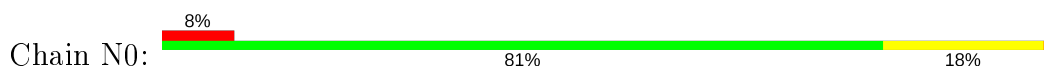
- Molecule 55: 60S ribosomal protein L19-A

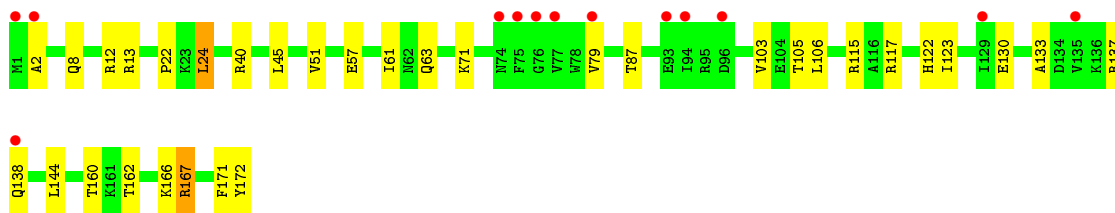


- Molecule 55: 60S ribosomal protein L19-A

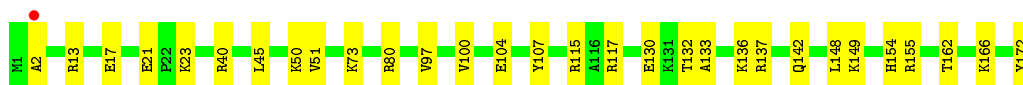
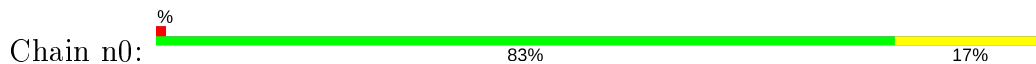


- Molecule 56: 60S ribosomal protein L20-A

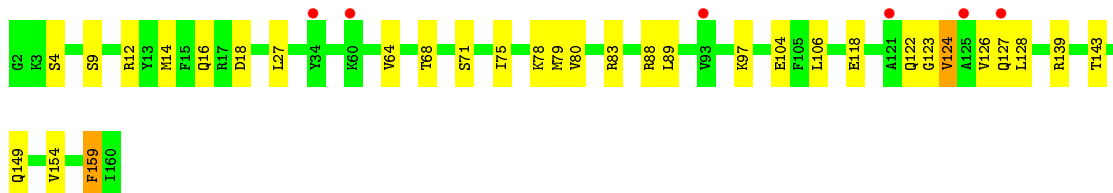
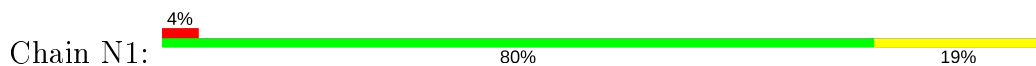




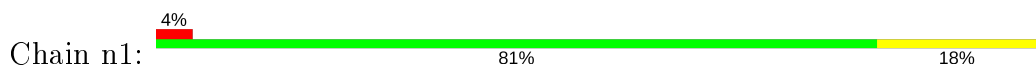
- Molecule 56: 60S ribosomal protein L20-A



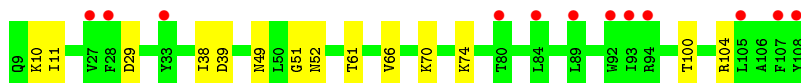
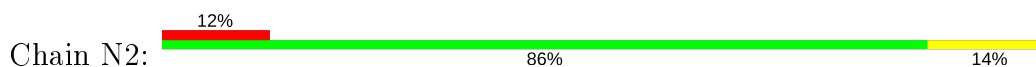
- Molecule 57: 60S ribosomal protein L21-A



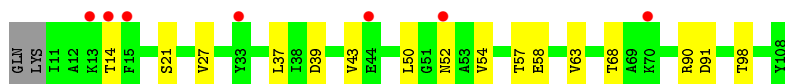
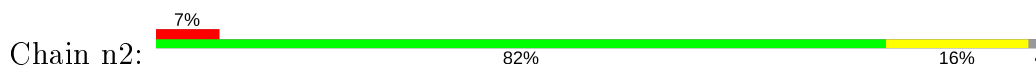
- Molecule 57: 60S ribosomal protein L21-A



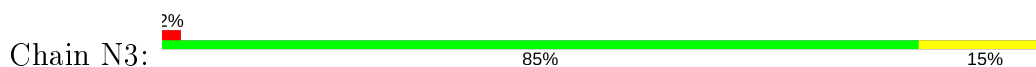
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A

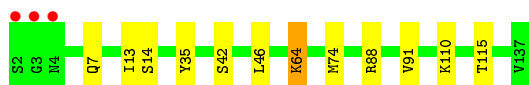
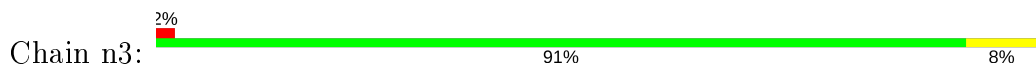


- Molecule 59: 60S ribosomal protein L23-A

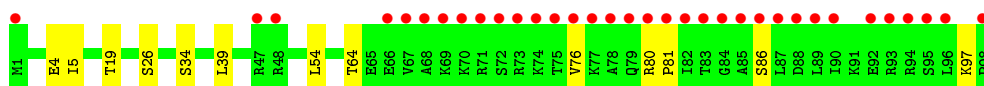
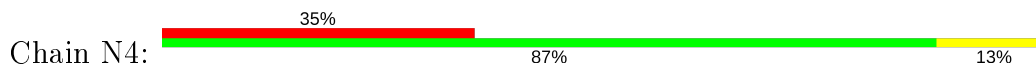




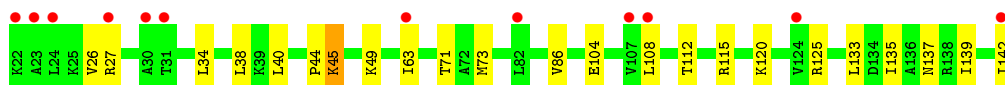
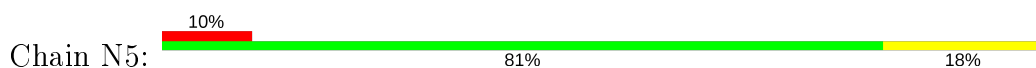
- Molecule 59: 60S ribosomal protein L23-A



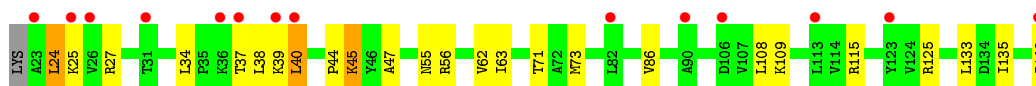
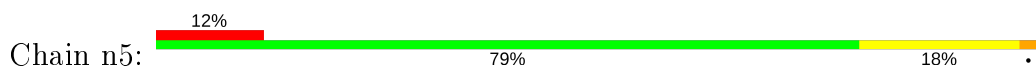
- Molecule 60: 60S ribosomal protein L24-A



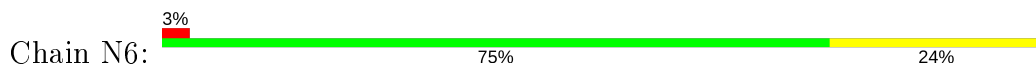
- Molecule 61: 60S ribosomal protein L25



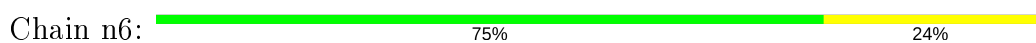
- Molecule 61: 60S ribosomal protein L25



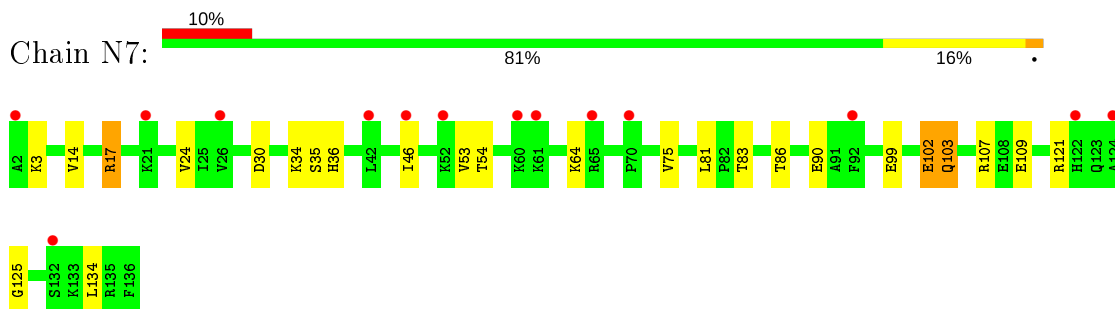
- Molecule 62: 60S ribosomal protein L26-A



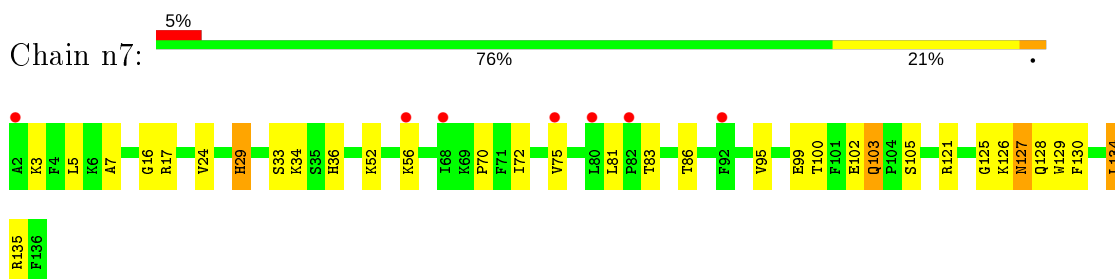
- Molecule 62: 60S ribosomal protein L26-A



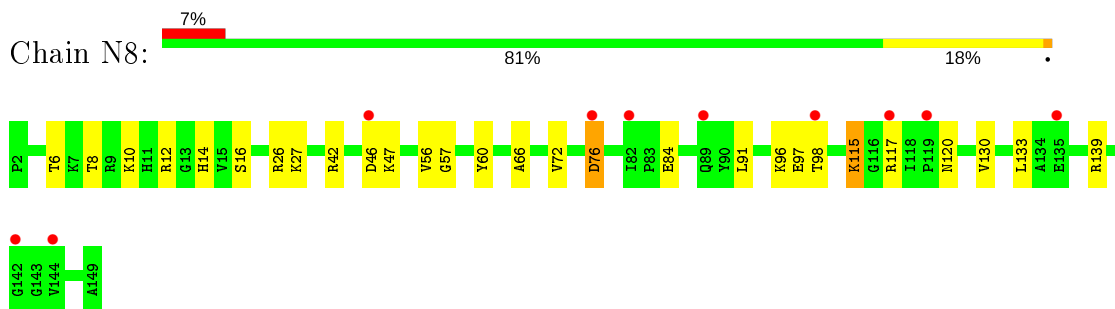
- Molecule 63: 60S ribosomal protein L27-A



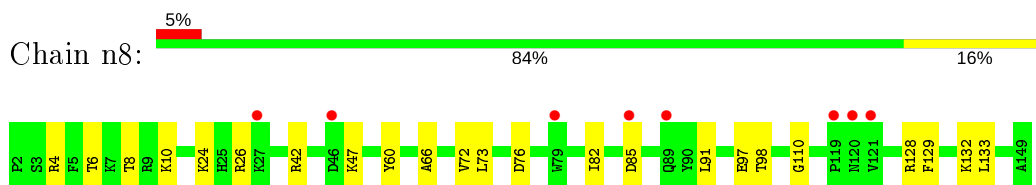
- Molecule 63: 60S ribosomal protein L27-A



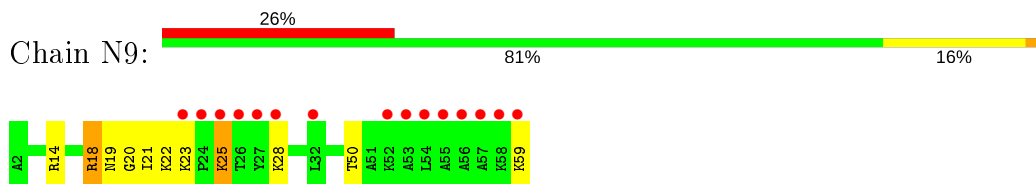
- Molecule 64: 60S ribosomal protein L28



- Molecule 64: 60S ribosomal protein L28

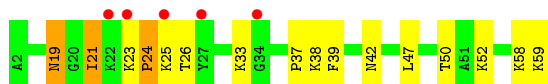


- Molecule 65: 60S ribosomal protein L29

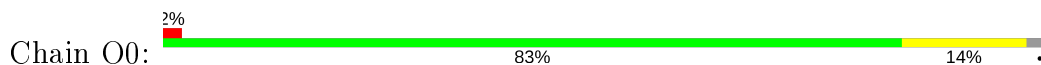


- Molecule 65: 60S ribosomal protein L29

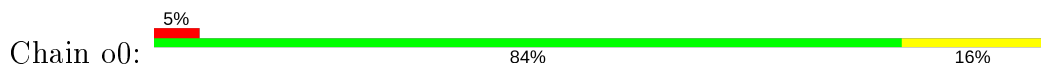




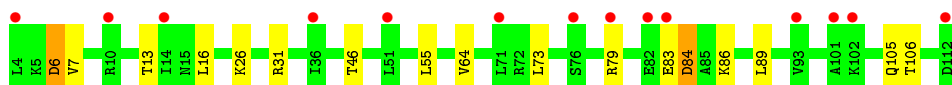
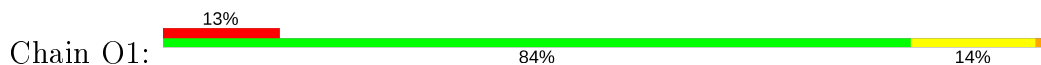
- Molecule 66: 60S ribosomal protein L30



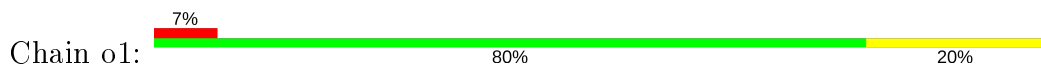
- Molecule 66: 60S ribosomal protein L30



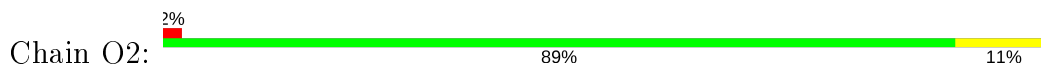
- Molecule 67: 60S ribosomal protein L31-A



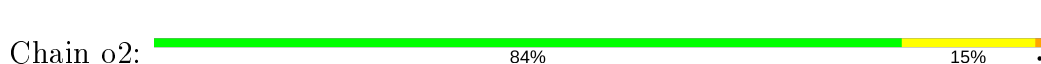
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32



- Molecule 68: 60S ribosomal protein L32




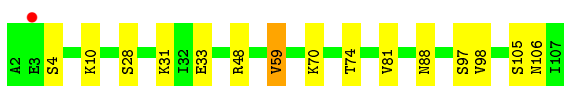
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:  89% 10%




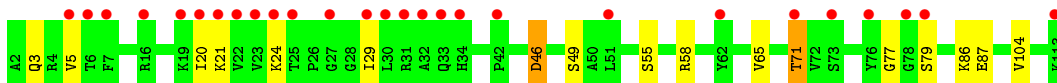
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:  86% 13%




• Molecule 70: 60S ribosomal protein L34-A

Chain O4:  24% 85% 13%




• Molecule 70: 60S ribosomal protein L34-A

Chain o4:  5% 87% 13%




• Molecule 71: 60S ribosomal protein L35-A

Chain O5:  3% 82% 18%




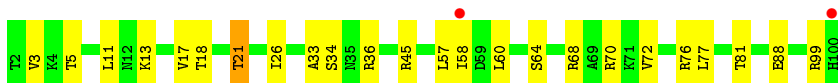
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:  1% 81% 18%

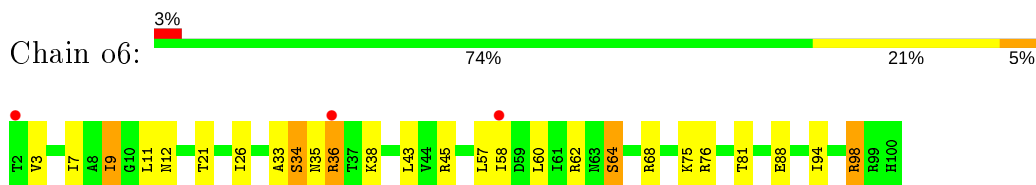


• Molecule 72: 60S ribosomal protein L36-A

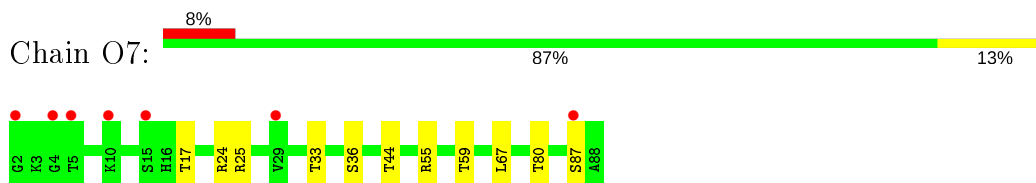
Chain O6:  2% 76% 23%



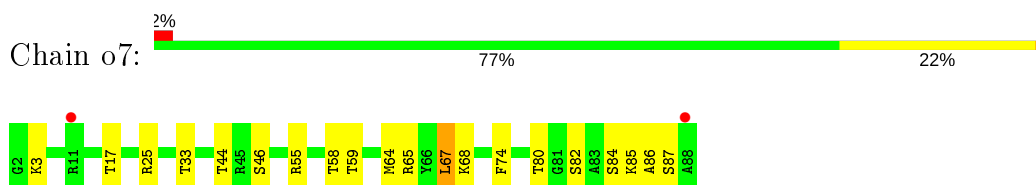
- Molecule 72: 60S ribosomal protein L36-A



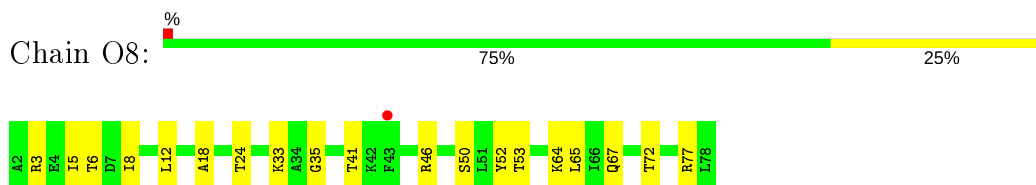
- Molecule 73: 60S ribosomal protein L37-A



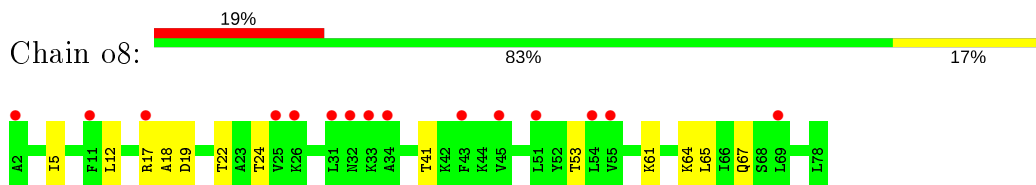
- Molecule 73: 60S ribosomal protein L37-A



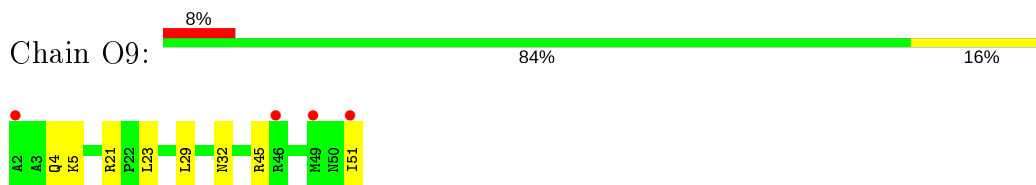
- Molecule 74: 60S ribosomal protein L38



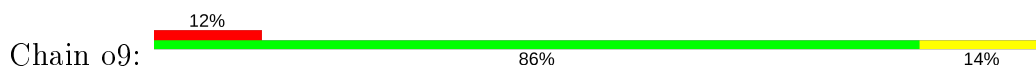
- Molecule 74: 60S ribosomal protein L38

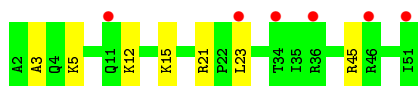


- Molecule 75: 60S ribosomal protein L39

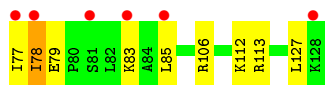
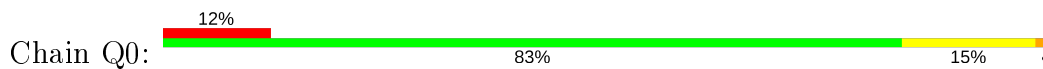


- Molecule 75: 60S ribosomal protein L39

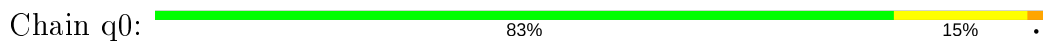




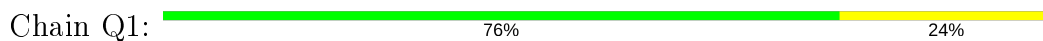
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



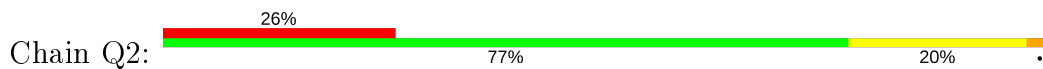
- Molecule 77: 60S ribosomal protein L41-A



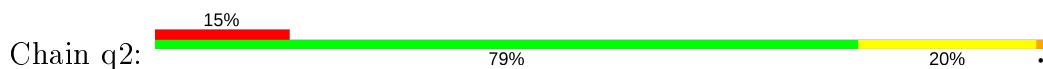
- Molecule 77: 60S ribosomal protein L41-A

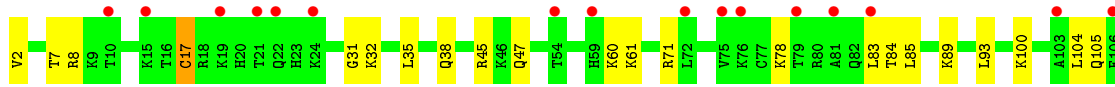


- Molecule 78: 60S ribosomal protein L42-A

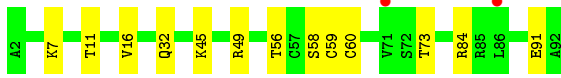
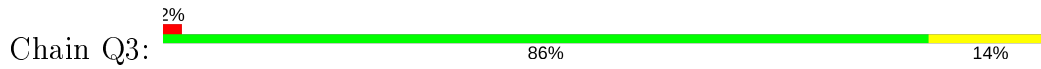


- Molecule 78: 60S ribosomal protein L42-A

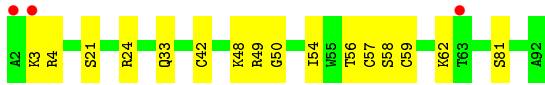
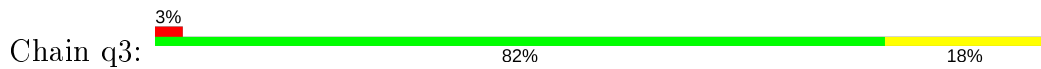




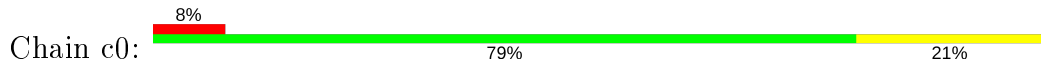
- Molecule 79: 60S ribosomal protein L43-A



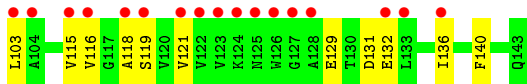
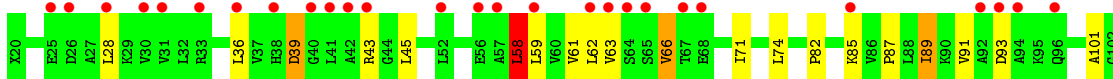
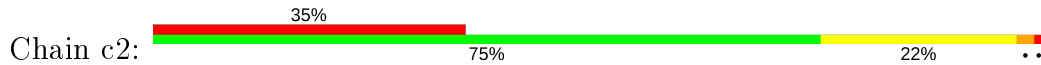
- Molecule 79: 60S ribosomal protein L43-A



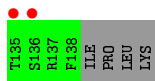
- Molecule 80: 40S ribosomal protein S10-A, 40S ribosomal protein S10-A, 40S Ribosomal Protein S10



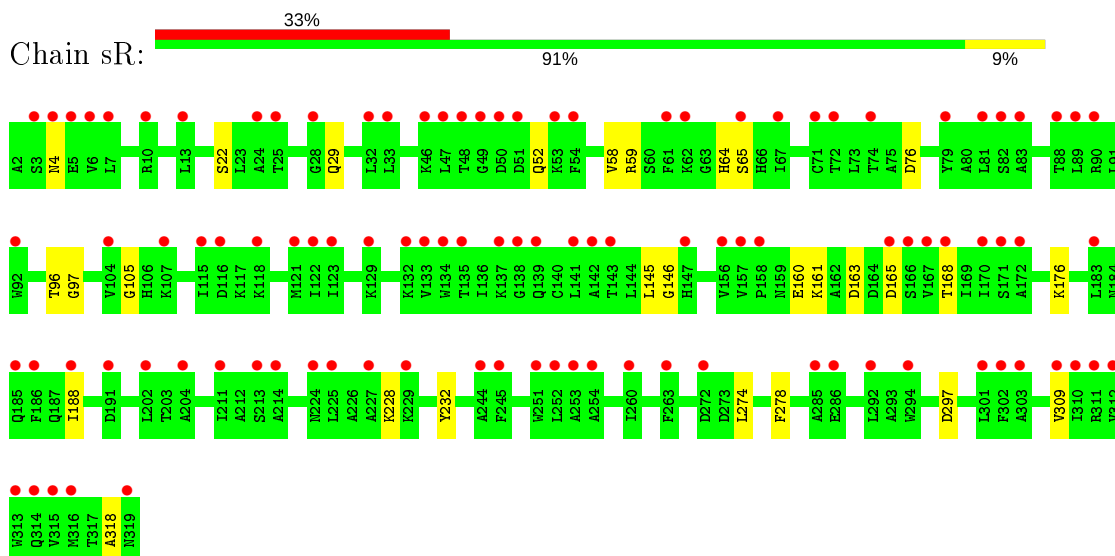
- Molecule 81: 40S Ribosomal Protein S12



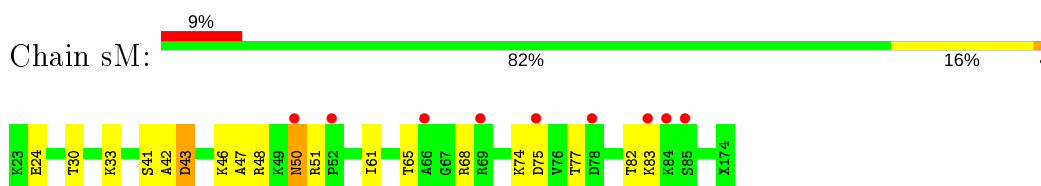
- Molecule 82: 40S ribosomal protein S15



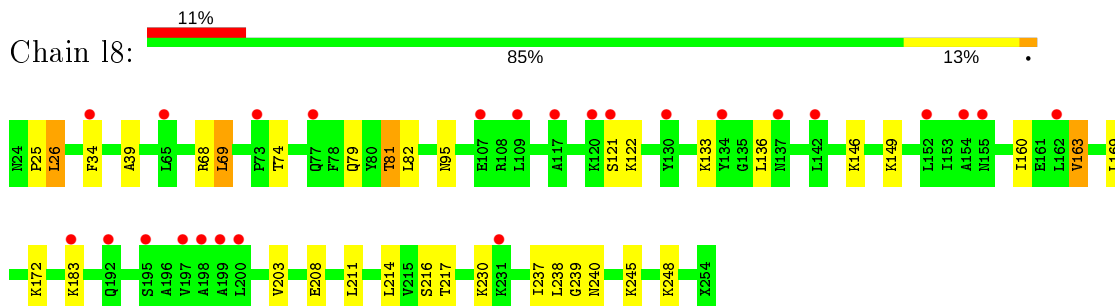
- Molecule 83: Guanine nucleotide-binding protein subunit beta-like protein



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



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

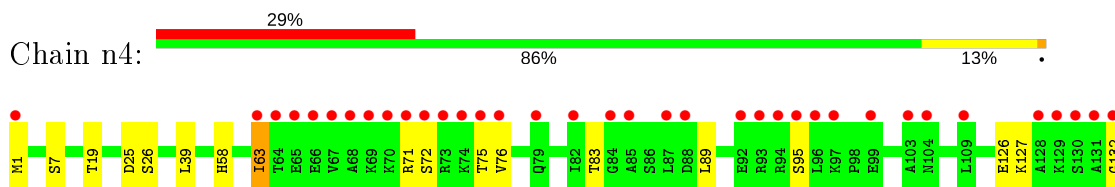


- Molecule 86: 60S Ribosomal Protein L12



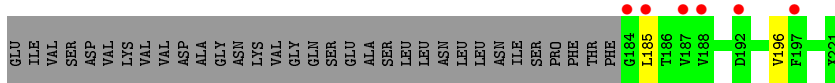
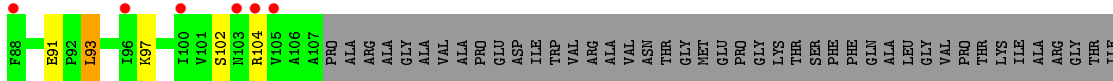
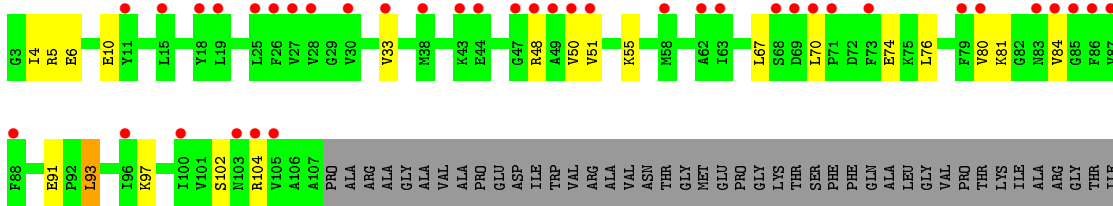
There are no outlier residues recorded for this chain.

- Molecule 87: 60S ribosomal protein L24-A





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



- Molecule 89: 60S Ribosomal Protein P1/2



There are no outlier residues recorded for this chain.

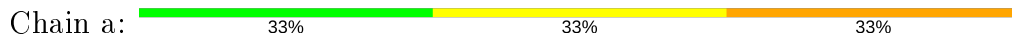
- Molecule 89: 60S Ribosomal Protein P1/2



- Molecule 90: aminoacyl-tRNA fragment ACCPmn



- Molecule 90: aminoacyl-tRNA fragment ACCPmn



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	436.18Å 288.24Å 303.58Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	172.59 – 3.25 172.59 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (172.59-3.25) 99.9 (172.59-3.25)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.26Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.208 , 0.249 0.210 , 0.251	Depositor DCC
R_{free} test set	23194 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtrriage
Anisotropy	0.116	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	414290	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	14.16	2.06	1.82
78	q2	17	CYS	CB-SG	11.98	2.02	1.82
36	5	2971	A	N9-C4	11.70	1.44	1.37
63	n7	36	HIS	C-N	9.18	1.51	1.34
36	5	1152	G	N9-C4	-8.42	1.31	1.38

The worst 5 of 1409 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	C1	145/155 (94%)	119 (82%)	19 (13%)	7 (5%)	2	14
13	c1	144/155 (93%)	120 (83%)	18 (12%)	6 (4%)	3	16
14	C2	122/124 (98%)	74 (61%)	26 (21%)	22 (18%)	0	1
15	C3	148/150 (99%)	127 (86%)	15 (10%)	6 (4%)	3	17
15	c3	148/150 (99%)	121 (82%)	19 (13%)	8 (5%)	2	12
16	C4	125/128 (98%)	97 (78%)	17 (14%)	11 (9%)	1	5
16	c4	126/128 (98%)	103 (82%)	17 (14%)	6 (5%)	2	14
17	C5	122/131 (93%)	96 (79%)	16 (13%)	10 (8%)	1	6
18	C6	139/142 (98%)	116 (84%)	15 (11%)	8 (6%)	1	10
18	c6	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	2	16
19	C7	116/125 (93%)	94 (81%)	14 (12%)	8 (7%)	1	8
19	c7	113/125 (90%)	92 (81%)	12 (11%)	9 (8%)	1	6
20	C8	143/145 (99%)	113 (79%)	22 (15%)	8 (6%)	2	11
20	c8	143/145 (99%)	121 (85%)	16 (11%)	6 (4%)	3	16
21	C9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	5	25
21	c9	141/143 (99%)	124 (88%)	14 (10%)	3 (2%)	7	32
22	D0	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	3	19
22	d0	108/110 (98%)	86 (80%)	12 (11%)	10 (9%)	0	4
23	D1	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	2
23	d1	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	1	10
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	6	28
24	d2	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	19	52
25	D3	142/144 (99%)	118 (83%)	14 (10%)	10 (7%)	1	7
25	d3	142/144 (99%)	128 (90%)	11 (8%)	3 (2%)	7	32
26	D4	132/134 (98%)	111 (84%)	13 (10%)	8 (6%)	1	10
26	d4	132/134 (98%)	106 (80%)	17 (13%)	9 (7%)	1	8
27	D5	68/70 (97%)	47 (69%)	12 (18%)	9 (13%)	0	1
27	d5	67/70 (96%)	53 (79%)	10 (15%)	4 (6%)	1	10
28	D6	95/97 (98%)	60 (63%)	22 (23%)	13 (14%)	0	1
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	5
29	D7	79/81 (98%)	65 (82%)	11 (14%)	3 (4%)	3	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	d7	79/81 (98%)	61 (77%)	11 (14%)	7 (9%)	1	4
30	D8	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	14
30	d8	61/63 (97%)	46 (75%)	12 (20%)	3 (5%)	2	14
31	D9	51/53 (96%)	40 (78%)	8 (16%)	3 (6%)	1	10
31	d9	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	1	10
32	E0	58/62 (94%)	46 (79%)	9 (16%)	3 (5%)	2	12
32	e0	60/62 (97%)	47 (78%)	7 (12%)	6 (10%)	0	3
33	E1	69/76 (91%)	38 (55%)	18 (26%)	13 (19%)	0	1
33	e1	74/76 (97%)	33 (45%)	23 (31%)	18 (24%)	0	0
34	SR	316/318 (99%)	275 (87%)	32 (10%)	9 (3%)	5	25
35	SM	131/159 (82%)	100 (76%)	17 (13%)	14 (11%)	0	3
39	L2	250/252 (99%)	229 (92%)	13 (5%)	8 (3%)	4	23
39	l2	250/252 (99%)	215 (86%)	26 (10%)	9 (4%)	3	20
40	L3	384/386 (100%)	334 (87%)	35 (9%)	15 (4%)	3	18
40	l3	384/386 (100%)	349 (91%)	25 (6%)	10 (3%)	5	27
41	L4	359/361 (99%)	301 (84%)	37 (10%)	21 (6%)	1	10
41	l4	359/361 (99%)	300 (84%)	41 (11%)	18 (5%)	2	13
42	L5	294/296 (99%)	239 (81%)	37 (13%)	18 (6%)	1	10
42	l5	292/296 (99%)	257 (88%)	28 (10%)	7 (2%)	6	28
43	L6	152/175 (87%)	132 (87%)	17 (11%)	3 (2%)	7	33
43	l6	153/175 (87%)	135 (88%)	14 (9%)	4 (3%)	5	27
44	L7	220/223 (99%)	199 (90%)	15 (7%)	6 (3%)	5	26
44	l7	221/223 (99%)	201 (91%)	14 (6%)	6 (3%)	5	26
45	L8	231/233 (99%)	194 (84%)	26 (11%)	11 (5%)	2	14
46	L9	189/191 (99%)	167 (88%)	17 (9%)	5 (3%)	5	27
46	l9	189/191 (99%)	175 (93%)	8 (4%)	6 (3%)	4	23
47	M0	207/220 (94%)	180 (87%)	18 (9%)	9 (4%)	2	16
47	m0	209/220 (95%)	168 (80%)	31 (15%)	10 (5%)	2	14
48	M1	167/169 (99%)	127 (76%)	26 (16%)	14 (8%)	1	5
48	m1	167/169 (99%)	140 (84%)	17 (10%)	10 (6%)	1	10
49	M3	191/194 (98%)	159 (83%)	21 (11%)	11 (6%)	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	m3	192/194 (99%)	156 (81%)	24 (12%)	12 (6%)	1	9
50	M4	134/137 (98%)	118 (88%)	10 (8%)	6 (4%)	2	15
50	m4	135/137 (98%)	123 (91%)	9 (7%)	3 (2%)	6	31
51	M5	201/203 (99%)	182 (90%)	12 (6%)	7 (4%)	3	21
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	4	24
52	M6	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	15	47
52	m6	195/197 (99%)	181 (93%)	12 (6%)	2 (1%)	15	47
53	M7	181/183 (99%)	152 (84%)	20 (11%)	9 (5%)	2	13
53	m7	153/183 (84%)	136 (89%)	12 (8%)	5 (3%)	4	22
54	M8	183/185 (99%)	161 (88%)	18 (10%)	4 (2%)	6	31
54	m8	183/185 (99%)	156 (85%)	21 (12%)	6 (3%)	4	22
55	M9	186/188 (99%)	173 (93%)	11 (6%)	2 (1%)	14	46
55	m9	186/188 (99%)	180 (97%)	4 (2%)	2 (1%)	14	46
56	N0	170/172 (99%)	153 (90%)	13 (8%)	4 (2%)	6	28
56	n0	170/172 (99%)	159 (94%)	8 (5%)	3 (2%)	8	35
57	N1	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	8	34
57	n1	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	12	41
58	N2	98/100 (98%)	80 (82%)	16 (16%)	2 (2%)	7	33
58	n2	96/100 (96%)	85 (88%)	10 (10%)	1 (1%)	15	47
59	N3	134/136 (98%)	122 (91%)	8 (6%)	4 (3%)	4	24
59	n3	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10	39
60	N4	96/98 (98%)	76 (79%)	14 (15%)	6 (6%)	1	9
61	N5	119/121 (98%)	105 (88%)	12 (10%)	2 (2%)	9	36
61	n5	118/121 (98%)	99 (84%)	10 (8%)	9 (8%)	1	6
62	N6	124/126 (98%)	111 (90%)	10 (8%)	3 (2%)	6	28
62	n6	124/126 (98%)	112 (90%)	7 (6%)	5 (4%)	3	17
63	N7	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	2	12
63	n7	133/135 (98%)	106 (80%)	15 (11%)	12 (9%)	1	4
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	2	11
64	n8	146/148 (99%)	121 (83%)	20 (14%)	5 (3%)	3	22
65	N9	56/58 (97%)	48 (86%)	5 (9%)	3 (5%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	n9	56/58 (97%)	40 (71%)	10 (18%)	6 (11%)	0	3
66	O0	95/100 (95%)	89 (94%)	5 (5%)	1 (1%)	14	46
66	o0	98/100 (98%)	88 (90%)	6 (6%)	4 (4%)	3	17
67	O1	107/109 (98%)	98 (92%)	5 (5%)	4 (4%)	3	19
67	o1	107/109 (98%)	94 (88%)	9 (8%)	4 (4%)	3	19
68	O2	125/127 (98%)	111 (89%)	11 (9%)	3 (2%)	6	28
68	o2	125/127 (98%)	108 (86%)	12 (10%)	5 (4%)	3	17
69	O3	104/106 (98%)	94 (90%)	8 (8%)	2 (2%)	8	34
69	o3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	4	25
70	O4	110/112 (98%)	97 (88%)	11 (10%)	2 (2%)	8	35
70	o4	110/112 (98%)	96 (87%)	11 (10%)	3 (3%)	5	26
71	O5	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	5	27
71	o5	117/119 (98%)	102 (87%)	11 (9%)	4 (3%)	3	22
72	O6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	1	7
72	o6	97/99 (98%)	83 (86%)	7 (7%)	7 (7%)	1	7
73	O7	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
73	o7	85/87 (98%)	76 (89%)	5 (6%)	4 (5%)	2	14
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	3	17
74	o8	75/77 (97%)	62 (83%)	12 (16%)	1 (1%)	12	41
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	32
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	32
76	Q0	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	3	17
76	q0	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	7	33
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	85 (82%)	12 (12%)	6 (6%)	1	10
78	q2	103/105 (98%)	94 (91%)	5 (5%)	4 (4%)	3	18
79	Q3	89/91 (98%)	79 (89%)	7 (8%)	3 (3%)	3	22
79	q3	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	14	46
80	c0	78/96 (81%)	61 (78%)	10 (13%)	7 (9%)	1	4
81	c2	108/124 (87%)	67 (62%)	26 (24%)	15 (14%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	c5	133/142 (94%)	96 (72%)	19 (14%)	18 (14%)	0	1
83	sR	316/318 (99%)	268 (85%)	39 (12%)	9 (3%)	5	25
84	sM	61/104 (59%)	43 (70%)	10 (16%)	8 (13%)	0	1
85	l8	224/231 (97%)	184 (82%)	25 (11%)	15 (7%)	1	8
87	n4	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	1	7
88	p0	117/219 (53%)	101 (86%)	12 (10%)	4 (3%)	3	22
All	All	22197/22912 (97%)	18787 (85%)	2314 (10%)	1096 (5%)	2	14

5 of 1096 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	5	ALA
2	S0	95	ALA
2	S0	158	VAL
2	S0	191	ARG
2	S0	203	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/173 (95%)	132 (80%)	32 (20%)	1	5
2	s0	165/173 (95%)	136 (82%)	29 (18%)	2	8
3	S1	191/192 (100%)	155 (81%)	36 (19%)	1	6
3	s1	192/192 (100%)	162 (84%)	30 (16%)	2	11
4	S2	176/176 (100%)	141 (80%)	35 (20%)	1	5
4	s2	176/176 (100%)	137 (78%)	39 (22%)	1	3
5	S3	182/182 (100%)	150 (82%)	32 (18%)	2	8
5	s3	182/182 (100%)	157 (86%)	25 (14%)	3	16
6	S4	221/221 (100%)	182 (82%)	39 (18%)	2	8
6	s4	221/221 (100%)	193 (87%)	28 (13%)	4	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	S5	173/173 (100%)	142 (82%)	31 (18%)	2	7
7	s5	173/173 (100%)	142 (82%)	31 (18%)	2	7
8	S6	188/193 (97%)	156 (83%)	32 (17%)	2	9
8	s6	187/193 (97%)	154 (82%)	33 (18%)	2	8
9	S7	165/166 (99%)	139 (84%)	26 (16%)	2	11
9	s7	165/166 (99%)	138 (84%)	27 (16%)	2	10
10	S8	150/160 (94%)	128 (85%)	22 (15%)	3	13
10	s8	150/160 (94%)	132 (88%)	18 (12%)	5	20
11	S9	158/158 (100%)	127 (80%)	31 (20%)	1	5
11	s9	158/158 (100%)	136 (86%)	22 (14%)	3	15
12	C0	77/77 (100%)	64 (83%)	13 (17%)	2	9
13	C1	129/129 (100%)	113 (88%)	16 (12%)	4	19
13	c1	129/129 (100%)	102 (79%)	27 (21%)	1	4
14	C2	88/100 (88%)	69 (78%)	19 (22%)	1	4
15	C3	127/127 (100%)	108 (85%)	19 (15%)	3	12
15	c3	127/127 (100%)	106 (84%)	21 (16%)	2	10
16	C4	81/97 (84%)	63 (78%)	18 (22%)	1	3
16	c4	97/97 (100%)	74 (76%)	23 (24%)	1	2
17	C5	101/107 (94%)	87 (86%)	14 (14%)	3	15
18	C6	117/118 (99%)	96 (82%)	21 (18%)	2	7
18	c6	118/118 (100%)	101 (86%)	17 (14%)	3	14
19	C7	94/113 (83%)	72 (77%)	22 (23%)	1	3
19	c7	92/113 (81%)	78 (85%)	14 (15%)	3	12
20	C8	128/128 (100%)	93 (73%)	35 (27%)	0	1
20	c8	128/128 (100%)	105 (82%)	23 (18%)	1	7
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	5
21	c9	115/115 (100%)	97 (84%)	18 (16%)	2	11
22	D0	100/103 (97%)	78 (78%)	22 (22%)	1	3
22	d0	103/103 (100%)	79 (77%)	24 (23%)	1	3
23	D1	74/74 (100%)	63 (85%)	11 (15%)	3	12
23	d1	74/74 (100%)	61 (82%)	13 (18%)	2	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	D2	110/110 (100%)	92 (84%)	18 (16%)	2	10
24	d2	110/110 (100%)	97 (88%)	13 (12%)	5	21
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	16
25	d3	119/119 (100%)	104 (87%)	15 (13%)	4	18
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1	6
26	d4	112/112 (100%)	96 (86%)	16 (14%)	3	14
27	D5	61/61 (100%)	44 (72%)	17 (28%)	0	1
27	d5	61/61 (100%)	53 (87%)	8 (13%)	4	17
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0	1
28	d6	83/83 (100%)	71 (86%)	12 (14%)	3	14
29	D7	70/70 (100%)	63 (90%)	7 (10%)	7	27
29	d7	70/70 (100%)	61 (87%)	9 (13%)	4	18
30	D8	56/56 (100%)	45 (80%)	11 (20%)	1	5
30	d8	56/56 (100%)	44 (79%)	12 (21%)	1	4
31	D9	47/47 (100%)	37 (79%)	10 (21%)	1	4
31	d9	47/47 (100%)	38 (81%)	9 (19%)	1	6
32	E0	51/53 (96%)	44 (86%)	7 (14%)	3	16
32	e0	53/53 (100%)	39 (74%)	14 (26%)	0	1
33	E1	62/66 (94%)	46 (74%)	16 (26%)	0	1
33	e1	66/66 (100%)	48 (73%)	18 (27%)	0	1
34	SR	259/260 (100%)	234 (90%)	25 (10%)	8	29
35	SM	97/107 (91%)	81 (84%)	16 (16%)	2	10
39	L2	193/194 (100%)	166 (86%)	27 (14%)	3	15
39	l2	192/194 (99%)	160 (83%)	32 (17%)	2	9
40	L3	321/322 (100%)	265 (83%)	56 (17%)	2	8
40	l3	321/322 (100%)	264 (82%)	57 (18%)	2	7
41	L4	288/288 (100%)	244 (85%)	44 (15%)	2	12
41	l4	288/288 (100%)	237 (82%)	51 (18%)	2	8
42	L5	244/244 (100%)	206 (84%)	38 (16%)	2	11
42	l5	243/244 (100%)	203 (84%)	40 (16%)	2	10
43	L6	134/152 (88%)	116 (87%)	18 (13%)	4	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	l6	135/152 (89%)	117 (87%)	18 (13%)	4	16
44	L7	186/187 (100%)	168 (90%)	18 (10%)	8	29
44	l7	187/187 (100%)	162 (87%)	25 (13%)	4	16
45	L8	187/191 (98%)	154 (82%)	33 (18%)	2	8
46	L9	171/171 (100%)	138 (81%)	33 (19%)	1	5
46	l9	171/171 (100%)	134 (78%)	37 (22%)	1	4
47	M0	177/186 (95%)	147 (83%)	30 (17%)	2	9
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	9
48	M1	147/147 (100%)	122 (83%)	25 (17%)	2	9
48	m1	147/147 (100%)	120 (82%)	27 (18%)	1	7
49	M3	154/154 (100%)	126 (82%)	28 (18%)	1	7
49	m3	154/154 (100%)	133 (86%)	21 (14%)	3	16
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	7
50	m4	108/108 (100%)	92 (85%)	16 (15%)	3	13
51	M5	175/175 (100%)	139 (79%)	36 (21%)	1	4
51	m5	175/175 (100%)	150 (86%)	25 (14%)	3	14
52	M6	160/160 (100%)	144 (90%)	16 (10%)	7	27
52	m6	160/160 (100%)	140 (88%)	20 (12%)	4	19
53	M7	140/145 (97%)	114 (81%)	26 (19%)	1	6
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	8
54	M8	150/150 (100%)	130 (87%)	20 (13%)	4	16
54	m8	150/150 (100%)	126 (84%)	24 (16%)	2	10
55	M9	153/153 (100%)	127 (83%)	26 (17%)	2	9
55	m9	153/153 (100%)	125 (82%)	28 (18%)	1	7
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	7
56	n0	156/156 (100%)	130 (83%)	26 (17%)	2	9
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	3
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	4
58	N2	87/87 (100%)	75 (86%)	12 (14%)	3	16
58	n2	85/87 (98%)	70 (82%)	15 (18%)	2	8
59	N3	104/104 (100%)	88 (85%)	16 (15%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	n3	104/104 (100%)	93 (89%)	11 (11%)	6	25
60	N4	57/86 (66%)	50 (88%)	7 (12%)	4	20
61	N5	104/105 (99%)	83 (80%)	21 (20%)	1	5
61	n5	104/105 (99%)	85 (82%)	19 (18%)	1	7
62	N6	109/109 (100%)	82 (75%)	27 (25%)	0	2
62	n6	109/109 (100%)	82 (75%)	27 (25%)	0	2
63	N7	115/115 (100%)	94 (82%)	21 (18%)	1	7
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	5
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	7
64	n8	118/118 (100%)	103 (87%)	15 (13%)	4	18
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	8
65	n9	46/46 (100%)	35 (76%)	11 (24%)	0	2
66	O0	81/84 (96%)	68 (84%)	13 (16%)	2	10
66	o0	84/84 (100%)	72 (86%)	12 (14%)	3	14
67	O1	92/96 (96%)	77 (84%)	15 (16%)	2	10
67	o1	94/96 (98%)	76 (81%)	18 (19%)	1	6
68	O2	109/109 (100%)	98 (90%)	11 (10%)	7	27
68	o2	109/109 (100%)	94 (86%)	15 (14%)	3	16
69	O3	90/90 (100%)	79 (88%)	11 (12%)	5	20
69	o3	90/90 (100%)	77 (86%)	13 (14%)	3	14
70	O4	95/95 (100%)	79 (83%)	16 (17%)	2	9
70	o4	95/95 (100%)	83 (87%)	12 (13%)	4	18
71	O5	104/104 (100%)	84 (81%)	20 (19%)	1	6
71	o5	103/104 (99%)	82 (80%)	21 (20%)	1	4
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	3
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	59 (84%)	11 (16%)	2	11
73	o7	70/70 (100%)	53 (76%)	17 (24%)	0	2
74	O8	68/68 (100%)	52 (76%)	16 (24%)	1	3
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	7
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	o9	45/45 (100%)	39 (87%)	6 (13%)	4	16
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	9
76	q0	47/47 (100%)	38 (81%)	9 (19%)	1	6
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0	1
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	70 (78%)	20 (22%)	1	3
78	q2	90/90 (100%)	72 (80%)	18 (20%)	1	5
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	3	15
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	4
80	c0	73/73 (100%)	60 (82%)	13 (18%)	2	7
81	c2	88/88 (100%)	68 (77%)	20 (23%)	1	3
82	c5	103/118 (87%)	85 (82%)	18 (18%)	2	8
83	sR	260/261 (100%)	241 (93%)	19 (7%)	14	40
84	sM	54/54 (100%)	41 (76%)	13 (24%)	0	2
85	l8	177/185 (96%)	154 (87%)	23 (13%)	4	17
87	n4	100/114 (88%)	91 (91%)	9 (9%)	9	32
88	p0	105/165 (64%)	85 (81%)	20 (19%)	1	6
All	All	18729/19106 (98%)	15556 (83%)	3173 (17%)	2	9

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

Mol	Chain	Res	Type
67	O1	16	LEU
7	s5	170	GLN
64	n8	26	ARG
70	O4	49	SER
2	s0	88	LYS

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

Mol	Chain	Res	Type
3	s1	209	ASN
22	d0	72	ASN
72	o6	63	ASN
11	s9	110	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	c0	32	HIS

5.3.3 RNA [i](#)

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

5 of 2305 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U

5 of 275 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3121	U
1	6	272	U
36	5	2818	U
36	1	3228	C
38	4	111	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
90	PPU	A	76	90,36	32,40,41	1.07	2 (6%)	33,57,60	1.74	8 (24%)
90	PPU	a	76	90,36	32,40,41	1.04	2 (6%)	33,57,60	1.74	6 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	PPU	A	76	90,36	-	3/21/43/44	0/4/4/4
90	PPU	a	76	90,36	-	4/21/43/44	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	a	76	PPU	C2'-C3'	-2.87	1.48	1.53
90	a	76	PPU	C5-C4	2.32	1.47	1.40
90	A	76	PPU	C2'-C3'	-2.23	1.49	1.53
90	A	76	PPU	C5-C4	2.19	1.46	1.40

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	a	76	PPU	C3'-N3'-C	-5.38	115.10	123.21
90	A	76	PPU	C3'-N3'-C	-4.92	115.79	123.21
90	a	76	PPU	CG-CB-CA	-4.45	104.87	114.13
90	A	76	PPU	CA-C-N3'	3.52	121.03	116.15
90	A	76	PPU	N3-C2-N1	-3.52	123.18	128.68

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	A	76	PPU	C3'-C4'-C5'-O5'
90	a	76	PPU	CE2-CZ-OC-CM

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3553 ligands modelled in this entry, 2208 are monoatomic - leaving 1345 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4324	92	0,6,6	0.00	-	-		
92	OHX	1	4305	92	0,6,6	0.00	-	-		
92	OHX	5	4405	-	0,6,6	0.00	-	-		
92	OHX	2	2165	-	0,6,6	0.00	-	-		
92	OHX	6	2168	-	0,6,6	0.00	-	-		
92	OHX	6	2233	-	0,6,6	0.00	-	-		
92	OHX	6	2161	92	0,6,6	0.00	-	-		
92	OHX	5	4209	92	0,6,6	0.00	-	-		
92	OHX	6	2216	92	0,6,6	0.00	-	-		
92	OHX	6	2319	-	0,6,6	0.00	-	-		
92	OHX	1	4325	-	0,6,6	0.00	-	-		
92	OHX	5	4477	-	0,6,6	0.00	-	-		
92	OHX	5	4409	36	0,6,6	0.00	-	-		
92	OHX	2	2166	92	0,6,6	0.00	-	-		
92	OHX	6	2152	-	0,6,6	0.00	-	-		
92	OHX	1	4360	-	0,6,6	0.00	-	-		
92	OHX	5	4440	92	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	8	223	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4389	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4250	-	0,6,6	0.00	-	-	-	-
92	OHX	7	232	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4568	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2263	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2268	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4462	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2158	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4226	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4101	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4304	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2084	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4311	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4108	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2190	1,92	0,6,6	0.00	-	-	-	-
92	OHX	6	2317	-	0,6,6	0.00	-	-	-	-
92	OHX	4	245	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4400	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2137	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4139	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2243	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4105	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4333	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2199	1	0,6,6	0.00	-	-	-	-
92	OHX	M0	308	92	0,6,6	0.00	-	-	-	-
92	OHX	M0	306	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4392	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2244	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4402	-	0,6,6	0.00	-	-	-	-
92	OHX	8	226	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2261	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4305	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2201	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4180	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4209	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4215	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4490	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2192	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4319	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2159	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4351	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2145	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4274	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4385	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2240	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4350	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2172	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2199	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4287	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2169	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4345	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4357	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4106	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4155	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4463	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2111	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4294	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4130	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4339	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4184	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4218	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2231	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4415	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2311	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4279	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4146	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2337	1,92	0,6,6	0.00	-	-	-	-
92	OHX	5	4322	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2226	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4204	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4436	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4356	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4265	-	0,6,6	0.00	-	-	-	-
92	OHX	8	230	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4338	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4433	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4542	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2245	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4179	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4376	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4267	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4309	36	0,6,6	0.00	-	-	-	-
92	OHX	1	4504	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2081	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4249	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4525	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2187	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4168	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2088	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4224	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2176	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4491	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2211	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4235	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2264	-	0,6,6	0.00	-	-	-	-
92	OHX	4	243	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2239	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4367	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2259	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4417	36	0,6,6	0.00	-	-	-	-
92	OHX	2	2152	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2276	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4319	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2151	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2208	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2305	-	0,6,6	0.00	-	-	-	-
92	OHX	8	235	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4170	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2248	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4451	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4221	-	0,6,6	0.00	-	-	-	-
92	OHX	4	239	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4398	-	0,6,6	0.00	-	-	-	-
92	OHX	m5	304	-	0,6,6	0.00	-	-	-	-
92	OHX	m0	304	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2335	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4154	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4459	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4480	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4522	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4348	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4419	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4388	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4279	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2219	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2225	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4445	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4287	92	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4252	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4186	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4437	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2202	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2144	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4487	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2188	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4371	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4214	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4465	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2072	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2245	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4353	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4324	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4347	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4229	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4444	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4213	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4200	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2166	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2169	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4509	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4182	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2130	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4242	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2208	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4171	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4213	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4483	-	0,6,6	0.00	-	-	-	-
92	OHX	4	246	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4391	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4495	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4336	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2239	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4427	36	0,6,6	0.00	-	-	-	-
92	OHX	2	2131	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4249	-	0,6,6	0.00	-	-	-	-
92	OHX	8	224	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4267	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4307	92	0,6,6	0.00	-	-	-	-
92	OHX	8	225	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2278	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2211	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4414	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4236	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2157	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4238	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2242	92	0,6,6	0.00	-	-	-	-
92	OHX	c5	202	-	0,6,6	0.00	-	-	-	-
92	OHX	N8	208	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4218	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4297	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4359	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2090	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4421	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4437	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4207	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4552	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4195	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2281	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4349	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4360	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4271	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4560	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4410	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4174	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2302	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4223	-	0,6,6	0.00	-	-	-	-
92	OHX	L2	305	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4312	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4250	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4475	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4339	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4164	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2249	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4113	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2243	1,92	0,6,6	0.00	-	-	-	-
92	OHX	1	4195	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4349	92	0,6,6	0.00	-	-	-	-
92	OHX	8	237	38	0,6,6	0.00	-	-	-	-
92	OHX	1	4354	-	0,6,6	0.00	-	-	-	-
92	OHX	S6	302	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4470	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4127	-	0,6,6	0.00	-	-	-	-
92	OHX	L3	409	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4226	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2163	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4444	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4498	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4419	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4230	-	0,6,6	0.00	-	-	-	-
92	OHX	4	235	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4295	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4488	-	0,6,6	0.00	-	-	-	-
92	OHX	7	240	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4501	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4160	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4334	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2144	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2286	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2273	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4403	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2206	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4185	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4157	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4302	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4156	-	0,6,6	0.00	-	-	-	-
92	OHX	4	236	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4303	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2315	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4254	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4517	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2078	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4573	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4171	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4304	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2146	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4313	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4240	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4448	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2162	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4425	-	0,6,6	0.00	-	-	-	-
92	OHX	7	201	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2177	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4143	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4421	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4341	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4355	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4426	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2289	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4484	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4129	-	0,6,6	0.00	-	-	-	-
92	OHX	n3	204	-	0,6,6	0.00	-	-	-	-
92	OHX	4	244	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2110	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4132	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4484	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2262	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4293	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4251	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4408	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4478	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4208	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4438	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2229	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2213	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4303	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2153	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4231	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4273	36	0,6,6	0.00	-	-	-	-
92	OHX	6	2316	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2116	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4288	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2327	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2164	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4337	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4212	-	0,6,6	0.00	-	-	-	-
92	OHX	m4	202	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4434	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4505	92,36	0,6,6	0.00	-	-	-	-
92	OHX	1	4317	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4536	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2291	1	0,6,6	0.00	-	-	-	-
92	OHX	2	2118	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4293	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2203	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4203	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2184	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2210	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4289	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2149	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2133	92	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2221	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2136	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2097	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4185	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4219	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4471	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4243	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4330	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4430	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2129	1,92	0,6,6	0.00	-	-	-	-
92	OHX	6	2146	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2227	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4544	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4446	92,36	0,6,6	0.00	-	-	-	-
92	OHX	5	4490	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4222	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2167	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4227	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4235	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2232	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4375	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4316	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2157	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4234	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2170	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4177	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4323	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2295	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4187	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2237	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2148	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4520	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2122	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4373	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4134	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4494	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4111	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4341	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2246	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2102	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4192	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4476	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4165	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4427	-	0,6,6	0.00	-	-	-	-
92	OHX	12	306	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4500	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4136	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2179	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2176	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2207	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2187	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2087	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4438	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4534	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4539	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2338	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4345	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4315	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4435	-	0,6,6	0.00	-	-	-	-
92	OHX	15	308	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4176	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4269	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4523	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4389	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4439	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4253	92	0,6,6	0.00	-	-	-	-
92	OHX	c8	204	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2175	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4281	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4330	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4167	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4384	-	0,6,6	0.00	-	-	-	-
92	OHX	4	233	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4449	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4326	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4208	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2283	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4336	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4432	92,36	0,6,6	0.00	-	-	-	-
92	OHX	1	4239	92	0,6,6	0.00	-	-	-	-
92	OHX	3	231	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2205	-	0,6,6	0.00	-	-	-	-
92	OHX	3	228	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2290	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4162	-	0,6,6	0.00	-	-	-	-
92	OHX	c3	201	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4363	-	0,6,6	0.00	-	-	-	-
92	OHX	8	222	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4556	92,36	0,6,6	0.00	-	-	-	-
92	OHX	1	4382	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4190	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4485	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4418	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4504	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2209	-	0,6,6	0.00	-	-	-	-
92	OHX	4	241	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2091	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4110	-	0,6,6	0.00	-	-	-	-
92	OHX	C5	202	17	0,6,6	0.00	-	-	-	-
92	OHX	5	4298	-	0,6,6	0.00	-	-	-	-
92	OHX	14	405	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2226	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4170	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4505	36	0,6,6	0.00	-	-	-	-
92	OHX	2	2156	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4357	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2093	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4429	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4499	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2232	92	0,6,6	0.00	-	-	-	-
92	OHX	8	229	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4258	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4308	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2191	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4380	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2230	-	0,6,6	0.00	-	-	-	-
92	OHX	5	3401	1	0,6,6	0.00	-	-	-	-
92	OHX	2	2195	92	0,6,6	0.00	-	-	-	-
92	OHX	c1	201	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4399	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4204	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4298	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2085	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4201	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2141	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4123	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2288	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2076	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4416	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2244	1,92	0,6,6	0.00	-	-	-	
92	OHX	5	4327	-	0,6,6	0.00	-	-	-	
92	OHX	6	2329	92	0,6,6	0.00	-	-	-	
92	OHX	6	2150	1	0,6,6	0.00	-	-	-	
92	OHX	5	4220	-	0,6,6	0.00	-	-	-	
92	OHX	5	4335	-	0,6,6	0.00	-	-	-	
92	OHX	2	2127	-	0,6,6	0.00	-	-	-	
92	OHX	7	234	-	0,6,6	0.00	-	-	-	
92	OHX	6	2201	92	0,6,6	0.00	-	-	-	
92	OHX	2	2242	-	0,6,6	0.00	-	-	-	
92	OHX	L4	408	-	0,6,6	0.00	-	-	-	
92	OHX	5	4266	92	0,6,6	0.00	-	-	-	
92	OHX	2	2128	-	0,6,6	0.00	-	-	-	
92	OHX	3	229	-	0,6,6	0.00	-	-	-	
92	OHX	1	4284	-	0,6,6	0.00	-	-	-	
92	OHX	1	4412	92	0,6,6	0.00	-	-	-	
92	OHX	1	4243	-	0,6,6	0.00	-	-	-	
92	OHX	5	4342	-	0,6,6	0.00	-	-	-	
92	OHX	7	230	-	0,6,6	0.00	-	-	-	
92	OHX	1	4199	-	0,6,6	0.00	-	-	-	
92	OHX	2	2177	-	0,6,6	0.00	-	-	-	
92	OHX	2	2074	92	0,6,6	0.00	-	-	-	
92	OHX	7	231	92	0,6,6	0.00	-	-	-	
92	OHX	N1	202	-	0,6,6	0.00	-	-	-	
92	OHX	1	4355	92,36	0,6,6	0.00	-	-	-	
92	OHX	1	4372	92	0,6,6	0.00	-	-	-	
92	OHX	5	4278	-	0,6,6	0.00	-	-	-	
92	OHX	6	2227	-	0,6,6	0.00	-	-	-	
92	OHX	1	4489	92	0,6,6	0.00	-	-	-	
92	OHX	2	2120	1	0,6,6	0.00	-	-	-	
92	OHX	5	4315	92	0,6,6	0.00	-	-	-	
92	OHX	1	4468	92	0,6,6	0.00	-	-	-	
92	OHX	2	2200	-	0,6,6	0.00	-	-	-	
92	OHX	5	4441	-	0,6,6	0.00	-	-	-	
92	OHX	6	2255	1,92	0,6,6	0.00	-	-	-	
92	OHX	1	4501	92	0,6,6	0.00	-	-	-	
92	OHX	1	4131	92	0,6,6	0.00	-	-	-	
92	OHX	1	4119	-	0,6,6	0.00	-	-	-	
92	OHX	2	2252	92	0,6,6	0.00	-	-	-	
92	OHX	5	4528	-	0,6,6	0.00	-	-	-	
92	OHX	1	4415	-	0,6,6	0.00	-	-	-	
92	OHX	5	4392	-	0,6,6	0.00	-	-	-	
92	OHX	6	2236	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2186	92	0,6,6	0.00	-	-	-	
92	OHX	5	4242	36	0,6,6	0.00	-	-	-	
92	OHX	2	2100	-	0,6,6	0.00	-	-	-	
92	OHX	5	4331	-	0,6,6	0.00	-	-	-	
92	OHX	6	2214	92	0,6,6	0.00	-	-	-	
92	OHX	1	4425	-	0,6,6	0.00	-	-	-	
92	OHX	2	2228	-	0,6,6	0.00	-	-	-	
92	OHX	5	4404	92	0,6,6	0.00	-	-	-	
92	OHX	6	2297	92	0,6,6	0.00	-	-	-	
92	OHX	1	4329	-	0,6,6	0.00	-	-	-	
92	OHX	1	4281	92	0,6,6	0.00	-	-	-	
92	OHX	5	4370	-	0,6,6	0.00	-	-	-	
92	OHX	5	4286	-	0,6,6	0.00	-	-	-	
92	OHX	6	2271	-	0,6,6	0.00	-	-	-	
92	OHX	5	4531	-	0,6,6	0.00	-	-	-	
92	OHX	6	2197	1	0,6,6	0.00	-	-	-	
92	OHX	5	4262	-	0,6,6	0.00	-	-	-	
92	OHX	6	2320	-	0,6,6	0.00	-	-	-	
92	OHX	2	2229	-	0,6,6	0.00	-	-	-	
92	OHX	n9	103	-	0,6,6	0.00	-	-	-	
92	OHX	5	4429	-	0,6,6	0.00	-	-	-	
92	OHX	o9	102	-	0,6,6	0.00	-	-	-	
92	OHX	5	4485	92	0,6,6	0.00	-	-	-	
92	OHX	1	4225	-	0,6,6	0.00	-	-	-	
92	OHX	5	4289	-	0,6,6	0.00	-	-	-	
92	OHX	6	2277	-	0,6,6	0.00	-	-	-	
92	OHX	1	4178	-	0,6,6	0.00	-	-	-	
92	OHX	6	2279	-	0,6,6	0.00	-	-	-	
92	OHX	1	4464	-	0,6,6	0.00	-	-	-	
92	OHX	1	4138	-	0,6,6	0.00	-	-	-	
92	OHX	5	4205	-	0,6,6	0.00	-	-	-	
92	OHX	5	4358	-	0,6,6	0.00	-	-	-	
92	OHX	5	4188	-	0,6,6	0.00	-	-	-	
92	OHX	2	2256	92	0,6,6	0.00	-	-	-	
92	OHX	2	2180	-	0,6,6	0.00	-	-	-	
92	OHX	5	4270	-	0,6,6	0.00	-	-	-	
92	OHX	2	2159	1,92	0,6,6	0.00	-	-	-	
92	OHX	5	4321	-	0,6,6	0.00	-	-	-	
92	OHX	M9	204	-	0,6,6	0.00	-	-	-	
92	OHX	1	4125	-	0,6,6	0.00	-	-	-	
92	OHX	5	4431	-	0,6,6	0.00	-	-	-	
92	OHX	5	4366	-	0,6,6	0.00	-	-	-	
92	OHX	3	230	92	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4434	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4299	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4296	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4103	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4206	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2175	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4483	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4460	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2178	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4310	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4256	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4473	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4395	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4246	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4502	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4220	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4378	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4452	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4199	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4288	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2138	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4282	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2223	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2195	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4524	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4451	-	0,6,6	0.00	-	-	-	-
92	OHX	L3	407	-	0,6,6	0.00	-	-	-	-
92	OHX	m0	305	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4472	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4255	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4284	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2105	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2153	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2266	1	0,6,6	0.00	-	-	-	-
92	OHX	2	2143	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2103	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2182	-	0,6,6	0.00	-	-	-	-
92	OHX	Q2	505	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2165	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4548	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2143	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2326	1	0,6,6	0.00	-	-	-	-
92	OHX	N9	102	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4137	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4503	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2299	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4422	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2205	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4275	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4128	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2196	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4387	36	0,6,6	0.00	-	-	-	-
92	OHX	2	2196	1	0,6,6	0.00	-	-	-	-
92	OHX	2	2207	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4467	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2224	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2287	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4406	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4430	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4292	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2313	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4489	36	0,6,6	0.00	-	-	-	-
92	OHX	1	4347	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4537	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4291	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4370	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4265	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2265	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2260	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2321	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4529	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2181	1	0,6,6	0.00	-	-	-	-
92	OHX	3	225	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4205	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4333	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4448	-	0,6,6	0.00	-	-	-	-
92	OHX	8	234	38	0,6,6	0.00	-	-	-	-
92	OHX	1	4496	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4452	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4372	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2190	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2228	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4433	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4189	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4417	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4436	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2270	-	0,6,6	0.00	-	-	-	-
92	OHX	o3	206	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4320	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2267	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2198	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4268	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2253	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4169	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4100	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4165	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4190	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2324	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4335	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4455	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4237	-	0,6,6	0.00	-	-	-	-
92	OHX	8	227	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4387	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4211	92	0,6,6	0.00	-	-	-	-
92	OHX	sR	401	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4358	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4363	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4422	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4461	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4378	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4224	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4366	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4379	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2220	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4216	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4414	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2318	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4232	36	0,6,6	0.00	-	-	-	-
92	OHX	6	2172	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4508	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4527	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2071	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4399	36	0,6,6	0.00	-	-	-	-
92	OHX	1	4365	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4397	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2274	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4259	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2334	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2079	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4413	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2275	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4301	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4151	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2123	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4420	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2250	-	0,6,6	0.00	-	-	-	-
92	OHX	A	101	90	0,6,6	0.00	-	-	-	-
92	OHX	5	4446	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4331	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2332	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2235	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4356	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4442	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2170	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4344	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4301	-	0,6,6	0.00	-	-	-	-
92	OHX	3	224	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2258	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4223	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2115	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2174	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4466	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2109	-	0,6,6	0.00	-	-	-	-
92	OHX	3	222	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4261	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4173	-	0,6,6	0.00	-	-	-	-
92	OHX	4	234	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4156	92	0,6,6	0.00	-	-	-	-
92	OHX	a	101	90,92	0,6,6	0.00	-	-	-	-
92	OHX	6	2206	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4384	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2234	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4497	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4192	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2082	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4547	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4214	-	0,6,6	0.00	-	-	-	-
92	OHX	S8	303	-	0,6,6	0.00	-	-	-	-
92	OHX	M5	310	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2225	-	0,6,6	0.00	-	-	-	-
92	OHX	O3	204	-	0,6,6	0.00	-	-	-	-
92	OHX	A	102	90,92	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4344	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4217	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4197	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4099	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2080	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4440	92,36	0,6,6	0.00	-	-	-	-
92	OHX	19	204	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2191	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2117	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4252	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2304	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4466	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4241	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4346	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2222	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4495	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4277	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4231	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2167	-	0,6,6	0.00	-	-	-	-
92	OHX	13	412	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4184	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2193	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2114	-	0,6,6	0.00	-	-	-	-
92	OHX	8	228	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4294	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4202	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2182	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4263	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4285	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2094	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2219	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2183	1,92	0,6,6	0.00	-	-	-	-
92	OHX	6	2296	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4377	-	0,6,6	0.00	-	-	-	-
92	OHX	4	240	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2284	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4277	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4115	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2255	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2254	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2149	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2218	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4461	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4397	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4412	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4530	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4172	92	0,6,6	0.00	-	-	-	-
92	OHX	7	233	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4285	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4327	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4229	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4174	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2280	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4468	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4203	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4256	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4282	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2269	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2339	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4238	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2236	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4225	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2164	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4317	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2214	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4270	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4443	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4566	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4263	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2173	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2247	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4326	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4482	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4473	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4329	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4332	-	0,6,6	0.00	-	-	-	-
92	OHX	4	242	-	0,6,6	0.00	-	-	-	-
92	OHX	D9	104	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4163	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4276	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4453	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4395	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4428	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4179	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4394	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4458	36	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4126	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2155	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4116	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4381	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4475	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2154	-	0,6,6	0.00	-	-	-	-
92	OHX	O7	107	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4296	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4196	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4454	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2238	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4314	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2086	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4460	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4161	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4312	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4271	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4390	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2132	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4266	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4512	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4391	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4121	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4297	-	0,6,6	0.00	-	-	-	-
92	OHX	15	310	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4313	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4385	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4206	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4508	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4292	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4396	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2293	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4480	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2112	-	0,6,6	0.00	-	-	-	-
92	OHX	3	223	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4450	36	0,6,6	0.00	-	-	-	-
92	OHX	6	2238	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4563	-	0,6,6	0.00	-	-	-	-
92	OHX	m7	208	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4198	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4197	92	0,6,6	0.00	-	-	-	-
92	OHX	4	247	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2282	92	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4350	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4441	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2218	1	0,6,6	0.00	-	-	-	-
92	OHX	5	4158	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2089	92	0,6,6	0.00	-	-	-	-
92	OHX	8	236	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4283	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4565	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4257	92,36	0,6,6	0.00	-	-	-	-
92	OHX	5	4488	-	0,6,6	0.00	-	-	-	-
92	OHX	8	232	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4507	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4299	36	0,6,6	0.00	-	-	-	-
92	OHX	2	2092	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4175	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2204	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4477	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4364	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4449	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4262	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4416	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4383	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2241	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2197	1	0,6,6	0.00	-	-	-	-
92	OHX	5	4541	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4320	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4187	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2248	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2221	1	0,6,6	0.00	-	-	-	-
92	OHX	5	4447	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2155	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2108	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2147	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4455	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2215	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4383	92	0,6,6	0.00	-	-	-	-
92	OHX	O7	108	-	0,6,6	0.00	-	-	-	-
92	OHX	s8	305	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2308	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4248	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4491	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4400	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4472	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	2	2185	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4164	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4532	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2294	1,92	0,6,6	0.00	-	-	-	-
92	OHX	5	4519	-	0,6,6	0.00	-	-	-	-
92	OHX	8	233	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2220	1	0,6,6	0.00	-	-	-	-
92	OHX	8	239	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4328	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2202	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2135	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4245	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2209	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4193	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2224	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4478	92	0,6,6	0.00	-	-	-	-
92	OHX	d9	104	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4167	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4272	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4469	-	0,6,6	0.00	-	-	-	-
92	OHX	7	238	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4325	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2069	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4176	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2181	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4321	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4300	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4381	92,36	0,6,6	0.00	-	-	-	-
92	OHX	5	4318	-	0,6,6	0.00	-	-	-	-
92	OHX	4	238	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4169	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4219	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4215	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4496	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4233	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2217	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4506	92	0,6,6	0.00	-	-	-	-
92	OHX	s4	302	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2140	1	0,6,6	0.00	-	-	-	-
92	OHX	5	4514	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4518	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4278	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4464	92	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2189	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4546	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4558	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4318	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2301	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4375	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4401	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2298	1,92	0,6,6	0.00	-	-	-	-
92	OHX	1	4233	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4183	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2184	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2168	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4104	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4361	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4462	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4158	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4109	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4191	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4561	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2312	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4481	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4398	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4253	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2178	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4457	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4458	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4275	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2192	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2333	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4240	36	0,6,6	0.00	-	-	-	-
92	OHX	6	2237	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4457	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4300	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4183	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4407	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2083	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4107	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4102	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4290	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2246	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4393	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4554	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4247	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4343	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4247	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4426	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4555	92	0,6,6	0.00	-	-	-	-
92	OHX	m0	303	92	0,6,6	0.00	-	-	-	-
92	OHX	3	220	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4369	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4515	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2119	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2150	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2077	1,92	0,6,6	0.00	-	-	-	-
92	OHX	6	2194	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4424	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2183	-	0,6,6	0.00	-	-	-	-
92	OHX	4	237	38	0,6,6	0.00	-	-	-	-
92	OHX	O1	202	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4141	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4559	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4459	92,36	0,6,6	0.00	-	-	-	-
92	OHX	5	4210	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2250	92	0,6,6	0.00	-	-	-	-
92	OHX	o7	105	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4352	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4148	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4112	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4342	36	0,6,6	0.00	-	-	-	-
92	OHX	1	4217	-	0,6,6	0.00	-	-	-	-
92	OHX	M0	307	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4295	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4177	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2106	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4368	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4405	92	0,6,6	0.00	-	-	-	-
92	OHX	3	227	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4567	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2257	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4194	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4492	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4273	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4120	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4114	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2251	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4545	92	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4308	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2145	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4364	-	0,6,6	0.00	-	-	-	-
92	OHX	7	229	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4258	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4526	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4386	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2231	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2240	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4521	36	0,6,6	0.00	-	-	-	-
92	OHX	2	2161	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4435	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2107	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2142	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4418	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4322	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2234	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4346	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4202	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4511	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4246	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2307	-	0,6,6	0.00	-	-	-	-
92	OHX	s1	302	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4340	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4497	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4431	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4338	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4382	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2210	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4180	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4228	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2099	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4244	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2303	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2104	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4499	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4142	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4362	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2222	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4352	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4538	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2075	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2241	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4290	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4178	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4307	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2256	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4343	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4463	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2073	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2233	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2158	92	0,6,6	0.00	-	-	-	-
92	OHX	O7	109	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4500	92,36	0,6,6	0.00	-	-	-	-
92	OHX	1	4157	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2173	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4379	-	0,6,6	0.00	-	-	-	-
92	OHX	8	221	-	0,6,6	0.00	-	-	-	-
92	OHX	3	221	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4564	92	0,6,6	0.00	-	-	-	-
92	OHX	d4	201	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4276	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4432	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4201	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4234	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2141	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4423	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4404	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4274	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2160	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4408	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4371	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4144	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2142	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4510	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2185	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4411	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4149	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2171	1	0,6,6	0.00	-	-	-	-
92	OHX	C8	203	92,36	0,6,6	0.00	-	-	-	-
92	OHX	5	4376	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2154	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2223	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4377	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4390	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4328	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	5	4550	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4188	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4260	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4543	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2251	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4513	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2160	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4196	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2098	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2156	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4373	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4396	-	0,6,6	0.00	-	-	-	-
92	OHX	c5	201	-	0,6,6	0.00	-	-	-	-
92	OHX	o2	204	-	0,6,6	0.00	-	-	-	-
92	OHX	n1	204	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4337	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4471	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4407	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4467	36	0,6,6	0.00	-	-	-	-
92	OHX	1	4394	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4445	-	0,6,6	0.00	-	-	-	-
92	OHX	l3	413	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4264	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4230	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2124	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4261	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2121	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4193	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4316	-	0,6,6	0.00	-	-	-	-
92	OHX	7	237	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4237	92	0,6,6	0.00	-	-	-	-
92	OHX	7	239	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2249	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4424	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4348	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4309	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4516	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4124	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2095	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4474	92	0,6,6	0.00	-	-	-	-
92	OHX	3	219	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2330	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4207	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2193	1	0,6,6	0.00	-	-	-	-
92	OHX	1	4283	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4374	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4162	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2113	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4241	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2147	92	0,6,6	0.00	-	-	-	-
92	OHX	8	238	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2200	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4351	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2126	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4411	-	0,6,6	0.00	-	-	-	-
92	OHX	M0	305	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4362	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4257	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4439	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4314	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4393	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2134	-	0,6,6	0.00	-	-	-	-
92	OHX	C3	201	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4492	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2314	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2189	1	0,6,6	0.00	-	-	-	-
92	OHX	2	2235	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4479	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4368	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4428	-	0,6,6	0.00	-	-	-	-
92	OHX	8	231	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4173	-	0,6,6	0.00	-	-	-	-
92	OHX	S2	303	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4493	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2285	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4562	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4163	-	0,6,6	0.00	-	-	-	-
92	OHX	3	226	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4402	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2215	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2292	-	0,6,6	0.00	-	-	-	-
92	OHX	8	240	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4493	-	0,6,6	0.00	-	-	-	-
92	OHX	15	309	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4248	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4403	92	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2217	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4175	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4161	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4423	92,36	0,6,6	0.00	-	-	-	-
92	OHX	6	2252	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4498	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4269	92	0,6,6	0.00	-	-	-	-
92	OHX	C8	202	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4470	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4244	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2322	-	0,6,6	0.00	-	-	-	-
92	OHX	4	248	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2253	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4456	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2188	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4245	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4239	-	0,6,6	0.00	-	-	-	-
92	OHX	7	235	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2328	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4456	-	0,6,6	0.00	-	-	-	-
92	OHX	M7	209	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4361	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4469	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4222	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4409	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4228	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2213	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4122	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4145	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4340	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4280	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4535	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4354	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4401	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4420	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2070	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4502	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4323	92,36	0,6,6	0.00	-	-	-	-
92	OHX	1	4181	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4260	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4186	-	0,6,6	0.00	-	-	-	-
92	OHX	L5	301	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4553	92,36	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	6	2323	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4310	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4255	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4450	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4311	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2179	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4380	36	0,6,6	0.00	-	-	-	-
92	OHX	1	4210	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4479	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4476	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2309	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4386	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2336	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4194	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2216	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2198	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2151	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4359	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4533	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4236	-	0,6,6	0.00	-	-	-	-
92	OHX	m9	202	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4482	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4153	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4413	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2212	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4166	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2162	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4227	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4374	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2174	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2096	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2204	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2180	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2203	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4147	92	0,6,6	0.00	-	-	-	-
92	OHX	m0	302	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2163	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2254	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4191	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4442	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4232	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2272	1,92	0,6,6	0.00	-	-	-	-
92	OHX	2	2194	92	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4447	-	0,6,6	0.00	-	-	-	-
92	OHX	14	404	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2101	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4286	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4168	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2212	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4306	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4549	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4353	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4280	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4465	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4367	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4135	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4140	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4212	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4117	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4453	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4216	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4369	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4182	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4443	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4159	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4406	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4540	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4181	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2310	92	0,6,6	0.00	-	-	-	-
92	OHX	M5	309	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4152	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4494	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4189	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4302	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4557	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4172	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4254	36	0,6,6	0.00	-	-	-	-
92	OHX	5	4332	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2125	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4198	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4160	-	0,6,6	0.00	-	-	-	-
92	OHX	q2	203	-	0,6,6	0.00	-	-	-	-
92	OHX	L3	408	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4221	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2331	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4251	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	OHX	1	4481	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4365	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4133	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2230	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2306	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4410	-	0,6,6	0.00	-	-	-	-
92	OHX	7	236	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4268	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4272	92	0,6,6	0.00	-	-	-	-
92	OHX	2	2247	92	0,6,6	0.00	-	-	-	-
92	OHX	SR	401	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4200	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4166	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4259	92	0,6,6	0.00	-	-	-	-
92	OHX	5	4551	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4150	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2171	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4291	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4454	-	0,6,6	0.00	-	-	-	-
92	OHX	m1	203	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4159	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2325	92	0,6,6	0.00	-	-	-	-
92	OHX	1	4334	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4388	36	0,6,6	0.00	-	-	-	-
92	OHX	1	4264	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4211	92	0,6,6	0.00	-	-	-	-
92	OHX	m5	303	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4486	-	0,6,6	0.00	-	-	-	-
92	OHX	6	2186	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4503	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2300	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4306	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4486	92	0,6,6	0.00	-	-	-	-
92	OHX	6	2148	-	0,6,6	0.00	-	-	-	-
92	OHX	5	4487	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4118	-	0,6,6	0.00	-	-	-	-
92	OHX	2	2139	-	0,6,6	0.00	-	-	-	-
92	OHX	1	4474	-	0,6,6	0.00	-	-	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

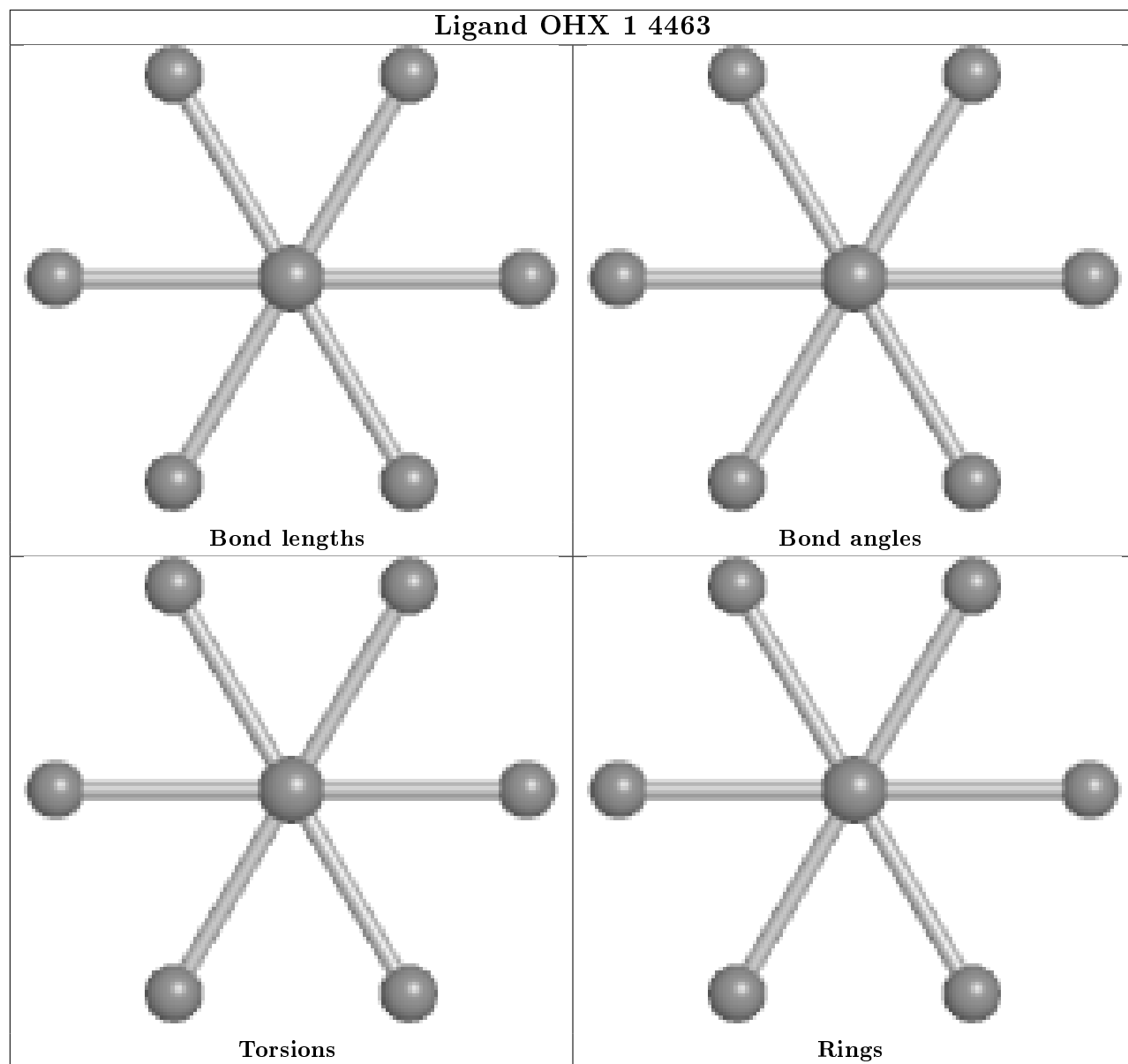
There are no torsion outliers.

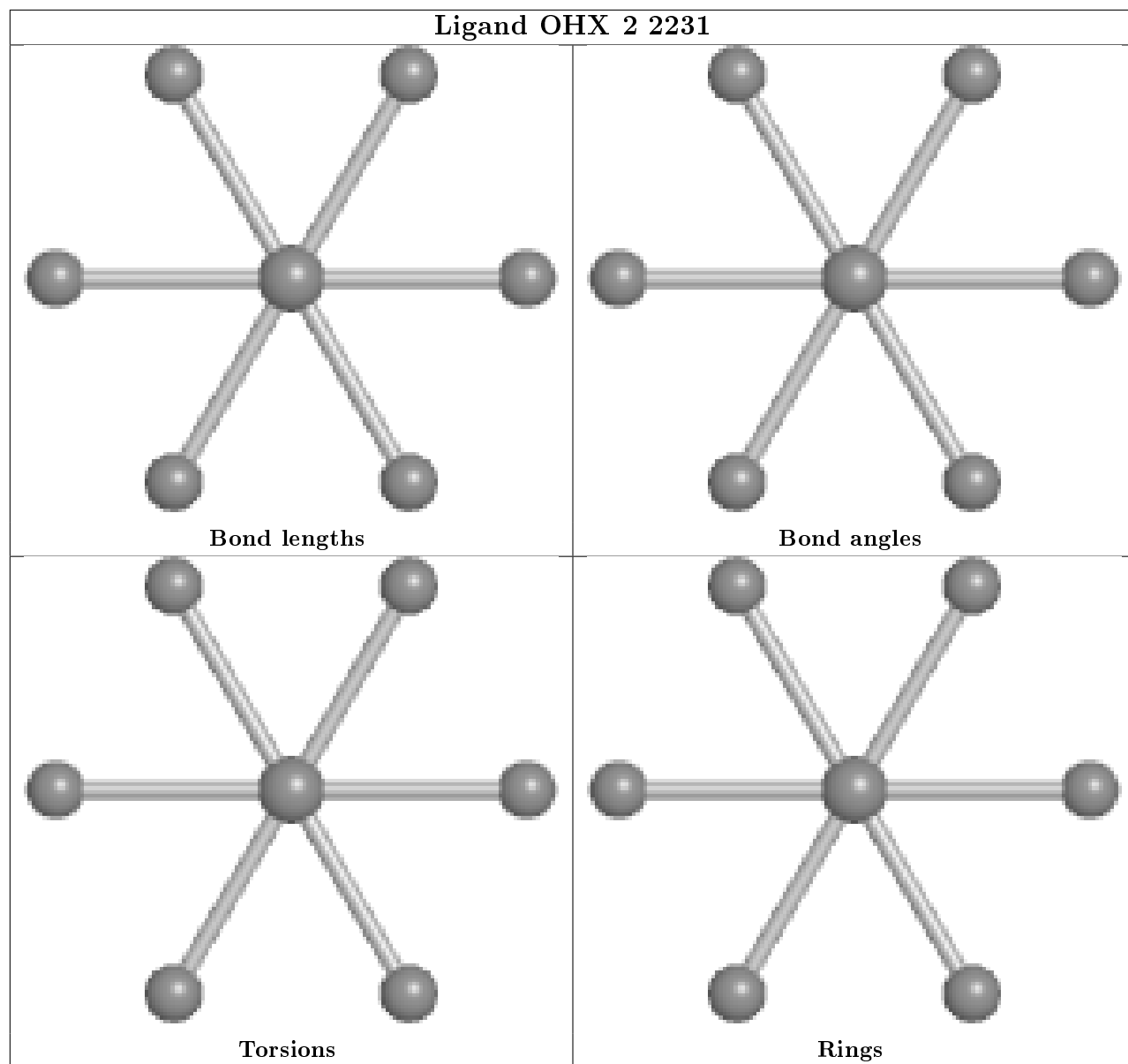
There are no ring outliers.

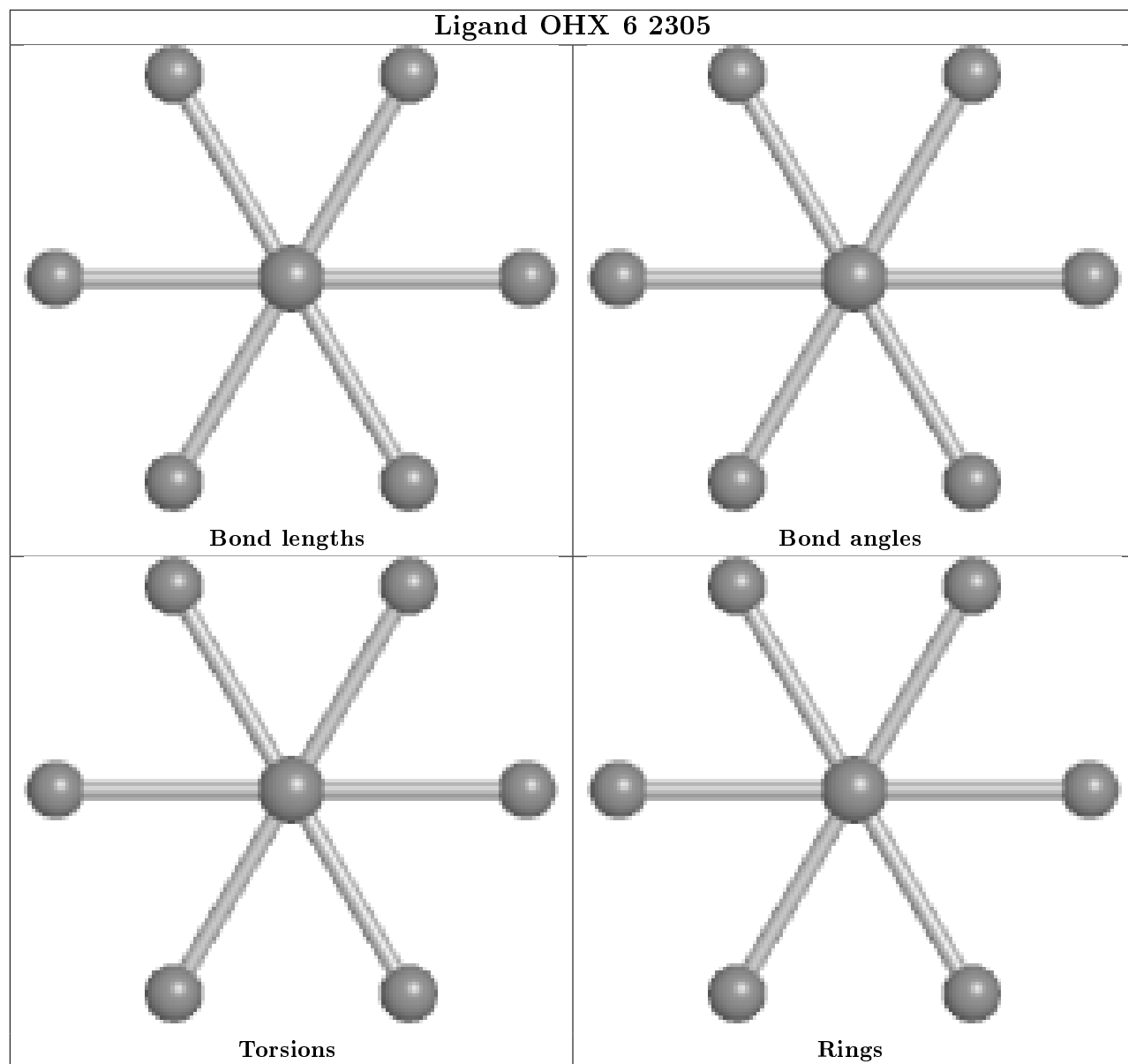
1 monomer is involved in 1 short contact:

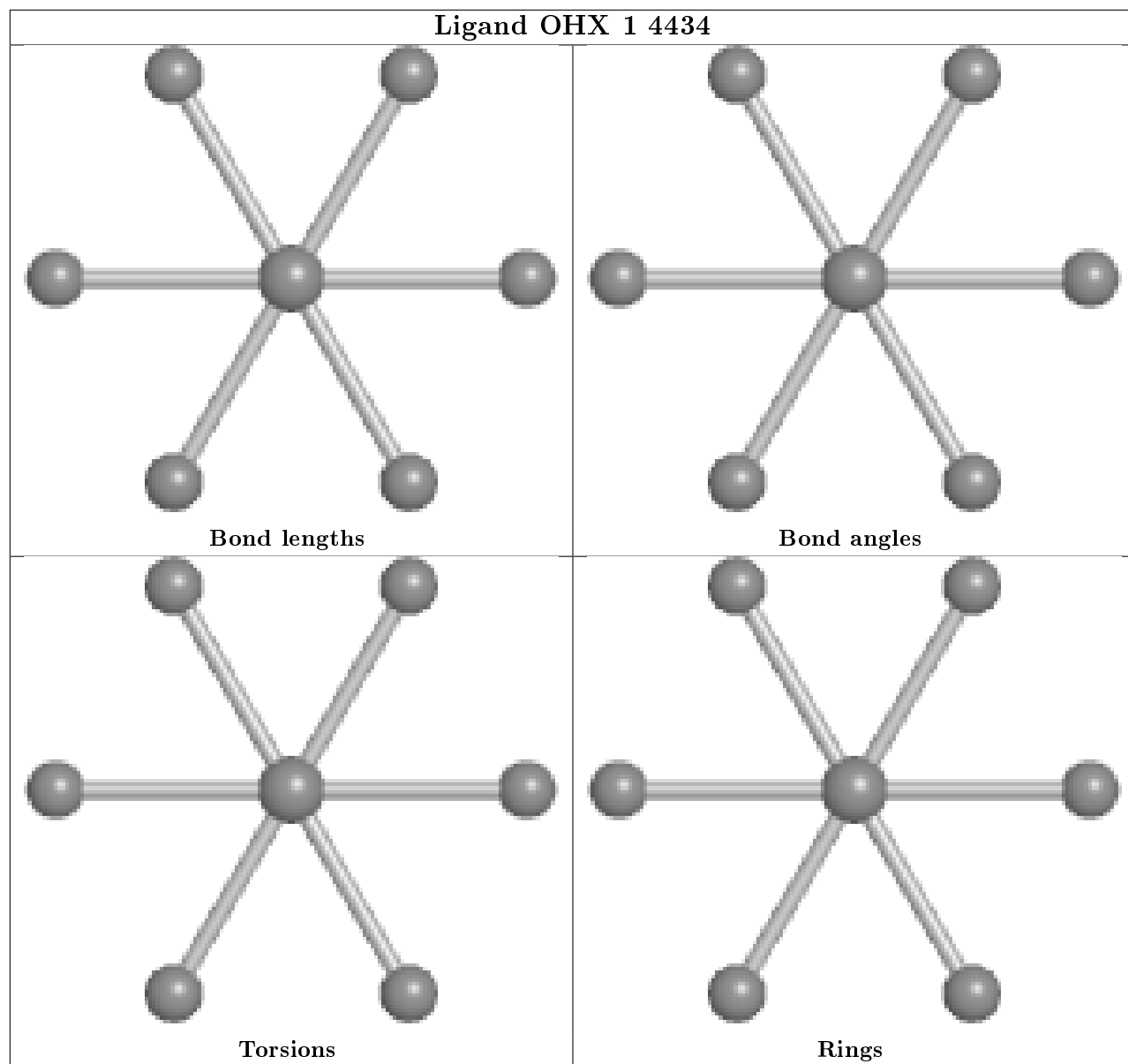
Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	19	204	OHX	0	1

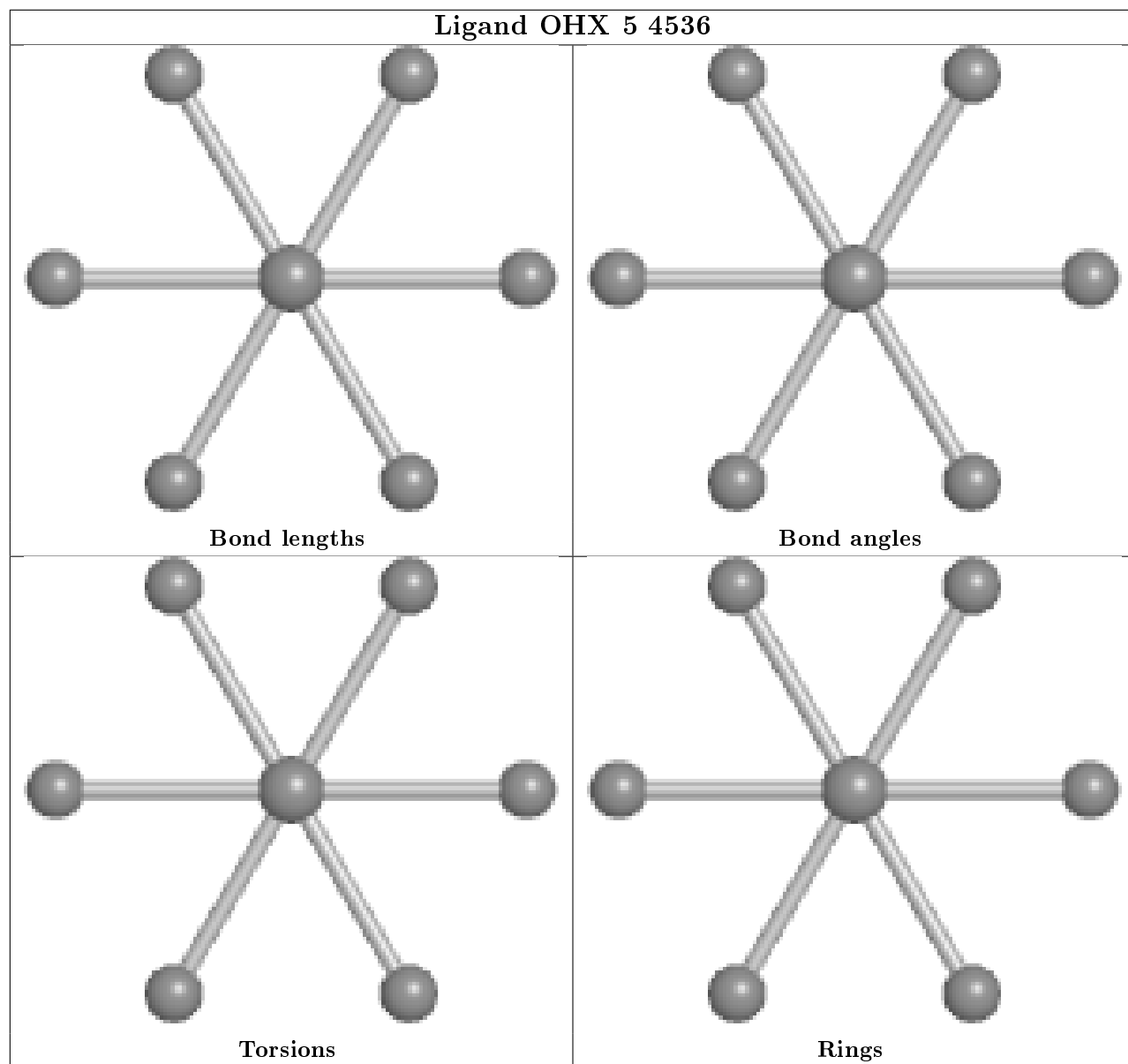
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

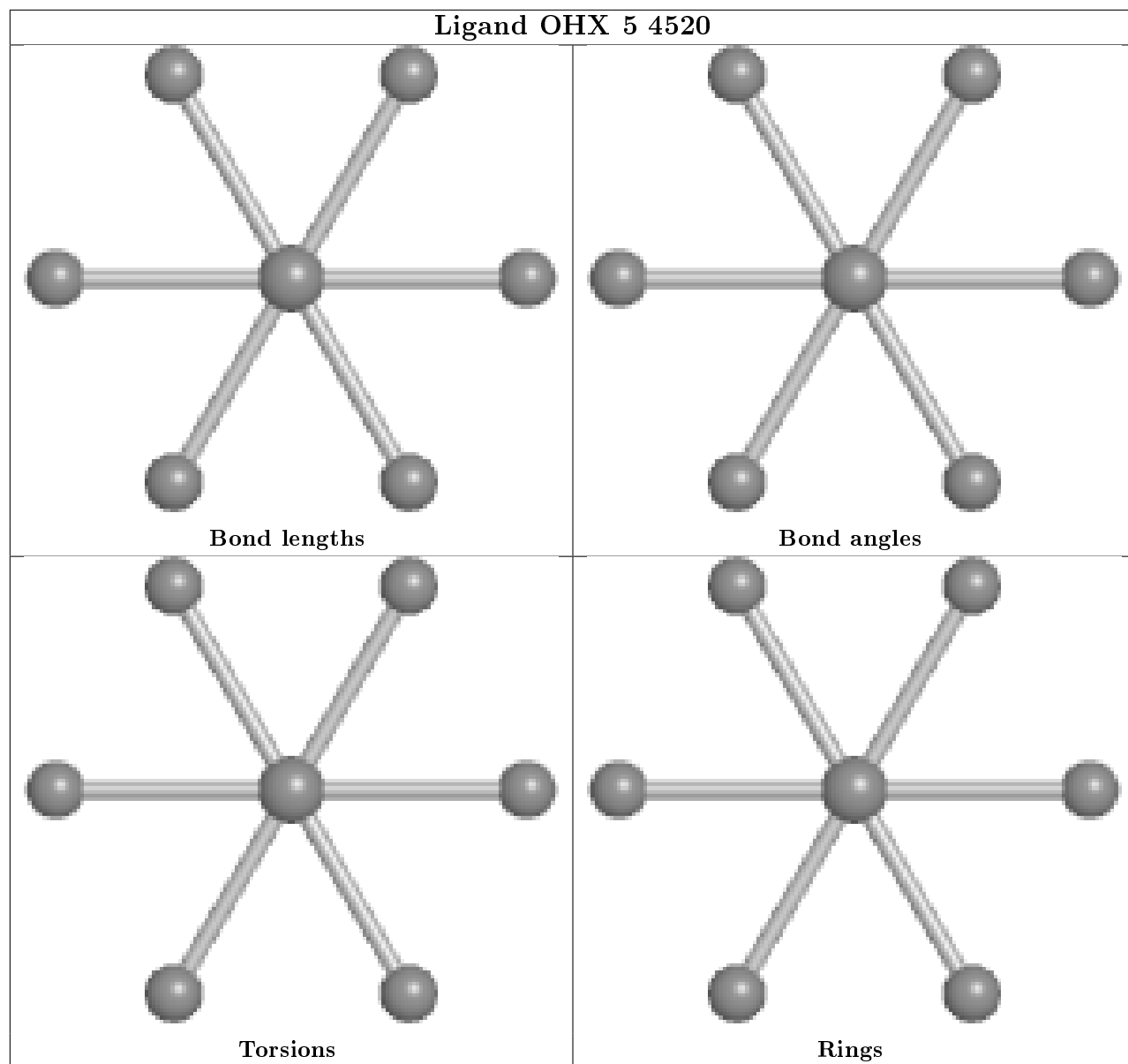


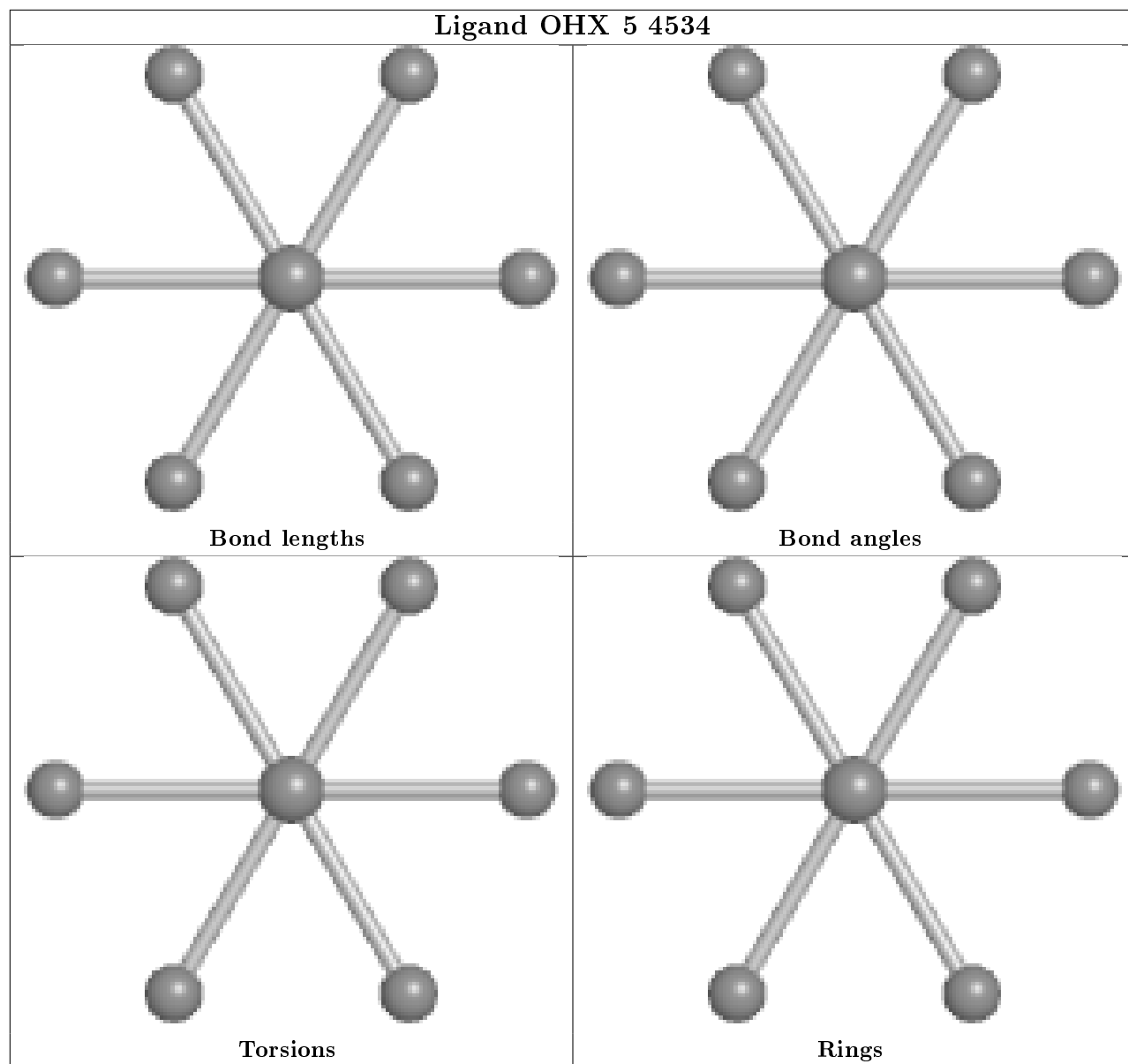


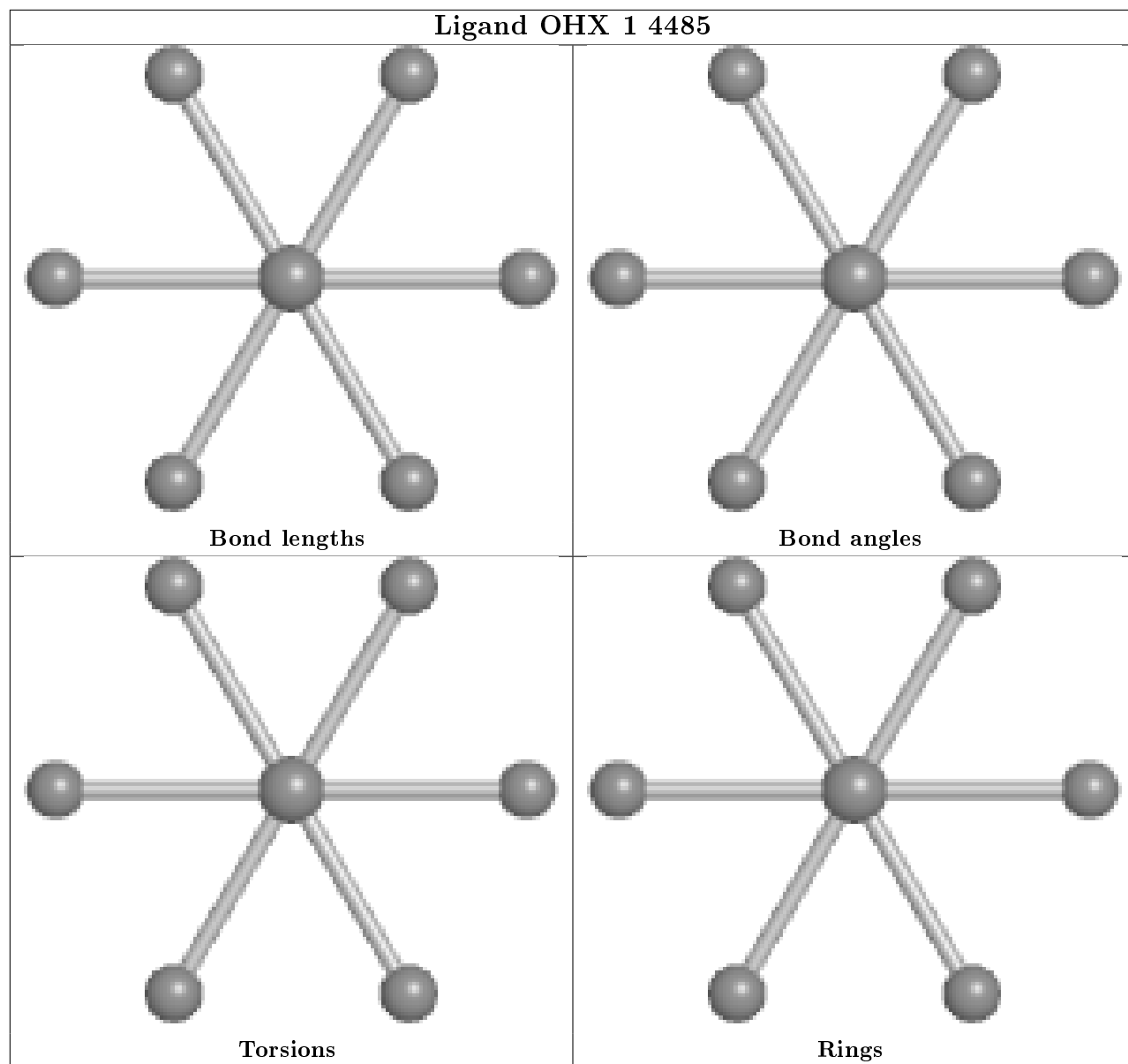


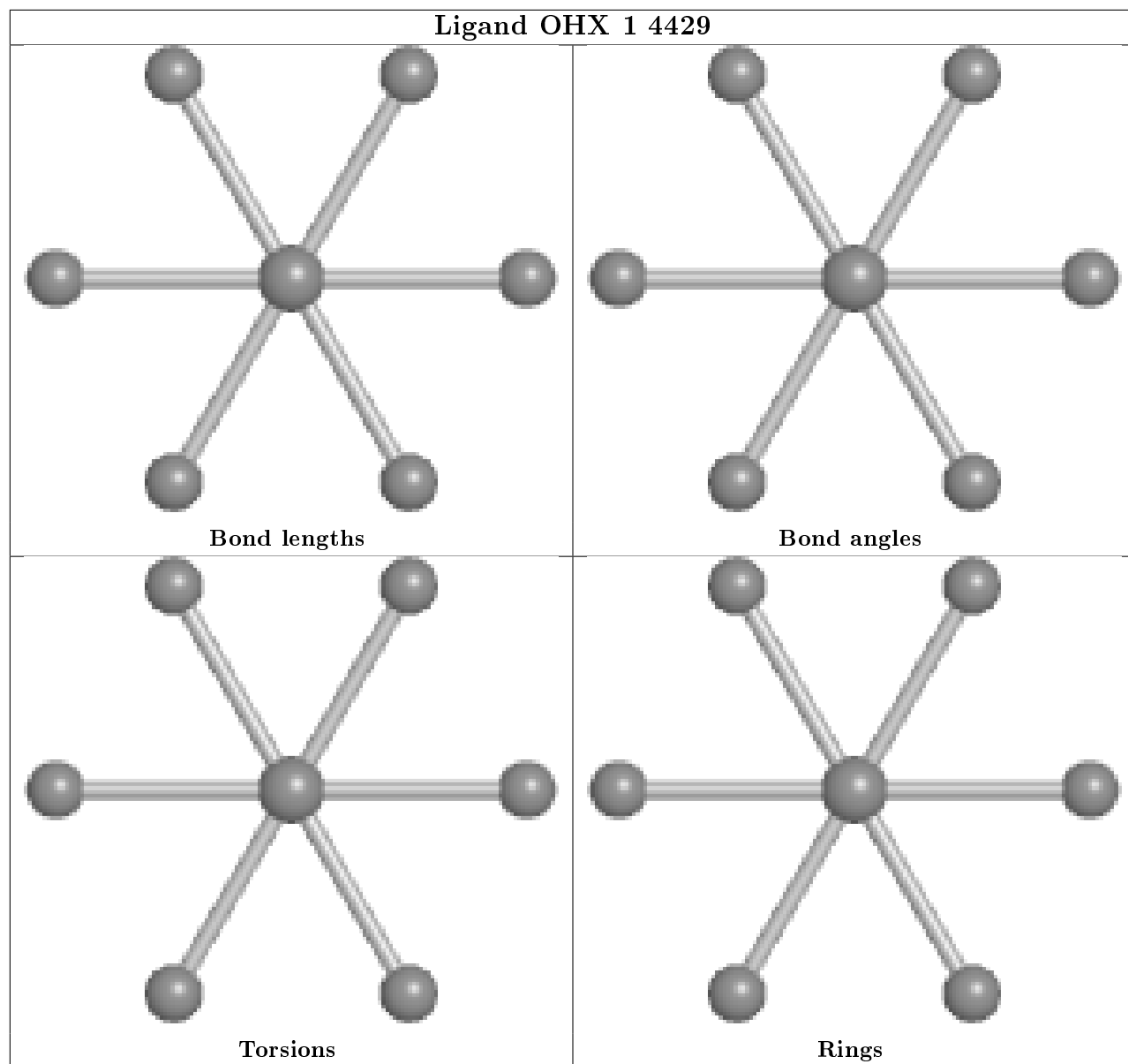


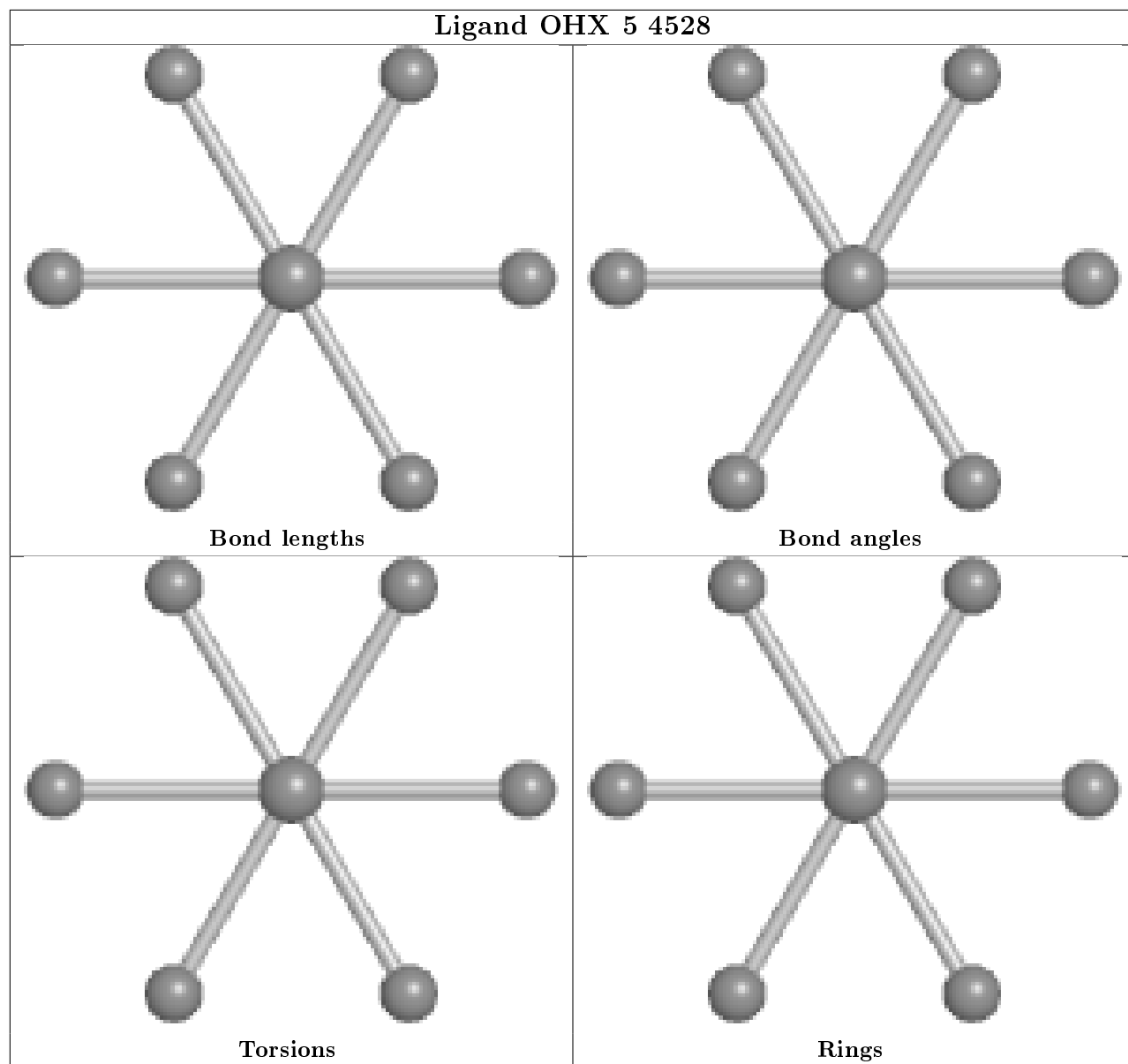


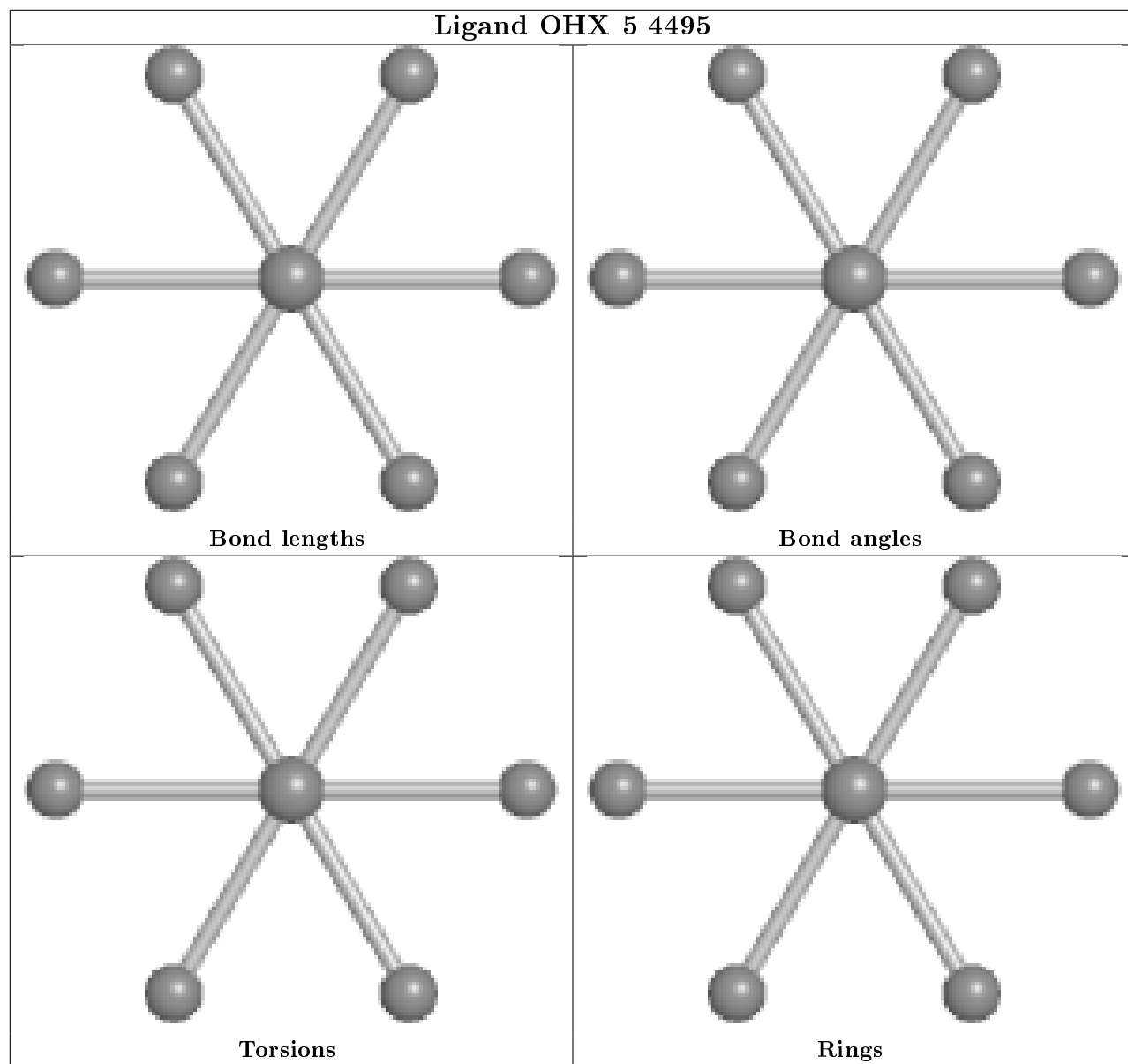


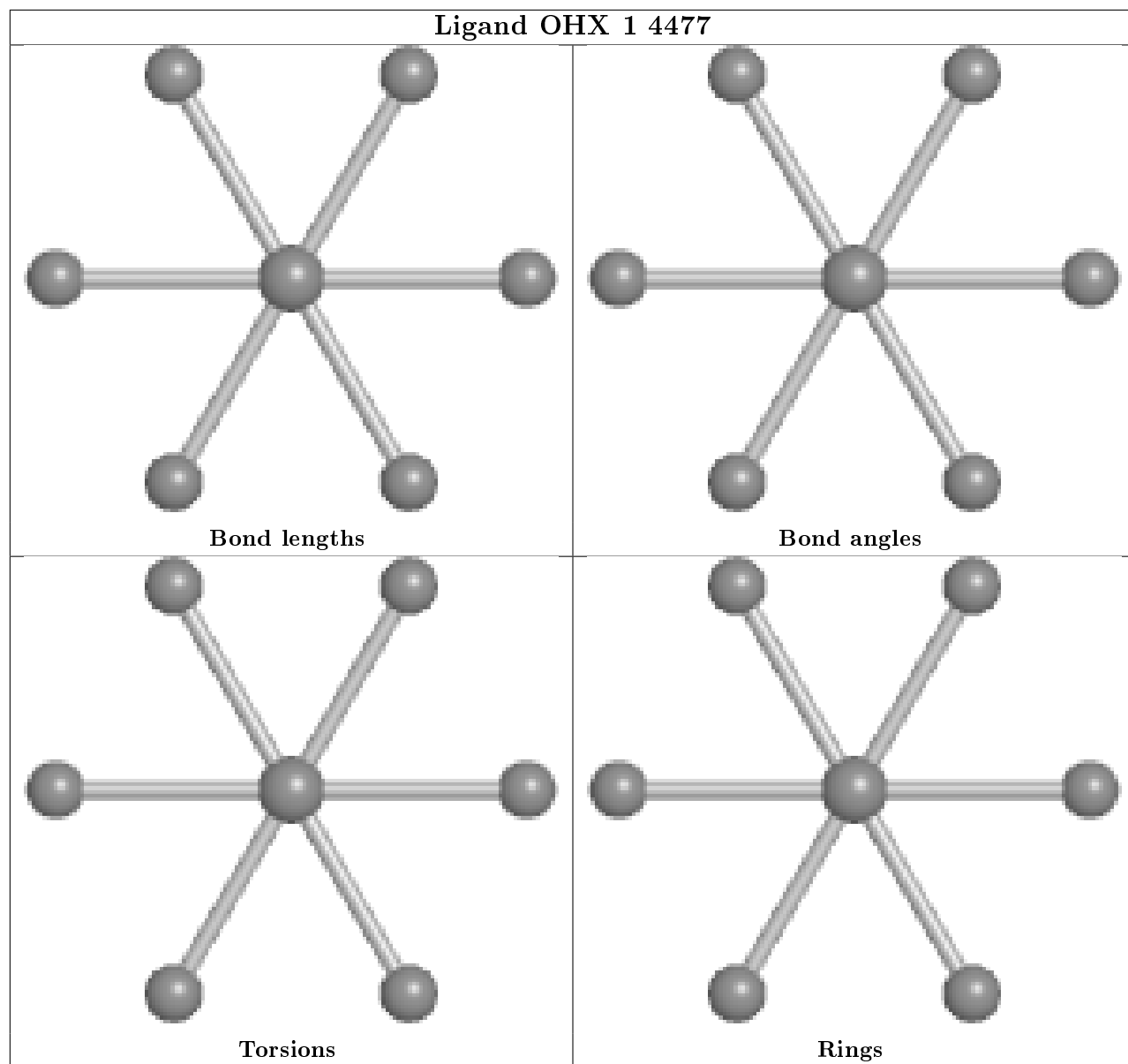


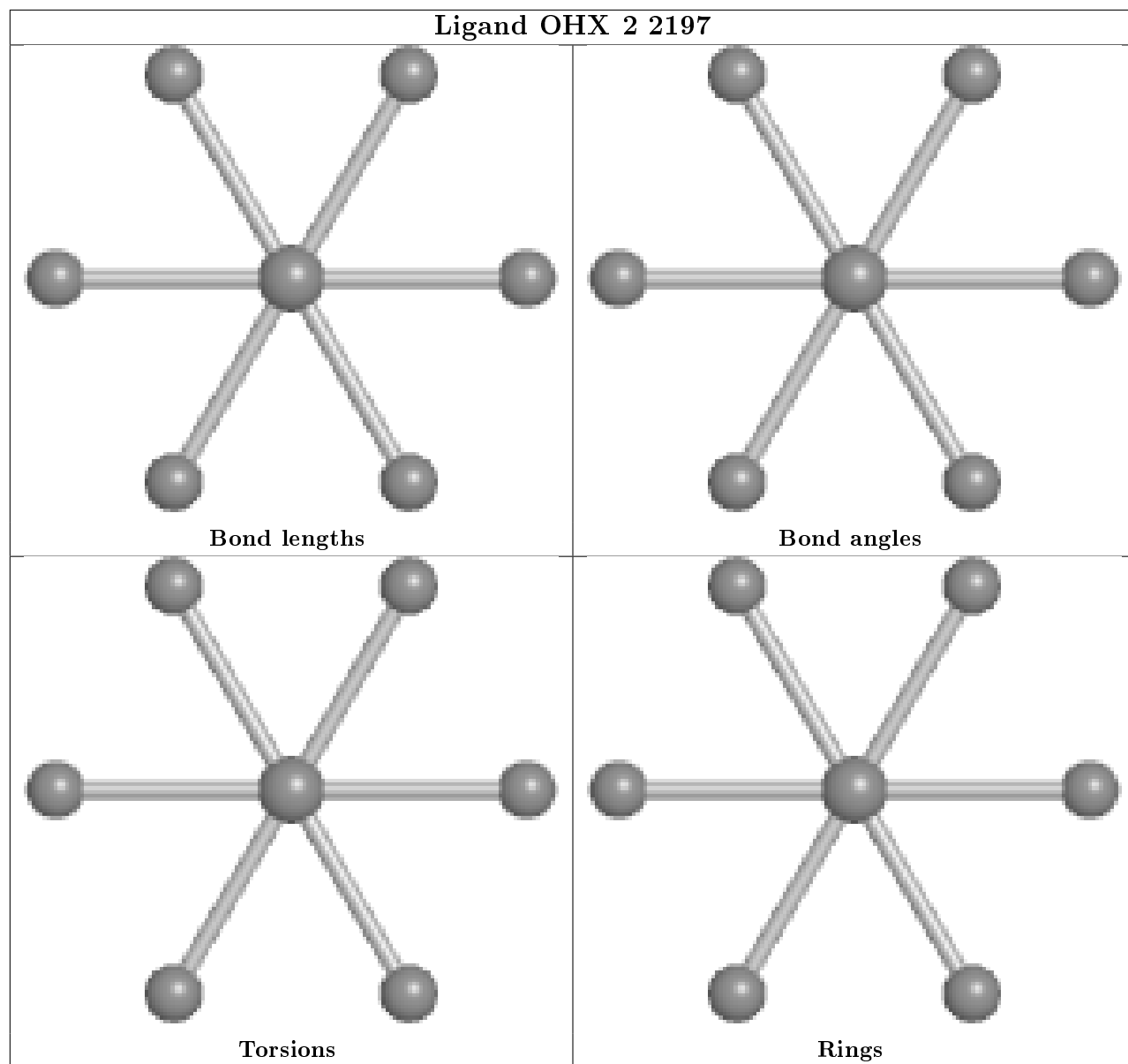


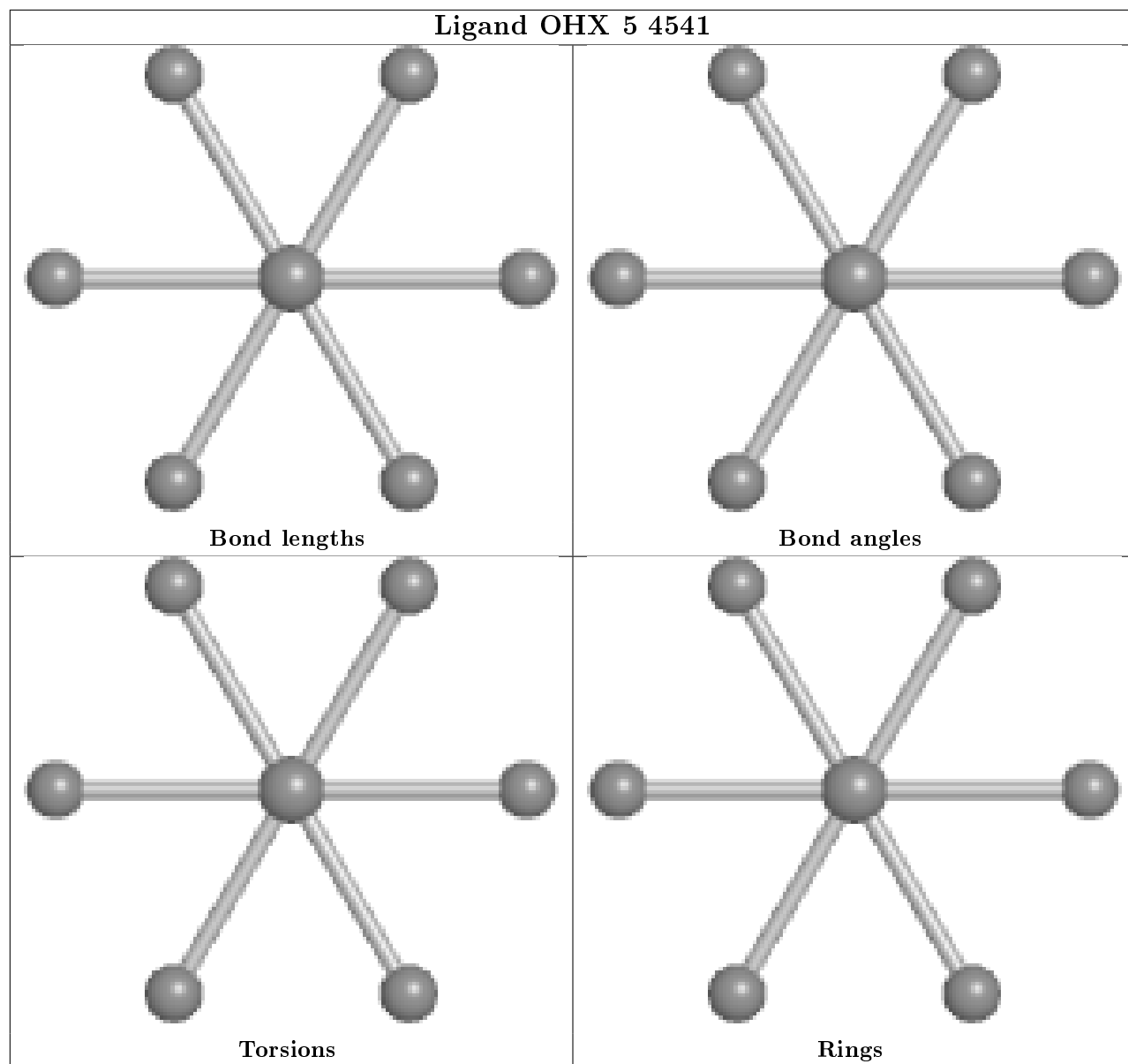


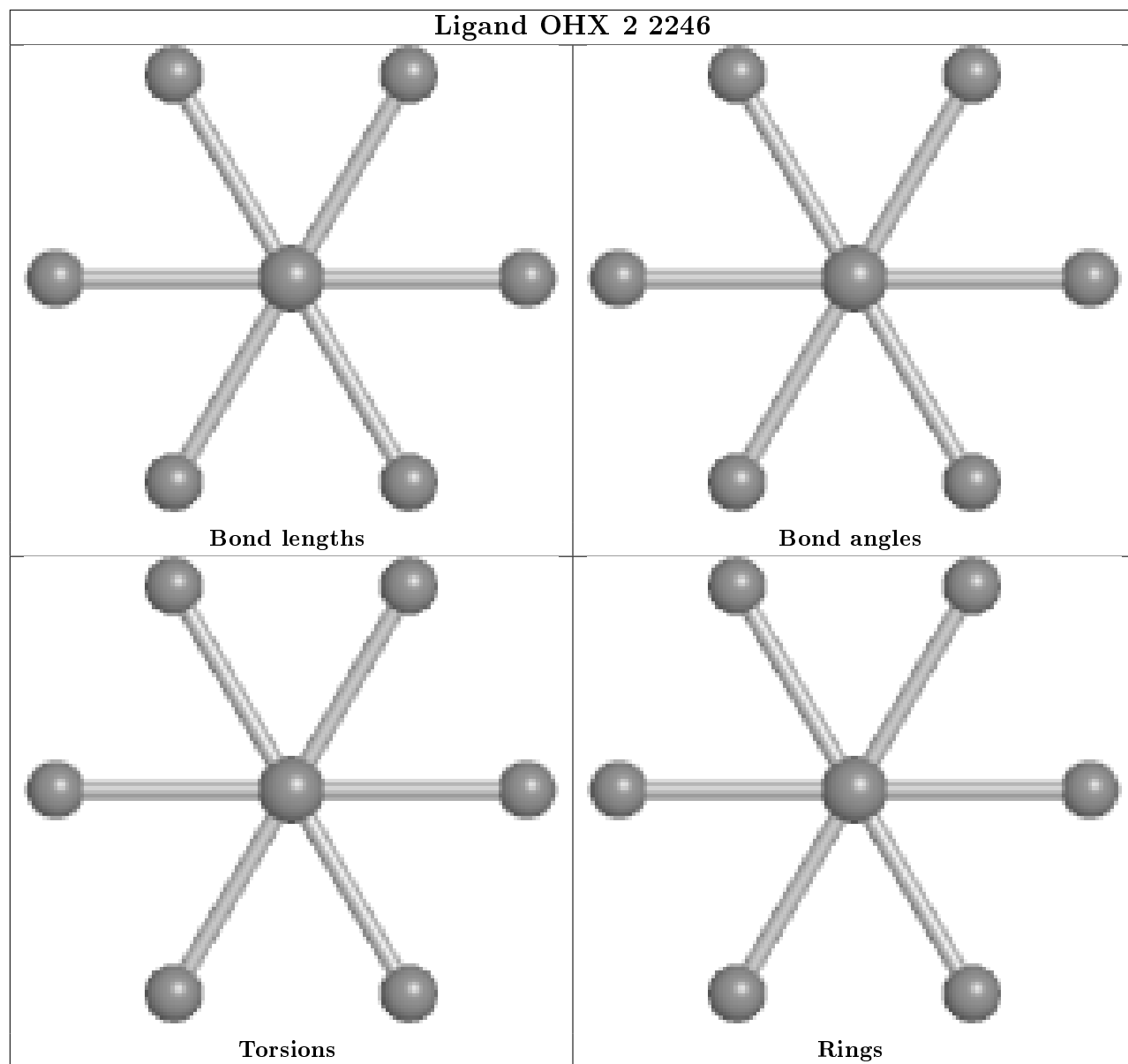


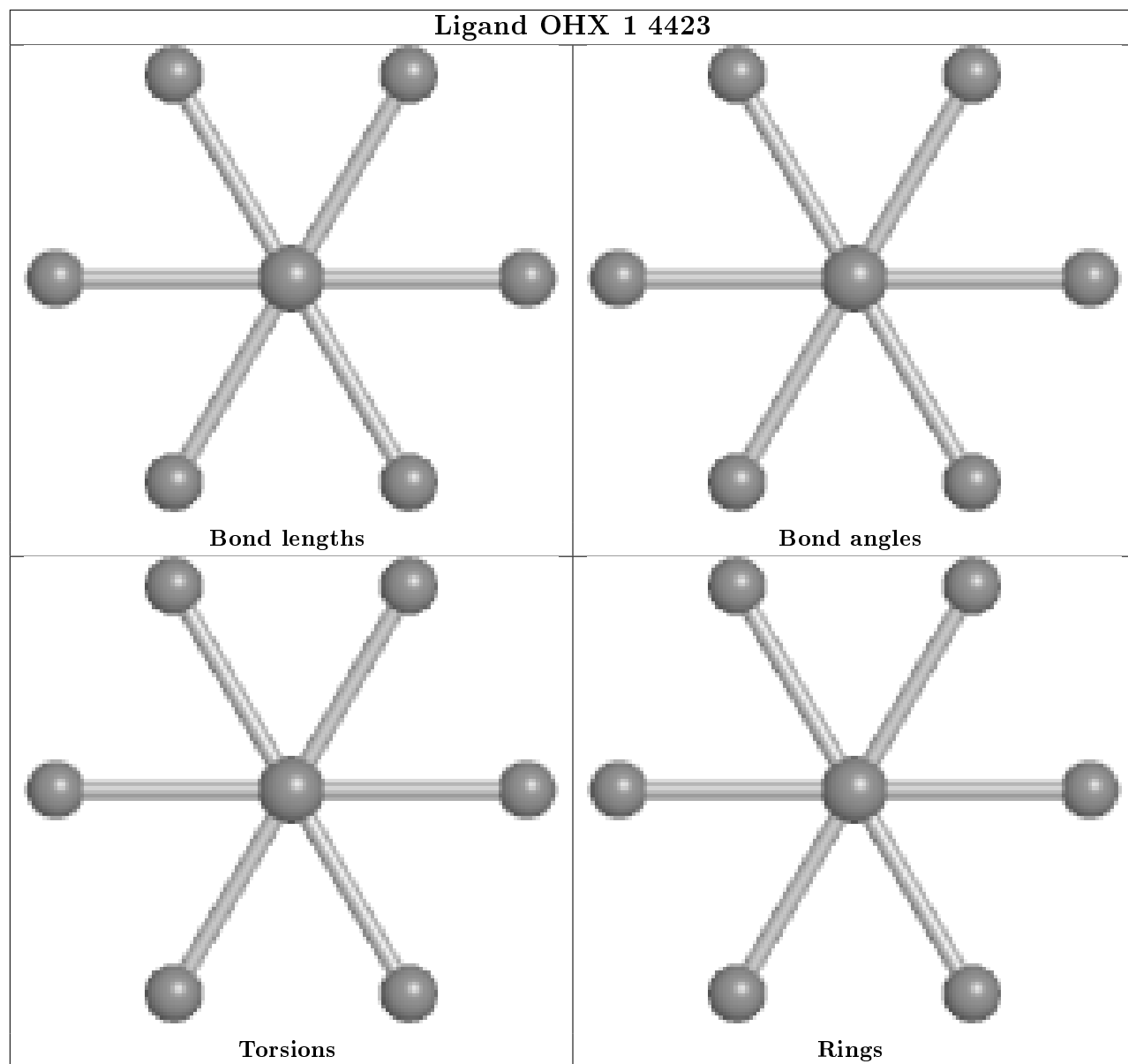


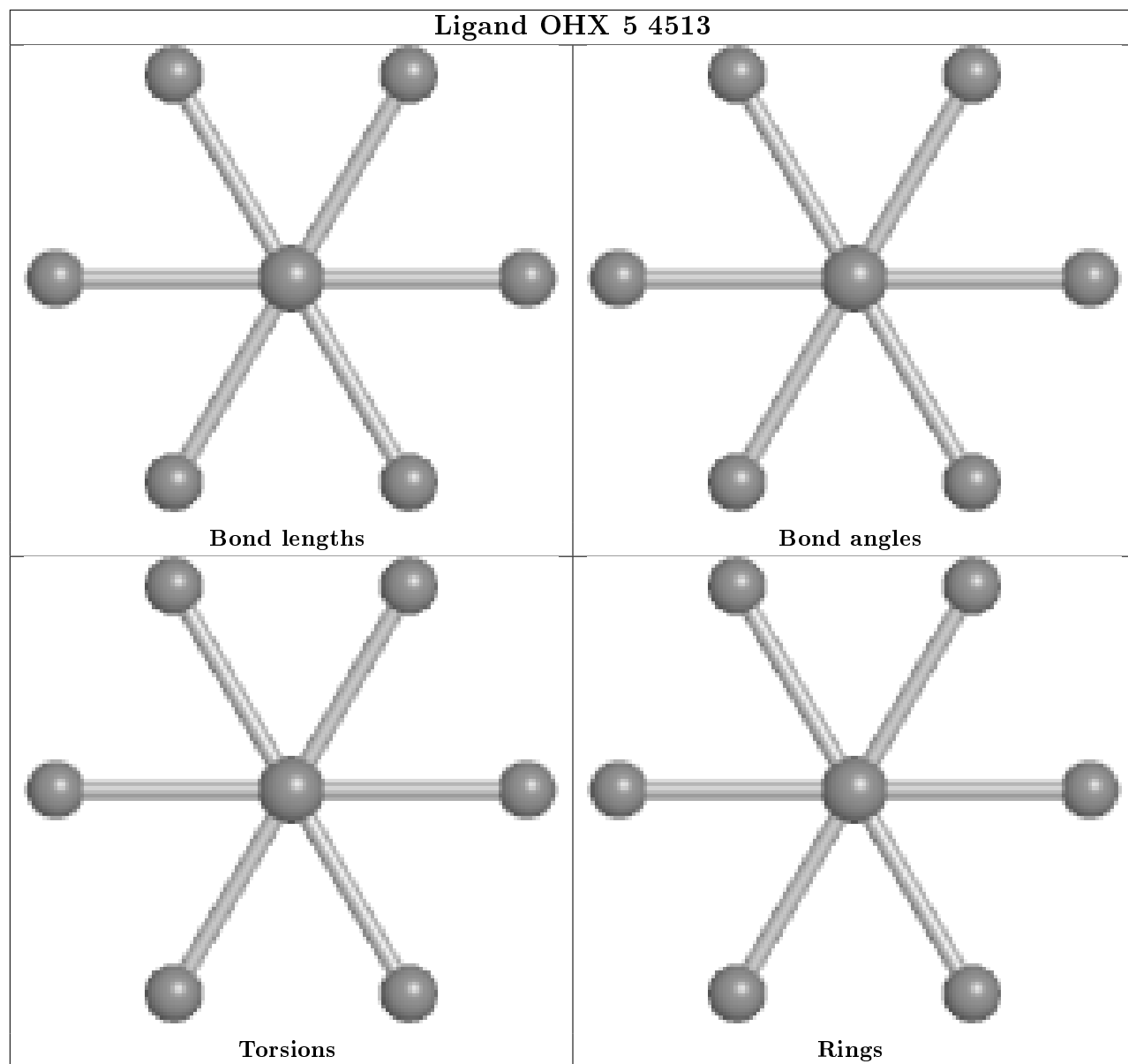


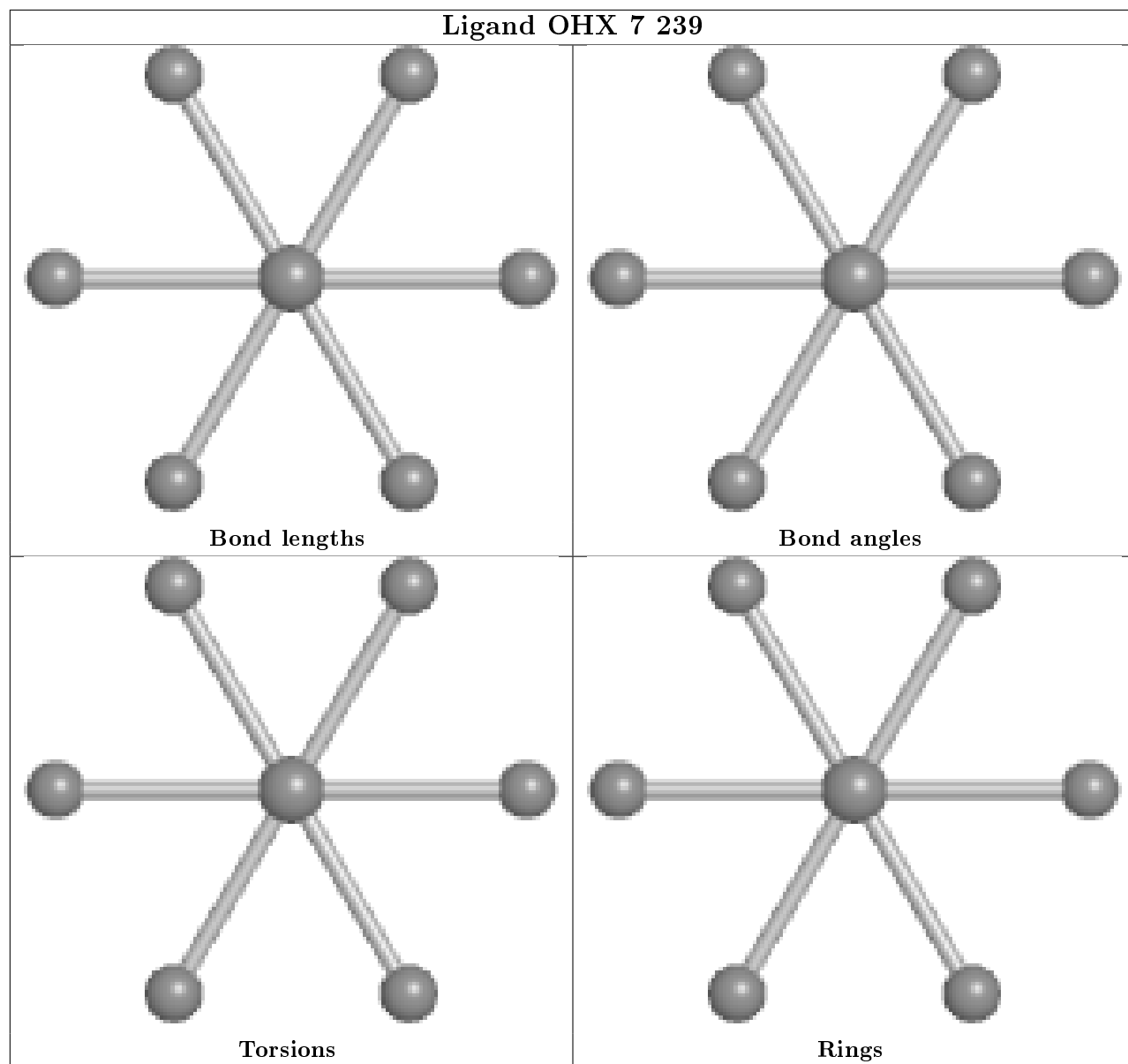


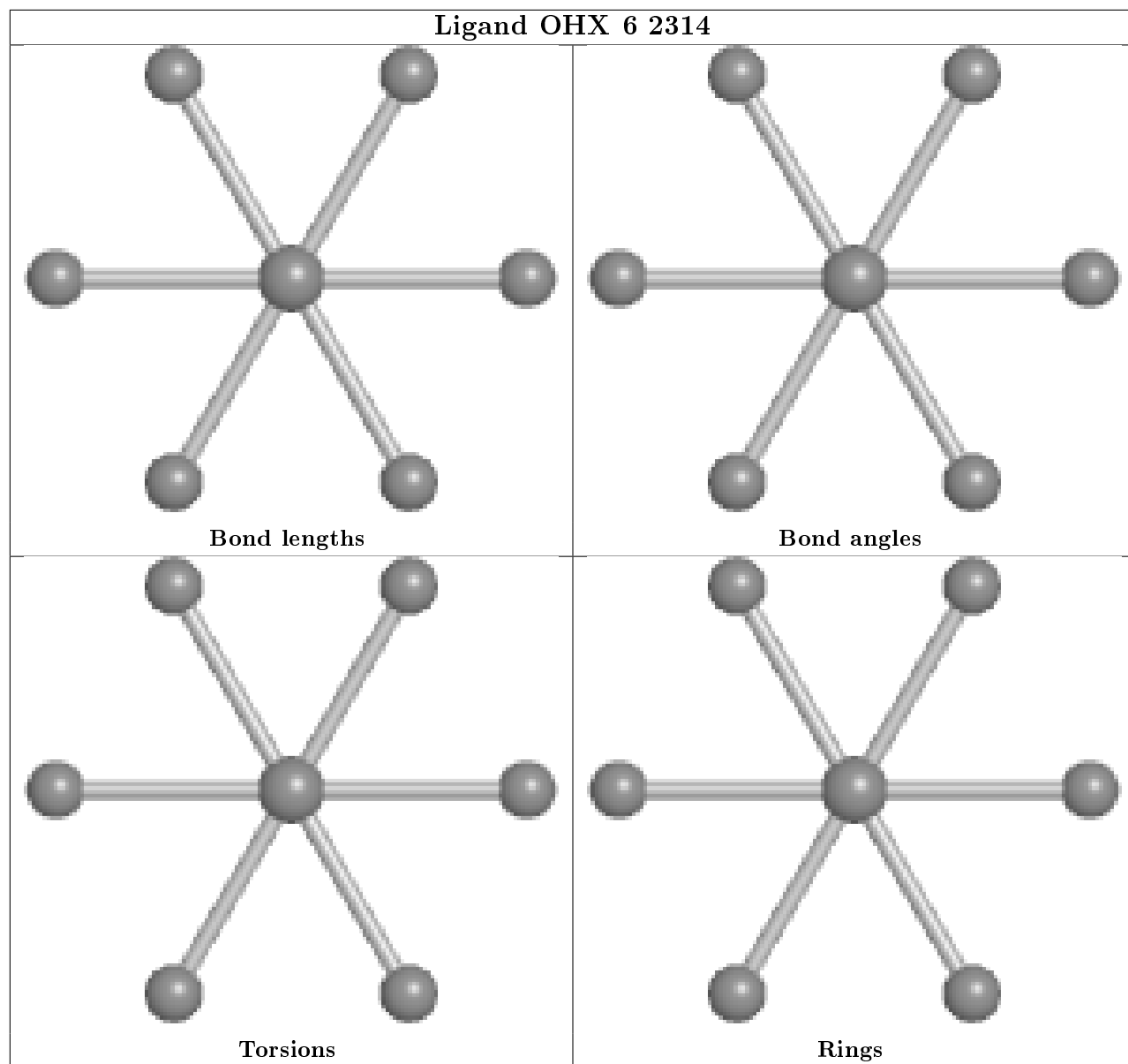


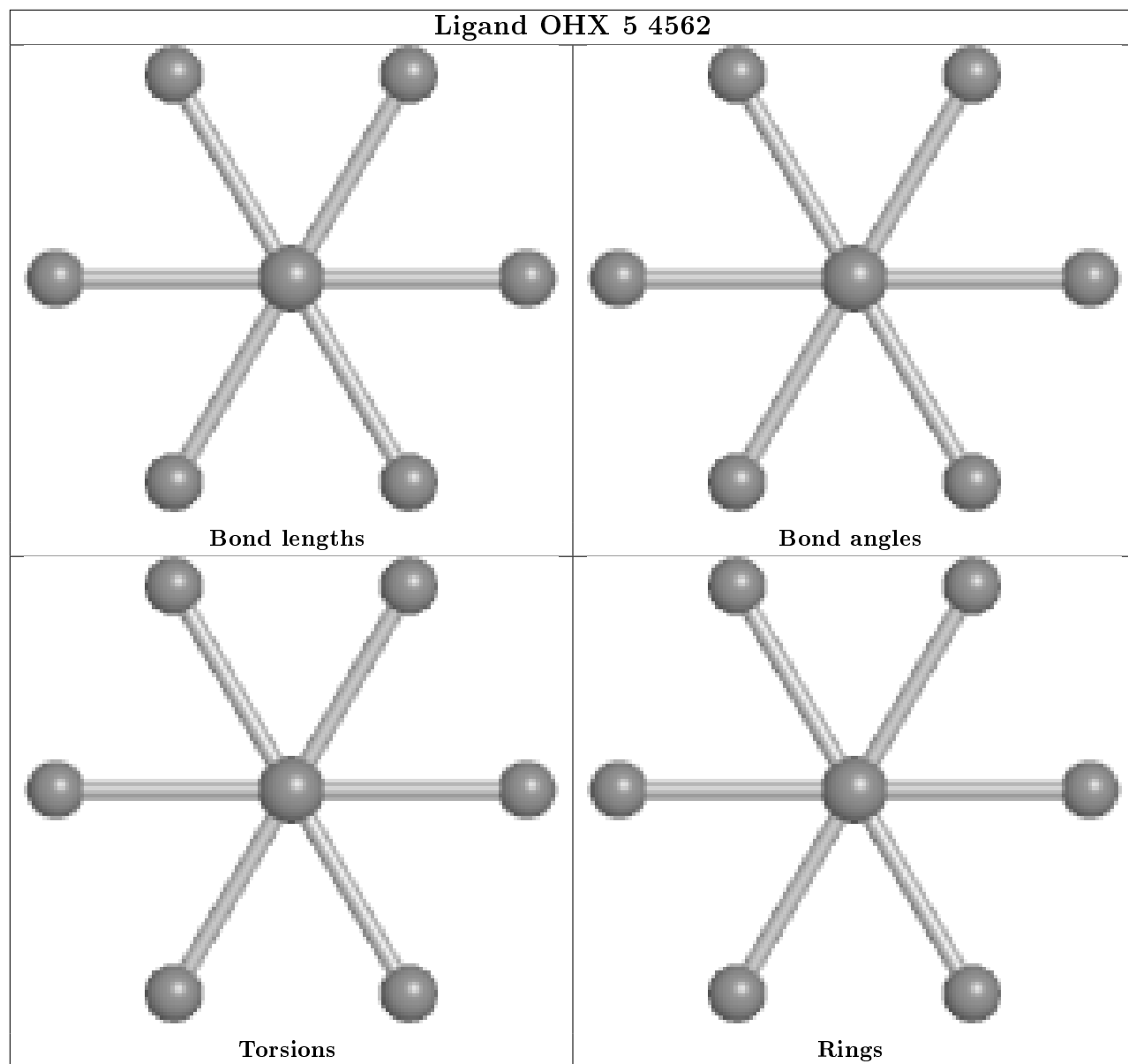


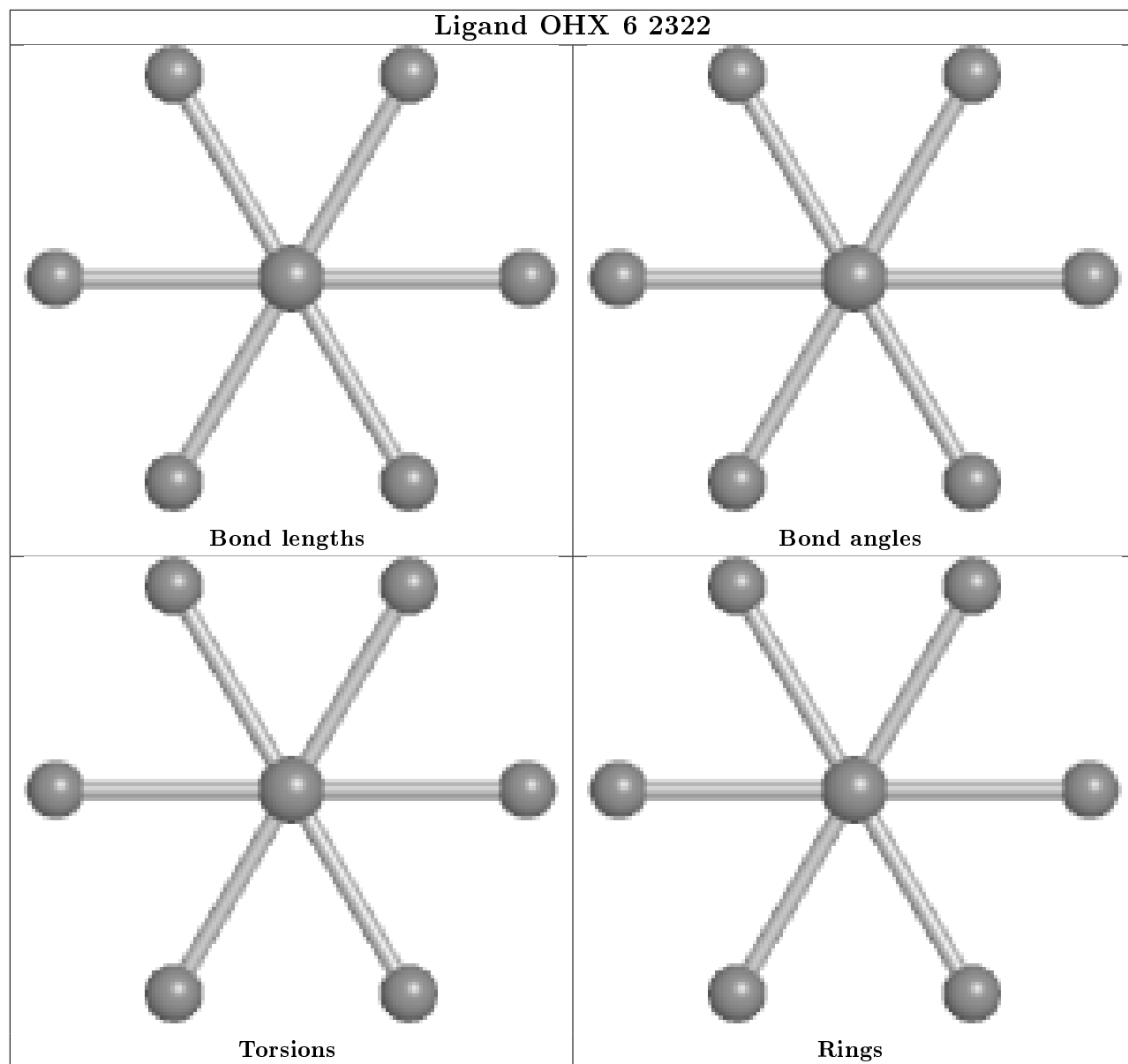


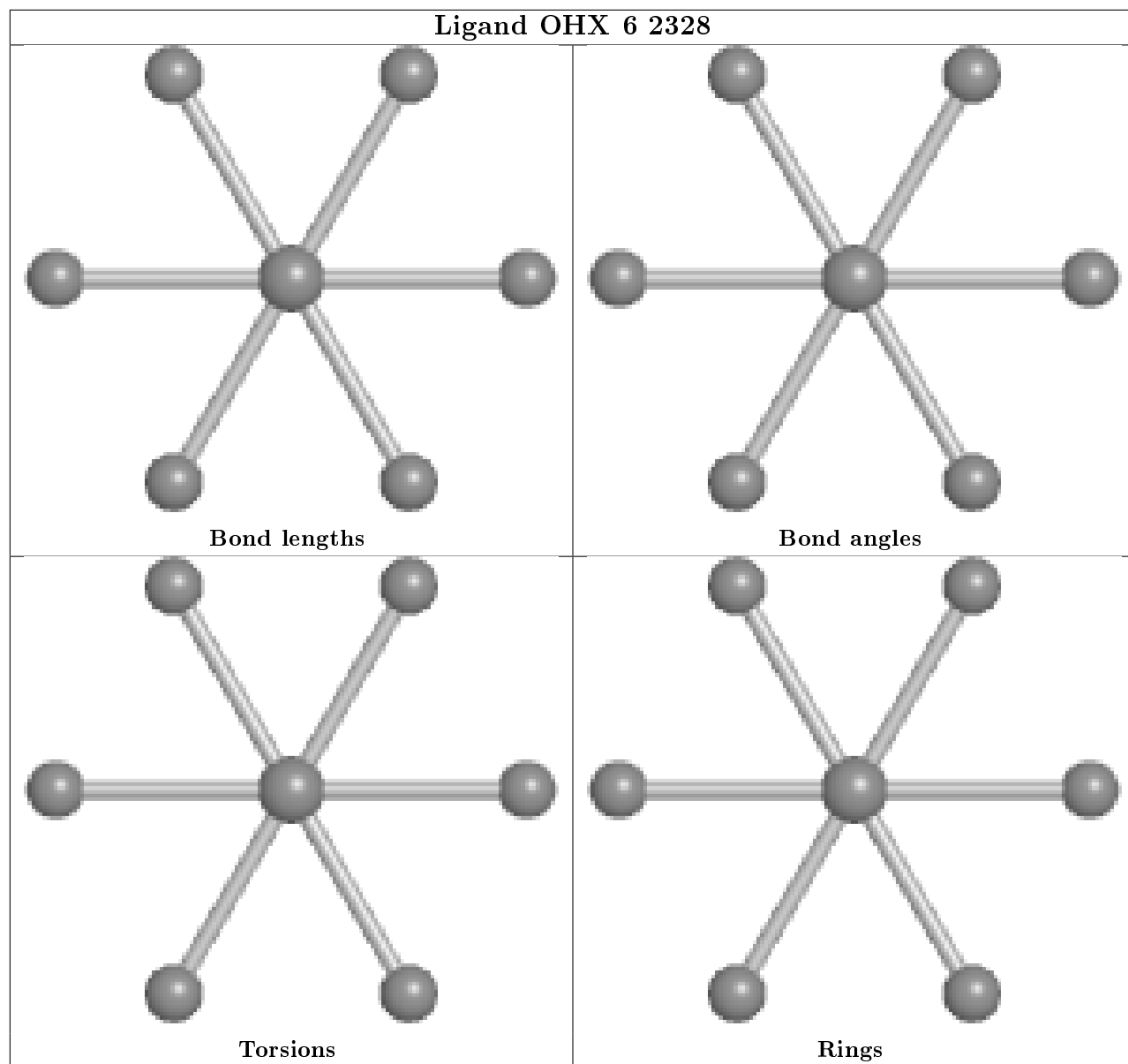


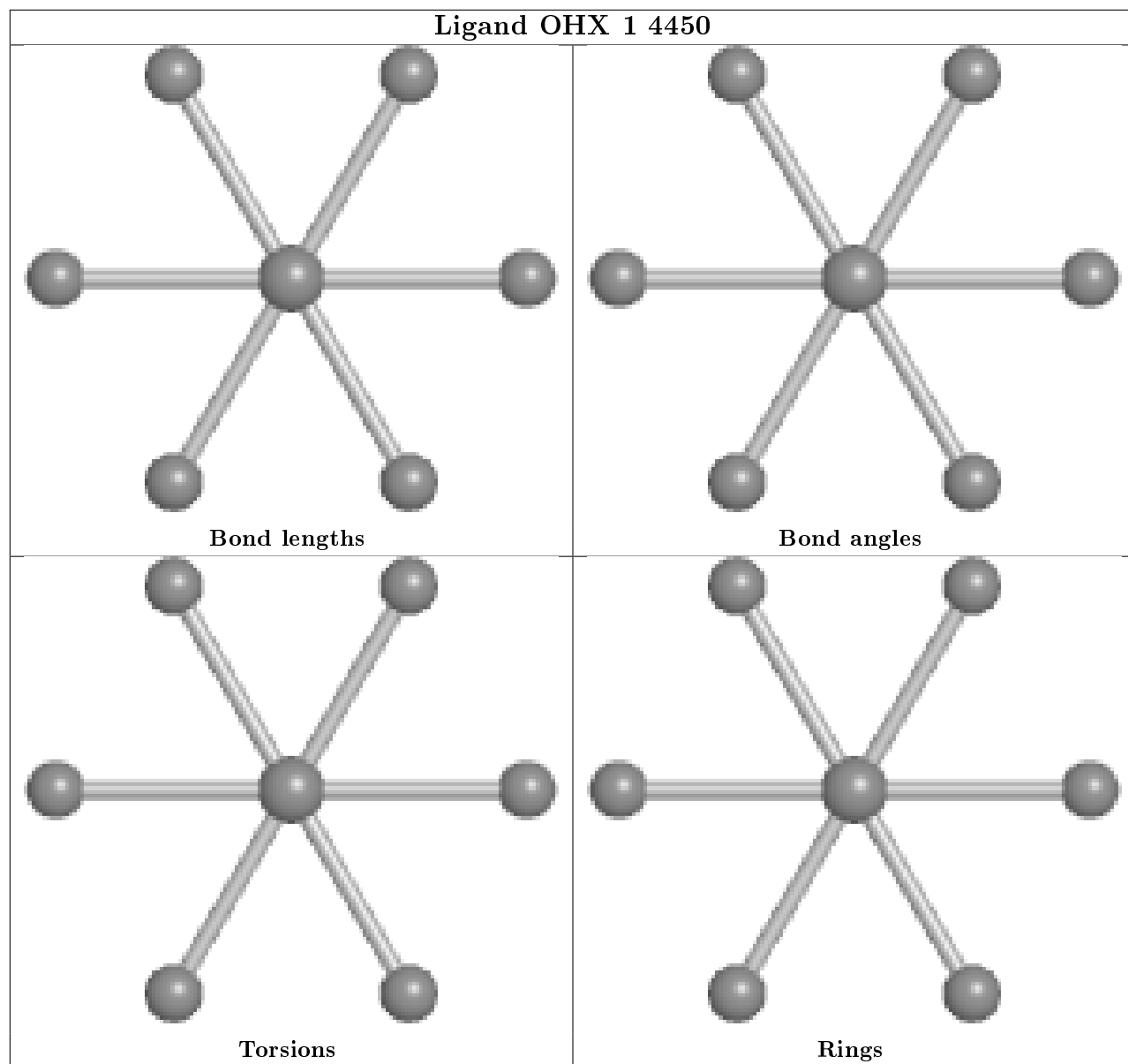


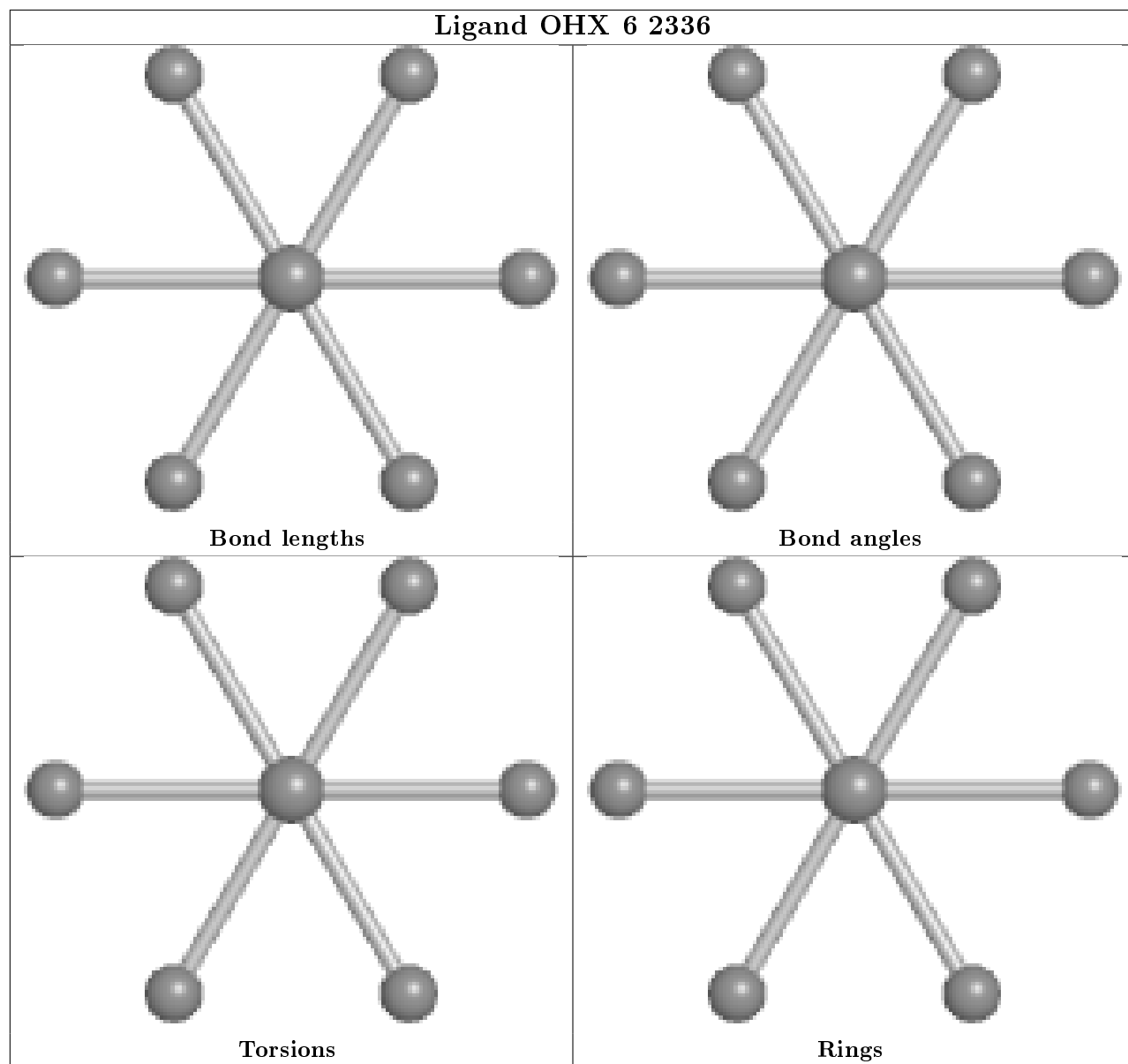


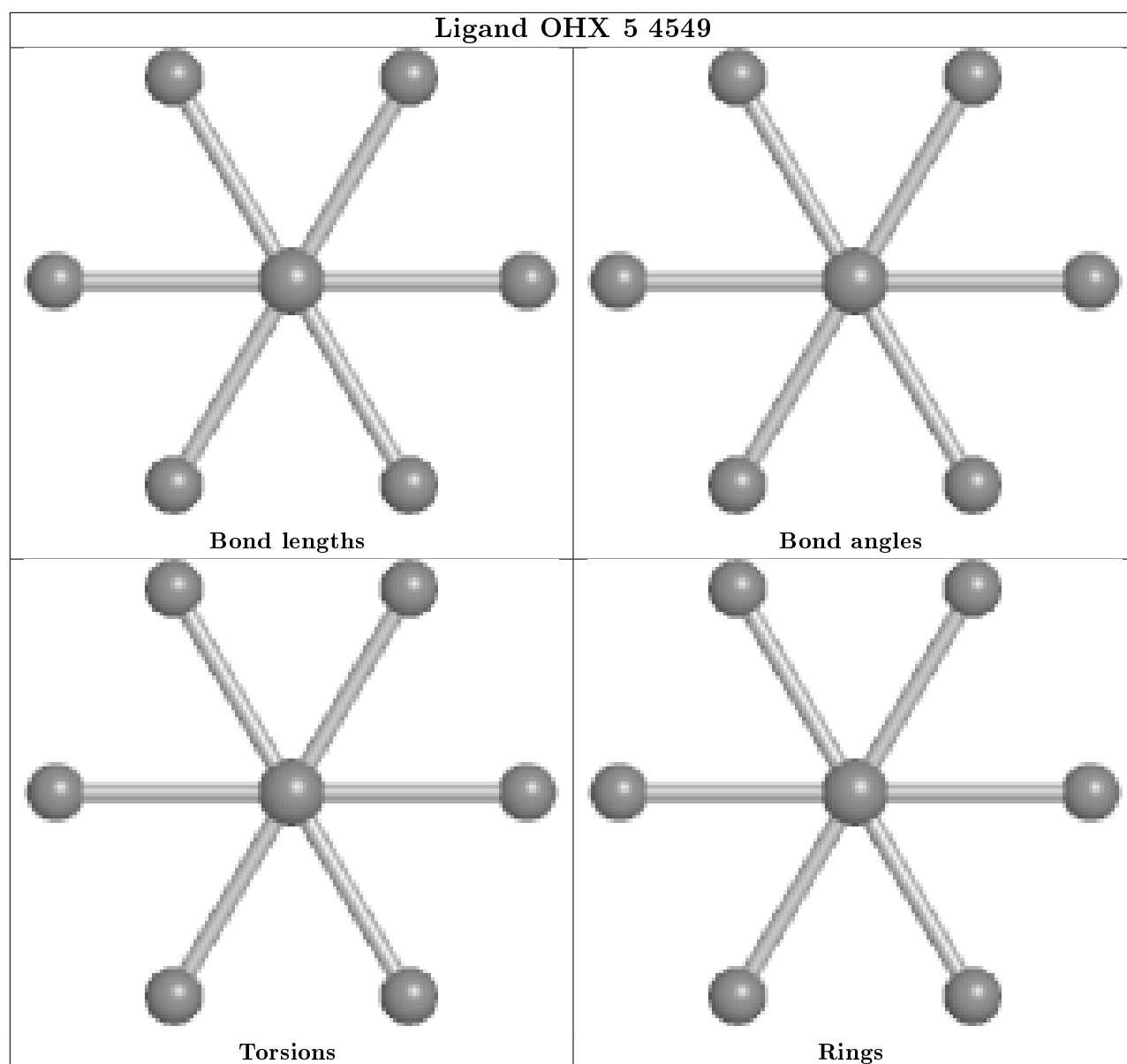












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
86	m2	2
84	sM	2
35	SM	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
80	c0	1
6	s4	1
1	2	1
42	l5	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	43.93
1	sM	139:UNK	C	155:UNK	N	38.21
1	SM	141:ALA	C	151:UNK	N	26.51
1	c0	84:UNK	C	87:UNK	N	7.82
1	2	1716:C	O3'	1717:G	P	3.78

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1781/1800 (98%)	0.31	109 (6%) 21 20	66, 101, 181, 226	0
1	6	1795/1800 (99%)	0.20	78 (4%) 35 33	55, 93, 167, 227	0
2	S0	206/206 (100%)	2.12	109 (52%) 0 0	106, 120, 129, 135	0
2	s0	206/206 (100%)	1.46	57 (27%) 0 0	91, 107, 119, 120	0
3	S1	214/216 (99%)	0.60	29 (13%) 3 3	112, 144, 166, 170	0
3	s1	216/216 (100%)	0.99	36 (16%) 1 1	89, 100, 117, 126	0
4	S2	217/217 (100%)	2.11	100 (46%) 0 0	88, 100, 114, 121	0
4	s2	217/217 (100%)	1.25	45 (20%) 1 1	75, 90, 101, 110	0
5	S3	223/223 (100%)	1.08	53 (23%) 0 0	95, 105, 125, 136	0
5	s3	223/223 (100%)	0.28	12 (5%) 25 24	93, 115, 133, 138	0
6	S4	260/260 (100%)	1.19	60 (23%) 0 1	77, 102, 112, 131	0
6	s4	260/260 (100%)	0.84	27 (10%) 6 6	62, 90, 105, 125	0
7	S5	206/206 (100%)	1.33	46 (22%) 0 1	105, 121, 131, 140	0
7	s5	206/206 (100%)	1.03	41 (19%) 1 1	97, 116, 131, 137	0
8	S6	226/226 (100%)	1.01	45 (19%) 1 1	80, 112, 126, 133	0
8	s6	218/226 (96%)	1.00	35 (16%) 1 2	65, 92, 110, 121	0
9	S7	184/186 (98%)	0.37	11 (5%) 21 21	100, 124, 149, 154	0
9	s7	186/186 (100%)	0.91	29 (15%) 2 2	84, 115, 139, 144	0
10	S8	188/199 (94%)	1.32	44 (23%) 0 1	74, 89, 121, 132	0
10	s8	188/199 (94%)	0.84	26 (13%) 2 2	61, 83, 121, 139	0
11	S9	185/185 (100%)	1.47	61 (32%) 0 0	92, 109, 138, 156	0
11	s9	185/185 (100%)	0.36	16 (8%) 10 10	77, 95, 122, 136	0
12	C0	83/96 (86%)	-0.07	2 (2%) 59 55	98, 116, 126, 129	0
13	C1	146/155 (94%)	1.61	37 (25%) 0 0	76, 86, 106, 118	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	c1	146/155 (94%)	1.58	36 (24%) 0 0	66, 81, 109, 129	0
14	C2	124/124 (100%)	0.48	12 (9%) 7 8	142, 150, 160, 163	0
15	C3	150/150 (100%)	0.29	6 (4%) 38 35	84, 99, 113, 118	0
15	c3	150/150 (100%)	0.39	8 (5%) 26 24	75, 88, 104, 107	0
16	C4	127/128 (99%)	0.59	20 (15%) 2 2	87, 145, 156, 158	0
16	c4	128/128 (100%)	1.75	56 (43%) 0 0	72, 104, 112, 117	0
17	C5	124/131 (94%)	0.75	14 (11%) 5 5	92, 105, 122, 138	0
18	C6	141/142 (99%)	1.31	37 (26%) 0 0	95, 114, 118, 121	0
18	c6	142/142 (100%)	1.30	42 (29%) 0 0	91, 111, 122, 135	0
19	C7	120/125 (96%)	1.43	39 (32%) 0 0	103, 116, 136, 138	0
19	c7	117/125 (93%)	0.65	12 (10%) 6 6	98, 111, 126, 134	0
20	C8	145/145 (100%)	0.91	24 (16%) 1 2	89, 109, 134, 139	0
20	c8	145/145 (100%)	0.91	26 (17%) 1 1	91, 105, 125, 130	0
21	C9	143/143 (100%)	1.26	27 (18%) 1 1	97, 109, 123, 130	0
21	c9	143/143 (100%)	1.20	36 (25%) 0 0	93, 105, 119, 128	0
22	D0	107/110 (97%)	1.12	24 (22%) 0 1	90, 117, 134, 136	0
22	d0	110/110 (100%)	1.43	33 (30%) 0 0	91, 121, 142, 148	0
23	D1	87/87 (100%)	2.20	47 (54%) 0 0	102, 110, 125, 131	0
23	d1	87/87 (100%)	1.56	28 (32%) 0 0	87, 96, 116, 122	0
24	D2	129/129 (100%)	1.52	39 (30%) 0 0	86, 97, 103, 115	0
24	d2	129/129 (100%)	1.54	39 (30%) 0 0	72, 82, 90, 98	0
25	D3	144/144 (100%)	0.81	12 (8%) 11 11	76, 81, 92, 104	0
25	d3	144/144 (100%)	0.62	11 (7%) 13 12	64, 69, 78, 90	0
26	D4	134/134 (100%)	0.24	6 (4%) 33 31	90, 110, 120, 125	0
26	d4	134/134 (100%)	0.33	7 (5%) 27 25	71, 94, 104, 110	0
27	D5	70/70 (100%)	0.56	5 (7%) 16 15	118, 130, 136, 138	0
27	d5	69/70 (98%)	0.80	9 (13%) 3 3	108, 121, 130, 131	0
28	D6	97/97 (100%)	2.17	42 (43%) 0 0	94, 110, 156, 157	0
28	d6	97/97 (100%)	2.94	72 (74%) 0 0	79, 92, 115, 120	0
29	D7	81/81 (100%)	0.43	5 (6%) 20 19	100, 113, 138, 141	0
29	d7	81/81 (100%)	0.73	12 (14%) 2 2	86, 100, 133, 135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	D8	63/63 (100%)	2.24	28 (44%) 0 0	115, 130, 137, 140	0
30	d8	63/63 (100%)	3.33	47 (74%) 0 0	111, 126, 132, 136	0
31	D9	53/53 (100%)	0.21	2 (3%) 40 37	89, 93, 112, 118	0
31	d9	53/53 (100%)	0.53	4 (7%) 14 13	90, 98, 126, 138	0
32	E0	60/62 (96%)	0.79	12 (20%) 1 1	82, 110, 134, 137	0
32	e0	62/62 (100%)	-0.09	1 (1%) 72 69	73, 97, 118, 122	0
33	E1	71/76 (93%)	1.05	15 (21%) 1 1	111, 138, 149, 152	0
33	e1	76/76 (100%)	1.89	31 (40%) 0 0	115, 163, 180, 182	0
34	SR	318/318 (100%)	1.62	109 (34%) 0 0	110, 122, 134, 155	0
35	SM	133/159 (83%)	1.47	34 (25%) 0 0	70, 100, 131, 138	0
36	1	3149/3394 (92%)	0.21	52 (1%) 70 67	44, 66, 136, 228	0
36	5	3150/3394 (92%)	0.20	39 (1%) 79 77	43, 64, 129, 201	0
37	3	121/121 (100%)	-0.19	0 100 100	52, 83, 98, 103	0
37	7	121/121 (100%)	-0.21	1 (0%) 86 86	48, 67, 79, 86	0
38	4	158/158 (100%)	0.09	2 (1%) 77 75	51, 67, 103, 140	0
38	8	158/158 (100%)	0.06	2 (1%) 77 75	53, 73, 107, 132	0
39	L2	252/252 (100%)	0.67	13 (5%) 27 25	51, 67, 83, 90	0
39	l2	252/252 (100%)	0.32	5 (1%) 65 63	52, 69, 84, 93	0
40	L3	386/386 (100%)	0.29	6 (1%) 72 69	49, 70, 82, 98	0
40	l3	386/386 (100%)	0.16	6 (1%) 72 69	44, 58, 71, 88	0
41	L4	361/361 (100%)	0.12	0 100 100	46, 62, 78, 81	0
41	l4	361/361 (100%)	0.27	10 (2%) 53 50	49, 66, 81, 90	0
42	L5	296/296 (100%)	0.98	54 (18%) 1 1	66, 90, 106, 125	0
42	l5	294/296 (99%)	0.28	6 (2%) 65 63	56, 70, 91, 107	0
43	L6	156/175 (89%)	0.36	1 (0%) 89 89	58, 66, 81, 92	0
43	l6	157/175 (89%)	0.31	3 (1%) 66 64	59, 66, 86, 97	0
44	L7	222/223 (99%)	0.10	2 (0%) 84 84	50, 58, 85, 115	0
44	l7	223/223 (100%)	0.01	0 100 100	49, 58, 91, 116	0
45	L8	233/233 (100%)	0.51	17 (7%) 15 14	74, 88, 117, 122	0
46	L9	191/191 (100%)	0.44	14 (7%) 15 14	68, 78, 88, 98	0
46	l9	191/191 (100%)	0.06	2 (1%) 82 82	54, 63, 79, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	M0	211/220 (95%)	0.09	3 (1%) 75 74	55, 70, 100, 113	0
47	m0	213/220 (96%)	0.28	9 (4%) 36 33	51, 69, 89, 101	0
48	M1	169/169 (100%)	1.12	39 (23%) 0 1	78, 94, 104, 110	0
48	m1	169/169 (100%)	-0.18	0 100 100	61, 76, 85, 88	0
49	M3	193/194 (99%)	0.14	1 (0%) 91 90	49, 71, 105, 128	0
49	m3	194/194 (100%)	0.32	7 (3%) 42 39	52, 78, 112, 125	0
50	M4	136/137 (99%)	0.07	2 (1%) 73 71	62, 69, 79, 88	0
50	m4	137/137 (100%)	0.08	4 (2%) 51 50	57, 64, 81, 88	0
51	M5	203/203 (100%)	0.58	6 (2%) 50 48	50, 63, 74, 77	0
51	m5	203/203 (100%)	1.18	37 (18%) 1 1	54, 71, 82, 87	0
52	M6	197/197 (100%)	0.06	0 100 100	50, 58, 77, 81	0
52	m6	197/197 (100%)	0.02	0 100 100	44, 51, 77, 82	0
53	M7	183/183 (100%)	0.89	23 (12%) 3 3	53, 61, 108, 127	0
53	m7	155/183 (84%)	0.23	1 (0%) 89 89	49, 55, 67, 93	0
54	M8	185/185 (100%)	0.50	7 (3%) 40 37	51, 62, 78, 93	0
54	m8	185/185 (100%)	0.56	6 (3%) 47 45	51, 66, 77, 81	0
55	M9	188/188 (100%)	0.71	14 (7%) 14 14	70, 84, 147, 155	0
55	m9	188/188 (100%)	0.42	5 (2%) 54 51	63, 76, 134, 143	0
56	N0	172/172 (100%)	0.58	13 (7%) 13 12	59, 65, 77, 83	0
56	n0	172/172 (100%)	0.00	1 (0%) 89 89	52, 59, 70, 79	0
57	N1	159/159 (100%)	0.58	6 (3%) 40 37	51, 65, 104, 111	0
57	n1	159/159 (100%)	0.50	6 (3%) 40 37	51, 57, 95, 99	0
58	N2	100/100 (100%)	0.63	12 (12%) 4 4	100, 111, 117, 125	0
58	n2	98/100 (98%)	0.48	7 (7%) 16 15	88, 98, 103, 106	0
59	N3	136/136 (100%)	0.18	3 (2%) 62 59	57, 67, 77, 83	0
59	n3	136/136 (100%)	0.43	3 (2%) 62 59	45, 55, 65, 70	0
60	N4	98/98 (100%)	2.82	34 (34%) 0 0	66, 78, 138, 139	0
61	N5	121/121 (100%)	0.77	12 (9%) 7 7	63, 75, 90, 110	0
61	n5	120/121 (99%)	0.73	14 (11%) 4 4	66, 79, 95, 105	0
62	N6	126/126 (100%)	0.39	4 (3%) 47 45	56, 72, 81, 90	0
62	n6	126/126 (100%)	0.33	0 100 100	60, 76, 88, 93	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
63	N7	135/135 (100%)	0.89	14 (10%) 6 6	88, 100, 110, 115	0
63	n7	135/135 (100%)	0.35	7 (5%) 27 25	93, 104, 116, 122	0
64	N8	148/148 (100%)	0.62	10 (6%) 17 16	44, 64, 84, 94	0
64	n8	148/148 (100%)	0.65	8 (5%) 25 24	44, 67, 84, 87	0
65	N9	58/58 (100%)	0.99	15 (25%) 0 0	48, 70, 103, 114	0
65	n9	58/58 (100%)	0.69	5 (8%) 10 10	48, 67, 86, 92	0
66	O0	97/100 (97%)	0.17	2 (2%) 63 61	87, 95, 113, 117	0
66	o0	100/100 (100%)	0.33	5 (5%) 28 26	84, 95, 111, 117	0
67	O1	109/109 (100%)	1.07	14 (12%) 3 3	67, 79, 99, 105	0
67	o1	109/109 (100%)	0.77	8 (7%) 15 14	57, 69, 96, 109	0
68	O2	127/127 (100%)	0.14	3 (2%) 59 55	46, 58, 72, 82	0
68	o2	127/127 (100%)	0.04	0 100 100	46, 62, 75, 82	0
69	O3	106/106 (100%)	0.27	0 100 100	49, 57, 77, 86	0
69	o3	106/106 (100%)	0.37	1 (0%) 84 84	49, 56, 80, 90	0
70	O4	112/112 (100%)	1.26	27 (24%) 0 0	63, 80, 115, 124	0
70	o4	112/112 (100%)	0.43	6 (5%) 25 24	62, 82, 116, 121	0
71	O5	119/119 (100%)	0.37	4 (3%) 45 42	61, 78, 86, 93	0
71	o5	119/119 (100%)	0.21	1 (0%) 86 86	68, 83, 96, 106	0
72	O6	99/99 (100%)	0.03	2 (2%) 65 63	68, 77, 102, 116	0
72	o6	99/99 (100%)	0.14	3 (3%) 50 48	76, 85, 101, 114	0
73	O7	87/87 (100%)	0.74	7 (8%) 12 11	51, 57, 76, 86	0
73	o7	87/87 (100%)	0.67	2 (2%) 60 58	49, 58, 85, 99	0
74	O8	77/77 (100%)	0.15	1 (1%) 77 75	89, 100, 114, 117	0
74	o8	77/77 (100%)	1.28	15 (19%) 1 1	88, 99, 108, 110	0
75	O9	50/50 (100%)	0.78	4 (8%) 12 11	60, 64, 69, 69	0
75	o9	50/50 (100%)	0.89	6 (12%) 4 4	59, 65, 72, 74	0
76	Q0	52/52 (100%)	0.68	6 (11%) 4 4	62, 67, 82, 91	0
76	q0	52/52 (100%)	-0.06	0 100 100	50, 54, 65, 68	0
77	Q1	25/25 (100%)	0.10	0 100 100	69, 74, 78, 79	0
77	q1	25/25 (100%)	0.03	0 100 100	62, 63, 65, 66	0
78	Q2	105/105 (100%)	1.41	27 (25%) 0 0	54, 67, 86, 109	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
78	q2	105/105 (100%)	1.07	16 (15%) 2 2	55, 66, 80, 100	0
79	Q3	91/91 (100%)	0.38	2 (2%) 62 59	58, 71, 85, 91	0
79	q3	91/91 (100%)	0.23	3 (3%) 46 43	54, 69, 81, 89	0
80	c0	79/96 (82%)	0.52	8 (10%) 7 7	108, 133, 143, 145	0
81	c2	109/124 (87%)	1.77	44 (40%) 0 0	173, 185, 191, 194	0
82	c5	135/142 (95%)	0.41	9 (6%) 17 17	84, 110, 123, 125	0
83	sR	318/318 (100%)	1.63	104 (32%) 0 0	117, 131, 143, 156	0
84	sM	63/104 (60%)	0.85	9 (14%) 2 2	61, 111, 117, 122	0
85	l8	225/231 (97%)	0.94	25 (11%) 5 5	83, 95, 118, 123	0
86	m2	0/150	-	-	-	-
87	n4	135/135 (100%)	1.31	39 (28%) 0 0	54, 97, 121, 135	0
88	p0	120/219 (54%)	1.69	45 (37%) 0 0	103, 120, 135, 142	0
89	p1	0/47	-	-	-	-
89	p2	0/47	-	-	-	-
90	A	2/3 (66%)	1.12	0 100 100	106, 106, 106, 107	0
90	a	2/3 (66%)	1.24	0 100 100	100, 100, 100, 102	0
All	All	32948/34108 (96%)	0.58	3198 (9%) 7 8	43, 82, 136, 228	0

The worst 5 of 3198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	86	SER	26.0
13	c1	3	THR	16.4
60	N4	75	THR	14.6
60	N4	84	GLY	14.3
60	N4	85	ALA	14.2

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

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
90	PPU	A	76	37/38	0.83	0.33	47,88,147,147	0
90	PPU	a	76	37/38	0.85	0.37	44,80,139,139	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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
91	MG	1	3960	1/1	-0.14	1.05	97,97,97,97	0
91	MG	5	3863	1/1	-0.01	1.00	53,53,53,53	1
91	MG	c6	202	1/1	0.03	0.45	110,110,110,110	0
91	MG	2	1966	1/1	0.13	0.45	100,100,100,100	0
91	MG	1	3936	1/1	0.15	0.28	192,192,192,192	0
91	MG	2	1976	1/1	0.15	0.26	101,101,101,101	0
91	MG	2	1967	1/1	0.15	0.32	103,103,103,103	0
91	MG	5	4093	1/1	0.19	0.50	76,76,76,76	1
91	MG	1	3685	1/1	0.20	0.40	58,58,58,58	1
91	MG	1	4066	1/1	0.21	0.34	93,93,93,93	0
91	MG	2	2038	1/1	0.22	0.46	134,134,134,134	0
91	MG	1	4082	1/1	0.29	0.95	64,64,64,64	1
91	MG	2	2053	1/1	0.30	1.36	85,85,85,85	1
91	MG	1	3838	1/1	0.30	0.43	69,69,69,69	0
91	MG	5	3961	1/1	0.31	0.34	94,94,94,94	0
91	MG	1	3712	1/1	0.32	0.55	79,79,79,79	0
91	MG	2	2057	1/1	0.33	0.54	113,113,113,113	0
91	MG	5	3745	1/1	0.33	0.26	95,95,95,95	0
91	MG	5	3957	1/1	0.34	0.29	88,88,88,88	0
91	MG	1	3906	1/1	0.35	0.23	119,119,119,119	0
91	MG	2	2009	1/1	0.36	0.73	71,71,71,71	0
91	MG	d5	201	1/1	0.36	0.22	106,106,106,106	0
91	MG	2	1983	1/1	0.37	0.36	102,102,102,102	0
91	MG	5	4063	1/1	0.39	0.53	49,49,49,49	1
91	MG	1	3954	1/1	0.40	0.63	52,52,52,52	1
91	MG	2	2063	1/1	0.40	0.38	95,95,95,95	0
91	MG	2	2055	1/1	0.40	0.74	123,123,123,123	0
91	MG	7	209	1/1	0.40	0.58	58,58,58,58	0
91	MG	6	2133	1/1	0.41	0.25	96,96,96,96	0
91	MG	c6	201	1/1	0.41	0.42	114,114,114,114	0
91	MG	5	4069	1/1	0.41	0.34	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	6	2083	1/1	0.42	0.41	98,98,98,98	0
91	MG	1	3734	1/1	0.42	0.51	63,63,63,63	1
91	MG	1	4076	1/1	0.42	0.71	55,55,55,55	1
91	MG	5	3948	1/1	0.43	0.89	57,57,57,57	1
91	MG	5	3832	1/1	0.43	0.73	64,64,64,64	0
91	MG	2	2052	1/1	0.43	0.28	88,88,88,88	1
91	MG	6	2111	1/1	0.43	0.76	115,115,115,115	0
91	MG	1	4014	1/1	0.44	0.22	83,83,83,83	1
91	MG	5	3931	1/1	0.44	0.45	55,55,55,55	1
91	MG	2	2016	1/1	0.44	0.48	86,86,86,86	0
91	MG	6	1992	1/1	0.44	0.39	106,106,106,106	0
91	MG	1	3736	1/1	0.46	0.34	88,88,88,88	0
91	MG	O2	202	1/1	0.46	0.59	47,47,47,47	1
91	MG	5	4138	1/1	0.46	0.41	98,98,98,98	0
91	MG	5	3904	1/1	0.47	0.75	72,72,72,72	1
91	MG	5	3688	1/1	0.47	0.41	66,66,66,66	0
91	MG	5	4007	1/1	0.48	0.70	77,77,77,77	0
91	MG	1	3844	1/1	0.49	0.63	91,91,91,91	0
91	MG	5	3747	1/1	0.50	0.66	59,59,59,59	1
91	MG	1	3830	1/1	0.50	0.30	85,85,85,85	0
91	MG	5	3767	1/1	0.50	0.70	142,142,142,142	0
91	MG	s8	303	1/1	0.50	0.92	75,75,75,75	0
91	MG	6	2045	1/1	0.51	0.21	91,91,91,91	0
91	MG	q1	101	1/1	0.51	0.72	63,63,63,63	0
91	MG	6	1919	1/1	0.51	0.33	79,79,79,79	0
91	MG	1	3484	1/1	0.52	0.50	60,60,60,60	1
91	MG	2	1972	1/1	0.52	0.59	93,93,93,93	0
91	MG	1	3881	1/1	0.52	0.28	75,75,75,75	0
91	MG	2	1927	1/1	0.52	0.50	89,89,89,89	0
91	MG	6	1972	1/1	0.52	1.02	73,73,73,73	0
91	MG	1	3872	1/1	0.52	0.66	72,72,72,72	0
91	MG	1	3760	1/1	0.52	0.47	54,54,54,54	1
91	MG	1	3768	1/1	0.52	1.08	68,68,68,68	1
91	MG	2	1912	1/1	0.53	0.41	95,95,95,95	0
91	MG	5	4120	1/1	0.53	0.79	52,52,52,52	1
91	MG	1	3922	1/1	0.53	0.94	58,58,58,58	0
91	MG	5	3970	1/1	0.53	0.56	52,52,52,52	1
91	MG	s8	304	1/1	0.54	0.32	74,74,74,74	0
91	MG	1	3749	1/1	0.54	0.47	79,79,79,79	0
91	MG	5	4054	1/1	0.54	0.49	71,71,71,71	0
91	MG	5	4106	1/1	0.54	0.52	49,49,49,49	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	1	3772	1/1	0.55	0.56	59,59,59,59	1
91	MG	6	1932	1/1	0.56	0.36	78,78,78,78	0
91	MG	o3	205	1/1	0.56	0.67	51,51,51,51	1
91	MG	6	1915	1/1	0.57	0.51	86,86,86,86	0
91	MG	5	4105	1/1	0.57	0.49	94,94,94,94	0
91	MG	2	1945	1/1	0.57	0.68	88,88,88,88	0
91	MG	L3	401	1/1	0.57	0.56	56,56,56,56	1
91	MG	1	3660	1/1	0.57	0.26	65,65,65,65	0
91	MG	2	1958	1/1	0.57	0.51	133,133,133,133	0
91	MG	1	3787	1/1	0.57	0.20	90,90,90,90	0
91	MG	2	2064	1/1	0.57	0.38	76,76,76,76	0
91	MG	5	3898	1/1	0.57	0.47	93,93,93,93	1
92	OHX	1	4429	7/7	0.58	0.70	66,66,66,66	7
91	MG	6	1999	1/1	0.58	0.21	108,108,108,108	0
91	MG	6	2077	1/1	0.58	0.33	111,111,111,111	0
91	MG	1	4092	1/1	0.58	0.21	105,105,105,105	0
91	MG	5	4140	1/1	0.58	0.48	50,50,50,50	1
91	MG	2	1947	1/1	0.58	0.49	80,80,80,80	0
91	MG	5	3914	1/1	0.59	0.10	121,121,121,121	0
91	MG	l3	404	1/1	0.59	0.98	48,48,48,48	1
91	MG	5	3409	1/1	0.60	0.22	62,62,62,62	0
91	MG	L8	301	1/1	0.60	0.38	83,83,83,83	0
91	MG	1	3668	1/1	0.60	0.53	61,61,61,61	0
91	MG	1	3930	1/1	0.60	0.41	79,79,79,79	0
91	MG	1	3421	1/1	0.60	0.57	88,88,88,88	0
91	MG	M0	301	1/1	0.60	0.24	70,70,70,70	0
91	MG	2	2029	1/1	0.60	0.57	74,74,74,74	0
91	MG	2	2002	1/1	0.60	0.50	85,85,85,85	0
91	MG	6	2086	1/1	0.61	0.52	93,93,93,93	0
91	MG	5	4033	1/1	0.61	0.84	53,53,53,53	1
91	MG	2	2021	1/1	0.61	0.24	91,91,91,91	0
91	MG	2	1955	1/1	0.61	0.61	103,103,103,103	0
91	MG	6	1997	1/1	0.61	0.58	62,62,62,62	1
91	MG	1	3497	1/1	0.61	0.35	63,63,63,63	0
91	MG	1	4051	1/1	0.61	0.59	127,127,127,127	0
91	MG	6	2341	1/1	0.61	0.50	77,77,77,77	0
92	OHX	1	4423	7/7	0.61	0.56	58,58,58,58	7
91	MG	6	2065	1/1	0.61	0.66	60,60,60,60	0
91	MG	2	2004	1/1	0.61	0.31	91,91,91,91	0
91	MG	5	4102	1/1	0.61	0.41	69,69,69,69	0
91	MG	5	3846	1/1	0.62	0.79	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	1	3665	1/1	0.62	0.78	67,67,67,67	0
91	MG	1	3845	1/1	0.62	0.24	73,73,73,73	0
91	MG	1	3961	1/1	0.62	0.25	82,82,82,82	0
91	MG	6	2049	1/1	0.62	0.25	71,71,71,71	0
91	MG	6	2089	1/1	0.62	0.26	77,77,77,77	1
92	OHX	6	2336	7/7	0.62	0.45	94,94,94,94	7
91	MG	6	2087	1/1	0.62	0.55	132,132,132,132	0
91	MG	6	2140	1/1	0.62	0.52	74,74,74,74	0
91	MG	1	3569	1/1	0.63	0.64	68,68,68,68	0
91	MG	5	3823	1/1	0.63	0.48	74,74,74,74	1
91	MG	4	226	1/1	0.63	0.30	66,66,66,66	0
91	MG	2	2007	1/1	0.63	1.44	79,79,79,79	1
91	MG	1	4084	1/1	0.63	0.40	73,73,73,73	0
91	MG	1	3575	1/1	0.63	0.60	50,50,50,50	0
91	MG	5	3819	1/1	0.63	0.56	47,47,47,47	1
91	MG	1	3784	1/1	0.63	0.19	69,69,69,69	0
91	MG	1	3427	1/1	0.64	0.36	55,55,55,55	0
91	MG	n0	205	1/1	0.64	0.30	60,60,60,60	0
91	MG	1	3480	1/1	0.64	0.58	57,57,57,57	0
91	MG	5	3676	1/1	0.64	0.67	86,86,86,86	0
91	MG	1	3766	1/1	0.64	0.48	77,77,77,77	0
91	MG	1	4063	1/1	0.64	0.80	61,61,61,61	0
91	MG	1	4021	1/1	0.64	0.75	62,62,62,62	1
91	MG	1	3788	1/1	0.64	0.65	62,62,62,62	1
91	MG	O4	201	1/1	0.64	0.16	83,83,83,83	0
91	MG	1	3916	1/1	0.64	0.17	89,89,89,89	0
91	MG	p0	301	1/1	0.64	0.12	105,105,105,105	0
91	MG	3	209	1/1	0.64	0.13	85,85,85,85	0
91	MG	O3	202	1/1	0.65	0.79	52,52,52,52	1
91	MG	6	2068	1/1	0.65	0.55	125,125,125,125	0
91	MG	1	3998	1/1	0.65	1.58	53,53,53,53	1
91	MG	M4	201	1/1	0.65	0.35	66,66,66,66	0
91	MG	5	3974	1/1	0.65	0.35	66,66,66,66	0
93	ZN	d7	101	1/1	0.65	0.36	154,154,154,154	0
91	MG	5	3532	1/1	0.65	0.73	47,47,47,47	0
91	MG	5	3656	1/1	0.65	0.30	52,52,52,52	0
91	MG	6	2119	1/1	0.65	0.65	88,88,88,88	1
91	MG	5	3798	1/1	0.65	0.67	78,78,78,78	0
91	MG	5	3788	1/1	0.65	0.54	49,49,49,49	0
91	MG	5	3492	1/1	0.65	0.27	67,67,67,67	0
91	MG	6	2050	1/1	0.66	0.32	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	4	229	1/1	0.66	1.36	68,68,68,68	1
91	MG	5	4004	1/1	0.66	0.43	69,69,69,69	0
91	MG	M5	308	1/1	0.66	0.85	69,69,69,69	1
91	MG	5	3941	1/1	0.66	0.29	86,86,86,86	0
91	MG	5	3810	1/1	0.66	0.37	68,68,68,68	1
91	MG	6	2088	1/1	0.66	0.91	87,87,87,87	0
91	MG	1	3895	1/1	0.66	1.32	66,66,66,66	1
91	MG	1	4083	1/1	0.66	0.70	53,53,53,53	0
91	MG	o3	203	1/1	0.66	0.43	67,67,67,67	0
92	OHX	6	2305	7/7	0.66	0.63	83,83,83,83	7
91	MG	1	3776	1/1	0.66	0.49	83,83,83,83	0
91	MG	6	2139	1/1	0.66	0.58	212,212,212,212	0
91	MG	5	4155	1/1	0.66	0.93	57,57,57,57	1
91	MG	5	3840	1/1	0.67	0.44	69,69,69,69	1
92	OHX	5	4458	7/7	0.67	0.30	51,51,51,51	7
91	MG	5	4068	1/1	0.67	0.47	58,58,58,58	0
92	OHX	6	2328	7/7	0.67	0.50	85,85,85,85	7
91	MG	18	301	1/1	0.67	0.60	87,87,87,87	0
91	MG	5	3440	1/1	0.67	0.52	63,63,63,63	0
91	MG	5	3768	1/1	0.67	0.71	79,79,79,79	0
91	MG	5	3989	1/1	0.67	0.46	68,68,68,68	1
91	MG	1	3651	1/1	0.67	0.40	63,63,63,63	0
91	MG	5	3966	1/1	0.67	0.49	51,51,51,51	1
91	MG	2	2030	1/1	0.67	0.38	95,95,95,95	1
91	MG	M7	208	1/1	0.67	0.26	86,86,86,86	0
91	MG	6	1939	1/1	0.67	0.14	100,100,100,100	0
91	MG	6	2112	1/1	0.67	0.28	96,96,96,96	0
91	MG	7	208	1/1	0.67	0.29	71,71,71,71	0
91	MG	1	3785	1/1	0.67	0.77	52,52,52,52	0
91	MG	1	3850	1/1	0.68	0.58	59,59,59,59	1
91	MG	1	4077	1/1	0.68	0.48	83,83,83,83	1
92	OHX	5	4513	7/7	0.68	0.62	72,72,72,72	7
91	MG	5	3804	1/1	0.68	0.71	70,70,70,70	0
91	MG	5	3999	1/1	0.68	0.34	76,76,76,76	0
91	MG	1	3827	1/1	0.68	0.30	69,69,69,69	0
91	MG	1	4049	1/1	0.68	0.30	67,67,67,67	0
91	MG	2	2035	1/1	0.68	0.50	78,78,78,78	0
91	MG	5	3926	1/1	0.68	0.30	82,82,82,82	1
91	MG	5	3744	1/1	0.68	0.43	76,76,76,76	0
91	MG	5	4030	1/1	0.68	0.50	67,67,67,67	0
91	MG	1	3721	1/1	0.68	1.18	65,65,65,65	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	1	3503	1/1	0.68	0.43	86,86,86,86	0
91	MG	2	1960	1/1	0.68	0.36	84,84,84,84	0
92	OHX	5	4524	7/7	0.69	0.33	154,154,154,154	7
91	MG	M5	306	1/1	0.69	0.80	52,52,52,52	1
91	MG	5	3971	1/1	0.69	0.51	65,65,65,65	0
91	MG	6	2131	1/1	0.69	0.60	64,64,64,64	1
92	OHX	6	2330	7/7	0.69	0.35	93,93,93,93	7
91	MG	1	4025	1/1	0.69	0.11	204,204,204,204	0
91	MG	1	4098	1/1	0.69	0.43	54,54,54,54	1
91	MG	1	4069	1/1	0.69	0.55	61,61,61,61	1
91	MG	8	202	1/1	0.69	0.27	56,56,56,56	0
91	MG	5	3802	1/1	0.69	0.16	71,71,71,71	0
91	MG	2	1962	1/1	0.69	0.36	100,100,100,100	0
91	MG	6	2037	1/1	0.69	0.32	98,98,98,98	0
91	MG	5	3678	1/1	0.69	0.66	49,49,49,49	0
91	MG	1	3512	1/1	0.69	0.51	61,61,61,61	0
91	MG	3	214	1/1	0.69	0.28	80,80,80,80	0
91	MG	5	4097	1/1	0.69	0.82	54,54,54,54	1
91	MG	6	2069	1/1	0.69	0.78	59,59,59,59	0
91	MG	5	4000	1/1	0.69	0.33	51,51,51,51	1
91	MG	5	3909	1/1	0.70	0.66	91,91,91,91	0
91	MG	1	3568	1/1	0.70	0.20	71,71,71,71	0
92	OHX	1	4434	7/7	0.70	0.41	84,84,84,84	7
91	MG	1	3978	1/1	0.70	0.84	50,50,50,50	1
91	MG	1	3723	1/1	0.70	0.69	64,64,64,64	0
91	MG	5	3703	1/1	0.70	0.68	63,63,63,63	0
91	MG	6	1940	1/1	0.70	0.27	85,85,85,85	0
91	MG	1	3993	1/1	0.70	0.84	62,62,62,62	1
91	MG	6	2074	1/1	0.70	0.33	98,98,98,98	0
91	MG	1	3748	1/1	0.70	0.47	57,57,57,57	0
91	MG	5	4112	1/1	0.70	0.29	59,59,59,59	1
91	MG	1	3823	1/1	0.70	0.40	60,60,60,60	0
91	MG	1	3808	1/1	0.70	0.40	59,59,59,59	0
91	MG	2	1926	1/1	0.71	0.30	101,101,101,101	0
91	MG	1	3700	1/1	0.71	0.23	81,81,81,81	0
91	MG	s8	301	1/1	0.71	0.39	68,68,68,68	0
91	MG	C5	201	1/1	0.71	0.46	91,91,91,91	0
91	MG	6	2036	1/1	0.71	0.47	97,97,97,97	0
91	MG	1	3640	1/1	0.71	0.51	107,107,107,107	0
91	MG	1	4073	1/1	0.71	0.22	68,68,68,68	0
91	MG	5	3891	1/1	0.71	0.62	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	7	222	1/1	0.71	0.54	63,63,63,63	0
91	MG	5	3900	1/1	0.71	0.15	83,83,83,83	0
92	OHX	8	237	7/7	0.71	0.32	102,102,102,102	7
91	MG	6	2043	1/1	0.71	0.66	83,83,83,83	0
91	MG	5	3795	1/1	0.71	0.31	68,68,68,68	0
91	MG	n6	201	1/1	0.71	0.30	72,72,72,72	0
92	OHX	2	2220	7/7	0.71	0.15	190,190,190,190	7
92	OHX	5	3401	7/7	0.71	0.30	170,170,170,170	7
91	MG	m6	204	1/1	0.71	0.41	55,55,55,55	1
92	OHX	1	4450	7/7	0.71	0.47	130,130,130,130	7
91	MG	1	4029	1/1	0.71	0.59	54,54,54,54	1
91	MG	1	3868	1/1	0.71	0.56	51,51,51,51	0
91	MG	2	1944	1/1	0.71	0.22	87,87,87,87	0
91	MG	2	2033	1/1	0.71	0.27	71,71,71,71	1
91	MG	5	3792	1/1	0.71	0.38	54,54,54,54	0
91	MG	2	2037	1/1	0.72	0.22	98,98,98,98	0
91	MG	1	3767	1/1	0.72	0.31	90,90,90,90	0
91	MG	1	3943	1/1	0.72	0.67	86,86,86,86	0
91	MG	1	3644	1/1	0.72	0.68	57,57,57,57	0
92	OHX	1	4421	7/7	0.72	0.26	106,106,106,106	7
91	MG	5	4151	1/1	0.72	0.46	68,68,68,68	0
91	MG	6	2026	1/1	0.72	0.52	70,70,70,70	0
91	MG	1	3670	1/1	0.72	0.38	71,71,71,71	1
91	MG	5	3829	1/1	0.72	0.39	75,75,75,75	0
91	MG	6	2039	1/1	0.72	0.30	100,100,100,100	0
91	MG	1	3797	1/1	0.72	0.34	81,81,81,81	1
92	OHX	6	2314	7/7	0.72	0.50	84,84,84,84	7
91	MG	5	4100	1/1	0.72	0.65	46,46,46,46	1
91	MG	S4	301	1/1	0.72	0.77	94,94,94,94	0
91	MG	1	3487	1/1	0.72	0.23	110,110,110,110	0
91	MG	5	3412	1/1	0.72	0.35	68,68,68,68	0
91	MG	1	3869	1/1	0.72	0.61	58,58,58,58	0
91	MG	5	3784	1/1	0.72	0.46	71,71,71,71	0
92	OHX	2	2253	7/7	0.72	0.39	113,113,113,113	7
91	MG	1	3634	1/1	0.72	0.21	86,86,86,86	0
91	MG	5	3803	1/1	0.72	0.43	64,64,64,64	0
91	MG	6	1930	1/1	0.72	0.28	94,94,94,94	0
91	MG	1	3656	1/1	0.72	0.16	75,75,75,75	0
91	MG	1	3933	1/1	0.72	0.30	56,56,56,56	1
91	MG	6	1995	1/1	0.72	0.48	68,68,68,68	0
91	MG	5	3899	1/1	0.72	0.22	117,117,117,117	0
92	OHX	5	4505	7/7	0.73	0.36	54,54,54,54	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	1	3910	1/1	0.73	0.33	77,77,77,77	0
91	MG	5	3668	1/1	0.73	0.45	52,52,52,52	0
91	MG	1	3792	1/1	0.73	0.35	70,70,70,70	0
91	MG	5	3969	1/1	0.73	0.48	79,79,79,79	0
91	MG	E1	502	1/1	0.73	0.22	137,137,137,137	0
91	MG	4	227	1/1	0.73	0.49	48,48,48,48	0
91	MG	6	2058	1/1	0.73	0.58	64,64,64,64	0
92	OHX	2	2228	7/7	0.73	0.37	110,110,110,110	7
91	MG	1	3966	1/1	0.73	0.77	56,56,56,56	1
91	MG	5	3507	1/1	0.73	0.39	78,78,78,78	0
91	MG	5	3944	1/1	0.73	0.59	53,53,53,53	0
91	MG	D3	201	1/1	0.73	0.52	75,75,75,75	0
91	MG	5	3842	1/1	0.73	0.64	59,59,59,59	1
91	MG	5	3645	1/1	0.73	0.34	51,51,51,51	0
91	MG	2	2059	1/1	0.73	0.41	75,75,75,75	0
91	MG	5	4003	1/1	0.73	0.49	53,53,53,53	0
91	MG	5	3861	1/1	0.73	0.55	52,52,52,52	1
91	MG	1	3857	1/1	0.74	0.47	60,60,60,60	0
91	MG	1	3629	1/1	0.74	0.38	72,72,72,72	0
92	OHX	2	2246	7/7	0.74	0.47	116,116,116,116	7
91	MG	6	2096	1/1	0.74	0.43	65,65,65,65	0
91	MG	1	3719	1/1	0.74	0.52	59,59,59,59	0
92	OHX	3	231	7/7	0.74	0.39	94,94,94,94	7
91	MG	1	3947	1/1	0.74	0.46	52,52,52,52	0
91	MG	1	4080	1/1	0.74	0.27	81,81,81,81	0
91	MG	5	4062	1/1	0.74	0.63	56,56,56,56	1
91	MG	1	3479	1/1	0.74	0.33	58,58,58,58	0
91	MG	15	304	1/1	0.74	0.25	77,77,77,77	0
91	MG	5	3567	1/1	0.74	0.57	55,55,55,55	0
91	MG	1	3693	1/1	0.74	0.47	68,68,68,68	0
91	MG	5	3964	1/1	0.74	0.65	46,46,46,46	1
91	MG	6	2114	1/1	0.74	1.14	69,69,69,69	1
91	MG	2	1904	1/1	0.74	0.39	87,87,87,87	0
91	MG	5	3965	1/1	0.74	0.48	46,46,46,46	1
91	MG	19	202	1/1	0.74	0.45	61,61,61,61	1
91	MG	5	3764	1/1	0.74	0.32	66,66,66,66	0
91	MG	1	4095	1/1	0.74	0.33	101,101,101,101	1
91	MG	1	4008	1/1	0.74	0.60	54,54,54,54	1
91	MG	2	1992	1/1	0.74	0.43	74,74,74,74	0
91	MG	6	2115	1/1	0.74	0.34	73,73,73,73	0
92	OHX	5	4534	7/7	0.74	0.61	72,72,72,72	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	5	4541	7/7	0.74	0.61	54,54,54,54	7
91	MG	5	4099	1/1	0.74	0.35	86,86,86,86	0
91	MG	6	2062	1/1	0.74	0.30	92,92,92,92	1
91	MG	1	4088	1/1	0.75	0.42	60,60,60,60	0
92	OHX	5	4495	7/7	0.75	0.69	51,51,51,51	7
91	MG	6	2126	1/1	0.75	0.36	84,84,84,84	0
91	MG	5	3690	1/1	0.75	0.77	56,56,56,56	0
91	MG	1	4071	1/1	0.75	0.28	63,63,63,63	0
91	MG	1	3623	1/1	0.75	0.30	58,58,58,58	0
91	MG	1	3939	1/1	0.75	0.76	60,60,60,60	1
92	OHX	5	4528	7/7	0.75	0.47	51,51,51,51	7
91	MG	1	3981	1/1	0.75	0.74	55,55,55,55	1
91	MG	6	1909	1/1	0.75	0.43	61,61,61,61	0
91	MG	o3	204	1/1	0.75	0.76	51,51,51,51	1
91	MG	5	3806	1/1	0.75	0.44	78,78,78,78	0
92	OHX	2	2238	7/7	0.75	0.30	107,107,107,107	7
91	MG	1	3671	1/1	0.75	0.70	112,112,112,112	0
91	MG	1	3853	1/1	0.75	0.33	56,56,56,56	0
91	MG	1	3710	1/1	0.75	0.47	59,59,59,59	0
91	MG	5	4088	1/1	0.75	0.50	44,44,44,44	1
91	MG	1	3864	1/1	0.75	0.35	53,53,53,53	0
91	MG	5	3650	1/1	0.75	0.41	61,61,61,61	1
91	MG	5	4154	1/1	0.75	0.63	61,61,61,61	1
92	OHX	6	2322	7/7	0.75	0.41	107,107,107,107	7
91	MG	5	3917	1/1	0.75	0.46	50,50,50,50	0
92	OHX	5	4521	7/7	0.75	0.31	104,104,104,104	7
91	MG	1	4044	1/1	0.75	0.56	56,56,56,56	0
91	MG	d2	201	1/1	0.75	0.41	67,67,67,67	0
91	MG	5	4142	1/1	0.75	0.52	51,51,51,51	1
91	MG	5	3664	1/1	0.76	0.61	54,54,54,54	1
91	MG	5	3643	1/1	0.76	0.38	49,49,49,49	0
92	OHX	2	2231	7/7	0.76	0.96	95,95,95,95	7
91	MG	5	3892	1/1	0.76	0.29	61,61,61,61	0
91	MG	5	4078	1/1	0.76	0.36	75,75,75,75	0
91	MG	5	3875	1/1	0.76	0.75	51,51,51,51	1
91	MG	6	2017	1/1	0.76	0.24	66,66,66,66	0
91	MG	1	3735	1/1	0.76	0.29	73,73,73,73	0
91	MG	8	206	1/1	0.76	0.31	63,63,63,63	0
91	MG	2	1993	1/1	0.76	0.48	87,87,87,87	0
91	MG	1	3980	1/1	0.76	0.27	65,65,65,65	0
91	MG	1	3893	1/1	0.76	0.32	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	4061	1/1	0.76	0.43	56,56,56,56	1
91	MG	3	211	1/1	0.76	0.13	80,80,80,80	0
91	MG	1	3846	1/1	0.76	0.35	51,51,51,51	0
91	MG	5	3476	1/1	0.76	0.68	53,53,53,53	0
91	MG	7	219	1/1	0.76	0.29	56,56,56,56	1
91	MG	2	1985	1/1	0.76	0.35	83,83,83,83	0
91	MG	5	3809	1/1	0.76	0.66	56,56,56,56	1
91	MG	6	2110	1/1	0.76	0.77	71,71,71,71	1
92	OHX	5	4562	7/7	0.76	0.92	68,68,68,68	7
92	OHX	5	4549	7/7	0.76	0.53	85,85,85,85	7
91	MG	1	4012	1/1	0.76	0.77	80,80,80,80	0
91	MG	6	2120	1/1	0.76	0.36	74,74,74,74	0
91	MG	1	3937	1/1	0.76	0.25	83,83,83,83	0
91	MG	S8	302	1/1	0.76	0.36	75,75,75,75	0
91	MG	6	2035	1/1	0.77	0.24	68,68,68,68	0
91	MG	5	3771	1/1	0.77	0.38	60,60,60,60	1
91	MG	1	3903	1/1	0.77	1.13	48,48,48,48	1
91	MG	1	3647	1/1	0.77	0.37	50,50,50,50	0
91	MG	1	3810	1/1	0.77	0.25	85,85,85,85	1
91	MG	1	3637	1/1	0.77	0.52	59,59,59,59	0
91	MG	5	3635	1/1	0.77	0.80	54,54,54,54	0
91	MG	2	1957	1/1	0.77	0.20	110,110,110,110	0
91	MG	6	2063	1/1	0.77	0.29	69,69,69,69	0
91	MG	5	3932	1/1	0.77	0.41	59,59,59,59	1
91	MG	1	3794	1/1	0.77	0.35	64,64,64,64	0
91	MG	1	3866	1/1	0.77	0.27	73,73,73,73	0
91	MG	2	1959	1/1	0.77	0.24	106,106,106,106	0
91	MG	6	2025	1/1	0.77	0.17	97,97,97,97	0
91	MG	7	225	1/1	0.77	0.49	63,63,63,63	1
91	MG	6	2001	1/1	0.77	0.74	90,90,90,90	0
91	MG	6	1971	1/1	0.77	0.26	101,101,101,101	0
91	MG	1	3860	1/1	0.77	0.90	55,55,55,55	1
91	MG	6	1974	1/1	0.77	0.43	91,91,91,91	0
91	MG	5	3724	1/1	0.77	0.36	49,49,49,49	1
91	MG	6	2003	1/1	0.77	0.67	97,97,97,97	0
91	MG	7	211	1/1	0.78	0.18	62,62,62,62	0
91	MG	6	2007	1/1	0.78	0.19	100,100,100,100	0
91	MG	5	3452	1/1	0.78	0.69	52,52,52,52	0
91	MG	6	1955	1/1	0.78	0.28	63,63,63,63	0
91	MG	5	4073	1/1	0.78	0.39	81,81,81,81	0
91	MG	1	3917	1/1	0.78	0.30	68,68,68,68	0
91	MG	5	3760	1/1	0.78	0.40	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	1	3716	1/1	0.78	0.32	52,52,52,52	1
91	MG	5	3881	1/1	0.78	0.81	61,61,61,61	0
92	OHX	1	4485	7/7	0.78	0.46	88,88,88,88	7
91	MG	2	1998	1/1	0.78	0.22	87,87,87,87	0
91	MG	6	2066	1/1	0.78	0.35	76,76,76,76	0
91	MG	5	3982	1/1	0.78	0.41	64,64,64,64	0
91	MG	6	2057	1/1	0.78	0.52	66,66,66,66	0
91	MG	1	3894	1/1	0.78	0.21	135,135,135,135	0
91	MG	4	225	1/1	0.78	0.31	69,69,69,69	0
91	MG	1	3499	1/1	0.78	0.31	62,62,62,62	0
91	MG	2	1978	1/1	0.78	0.34	101,101,101,101	0
91	MG	1	3686	1/1	0.78	0.15	68,68,68,68	0
91	MG	6	2027	1/1	0.78	0.87	68,68,68,68	0
91	MG	1	3791	1/1	0.78	0.84	55,55,55,55	1
91	MG	M7	205	1/1	0.78	0.40	56,56,56,56	0
91	MG	1	3741	1/1	0.78	0.54	69,69,69,69	0
91	MG	1	3648	1/1	0.78	0.44	47,47,47,47	1
91	MG	1	3733	1/1	0.78	0.27	64,64,64,64	0
91	MG	1	3892	1/1	0.78	0.25	75,75,75,75	0
91	MG	O2	201	1/1	0.78	1.14	60,60,60,60	1
91	MG	1	3975	1/1	0.78	0.70	50,50,50,50	1
91	MG	5	3752	1/1	0.78	0.54	57,57,57,57	0
91	MG	6	2121	1/1	0.79	0.32	71,71,71,71	0
91	MG	5	3958	1/1	0.79	0.40	50,50,50,50	1
91	MG	2	1923	1/1	0.79	0.32	79,79,79,79	0
92	OHX	1	4448	7/7	0.79	0.35	60,60,60,60	7
91	MG	5	3730	1/1	0.79	0.48	60,60,60,60	0
91	MG	5	3936	1/1	0.79	0.60	75,75,75,75	0
91	MG	2	1918	1/1	0.79	0.67	78,78,78,78	0
91	MG	c6	203	1/1	0.79	0.42	108,108,108,108	0
91	MG	1	3745	1/1	0.79	0.30	59,59,59,59	0
92	OHX	2	2247	7/7	0.79	0.40	80,80,80,80	7
91	MG	5	3468	1/1	0.79	0.40	67,67,67,67	0
91	MG	6	2137	1/1	0.79	0.87	71,71,71,71	1
91	MG	l5	306	1/1	0.79	0.75	64,64,64,64	0
91	MG	5	4035	1/1	0.79	0.30	62,62,62,62	0
93	ZN	D7	101	1/1	0.79	0.39	159,159,159,159	0
91	MG	L4	406	1/1	0.79	1.65	54,54,54,54	1
91	MG	5	3953	1/1	0.79	0.40	52,52,52,52	1
91	MG	m1	201	1/1	0.79	0.38	80,80,80,80	0
91	MG	1	3889	1/1	0.79	0.42	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	12	304	1/1	0.79	0.68	68,68,68,68	0
91	MG	3	217	1/1	0.79	0.49	64,64,64,64	1
91	MG	1	3935	1/1	0.79	0.36	56,56,56,56	1
91	MG	5	4119	1/1	0.79	0.26	58,58,58,58	0
91	MG	5	3992	1/1	0.79	0.86	70,70,70,70	1
92	OHX	1	4387	7/7	0.79	0.20	218,218,218,218	7
91	MG	5	3653	1/1	0.79	0.84	65,65,65,65	0
91	MG	6	2052	1/1	0.79	0.28	66,66,66,66	1
91	MG	1	4027	1/1	0.79	0.22	57,57,57,57	1
92	OHX	2	2197	7/7	0.79	0.45	105,105,105,105	7
92	OHX	1	4464	7/7	0.80	0.51	86,86,86,86	7
92	OHX	6	2291	7/7	0.80	0.29	109,109,109,109	7
92	OHX	5	4469	7/7	0.80	0.38	88,88,88,88	7
91	MG	5	3472	1/1	0.80	0.12	123,123,123,123	0
91	MG	5	3648	1/1	0.80	0.52	66,66,66,66	0
91	MG	1	3673	1/1	0.80	0.28	59,59,59,59	0
91	MG	1	3842	1/1	0.80	0.24	74,74,74,74	0
91	MG	5	3669	1/1	0.80	0.45	56,56,56,56	1
91	MG	2	1949	1/1	0.80	0.30	87,87,87,87	0
91	MG	1	3949	1/1	0.80	0.54	66,66,66,66	1
91	MG	1	3986	1/1	0.80	0.67	66,66,66,66	0
91	MG	M5	307	1/1	0.80	0.88	77,77,77,77	0
91	MG	5	3506	1/1	0.80	0.36	56,56,56,56	0
91	MG	5	3705	1/1	0.80	0.28	79,79,79,79	0
91	MG	5	3564	1/1	0.80	0.35	61,61,61,61	0
91	MG	1	3786	1/1	0.80	0.31	59,59,59,59	0
91	MG	1	3715	1/1	0.80	0.45	58,58,58,58	0
91	MG	1	3474	1/1	0.80	0.32	49,49,49,49	0
91	MG	1	3953	1/1	0.80	0.80	77,77,77,77	0
91	MG	6	1984	1/1	0.80	1.10	73,73,73,73	1
91	MG	1	3940	1/1	0.80	0.40	67,67,67,67	0
91	MG	6	2125	1/1	0.80	0.31	79,79,79,79	0
91	MG	3	212	1/1	0.80	0.44	59,59,59,59	0
91	MG	8	218	1/1	0.80	0.36	79,79,79,79	0
91	MG	s8	302	1/1	0.80	0.41	59,59,59,59	0
91	MG	5	3681	1/1	0.80	0.52	54,54,54,54	0
91	MG	1	3444	1/1	0.80	0.47	75,75,75,75	0
91	MG	2	2025	1/1	0.80	0.47	79,79,79,79	0
91	MG	6	2010	1/1	0.80	0.15	84,84,84,84	0
91	MG	6	2053	1/1	0.80	0.33	74,74,74,74	0
91	MG	5	4071	1/1	0.80	0.30	52,52,52,52	1
91	MG	5	3502	1/1	0.80	0.23	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3779	1/1	0.80	0.43	53,53,53,53	0
92	OHX	N8	208	7/7	0.80	0.31	112,112,112,112	7
91	MG	D9	101	1/1	0.80	0.21	90,90,90,90	0
91	MG	5	4090	1/1	0.80	0.22	106,106,106,106	0
92	OHX	1	4477	7/7	0.80	0.42	75,75,75,75	7
92	OHX	1	4455	7/7	0.80	0.35	69,69,69,69	7
91	MG	2	1946	1/1	0.80	0.44	87,87,87,87	0
91	MG	5	4150	1/1	0.80	0.74	45,45,45,45	0
92	OHX	6	2300	7/7	0.80	0.40	76,76,76,76	7
91	MG	1	3932	1/1	0.80	0.40	52,52,52,52	0
91	MG	17	304	1/1	0.80	0.78	52,52,52,52	1
91	MG	5	3998	1/1	0.80	0.21	67,67,67,67	0
91	MG	5	3934	1/1	0.80	1.04	67,67,67,67	1
91	MG	5	3754	1/1	0.81	0.41	64,64,64,64	0
91	MG	5	4020	1/1	0.81	0.39	54,54,54,54	0
91	MG	6	2005	1/1	0.81	0.16	88,88,88,88	0
92	OHX	1	4446	7/7	0.81	0.38	65,65,65,65	7
91	MG	N3	203	1/1	0.81	0.39	80,80,80,80	0
91	MG	6	2008	1/1	0.81	0.46	93,93,93,93	0
91	MG	5	3620	1/1	0.81	0.46	52,52,52,52	0
91	MG	2	2018	1/1	0.81	0.22	84,84,84,84	0
91	MG	1	4072	1/1	0.81	0.35	72,72,72,72	0
91	MG	1	3545	1/1	0.81	0.54	40,40,40,40	0
91	MG	5	4144	1/1	0.81	0.49	53,53,53,53	1
91	MG	M9	202	1/1	0.81	0.31	84,84,84,84	0
91	MG	1	3672	1/1	0.81	0.22	68,68,68,68	0
92	OHX	1	4352	7/7	0.81	0.25	135,135,135,135	7
91	MG	2	1911	1/1	0.81	0.32	88,88,88,88	0
92	OHX	A	102	7/7	0.81	0.51	75,75,75,75	7
91	MG	6	1945	1/1	0.81	0.73	103,103,103,103	0
92	OHX	1	4459	7/7	0.81	0.27	68,68,68,68	7
91	MG	6	2055	1/1	0.81	0.71	59,59,59,59	0
92	OHX	5	4398	7/7	0.81	0.53	58,58,58,58	7
91	MG	1	3489	1/1	0.81	0.31	56,56,56,56	0
91	MG	1	4097	1/1	0.81	0.38	66,66,66,66	0
91	MG	5	4149	1/1	0.81	0.37	49,49,49,49	1
91	MG	1	3995	1/1	0.81	0.90	70,70,70,70	1
92	OHX	2	2251	7/7	0.81	0.16	191,191,191,191	7
91	MG	5	4094	1/1	0.81	0.28	68,68,68,68	0
92	OHX	2	2224	7/7	0.81	0.15	164,164,164,164	7
91	MG	15	301	1/1	0.81	1.23	64,64,64,64	1
91	MG	2	2046	1/1	0.81	0.32	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3816	1/1	0.81	0.36	53,53,53,53	0
91	MG	l3	406	1/1	0.81	0.52	53,53,53,53	1
91	MG	1	3687	1/1	0.81	0.49	59,59,59,59	0
91	MG	3	202	1/1	0.81	0.33	62,62,62,62	0
92	OHX	2	2209	7/7	0.81	0.34	96,96,96,96	7
91	MG	1	3681	1/1	0.81	0.74	87,87,87,87	0
91	MG	5	3739	1/1	0.81	0.37	64,64,64,64	0
92	OHX	1	4436	7/7	0.81	0.30	55,55,55,55	7
91	MG	1	4087	1/1	0.81	0.21	71,71,71,71	0
91	MG	2	1979	1/1	0.81	0.14	90,90,90,90	0
91	MG	6	2078	1/1	0.81	0.35	98,98,98,98	0
91	MG	n9	102	1/1	0.81	0.19	68,68,68,68	0
91	MG	1	3761	1/1	0.81	0.93	59,59,59,59	0
92	OHX	2	2152	7/7	0.81	0.16	186,186,186,186	7
91	MG	1	3873	1/1	0.81	0.37	54,54,54,54	0
91	MG	5	4569	1/1	0.81	0.36	60,60,60,60	0
91	MG	1	3973	1/1	0.81	0.60	82,82,82,82	0
91	MG	5	3434	1/1	0.81	0.49	50,50,50,50	1
91	MG	5	3508	1/1	0.81	0.49	53,53,53,53	0
91	MG	1	4068	1/1	0.81	0.44	74,74,74,74	0
91	MG	1	3781	1/1	0.81	0.73	59,59,59,59	1
92	OHX	2	2227	7/7	0.81	0.47	82,82,82,82	7
91	MG	6	2046	1/1	0.81	0.29	84,84,84,84	0
91	MG	4	216	1/1	0.81	0.36	54,54,54,54	0
91	MG	5	3993	1/1	0.81	0.54	56,56,56,56	0
92	OHX	1	4470	7/7	0.82	0.38	56,56,56,56	7
91	MG	1	3757	1/1	0.82	0.19	69,69,69,69	0
91	MG	1	3593	1/1	0.82	0.57	46,46,46,46	0
92	OHX	5	4512	7/7	0.82	0.36	75,75,75,75	7
91	MG	5	3467	1/1	0.82	0.31	52,52,52,52	0
91	MG	1	3732	1/1	0.82	0.32	63,63,63,63	0
92	OHX	1	4494	7/7	0.82	0.39	61,61,61,61	7
91	MG	1	3919	1/1	0.82	1.09	50,50,50,50	1
92	OHX	5	4397	7/7	0.82	0.29	88,88,88,88	7
91	MG	1	4010	1/1	0.82	0.57	53,53,53,53	1
91	MG	5	3529	1/1	0.82	0.55	38,38,38,38	0
92	OHX	5	4490	7/7	0.82	0.34	71,71,71,71	7
92	OHX	1	4471	7/7	0.82	0.41	75,75,75,75	7
91	MG	5	3695	1/1	0.82	0.40	58,58,58,58	0
91	MG	5	3913	1/1	0.82	0.43	75,75,75,75	0
91	MG	8	215	1/1	0.82	0.71	53,53,53,53	1
91	MG	5	4031	1/1	0.82	0.61	55,55,55,55	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3658	1/1	0.82	0.22	65,65,65,65	0
91	MG	1	3914	1/1	0.82	0.29	57,57,57,57	1
91	MG	5	3640	1/1	0.82	0.33	61,61,61,61	0
91	MG	4	222	1/1	0.82	0.32	77,77,77,77	0
92	OHX	6	2292	7/7	0.82	0.28	136,136,136,136	7
91	MG	5	3537	1/1	0.82	0.31	58,58,58,58	0
91	MG	1	3435	1/1	0.82	0.36	58,58,58,58	0
92	OHX	6	2337	7/7	0.82	0.31	97,97,97,97	7
91	MG	1	3934	1/1	0.82	0.47	62,62,62,62	0
91	MG	5	3720	1/1	0.82	0.29	116,116,116,116	0
91	MG	5	3628	1/1	0.82	0.45	50,50,50,50	0
92	OHX	M7	209	7/7	0.82	0.39	70,70,70,70	7
91	MG	5	3570	1/1	0.82	0.32	62,62,62,62	0
91	MG	2	1984	1/1	0.82	0.99	97,97,97,97	0
91	MG	12	302	1/1	0.82	0.66	61,61,61,61	0
91	MG	6	1905	1/1	0.82	0.20	86,86,86,86	0
91	MG	5	3469	1/1	0.82	0.14	117,117,117,117	0
91	MG	1	3888	1/1	0.82	1.03	64,64,64,64	1
92	OHX	1	4466	7/7	0.82	0.30	93,93,93,93	7
91	MG	1	3988	1/1	0.82	0.65	48,48,48,48	1
92	OHX	5	4460	7/7	0.82	0.40	98,98,98,98	7
91	MG	2	2068	1/1	0.82	0.17	105,105,105,105	0
91	MG	5	3933	1/1	0.82	0.44	76,76,76,76	0
91	MG	5	3710	1/1	0.82	0.41	57,57,57,57	0
91	MG	1	3799	1/1	0.82	0.56	70,70,70,70	0
91	MG	5	3617	1/1	0.82	0.59	50,50,50,50	0
91	MG	1	4059	1/1	0.82	0.40	62,62,62,62	0
91	MG	1	3551	1/1	0.82	0.73	67,67,67,67	0
91	MG	5	3975	1/1	0.82	0.63	81,81,81,81	0
92	OHX	5	4540	7/7	0.83	0.26	101,101,101,101	7
91	MG	1	3502	1/1	0.83	0.73	64,64,64,64	0
91	MG	5	4038	1/1	0.83	0.32	67,67,67,67	1
91	MG	1	3441	1/1	0.83	0.31	56,56,56,56	0
92	OHX	M0	307	7/7	0.83	0.21	108,108,108,108	7
91	MG	1	3871	1/1	0.83	0.22	63,63,63,63	0
91	MG	1	4078	1/1	0.83	0.43	57,57,57,57	0
91	MG	1	3725	1/1	0.83	0.41	57,57,57,57	0
91	MG	2	2043	1/1	0.83	0.26	105,105,105,105	1
91	MG	1	3780	1/1	0.83	0.40	55,55,55,55	0
91	MG	4	230	1/1	0.83	0.74	52,52,52,52	1
92	OHX	5	4556	7/7	0.83	0.43	96,96,96,96	7
91	MG	2	2050	1/1	0.83	0.27	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	6	1914	1/1	0.83	0.44	56,56,56,56	0
91	MG	1	3655	1/1	0.83	0.32	71,71,71,71	0
91	MG	2	2060	1/1	0.83	0.15	138,138,138,138	0
92	OHX	6	2263	7/7	0.83	0.24	101,101,101,101	7
91	MG	5	3949	1/1	0.83	0.20	61,61,61,61	0
91	MG	5	3880	1/1	0.83	0.43	111,111,111,111	0
91	MG	5	3789	1/1	0.83	0.22	64,64,64,64	1
91	MG	1	4041	1/1	0.83	0.54	62,62,62,62	0
91	MG	5	4021	1/1	0.83	0.24	54,54,54,54	0
91	MG	5	4074	1/1	0.83	0.33	67,67,67,67	0
91	MG	1	3762	1/1	0.83	0.31	89,89,89,89	0
91	MG	5	3449	1/1	0.83	0.37	57,57,57,57	0
91	MG	N3	201	1/1	0.83	0.94	62,62,62,62	1
91	MG	2	1925	1/1	0.83	0.63	81,81,81,81	0
91	MG	1	3801	1/1	0.83	0.41	53,53,53,53	0
91	MG	2	2032	1/1	0.83	0.58	94,94,94,94	0
91	MG	5	3465	1/1	0.83	0.34	55,55,55,55	0
91	MG	2	1950	1/1	0.83	0.35	87,87,87,87	0
92	OHX	o9	102	7/7	0.83	0.42	64,64,64,64	7
91	MG	5	4092	1/1	0.83	0.28	49,49,49,49	0
91	MG	6	2056	1/1	0.83	0.39	89,89,89,89	0
92	OHX	M0	308	7/7	0.83	0.23	108,108,108,108	7
92	OHX	5	4496	7/7	0.83	0.28	159,159,159,159	7
91	MG	1	3737	1/1	0.83	0.27	87,87,87,87	0
91	MG	5	3986	1/1	0.83	1.49	77,77,77,77	0
91	MG	7	223	1/1	0.83	0.45	77,77,77,77	0
91	MG	5	3439	1/1	0.83	0.35	50,50,50,50	0
92	OHX	5	4399	7/7	0.83	0.36	62,62,62,62	7
92	OHX	5	4510	7/7	0.84	0.55	64,64,64,64	7
91	MG	5	3734	1/1	0.84	0.57	57,57,57,57	1
91	MG	5	4058	1/1	0.84	0.82	47,47,47,47	1
91	MG	6	2082	1/1	0.84	0.33	62,62,62,62	0
91	MG	2	1905	1/1	0.84	0.58	72,72,72,72	0
91	MG	1	3460	1/1	0.84	0.73	67,67,67,67	0
91	MG	5	3808	1/1	0.84	0.37	60,60,60,60	0
91	MG	1	3591	1/1	0.84	0.46	57,57,57,57	0
91	MG	5	3769	1/1	0.84	0.44	60,60,60,60	0
91	MG	m3	202	1/1	0.84	0.64	57,57,57,57	0
91	MG	1	3661	1/1	0.84	0.23	61,61,61,61	0
92	OHX	5	4533	7/7	0.84	0.68	66,66,66,66	7
92	OHX	1	4427	7/7	0.84	0.31	54,54,54,54	7
91	MG	1	3839	1/1	0.84	0.32	80,80,80,80	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	6	1937	1/1	0.84	0.71	69,69,69,69	0
91	MG	1	3432	1/1	0.84	0.49	62,62,62,62	0
91	MG	5	3746	1/1	0.84	0.29	67,67,67,67	0
91	MG	2	1906	1/1	0.84	0.29	73,73,73,73	0
92	OHX	7	240	7/7	0.84	0.31	73,73,73,73	7
91	MG	1	3482	1/1	0.84	0.40	53,53,53,53	0
91	MG	1	3849	1/1	0.84	0.39	57,57,57,57	0
91	MG	1	3667	1/1	0.84	0.33	63,63,63,63	1
92	OHX	6	2285	7/7	0.84	0.34	81,81,81,81	7
91	MG	1	3620	1/1	0.84	0.65	66,66,66,66	0
92	OHX	5	4531	7/7	0.84	0.23	122,122,122,122	7
91	MG	n8	203	1/1	0.84	0.45	51,51,51,51	0
91	MG	5	3894	1/1	0.84	0.41	46,46,46,46	0
91	MG	1	3619	1/1	0.84	0.50	60,60,60,60	0
92	OHX	c5	202	7/7	0.84	0.27	112,112,112,112	7
91	MG	1	3698	1/1	0.84	1.14	63,63,63,63	0
92	OHX	5	4543	7/7	0.84	0.47	63,63,63,63	7
91	MG	5	3652	1/1	0.84	0.84	108,108,108,108	0
91	MG	1	3756	1/1	0.84	0.36	60,60,60,60	1
91	MG	M7	204	1/1	0.84	0.50	52,52,52,52	0
91	MG	1	3662	1/1	0.84	0.15	85,85,85,85	0
91	MG	1	3628	1/1	0.84	0.53	53,53,53,53	0
91	MG	1	3638	1/1	0.84	0.44	62,62,62,62	0
91	MG	5	3736	1/1	0.84	0.53	84,84,84,84	0
92	OHX	5	4387	7/7	0.84	0.38	89,89,89,89	7
91	MG	7	205	1/1	0.84	0.67	58,58,58,58	0
91	MG	5	3486	1/1	0.84	0.36	55,55,55,55	0
91	MG	1	3987	1/1	0.84	0.49	70,70,70,70	0
91	MG	6	1963	1/1	0.84	0.44	71,71,71,71	0
91	MG	6	2013	1/1	0.84	0.33	66,66,66,66	1
91	MG	M3	204	1/1	0.84	0.80	114,114,114,114	0
91	MG	6	1916	1/1	0.84	0.74	62,62,62,62	0
91	MG	1	3546	1/1	0.84	0.37	61,61,61,61	0
91	MG	4	205	1/1	0.84	0.56	62,62,62,62	0
92	OHX	2	2239	7/7	0.84	0.40	106,106,106,106	7
91	MG	1	3457	1/1	0.84	0.34	74,74,74,74	0
91	MG	5	3922	1/1	0.84	1.28	66,66,66,66	1
91	MG	1	3531	1/1	0.84	0.43	59,59,59,59	0
91	MG	M5	305	1/1	0.84	0.42	69,69,69,69	0
91	MG	5	3471	1/1	0.84	0.41	54,54,54,54	0
91	MG	5	4146	1/1	0.84	0.40	63,63,63,63	0
92	OHX	6	2283	7/7	0.85	0.25	104,104,104,104	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3665	1/1	0.85	0.29	53,53,53,53	0
91	MG	3	216	1/1	0.85	0.34	93,93,93,93	0
91	MG	1	3635	1/1	0.85	0.30	58,58,58,58	0
92	OHX	1	4375	7/7	0.85	0.39	91,91,91,91	7
92	OHX	5	4431	7/7	0.85	0.49	80,80,80,80	7
91	MG	5	4045	1/1	0.85	0.30	58,58,58,58	0
92	OHX	1	4492	7/7	0.85	0.47	64,64,64,64	7
91	MG	n0	204	1/1	0.85	0.47	57,57,57,57	0
92	OHX	1	4499	7/7	0.85	0.38	70,70,70,70	7
91	MG	5	3955	1/1	0.85	0.26	51,51,51,51	1
92	OHX	m4	202	7/7	0.85	0.62	104,104,104,104	7
91	MG	1	3957	1/1	0.85	0.35	62,62,62,62	0
91	MG	6	1921	1/1	0.85	0.40	72,72,72,72	0
91	MG	1	3727	1/1	0.85	0.36	50,50,50,50	0
91	MG	17	303	1/1	0.85	0.41	54,54,54,54	0
91	MG	6	2117	1/1	0.85	0.67	74,74,74,74	1
92	OHX	5	4509	7/7	0.85	0.19	101,101,101,101	7
91	MG	2	1951	1/1	0.85	0.51	95,95,95,95	0
91	MG	7	221	1/1	0.85	0.19	63,63,63,63	0
91	MG	1	4506	1/1	0.85	0.32	60,60,60,60	0
91	MG	5	3543	1/1	0.85	0.87	60,60,60,60	0
91	MG	1	3414	1/1	0.85	0.27	75,75,75,75	0
91	MG	5	3930	1/1	0.85	0.56	50,50,50,50	0
92	OHX	2	2245	7/7	0.85	0.23	112,112,112,112	7
91	MG	1	3770	1/1	0.85	0.40	76,76,76,76	0
91	MG	1	3589	1/1	0.85	0.36	42,42,42,42	0
91	MG	2	2066	1/1	0.85	1.35	85,85,85,85	1
91	MG	l3	411	1/1	0.85	1.21	51,51,51,51	1
92	OHX	1	4378	7/7	0.85	0.31	76,76,76,76	7
91	MG	6	2128	1/1	0.85	0.48	89,89,89,89	0
91	MG	1	3982	1/1	0.85	1.09	46,46,46,46	1
92	OHX	1	4304	7/7	0.85	0.55	66,66,66,66	7
91	MG	2	1934	1/1	0.85	0.53	89,89,89,89	0
91	MG	6	2091	1/1	0.85	0.19	81,81,81,81	0
91	MG	5	3701	1/1	0.85	0.74	58,58,58,58	0
91	MG	6	1958	1/1	0.85	0.58	79,79,79,79	0
91	MG	5	4148	1/1	0.85	0.51	82,82,82,82	0
92	OHX	5	4451	7/7	0.85	0.27	93,93,93,93	7
91	MG	5	3448	1/1	0.85	0.58	49,49,49,49	0
91	MG	1	3544	1/1	0.85	0.62	48,48,48,48	0
92	OHX	5	4413	7/7	0.85	0.33	72,72,72,72	7
92	OHX	6	2321	7/7	0.85	0.39	138,138,138,138	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	2	2250	7/7	0.85	0.28	120,120,120,120	7
91	MG	6	1978	1/1	0.85	0.17	96,96,96,96	0
91	MG	1	3630	1/1	0.85	0.15	78,78,78,78	0
91	MG	1	3755	1/1	0.85	0.42	58,58,58,58	0
91	MG	5	3408	1/1	0.85	0.47	53,53,53,53	0
91	MG	5	3555	1/1	0.85	0.34	84,84,84,84	0
91	MG	1	4056	1/1	0.85	0.41	48,48,48,48	1
91	MG	5	3726	1/1	0.85	0.53	58,58,58,58	0
91	MG	Q0	201	1/1	0.85	0.89	68,68,68,68	1
92	OHX	2	2217	7/7	0.85	0.31	92,92,92,92	7
92	OHX	6	2301	7/7	0.85	0.55	68,68,68,68	7
91	MG	5	4113	1/1	0.85	0.35	52,52,52,52	1
91	MG	2	2067	1/1	0.85	0.26	83,83,83,83	0
92	OHX	1	4493	7/7	0.85	0.41	75,75,75,75	7
91	MG	1	3942	1/1	0.85	0.18	74,74,74,74	1
91	MG	M7	206	1/1	0.85	0.27	59,59,59,59	0
91	MG	5	4082	1/1	0.85	0.30	60,60,60,60	0
91	MG	5	3470	1/1	0.85	0.49	51,51,51,51	0
91	MG	5	3887	1/1	0.86	0.65	46,46,46,46	1
91	MG	6	1976	1/1	0.86	0.43	74,74,74,74	0
91	MG	5	3420	1/1	0.86	0.57	44,44,44,44	0
91	MG	5	3513	1/1	0.86	0.29	52,52,52,52	0
91	MG	8	204	1/1	0.86	0.24	67,67,67,67	0
91	MG	12	303	1/1	0.86	0.47	56,56,56,56	0
91	MG	3	218	1/1	0.86	0.26	70,70,70,70	0
91	MG	6	1908	1/1	0.86	0.29	88,88,88,88	0
91	MG	6	1947	1/1	0.86	0.64	49,49,49,49	0
91	MG	5	3783	1/1	0.86	0.32	52,52,52,52	1
91	MG	2	2017	1/1	0.86	0.29	85,85,85,85	0
92	OHX	2	2213	7/7	0.86	0.55	82,82,82,82	7
91	MG	6	1979	1/1	0.86	0.41	72,72,72,72	0
91	MG	5	3562	1/1	0.86	0.41	65,65,65,65	0
92	OHX	6	2253	7/7	0.86	0.32	99,99,99,99	7
91	MG	5	3735	1/1	0.86	0.25	59,59,59,59	0
91	MG	Q2	503	1/1	0.86	0.36	66,66,66,66	0
91	MG	5	3531	1/1	0.86	0.62	50,50,50,50	0
92	OHX	5	4535	7/7	0.86	0.42	63,63,63,63	7
91	MG	l3	410	1/1	0.86	0.97	47,47,47,47	1
91	MG	5	3721	1/1	0.86	0.55	51,51,51,51	1
91	MG	6	2022	1/1	0.86	0.65	63,63,63,63	0
92	OHX	2	2168	7/7	0.86	0.47	112,112,112,112	7
91	MG	8	211	1/1	0.86	0.27	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	8	238	7/7	0.86	0.31	85,85,85,85	7
92	OHX	2	2186	7/7	0.86	0.26	113,113,113,113	7
91	MG	Q2	502	1/1	0.86	0.17	80,80,80,80	0
91	MG	5	3483	1/1	0.86	0.24	82,82,82,82	0
91	MG	1	3989	1/1	0.86	0.34	62,62,62,62	1
92	OHX	5	4542	7/7	0.86	0.32	81,81,81,81	7
91	MG	1	3841	1/1	0.86	0.89	62,62,62,62	0
91	MG	6	1902	1/1	0.86	0.12	78,78,78,78	0
91	MG	2	1909	1/1	0.86	0.44	88,88,88,88	0
91	MG	1	3832	1/1	0.86	0.36	57,57,57,57	0
91	MG	5	3685	1/1	0.86	0.31	53,53,53,53	0
91	MG	6	1953	1/1	0.86	0.54	61,61,61,61	0
91	MG	5	4059	1/1	0.86	0.31	70,70,70,70	1
91	MG	5	3661	1/1	0.86	0.30	53,53,53,53	1
92	OHX	1	4452	7/7	0.86	0.31	83,83,83,83	7
91	MG	1	3912	1/1	0.86	0.55	65,65,65,65	0
92	OHX	6	2307	7/7	0.86	0.32	86,86,86,86	7
92	OHX	m1	203	7/7	0.86	0.51	92,92,92,92	7
91	MG	1	3592	1/1	0.86	0.38	57,57,57,57	0
91	MG	5	3444	1/1	0.86	0.46	54,54,54,54	0
91	MG	5	3679	1/1	0.86	0.60	66,66,66,66	0
92	OHX	2	2233	7/7	0.86	0.34	92,92,92,92	7
92	OHX	6	2265	7/7	0.86	0.21	132,132,132,132	7
91	MG	5	4101	1/1	0.86	0.27	57,57,57,57	1
92	OHX	5	4519	7/7	0.86	0.33	85,85,85,85	7
91	MG	5	3906	1/1	0.86	0.25	56,56,56,56	1
92	OHX	1	4461	7/7	0.86	0.26	144,144,144,144	7
92	OHX	1	4426	7/7	0.87	0.20	119,119,119,119	7
91	MG	m8	202	1/1	0.87	1.51	56,56,56,56	1
92	OHX	5	4544	7/7	0.87	0.47	69,69,69,69	7
91	MG	2	1997	1/1	0.87	0.41	97,97,97,97	0
91	MG	M7	203	1/1	0.87	0.77	76,76,76,76	0
91	MG	5	3815	1/1	0.87	0.29	52,52,52,52	0
92	OHX	6	2313	7/7	0.87	0.34	85,85,85,85	7
91	MG	5	4084	1/1	0.87	0.32	52,52,52,52	1
91	MG	5	3559	1/1	0.87	0.49	62,62,62,62	0
91	MG	5	3629	1/1	0.87	0.20	64,64,64,64	0
91	MG	2	1956	1/1	0.87	0.22	101,101,101,101	0
91	MG	5	3606	1/1	0.87	0.53	54,54,54,54	0
91	MG	5	3836	1/1	0.87	0.56	62,62,62,62	0
92	OHX	6	2332	7/7	0.87	0.22	116,116,116,116	7
92	OHX	6	2262	7/7	0.87	0.16	150,150,150,150	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	5	4529	7/7	0.87	0.16	126,126,126,126	7
91	MG	6	2108	1/1	0.87	0.13	125,125,125,125	0
92	OHX	5	4492	7/7	0.87	0.31	66,66,66,66	7
91	MG	6	1996	1/1	0.87	0.23	62,62,62,62	0
91	MG	2	1974	1/1	0.87	0.27	106,106,106,106	0
91	MG	1	3601	1/1	0.87	0.70	60,60,60,60	0
91	MG	2	1961	1/1	0.87	0.28	70,70,70,70	0
92	OHX	5	4475	7/7	0.87	0.25	79,79,79,79	7
91	MG	1	4075	1/1	0.87	0.55	110,110,110,110	0
91	MG	5	4005	1/1	0.87	0.30	77,77,77,77	0
92	OHX	2	2206	7/7	0.87	0.33	98,98,98,98	7
91	MG	1	3730	1/1	0.87	1.20	49,49,49,49	1
91	MG	1	3707	1/1	0.87	0.41	56,56,56,56	0
91	MG	5	3494	1/1	0.87	0.33	64,64,64,64	0
91	MG	6	1943	1/1	0.87	0.53	55,55,55,55	0
91	MG	5	3748	1/1	0.87	0.68	54,54,54,54	0
92	OHX	2	2210	7/7	0.87	0.19	123,123,123,123	7
91	MG	2	2065	1/1	0.87	0.76	136,136,136,136	0
91	MG	6	2018	1/1	0.87	0.11	105,105,105,105	0
91	MG	5	3893	1/1	0.87	0.44	50,50,50,50	1
91	MG	5	3406	1/1	0.87	0.33	59,59,59,59	0
92	OHX	1	4379	7/7	0.87	0.34	69,69,69,69	7
91	MG	5	3512	1/1	0.87	0.35	55,55,55,55	0
92	OHX	2	2230	7/7	0.87	0.23	97,97,97,97	7
91	MG	6	1988	1/1	0.87	0.15	96,96,96,96	0
91	MG	5	3972	1/1	0.87	0.52	133,133,133,133	0
91	MG	5	3671	1/1	0.87	0.09	64,64,64,64	0
91	MG	1	3816	1/1	0.87	0.60	52,52,52,52	1
91	MG	1	3991	1/1	0.87	0.31	71,71,71,71	0
91	MG	5	4121	1/1	0.87	0.48	52,52,52,52	0
91	MG	1	3689	1/1	0.87	0.63	64,64,64,64	0
91	MG	4	204	1/1	0.87	0.62	66,66,66,66	0
91	MG	5	3516	1/1	0.87	0.33	67,67,67,67	0
91	MG	5	3489	1/1	0.87	0.20	85,85,85,85	0
92	OHX	6	2309	7/7	0.87	0.30	98,98,98,98	7
91	MG	1	4079	1/1	0.87	0.57	74,74,74,74	0
92	OHX	6	2334	7/7	0.87	0.32	105,105,105,105	7
91	MG	5	3984	1/1	0.87	0.58	53,53,53,53	1
92	OHX	6	2276	7/7	0.87	0.31	68,68,68,68	7
91	MG	1	4030	1/1	0.87	1.02	53,53,53,53	1
91	MG	5	3618	1/1	0.87	0.39	46,46,46,46	0
92	OHX	6	2231	7/7	0.87	0.35	83,83,83,83	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	2	2020	1/1	0.87	0.38	89,89,89,89	0
91	MG	5	4128	1/1	0.87	0.29	45,45,45,45	1
91	MG	1	3994	1/1	0.87	0.30	60,60,60,60	1
91	MG	c9	201	1/1	0.87	0.09	96,96,96,96	0
91	MG	5	3611	1/1	0.87	0.14	60,60,60,60	0
91	MG	5	3453	1/1	0.87	0.38	73,73,73,73	0
91	MG	5	3421	1/1	0.87	0.25	53,53,53,53	0
91	MG	1	3538	1/1	0.87	0.71	50,50,50,50	0
91	MG	1	4067	1/1	0.87	0.67	70,70,70,70	0
91	MG	2	1938	1/1	0.87	0.38	75,75,75,75	0
91	MG	5	3571	1/1	0.88	0.49	49,49,49,49	0
91	MG	1	3690	1/1	0.88	0.57	54,54,54,54	0
91	MG	6	1983	1/1	0.88	0.35	68,68,68,68	0
92	OHX	1	4397	7/7	0.88	0.22	107,107,107,107	7
91	MG	5	3820	1/1	0.88	0.48	52,52,52,52	1
92	OHX	5	4432	7/7	0.88	0.32	70,70,70,70	7
91	MG	5	4008	1/1	0.88	0.41	54,54,54,54	0
91	MG	5	3757	1/1	0.88	0.46	57,57,57,57	0
91	MG	S2	302	1/1	0.88	0.41	85,85,85,85	0
91	MG	2	1990	1/1	0.88	0.53	98,98,98,98	0
91	MG	6	1994	1/1	0.88	0.55	72,72,72,72	0
91	MG	5	3947	1/1	0.88	0.21	61,61,61,61	0
92	OHX	5	4405	7/7	0.88	0.48	72,72,72,72	7
91	MG	6	1962	1/1	0.88	0.52	75,75,75,75	0
91	MG	L4	407	1/1	0.88	0.79	45,45,45,45	1
91	MG	5	3696	1/1	0.88	0.27	49,49,49,49	0
91	MG	5	3722	1/1	0.88	0.13	91,91,91,91	0
91	MG	1	3450	1/1	0.88	0.41	55,55,55,55	0
91	MG	1	3411	1/1	0.88	0.41	63,63,63,63	0
91	MG	5	4040	1/1	0.88	0.58	52,52,52,52	1
91	MG	2	1910	1/1	0.88	0.64	76,76,76,76	0
92	OHX	6	2298	7/7	0.88	0.24	162,162,162,162	7
91	MG	1	4096	1/1	0.88	0.42	62,62,62,62	0
92	OHX	2	2223	7/7	0.88	0.25	81,81,81,81	7
91	MG	6	2340	1/1	0.88	0.29	85,85,85,85	0
92	OHX	3	228	7/7	0.88	0.32	93,93,93,93	7
91	MG	5	3704	1/1	0.88	0.21	58,58,58,58	0
91	MG	1	3948	1/1	0.88	0.38	63,63,63,63	1
91	MG	5	3848	1/1	0.88	0.44	50,50,50,50	0
91	MG	5	3660	1/1	0.88	0.40	53,53,53,53	0
92	OHX	6	2317	7/7	0.88	0.28	107,107,107,107	7
91	MG	n0	203	1/1	0.88	0.19	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	2	2010	1/1	0.88	0.44	87,87,87,87	0
91	MG	L4	405	1/1	0.88	0.49	51,51,51,51	0
92	OHX	1	4312	7/7	0.88	0.30	70,70,70,70	7
92	OHX	2	2234	7/7	0.88	0.28	106,106,106,106	7
91	MG	19	201	1/1	0.88	0.33	58,58,58,58	0
91	MG	5	3633	1/1	0.88	0.41	55,55,55,55	0
91	MG	5	3856	1/1	0.88	0.51	49,49,49,49	1
92	OHX	2	2198	7/7	0.88	0.26	125,125,125,125	7
91	MG	2	2061	1/1	0.88	0.18	90,90,90,90	0
91	MG	8	217	1/1	0.88	0.45	68,68,68,68	0
91	MG	2	2040	1/1	0.88	0.12	97,97,97,97	0
92	OHX	2	2256	7/7	0.88	0.23	130,130,130,130	7
91	MG	5	3407	1/1	0.88	0.25	48,48,48,48	0
91	MG	5	3411	1/1	0.88	0.52	52,52,52,52	0
91	MG	1	3938	1/1	0.88	0.86	51,51,51,51	1
92	OHX	1	4456	7/7	0.88	0.33	56,56,56,56	7
91	MG	3	208	1/1	0.88	0.20	64,64,64,64	1
92	OHX	6	2304	7/7	0.88	0.52	84,84,84,84	7
91	MG	5	4072	1/1	0.88	0.39	51,51,51,51	0
91	MG	1	3750	1/1	0.88	0.16	68,68,68,68	0
92	OHX	1	4444	7/7	0.88	0.27	85,85,85,85	7
91	MG	5	3919	1/1	0.88	1.16	53,53,53,53	1
91	MG	6	1923	1/1	0.88	0.35	80,80,80,80	0
92	OHX	4	247	7/7	0.88	0.32	82,82,82,82	7
91	MG	14	403	1/1	0.88	0.40	69,69,69,69	1
92	OHX	6	2287	7/7	0.88	0.29	85,85,85,85	7
91	MG	1	3782	1/1	0.88	0.24	70,70,70,70	0
91	MG	5	3862	1/1	0.88	0.64	57,57,57,57	1
92	OHX	2	2215	7/7	0.88	0.34	115,115,115,115	7
91	MG	1	3434	1/1	0.88	0.13	65,65,65,65	0
91	MG	1	3837	1/1	0.88	0.36	59,59,59,59	1
91	MG	1	3812	1/1	0.88	0.21	79,79,79,79	0
91	MG	7	217	1/1	0.88	0.29	55,55,55,55	1
91	MG	5	3732	1/1	0.88	0.48	70,70,70,70	1
91	MG	6	1964	1/1	0.88	0.52	69,69,69,69	0
91	MG	5	3624	1/1	0.88	0.53	51,51,51,51	0
92	OHX	1	4488	7/7	0.88	0.40	102,102,102,102	7
91	MG	5	3417	1/1	0.88	0.34	73,73,73,73	0
91	MG	O7	103	1/1	0.88	0.26	84,84,84,84	0
91	MG	Q2	504	1/1	0.88	0.80	60,60,60,60	1
91	MG	5	3742	1/1	0.88	0.35	49,49,49,49	0
91	MG	7	220	1/1	0.88	0.72	63,63,63,63	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	1	3622	1/1	0.88	0.23	65,65,65,65	0
91	MG	2	2257	1/1	0.88	0.57	80,80,80,80	0
91	MG	7	207	1/1	0.88	0.38	48,48,48,48	0
91	MG	2	1980	1/1	0.88	0.14	104,104,104,104	1
92	OHX	1	4398	7/7	0.88	0.23	117,117,117,117	7
91	MG	1	3945	1/1	0.88	0.19	62,62,62,62	0
92	OHX	5	4439	7/7	0.88	0.33	93,93,93,93	7
91	MG	5	3642	1/1	0.88	0.44	53,53,53,53	0
92	OHX	8	236	7/7	0.89	0.39	91,91,91,91	7
91	MG	2	1942	1/1	0.89	0.56	79,79,79,79	0
92	OHX	1	4321	7/7	0.89	0.38	71,71,71,71	7
91	MG	q3	502	1/1	0.89	0.38	71,71,71,71	0
91	MG	5	3495	1/1	0.89	0.51	45,45,45,45	0
91	MG	5	3455	1/1	0.89	0.26	52,52,52,52	0
92	OHX	s1	302	7/7	0.89	0.22	109,109,109,109	7
91	MG	1	3929	1/1	0.89	0.49	70,70,70,70	0
92	OHX	6	2248	7/7	0.89	0.41	97,97,97,97	7
91	MG	2	1943	1/1	0.89	0.19	87,87,87,87	0
91	MG	1	3407	1/1	0.89	0.36	56,56,56,56	0
91	MG	1	4004	1/1	0.89	0.49	60,60,60,60	1
92	OHX	1	4480	7/7	0.89	0.28	85,85,85,85	7
91	MG	2	1940	1/1	0.89	0.33	86,86,86,86	0
92	OHX	1	4478	7/7	0.89	0.22	112,112,112,112	7
92	OHX	6	2286	7/7	0.89	0.17	120,120,120,120	7
91	MG	5	3451	1/1	0.89	0.14	55,55,55,55	0
92	OHX	1	4418	7/7	0.89	0.48	53,53,53,53	7
92	OHX	5	4275	7/7	0.89	0.25	128,128,128,128	7
91	MG	5	3995	1/1	0.89	0.30	51,51,51,51	1
92	OHX	6	2270	7/7	0.89	0.23	118,118,118,118	7
91	MG	4	219	1/1	0.89	0.46	76,76,76,76	0
91	MG	D9	103	1/1	0.89	0.26	93,93,93,93	0
92	OHX	2	2190	7/7	0.89	0.29	79,79,79,79	7
91	MG	1	3769	1/1	0.89	0.28	50,50,50,50	0
91	MG	1	3485	1/1	0.89	0.44	56,56,56,56	0
91	MG	1	3718	1/1	0.89	0.31	75,75,75,75	0
91	MG	d9	103	1/1	0.89	0.24	118,118,118,118	0
91	MG	5	3632	1/1	0.89	0.43	54,54,54,54	0
91	MG	2	2022	1/1	0.89	0.38	67,67,67,67	0
92	OHX	1	4389	7/7	0.89	0.29	61,61,61,61	7
92	OHX	1	4457	7/7	0.89	0.32	61,61,61,61	7
92	OHX	1	4458	7/7	0.89	0.33	66,66,66,66	7
92	OHX	2	2194	7/7	0.89	0.22	104,104,104,104	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	2	1969	1/1	0.89	0.41	86,86,86,86	0
92	OHX	1	4428	7/7	0.89	0.30	79,79,79,79	7
92	OHX	5	4384	7/7	0.89	0.22	101,101,101,101	7
92	OHX	6	2288	7/7	0.89	0.33	72,72,72,72	7
91	MG	6	1941	1/1	0.89	0.68	84,84,84,84	0
91	MG	1	3795	1/1	0.89	0.20	64,64,64,64	0
92	OHX	5	4498	7/7	0.89	0.63	74,74,74,74	7
91	MG	5	3723	1/1	0.89	0.37	78,78,78,78	0
92	OHX	1	4497	7/7	0.89	0.35	67,67,67,67	7
92	OHX	5	4502	7/7	0.89	0.34	67,67,67,67	7
91	MG	o2	202	1/1	0.89	0.64	47,47,47,47	1
91	MG	5	3700	1/1	0.89	0.32	75,75,75,75	0
91	MG	1	4039	1/1	0.89	0.22	95,95,95,95	0
91	MG	1	3809	1/1	0.89	0.51	56,56,56,56	1
91	MG	5	4067	1/1	0.89	0.44	48,48,48,48	0
92	OHX	5	4532	7/7	0.89	0.28	66,66,66,66	7
91	MG	N8	207	1/1	0.89	0.94	58,58,58,58	1
91	MG	1	4058	1/1	0.89	0.49	72,72,72,72	0
92	OHX	7	237	7/7	0.89	0.28	77,77,77,77	7
91	MG	2	1913	1/1	0.89	0.18	75,75,75,75	0
91	MG	c8	202	1/1	0.89	0.36	97,97,97,97	0
92	OHX	2	2115	7/7	0.89	0.27	132,132,132,132	7
91	MG	5	3663	1/1	0.89	0.13	64,64,64,64	0
91	MG	1	3547	1/1	0.89	0.60	60,60,60,60	0
91	MG	1	3865	1/1	0.89	0.29	62,62,62,62	1
91	MG	5	3657	1/1	0.89	0.35	63,63,63,63	0
91	MG	5	3807	1/1	0.89	0.40	53,53,53,53	0
91	MG	5	3996	1/1	0.89	0.58	48,48,48,48	1
91	MG	6	2000	1/1	0.89	0.62	99,99,99,99	0
91	MG	5	3714	1/1	0.89	0.29	49,49,49,49	1
91	MG	1	4038	1/1	0.89	0.29	55,55,55,55	0
91	MG	7	218	1/1	0.89	0.31	54,54,54,54	1
91	MG	6	1949	1/1	0.89	0.52	91,91,91,91	0
91	MG	1	3884	1/1	0.89	0.30	59,59,59,59	0
91	MG	5	3475	1/1	0.89	0.31	60,60,60,60	0
92	OHX	5	4430	7/7	0.89	0.52	89,89,89,89	7
91	MG	5	3501	1/1	0.89	0.26	62,62,62,62	0
91	MG	5	3619	1/1	0.89	0.44	76,76,76,76	0
91	MG	15	307	1/1	0.89	0.61	59,59,59,59	1
92	OHX	2	2226	7/7	0.89	0.28	215,215,215,215	7
92	OHX	1	4400	7/7	0.89	0.25	70,70,70,70	7
91	MG	5	3997	1/1	0.89	0.38	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	3515	1/1	0.89	0.56	45,45,45,45	0
91	MG	1	3724	1/1	0.89	0.36	50,50,50,50	0
91	MG	M3	203	1/1	0.89	0.25	65,65,65,65	0
91	MG	5	4056	1/1	0.89	0.37	60,60,60,60	0
92	OHX	2	2214	7/7	0.89	0.20	125,125,125,125	7
92	OHX	1	4475	7/7	0.89	0.28	61,61,61,61	7
91	MG	1	3505	1/1	0.89	0.23	63,63,63,63	0
91	MG	5	3833	1/1	0.89	0.27	57,57,57,57	0
91	MG	5	3485	1/1	0.89	0.61	71,71,71,71	0
91	MG	d6	102	1/1	0.89	0.70	81,81,81,81	0
92	OHX	1	4377	7/7	0.89	0.28	130,130,130,130	7
91	MG	1	3616	1/1	0.89	0.38	59,59,59,59	0
91	MG	2	2027	1/1	0.89	0.17	90,90,90,90	0
91	MG	5	3895	1/1	0.89	0.15	72,72,72,72	0
92	OHX	1	4472	7/7	0.89	0.47	67,67,67,67	7
92	OHX	6	2240	7/7	0.89	0.35	82,82,82,82	7
92	OHX	1	4486	7/7	0.89	0.38	86,86,86,86	7
91	MG	2	1917	1/1	0.89	0.52	71,71,71,71	0
91	MG	2	2015	1/1	0.89	1.31	74,74,74,74	1
91	MG	6	1935	1/1	0.89	0.43	75,75,75,75	0
91	MG	1	3913	1/1	0.89	0.30	56,56,56,56	0
91	MG	5	3838	1/1	0.89	0.20	67,67,67,67	0
92	OHX	2	2187	7/7	0.89	0.40	118,118,118,118	7
91	MG	2	1928	1/1	0.89	1.13	64,64,64,64	0
91	MG	5	3699	1/1	0.89	0.31	45,45,45,45	0
92	OHX	6	2238	7/7	0.89	0.26	114,114,114,114	7
91	MG	5	3946	1/1	0.89	0.26	48,48,48,48	1
91	MG	1	3521	1/1	0.89	0.43	43,43,43,43	0
91	MG	6	2100	1/1	0.90	0.21	78,78,78,78	0
91	MG	5	3561	1/1	0.90	0.55	58,58,58,58	0
91	MG	5	3907	1/1	0.90	0.22	83,83,83,83	0
92	OHX	5	4485	7/7	0.90	0.32	65,65,65,65	7
91	MG	6	1956	1/1	0.90	0.47	90,90,90,90	0
91	MG	5	3677	1/1	0.90	0.36	48,48,48,48	0
91	MG	5	4098	1/1	0.90	0.56	74,74,74,74	0
91	MG	1	3701	1/1	0.90	0.55	59,59,59,59	0
91	MG	1	3404	1/1	0.90	0.33	52,52,52,52	0
91	MG	2	1919	1/1	0.90	0.66	80,80,80,80	0
91	MG	N8	206	1/1	0.90	1.20	52,52,52,52	0
92	OHX	1	4468	7/7	0.90	0.34	78,78,78,78	7
92	OHX	5	4467	7/7	0.90	0.13	143,143,143,143	7
91	MG	1	3624	1/1	0.90	0.35	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	1	4393	7/7	0.90	0.25	121,121,121,121	7
91	MG	5	3524	1/1	0.90	0.43	60,60,60,60	0
92	OHX	5	4500	7/7	0.90	0.16	147,147,147,147	7
92	OHX	1	4503	7/7	0.90	0.39	96,96,96,96	7
92	OHX	5	4461	7/7	0.90	1.10	53,53,53,53	7
92	OHX	2	2199	7/7	0.90	0.23	107,107,107,107	7
92	OHX	6	2296	7/7	0.90	0.16	115,115,115,115	7
91	MG	1	3813	1/1	0.90	0.83	54,54,54,54	0
91	MG	1	3401	1/1	0.90	0.15	71,71,71,71	0
92	OHX	3	230	7/7	0.90	0.25	92,92,92,92	7
91	MG	1	3490	1/1	0.90	0.41	65,65,65,65	0
91	MG	n8	202	1/1	0.90	0.19	67,67,67,67	0
91	MG	2	1954	1/1	0.90	0.31	74,74,74,74	0
91	MG	5	4087	1/1	0.90	0.30	49,49,49,49	0
91	MG	1	3675	1/1	0.90	0.43	67,67,67,67	0
91	MG	6	2030	1/1	0.90	0.85	71,71,71,71	0
92	OHX	5	4511	7/7	0.90	0.30	81,81,81,81	7
91	MG	5	3631	1/1	0.90	0.49	47,47,47,47	0
91	MG	2	1939	1/1	0.90	0.34	75,75,75,75	0
91	MG	1	3821	1/1	0.90	0.41	62,62,62,62	1
91	MG	5	4001	1/1	0.90	0.52	54,54,54,54	1
92	OHX	d4	201	7/7	0.90	0.33	98,98,98,98	7
91	MG	5	4006	1/1	0.90	0.69	61,61,61,61	1
92	OHX	1	4320	7/7	0.90	0.12	190,190,190,190	0
91	MG	5	3716	1/1	0.90	0.30	51,51,51,51	0
91	MG	1	3529	1/1	0.90	0.60	51,51,51,51	0
91	MG	5	4147	1/1	0.90	0.62	46,46,46,46	1
91	MG	1	3590	1/1	0.90	0.56	50,50,50,50	0
91	MG	2	1936	1/1	0.90	0.65	75,75,75,75	0
92	OHX	1	4438	7/7	0.90	0.49	81,81,81,81	7
91	MG	6	2130	1/1	0.90	0.41	91,91,91,91	0
92	OHX	5	4514	7/7	0.90	0.26	83,83,83,83	7
92	OHX	1	4342	7/7	0.90	0.24	201,201,201,201	0
91	MG	1	3896	1/1	0.90	0.37	70,70,70,70	0
92	OHX	5	4411	7/7	0.90	0.30	61,61,61,61	7
92	OHX	5	4435	7/7	0.90	0.27	73,73,73,73	7
91	MG	5	3978	1/1	0.90	0.27	54,54,54,54	1
92	OHX	1	4437	7/7	0.90	0.32	105,105,105,105	7
91	MG	5	3428	1/1	0.90	0.35	57,57,57,57	0
91	MG	4	212	1/1	0.90	0.28	67,67,67,67	0
91	MG	5	3491	1/1	0.90	0.47	92,92,92,92	0
92	OHX	2	2181	7/7	0.90	0.15	165,165,165,165	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	5	4452	7/7	0.90	0.22	111,111,111,111	7
91	MG	5	3890	1/1	0.90	0.19	73,73,73,73	0
91	MG	7	227	1/1	0.90	0.38	64,64,64,64	1
91	MG	5	3638	1/1	0.90	0.68	55,55,55,55	0
92	OHX	5	4517	7/7	0.90	0.40	54,54,54,54	7
91	MG	5	4153	1/1	0.90	1.11	55,55,55,55	1
92	OHX	8	234	7/7	0.90	0.37	60,60,60,60	7
91	MG	1	3440	1/1	0.90	0.46	50,50,50,50	0
91	MG	1	3418	1/1	0.90	0.26	59,59,59,59	0
91	MG	5	3534	1/1	0.90	0.52	51,51,51,51	0
91	MG	2	1953	1/1	0.90	0.25	97,97,97,97	0
91	MG	1	3941	1/1	0.90	0.34	70,70,70,70	0
92	OHX	5	4357	7/7	0.90	0.26	126,126,126,126	7
92	OHX	6	2264	7/7	0.90	0.17	110,110,110,110	7
92	OHX	5	4425	7/7	0.90	0.52	58,58,58,58	7
91	MG	1	4048	1/1	0.90	1.07	66,66,66,66	1
91	MG	7	224	1/1	0.90	0.19	62,62,62,62	0
91	MG	1	3738	1/1	0.90	0.33	60,60,60,60	0
91	MG	1	3509	1/1	0.90	0.43	67,67,67,67	0
91	MG	1	4035	1/1	0.90	0.43	62,62,62,62	1
91	MG	1	4009	1/1	0.90	0.31	72,72,72,72	0
91	MG	2	2031	1/1	0.90	0.35	82,82,82,82	0
91	MG	N8	202	1/1	0.90	0.31	45,45,45,45	1
91	MG	1	3803	1/1	0.90	0.18	66,66,66,66	0
92	OHX	15	310	7/7	0.90	0.23	83,83,83,83	7
91	MG	1	3652	1/1	0.90	0.34	71,71,71,71	0
92	OHX	2	2204	7/7	0.90	0.28	134,134,134,134	7
91	MG	1	3739	1/1	0.90	0.29	87,87,87,87	0
92	OHX	5	4546	7/7	0.90	0.25	68,68,68,68	7
91	MG	5	3433	1/1	0.90	0.46	76,76,76,76	0
92	OHX	6	2256	7/7	0.90	0.17	109,109,109,109	7
91	MG	4	210	1/1	0.90	0.30	53,53,53,53	0
91	MG	5	3616	1/1	0.90	0.40	42,42,42,42	0
92	OHX	1	4413	7/7	0.90	0.51	68,68,68,68	7
91	MG	5	3674	1/1	0.90	0.90	56,56,56,56	0
91	MG	5	3753	1/1	0.90	0.34	88,88,88,88	0
91	MG	13	408	1/1	0.90	0.53	45,45,45,45	1
91	MG	1	3833	1/1	0.90	0.19	61,61,61,61	0
91	MG	5	4010	1/1	0.90	0.09	83,83,83,83	0
91	MG	1	3778	1/1	0.90	0.38	62,62,62,62	0
91	MG	5	4079	1/1	0.90	0.27	68,68,68,68	0
92	OHX	6	2277	7/7	0.90	0.28	96,96,96,96	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	1	3473	1/1	0.90	0.15	56,56,56,56	0
91	MG	5	3844	1/1	0.90	0.22	45,45,45,45	1
91	MG	1	3885	1/1	0.90	0.54	66,66,66,66	0
91	MG	1	3908	1/1	0.90	0.81	49,49,49,49	1
92	OHX	d9	104	7/7	0.90	0.25	109,109,109,109	7
92	OHX	5	4388	7/7	0.90	0.32	136,136,136,136	7
92	OHX	6	2284	7/7	0.90	0.43	94,94,94,94	7
91	MG	1	3694	1/1	0.90	0.16	59,59,59,59	0
91	MG	2	1952	1/1	0.90	0.45	79,79,79,79	0
92	OHX	5	4450	7/7	0.90	0.14	126,126,126,126	7
91	MG	m7	205	1/1	0.91	0.24	62,62,62,62	0
92	OHX	5	4567	7/7	0.91	0.28	100,100,100,100	7
91	MG	6	1925	1/1	0.91	0.26	88,88,88,88	0
91	MG	6	2059	1/1	0.91	0.22	70,70,70,70	0
91	MG	1	3588	1/1	0.91	0.22	50,50,50,50	0
91	MG	6	2135	1/1	0.91	1.43	72,72,72,72	1
91	MG	5	3464	1/1	0.91	0.35	48,48,48,48	0
91	MG	5	3991	1/1	0.91	0.52	60,60,60,60	1
91	MG	1	4011	1/1	0.91	0.27	58,58,58,58	0
91	MG	1	3420	1/1	0.91	0.33	85,85,85,85	0
91	MG	1	3643	1/1	0.91	0.32	58,58,58,58	0
91	MG	5	4130	1/1	0.91	0.29	61,61,61,61	0
91	MG	5	3672	1/1	0.91	0.69	64,64,64,64	0
91	MG	1	3804	1/1	0.91	0.65	49,49,49,49	0
91	MG	5	3775	1/1	0.91	0.31	52,52,52,52	0
92	OHX	2	2159	7/7	0.91	0.17	112,112,112,112	7
92	OHX	5	4417	7/7	0.91	0.29	54,54,54,54	7
91	MG	6	2098	1/1	0.91	0.38	68,68,68,68	1
91	MG	6	2042	1/1	0.91	0.36	70,70,70,70	0
91	MG	n0	202	1/1	0.91	0.24	61,61,61,61	0
92	OHX	1	4203	7/7	0.91	0.31	75,75,75,75	7
91	MG	6	2092	1/1	0.91	0.21	79,79,79,79	0
91	MG	5	3459	1/1	0.91	0.28	58,58,58,58	0
91	MG	1	3717	1/1	0.91	0.60	72,72,72,72	0
91	MG	5	4132	1/1	0.91	0.31	57,57,57,57	1
91	MG	5	3554	1/1	0.91	0.21	49,49,49,49	0
91	MG	5	4042	1/1	0.91	0.39	65,65,65,65	0
91	MG	1	3598	1/1	0.91	0.51	52,52,52,52	0
91	MG	5	3903	1/1	0.91	0.38	75,75,75,75	1
91	MG	5	3709	1/1	0.91	0.65	69,69,69,69	0
91	MG	2	2049	1/1	0.91	0.71	73,73,73,73	0
91	MG	1	3726	1/1	0.91	0.64	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3530	1/1	0.91	0.62	44,44,44,44	0
91	MG	2	1933	1/1	0.91	0.55	82,82,82,82	0
91	MG	5	4125	1/1	0.91	0.42	91,91,91,91	0
92	OHX	sR	401	7/7	0.91	0.19	137,137,137,137	7
92	OHX	5	4351	7/7	0.91	0.17	97,97,97,97	7
91	MG	1	3905	1/1	0.91	1.05	53,53,53,53	1
91	MG	5	4050	1/1	0.91	0.56	47,47,47,47	1
91	MG	6	2034	1/1	0.91	0.35	103,103,103,103	0
91	MG	5	3731	1/1	0.91	0.27	54,54,54,54	0
91	MG	2	1930	1/1	0.91	0.43	82,82,82,82	0
91	MG	1	4089	1/1	0.91	0.44	61,61,61,61	0
92	OHX	2	2248	7/7	0.91	0.14	129,129,129,129	7
91	MG	1	3449	1/1	0.91	0.40	47,47,47,47	0
91	MG	5	3942	1/1	0.91	0.63	63,63,63,63	0
91	MG	6	2067	1/1	0.91	0.83	80,80,80,80	1
91	MG	1	3664	1/1	0.91	0.46	50,50,50,50	0
92	OHX	O7	109	7/7	0.91	0.28	62,62,62,62	7
92	OHX	5	4497	7/7	0.91	0.25	85,85,85,85	7
92	OHX	5	4499	7/7	0.91	0.38	54,54,54,54	7
91	MG	5	4139	1/1	0.91	0.64	55,55,55,55	1
92	OHX	1	4498	7/7	0.91	0.24	109,109,109,109	7
91	MG	1	3666	1/1	0.91	0.94	62,62,62,62	0
91	MG	6	2041	1/1	0.91	0.32	82,82,82,82	0
91	MG	1	4020	1/1	0.91	0.43	54,54,54,54	0
92	OHX	l3	413	7/7	0.91	0.20	81,81,81,81	7
92	OHX	5	4407	7/7	0.91	0.45	63,63,63,63	7
91	MG	1	3481	1/1	0.91	0.39	69,69,69,69	0
91	MG	1	3815	1/1	0.91	0.29	69,69,69,69	0
92	OHX	5	4459	7/7	0.91	0.21	86,86,86,86	7
92	OHX	8	235	7/7	0.91	0.26	76,76,76,76	7
92	OHX	1	4383	7/7	0.91	0.23	94,94,94,94	7
92	OHX	1	4451	7/7	0.91	0.18	74,74,74,74	7
92	OHX	5	4374	7/7	0.91	0.35	65,65,65,65	7
92	OHX	5	4423	7/7	0.91	0.43	55,55,55,55	7
92	OHX	C5	202	7/7	0.91	0.24	123,123,123,123	7
91	MG	o4	202	1/1	0.91	0.36	71,71,71,71	0
91	MG	1	3603	1/1	0.91	0.53	69,69,69,69	0
91	MG	1	3877	1/1	0.91	0.34	53,53,53,53	1
92	OHX	6	2230	7/7	0.91	0.23	105,105,105,105	7
92	OHX	6	2274	7/7	0.91	0.21	145,145,145,145	7
92	OHX	2	2129	7/7	0.91	0.19	121,121,121,121	7
91	MG	1	3467	1/1	0.91	0.51	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	2	1924	1/1	0.91	0.23	92,92,92,92	0
92	OHX	4	244	7/7	0.91	0.31	69,69,69,69	7
91	MG	5	3759	1/1	0.91	0.56	54,54,54,54	0
91	MG	1	3946	1/1	0.91	0.25	63,63,63,63	0
91	MG	5	3484	1/1	0.91	0.29	75,75,75,75	0
91	MG	5	4107	1/1	0.91	0.42	58,58,58,58	0
92	OHX	s8	305	7/7	0.91	0.21	114,114,114,114	7
91	MG	1	3901	1/1	0.91	0.70	54,54,54,54	1
92	OHX	6	2273	7/7	0.91	0.22	90,90,90,90	7
92	OHX	2	2192	7/7	0.91	0.26	107,107,107,107	7
91	MG	6	2002	1/1	0.91	0.20	100,100,100,100	0
92	OHX	2	2225	7/7	0.91	0.26	80,80,80,80	7
91	MG	5	3828	1/1	0.91	0.38	52,52,52,52	1
91	MG	S6	301	1/1	0.91	0.15	106,106,106,106	0
92	OHX	5	4437	7/7	0.91	0.49	49,49,49,49	7
91	MG	5	3487	1/1	0.91	0.53	54,54,54,54	0
91	MG	1	3431	1/1	0.91	0.73	57,57,57,57	0
91	MG	1	3883	1/1	0.91	0.14	87,87,87,87	0
91	MG	5	4136	1/1	0.91	0.25	59,59,59,59	0
92	OHX	1	4355	7/7	0.91	0.38	60,60,60,60	7
91	MG	5	3599	1/1	0.91	0.50	43,43,43,43	0
92	OHX	2	2148	7/7	0.91	0.20	106,106,106,106	7
92	OHX	1	4411	7/7	0.91	0.22	104,104,104,104	7
91	MG	8	210	1/1	0.91	0.41	60,60,60,60	0
92	OHX	8	240	7/7	0.91	0.32	82,82,82,82	7
91	MG	2	2001	1/1	0.91	0.17	85,85,85,85	0
92	OHX	5	4453	7/7	0.91	0.35	84,84,84,84	7
92	OHX	1	4483	7/7	0.91	0.41	63,63,63,63	7
91	MG	M0	304	1/1	0.91	0.31	62,62,62,62	0
92	OHX	5	4479	7/7	0.91	0.47	58,58,58,58	7
91	MG	4	213	1/1	0.91	0.34	70,70,70,70	0
91	MG	1	3576	1/1	0.91	0.34	50,50,50,50	0
91	MG	5	3940	1/1	0.91	0.29	57,57,57,57	0
91	MG	L7	301	1/1	0.91	0.25	53,53,53,53	0
91	MG	5	3879	1/1	0.91	0.75	47,47,47,47	1
91	MG	5	3694	1/1	0.91	0.31	42,42,42,42	0
91	MG	4	223	1/1	0.91	0.35	60,60,60,60	0
92	OHX	2	2252	7/7	0.91	0.35	106,106,106,106	7
91	MG	1	3462	1/1	0.91	0.58	44,44,44,44	0
92	OHX	2	2157	7/7	0.91	0.27	113,113,113,113	7
91	MG	5	3841	1/1	0.91	0.25	73,73,73,73	0
91	MG	4	208	1/1	0.91	0.35	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	4019	1/1	0.91	0.40	51,51,51,51	1
91	MG	1	3743	1/1	0.91	0.34	58,58,58,58	0
91	MG	6	1924	1/1	0.91	0.24	67,67,67,67	0
91	MG	6	2060	1/1	0.91	0.42	71,71,71,71	0
92	OHX	2	2201	7/7	0.92	0.19	127,127,127,127	7
91	MG	1	3771	1/1	0.92	1.14	53,53,53,53	1
92	OHX	1	4235	7/7	0.92	0.27	70,70,70,70	7
91	MG	1	3555	1/1	0.92	0.45	50,50,50,50	0
92	OHX	5	4328	7/7	0.92	0.40	69,69,69,69	7
91	MG	1	3879	1/1	0.92	0.36	51,51,51,51	0
92	OHX	19	204	7/7	0.92	0.47	79,79,79,79	7
91	MG	5	3811	1/1	0.92	0.53	48,48,48,48	1
91	MG	1	3972	1/1	0.92	0.19	76,76,76,76	0
91	MG	5	3527	1/1	0.92	0.42	44,44,44,44	0
91	MG	8	214	1/1	0.92	0.21	101,101,101,101	0
91	MG	5	3911	1/1	0.92	0.59	60,60,60,60	1
91	MG	1	3867	1/1	0.92	0.35	81,81,81,81	0
92	OHX	1	4343	7/7	0.92	0.45	70,70,70,70	7
92	OHX	2	2111	7/7	0.92	0.26	106,106,106,106	7
91	MG	2	2062	1/1	0.92	0.17	112,112,112,112	0
92	OHX	6	2281	7/7	0.92	0.26	82,82,82,82	7
91	MG	5	3574	1/1	0.92	0.74	42,42,42,42	0
92	OHX	5	4441	7/7	0.92	0.33	53,53,53,53	7
91	MG	1	3491	1/1	0.92	0.34	55,55,55,55	0
92	OHX	c3	201	7/7	0.92	0.32	100,100,100,100	7
91	MG	1	3409	1/1	0.92	0.51	48,48,48,48	0
91	MG	M0	302	1/1	0.92	0.29	60,60,60,60	0
92	OHX	2	2173	7/7	0.92	0.33	97,97,97,97	7
91	MG	1	4057	1/1	0.92	0.45	45,45,45,45	1
92	OHX	2	2167	7/7	0.92	0.20	104,104,104,104	7
92	OHX	5	4526	7/7	0.92	0.38	71,71,71,71	7
92	OHX	6	2222	7/7	0.92	0.55	64,64,64,64	7
92	OHX	2	2207	7/7	0.92	0.24	113,113,113,113	7
91	MG	N9	101	1/1	0.92	0.18	50,50,50,50	0
91	MG	6	1929	1/1	0.92	0.51	61,61,61,61	0
92	OHX	4	248	7/7	0.92	0.36	75,75,75,75	7
91	MG	5	3954	1/1	0.92	0.58	51,51,51,51	1
91	MG	5	3431	1/1	0.92	0.38	44,44,44,44	0
91	MG	5	3801	1/1	0.92	0.39	60,60,60,60	1
91	MG	1	3582	1/1	0.92	0.56	62,62,62,62	0
91	MG	1	3433	1/1	0.92	0.40	48,48,48,48	0
91	MG	1	3952	1/1	0.92	0.39	58,58,58,58	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3460	1/1	0.92	0.64	48,48,48,48	0
92	OHX	15	308	7/7	0.92	0.16	107,107,107,107	7
91	MG	6	1927	1/1	0.92	0.59	54,54,54,54	0
92	OHX	1	4287	7/7	0.92	0.27	80,80,80,80	7
92	OHX	1	4380	7/7	0.92	0.22	74,74,74,74	7
91	MG	2	2000	1/1	0.92	0.43	75,75,75,75	0
91	MG	1	3558	1/1	0.92	0.38	56,56,56,56	0
91	MG	1	4065	1/1	0.92	0.81	62,62,62,62	1
92	OHX	1	4365	7/7	0.92	0.28	61,61,61,61	7
92	OHX	5	4322	7/7	0.92	0.29	73,73,73,73	7
91	MG	5	3584	1/1	0.92	0.57	53,53,53,53	0
91	MG	1	3691	1/1	0.92	0.36	59,59,59,59	0
91	MG	2	2011	1/1	0.92	0.19	91,91,91,91	0
91	MG	1	3965	1/1	0.92	0.82	48,48,48,48	1
91	MG	5	3654	1/1	0.92	0.41	49,49,49,49	0
91	MG	4	214	1/1	0.92	0.11	62,62,62,62	0
91	MG	1	3971	1/1	0.92	0.72	46,46,46,46	1
92	OHX	5	4462	7/7	0.92	0.31	80,80,80,80	7
92	OHX	5	4516	7/7	0.92	0.19	82,82,82,82	7
92	OHX	5	4420	7/7	0.92	0.22	72,72,72,72	7
91	MG	5	3636	1/1	0.92	0.50	56,56,56,56	0
91	MG	1	3439	1/1	0.92	0.74	42,42,42,42	0
92	OHX	2	2212	7/7	0.92	0.17	148,148,148,148	7
92	OHX	1	4351	7/7	0.92	0.36	64,64,64,64	7
91	MG	1	3403	1/1	0.92	0.82	65,65,65,65	0
92	OHX	2	2232	7/7	0.92	0.14	139,139,139,139	7
91	MG	1	3674	1/1	0.92	0.35	45,45,45,45	0
91	MG	1	3627	1/1	0.92	0.59	51,51,51,51	0
91	MG	M5	302	1/1	0.92	1.11	52,52,52,52	1
91	MG	1	3974	1/1	0.92	1.33	60,60,60,60	1
91	MG	5	3683	1/1	0.92	0.64	63,63,63,63	0
91	MG	1	3583	1/1	0.92	0.57	49,49,49,49	0
92	OHX	6	2234	7/7	0.92	0.31	97,97,97,97	7
91	MG	4	224	1/1	0.92	1.24	62,62,62,62	1
91	MG	7	212	1/1	0.92	0.11	69,69,69,69	0
91	MG	5	3461	1/1	0.92	0.43	45,45,45,45	0
91	MG	5	3402	1/1	0.92	0.16	60,60,60,60	0
92	OHX	D9	104	7/7	0.92	0.36	97,97,97,97	7
91	MG	1	4017	1/1	0.92	0.88	53,53,53,53	1
91	MG	1	3519	1/1	0.92	0.63	58,58,58,58	0
91	MG	5	3536	1/1	0.92	0.54	45,45,45,45	0
91	MG	1	3416	1/1	0.92	0.39	64,64,64,64	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	S2	301	1/1	0.92	0.57	76,76,76,76	0
92	OHX	1	4445	7/7	0.92	0.30	72,72,72,72	7
91	MG	1	3448	1/1	0.92	0.32	63,63,63,63	0
92	OHX	1	4358	7/7	0.92	0.43	75,75,75,75	7
92	OHX	1	4390	7/7	0.92	0.32	60,60,60,60	7
91	MG	2	2051	1/1	0.92	0.27	74,74,74,74	1
92	OHX	1	4362	7/7	0.92	0.35	64,64,64,64	7
91	MG	5	4026	1/1	0.92	0.26	62,62,62,62	0
92	OHX	1	4385	7/7	0.92	0.49	68,68,68,68	7
92	OHX	5	4456	7/7	0.92	0.24	58,58,58,58	7
91	MG	5	3824	1/1	0.92	0.38	67,67,67,67	0
91	MG	2	2012	1/1	0.92	0.32	116,116,116,116	0
91	MG	5	3662	1/1	0.92	0.65	52,52,52,52	0
91	MG	5	3456	1/1	0.92	0.50	50,50,50,50	0
92	OHX	1	4414	7/7	0.92	0.28	112,112,112,112	7
92	OHX	5	4385	7/7	0.92	0.47	59,59,59,59	7
92	OHX	1	4479	7/7	0.92	0.37	71,71,71,71	7
92	OHX	5	4403	7/7	0.92	0.44	67,67,67,67	7
92	OHX	5	4488	7/7	0.92	0.33	69,69,69,69	7
91	MG	3	205	1/1	0.92	0.59	47,47,47,47	0
91	MG	1	3584	1/1	0.92	0.58	43,43,43,43	0
91	MG	1	3413	1/1	0.92	0.36	55,55,55,55	0
92	OHX	6	2217	7/7	0.92	0.19	114,114,114,114	7
91	MG	1	3704	1/1	0.92	0.70	53,53,53,53	0
92	OHX	1	4404	7/7	0.92	0.35	58,58,58,58	7
91	MG	1	3496	1/1	0.92	0.34	54,54,54,54	0
91	MG	o7	103	1/1	0.92	0.81	48,48,48,48	1
91	MG	6	1990	1/1	0.92	0.46	78,78,78,78	0
92	OHX	5	4473	7/7	0.92	0.42	70,70,70,70	7
91	MG	Q0	203	1/1	0.92	0.30	70,70,70,70	0
91	MG	5	4044	1/1	0.92	0.14	85,85,85,85	0
91	MG	n0	201	1/1	0.92	0.81	55,55,55,55	1
91	MG	1	4006	1/1	0.92	0.52	46,46,46,46	0
92	OHX	8	232	7/7	0.92	0.31	87,87,87,87	7
92	OHX	1	4252	7/7	0.92	0.26	92,92,92,92	7
91	MG	1	3581	1/1	0.92	0.24	42,42,42,42	0
91	MG	1	3752	1/1	0.92	0.64	50,50,50,50	0
92	OHX	5	4470	7/7	0.92	0.21	66,66,66,66	7
92	OHX	3	227	7/7	0.92	0.41	89,89,89,89	7
92	OHX	1	4447	7/7	0.92	0.26	68,68,68,68	7
92	OHX	6	2266	7/7	0.92	0.18	162,162,162,162	7
91	MG	3	207	1/1	0.92	0.49	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	3973	1/1	0.92	0.65	52,52,52,52	0
92	OHX	5	4493	7/7	0.92	0.26	111,111,111,111	7
91	MG	5	3480	1/1	0.92	0.35	53,53,53,53	0
91	MG	5	3579	1/1	0.92	0.85	44,44,44,44	0
91	MG	5	3496	1/1	0.93	0.31	50,50,50,50	0
91	MG	2	2048	1/1	0.93	0.56	80,80,80,80	0
92	OHX	6	2258	7/7	0.93	0.44	72,72,72,72	7
92	OHX	5	4400	7/7	0.93	0.26	79,79,79,79	7
92	OHX	2	2185	7/7	0.93	0.20	115,115,115,115	7
92	OHX	1	4261	7/7	0.93	0.44	55,55,55,55	7
91	MG	5	3825	1/1	0.93	0.11	77,77,77,77	0
91	MG	17	302	1/1	0.93	0.71	48,48,48,48	1
91	MG	5	3403	1/1	0.93	0.73	48,48,48,48	0
91	MG	m6	203	1/1	0.93	0.70	50,50,50,50	1
91	MG	1	3541	1/1	0.93	0.94	62,62,62,62	0
92	OHX	6	2271	7/7	0.93	0.17	94,94,94,94	7
91	MG	7	215	1/1	0.93	0.48	64,64,64,64	1
92	OHX	1	4327	7/7	0.93	0.37	87,87,87,87	7
91	MG	1	3758	1/1	0.93	0.32	66,66,66,66	0
91	MG	c8	201	1/1	0.93	0.07	102,102,102,102	0
92	OHX	1	4367	7/7	0.93	0.23	80,80,80,80	7
92	OHX	5	4414	7/7	0.93	0.64	63,63,63,63	7
92	OHX	1	4406	7/7	0.93	0.35	70,70,70,70	7
92	OHX	2	2114	7/7	0.93	0.17	120,120,120,120	7
91	MG	5	3463	1/1	0.93	0.32	68,68,68,68	0
91	MG	1	3451	1/1	0.93	0.51	50,50,50,50	0
92	OHX	5	4428	7/7	0.93	0.28	58,58,58,58	7
91	MG	5	3693	1/1	0.93	0.32	49,49,49,49	0
92	OHX	5	4371	7/7	0.93	0.38	91,91,91,91	7
91	MG	1	4016	1/1	0.93	0.29	63,63,63,63	0
91	MG	5	3908	1/1	0.93	0.89	68,68,68,68	1
91	MG	5	3404	1/1	0.93	0.38	47,47,47,47	0
92	OHX	a	101	7/7	0.93	0.39	73,73,73,73	7
91	MG	6	1952	1/1	0.93	0.58	73,73,73,73	0
92	OHX	5	4449	7/7	0.93	0.33	61,61,61,61	7
91	MG	1	3405	1/1	0.93	0.47	62,62,62,62	0
92	OHX	6	2329	7/7	0.93	0.25	89,89,89,89	7
92	OHX	1	4310	7/7	0.93	0.32	73,73,73,73	7
92	OHX	5	4486	7/7	0.93	0.23	108,108,108,108	7
91	MG	5	3852	1/1	0.93	0.35	52,52,52,52	1
91	MG	5	3426	1/1	0.93	0.28	73,73,73,73	0
92	OHX	5	4415	7/7	0.93	0.47	80,80,80,80	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3666	1/1	0.93	0.28	66,66,66,66	0
91	MG	1	3951	1/1	0.93	0.29	55,55,55,55	1
92	OHX	1	4410	7/7	0.93	0.23	116,116,116,116	7
92	OHX	1	4374	7/7	0.93	0.50	77,77,77,77	7
91	MG	1	3443	1/1	0.93	0.40	77,77,77,77	0
92	OHX	5	4395	7/7	0.93	0.30	67,67,67,67	7
91	MG	n3	201	1/1	0.93	0.54	42,42,42,42	0
91	MG	5	3519	1/1	0.93	0.63	40,40,40,40	0
92	OHX	1	4409	7/7	0.93	0.23	90,90,90,90	7
91	MG	1	3807	1/1	0.93	0.64	52,52,52,52	0
91	MG	6	2076	1/1	0.93	0.44	59,59,59,59	0
91	MG	6	2004	1/1	0.93	0.60	56,56,56,56	0
92	OHX	6	2201	7/7	0.93	0.35	72,72,72,72	7
91	MG	5	3594	1/1	0.93	0.37	50,50,50,50	0
92	OHX	8	231	7/7	0.93	0.25	94,94,94,94	7
91	MG	1	4046	1/1	0.93	0.51	59,59,59,59	1
92	OHX	1	4473	7/7	0.93	0.35	64,64,64,64	7
91	MG	5	3925	1/1	0.93	0.12	113,113,113,113	0
91	MG	1	3900	1/1	0.93	0.20	54,54,54,54	0
91	MG	2	2008	1/1	0.93	1.11	91,91,91,91	0
92	OHX	2	2133	7/7	0.93	0.20	107,107,107,107	7
91	MG	1	3843	1/1	0.93	0.80	57,57,57,57	1
91	MG	5	3634	1/1	0.93	0.68	65,65,65,65	0
91	MG	1	3579	1/1	0.93	0.31	50,50,50,50	0
92	OHX	6	2245	7/7	0.93	0.20	100,100,100,100	7
92	OHX	1	4337	7/7	0.93	0.54	71,71,71,71	7
92	OHX	5	4320	7/7	0.93	0.31	91,91,91,91	7
91	MG	l5	302	1/1	0.93	0.49	68,68,68,68	1
91	MG	5	3435	1/1	0.93	0.36	58,58,58,58	0
91	MG	1	3587	1/1	0.93	0.46	43,43,43,43	0
91	MG	1	3999	1/1	0.93	0.63	45,45,45,45	1
92	OHX	1	4391	7/7	0.93	0.36	80,80,80,80	7
92	OHX	6	2280	7/7	0.93	0.35	72,72,72,72	7
92	OHX	5	4477	7/7	0.93	0.34	70,70,70,70	7
92	OHX	5	4504	7/7	0.93	0.56	69,69,69,69	7
92	OHX	1	4420	7/7	0.93	0.31	71,71,71,71	7
92	OHX	1	4354	7/7	0.93	0.21	76,76,76,76	7
91	MG	4	231	1/1	0.93	0.64	98,98,98,98	1
91	MG	o2	201	1/1	0.93	0.31	47,47,47,47	0
91	MG	5	3410	1/1	0.93	0.22	48,48,48,48	0
91	MG	m6	206	1/1	0.93	0.76	48,48,48,48	1
91	MG	5	3627	1/1	0.93	0.22	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	5	4443	7/7	0.93	0.35	68,68,68,68	7
91	MG	6	1904	1/1	0.93	0.29	96,96,96,96	0
93	ZN	q2	202	1/1	0.93	0.07	88,88,88,88	0
91	MG	5	3728	1/1	0.93	0.53	67,67,67,67	0
91	MG	1	4040	1/1	0.93	0.34	62,62,62,62	0
92	OHX	5	4463	7/7	0.93	0.23	97,97,97,97	7
92	OHX	1	4316	7/7	0.93	0.32	94,94,94,94	7
91	MG	4	217	1/1	0.93	0.27	67,67,67,67	0
92	OHX	6	2249	7/7	0.93	0.37	72,72,72,72	7
92	OHX	O1	202	7/7	0.93	0.28	89,89,89,89	7
91	MG	5	3592	1/1	0.93	0.62	50,50,50,50	0
92	OHX	6	2293	7/7	0.93	0.28	103,103,103,103	7
91	MG	5	4115	1/1	0.93	0.37	72,72,72,72	0
91	MG	5	3573	1/1	0.93	0.42	43,43,43,43	0
92	OHX	1	4449	7/7	0.93	0.53	62,62,62,62	7
91	MG	1	3642	1/1	0.93	0.54	57,57,57,57	0
91	MG	5	3950	1/1	0.93	0.39	66,66,66,66	1
91	MG	8	212	1/1	0.93	0.46	70,70,70,70	0
91	MG	5	3548	1/1	0.93	0.69	43,43,43,43	0
92	OHX	6	2257	7/7	0.93	0.25	70,70,70,70	7
91	MG	l3	401	1/1	0.93	0.54	45,45,45,45	1
91	MG	5	3799	1/1	0.93	0.30	55,55,55,55	1
92	OHX	1	4254	7/7	0.93	0.46	65,65,65,65	7
91	MG	1	3554	1/1	0.93	0.56	48,48,48,48	0
92	OHX	8	229	7/7	0.93	0.32	59,59,59,59	7
91	MG	1	3426	1/1	0.93	0.70	62,62,62,62	0
92	OHX	3	229	7/7	0.93	0.32	65,65,65,65	7
91	MG	6	2094	1/1	0.93	0.18	88,88,88,88	0
91	MG	5	4109	1/1	0.93	0.26	57,57,57,57	0
91	MG	2	1971	1/1	0.93	0.47	76,76,76,76	0
92	OHX	1	4350	7/7	0.93	0.27	55,55,55,55	7
92	OHX	L4	408	7/7	0.93	0.32	76,76,76,76	7
91	MG	5	3558	1/1	0.93	0.35	56,56,56,56	0
92	OHX	5	4565	7/7	0.93	0.38	77,77,77,77	7
91	MG	1	3633	1/1	0.93	0.40	70,70,70,70	0
91	MG	5	3503	1/1	0.93	0.49	47,47,47,47	0
91	MG	5	3523	1/1	0.93	0.20	52,52,52,52	0
91	MG	1	3744	1/1	0.93	0.31	55,55,55,55	0
91	MG	4	207	1/1	0.93	0.60	51,51,51,51	0
92	OHX	6	2212	7/7	0.93	0.26	105,105,105,105	7
92	OHX	6	2255	7/7	0.93	0.24	82,82,82,82	7
92	OHX	c5	201	7/7	0.93	0.29	127,127,127,127	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	2	1932	1/1	0.93	0.54	74,74,74,74	0
92	OHX	1	4214	7/7	0.93	0.44	69,69,69,69	7
91	MG	1	3556	1/1	0.93	0.42	60,60,60,60	0
91	MG	6	2138	1/1	0.93	0.18	94,94,94,94	0
92	OHX	1	4370	7/7	0.93	0.25	57,57,57,57	7
91	MG	1	3763	1/1	0.93	1.15	58,58,58,58	1
91	MG	5	3822	1/1	0.93	0.40	56,56,56,56	0
92	OHX	1	4394	7/7	0.93	0.68	72,72,72,72	7
91	MG	1	3847	1/1	0.93	0.52	54,54,54,54	1
91	MG	1	3594	1/1	0.93	0.53	44,44,44,44	0
92	OHX	5	4364	7/7	0.93	0.34	74,74,74,74	7
91	MG	5	4131	1/1	0.93	0.20	64,64,64,64	0
92	OHX	2	2175	7/7	0.93	0.22	113,113,113,113	7
91	MG	1	3702	1/1	0.93	0.43	45,45,45,45	0
91	MG	5	3689	1/1	0.93	0.49	61,61,61,61	0
91	MG	5	3787	1/1	0.93	0.46	80,80,80,80	0
91	MG	1	4047	1/1	0.93	0.40	89,89,89,89	0
91	MG	5	4060	1/1	0.93	0.88	60,60,60,60	1
91	MG	5	4110	1/1	0.93	0.72	49,49,49,49	1
91	MG	5	3702	1/1	0.93	0.10	67,67,67,67	0
91	MG	5	3545	1/1	0.93	0.26	68,68,68,68	0
92	OHX	1	4408	7/7	0.93	0.31	91,91,91,91	7
92	OHX	5	4375	7/7	0.93	0.28	82,82,82,82	7
91	MG	13	407	1/1	0.93	0.32	54,54,54,54	0
92	OHX	5	4355	7/7	0.93	0.51	63,63,63,63	7
92	OHX	5	4380	7/7	0.93	0.35	105,105,105,105	7
91	MG	5	3675	1/1	0.93	0.36	71,71,71,71	0
91	MG	1	4001	1/1	0.93	0.31	67,67,67,67	1
91	MG	5	3860	1/1	0.93	0.41	49,49,49,49	1
91	MG	1	3944	1/1	0.93	0.51	104,104,104,104	0
91	MG	1	4032	1/1	0.93	0.25	58,58,58,58	1
91	MG	5	3488	1/1	0.93	0.73	38,38,38,38	0
92	OHX	6	2210	7/7	0.93	0.35	90,90,90,90	7
91	MG	2	1922	1/1	0.93	0.83	81,81,81,81	0
91	MG	6	2073	1/1	0.93	0.33	73,73,73,73	0
91	MG	1	3535	1/1	0.93	0.27	47,47,47,47	0
91	MG	5	3959	1/1	0.93	0.19	68,68,68,68	0
91	MG	04	201	1/1	0.93	0.86	79,79,79,79	1
91	MG	1	3543	1/1	0.93	0.59	55,55,55,55	0
91	MG	6	1906	1/1	0.93	0.36	66,66,66,66	0
92	OHX	1	4474	7/7	0.93	0.21	77,77,77,77	7
92	OHX	1	4144	7/7	0.94	0.40	86,86,86,86	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	5	4379	7/7	0.94	0.24	88,88,88,88	7
91	MG	1	3657	1/1	0.94	0.34	57,57,57,57	0
92	OHX	6	2318	7/7	0.94	0.26	99,99,99,99	7
91	MG	5	3590	1/1	0.94	0.55	53,53,53,53	0
92	OHX	2	2193	7/7	0.94	0.20	109,109,109,109	7
91	MG	M3	202	1/1	0.94	0.97	58,58,58,58	1
92	OHX	5	4484	7/7	0.94	0.25	76,76,76,76	7
92	OHX	1	4225	7/7	0.94	0.38	67,67,67,67	7
91	MG	6	1931	1/1	0.94	0.39	77,77,77,77	0
91	MG	2	1915	1/1	0.94	0.44	87,87,87,87	0
92	OHX	2	2127	7/7	0.94	0.23	134,134,134,134	7
91	MG	1	3819	1/1	0.94	0.15	70,70,70,70	0
92	OHX	1	4373	7/7	0.94	0.21	86,86,86,86	7
91	MG	5	3414	1/1	0.94	0.31	51,51,51,51	0
91	MG	5	3827	1/1	0.94	0.46	51,51,51,51	0
92	OHX	1	4340	7/7	0.94	0.23	67,67,67,67	7
91	MG	1	3566	1/1	0.94	0.76	45,45,45,45	0
91	MG	5	3609	1/1	0.94	0.61	49,49,49,49	0
91	MG	5	4055	1/1	0.94	0.34	55,55,55,55	1
91	MG	1	3731	1/1	0.94	0.37	55,55,55,55	0
92	OHX	5	4363	7/7	0.94	0.25	77,77,77,77	7
91	MG	5	4025	1/1	0.94	0.37	45,45,45,45	0
92	OHX	2	2169	7/7	0.94	0.30	96,96,96,96	7
92	OHX	6	2247	7/7	0.94	0.29	89,89,89,89	7
92	OHX	1	4348	7/7	0.94	0.28	54,54,54,54	7
91	MG	5	3500	1/1	0.94	0.71	60,60,60,60	0
92	OHX	1	4403	7/7	0.94	0.41	70,70,70,70	7
91	MG	1	3904	1/1	0.94	0.28	66,66,66,66	1
92	OHX	5	4464	7/7	0.94	0.26	79,79,79,79	7
91	MG	5	3889	1/1	0.94	0.44	54,54,54,54	1
91	MG	6	1920	1/1	0.94	0.45	54,54,54,54	0
91	MG	m7	201	1/1	0.94	0.44	52,52,52,52	1
92	OHX	5	4390	7/7	0.94	0.27	66,66,66,66	7
92	OHX	5	4370	7/7	0.94	0.33	60,60,60,60	7
92	OHX	5	4426	7/7	0.94	0.36	64,64,64,64	7
92	OHX	1	4296	7/7	0.94	0.20	80,80,80,80	7
91	MG	5	3596	1/1	0.94	0.81	42,42,42,42	0
92	OHX	5	4561	7/7	0.94	0.43	62,62,62,62	7
92	OHX	6	2324	7/7	0.94	0.25	99,99,99,99	7
91	MG	5	3424	1/1	0.94	0.47	52,52,52,52	0
92	OHX	1	4369	7/7	0.94	0.31	59,59,59,59	7
91	MG	5	3647	1/1	0.94	0.30	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	1	3811	1/1	0.94	0.76	50,50,50,50	1
91	MG	6	1982	1/1	0.94	1.01	73,73,73,73	0
91	MG	1	3455	1/1	0.94	0.76	56,56,56,56	0
91	MG	5	3912	1/1	0.94	0.15	89,89,89,89	0
91	MG	n1	202	1/1	0.94	0.53	59,59,59,59	1
91	MG	1	3540	1/1	0.94	0.78	50,50,50,50	0
91	MG	1	3909	1/1	0.94	0.37	57,57,57,57	1
92	OHX	1	4405	7/7	0.94	0.19	86,86,86,86	7
91	MG	5	3446	1/1	0.94	0.41	45,45,45,45	0
91	MG	1	3924	1/1	0.94	0.20	52,52,52,52	0
92	OHX	1	4247	7/7	0.94	0.26	94,94,94,94	7
92	OHX	1	4280	7/7	0.94	0.28	65,65,65,65	7
91	MG	5	3960	1/1	0.94	0.27	55,55,55,55	0
91	MG	5	3882	1/1	0.94	0.41	46,46,46,46	0
92	OHX	5	4434	7/7	0.94	0.28	99,99,99,99	7
92	OHX	5	4354	7/7	0.94	0.32	79,79,79,79	7
92	OHX	5	4454	7/7	0.94	0.26	63,63,63,63	7
91	MG	5	3929	1/1	0.94	0.60	55,55,55,55	0
92	OHX	1	4453	7/7	0.94	0.51	65,65,65,65	7
91	MG	1	3564	1/1	0.94	0.37	72,72,72,72	0
91	MG	1	3500	1/1	0.94	0.20	60,60,60,60	1
92	OHX	2	2195	7/7	0.94	0.23	115,115,115,115	7
91	MG	5	3509	1/1	0.94	0.23	50,50,50,50	0
91	MG	7	204	1/1	0.94	0.36	65,65,65,65	0
91	MG	1	3612	1/1	0.94	0.22	47,47,47,47	0
92	OHX	5	4446	7/7	0.94	0.49	56,56,56,56	7
91	MG	1	3959	1/1	0.94	0.66	57,57,57,57	1
91	MG	1	3679	1/1	0.94	0.60	55,55,55,55	0
91	MG	1	3963	1/1	0.94	0.78	57,57,57,57	1
91	MG	1	3659	1/1	0.94	0.25	52,52,52,52	0
91	MG	6	1959	1/1	0.94	0.39	71,71,71,71	0
91	MG	5	4015	1/1	0.94	0.67	58,58,58,58	1
91	MG	1	3706	1/1	0.94	0.40	63,63,63,63	0
91	MG	1	3854	1/1	0.94	0.39	45,45,45,45	0
91	MG	5	3539	1/1	0.94	0.65	48,48,48,48	0
92	OHX	2	2189	7/7	0.94	0.41	85,85,85,85	7
92	OHX	8	227	7/7	0.94	0.27	76,76,76,76	7
91	MG	5	4066	1/1	0.94	0.43	59,59,59,59	1
92	OHX	5	4436	7/7	0.94	0.34	58,58,58,58	7
91	MG	5	3740	1/1	0.94	0.28	51,51,51,51	0
91	MG	M6	204	1/1	0.94	0.93	52,52,52,52	1
91	MG	1	3927	1/1	0.94	0.50	62,62,62,62	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	5	4538	7/7	0.94	0.15	120,120,120,120	7
91	MG	1	3874	1/1	0.94	0.23	52,52,52,52	1
91	MG	2	1908	1/1	0.94	0.28	90,90,90,90	0
91	MG	6	1968	1/1	0.94	0.52	100,100,100,100	0
91	MG	1	3886	1/1	0.94	0.71	58,58,58,58	1
92	OHX	5	4393	7/7	0.94	0.36	67,67,67,67	7
92	OHX	1	4302	7/7	0.94	0.39	60,60,60,60	7
91	MG	2	1935	1/1	0.94	0.16	106,106,106,106	0
91	MG	2	1937	1/1	0.94	0.53	70,70,70,70	0
92	OHX	C3	201	7/7	0.94	0.33	109,109,109,109	7
92	OHX	1	4392	7/7	0.94	0.28	55,55,55,55	7
91	MG	5	3522	1/1	0.94	0.52	40,40,40,40	0
91	MG	5	4111	1/1	0.94	0.57	64,64,64,64	0
91	MG	1	3452	1/1	0.94	0.56	59,59,59,59	0
92	OHX	1	4314	7/7	0.94	0.27	74,74,74,74	7
91	MG	1	3454	1/1	0.94	0.40	62,62,62,62	0
91	MG	O7	104	1/1	0.94	0.86	52,52,52,52	1
91	MG	S1	301	1/1	0.94	0.30	113,113,113,113	0
91	MG	1	3463	1/1	0.94	0.58	45,45,45,45	0
91	MG	1	4091	1/1	0.94	0.44	64,64,64,64	0
91	MG	1	3831	1/1	0.94	0.67	59,59,59,59	1
92	OHX	1	4257	7/7	0.94	0.19	109,109,109,109	7
92	OHX	1	4363	7/7	0.94	0.39	87,87,87,87	7
91	MG	m0	301	1/1	0.94	0.50	47,47,47,47	0
91	MG	7	210	1/1	0.94	0.12	75,75,75,75	0
92	OHX	6	2226	7/7	0.94	0.27	105,105,105,105	7
92	OHX	5	4559	7/7	0.94	0.27	100,100,100,100	7
92	OHX	L5	301	7/7	0.94	0.16	94,94,94,94	7
92	OHX	1	4381	7/7	0.94	0.24	75,75,75,75	7
91	MG	1	3964	1/1	0.94	1.06	47,47,47,47	1
91	MG	5	3843	1/1	0.94	0.47	54,54,54,54	0
91	MG	1	3417	1/1	0.94	0.20	54,54,54,54	0
91	MG	1	3429	1/1	0.94	0.88	62,62,62,62	0
91	MG	5	3612	1/1	0.94	0.36	58,58,58,58	0
92	OHX	5	4518	7/7	0.94	0.23	61,61,61,61	7
91	MG	5	3565	1/1	0.94	0.64	58,58,58,58	0
92	OHX	5	4472	7/7	0.94	0.34	71,71,71,71	7
92	OHX	5	4433	7/7	0.94	0.73	59,59,59,59	7
91	MG	5	3499	1/1	0.94	0.20	64,64,64,64	0
92	OHX	5	4404	7/7	0.94	0.29	62,62,62,62	7
91	MG	5	3915	1/1	0.94	0.24	55,55,55,55	0
91	MG	L2	304	1/1	0.94	0.68	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	5	4369	7/7	0.94	0.41	57,57,57,57	7
92	OHX	2	2235	7/7	0.94	0.27	78,78,78,78	7
92	OHX	1	4432	7/7	0.94	0.43	56,56,56,56	7
91	MG	5	4080	1/1	0.94	0.41	45,45,45,45	1
92	OHX	1	4324	7/7	0.94	0.27	90,90,90,90	7
91	MG	M9	203	1/1	0.94	0.80	79,79,79,79	1
92	OHX	15	309	7/7	0.94	0.20	100,100,100,100	7
91	MG	1	3412	1/1	0.94	0.60	49,49,49,49	0
91	MG	5	3713	1/1	0.94	0.26	49,49,49,49	1
91	MG	5	3430	1/1	0.94	0.69	47,47,47,47	0
91	MG	5	3687	1/1	0.94	0.65	54,54,54,54	0
92	OHX	2	2200	7/7	0.94	0.19	91,91,91,91	7
92	OHX	2	2128	7/7	0.94	0.27	107,107,107,107	7
91	MG	1	3436	1/1	0.94	0.51	59,59,59,59	0
92	OHX	1	4245	7/7	0.94	0.27	70,70,70,70	7
91	MG	6	1946	1/1	0.94	0.22	70,70,70,70	0
91	MG	L2	302	1/1	0.94	1.02	57,57,57,57	1
91	MG	1	4043	1/1	0.94	0.61	53,53,53,53	1
92	OHX	6	2310	7/7	0.94	0.19	93,93,93,93	7
91	MG	8	209	1/1	0.94	0.21	61,61,61,61	0
92	OHX	5	4553	7/7	0.94	0.27	80,80,80,80	7
91	MG	1	3773	1/1	0.94	0.38	62,62,62,62	0
91	MG	5	3493	1/1	0.94	0.68	61,61,61,61	0
91	MG	5	4141	1/1	0.94	0.34	50,50,50,50	0
91	MG	1	3468	1/1	0.94	0.25	67,67,67,67	0
92	OHX	2	2161	7/7	0.94	0.24	94,94,94,94	7
91	MG	5	3737	1/1	0.94	0.24	56,56,56,56	0
92	OHX	6	2302	7/7	0.94	0.21	124,124,124,124	7
92	OHX	5	4301	7/7	0.94	0.52	69,69,69,69	7
91	MG	L3	406	1/1	0.94	0.26	65,65,65,65	1
91	MG	1	3764	1/1	0.94	0.26	106,106,106,106	0
92	OHX	5	4566	7/7	0.94	0.35	57,57,57,57	7
91	MG	1	4060	1/1	0.94	0.51	71,71,71,71	0
91	MG	1	3422	1/1	0.94	0.44	51,51,51,51	0
92	OHX	5	4316	7/7	0.94	0.48	87,87,87,87	7
91	MG	4	215	1/1	0.94	0.60	77,77,77,77	0
91	MG	6	2048	1/1	0.94	0.47	84,84,84,84	0
92	OHX	2	2122	7/7	0.94	0.20	103,103,103,103	7
92	OHX	1	4368	7/7	0.94	0.60	86,86,86,86	7
92	OHX	5	4412	7/7	0.94	0.24	71,71,71,71	7
91	MG	1	3514	1/1	0.94	0.82	54,54,54,54	0
92	OHX	1	4508	7/7	0.94	0.41	72,72,72,72	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	1	4315	7/7	0.94	0.30	72,72,72,72	7
91	MG	2	1977	1/1	0.94	0.53	82,82,82,82	0
92	OHX	5	4424	7/7	0.94	0.35	67,67,67,67	7
92	OHX	1	4422	7/7	0.94	0.37	65,65,65,65	7
91	MG	5	3770	1/1	0.94	0.31	49,49,49,49	1
92	OHX	5	4359	7/7	0.94	0.22	112,112,112,112	7
92	OHX	c1	201	7/7	0.94	0.24	99,99,99,99	7
92	OHX	1	4259	7/7	0.94	0.20	91,91,91,91	7
92	OHX	5	4494	7/7	0.94	0.40	70,70,70,70	7
92	OHX	5	4468	7/7	0.94	0.25	82,82,82,82	7
91	MG	5	4065	1/1	0.94	0.14	104,104,104,104	0
91	MG	1	3604	1/1	0.94	0.61	47,47,47,47	0
92	OHX	6	2254	7/7	0.94	0.38	92,92,92,92	7
91	MG	5	3837	1/1	0.94	0.65	43,43,43,43	0
92	OHX	5	4315	7/7	0.94	0.31	93,93,93,93	7
91	MG	6	2047	1/1	0.94	0.17	72,72,72,72	0
92	OHX	1	4293	7/7	0.94	0.36	141,141,141,141	7
91	MG	2	2056	1/1	0.94	0.19	88,88,88,88	0
92	OHX	1	4292	7/7	0.94	0.10	157,157,157,157	7
91	MG	6	2081	1/1	0.94	0.37	67,67,67,67	0
91	MG	5	4009	1/1	0.94	0.46	48,48,48,48	1
92	OHX	5	4568	7/7	0.94	0.31	74,74,74,74	7
91	MG	1	3852	1/1	0.94	0.65	45,45,45,45	1
91	MG	5	4011	1/1	0.94	0.24	53,53,53,53	0
91	MG	5	3478	1/1	0.94	0.37	60,60,60,60	0
92	OHX	1	4306	7/7	0.95	0.38	72,72,72,72	7
92	OHX	1	4317	7/7	0.95	0.21	57,57,57,57	7
91	MG	1	3617	1/1	0.95	0.13	71,71,71,71	0
91	MG	N8	203	1/1	0.95	0.35	46,46,46,46	0
92	OHX	1	4277	7/7	0.95	0.25	62,62,62,62	7
92	OHX	6	2289	7/7	0.95	0.29	93,93,93,93	7
92	OHX	1	4294	7/7	0.95	0.40	73,73,73,73	7
92	OHX	2	2137	7/7	0.95	0.38	76,76,76,76	7
92	OHX	2	2243	7/7	0.95	0.20	130,130,130,130	7
92	OHX	1	4271	7/7	0.95	0.23	96,96,96,96	7
91	MG	5	3588	1/1	0.95	0.53	51,51,51,51	0
91	MG	5	3458	1/1	0.95	0.36	48,48,48,48	0
91	MG	5	3589	1/1	0.95	0.68	53,53,53,53	0
91	MG	1	3532	1/1	0.95	0.60	49,49,49,49	0
92	OHX	2	2099	7/7	0.95	0.27	118,118,118,118	7
92	OHX	2	2162	7/7	0.95	0.12	116,116,116,116	7
92	OHX	1	4276	7/7	0.95	0.28	68,68,68,68	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3457	1/1	0.95	0.60	53,53,53,53	0
92	OHX	5	4406	7/7	0.95	0.38	55,55,55,55	7
91	MG	L2	301	1/1	0.95	0.36	50,50,50,50	0
91	MG	1	3836	1/1	0.95	0.62	66,66,66,66	1
92	OHX	5	4345	7/7	0.95	0.45	58,58,58,58	7
91	MG	7	206	1/1	0.95	0.59	43,43,43,43	0
91	MG	1	3425	1/1	0.95	0.23	66,66,66,66	0
92	OHX	s4	302	7/7	0.95	0.27	95,95,95,95	7
92	OHX	1	4334	7/7	0.95	0.32	66,66,66,66	7
92	OHX	6	2261	7/7	0.95	0.22	72,72,72,72	7
91	MG	1	3567	1/1	0.95	0.59	54,54,54,54	0
91	MG	6	1981	1/1	0.95	0.42	71,71,71,71	0
92	OHX	6	2195	7/7	0.95	0.20	149,149,149,149	7
92	OHX	5	4503	7/7	0.95	0.34	64,64,64,64	7
91	MG	6	1922	1/1	0.95	0.41	61,61,61,61	0
91	MG	5	3551	1/1	0.95	0.49	40,40,40,40	0
91	MG	1	3926	1/1	0.95	0.58	84,84,84,84	1
92	OHX	5	4501	7/7	0.95	0.29	75,75,75,75	7
91	MG	5	3625	1/1	0.95	0.28	53,53,53,53	0
92	OHX	5	4515	7/7	0.95	0.38	58,58,58,58	7
92	OHX	2	2124	7/7	0.95	0.15	107,107,107,107	7
91	MG	5	3549	1/1	0.95	0.40	53,53,53,53	0
91	MG	5	4124	1/1	0.95	0.39	54,54,54,54	1
92	OHX	5	4294	7/7	0.95	0.34	102,102,102,102	7
91	MG	6	1901	1/1	0.95	0.42	63,63,63,63	0
91	MG	1	3920	1/1	0.95	0.35	59,59,59,59	1
92	OHX	5	4410	7/7	0.95	0.38	63,63,63,63	7
92	OHX	2	2130	7/7	0.95	0.16	111,111,111,111	7
91	MG	2	1931	1/1	0.95	0.29	85,85,85,85	0
92	OHX	5	4386	7/7	0.95	0.19	114,114,114,114	7
91	MG	1	3609	1/1	0.95	0.67	48,48,48,48	0
92	OHX	6	2323	7/7	0.95	0.38	71,71,71,71	7
91	MG	6	1907	1/1	0.95	0.42	65,65,65,65	0
91	MG	m5	301	1/1	0.95	0.56	69,69,69,69	0
91	MG	5	3698	1/1	0.95	0.68	61,61,61,61	0
92	OHX	2	2236	7/7	0.95	0.32	86,86,86,86	7
92	OHX	6	2190	7/7	0.95	0.20	100,100,100,100	7
91	MG	5	3901	1/1	0.95	0.50	72,72,72,72	0
92	OHX	c8	204	7/7	0.95	0.23	110,110,110,110	7
92	OHX	1	4329	7/7	0.95	0.19	87,87,87,87	7
91	MG	1	3618	1/1	0.95	0.30	60,60,60,60	0
91	MG	1	3507	1/1	0.95	0.36	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	4046	1/1	0.95	0.29	51,51,51,51	0
92	OHX	5	4240	7/7	0.95	0.26	68,68,68,68	7
91	MG	1	3580	1/1	0.95	0.50	41,41,41,41	0
92	OHX	5	4352	7/7	0.95	0.26	100,100,100,100	7
93	ZN	E1	501	1/1	0.95	0.08	142,142,142,142	0
92	OHX	6	2252	7/7	0.95	0.30	86,86,86,86	7
92	OHX	5	4360	7/7	0.95	0.58	74,74,74,74	7
92	OHX	5	4362	7/7	0.95	0.45	57,57,57,57	7
91	MG	2	2019	1/1	0.95	0.27	115,115,115,115	0
91	MG	5	3979	1/1	0.95	0.56	48,48,48,48	1
91	MG	8	219	1/1	0.95	0.40	79,79,79,79	0
92	OHX	5	4447	7/7	0.95	0.26	74,74,74,74	7
92	OHX	1	4298	7/7	0.95	0.32	63,63,63,63	7
91	MG	6	2015	1/1	0.95	0.30	87,87,87,87	0
91	MG	1	3829	1/1	0.95	0.22	59,59,59,59	0
91	MG	1	3494	1/1	0.95	0.33	67,67,67,67	0
92	OHX	6	2180	7/7	0.95	0.25	90,90,90,90	7
91	MG	5	3743	1/1	0.95	0.22	60,60,60,60	0
92	OHX	5	4265	7/7	0.95	0.14	123,123,123,123	7
92	OHX	5	4487	7/7	0.95	0.16	87,87,87,87	7
91	MG	6	1989	1/1	0.95	0.21	70,70,70,70	0
92	OHX	5	4373	7/7	0.95	0.31	70,70,70,70	7
91	MG	n8	204	1/1	0.95	0.59	53,53,53,53	1
91	MG	5	3639	1/1	0.95	0.53	51,51,51,51	0
92	OHX	1	4241	7/7	0.95	0.33	68,68,68,68	7
92	OHX	1	4345	7/7	0.95	0.38	76,76,76,76	7
92	OHX	1	4231	7/7	0.95	0.15	151,151,151,151	7
92	OHX	1	4322	7/7	0.95	0.46	65,65,65,65	7
91	MG	1	3645	1/1	0.95	0.35	51,51,51,51	0
92	OHX	8	228	7/7	0.95	0.26	91,91,91,91	7
92	OHX	2	2141	7/7	0.95	0.26	112,112,112,112	7
92	OHX	5	4261	7/7	0.95	0.24	82,82,82,82	7
91	MG	5	3692	1/1	0.95	0.26	62,62,62,62	0
91	MG	o9	101	1/1	0.95	0.83	64,64,64,64	1
91	MG	1	3676	1/1	0.95	0.31	52,52,52,52	0
91	MG	5	3751	1/1	0.95	0.09	129,129,129,129	0
91	MG	1	3796	1/1	0.95	0.52	60,60,60,60	1
92	OHX	1	4388	7/7	0.95	0.36	65,65,65,65	7
91	MG	5	3511	1/1	0.95	0.63	48,48,48,48	0
92	OHX	2	2113	7/7	0.95	0.20	115,115,115,115	7
91	MG	1	3747	1/1	0.95	0.40	57,57,57,57	0
92	OHX	6	2224	7/7	0.95	0.24	114,114,114,114	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	1	4384	7/7	0.95	0.22	90,90,90,90	7
91	MG	6	2031	1/1	0.95	0.49	82,82,82,82	1
91	MG	1	4023	1/1	0.95	1.05	50,50,50,50	1
92	OHX	5	4338	7/7	0.95	0.33	67,67,67,67	7
91	MG	2	1941	1/1	0.95	0.14	87,87,87,87	0
91	MG	1	3597	1/1	0.95	0.62	59,59,59,59	0
92	OHX	6	2228	7/7	0.95	0.23	88,88,88,88	7
92	OHX	6	2269	7/7	0.95	0.32	100,100,100,100	7
91	MG	5	3886	1/1	0.95	0.22	80,80,80,80	0
92	OHX	1	4238	7/7	0.95	0.32	67,67,67,67	7
92	OHX	5	4349	7/7	0.95	0.23	72,72,72,72	7
92	OHX	1	4372	7/7	0.95	0.34	67,67,67,67	7
91	MG	6	2024	1/1	0.95	0.28	71,71,71,71	1
92	OHX	2	2140	7/7	0.95	0.21	95,95,95,95	7
92	OHX	5	4381	7/7	0.95	0.24	77,77,77,77	7
91	MG	1	3498	1/1	0.95	0.30	52,52,52,52	0
92	OHX	1	4396	7/7	0.95	0.82	72,72,72,72	7
91	MG	1	3442	1/1	0.95	0.32	44,44,44,44	0
91	MG	7	213	1/1	0.95	0.40	52,52,52,52	0
92	OHX	2	2105	7/7	0.95	0.20	106,106,106,106	7
92	OHX	1	4328	7/7	0.95	0.28	86,86,86,86	7
92	OHX	5	4382	7/7	0.95	0.55	63,63,63,63	7
91	MG	7	226	1/1	0.95	0.45	64,64,64,64	1
91	MG	C8	201	1/1	0.95	0.07	107,107,107,107	0
91	MG	5	3582	1/1	0.95	0.40	47,47,47,47	0
91	MG	6	2127	1/1	0.95	1.20	102,102,102,102	1
91	MG	5	3847	1/1	0.95	0.56	55,55,55,55	1
92	OHX	5	4341	7/7	0.95	0.22	98,98,98,98	7
91	MG	5	3729	1/1	0.95	0.63	55,55,55,55	0
91	MG	5	3538	1/1	0.95	0.42	44,44,44,44	0
91	MG	5	3670	1/1	0.95	0.31	51,51,51,51	0
92	OHX	1	4263	7/7	0.95	0.24	101,101,101,101	7
91	MG	5	4076	1/1	0.95	0.29	58,58,58,58	1
92	OHX	5	4401	7/7	0.95	0.23	73,73,73,73	7
91	MG	5	3778	1/1	0.95	0.41	51,51,51,51	1
91	MG	1	3596	1/1	0.95	0.35	65,65,65,65	0
92	OHX	1	4220	7/7	0.95	0.31	95,95,95,95	7
92	OHX	6	2239	7/7	0.95	0.20	82,82,82,82	7
91	MG	1	3447	1/1	0.95	0.25	108,108,108,108	0
92	OHX	1	4347	7/7	0.95	0.39	86,86,86,86	7
92	OHX	5	4350	7/7	0.95	0.28	72,72,72,72	7
92	OHX	7	235	7/7	0.95	0.27	89,89,89,89	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	1	3703	1/1	0.95	0.78	75,75,75,75	0
91	MG	6	2106	1/1	0.95	0.09	100,100,100,100	0
92	OHX	1	4402	7/7	0.95	0.24	72,72,72,72	7
91	MG	6	2104	1/1	0.95	0.25	100,100,100,100	0
92	OHX	6	2295	7/7	0.95	0.48	75,75,75,75	7
91	MG	1	3415	1/1	0.95	0.48	53,53,53,53	0
91	MG	1	4050	1/1	0.95	0.14	68,68,68,68	0
91	MG	5	3916	1/1	0.95	0.28	51,51,51,51	0
91	MG	1	3992	1/1	0.95	0.24	59,59,59,59	0
92	OHX	1	4311	7/7	0.95	0.17	83,83,83,83	7
92	OHX	1	4210	7/7	0.95	0.29	70,70,70,70	7
92	OHX	5	4545	7/7	0.95	0.19	73,73,73,73	7
92	OHX	2	2151	7/7	0.95	0.50	81,81,81,81	7
92	OHX	6	2282	7/7	0.95	0.50	73,73,73,73	7
92	OHX	1	4297	7/7	0.95	0.32	69,69,69,69	7
92	OHX	1	4416	7/7	0.95	0.23	65,65,65,65	7
91	MG	1	3915	1/1	0.95	0.60	67,67,67,67	0
92	OHX	6	2232	7/7	0.95	0.15	102,102,102,102	7
91	MG	5	3980	1/1	0.95	0.92	64,64,64,64	1
91	MG	1	4054	1/1	0.95	0.27	83,83,83,83	1
91	MG	13	402	1/1	0.95	0.30	45,45,45,45	1
91	MG	1	4093	1/1	0.95	0.92	50,50,50,50	1
92	OHX	6	2216	7/7	0.95	0.27	80,80,80,80	7
91	MG	1	4086	1/1	0.95	0.88	66,66,66,66	1
92	OHX	6	2236	7/7	0.95	0.19	122,122,122,122	7
92	OHX	4	242	7/7	0.95	0.20	107,107,107,107	7
91	MG	1	3990	1/1	0.95	0.20	84,84,84,84	0
91	MG	1	3682	1/1	0.95	0.27	52,52,52,52	0
91	MG	5	3597	1/1	0.95	0.65	44,44,44,44	0
92	OHX	1	4272	7/7	0.95	0.22	68,68,68,68	7
91	MG	6	2072	1/1	0.95	0.36	91,91,91,91	0
92	OHX	5	4560	7/7	0.95	0.25	75,75,75,75	7
91	MG	1	3527	1/1	0.95	0.52	47,47,47,47	0
91	MG	6	1957	1/1	0.95	0.36	89,89,89,89	0
92	OHX	6	2203	7/7	0.95	0.27	79,79,79,79	7
92	OHX	5	4491	7/7	0.95	0.36	65,65,65,65	7
92	OHX	2	2183	7/7	0.95	0.20	99,99,99,99	7
91	MG	5	3924	1/1	0.95	0.47	66,66,66,66	1
92	OHX	5	4377	7/7	0.95	0.32	82,82,82,82	7
92	OHX	m0	304	7/7	0.96	0.20	100,100,100,100	7
92	OHX	O7	107	7/7	0.96	0.24	83,83,83,83	7
91	MG	5	4126	1/1	0.96	0.52	56,56,56,56	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	8	226	7/7	0.96	0.24	86,86,86,86	7
91	MG	5	3818	1/1	0.96	0.23	47,47,47,47	1
92	OHX	1	4226	7/7	0.96	0.29	140,140,140,140	7
91	MG	5	4117	1/1	0.96	0.96	50,50,50,50	1
91	MG	5	3622	1/1	0.96	0.47	45,45,45,45	0
92	OHX	1	4239	7/7	0.96	0.38	70,70,70,70	7
91	MG	5	3442	1/1	0.96	0.46	69,69,69,69	0
91	MG	5	3595	1/1	0.96	0.56	56,56,56,56	0
91	MG	5	3576	1/1	0.96	0.64	44,44,44,44	0
91	MG	O7	106	1/1	0.96	0.86	57,57,57,57	1
92	OHX	5	4325	7/7	0.96	0.20	70,70,70,70	7
91	MG	5	3976	1/1	0.96	0.35	48,48,48,48	0
92	OHX	1	4333	7/7	0.96	0.28	66,66,66,66	7
92	OHX	1	4307	7/7	0.96	0.34	50,50,50,50	7
92	OHX	5	4291	7/7	0.96	0.35	66,66,66,66	7
92	OHX	6	2206	7/7	0.96	0.30	66,66,66,66	7
91	MG	l2	301	1/1	0.96	0.84	58,58,58,58	1
91	MG	1	3402	1/1	0.96	0.35	59,59,59,59	0
92	OHX	6	2279	7/7	0.96	0.31	64,64,64,64	7
91	MG	1	4013	1/1	0.96	0.57	67,67,67,67	1
92	OHX	1	4184	7/7	0.96	0.24	124,124,124,124	7
92	OHX	1	4424	7/7	0.96	0.29	67,67,67,67	7
92	OHX	5	4270	7/7	0.96	0.17	78,78,78,78	7
92	OHX	6	2227	7/7	0.96	0.18	92,92,92,92	7
92	OHX	5	4285	7/7	0.96	0.25	62,62,62,62	7
93	ZN	Q2	501	1/1	0.96	0.09	90,90,90,90	0
91	MG	5	3987	1/1	0.96	0.57	52,52,52,52	0
92	OHX	1	4246	7/7	0.96	0.34	88,88,88,88	7
91	MG	1	4034	1/1	0.96	0.58	50,50,50,50	1
92	OHX	5	4483	7/7	0.96	0.23	81,81,81,81	7
91	MG	m7	207	1/1	0.96	0.88	53,53,53,53	1
91	MG	2	1995	1/1	0.96	0.29	93,93,93,93	1
92	OHX	5	4457	7/7	0.96	0.32	58,58,58,58	7
91	MG	6	2105	1/1	0.96	0.55	72,72,72,72	0
92	OHX	1	4230	7/7	0.96	0.26	73,73,73,73	7
92	OHX	5	4307	7/7	0.96	0.26	71,71,71,71	7
92	OHX	5	4257	7/7	0.96	0.34	56,56,56,56	7
91	MG	4	209	1/1	0.96	0.48	50,50,50,50	0
91	MG	5	4081	1/1	0.96	0.76	53,53,53,53	1
92	OHX	6	2259	7/7	0.96	0.22	74,74,74,74	7
91	MG	5	3462	1/1	0.96	0.75	49,49,49,49	0
92	OHX	5	4481	7/7	0.96	0.29	63,63,63,63	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	1	4433	7/7	0.96	0.26	87,87,87,87	7
92	OHX	6	2196	7/7	0.96	0.17	163,163,163,163	7
92	OHX	6	2272	7/7	0.96	0.22	80,80,80,80	7
91	MG	5	3419	1/1	0.96	0.32	47,47,47,47	0
92	OHX	1	4382	7/7	0.96	0.23	71,71,71,71	7
91	MG	d3	201	1/1	0.96	1.62	68,68,68,68	1
92	OHX	1	4265	7/7	0.96	0.30	73,73,73,73	7
92	OHX	5	4343	7/7	0.96	0.14	77,77,77,77	7
91	MG	6	1951	1/1	0.96	0.28	84,84,84,84	0
91	MG	5	3623	1/1	0.96	0.34	49,49,49,49	0
91	MG	1	3585	1/1	0.96	0.60	54,54,54,54	0
92	OHX	1	4366	7/7	0.96	0.42	78,78,78,78	7
91	MG	6	2064	1/1	0.96	0.46	103,103,103,103	0
92	OHX	2	2171	7/7	0.96	0.15	116,116,116,116	7
92	OHX	6	2213	7/7	0.96	0.20	103,103,103,103	7
92	OHX	5	4310	7/7	0.96	0.32	65,65,65,65	7
92	OHX	4	246	7/7	0.96	0.28	82,82,82,82	7
91	MG	1	3511	1/1	0.96	0.62	43,43,43,43	0
92	OHX	2	2101	7/7	0.96	0.26	82,82,82,82	7
91	MG	2	2042	1/1	0.96	0.24	90,90,90,90	0
92	OHX	5	4288	7/7	0.96	0.43	65,65,65,65	7
92	OHX	2	2123	7/7	0.96	0.20	98,98,98,98	7
92	OHX	8	224	7/7	0.96	0.28	75,75,75,75	7
91	MG	6	2116	1/1	0.96	1.04	65,65,65,65	1
91	MG	n8	201	1/1	0.96	0.41	69,69,69,69	1
92	OHX	2	2142	7/7	0.96	0.24	150,150,150,150	7
91	MG	1	3834	1/1	0.96	0.26	71,71,71,71	0
92	OHX	1	4202	7/7	0.96	0.29	107,107,107,107	7
91	MG	5	3857	1/1	0.96	0.74	46,46,46,46	1
92	OHX	1	4357	7/7	0.96	0.43	69,69,69,69	7
92	OHX	6	2229	7/7	0.96	0.28	77,77,77,77	7
91	MG	5	3851	1/1	0.96	0.11	60,60,60,60	0
91	MG	1	3931	1/1	0.96	1.00	71,71,71,71	1
91	MG	1	3428	1/1	0.96	0.27	66,66,66,66	0
92	OHX	5	4281	7/7	0.96	0.29	65,65,65,65	7
92	OHX	2	2174	7/7	0.96	0.24	83,83,83,83	7
92	OHX	3	224	7/7	0.96	0.28	92,92,92,92	7
92	OHX	2	2222	7/7	0.96	0.28	101,101,101,101	7
91	MG	M8	202	1/1	0.96	0.99	61,61,61,61	1
91	MG	5	3938	1/1	0.96	0.79	64,64,64,64	0
92	OHX	1	4364	7/7	0.96	0.32	60,60,60,60	7
92	OHX	1	4505	7/7	0.96	0.14	155,155,155,155	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	1	4500	7/7	0.96	0.29	89,89,89,89	7
92	OHX	7	236	7/7	0.96	0.27	64,64,64,64	7
92	OHX	5	4408	7/7	0.96	0.23	79,79,79,79	7
92	OHX	5	4264	7/7	0.96	0.26	80,80,80,80	7
91	MG	5	3510	1/1	0.96	0.49	50,50,50,50	0
92	OHX	2	2120	7/7	0.96	0.10	134,134,134,134	7
92	OHX	5	4550	7/7	0.96	0.24	96,96,96,96	7
91	MG	8	208	1/1	0.96	0.16	74,74,74,74	0
92	OHX	5	4254	7/7	0.96	0.22	114,114,114,114	7
91	MG	5	4027	1/1	0.96	0.73	45,45,45,45	1
91	MG	1	3526	1/1	0.96	0.50	54,54,54,54	0
91	MG	15	303	1/1	0.96	0.52	53,53,53,53	0
91	MG	5	3557	1/1	0.96	0.51	64,64,64,64	0
92	OHX	5	4304	7/7	0.96	0.24	62,62,62,62	7
91	MG	1	3863	1/1	0.96	0.23	51,51,51,51	1
91	MG	1	3621	1/1	0.96	0.43	77,77,77,77	0
92	OHX	1	4412	7/7	0.96	0.29	79,79,79,79	7
91	MG	1	4018	1/1	0.96	0.78	55,55,55,55	1
91	MG	6	1961	1/1	0.96	0.50	64,64,64,64	0
91	MG	5	3593	1/1	0.96	0.46	48,48,48,48	0
92	OHX	1	4401	7/7	0.96	0.27	75,75,75,75	7
91	MG	O1	201	1/1	0.96	0.79	81,81,81,81	1
92	OHX	1	4386	7/7	0.96	0.36	76,76,76,76	7
92	OHX	3	225	7/7	0.96	0.23	96,96,96,96	7
91	MG	1	3501	1/1	0.96	0.47	48,48,48,48	0
92	OHX	5	4293	7/7	0.96	0.23	71,71,71,71	7
91	MG	1	3658	1/1	0.96	0.28	53,53,53,53	0
91	MG	5	4036	1/1	0.96	0.42	50,50,50,50	1
91	MG	5	3603	1/1	0.96	0.75	49,49,49,49	0
92	OHX	5	4356	7/7	0.96	0.20	83,83,83,83	7
92	OHX	5	4235	7/7	0.96	0.28	70,70,70,70	7
91	MG	6	1912	1/1	0.96	0.36	98,98,98,98	0
92	OHX	5	4557	7/7	0.96	0.20	156,156,156,156	7
92	OHX	6	2193	7/7	0.96	0.16	143,143,143,143	7
91	MG	1	3890	1/1	0.96	1.31	56,56,56,56	1
92	OHX	5	4321	7/7	0.96	0.13	119,119,119,119	7
92	OHX	2	2254	7/7	0.96	0.28	82,82,82,82	7
92	OHX	6	2200	7/7	0.96	0.19	98,98,98,98	7
92	OHX	2	2139	7/7	0.96	0.31	93,93,93,93	7
91	MG	5	3797	1/1	0.96	0.20	59,59,59,59	0
91	MG	N8	204	1/1	0.96	0.90	47,47,47,47	1
91	MG	o3	202	1/1	0.96	0.40	49,49,49,49	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	1	3561	1/1	0.96	0.37	59,59,59,59	0
92	OHX	2	2134	7/7	0.96	0.27	72,72,72,72	7
91	MG	5	3869	1/1	0.96	0.87	51,51,51,51	1
92	OHX	6	2219	7/7	0.96	0.27	71,71,71,71	7
92	OHX	5	4326	7/7	0.96	0.30	79,79,79,79	7
91	MG	6	1973	1/1	0.96	0.20	95,95,95,95	0
92	OHX	5	4306	7/7	0.96	0.28	67,67,67,67	7
92	OHX	5	4358	7/7	0.96	0.35	55,55,55,55	7
91	MG	6	2009	1/1	0.96	0.42	111,111,111,111	0
91	MG	1	3483	1/1	0.96	0.56	82,82,82,82	0
92	OHX	2	2136	7/7	0.96	0.41	87,87,87,87	7
92	OHX	1	4309	7/7	0.96	0.37	83,83,83,83	7
91	MG	5	3988	1/1	0.96	0.31	65,65,65,65	0
91	MG	5	4075	1/1	0.96	0.36	60,60,60,60	0
91	MG	1	3608	1/1	0.96	0.45	43,43,43,43	0
91	MG	C1	202	1/1	0.96	1.40	83,83,83,83	1
92	OHX	1	4305	7/7	0.96	0.25	86,86,86,86	7
92	OHX	4	241	7/7	0.96	0.34	57,57,57,57	7
92	OHX	5	4287	7/7	0.96	0.34	56,56,56,56	7
92	OHX	1	4256	7/7	0.96	0.37	92,92,92,92	7
91	MG	6	1910	1/1	0.96	0.37	114,114,114,114	0
91	MG	6	1903	1/1	0.96	0.71	59,59,59,59	0
92	OHX	5	4336	7/7	0.96	0.48	58,58,58,58	7
92	OHX	5	4272	7/7	0.96	0.35	56,56,56,56	7
92	OHX	2	2144	7/7	0.96	0.20	101,101,101,101	7
91	MG	1	4507	1/1	0.96	0.43	54,54,54,54	1
92	OHX	1	4275	7/7	0.96	0.17	113,113,113,113	7
91	MG	1	4028	1/1	0.96	0.27	69,69,69,69	0
91	MG	M5	304	1/1	0.96	0.93	54,54,54,54	1
92	OHX	6	2207	7/7	0.96	0.29	100,100,100,100	7
91	MG	1	3577	1/1	0.96	0.83	51,51,51,51	0
92	OHX	2	2176	7/7	0.96	0.19	96,96,96,96	7
92	OHX	5	4396	7/7	0.96	0.60	52,52,52,52	7
92	OHX	14	404	7/7	0.96	0.22	83,83,83,83	7
91	MG	5	3781	1/1	0.96	0.69	58,58,58,58	1
91	MG	8	203	1/1	0.96	0.34	55,55,55,55	0
92	OHX	8	225	7/7	0.96	0.24	99,99,99,99	7
91	MG	5	3952	1/1	0.96	1.55	60,60,60,60	1
92	OHX	1	4395	7/7	0.96	0.23	76,76,76,76	7
92	OHX	5	4331	7/7	0.96	0.32	75,75,75,75	7
91	MG	1	3560	1/1	0.96	0.43	44,44,44,44	0
92	OHX	8	223	7/7	0.96	0.26	75,75,75,75	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	6	2208	7/7	0.96	0.25	76,76,76,76	7
91	MG	2	1994	1/1	0.96	0.35	76,76,76,76	0
92	OHX	1	4249	7/7	0.96	0.23	87,87,87,87	7
92	OHX	5	4230	7/7	0.96	0.25	91,91,91,91	7
91	MG	o2	203	1/1	0.96	0.71	45,45,45,45	1
92	OHX	2	2096	7/7	0.96	0.35	84,84,84,84	7
91	MG	5	3776	1/1	0.96	0.32	48,48,48,48	1
92	OHX	1	4431	7/7	0.96	0.26	67,67,67,67	7
91	MG	m9	201	1/1	0.96	1.04	68,68,68,68	1
92	OHX	C8	203	7/7	0.96	0.19	107,107,107,107	7
91	MG	6	1944	1/1	0.96	0.50	86,86,86,86	0
91	MG	1	3445	1/1	0.96	0.38	60,60,60,60	0
92	OHX	5	4299	7/7	0.96	0.14	148,148,148,148	7
91	MG	8	213	1/1	0.96	0.50	62,62,62,62	0
92	OHX	5	4353	7/7	0.96	0.34	59,59,59,59	7
92	OHX	5	4247	7/7	0.96	0.29	61,61,61,61	7
91	MG	l3	405	1/1	0.96	0.57	46,46,46,46	1
92	OHX	5	4445	7/7	0.96	0.37	69,69,69,69	7
92	OHX	6	2167	7/7	0.96	0.24	107,107,107,107	7
91	MG	5	3610	1/1	0.96	0.68	45,45,45,45	0
92	OHX	1	4313	7/7	0.96	0.27	67,67,67,67	7
92	OHX	6	2331	7/7	0.96	0.26	90,90,90,90	7
91	MG	5	3814	1/1	0.96	0.55	51,51,51,51	0
92	OHX	2	2112	7/7	0.96	0.24	86,86,86,86	7
92	OHX	1	4284	7/7	0.96	0.32	73,73,73,73	7
91	MG	5	3796	1/1	0.96	0.39	50,50,50,50	0
92	OHX	5	4421	7/7	0.96	0.40	87,87,87,87	7
92	OHX	O7	108	7/7	0.96	0.31	70,70,70,70	7
91	MG	1	3997	1/1	0.96	0.30	69,69,69,69	1
92	OHX	1	4308	7/7	0.96	0.31	92,92,92,92	7
91	MG	5	3607	1/1	0.96	0.43	50,50,50,50	0
91	MG	1	3552	1/1	0.96	0.45	44,44,44,44	0
91	MG	5	3708	1/1	0.96	0.92	59,59,59,59	1
91	MG	5	3520	1/1	0.96	0.32	53,53,53,53	0
91	MG	o7	101	1/1	0.96	0.26	52,52,52,52	0
92	OHX	SR	401	7/7	0.96	0.11	139,139,139,139	7
91	MG	1	3565	1/1	0.96	0.29	52,52,52,52	0
91	MG	5	4049	1/1	0.96	0.72	51,51,51,51	1
92	OHX	1	4168	7/7	0.96	0.21	84,84,84,84	7
91	MG	6	2109	1/1	0.96	0.13	97,97,97,97	0
91	MG	5	3923	1/1	0.96	0.58	48,48,48,48	0
91	MG	5	4085	1/1	0.96	0.53	62,62,62,62	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	3706	1/1	0.96	0.40	49,49,49,49	0
91	MG	1	3759	1/1	0.96	0.47	48,48,48,48	0
91	MG	N3	202	1/1	0.96	0.66	52,52,52,52	0
91	MG	1	3528	1/1	0.97	0.62	42,42,42,42	0
91	MG	5	3436	1/1	0.97	0.53	58,58,58,58	0
92	OHX	5	4283	7/7	0.97	0.28	80,80,80,80	7
91	MG	1	3684	1/1	0.97	0.16	66,66,66,66	0
91	MG	1	3571	1/1	0.97	0.49	51,51,51,51	0
92	OHX	5	4329	7/7	0.97	0.27	76,76,76,76	7
92	OHX	2	2094	7/7	0.97	0.29	92,92,92,92	7
92	OHX	5	4263	7/7	0.97	0.28	74,74,74,74	7
92	OHX	1	4213	7/7	0.97	0.28	65,65,65,65	7
91	MG	1	3437	1/1	0.97	0.29	51,51,51,51	0
91	MG	1	3493	1/1	0.97	0.30	56,56,56,56	1
92	OHX	1	4262	7/7	0.97	0.24	76,76,76,76	7
92	OHX	5	4376	7/7	0.97	0.11	90,90,90,90	7
91	MG	5	4043	1/1	0.97	0.80	49,49,49,49	1
91	MG	1	3789	1/1	0.97	0.23	53,53,53,53	0
92	OHX	6	2184	7/7	0.97	0.28	93,93,93,93	7
91	MG	5	3498	1/1	0.97	0.38	53,53,53,53	0
92	OHX	2	2177	7/7	0.97	0.27	81,81,81,81	7
92	OHX	7	201	7/7	0.97	0.42	56,56,56,56	7
91	MG	1	3979	1/1	0.97	0.72	50,50,50,50	1
92	OHX	m5	304	7/7	0.97	0.26	90,90,90,90	7
92	OHX	6	2308	7/7	0.97	0.23	90,90,90,90	7
92	OHX	1	4489	7/7	0.97	0.26	63,63,63,63	7
91	MG	5	3563	1/1	0.97	0.68	46,46,46,46	0
91	MG	1	3798	1/1	0.97	0.42	59,59,59,59	0
91	MG	4	202	1/1	0.97	0.40	56,56,56,56	1
92	OHX	1	4260	7/7	0.97	0.18	94,94,94,94	7
92	OHX	2	2118	7/7	0.97	0.20	106,106,106,106	7
92	OHX	4	239	7/7	0.97	0.22	71,71,71,71	7
91	MG	5	4095	1/1	0.97	0.71	54,54,54,54	0
91	MG	5	3572	1/1	0.97	0.59	48,48,48,48	0
91	MG	1	3711	1/1	0.97	0.49	51,51,51,51	0
92	OHX	2	2154	7/7	0.97	0.28	90,90,90,90	7
92	OHX	6	2246	7/7	0.97	0.23	72,72,72,72	7
92	OHX	2	2095	7/7	0.97	0.22	100,100,100,100	7
92	OHX	2	2121	7/7	0.97	0.19	78,78,78,78	7
92	OHX	6	2275	7/7	0.97	0.13	102,102,102,102	7
92	OHX	1	4197	7/7	0.97	0.38	66,66,66,66	7
91	MG	6	1967	1/1	0.97	0.32	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	5	4573	7/7	0.97	0.39	69,69,69,69	7
92	OHX	5	4311	7/7	0.97	0.24	66,66,66,66	7
92	OHX	2	2182	7/7	0.97	0.25	88,88,88,88	7
92	OHX	1	4290	7/7	0.97	0.26	54,54,54,54	7
92	OHX	6	2189	7/7	0.97	0.26	76,76,76,76	7
92	OHX	5	4555	7/7	0.97	0.23	97,97,97,97	7
91	MG	5	3854	1/1	0.97	0.62	48,48,48,48	1
92	OHX	5	4237	7/7	0.97	0.22	74,74,74,74	7
91	MG	1	3534	1/1	0.97	0.62	48,48,48,48	0
92	OHX	1	4371	7/7	0.97	0.46	76,76,76,76	7
92	OHX	5	4214	7/7	0.97	0.23	73,73,73,73	7
92	OHX	5	4297	7/7	0.97	0.24	60,60,60,60	7
91	MG	1	3513	1/1	0.97	0.41	45,45,45,45	0
92	OHX	5	4276	7/7	0.97	0.22	97,97,97,97	7
91	MG	5	3877	1/1	0.97	0.34	63,63,63,63	0
92	OHX	1	4209	7/7	0.97	0.20	80,80,80,80	7
91	MG	L4	404	1/1	0.97	0.98	53,53,53,53	1
92	OHX	5	4241	7/7	0.97	0.33	66,66,66,66	7
91	MG	1	3614	1/1	0.97	0.31	52,52,52,52	0
92	OHX	6	2194	7/7	0.97	0.21	98,98,98,98	7
91	MG	C1	201	1/1	0.97	1.45	79,79,79,79	1
91	MG	1	3606	1/1	0.97	0.64	42,42,42,42	0
91	MG	5	3859	1/1	0.97	0.78	47,47,47,47	1
92	OHX	6	2220	7/7	0.97	0.15	98,98,98,98	7
91	MG	5	3659	1/1	0.97	0.26	41,41,41,41	0
91	MG	5	3604	1/1	0.97	0.46	41,41,41,41	0
91	MG	6	2118	1/1	0.97	0.42	96,96,96,96	0
92	OHX	5	4258	7/7	0.97	0.34	77,77,77,77	7
91	MG	1	3553	1/1	0.97	0.49	51,51,51,51	0
92	OHX	6	2175	7/7	0.97	0.19	101,101,101,101	7
92	OHX	5	4225	7/7	0.97	0.25	90,90,90,90	7
92	OHX	2	2089	7/7	0.97	0.20	102,102,102,102	7
91	MG	1	3475	1/1	0.97	0.55	40,40,40,40	0
91	MG	N8	201	1/1	0.97	0.61	44,44,44,44	1
92	OHX	2	2145	7/7	0.97	0.16	146,146,146,146	7
91	MG	5	3641	1/1	0.97	0.27	59,59,59,59	0
92	OHX	2	2160	7/7	0.97	0.24	87,87,87,87	7
92	OHX	2	2172	7/7	0.97	0.24	102,102,102,102	7
92	OHX	1	4502	7/7	0.97	0.15	102,102,102,102	7
92	OHX	1	4172	7/7	0.97	0.20	88,88,88,88	7
91	MG	1	3550	1/1	0.97	0.50	43,43,43,43	0
92	OHX	2	2102	7/7	0.97	0.22	106,106,106,106	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	4	240	7/7	0.97	0.24	90,90,90,90	7
92	OHX	2	2165	7/7	0.97	0.15	102,102,102,102	7
92	OHX	6	2223	7/7	0.97	0.23	111,111,111,111	7
91	MG	1	3523	1/1	0.97	0.60	42,42,42,42	0
92	OHX	6	2181	7/7	0.97	0.22	124,124,124,124	7
91	MG	1	3923	1/1	0.97	0.25	56,56,56,56	0
92	OHX	2	2106	7/7	0.97	0.34	82,82,82,82	7
92	OHX	5	4286	7/7	0.97	0.26	59,59,59,59	7
92	OHX	5	4368	7/7	0.97	0.28	53,53,53,53	7
92	OHX	5	4309	7/7	0.97	0.33	66,66,66,66	7
91	MG	2	2036	1/1	0.97	0.63	70,70,70,70	0
92	OHX	5	4245	7/7	0.97	0.27	102,102,102,102	7
92	OHX	1	4216	7/7	0.97	0.19	96,96,96,96	7
91	MG	6	2075	1/1	0.97	0.21	107,107,107,107	0
92	OHX	2	2108	7/7	0.97	0.27	97,97,97,97	7
92	OHX	5	4465	7/7	0.97	0.34	75,75,75,75	7
92	OHX	5	4252	7/7	0.97	0.25	70,70,70,70	7
92	OHX	6	2260	7/7	0.97	0.24	68,68,68,68	7
91	MG	6	1933	1/1	0.97	0.22	76,76,76,76	0
91	MG	5	3602	1/1	0.97	0.67	46,46,46,46	0
92	OHX	1	4242	7/7	0.97	0.23	69,69,69,69	7
92	OHX	7	238	7/7	0.97	0.30	63,63,63,63	7
91	MG	1	3607	1/1	0.97	0.64	39,39,39,39	0
92	OHX	1	4346	7/7	0.97	0.32	76,76,76,76	7
92	OHX	5	4300	7/7	0.97	0.35	65,65,65,65	7
91	MG	5	3963	1/1	0.97	0.22	71,71,71,71	0
92	OHX	1	4193	7/7	0.97	0.26	92,92,92,92	7
92	OHX	5	4551	7/7	0.97	0.27	77,77,77,77	7
92	OHX	5	4372	7/7	0.97	0.29	63,63,63,63	7
92	OHX	1	4496	7/7	0.97	0.20	86,86,86,86	7
92	OHX	5	4296	7/7	0.97	0.11	108,108,108,108	7
91	MG	5	4023	1/1	0.97	0.33	48,48,48,48	1
92	OHX	1	4349	7/7	0.97	0.20	63,63,63,63	7
92	OHX	5	4323	7/7	0.97	0.20	74,74,74,74	7
91	MG	6	2103	1/1	0.97	0.16	91,91,91,91	0
92	OHX	3	223	7/7	0.97	0.15	92,92,92,92	7
91	MG	1	3410	1/1	0.97	0.49	41,41,41,41	0
91	MG	5	4013	1/1	0.97	0.56	57,57,57,57	1
92	OHX	1	4469	7/7	0.97	0.33	66,66,66,66	7
91	MG	5	4028	1/1	0.97	0.57	47,47,47,47	1
92	OHX	6	2339	7/7	0.97	0.23	126,126,126,126	7
92	OHX	1	4222	7/7	0.97	0.31	80,80,80,80	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	2	2179	7/7	0.97	0.17	80,80,80,80	7
91	MG	5	3566	1/1	0.97	0.36	48,48,48,48	0
92	OHX	5	4340	7/7	0.97	0.29	60,60,60,60	7
92	OHX	1	4228	7/7	0.97	0.32	62,62,62,62	7
92	OHX	1	4278	7/7	0.97	0.24	90,90,90,90	7
91	MG	5	3793	1/1	0.97	0.22	66,66,66,66	0
92	OHX	1	4359	7/7	0.97	0.36	64,64,64,64	7
91	MG	1	3828	1/1	0.97	0.45	48,48,48,48	0
91	MG	1	3898	1/1	0.97	0.16	59,59,59,59	1
92	OHX	5	4289	7/7	0.97	0.19	121,121,121,121	7
91	MG	1	3524	1/1	0.97	0.69	47,47,47,47	0
93	ZN	D9	102	1/1	0.97	0.10	93,93,93,93	0
92	OHX	1	4188	7/7	0.97	0.29	58,58,58,58	7
91	MG	5	3821	1/1	0.97	0.43	51,51,51,51	1
92	OHX	1	4270	7/7	0.97	0.33	67,67,67,67	7
91	MG	5	3429	1/1	0.97	0.33	52,52,52,52	0
92	OHX	1	4484	7/7	0.97	0.21	82,82,82,82	7
91	MG	1	3840	1/1	0.97	0.28	65,65,65,65	0
91	MG	1	4015	1/1	0.97	0.70	60,60,60,60	1
92	OHX	L2	305	7/7	0.97	0.27	73,73,73,73	7
92	OHX	1	4208	7/7	0.97	0.26	100,100,100,100	7
92	OHX	5	4342	7/7	0.97	0.37	70,70,70,70	7
92	OHX	1	4183	7/7	0.97	0.16	124,124,124,124	7
92	OHX	5	4312	7/7	0.97	0.36	64,64,64,64	7
91	MG	5	3985	1/1	0.97	0.41	51,51,51,51	1
91	MG	5	3450	1/1	0.97	0.63	43,43,43,43	0
92	OHX	o3	206	7/7	0.97	0.34	68,68,68,68	7
91	MG	1	3817	1/1	0.97	0.15	53,53,53,53	0
91	MG	8	220	1/1	0.97	0.24	79,79,79,79	0
91	MG	6	2071	1/1	0.97	0.54	59,59,59,59	0
92	OHX	5	4455	7/7	0.97	0.18	81,81,81,81	7
92	OHX	2	2135	7/7	0.97	0.25	105,105,105,105	7
92	OHX	6	2173	7/7	0.97	0.21	91,91,91,91	7
91	MG	2	2045	1/1	0.97	0.26	95,95,95,95	0
92	OHX	5	4348	7/7	0.97	0.18	84,84,84,84	7
92	OHX	6	2235	7/7	0.97	0.13	96,96,96,96	7
91	MG	1	3470	1/1	0.97	0.42	57,57,57,57	0
92	OHX	6	2241	7/7	0.97	0.22	87,87,87,87	7
91	MG	1	3928	1/1	0.97	0.72	49,49,49,49	1
91	MG	1	3495	1/1	0.97	0.58	55,55,55,55	0
92	OHX	6	2225	7/7	0.97	0.24	100,100,100,100	7
91	MG	O3	201	1/1	0.97	0.79	50,50,50,50	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	1	4250	7/7	0.97	0.20	77,77,77,77	7
92	OHX	2	2085	7/7	0.97	0.18	95,95,95,95	7
93	ZN	e1	501	1/1	0.97	0.07	168,168,168,168	0
92	OHX	6	2170	7/7	0.97	0.17	135,135,135,135	7
92	OHX	5	4478	7/7	0.97	0.30	78,78,78,78	7
92	OHX	5	4365	7/7	0.97	0.30	57,57,57,57	7
91	MG	5	3733	1/1	0.97	0.21	59,59,59,59	1
92	OHX	6	2183	7/7	0.97	0.16	101,101,101,101	7
91	MG	5	3928	1/1	0.97	1.36	59,59,59,59	1
92	OHX	6	2174	7/7	0.97	0.29	63,63,63,63	7
91	MG	4	211	1/1	0.97	0.33	58,58,58,58	0
91	MG	7	228	1/1	0.97	0.26	66,66,66,66	1
91	MG	5	3479	1/1	0.97	0.39	76,76,76,76	0
92	OHX	2	2117	7/7	0.97	0.16	116,116,116,116	7
91	MG	5	3790	1/1	0.97	0.96	47,47,47,47	1
91	MG	6	2093	1/1	0.97	0.59	62,62,62,62	1
92	OHX	3	226	7/7	0.97	0.30	64,64,64,64	7
92	OHX	3	219	7/7	0.97	0.24	85,85,85,85	7
92	OHX	2	2155	7/7	0.97	0.23	83,83,83,83	7
91	MG	1	3599	1/1	0.97	0.64	44,44,44,44	0
91	MG	5	4037	1/1	0.97	0.20	109,109,109,109	0
92	OHX	5	4184	7/7	0.97	0.25	75,75,75,75	7
91	MG	6	1987	1/1	0.97	0.34	67,67,67,67	0
91	MG	5	3601	1/1	0.97	0.42	44,44,44,44	0
91	MG	2	2041	1/1	0.97	0.30	84,84,84,84	0
91	MG	1	3438	1/1	0.97	0.34	67,67,67,67	0
92	OHX	6	2182	7/7	0.97	0.29	81,81,81,81	7
92	OHX	2	2079	7/7	0.97	0.19	120,120,120,120	7
92	OHX	C8	202	7/7	0.97	0.17	108,108,108,108	7
92	OHX	1	4244	7/7	0.97	0.39	73,73,73,73	7
92	OHX	5	4302	7/7	0.97	0.24	61,61,61,61	7
92	OHX	1	4187	7/7	0.97	0.28	59,59,59,59	7
93	ZN	d6	101	1/1	0.97	0.09	85,85,85,85	0
92	OHX	5	4290	7/7	0.97	0.39	59,59,59,59	7
91	MG	7	202	1/1	0.97	0.40	56,56,56,56	0
92	OHX	2	2146	7/7	0.97	0.14	129,129,129,129	7
92	OHX	5	4256	7/7	0.97	0.18	80,80,80,80	7
92	OHX	5	4361	7/7	0.97	0.22	65,65,65,65	7
92	OHX	1	4196	7/7	0.97	0.14	102,102,102,102	7
92	OHX	6	2218	7/7	0.97	0.23	106,106,106,106	7
92	OHX	1	4286	7/7	0.97	0.16	102,102,102,102	7
92	OHX	5	4305	7/7	0.97	0.21	89,89,89,89	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	1	4145	7/7	0.97	0.33	82,82,82,82	7
92	OHX	2	2205	7/7	0.97	0.21	73,73,73,73	7
92	OHX	1	4318	7/7	0.97	0.13	86,86,86,86	7
92	OHX	n3	204	7/7	0.97	0.27	73,73,73,73	7
92	OHX	1	4229	7/7	0.97	0.23	116,116,116,116	7
92	OHX	6	2179	7/7	0.97	0.20	101,101,101,101	7
91	MG	L3	404	1/1	0.97	0.29	57,57,57,57	0
92	OHX	5	4344	7/7	0.97	0.33	59,59,59,59	7
91	MG	1	3669	1/1	0.97	0.54	57,57,57,57	0
92	OHX	5	4298	7/7	0.97	0.32	71,71,71,71	7
92	OHX	1	4264	7/7	0.97	0.28	67,67,67,67	7
92	OHX	5	4367	7/7	0.97	0.41	68,68,68,68	7
92	OHX	1	4212	7/7	0.97	0.22	62,62,62,62	7
92	OHX	5	4337	7/7	0.97	0.19	92,92,92,92	7
92	OHX	6	2198	7/7	0.97	0.19	104,104,104,104	7
91	MG	1	3506	1/1	0.97	0.56	55,55,55,55	0
92	OHX	2	2164	7/7	0.97	0.32	100,100,100,100	7
91	MG	5	4091	1/1	0.97	0.49	45,45,45,45	1
92	OHX	1	4338	7/7	0.97	0.27	75,75,75,75	7
92	OHX	1	4253	7/7	0.97	0.21	80,80,80,80	7
92	OHX	5	4267	7/7	0.97	0.32	53,53,53,53	7
92	OHX	1	4221	7/7	0.97	0.34	77,77,77,77	7
92	OHX	1	4139	7/7	0.97	0.24	82,82,82,82	7
92	OHX	1	4326	7/7	0.97	0.37	61,61,61,61	7
92	OHX	2	2100	7/7	0.97	0.18	103,103,103,103	7
91	MG	1	3446	1/1	0.97	0.11	62,62,62,62	0
91	MG	1	3613	1/1	0.97	0.32	50,50,50,50	0
91	MG	1	3520	1/1	0.97	0.58	49,49,49,49	0
91	MG	6	1918	1/1	0.97	0.38	80,80,80,80	0
91	MG	q3	503	1/1	0.97	0.75	56,56,56,56	1
92	OHX	1	4162	7/7	0.97	0.31	95,95,95,95	7
92	OHX	6	2187	7/7	0.97	0.30	77,77,77,77	7
91	MG	5	3541	1/1	0.97	0.56	35,35,35,35	0
91	MG	6	2006	1/1	0.97	0.27	69,69,69,69	0
91	MG	5	3605	1/1	0.97	0.59	46,46,46,46	0
91	MG	1	3573	1/1	0.97	0.71	44,44,44,44	0
91	MG	5	3921	1/1	0.97	0.71	50,50,50,50	0
91	MG	3	203	1/1	0.97	0.43	66,66,66,66	0
91	MG	6	2113	1/1	0.97	0.32	86,86,86,86	0
91	MG	5	3585	1/1	0.97	0.47	45,45,45,45	0
92	OHX	1	4149	7/7	0.97	0.32	65,65,65,65	7
91	MG	L3	403	1/1	0.97	0.49	51,51,51,51	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3514	1/1	0.97	0.31	57,57,57,57	0
92	OHX	5	4303	7/7	0.97	0.27	79,79,79,79	7
91	MG	5	3521	1/1	0.97	0.75	45,45,45,45	0
92	OHX	2	2255	7/7	0.97	0.27	106,106,106,106	7
92	OHX	5	4212	7/7	0.97	0.31	86,86,86,86	7
91	MG	1	3504	1/1	0.97	0.23	59,59,59,59	0
92	OHX	1	4288	7/7	0.97	0.25	53,53,53,53	7
91	MG	5	3591	1/1	0.97	0.51	45,45,45,45	0
92	OHX	1	4232	7/7	0.97	0.13	131,131,131,131	7
92	OHX	1	4150	7/7	0.97	0.24	88,88,88,88	7
91	MG	1	3921	1/1	0.97	0.32	67,67,67,67	0
92	OHX	5	4249	7/7	0.97	0.19	76,76,76,76	7
91	MG	5	3883	1/1	0.97	0.35	52,52,52,52	1
92	OHX	1	4319	7/7	0.97	0.22	86,86,86,86	7
92	OHX	6	2221	7/7	0.97	0.22	79,79,79,79	7
91	MG	1	3765	1/1	0.97	0.81	69,69,69,69	1
91	MG	6	2029	1/1	0.97	0.25	114,114,114,114	0
91	MG	5	3651	1/1	0.97	0.32	59,59,59,59	0
91	MG	6	1965	1/1	0.98	0.56	54,54,54,54	0
91	MG	5	3587	1/1	0.98	0.58	44,44,44,44	0
92	OHX	7	230	7/7	0.98	0.20	74,74,74,74	7
92	OHX	1	4207	7/7	0.98	0.25	64,64,64,64	7
91	MG	5	3850	1/1	0.98	0.33	53,53,53,53	1
92	OHX	5	4319	7/7	0.98	0.35	68,68,68,68	7
92	OHX	1	4191	7/7	0.98	0.33	67,67,67,67	7
92	OHX	1	4182	7/7	0.98	0.34	65,65,65,65	7
92	OHX	1	4467	7/7	0.98	0.27	74,74,74,74	7
92	OHX	1	4148	7/7	0.98	0.23	91,91,91,91	7
91	MG	5	3482	1/1	0.98	0.26	56,56,56,56	0
91	MG	6	2102	1/1	0.98	1.03	69,69,69,69	1
92	OHX	2	2147	7/7	0.98	0.24	85,85,85,85	7
91	MG	1	3740	1/1	0.98	0.20	90,90,90,90	0
91	MG	n9	101	1/1	0.98	0.99	53,53,53,53	1
91	MG	1	3859	1/1	0.98	0.55	58,58,58,58	1
92	OHX	1	4152	7/7	0.98	0.32	71,71,71,71	7
91	MG	1	3754	1/1	0.98	0.27	49,49,49,49	1
91	MG	5	3867	1/1	0.98	0.56	46,46,46,46	1
92	OHX	2	2131	7/7	0.98	0.20	92,92,92,92	7
92	OHX	7	231	7/7	0.98	0.27	64,64,64,64	7
92	OHX	2	2083	7/7	0.98	0.15	130,130,130,130	7
92	OHX	5	4332	7/7	0.98	0.43	63,63,63,63	7
92	OHX	2	2125	7/7	0.98	0.22	89,89,89,89	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3758	1/1	0.98	0.34	55,55,55,55	0
92	OHX	5	4231	7/7	0.98	0.25	76,76,76,76	7
92	OHX	2	2116	7/7	0.98	0.23	81,81,81,81	7
92	OHX	6	2149	7/7	0.98	0.18	98,98,98,98	7
91	MG	1	3515	1/1	0.98	0.62	54,54,54,54	0
92	OHX	5	4554	7/7	0.98	0.25	67,67,67,67	7
92	OHX	5	4232	7/7	0.98	0.25	82,82,82,82	7
91	MG	5	3750	1/1	0.98	0.72	47,47,47,47	1
91	MG	1	3996	1/1	0.98	0.19	57,57,57,57	1
91	MG	5	4052	1/1	0.98	0.27	56,56,56,56	1
92	OHX	1	4114	7/7	0.98	0.21	75,75,75,75	7
91	MG	5	4070	1/1	0.98	0.22	63,63,63,63	0
91	MG	5	3935	1/1	0.98	0.27	52,52,52,52	1
91	MG	4	232	1/1	0.98	0.50	60,60,60,60	0
92	OHX	6	2244	7/7	0.98	0.32	73,73,73,73	7
92	OHX	1	4194	7/7	0.98	0.28	78,78,78,78	7
92	OHX	1	4170	7/7	0.98	0.24	68,68,68,68	7
92	OHX	1	4481	7/7	0.98	0.28	78,78,78,78	7
91	MG	1	3492	1/1	0.98	0.24	58,58,58,58	0
91	MG	1	3751	1/1	0.98	0.49	64,64,64,64	0
91	MG	1	3639	1/1	0.98	0.23	57,57,57,57	0
92	OHX	1	4195	7/7	0.98	0.28	71,71,71,71	7
92	OHX	L3	408	7/7	0.98	0.19	84,84,84,84	7
92	OHX	2	2107	7/7	0.98	0.21	110,110,110,110	7
92	OHX	5	4190	7/7	0.98	0.22	109,109,109,109	0
92	OHX	5	4278	7/7	0.98	0.34	65,65,65,65	7
92	OHX	M5	310	7/7	0.98	0.25	81,81,81,81	7
91	MG	1	3461	1/1	0.98	0.47	52,52,52,52	0
92	OHX	l3	412	7/7	0.98	0.26	70,70,70,70	7
92	OHX	2	2091	7/7	0.98	0.25	90,90,90,90	7
91	MG	1	3722	1/1	0.98	0.41	47,47,47,47	0
91	MG	5	4123	1/1	0.98	0.49	49,49,49,49	1
91	MG	5	3454	1/1	0.98	0.39	46,46,46,46	0
92	OHX	1	4173	7/7	0.98	0.28	106,106,106,106	7
92	OHX	6	2168	7/7	0.98	0.20	72,72,72,72	7
92	OHX	1	4156	7/7	0.98	0.45	63,63,63,63	7
92	OHX	1	4266	7/7	0.98	0.34	62,62,62,62	7
92	OHX	5	4339	7/7	0.98	0.26	58,58,58,58	7
91	MG	5	3447	1/1	0.98	0.42	44,44,44,44	0
92	OHX	5	4244	7/7	0.98	0.25	81,81,81,81	7
91	MG	8	207	1/1	0.98	0.24	73,73,73,73	0
91	MG	1	3570	1/1	0.98	0.37	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	M0	303	1/1	0.98	0.68	60,60,60,60	1
92	OHX	1	4219	7/7	0.98	0.19	60,60,60,60	7
92	OHX	2	2104	7/7	0.98	0.28	83,83,83,83	7
91	MG	5	3813	1/1	0.98	0.39	59,59,59,59	0
92	OHX	5	4474	7/7	0.98	0.19	90,90,90,90	7
92	OHX	8	222	7/7	0.98	0.20	95,95,95,95	7
92	OHX	5	4268	7/7	0.98	0.24	73,73,73,73	7
92	OHX	6	2242	7/7	0.98	0.26	71,71,71,71	7
91	MG	2	2006	1/1	0.98	0.37	96,96,96,96	0
92	OHX	5	4201	7/7	0.98	0.25	81,81,81,81	7
92	OHX	5	4335	7/7	0.98	0.21	65,65,65,65	7
92	OHX	1	4159	7/7	0.98	0.17	109,109,109,109	7
91	MG	5	4017	1/1	0.98	0.27	63,63,63,63	0
92	OHX	O3	204	7/7	0.98	0.28	62,62,62,62	7
91	MG	1	3453	1/1	0.98	0.35	51,51,51,51	0
92	OHX	2	2126	7/7	0.98	0.24	86,86,86,86	7
92	OHX	6	2177	7/7	0.98	0.28	74,74,74,74	7
92	OHX	2	2093	7/7	0.98	0.16	123,123,123,123	7
91	MG	1	3925	1/1	0.98	0.41	52,52,52,52	1
91	MG	2	2054	1/1	0.98	0.14	92,92,92,92	1
91	MG	5	3542	1/1	0.98	0.41	50,50,50,50	0
91	MG	5	3547	1/1	0.98	0.77	46,46,46,46	0
92	OHX	5	4419	7/7	0.98	0.15	69,69,69,69	7
92	OHX	1	4283	7/7	0.98	0.36	65,65,65,65	7
92	OHX	5	4172	7/7	0.98	0.27	71,71,71,71	7
91	MG	5	3423	1/1	0.98	0.50	65,65,65,65	0
92	OHX	q2	203	7/7	0.98	0.22	64,64,64,64	7
92	OHX	1	4258	7/7	0.98	0.35	60,60,60,60	7
92	OHX	n9	103	7/7	0.98	0.25	74,74,74,74	7
92	OHX	1	4360	7/7	0.98	0.28	64,64,64,64	7
91	MG	1	3530	1/1	0.98	0.51	47,47,47,47	0
92	OHX	1	4185	7/7	0.98	0.23	71,71,71,71	7
91	MG	1	3862	1/1	0.98	0.40	61,61,61,61	1
92	OHX	6	2204	7/7	0.98	0.26	79,79,79,79	7
92	OHX	4	238	7/7	0.98	0.23	94,94,94,94	7
92	OHX	1	4282	7/7	0.98	0.25	102,102,102,102	7
91	MG	L4	403	1/1	0.98	0.49	68,68,68,68	1
92	OHX	1	4177	7/7	0.98	0.26	94,94,94,94	7
92	OHX	5	4402	7/7	0.98	0.24	79,79,79,79	7
92	OHX	5	4208	7/7	0.98	0.14	128,128,128,128	0
92	OHX	2	2071	7/7	0.98	0.18	106,106,106,106	0
92	OHX	M0	305	7/7	0.98	0.40	66,66,66,66	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	2	2098	7/7	0.98	0.29	88,88,88,88	7
92	OHX	7	229	7/7	0.98	0.26	84,84,84,84	7
91	MG	5	3918	1/1	0.98	0.11	62,62,62,62	0
92	OHX	6	2185	7/7	0.98	0.14	123,123,123,123	7
92	OHX	1	4285	7/7	0.98	0.25	82,82,82,82	7
92	OHX	2	2092	7/7	0.98	0.20	96,96,96,96	7
92	OHX	2	2084	7/7	0.98	0.24	97,97,97,97	7
91	MG	5	3849	1/1	0.98	0.18	62,62,62,62	0
92	OHX	1	4178	7/7	0.98	0.24	76,76,76,76	7
91	MG	7	216	1/1	0.98	0.39	62,62,62,62	1
92	OHX	2	2080	7/7	0.98	0.17	114,114,114,114	7
91	MG	m6	205	1/1	0.98	0.15	54,54,54,54	0
91	MG	1	3459	1/1	0.98	0.39	57,57,57,57	0
92	OHX	1	4227	7/7	0.98	0.29	81,81,81,81	7
92	OHX	2	2077	7/7	0.98	0.18	105,105,105,105	7
92	OHX	1	4138	7/7	0.98	0.37	60,60,60,60	7
92	OHX	6	2159	7/7	0.98	0.29	73,73,73,73	7
92	OHX	6	2153	7/7	0.98	0.22	91,91,91,91	7
92	OHX	6	2171	7/7	0.98	0.33	70,70,70,70	7
92	OHX	6	2197	7/7	0.98	0.14	156,156,156,156	7
92	OHX	2	2150	7/7	0.98	0.12	106,106,106,106	7
92	OHX	5	4205	7/7	0.98	0.27	92,92,92,92	7
92	OHX	2	2075	7/7	0.98	0.20	105,105,105,105	7
91	MG	2	1914	1/1	0.98	0.54	79,79,79,79	0
92	OHX	1	4224	7/7	0.98	0.30	67,67,67,67	7
92	OHX	5	4333	7/7	0.98	0.18	79,79,79,79	7
92	OHX	5	4259	7/7	0.98	0.38	62,62,62,62	7
92	OHX	1	4153	7/7	0.98	0.19	102,102,102,102	7
91	MG	1	4037	1/1	0.98	0.60	69,69,69,69	1
92	OHX	5	4207	7/7	0.98	0.27	68,68,68,68	7
91	MG	5	3422	1/1	0.98	0.71	57,57,57,57	0
92	OHX	6	2215	7/7	0.98	0.36	85,85,85,85	7
92	OHX	1	4175	7/7	0.98	0.23	64,64,64,64	7
92	OHX	6	2151	7/7	0.98	0.19	99,99,99,99	7
91	MG	5	3552	1/1	0.98	0.43	46,46,46,46	0
92	OHX	1	4200	7/7	0.98	0.15	86,86,86,86	7
92	OHX	1	4186	7/7	0.98	0.21	78,78,78,78	7
92	OHX	1	4171	7/7	0.98	0.26	64,64,64,64	7
92	OHX	5	4442	7/7	0.98	0.22	59,59,59,59	7
92	OHX	5	4482	7/7	0.98	0.23	67,67,67,67	7
92	OHX	5	4187	7/7	0.98	0.28	50,50,50,50	7
91	MG	N6	201	1/1	0.98	0.61	68,68,68,68	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	4057	1/1	0.98	0.49	52,52,52,52	1
92	OHX	5	4564	7/7	0.98	0.27	80,80,80,80	7
92	OHX	5	4206	7/7	0.98	0.21	92,92,92,92	7
92	OHX	5	4522	7/7	0.98	0.26	69,69,69,69	7
92	OHX	6	2147	7/7	0.98	0.17	97,97,97,97	0
92	OHX	6	2162	7/7	0.98	0.16	127,127,127,127	7
92	OHX	5	4238	7/7	0.98	0.25	57,57,57,57	7
92	OHX	5	4189	7/7	0.98	0.25	68,68,68,68	7
91	MG	M3	201	1/1	0.98	0.64	61,61,61,61	1
91	MG	5	4114	1/1	0.98	1.11	59,59,59,59	1
93	ZN	D6	101	1/1	0.98	0.06	106,106,106,106	0
92	OHX	4	243	7/7	0.98	0.15	104,104,104,104	7
92	OHX	6	2145	7/7	0.98	0.19	89,89,89,89	7
92	OHX	1	4180	7/7	0.98	0.34	65,65,65,65	7
92	OHX	2	2203	7/7	0.98	0.17	105,105,105,105	7
92	OHX	2	2143	7/7	0.98	0.12	124,124,124,124	7
91	MG	5	3826	1/1	0.98	0.21	60,60,60,60	1
91	MG	1	3578	1/1	0.98	0.60	42,42,42,42	0
92	OHX	5	4248	7/7	0.98	0.21	72,72,72,72	7
92	OHX	6	2188	7/7	0.98	0.26	89,89,89,89	7
91	MG	1	3476	1/1	0.98	0.27	83,83,83,83	0
91	MG	5	3866	1/1	0.98	0.25	55,55,55,55	1
91	MG	1	4022	1/1	0.98	0.81	53,53,53,53	1
92	OHX	5	4250	7/7	0.98	0.22	60,60,60,60	7
92	OHX	8	239	7/7	0.98	0.26	87,87,87,87	7
92	OHX	5	4226	7/7	0.98	0.22	91,91,91,91	7
92	OHX	1	4199	7/7	0.98	0.32	73,73,73,73	7
92	OHX	6	2178	7/7	0.98	0.30	79,79,79,79	7
91	MG	1	3537	1/1	0.98	0.48	43,43,43,43	0
92	OHX	5	4313	7/7	0.98	0.20	63,63,63,63	7
92	OHX	1	4215	7/7	0.98	0.30	55,55,55,55	7
91	MG	5	3525	1/1	0.98	0.55	41,41,41,41	0
92	OHX	1	4142	7/7	0.98	0.22	95,95,95,95	7
92	OHX	5	4260	7/7	0.98	0.25	52,52,52,52	7
92	OHX	4	235	7/7	0.98	0.25	69,69,69,69	7
91	MG	1	3542	1/1	0.98	0.55	46,46,46,46	0
92	OHX	5	4269	7/7	0.98	0.20	66,66,66,66	7
91	MG	5	3876	1/1	0.98	0.40	54,54,54,54	0
92	OHX	1	4164	7/7	0.98	0.28	68,68,68,68	7
92	OHX	5	4327	7/7	0.98	0.26	74,74,74,74	7
91	MG	5	3535	1/1	0.98	0.50	48,48,48,48	0
92	OHX	6	2161	7/7	0.98	0.22	88,88,88,88	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	3782	1/1	0.98	0.23	48,48,48,48	1
91	MG	l3	403	1/1	0.98	0.71	43,43,43,43	0
92	OHX	1	4248	7/7	0.98	0.29	83,83,83,83	7
91	MG	1	3600	1/1	0.98	0.47	47,47,47,47	0
92	OHX	1	4181	7/7	0.98	0.15	96,96,96,96	7
91	MG	1	3984	1/1	0.98	0.89	50,50,50,50	1
92	OHX	1	4236	7/7	0.98	0.28	63,63,63,63	7
92	OHX	6	2176	7/7	0.98	0.28	74,74,74,74	7
91	MG	5	3505	1/1	0.98	0.46	47,47,47,47	0
91	MG	6	2097	1/1	0.98	0.19	86,86,86,86	0
92	OHX	2	2221	7/7	0.98	0.24	87,87,87,87	7
91	MG	M6	202	1/1	0.98	0.84	53,53,53,53	1
91	MG	1	3902	1/1	0.98	0.27	54,54,54,54	1
92	OHX	1	4166	7/7	0.98	0.32	99,99,99,99	7
92	OHX	5	4282	7/7	0.98	0.18	100,100,100,100	7
92	OHX	1	4279	7/7	0.98	0.29	61,61,61,61	7
92	OHX	6	2325	7/7	0.98	0.21	99,99,99,99	7
92	OHX	m0	302	7/7	0.98	0.15	99,99,99,99	7
92	OHX	2	2109	7/7	0.98	0.25	100,100,100,100	7
91	MG	1	3970	1/1	0.98	0.30	83,83,83,83	0
91	MG	5	3990	1/1	0.98	0.19	53,53,53,53	0
92	OHX	1	4255	7/7	0.98	0.29	66,66,66,66	7
92	OHX	5	4539	7/7	0.98	0.23	73,73,73,73	7
92	OHX	2	2158	7/7	0.98	0.13	123,123,123,123	7
92	OHX	1	4190	7/7	0.98	0.28	74,74,74,74	7
91	MG	1	3548	1/1	0.98	0.60	45,45,45,45	0
92	OHX	1	4176	7/7	0.98	0.19	69,69,69,69	7
92	OHX	6	2144	7/7	0.98	0.20	87,87,87,87	7
92	OHX	8	221	7/7	0.98	0.25	68,68,68,68	7
91	MG	6	2033	1/1	0.98	0.39	75,75,75,75	0
92	OHX	1	4442	7/7	0.98	0.28	65,65,65,65	7
92	OHX	6	2192	7/7	0.98	0.11	120,120,120,120	7
92	OHX	3	221	7/7	0.98	0.31	69,69,69,69	7
91	MG	M8	203	1/1	0.98	1.11	56,56,56,56	1
92	OHX	6	2237	7/7	0.98	0.13	108,108,108,108	7
92	OHX	5	4243	7/7	0.98	0.30	59,59,59,59	7
91	MG	2	2039	1/1	0.98	0.18	100,100,100,100	0
92	OHX	6	2172	7/7	0.98	0.35	82,82,82,82	7
92	OHX	o2	204	7/7	0.98	0.30	58,58,58,58	7
91	MG	1	3430	1/1	0.98	0.65	59,59,59,59	0
91	MG	1	4033	1/1	0.98	0.21	57,57,57,57	0
91	MG	L4	402	1/1	0.98	0.66	52,52,52,52	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	1	4169	7/7	0.98	0.25	74,74,74,74	7
91	MG	5	3613	1/1	0.98	0.13	60,60,60,60	0
91	MG	6	1938	1/1	0.98	0.21	72,72,72,72	0
92	OHX	3	220	7/7	0.98	0.35	63,63,63,63	7
92	OHX	5	4273	7/7	0.98	0.23	71,71,71,71	7
92	OHX	m5	303	7/7	0.98	0.20	89,89,89,89	7
92	OHX	2	2103	7/7	0.98	0.17	103,103,103,103	7
91	MG	5	4034	1/1	0.98	0.26	48,48,48,48	1
91	MG	1	3572	1/1	0.98	0.60	45,45,45,45	0
92	OHX	1	4151	7/7	0.98	0.20	90,90,90,90	7
92	OHX	5	4324	7/7	0.98	0.35	75,75,75,75	7
92	OHX	1	4487	7/7	0.99	0.23	91,91,91,91	7
91	MG	1	3610	1/1	0.99	0.70	28,28,28,28	0
92	OHX	5	4422	7/7	0.99	0.22	59,59,59,59	7
91	MG	5	3865	1/1	0.99	0.55	54,54,54,54	1
92	OHX	5	4202	7/7	0.99	0.27	59,59,59,59	7
92	OHX	1	4141	7/7	0.99	0.26	75,75,75,75	7
92	OHX	5	4170	7/7	0.99	0.19	75,75,75,75	7
91	MG	5	3756	1/1	0.99	0.21	98,98,98,98	0
92	OHX	5	4163	7/7	0.99	0.25	62,62,62,62	2
91	MG	1	3793	1/1	0.99	0.33	64,64,64,64	1
91	MG	5	3466	1/1	0.99	0.48	51,51,51,51	0
92	OHX	1	4234	7/7	0.99	0.24	60,60,60,60	7
92	OHX	5	4182	7/7	0.99	0.21	62,62,62,62	7
92	OHX	5	4255	7/7	0.99	0.23	89,89,89,89	7
91	MG	1	3605	1/1	0.99	0.55	47,47,47,47	0
92	OHX	1	4161	7/7	0.99	0.19	86,86,86,86	7
92	OHX	1	4111	7/7	0.99	0.24	71,71,71,71	7
91	MG	s1	301	1/1	0.99	0.21	93,93,93,93	0
92	OHX	2	2097	7/7	0.99	0.23	76,76,76,76	7
92	OHX	5	4185	7/7	0.99	0.24	73,73,73,73	7
92	OHX	5	4476	7/7	0.99	0.28	65,65,65,65	7
92	OHX	5	4227	7/7	0.99	0.28	59,59,59,59	7
92	OHX	5	4175	7/7	0.99	0.22	65,65,65,65	7
92	OHX	1	4109	7/7	0.99	0.26	67,67,67,67	7
91	MG	5	3673	1/1	0.99	0.21	49,49,49,49	0
93	ZN	q3	501	1/1	0.99	0.18	77,77,77,77	0
92	OHX	5	4213	7/7	0.99	0.21	71,71,71,71	7
92	OHX	1	4106	7/7	0.99	0.23	61,61,61,61	7
92	OHX	5	4217	7/7	0.99	0.22	75,75,75,75	7
92	OHX	5	4164	7/7	0.99	0.24	67,67,67,67	7
92	OHX	5	4222	7/7	0.99	0.18	91,91,91,91	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	6	2156	7/7	0.99	0.27	79,79,79,79	7
92	OHX	5	4158	7/7	0.99	0.27	59,59,59,59	3
92	OHX	5	4215	7/7	0.99	0.18	60,60,60,60	7
92	OHX	6	2251	7/7	0.99	0.20	76,76,76,76	7
92	OHX	6	2186	7/7	0.99	0.21	82,82,82,82	7
92	OHX	5	4223	7/7	0.99	0.27	70,70,70,70	7
92	OHX	1	4158	7/7	0.99	0.20	57,57,57,57	7
92	OHX	6	2148	7/7	0.99	0.23	88,88,88,88	7
91	MG	1	4090	1/1	0.99	0.19	76,76,76,76	0
91	MG	5	3443	1/1	0.99	0.46	44,44,44,44	0
92	OHX	7	232	7/7	0.99	0.25	58,58,58,58	7
91	MG	2	2044	1/1	0.99	0.27	75,75,75,75	0
92	OHX	2	2090	7/7	0.99	0.20	84,84,84,84	7
92	OHX	6	2158	7/7	0.99	0.24	79,79,79,79	7
92	OHX	5	4183	7/7	0.99	0.28	56,56,56,56	7
92	OHX	1	4110	7/7	0.99	0.21	75,75,75,75	7
92	OHX	5	4193	7/7	0.99	0.25	69,69,69,69	7
93	ZN	Q3	501	1/1	0.99	0.13	79,79,79,79	0
91	MG	5	4108	1/1	0.99	0.25	59,59,59,59	0
92	OHX	6	2160	7/7	0.99	0.27	70,70,70,70	7
91	MG	5	3528	1/1	0.99	0.40	54,54,54,54	0
92	OHX	1	4124	7/7	0.99	0.22	92,92,92,92	7
92	OHX	6	2143	7/7	0.99	0.24	78,78,78,78	3
92	OHX	5	4216	7/7	0.99	0.35	56,56,56,56	7
91	MG	5	3445	1/1	0.99	0.59	47,47,47,47	0
92	OHX	5	4156	7/7	0.99	0.20	65,65,65,65	0
91	MG	5	3765	1/1	0.99	0.86	51,51,51,51	1
92	OHX	5	4165	7/7	0.99	0.21	72,72,72,72	7
92	OHX	S2	303	7/7	0.99	0.24	98,98,98,98	7
92	OHX	N9	102	7/7	0.99	0.24	74,74,74,74	7
92	OHX	1	4140	7/7	0.99	0.24	84,84,84,84	7
92	OHX	5	4218	7/7	0.99	0.20	80,80,80,80	7
92	OHX	5	4174	7/7	0.99	0.24	64,64,64,64	7
91	MG	2	2028	1/1	0.99	0.21	80,80,80,80	1
91	MG	5	3540	1/1	0.99	0.35	45,45,45,45	0
92	OHX	1	4116	7/7	0.99	0.29	70,70,70,70	7
92	OHX	1	4113	7/7	0.99	0.18	78,78,78,78	7
91	MG	5	4152	1/1	0.99	0.56	60,60,60,60	1
92	OHX	4	234	7/7	0.99	0.23	71,71,71,71	7
92	OHX	1	4131	7/7	0.99	0.26	72,72,72,72	7
92	OHX	1	4121	7/7	0.99	0.24	75,75,75,75	7
92	OHX	5	4169	7/7	0.99	0.23	60,60,60,60	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
92	OHX	1	4167	7/7	0.99	0.20	65,65,65,65	7
92	OHX	5	4318	7/7	0.99	0.38	55,55,55,55	7
92	OHX	5	4220	7/7	0.99	0.21	57,57,57,57	7
91	MG	1	3969	1/1	0.99	0.18	75,75,75,75	0
92	OHX	n1	204	7/7	0.99	0.20	63,63,63,63	7
92	OHX	5	4253	7/7	0.99	0.29	61,61,61,61	7
92	OHX	5	4233	7/7	0.99	0.28	65,65,65,65	7
92	OHX	6	2150	7/7	0.99	0.20	74,74,74,74	7
92	OHX	5	4161	7/7	0.99	0.22	72,72,72,72	0
92	OHX	5	4280	7/7	0.99	0.31	74,74,74,74	7
91	MG	m7	202	1/1	0.99	0.84	52,52,52,52	1
92	OHX	1	4160	7/7	0.99	0.21	78,78,78,78	7
91	MG	1	3477	1/1	0.99	0.29	50,50,50,50	0
92	OHX	1	4223	7/7	0.99	0.23	81,81,81,81	7
92	OHX	5	4180	7/7	0.99	0.20	74,74,74,74	7
92	OHX	5	4173	7/7	0.99	0.24	75,75,75,75	7
92	OHX	5	4277	7/7	0.99	0.33	56,56,56,56	7
92	OHX	1	4157	7/7	0.99	0.26	73,73,73,73	7
92	OHX	1	4192	7/7	0.99	0.23	55,55,55,55	7
92	OHX	2	2082	7/7	0.99	0.24	81,81,81,81	7
91	MG	5	4104	1/1	0.99	0.27	62,62,62,62	0
92	OHX	5	4200	7/7	0.99	0.31	60,60,60,60	7
92	OHX	1	4115	7/7	0.99	0.28	64,64,64,64	7
92	OHX	5	4228	7/7	0.99	0.28	60,60,60,60	7
92	OHX	1	4120	7/7	0.99	0.18	80,80,80,80	7
92	OHX	1	4127	7/7	0.99	0.20	80,80,80,80	7
92	OHX	2	2069	7/7	0.99	0.22	92,92,92,92	0
92	OHX	2	2081	7/7	0.99	0.31	101,101,101,101	7
92	OHX	2	2070	7/7	0.99	0.25	96,96,96,96	7
92	OHX	1	4240	7/7	0.99	0.18	73,73,73,73	7
91	MG	5	4077	1/1	0.99	0.95	60,60,60,60	1
92	OHX	2	2072	7/7	0.99	0.20	97,97,97,97	7
92	OHX	1	4206	7/7	0.99	0.27	63,63,63,63	7
92	OHX	1	4189	7/7	0.99	0.29	67,67,67,67	7
93	ZN	O7	102	1/1	0.99	0.14	59,59,59,59	0
91	MG	5	3773	1/1	0.99	0.24	49,49,49,49	1
92	OHX	5	4219	7/7	0.99	0.28	70,70,70,70	7
92	OHX	N1	202	7/7	0.99	0.22	69,69,69,69	7
92	OHX	1	4112	7/7	0.99	0.27	63,63,63,63	7
92	OHX	2	2073	7/7	0.99	0.22	82,82,82,82	7
92	OHX	6	2142	7/7	0.99	0.21	98,98,98,98	2
91	MG	1	3775	1/1	0.99	0.26	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	3577	1/1	0.99	0.29	43,43,43,43	0
91	MG	5	4032	1/1	0.99	0.25	55,55,55,55	1
92	OHX	5	4198	7/7	0.99	0.28	71,71,71,71	7
92	OHX	5	4246	7/7	0.99	0.24	65,65,65,65	7
91	MG	5	3884	1/1	0.99	0.43	57,57,57,57	1
92	OHX	1	4490	7/7	0.99	0.23	54,54,54,54	7
92	OHX	1	4143	7/7	0.99	0.22	61,61,61,61	7
92	OHX	2	2110	7/7	0.99	0.19	85,85,85,85	7
92	OHX	1	4128	7/7	0.99	0.26	60,60,60,60	7
93	ZN	o7	104	1/1	0.99	0.15	61,61,61,61	0
91	MG	5	4012	1/1	0.99	0.20	62,62,62,62	0
92	OHX	6	2146	7/7	0.99	0.24	74,74,74,74	7
92	OHX	6	2165	7/7	0.99	0.17	92,92,92,92	7
91	MG	3	210	1/1	0.99	0.34	64,64,64,64	0
93	ZN	Q0	202	1/1	0.99	0.13	64,64,64,64	0
92	OHX	1	4107	7/7	0.99	0.23	69,69,69,69	1
92	OHX	5	4203	7/7	0.99	0.28	59,59,59,59	7
92	OHX	1	4117	7/7	0.99	0.25	71,71,71,71	7
92	OHX	1	4163	7/7	0.99	0.24	60,60,60,60	7
91	MG	5	4133	1/1	0.99	0.23	70,70,70,70	0
92	OHX	1	4133	7/7	0.99	0.21	92,92,92,92	7
92	OHX	1	4135	7/7	0.99	0.24	67,67,67,67	7
92	OHX	5	4168	7/7	0.99	0.22	83,83,83,83	2
92	OHX	7	233	7/7	0.99	0.27	80,80,80,80	7
92	OHX	5	4506	7/7	0.99	0.19	91,91,91,91	7
92	OHX	2	2087	7/7	0.99	0.27	91,91,91,91	7
92	OHX	1	4174	7/7	0.99	0.20	74,74,74,74	7
92	OHX	1	4501	7/7	0.99	0.24	72,72,72,72	7
91	MG	1	4003	1/1	0.99	0.23	76,76,76,76	0
92	OHX	5	4177	7/7	0.99	0.25	80,80,80,80	7
92	OHX	6	2154	7/7	0.99	0.15	105,105,105,105	7
92	OHX	5	4157	7/7	0.99	0.23	61,61,61,61	1
92	OHX	3	222	7/7	0.99	0.23	94,94,94,94	7
91	MG	M5	303	1/1	0.99	0.31	50,50,50,50	1
92	OHX	1	4130	7/7	0.99	0.23	77,77,77,77	7
92	OHX	5	4178	7/7	0.99	0.25	68,68,68,68	7
92	OHX	5	4181	7/7	0.99	0.27	76,76,76,76	7
91	MG	o7	102	1/1	0.99	0.62	56,56,56,56	1
92	OHX	6	2157	7/7	0.99	0.22	81,81,81,81	7
91	MG	6	2070	1/1	0.99	0.14	62,62,62,62	1
92	OHX	1	4211	7/7	0.99	0.23	54,54,54,54	7
92	OHX	5	4209	7/7	0.99	0.27	79,79,79,79	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	1	4147	7/7	0.99	0.25	78,78,78,78	7
92	OHX	1	4198	7/7	0.99	0.24	51,51,51,51	7
91	MG	5	3968	1/1	0.99	0.11	53,53,53,53	1
92	OHX	5	4191	7/7	0.99	0.26	67,67,67,67	7
91	MG	5	3580	1/1	0.99	0.48	46,46,46,46	0
92	OHX	1	4125	7/7	0.99	0.20	79,79,79,79	7
92	OHX	M5	309	7/7	0.99	0.22	84,84,84,84	7
92	OHX	2	2086	7/7	0.99	0.23	87,87,87,87	7
92	OHX	2	2119	7/7	0.99	0.30	93,93,93,93	7
91	MG	1	3632	1/1	0.99	0.20	49,49,49,49	0
92	OHX	5	4166	7/7	0.99	0.19	68,68,68,68	7
92	OHX	1	4122	7/7	0.99	0.18	93,93,93,93	7
92	OHX	1	4201	7/7	0.99	0.34	57,57,57,57	7
92	OHX	5	4199	7/7	0.99	0.24	75,75,75,75	7
93	ZN	d9	102	1/1	0.99	0.18	96,96,96,96	0
92	OHX	5	4179	7/7	0.99	0.20	74,74,74,74	7
91	MG	1	3870	1/1	0.99	0.52	49,49,49,49	1
92	OHX	6	2155	7/7	0.99	0.28	71,71,71,71	7
92	OHX	1	4126	7/7	0.99	0.22	65,65,65,65	7
92	OHX	5	4234	7/7	0.99	0.32	63,63,63,63	7
91	MG	5	3902	1/1	0.99	0.20	48,48,48,48	1
91	MG	6	2129	1/1	0.99	0.31	78,78,78,78	0
92	OHX	1	4118	7/7	0.99	0.23	60,60,60,60	7
92	OHX	5	4192	7/7	0.99	0.23	68,68,68,68	7
92	OHX	1	4100	7/7	1.00	0.22	68,68,68,68	2
92	OHX	5	4188	7/7	1.00	0.22	62,62,62,62	7
92	OHX	5	4159	7/7	1.00	0.27	57,57,57,57	2
92	OHX	5	4160	7/7	1.00	0.23	72,72,72,72	0
91	MG	5	4134	1/1	1.00	0.15	66,66,66,66	0
91	MG	1	4061	1/1	1.00	0.28	73,73,73,73	0
92	OHX	1	4123	7/7	1.00	0.25	73,73,73,73	7
92	OHX	1	4102	7/7	1.00	0.21	73,73,73,73	1
92	OHX	5	4171	7/7	1.00	0.27	72,72,72,72	7
92	OHX	5	4186	7/7	1.00	0.30	62,62,62,62	7
92	OHX	5	4167	7/7	1.00	0.25	57,57,57,57	7
92	OHX	5	4239	7/7	1.00	0.25	61,61,61,61	7
92	OHX	1	4099	7/7	1.00	0.23	63,63,63,63	1
91	MG	1	4002	1/1	-	-	72,72,72,72	1
91	MG	5	3717	1/1	0.05	0.40	95,95,95,95	0
91	MG	5	3983	1/1	0.24	0.45	58,58,58,58	1
91	MG	1	3822	1/1	0.26	1.23	70,70,70,70	1
91	MG	1	4094	1/1	0.26	0.92	49,49,49,49	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	6	1970	1/1	0.30	0.81	77,77,77,77	0
91	MG	6	1934	1/1	0.33	0.44	88,88,88,88	0
91	MG	5	3870	1/1	0.37	0.56	69,69,69,69	1
91	MG	2	2005	1/1	0.38	0.50	131,131,131,131	0
91	MG	1	3814	1/1	0.42	0.33	73,73,73,73	0
91	MG	5	4014	1/1	0.47	0.59	49,49,49,49	1
91	MG	1	3720	1/1	0.48	0.25	93,93,93,93	0
91	MG	19	203	1/1	0.49	0.47	55,55,55,55	1
91	MG	1	3875	1/1	0.50	0.47	65,65,65,65	0
91	MG	5	4016	1/1	0.50	0.38	101,101,101,101	0
91	MG	1	4070	1/1	0.53	0.35	77,77,77,77	0
91	MG	1	3955	1/1	0.53	0.79	105,105,105,105	0
91	MG	2	2024	1/1	0.54	0.70	97,97,97,97	0
91	MG	2	2013	1/1	0.55	0.54	90,90,90,90	0
91	MG	2	1981	1/1	0.55	0.62	119,119,119,119	0
91	MG	M6	201	1/1	0.56	0.39	51,51,51,51	1
91	MG	5	4103	1/1	0.56	1.12	54,54,54,54	1
91	MG	1	3472	1/1	0.56	0.58	63,63,63,63	0
91	MG	1	3728	1/1	0.57	0.33	64,64,64,64	0
91	MG	5	3920	1/1	0.57	1.44	58,58,58,58	1
91	MG	2	1920	1/1	0.57	0.71	79,79,79,79	0
91	MG	1	4055	1/1	0.58	0.43	67,67,67,67	0
91	MG	6	1917	1/1	0.58	0.49	91,91,91,91	0
91	MG	1	4019	1/1	0.60	0.75	53,53,53,53	1
91	MG	M9	201	1/1	0.60	0.30	79,79,79,79	0
91	MG	6	1993	1/1	0.60	0.28	91,91,91,91	0
91	MG	1	3641	1/1	0.60	0.44	66,66,66,66	0
91	MG	6	1985	1/1	0.61	0.30	90,90,90,90	0
91	MG	6	1926	1/1	0.62	0.49	90,90,90,90	0
91	MG	1	3680	1/1	0.63	0.58	56,56,56,56	0
91	MG	1	3962	1/1	0.64	0.59	56,56,56,56	0
91	MG	6	2054	1/1	0.64	0.33	77,77,77,77	0
91	MG	5	4047	1/1	0.65	0.53	51,51,51,51	1
92	OHX	6	2326	7/7	0.66	0.39	148,148,148,148	7
91	MG	5	4051	1/1	0.66	0.86	71,71,71,71	1
91	MG	1	3950	1/1	0.67	0.23	82,82,82,82	0
91	MG	D0	201	1/1	0.67	0.42	88,88,88,88	0
91	MG	1	3697	1/1	0.68	0.42	51,51,51,51	0
91	MG	5	3871	1/1	0.68	0.18	82,82,82,82	0
91	MG	6	2123	1/1	0.68	0.36	72,72,72,72	0
91	MG	m7	206	1/1	0.68	0.42	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	1	3882	1/1	0.69	0.49	55,55,55,55	1
91	MG	c8	203	1/1	0.69	0.30	113,113,113,113	0
91	MG	1	3876	1/1	0.69	0.41	73,73,73,73	1
91	MG	2	1964	1/1	0.69	0.92	75,75,75,75	0
91	MG	2	2026	1/1	0.69	0.46	101,101,101,101	0
91	MG	N3	204	1/1	0.69	0.47	80,80,80,80	0
91	MG	1	4000	1/1	0.69	0.28	63,63,63,63	1
91	MG	5	4135	1/1	0.71	0.71	82,82,82,82	1
92	OHX	5	4563	7/7	0.71	0.26	174,174,174,174	7
91	MG	5	3418	1/1	0.71	0.55	51,51,51,51	0
91	MG	1	3779	1/1	0.71	0.49	55,55,55,55	0
91	MG	5	4064	1/1	0.71	0.49	50,50,50,50	1
91	MG	6	2099	1/1	0.72	0.67	61,61,61,61	1
92	OHX	1	4417	7/7	0.72	0.29	143,143,143,143	7
91	MG	5	3927	1/1	0.72	0.52	70,70,70,70	0
91	MG	1	3880	1/1	0.72	0.31	115,115,115,115	0
91	MG	1	3714	1/1	0.72	0.40	62,62,62,62	0
91	MG	n3	203	1/1	0.72	0.43	49,49,49,49	1
91	MG	6	2107	1/1	0.72	0.41	76,76,76,76	0
91	MG	2	1968	1/1	0.72	0.35	78,78,78,78	0
91	MG	2	2023	1/1	0.72	0.70	98,98,98,98	0
92	OHX	5	4536	7/7	0.72	0.48	67,67,67,67	7
91	MG	5	3835	1/1	0.73	0.39	50,50,50,50	1
91	MG	2	1999	1/1	0.73	0.48	115,115,115,115	0
91	MG	2	2014	1/1	0.73	0.47	71,71,71,71	0
91	MG	5	3780	1/1	0.74	0.34	53,53,53,53	0
91	MG	6	2020	1/1	0.74	0.42	86,86,86,86	0
92	OHX	7	239	7/7	0.74	0.42	75,75,75,75	7
91	MG	5	4145	1/1	0.75	0.39	120,120,120,120	0
91	MG	6	2061	1/1	0.75	0.25	82,82,82,82	0
91	MG	14	401	1/1	0.76	1.32	62,62,62,62	0
91	MG	5	3834	1/1	0.76	0.50	53,53,53,53	1
91	MG	6	2044	1/1	0.76	0.43	72,72,72,72	0
91	MG	5	3777	1/1	0.76	0.17	69,69,69,69	0
91	MG	5	3715	1/1	0.76	0.41	67,67,67,67	0
92	OHX	m9	202	7/7	0.76	0.34	83,83,83,83	7
91	MG	2	1989	1/1	0.76	0.29	91,91,91,91	0
91	MG	5	3967	1/1	0.76	0.32	61,61,61,61	0
91	MG	8	216	1/1	0.76	0.70	68,68,68,68	0
91	MG	1	3646	1/1	0.76	0.25	55,55,55,55	0
91	MG	1	3510	1/1	0.77	0.61	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	6	2095	1/1	0.77	0.17	78,78,78,78	0
91	MG	5	3977	1/1	0.77	1.14	64,64,64,64	1
91	MG	1	3557	1/1	0.77	0.41	77,77,77,77	0
91	MG	1	3918	1/1	0.78	0.23	88,88,88,88	0
91	MG	2	1988	1/1	0.78	0.35	77,77,77,77	0
91	MG	5	3897	1/1	0.78	0.39	50,50,50,50	1
91	MG	5	3719	1/1	0.78	0.55	73,73,73,73	0
91	MG	1	3602	1/1	0.78	0.43	48,48,48,48	0
91	MG	1	3705	1/1	0.78	0.38	61,61,61,61	0
91	MG	5	3738	1/1	0.78	0.33	66,66,66,66	0
91	MG	5	4086	1/1	0.78	0.96	53,53,53,53	1
91	MG	5	4029	1/1	0.78	1.01	54,54,54,54	1
91	MG	1	3958	1/1	0.78	0.37	56,56,56,56	1
91	MG	2	1948	1/1	0.79	0.31	143,143,143,143	0
91	MG	1	4026	1/1	0.79	0.44	58,58,58,58	0
91	MG	6	2132	1/1	0.79	0.50	77,77,77,77	0
91	MG	5	3766	1/1	0.79	0.26	63,63,63,63	1
91	MG	5	4572	1/1	0.79	0.40	50,50,50,50	0
91	MG	5	3727	1/1	0.79	0.29	61,61,61,61	0
91	MG	5	3655	1/1	0.79	0.36	99,99,99,99	0
91	MG	6	2021	1/1	0.79	0.18	75,75,75,75	0
91	MG	14	402	1/1	0.79	0.53	60,60,60,60	0
92	OHX	6	2306	7/7	0.79	0.22	142,142,142,142	7
91	MG	4	218	1/1	0.79	0.24	68,68,68,68	0
91	MG	1	3456	1/1	0.79	0.26	74,74,74,74	0
92	OHX	6	2327	7/7	0.79	0.30	160,160,160,160	7
92	OHX	1	4463	7/7	0.79	0.45	77,77,77,77	7
92	OHX	2	2242	7/7	0.79	0.38	97,97,97,97	7
91	MG	6	2079	1/1	0.79	1.12	61,61,61,61	1
91	MG	5	3621	1/1	0.79	0.41	67,67,67,67	0
91	MG	1	3774	1/1	0.80	0.32	62,62,62,62	0
91	MG	m4	201	1/1	0.80	0.35	68,68,68,68	0
91	MG	5	3718	1/1	0.80	0.46	62,62,62,62	0
91	MG	1	3424	1/1	0.80	0.24	56,56,56,56	0
91	MG	1	3695	1/1	0.80	0.78	75,75,75,75	0
92	OHX	5	4520	7/7	0.80	0.66	97,97,97,97	7
91	MG	M7	207	1/1	0.80	0.38	59,59,59,59	0
91	MG	2	2047	1/1	0.80	0.97	99,99,99,99	0
92	OHX	1	4425	7/7	0.80	0.59	94,94,94,94	7
91	MG	L3	405	1/1	0.81	0.35	71,71,71,71	0
91	MG	1	3729	1/1	0.81	0.51	58,58,58,58	1
91	MG	M1	300	1/1	0.81	0.17	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3711	1/1	0.81	0.67	96,96,96,96	0
91	MG	m5	302	1/1	0.81	0.27	66,66,66,66	0
91	MG	3	215	1/1	0.81	0.20	90,90,90,90	0
91	MG	1	3688	1/1	0.81	0.45	92,92,92,92	0
92	OHX	L3	409	7/7	0.81	0.40	94,94,94,94	7
91	MG	2	1975	1/1	0.81	0.66	79,79,79,79	0
91	MG	5	3437	1/1	0.81	0.36	93,93,93,93	0
92	OHX	5	4489	7/7	0.81	0.34	86,86,86,86	7
91	MG	m7	204	1/1	0.81	0.41	51,51,51,51	0
91	MG	5	3951	1/1	0.81	0.83	64,64,64,64	0
91	MG	2	1996	1/1	0.82	0.16	95,95,95,95	0
91	MG	6	2085	1/1	0.82	0.52	67,67,67,67	1
91	MG	5	3497	1/1	0.82	0.25	70,70,70,70	0
91	MG	5	3691	1/1	0.82	0.47	60,60,60,60	1
91	MG	1	3408	1/1	0.82	0.35	61,61,61,61	0
91	MG	5	3761	1/1	0.82	0.26	63,63,63,63	0
91	MG	6	2028	1/1	0.82	0.47	70,70,70,70	0
91	MG	5	3805	1/1	0.82	0.39	53,53,53,53	0
91	MG	N0	202	1/1	0.82	0.19	60,60,60,60	0
91	MG	1	3486	1/1	0.82	0.32	51,51,51,51	0
91	MG	1	3625	1/1	0.82	0.53	61,61,61,61	0
91	MG	1	3465	1/1	0.82	0.69	51,51,51,51	0
91	MG	1	3677	1/1	0.83	0.58	52,52,52,52	0
91	MG	m1	202	1/1	0.83	0.26	76,76,76,76	0
91	MG	5	4127	1/1	0.83	0.35	54,54,54,54	1
92	OHX	1	4465	7/7	0.83	0.38	67,67,67,67	7
91	MG	o6	201	1/1	0.83	0.20	80,80,80,80	1
91	MG	s4	301	1/1	0.83	0.23	73,73,73,73	0
91	MG	5	3962	1/1	0.83	0.54	50,50,50,50	0
91	MG	1	3692	1/1	0.83	0.22	82,82,82,82	0
91	MG	6	2032	1/1	0.83	0.68	67,67,67,67	0
92	OHX	2	2241	7/7	0.83	0.32	104,104,104,104	7
91	MG	5	3578	1/1	0.84	0.64	54,54,54,54	0
91	MG	1	3806	1/1	0.84	0.34	65,65,65,65	0
91	MG	2	1965	1/1	0.84	0.51	83,83,83,83	0
91	MG	n3	202	1/1	0.84	0.51	58,58,58,58	0
91	MG	5	4118	1/1	0.84	0.19	72,72,72,72	0
92	OHX	1	4415	7/7	0.84	0.34	83,83,83,83	7
92	OHX	2	2202	7/7	0.84	0.48	100,100,100,100	7
92	OHX	6	2290	7/7	0.84	0.20	148,148,148,148	7
92	OHX	5	4537	7/7	0.84	0.57	56,56,56,56	7
91	MG	5	3682	1/1	0.84	0.31	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3830	1/1	0.84	0.30	70,70,70,70	0
91	MG	15	305	1/1	0.84	0.10	79,79,79,79	0
91	MG	4	228	1/1	0.84	0.33	58,58,58,58	0
92	OHX	5	4548	7/7	0.84	0.75	58,58,58,58	7
91	MG	6	1928	1/1	0.84	0.53	60,60,60,60	0
92	OHX	2	2196	7/7	0.84	0.23	139,139,139,139	7
92	OHX	2	2188	7/7	0.85	0.31	93,93,93,93	7
91	MG	5	3637	1/1	0.85	0.37	63,63,63,63	0
92	OHX	5	4530	7/7	0.85	0.31	130,130,130,130	7
92	OHX	6	2320	7/7	0.85	0.40	77,77,77,77	7
91	MG	5	3425	1/1	0.85	0.12	57,57,57,57	0
91	MG	1	3653	1/1	0.85	0.27	86,86,86,86	0
91	MG	5	3630	1/1	0.85	0.57	57,57,57,57	0
91	MG	N8	205	1/1	0.85	0.20	63,63,63,63	0
92	OHX	6	2267	7/7	0.85	0.31	100,100,100,100	7
91	MG	5	3981	1/1	0.85	0.57	56,56,56,56	1
91	MG	L2	303	1/1	0.85	0.30	54,54,54,54	0
91	MG	8	241	1/1	0.85	0.44	56,56,56,56	0
91	MG	d9	101	1/1	0.85	0.21	96,96,96,96	0
91	MG	1	3835	1/1	0.85	0.35	68,68,68,68	0
91	MG	6	1948	1/1	0.85	0.47	53,53,53,53	0
91	MG	7	214	1/1	0.85	0.36	80,80,80,80	0
91	MG	5	3910	1/1	0.85	0.42	64,64,64,64	0
92	OHX	5	4391	7/7	0.86	0.36	52,52,52,52	7
91	MG	5	3786	1/1	0.86	0.61	49,49,49,49	0
91	MG	1	3805	1/1	0.86	0.37	61,61,61,61	0
91	MG	1	3522	1/1	0.86	0.64	42,42,42,42	0
91	MG	1	3471	1/1	0.86	0.47	58,58,58,58	0
91	MG	5	3474	1/1	0.86	0.27	62,62,62,62	0
91	MG	6	2011	1/1	0.86	0.28	64,64,64,64	1
91	MG	5	3646	1/1	0.86	0.35	46,46,46,46	0
91	MG	1	3826	1/1	0.86	0.56	58,58,58,58	0
92	OHX	14	405	7/7	0.86	0.39	73,73,73,73	7
91	MG	5	3845	1/1	0.86	0.44	68,68,68,68	0
91	MG	1	3878	1/1	0.86	0.71	55,55,55,55	0
92	OHX	6	2333	7/7	0.86	0.15	123,123,123,123	7
91	MG	5	3762	1/1	0.86	0.27	67,67,67,67	0
91	MG	5	4022	1/1	0.86	0.55	52,52,52,52	0
91	MG	5	3712	1/1	0.86	0.38	48,48,48,48	1
91	MG	3	213	1/1	0.86	0.20	79,79,79,79	0
91	MG	1	3777	1/1	0.86	0.23	102,102,102,102	0
91	MG	5	3684	1/1	0.86	0.47	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	5	4427	7/7	0.86	0.33	66,66,66,66	7
91	MG	5	3517	1/1	0.86	0.54	44,44,44,44	0
91	MG	1	4042	1/1	0.86	1.09	67,67,67,67	1
91	MG	6	1998	1/1	0.86	0.19	79,79,79,79	0
91	MG	6	1969	1/1	0.86	0.20	73,73,73,73	0
91	MG	5	4048	1/1	0.87	0.35	57,57,57,57	1
91	MG	5	4053	1/1	0.87	0.29	62,62,62,62	0
92	OHX	5	4523	7/7	0.87	0.31	125,125,125,125	7
91	MG	1	3911	1/1	0.87	0.31	62,62,62,62	0
91	MG	5	4137	1/1	0.87	0.32	55,55,55,55	0
91	MG	1	4085	1/1	0.87	0.14	62,62,62,62	1
92	OHX	5	4558	7/7	0.87	0.33	97,97,97,97	7
91	MG	O7	105	1/1	0.87	0.20	81,81,81,81	0
91	MG	2	1901	1/1	0.87	0.42	86,86,86,86	0
91	MG	M8	201	1/1	0.87	1.88	53,53,53,53	1
91	MG	5	3755	1/1	0.87	0.60	56,56,56,56	0
91	MG	1	3423	1/1	0.87	0.18	50,50,50,50	0
92	OHX	6	2243	7/7	0.87	0.46	80,80,80,80	7
91	MG	5	3791	1/1	0.87	0.18	66,66,66,66	0
91	MG	4	203	1/1	0.87	0.67	66,66,66,66	0
91	MG	1	3525	1/1	0.87	0.51	53,53,53,53	0
91	MG	5	3888	1/1	0.87	0.46	50,50,50,50	0
91	MG	1	4052	1/1	0.88	0.26	55,55,55,55	0
91	MG	5	3872	1/1	0.88	0.49	47,47,47,47	1
91	MG	5	3626	1/1	0.88	0.39	62,62,62,62	0
91	MG	5	3774	1/1	0.88	0.30	54,54,54,54	0
92	OHX	5	4409	7/7	0.88	0.26	59,59,59,59	7
92	OHX	6	2294	7/7	0.88	0.25	81,81,81,81	7
91	MG	5	3649	1/1	0.88	0.44	53,53,53,53	0
91	MG	D6	102	1/1	0.88	0.53	92,92,92,92	0
92	OHX	1	4295	7/7	0.88	0.17	116,116,116,116	7
92	OHX	2	2208	7/7	0.88	0.29	106,106,106,106	7
91	MG	1	3820	1/1	0.88	0.80	61,61,61,61	0
91	MG	6	1954	1/1	0.88	0.46	67,67,67,67	0
92	OHX	m7	208	7/7	0.88	0.30	63,63,63,63	7
91	MG	1	3699	1/1	0.88	0.41	65,65,65,65	0
91	MG	7	203	1/1	0.88	0.60	39,39,39,39	0
91	MG	6	2124	1/1	0.88	1.13	73,73,73,73	0
91	MG	5	3568	1/1	0.88	0.70	43,43,43,43	0
92	OHX	5	4547	7/7	0.89	0.29	79,79,79,79	7
91	MG	5	3725	1/1	0.89	0.76	46,46,46,46	1
91	MG	6	2136	1/1	0.89	0.33	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	8	201	1/1	0.89	0.25	56,56,56,56	0
91	MG	5	4116	1/1	0.89	0.35	64,64,64,64	1
91	MG	2	1987	1/1	0.89	0.19	98,98,98,98	0
91	MG	1	3709	1/1	0.89	0.77	65,65,65,65	0
91	MG	1	3713	1/1	0.89	0.35	66,66,66,66	0
91	MG	1	3696	1/1	0.89	1.15	70,70,70,70	1
91	MG	5	3749	1/1	0.89	0.25	61,61,61,61	0
91	MG	1	3518	1/1	0.89	0.47	40,40,40,40	0
91	MG	1	3683	1/1	0.89	0.60	59,59,59,59	0
91	MG	4	220	1/1	0.89	0.28	102,102,102,102	1
91	MG	5	3405	1/1	0.89	0.62	70,70,70,70	0
91	MG	6	2019	1/1	0.89	1.37	86,86,86,86	1
91	MG	2	1903	1/1	0.89	0.67	59,59,59,59	0
91	MG	8	205	1/1	0.89	0.54	61,61,61,61	0
92	OHX	S6	302	7/7	0.89	0.14	117,117,117,117	7
91	MG	L6	201	1/1	0.89	0.29	59,59,59,59	0
91	MG	5	3858	1/1	0.89	0.28	48,48,48,48	1
92	OHX	6	2335	7/7	0.89	0.23	124,124,124,124	7
91	MG	5	3874	1/1	0.89	0.27	54,54,54,54	0
91	MG	4	201	1/1	0.89	0.37	47,47,47,47	0
92	OHX	M0	306	7/7	0.90	0.53	64,64,64,64	7
91	MG	6	2016	1/1	0.90	0.35	97,97,97,97	0
92	OHX	6	2299	7/7	0.90	0.23	125,125,125,125	7
92	OHX	2	2244	7/7	0.90	0.27	147,147,147,147	7
91	MG	5	3544	1/1	0.90	0.58	47,47,47,47	0
92	OHX	6	2268	7/7	0.90	0.30	78,78,78,78	7
91	MG	6	1991	1/1	0.90	0.37	63,63,63,63	0
91	MG	17	301	1/1	0.90	0.34	47,47,47,47	0
91	MG	5	3432	1/1	0.90	0.38	49,49,49,49	0
91	MG	1	3650	1/1	0.90	0.26	65,65,65,65	0
92	OHX	5	4508	7/7	0.90	0.16	117,117,117,117	7
91	MG	1	4053	1/1	0.90	0.35	71,71,71,71	0
92	OHX	5	4471	7/7	0.90	0.35	89,89,89,89	7
91	MG	1	3887	1/1	0.90	0.45	62,62,62,62	0
91	MG	5	3615	1/1	0.90	0.80	51,51,51,51	0
92	OHX	2	2249	7/7	0.90	0.16	144,144,144,144	7
91	MG	5	3680	1/1	0.90	0.29	70,70,70,70	0
92	OHX	2	2216	7/7	0.90	0.31	95,95,95,95	7
91	MG	6	2134	1/1	0.90	0.74	97,97,97,97	0
91	MG	2	1902	1/1	0.90	0.83	56,56,56,56	0
92	OHX	6	2214	7/7	0.90	0.25	105,105,105,105	7
91	MG	5	3644	1/1	0.90	0.37	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	6	1980	1/1	0.90	0.12	85,85,85,85	0
91	MG	5	3873	1/1	0.90	0.35	54,54,54,54	0
92	OHX	2	2211	7/7	0.90	0.17	124,124,124,124	7
92	OHX	1	4430	7/7	0.90	0.40	85,85,85,85	7
91	MG	1	3899	1/1	0.90	0.14	67,67,67,67	1
91	MG	5	3896	1/1	0.90	0.27	45,45,45,45	0
91	MG	6	2101	1/1	0.90	0.36	75,75,75,75	1
91	MG	5	3427	1/1	0.91	0.36	55,55,55,55	0
91	MG	5	3945	1/1	0.91	0.56	56,56,56,56	0
92	OHX	1	4441	7/7	0.91	0.15	186,186,186,186	7
91	MG	2	1970	1/1	0.91	0.20	79,79,79,79	0
91	MG	m6	202	1/1	0.91	1.27	51,51,51,51	1
91	MG	1	3678	1/1	0.91	0.78	57,57,57,57	0
91	MG	2	1986	1/1	0.91	0.34	89,89,89,89	0
92	OHX	1	4504	7/7	0.91	0.34	73,73,73,73	7
92	OHX	S8	303	7/7	0.91	0.15	115,115,115,115	7
91	MG	1	3818	1/1	0.91	0.73	73,73,73,73	0
91	MG	1	3977	1/1	0.91	0.23	48,48,48,48	0
91	MG	5	3741	1/1	0.91	0.19	75,75,75,75	1
91	MG	6	2038	1/1	0.91	0.13	99,99,99,99	0
91	MG	1	3783	1/1	0.91	0.34	66,66,66,66	0
91	MG	l2	305	1/1	0.91	0.91	59,59,59,59	1
92	OHX	M9	204	7/7	0.91	0.20	94,94,94,94	7
91	MG	1	3824	1/1	0.91	0.53	74,74,74,74	0
91	MG	5	3763	1/1	0.91	0.31	79,79,79,79	0
91	MG	5	3550	1/1	0.91	0.63	58,58,58,58	0
91	MG	1	3742	1/1	0.91	0.21	69,69,69,69	0
92	OHX	6	2303	7/7	0.91	0.36	88,88,88,88	7
92	OHX	1	4443	7/7	0.91	0.30	108,108,108,108	7
92	OHX	2	2132	7/7	0.92	0.18	114,114,114,114	7
91	MG	sM	201	1/1	0.92	0.56	59,59,59,59	0
92	OHX	6	2278	7/7	0.92	0.15	110,110,110,110	7
91	MG	6	2051	1/1	0.92	1.06	67,67,67,67	1
91	MG	5	3416	1/1	0.92	0.52	49,49,49,49	0
91	MG	q2	201	1/1	0.92	0.97	55,55,55,55	1
91	MG	1	3649	1/1	0.92	0.31	69,69,69,69	0
91	MG	1	3654	1/1	0.92	0.18	72,72,72,72	0
91	MG	1	4031	1/1	0.92	0.23	55,55,55,55	0
91	MG	5	3583	1/1	0.92	0.81	42,42,42,42	0
91	MG	5	3905	1/1	0.92	0.96	49,49,49,49	1
91	MG	O7	101	1/1	0.92	0.95	67,67,67,67	1
91	MG	1	4074	1/1	0.92	0.79	63,63,63,63	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	5	3614	1/1	0.92	0.27	63,63,63,63	0
92	OHX	8	233	7/7	0.92	0.21	103,103,103,103	7
92	OHX	2	2219	7/7	0.92	0.23	99,99,99,99	7
91	MG	5	3586	1/1	0.92	0.67	50,50,50,50	0
91	MG	1	3517	1/1	0.92	0.30	51,51,51,51	0
91	MG	1	3458	1/1	0.92	0.36	48,48,48,48	0
91	MG	1	3559	1/1	0.92	0.56	53,53,53,53	0
91	MG	5	3667	1/1	0.92	0.39	56,56,56,56	0
92	OHX	1	4462	7/7	0.92	0.61	66,66,66,66	7
92	OHX	1	4419	7/7	0.92	0.48	71,71,71,71	7
91	MG	m7	203	1/1	0.92	0.66	48,48,48,48	0
91	MG	1	4024	1/1	0.92	0.28	79,79,79,79	0
91	MG	q0	202	1/1	0.92	0.25	56,56,56,56	0
91	MG	3	204	1/1	0.92	0.52	63,63,63,63	0
91	MG	3	201	1/1	0.92	0.32	92,92,92,92	0
92	OHX	1	4460	7/7	0.92	0.58	60,60,60,60	7
91	MG	1	3802	1/1	0.92	0.27	49,49,49,49	0
91	MG	5	3526	1/1	0.92	0.41	53,53,53,53	0
92	OHX	5	4527	7/7	0.92	0.25	94,94,94,94	7
92	OHX	2	2149	7/7	0.92	0.29	112,112,112,112	7
91	MG	1	3508	1/1	0.92	0.45	50,50,50,50	0
92	OHX	2	2170	7/7	0.92	0.27	94,94,94,94	7
91	MG	2	1929	1/1	0.92	0.53	103,103,103,103	0
91	MG	5	3772	1/1	0.92	0.28	58,58,58,58	1
91	MG	6	1975	1/1	0.92	0.48	74,74,74,74	0
91	MG	5	4018	1/1	0.92	0.52	55,55,55,55	0
91	MG	5	3994	1/1	0.93	0.23	78,78,78,78	0
91	MG	1	3968	1/1	0.93	0.46	44,44,44,44	1
92	OHX	A	101	7/7	0.93	0.35	112,112,112,112	7
92	OHX	5	4444	7/7	0.93	0.29	66,66,66,66	7
91	MG	6	2014	1/1	0.93	0.17	98,98,98,98	0
91	MG	5	3560	1/1	0.93	0.46	66,66,66,66	0
91	MG	6	2122	1/1	0.93	0.94	75,75,75,75	1
91	MG	5	3943	1/1	0.93	0.52	61,61,61,61	1
92	OHX	5	4392	7/7	0.93	0.36	66,66,66,66	7
91	MG	6	1977	1/1	0.93	0.20	95,95,95,95	0
91	MG	1	3708	1/1	0.93	0.40	63,63,63,63	0
91	MG	5	3812	1/1	0.93	0.27	73,73,73,73	1
92	OHX	1	4274	7/7	0.93	0.49	67,67,67,67	7
91	MG	6	2012	1/1	0.93	0.34	95,95,95,95	0
92	OHX	6	2315	7/7	0.93	0.14	120,120,120,120	7
91	MG	5	3533	1/1	0.93	0.52	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3546	1/1	0.93	0.63	49,49,49,49	0
91	MG	5	3853	1/1	0.93	0.39	66,66,66,66	0
92	OHX	1	4325	7/7	0.93	0.13	124,124,124,124	7
92	OHX	1	4440	7/7	0.93	0.14	152,152,152,152	7
91	MG	2	2058	1/1	0.93	0.16	88,88,88,88	0
91	MG	O3	203	1/1	0.93	0.57	59,59,59,59	1
91	MG	5	3800	1/1	0.93	0.72	59,59,59,59	0
91	MG	2	2034	1/1	0.93	0.40	85,85,85,85	1
92	OHX	m0	305	7/7	0.94	0.59	59,59,59,59	7
92	OHX	4	245	7/7	0.94	0.36	60,60,60,60	7
91	MG	m6	201	1/1	0.94	0.59	48,48,48,48	1
92	OHX	1	4251	7/7	0.94	0.28	107,107,107,107	7
92	OHX	1	4361	7/7	0.94	0.45	68,68,68,68	7
91	MG	1	3539	1/1	0.94	0.53	60,60,60,60	0
92	OHX	2	2229	7/7	0.94	0.18	90,90,90,90	7
92	OHX	1	4237	7/7	0.94	0.27	97,97,97,97	7
92	OHX	6	2312	7/7	0.94	0.29	70,70,70,70	7
91	MG	n1	203	1/1	0.94	0.51	73,73,73,73	0
91	MG	1	3611	1/1	0.94	0.24	57,57,57,57	0
91	MG	N0	201	1/1	0.94	1.17	60,60,60,60	1
92	OHX	1	4330	7/7	0.94	0.17	93,93,93,93	7
92	OHX	5	4394	7/7	0.94	0.23	80,80,80,80	7
91	MG	1	3419	1/1	0.94	0.87	54,54,54,54	0
91	MG	1	3626	1/1	0.94	0.49	49,49,49,49	0
92	OHX	6	2319	7/7	0.94	0.23	105,105,105,105	7
91	MG	5	3885	1/1	0.94	0.52	56,56,56,56	1
92	OHX	5	4346	7/7	0.94	0.36	60,60,60,60	7
91	MG	M7	201	1/1	0.94	0.67	55,55,55,55	1
91	MG	1	3800	1/1	0.94	0.28	55,55,55,55	1
91	MG	5	3937	1/1	0.94	0.42	70,70,70,70	0
91	MG	o4	203	1/1	0.94	1.35	80,80,80,80	1
92	OHX	5	4552	7/7	0.94	0.24	71,71,71,71	7
91	MG	6	1986	1/1	0.94	0.30	61,61,61,61	0
92	OHX	5	4525	7/7	0.94	0.22	81,81,81,81	7
91	MG	1	3464	1/1	0.94	0.50	41,41,41,41	0
92	OHX	2	2218	7/7	0.94	0.12	111,111,111,111	7
91	MG	5	3707	1/1	0.94	0.17	69,69,69,69	0
92	OHX	6	2250	7/7	0.94	0.32	98,98,98,98	7
92	OHX	6	2316	7/7	0.94	0.35	72,72,72,72	7
91	MG	6	2023	1/1	0.94	0.19	85,85,85,85	0
91	MG	S8	301	1/1	0.94	1.61	79,79,79,79	1
92	OHX	1	4243	7/7	0.94	0.38	76,76,76,76	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	5	4378	7/7	0.94	0.38	87,87,87,87	7
92	OHX	5	4507	7/7	0.94	0.22	61,61,61,61	7
91	MG	5	4571	1/1	0.94	0.65	53,53,53,53	1
91	MG	1	3563	1/1	0.94	0.69	52,52,52,52	0
91	MG	5	3504	1/1	0.94	0.20	51,51,51,51	0
91	MG	2	2003	1/1	0.94	0.59	77,77,77,77	0
92	OHX	6	2297	7/7	0.94	0.23	99,99,99,99	7
91	MG	5	3490	1/1	0.94	0.22	62,62,62,62	0
92	OHX	1	4291	7/7	0.94	0.22	77,77,77,77	7
92	OHX	1	4495	7/7	0.94	0.29	77,77,77,77	7
91	MG	m8	201	1/1	0.94	0.35	66,66,66,66	0
92	OHX	1	4356	7/7	0.94	0.45	74,74,74,74	7
91	MG	1	3466	1/1	0.94	0.48	54,54,54,54	0
92	OHX	1	4301	7/7	0.94	0.26	57,57,57,57	7
91	MG	1	3861	1/1	0.94	0.33	48,48,48,48	0
91	MG	M7	202	1/1	0.94	0.41	58,58,58,58	1
92	OHX	5	4466	7/7	0.94	0.25	70,70,70,70	7
91	MG	1	3636	1/1	0.94	0.30	54,54,54,54	0
92	OHX	5	4295	7/7	0.94	0.30	79,79,79,79	7
91	MG	1	3956	1/1	0.94	0.39	48,48,48,48	0
91	MG	1	4062	1/1	0.94	0.25	91,91,91,91	1
91	MG	5	4039	1/1	0.95	0.28	51,51,51,51	1
91	MG	1	3488	1/1	0.95	0.29	69,69,69,69	0
91	MG	2	1973	1/1	0.95	0.63	118,118,118,118	0
91	MG	1	4081	1/1	0.95	0.81	67,67,67,67	1
92	OHX	6	2202	7/7	0.95	0.26	89,89,89,89	7
91	MG	1	3825	1/1	0.95	0.14	59,59,59,59	0
91	MG	6	1966	1/1	0.95	0.52	95,95,95,95	0
92	OHX	1	4454	7/7	0.95	0.20	98,98,98,98	7
91	MG	5	4570	1/1	0.95	0.27	59,59,59,59	0
92	OHX	2	2191	7/7	0.95	0.24	85,85,85,85	7
91	MG	6	1936	1/1	0.95	0.42	61,61,61,61	0
91	MG	M6	203	1/1	0.95	1.24	59,59,59,59	1
92	OHX	2	2184	7/7	0.95	0.11	111,111,111,111	7
91	MG	5	3569	1/1	0.95	0.54	44,44,44,44	0
91	MG	1	3406	1/1	0.95	0.41	113,113,113,113	0
91	MG	5	3553	1/1	0.95	0.55	51,51,51,51	0
92	OHX	2	2178	7/7	0.95	0.20	107,107,107,107	7
91	MG	4	206	1/1	0.95	0.52	71,71,71,71	0
92	OHX	m0	303	7/7	0.95	0.68	61,61,61,61	7
92	OHX	6	2338	7/7	0.95	0.28	89,89,89,89	7
91	MG	6	1911	1/1	0.95	0.49	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3600	1/1	0.95	0.65	50,50,50,50	0
91	MG	1	3897	1/1	0.95	0.27	56,56,56,56	1
92	OHX	6	2191	7/7	0.95	0.21	91,91,91,91	7
92	OHX	2	2237	7/7	0.95	0.32	86,86,86,86	7
92	OHX	5	4383	7/7	0.95	0.33	56,56,56,56	7
91	MG	1	3595	1/1	0.95	0.47	59,59,59,59	0
92	OHX	1	4281	7/7	0.95	0.17	98,98,98,98	7
91	MG	1	3549	1/1	0.95	0.26	56,56,56,56	0
92	OHX	5	4438	7/7	0.95	0.11	133,133,133,133	7
91	MG	6	1950	1/1	0.95	0.57	54,54,54,54	0
91	MG	M5	301	1/1	0.95	0.28	55,55,55,55	0
91	MG	1	3855	1/1	0.95	0.16	78,78,78,78	0
92	OHX	5	4279	7/7	0.95	0.31	64,64,64,64	7
91	MG	6	1942	1/1	0.95	0.38	54,54,54,54	0
91	MG	l3	409	1/1	0.95	0.35	49,49,49,49	0
91	MG	5	4083	1/1	0.95	0.37	54,54,54,54	1
91	MG	2	1991	1/1	0.95	0.28	80,80,80,80	0
92	OHX	5	4347	7/7	0.95	0.28	62,62,62,62	7
91	MG	5	4002	1/1	0.95	0.20	63,63,63,63	0
92	OHX	1	4300	7/7	0.95	0.23	122,122,122,122	7
92	OHX	5	4314	7/7	0.95	0.20	105,105,105,105	7
91	MG	1	3985	1/1	0.95	0.20	82,82,82,82	0
92	OHX	5	4284	7/7	0.95	0.36	52,52,52,52	7
91	MG	5	3785	1/1	0.95	0.09	71,71,71,71	0
91	MG	5	4129	1/1	0.95	0.46	62,62,62,62	1
92	OHX	1	4335	7/7	0.95	0.15	106,106,106,106	7
91	MG	o3	201	1/1	0.96	0.69	49,49,49,49	1
91	MG	5	3481	1/1	0.96	0.51	45,45,45,45	0
92	OHX	1	4217	7/7	0.96	0.18	69,69,69,69	7
91	MG	1	3615	1/1	0.96	0.33	55,55,55,55	0
91	MG	5	3477	1/1	0.96	0.25	72,72,72,72	0
92	OHX	5	4242	7/7	0.96	0.34	66,66,66,66	7
91	MG	1	3533	1/1	0.96	0.29	58,58,58,58	0
92	OHX	1	4289	7/7	0.96	0.27	111,111,111,111	7
92	OHX	5	4389	7/7	0.96	0.22	83,83,83,83	7
91	MG	1	3516	1/1	0.96	0.56	47,47,47,47	0
91	MG	1	4036	1/1	0.96	0.15	68,68,68,68	0
91	MG	1	3663	1/1	0.96	0.24	66,66,66,66	0
92	OHX	1	4439	7/7	0.96	0.27	60,60,60,60	7
91	MG	2	1982	1/1	0.96	0.56	74,74,74,74	0
91	MG	5	3441	1/1	0.96	0.29	62,62,62,62	0
91	MG	3	206	1/1	0.96	0.55	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	1	4344	7/7	0.96	0.17	74,74,74,74	7
92	OHX	1	4268	7/7	0.96	0.37	123,123,123,123	7
92	OHX	1	4165	7/7	0.96	0.31	76,76,76,76	7
91	MG	2	1921	1/1	0.96	0.55	70,70,70,70	0
91	MG	1	4005	1/1	0.96	0.45	69,69,69,69	0
92	OHX	1	4482	7/7	0.96	0.16	153,153,153,153	7
92	OHX	5	4317	7/7	0.96	0.37	103,103,103,103	7
92	OHX	6	2233	7/7	0.96	0.20	90,90,90,90	7
92	OHX	1	4339	7/7	0.96	0.27	78,78,78,78	7
92	OHX	5	4271	7/7	0.96	0.15	145,145,145,145	7
92	OHX	8	230	7/7	0.96	0.22	108,108,108,108	7
92	OHX	1	4273	7/7	0.96	0.20	80,80,80,80	7
92	OHX	2	2166	7/7	0.96	0.14	103,103,103,103	7
91	MG	1	3469	1/1	0.96	0.30	58,58,58,58	0
92	OHX	2	2240	7/7	0.96	0.21	104,104,104,104	7
92	OHX	1	4476	7/7	0.96	0.31	84,84,84,84	7
91	MG	5	3518	1/1	0.96	0.88	45,45,45,45	0
91	MG	2	1916	1/1	0.96	0.38	69,69,69,69	0
91	MG	1	4064	1/1	0.96	0.91	63,63,63,63	1
92	OHX	5	4440	7/7	0.96	0.26	68,68,68,68	7
91	MG	6	2090	1/1	0.96	0.21	84,84,84,84	1
91	MG	5	4024	1/1	0.96	0.25	47,47,47,47	1
91	MG	1	3967	1/1	0.96	1.00	48,48,48,48	1
91	MG	L4	401	1/1	0.96	0.64	49,49,49,49	1
91	MG	5	3598	1/1	0.96	0.65	37,37,37,37	0
92	OHX	5	4229	7/7	0.96	0.46	58,58,58,58	7
91	MG	5	3855	1/1	0.96	0.10	60,60,60,60	0
92	OHX	1	4303	7/7	0.96	0.40	74,74,74,74	7
91	MG	1	3891	1/1	0.96	0.25	58,58,58,58	0
92	OHX	2	2163	7/7	0.96	0.18	100,100,100,100	7
91	MG	5	3473	1/1	0.96	0.49	51,51,51,51	0
92	OHX	5	4418	7/7	0.96	0.58	53,53,53,53	7
92	OHX	4	237	7/7	0.96	0.25	83,83,83,83	7
92	OHX	12	306	7/7	0.97	0.26	77,77,77,77	7
92	OHX	6	2205	7/7	0.97	0.28	88,88,88,88	7
92	OHX	5	4334	7/7	0.97	0.25	157,157,157,157	7
92	OHX	1	4331	7/7	0.97	0.28	95,95,95,95	7
92	OHX	1	4407	7/7	0.97	0.25	64,64,64,64	7
92	OHX	2	2180	7/7	0.97	0.12	113,113,113,113	7
92	OHX	1	4323	7/7	0.97	0.26	56,56,56,56	7
91	MG	1	3478	1/1	0.97	0.45	62,62,62,62	1
91	MG	6	1960	1/1	0.97	0.56	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3686	1/1	0.97	0.35	49,49,49,49	0
91	MG	5	4122	1/1	0.97	0.65	44,44,44,44	1
92	OHX	1	4218	7/7	0.97	0.30	56,56,56,56	7
91	MG	5	3697	1/1	0.97	0.51	49,49,49,49	1
92	OHX	5	4366	7/7	0.97	0.12	90,90,90,90	7
91	MG	5	3878	1/1	0.97	0.22	61,61,61,61	0
91	MG	5	3415	1/1	0.97	0.23	55,55,55,55	0
92	OHX	1	4129	7/7	0.97	0.35	64,64,64,64	7
92	OHX	1	4332	7/7	0.97	0.24	101,101,101,101	7
92	OHX	5	4429	7/7	0.97	0.52	52,52,52,52	7
91	MG	6	1913	1/1	0.97	0.46	65,65,65,65	0
92	OHX	1	4353	7/7	0.97	0.30	59,59,59,59	7
92	OHX	5	4251	7/7	0.97	0.22	89,89,89,89	7
91	MG	5	3939	1/1	0.97	0.29	48,48,48,48	0
91	MG	5	3575	1/1	0.97	0.63	46,46,46,46	0
91	MG	L3	402	1/1	0.97	0.56	53,53,53,53	0
91	MG	2	1907	1/1	0.97	0.61	67,67,67,67	0
91	MG	5	3839	1/1	0.97	0.98	50,50,50,50	1
92	OHX	1	4336	7/7	0.97	0.39	70,70,70,70	7
91	MG	1	3586	1/1	0.97	0.56	38,38,38,38	0
92	OHX	5	4330	7/7	0.97	0.35	71,71,71,71	7
92	OHX	1	4205	7/7	0.97	0.23	79,79,79,79	7
92	OHX	5	4448	7/7	0.97	0.28	54,54,54,54	7
91	MG	5	4143	1/1	0.97	0.79	63,63,63,63	1
92	OHX	5	4292	7/7	0.97	0.26	72,72,72,72	7
91	MG	5	3831	1/1	0.97	0.17	71,71,71,71	0
91	MG	1	3976	1/1	0.97	0.39	68,68,68,68	1
92	OHX	2	2153	7/7	0.97	0.37	72,72,72,72	7
92	OHX	2	2138	7/7	0.97	0.26	100,100,100,100	7
92	OHX	1	4435	7/7	0.97	0.15	87,87,87,87	7
91	MG	2	1963	1/1	0.97	0.26	83,83,83,83	0
92	OHX	2	2156	7/7	0.97	0.33	88,88,88,88	7
92	OHX	1	4341	7/7	0.97	0.19	112,112,112,112	7
91	MG	5	3956	1/1	0.97	0.43	59,59,59,59	1
91	MG	1	3851	1/1	0.97	0.23	70,70,70,70	0
92	OHX	1	4179	7/7	0.97	0.25	86,86,86,86	7
91	MG	1	3848	1/1	0.97	0.21	83,83,83,83	0
92	OHX	1	4267	7/7	0.97	0.20	62,62,62,62	7
92	OHX	6	2211	7/7	0.97	0.20	88,88,88,88	7
91	MG	1	3631	1/1	0.97	0.47	66,66,66,66	0
92	OHX	2	2076	7/7	0.97	0.19	111,111,111,111	7
92	OHX	6	2311	7/7	0.97	0.26	92,92,92,92	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
91	MG	5	3438	1/1	0.97	0.51	50,50,50,50	0
91	MG	n1	201	1/1	0.97	0.34	51,51,51,51	1
91	MG	1	3746	1/1	0.98	0.62	58,58,58,58	0
92	OHX	2	2088	7/7	0.98	0.28	91,91,91,91	7
91	MG	5	3817	1/1	0.98	0.35	51,51,51,51	1
92	OHX	7	234	7/7	0.98	0.26	79,79,79,79	7
92	OHX	5	4236	7/7	0.98	0.34	62,62,62,62	7
92	OHX	5	4274	7/7	0.98	0.30	71,71,71,71	7
92	OHX	5	4197	7/7	0.98	0.28	78,78,78,78	7
92	OHX	6	2209	7/7	0.98	0.19	67,67,67,67	7
91	MG	5	3413	1/1	0.98	0.57	51,51,51,51	0
91	MG	m3	201	1/1	0.98	0.27	66,66,66,66	1
91	MG	5	3868	1/1	0.98	0.27	54,54,54,54	0
91	MG	4	221	1/1	0.98	0.21	103,103,103,103	0
92	OHX	5	4204	7/7	0.98	0.28	82,82,82,82	7
92	OHX	1	4299	7/7	0.98	0.33	62,62,62,62	7
91	MG	5	3581	1/1	0.98	0.54	47,47,47,47	0
91	MG	5	3864	1/1	0.98	0.33	56,56,56,56	0
91	MG	1	4045	1/1	0.98	0.21	59,59,59,59	1
92	OHX	L3	407	7/7	0.98	0.25	70,70,70,70	7
92	OHX	5	4210	7/7	0.98	0.44	54,54,54,54	7
92	OHX	6	2163	7/7	0.98	0.29	70,70,70,70	7
92	OHX	o7	105	7/7	0.98	0.28	74,74,74,74	7
92	OHX	5	4480	7/7	0.98	0.30	61,61,61,61	7
91	MG	5	3556	1/1	0.98	0.33	51,51,51,51	0
91	MG	1	3858	1/1	0.98	0.28	57,57,57,57	1
92	OHX	1	4491	7/7	0.98	0.25	70,70,70,70	7
92	OHX	4	236	7/7	0.98	0.24	66,66,66,66	7
92	OHX	1	4233	7/7	0.98	0.20	68,68,68,68	7
92	OHX	1	4399	7/7	0.98	0.29	70,70,70,70	7
91	MG	1	3536	1/1	0.98	0.43	46,46,46,46	0
92	OHX	1	4204	7/7	0.98	0.15	86,86,86,86	7
92	OHX	5	4308	7/7	0.98	0.16	114,114,114,114	7
92	OHX	1	4134	7/7	0.98	0.27	66,66,66,66	7
91	MG	6	2080	1/1	0.98	0.13	80,80,80,80	1
92	OHX	1	4376	7/7	0.98	0.17	102,102,102,102	7
92	OHX	5	4211	7/7	0.98	0.25	79,79,79,79	7
92	OHX	2	2074	7/7	0.98	0.17	97,97,97,97	7
92	OHX	5	4416	7/7	0.98	0.28	56,56,56,56	7
92	OHX	6	2169	7/7	0.98	0.18	120,120,120,120	7
91	MG	1	3753	1/1	0.98	0.52	58,58,58,58	1
91	MG	1	3562	1/1	0.98	0.75	48,48,48,48	0

Continued on next page...

Continued from previous page...

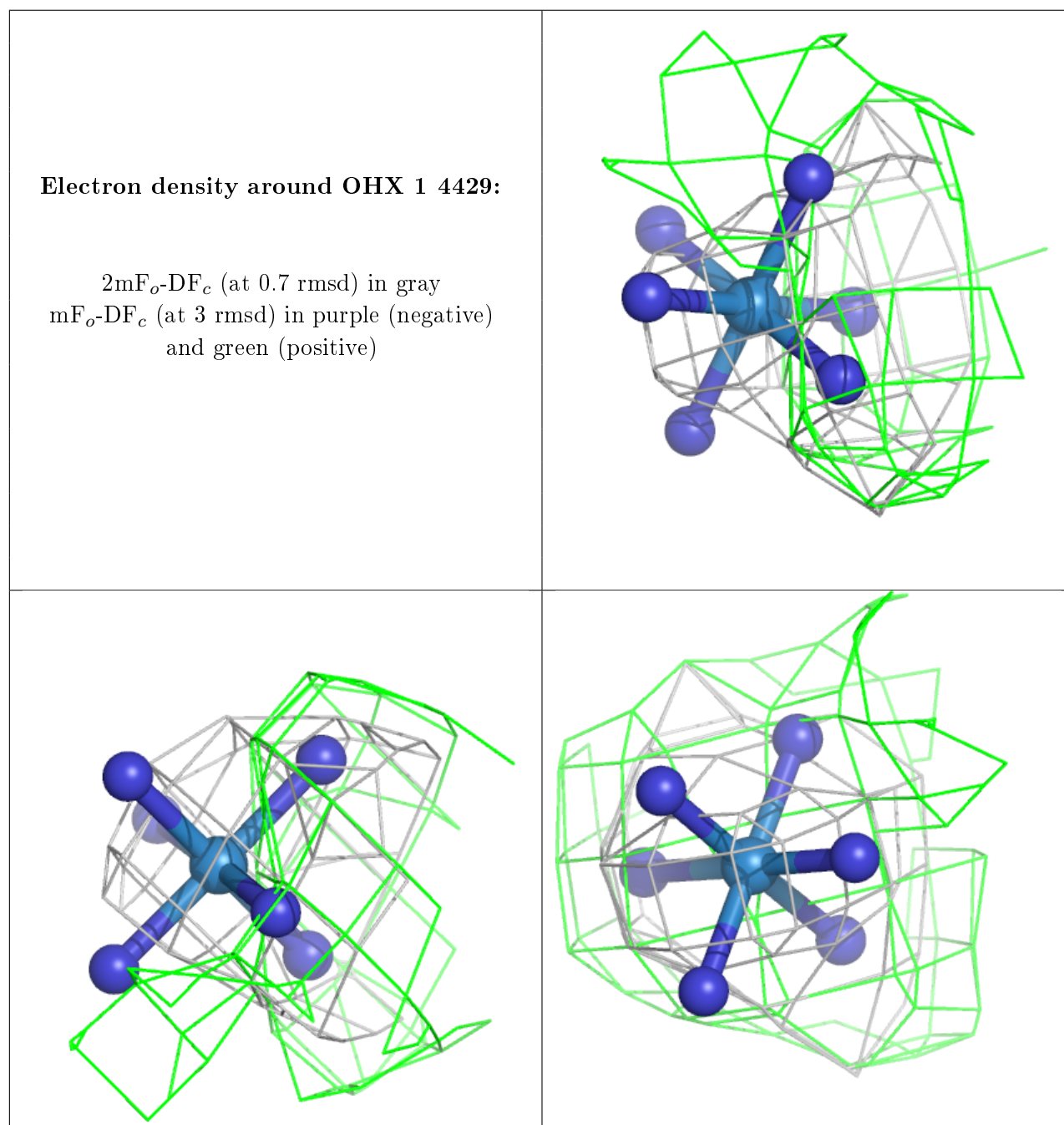
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
91	MG	1	3574	1/1	0.98	0.19	66,66,66,66	0
91	MG	1	3790	1/1	0.98	0.23	71,71,71,71	0
92	OHX	5	4224	7/7	0.98	0.18	73,73,73,73	7
92	OHX	2	2078	7/7	0.98	0.21	102,102,102,102	7
92	OHX	5	4196	7/7	0.98	0.30	88,88,88,88	7
91	MG	5	3794	1/1	0.98	0.84	52,52,52,52	1
92	OHX	6	2199	7/7	0.98	0.20	81,81,81,81	7
91	MG	6	2040	1/1	0.99	0.29	69,69,69,69	0
92	OHX	6	2141	7/7	0.99	0.23	77,77,77,77	1
92	OHX	6	2166	7/7	0.99	0.20	72,72,72,72	7
92	OHX	1	4155	7/7	0.99	0.22	87,87,87,87	7
92	OHX	5	4162	7/7	0.99	0.21	70,70,70,70	0
92	OHX	Q2	505	7/7	0.99	0.22	58,58,58,58	7
92	OHX	5	4262	7/7	0.99	0.36	60,60,60,60	7
91	MG	N1	201	1/1	0.99	0.36	56,56,56,56	1
92	OHX	5	4221	7/7	0.99	0.18	101,101,101,101	7
92	OHX	1	4137	7/7	0.99	0.26	77,77,77,77	7
91	MG	6	2084	1/1	0.99	0.29	99,99,99,99	0
92	OHX	1	4136	7/7	0.99	0.32	73,73,73,73	7
92	OHX	4	233	7/7	0.99	0.26	63,63,63,63	1
91	MG	1	3983	1/1	0.99	0.98	60,60,60,60	1
92	OHX	5	4176	7/7	0.99	0.21	76,76,76,76	7
92	OHX	6	2164	7/7	0.99	0.21	71,71,71,71	7
92	OHX	5	4195	7/7	0.99	0.14	93,93,93,93	7
92	OHX	1	4119	7/7	0.99	0.24	81,81,81,81	7
92	OHX	1	4146	7/7	0.99	0.33	76,76,76,76	7
91	MG	5	3608	1/1	0.99	0.64	38,38,38,38	0
92	OHX	1	4103	7/7	0.99	0.19	72,72,72,72	3
92	OHX	6	2152	7/7	0.99	0.22	76,76,76,76	7
92	OHX	1	4132	7/7	0.99	0.27	77,77,77,77	7
91	MG	1	3856	1/1	0.99	0.25	90,90,90,90	0
92	OHX	1	4104	7/7	0.99	0.24	64,64,64,64	2
91	MG	5	4041	1/1	0.99	0.23	76,76,76,76	0
91	MG	O9	101	1/1	0.99	0.53	63,63,63,63	0
92	OHX	1	4101	7/7	0.99	0.28	63,63,63,63	2
92	OHX	1	4269	7/7	0.99	0.24	55,55,55,55	7
91	MG	5	4089	1/1	0.99	0.67	64,64,64,64	1
92	OHX	1	4154	7/7	0.99	0.22	70,70,70,70	7
92	OHX	1	4105	7/7	0.99	0.21	74,74,74,74	7
91	MG	1	3907	1/1	0.99	0.29	70,70,70,70	0
92	OHX	5	4266	7/7	0.99	0.25	54,54,54,54	7
91	MG	5	4096	1/1	0.99	0.84	56,56,56,56	1

Continued on next page...

Continued from previous page...

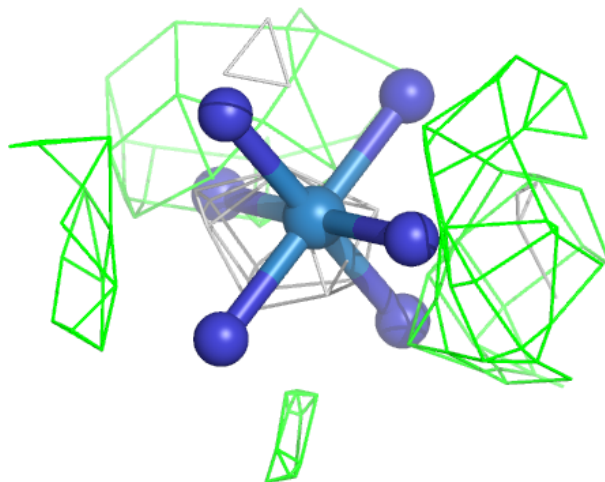
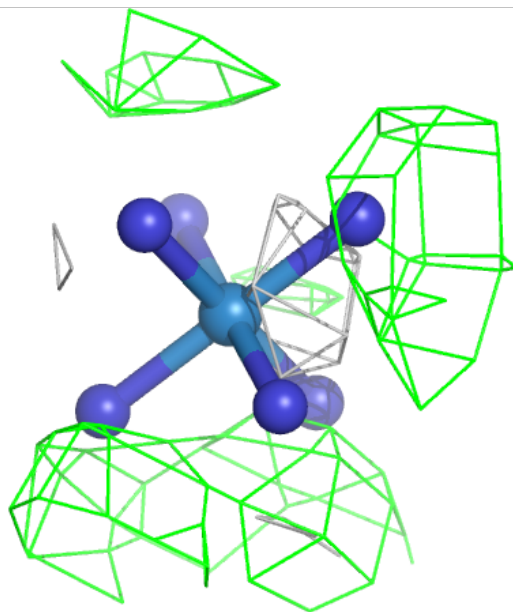
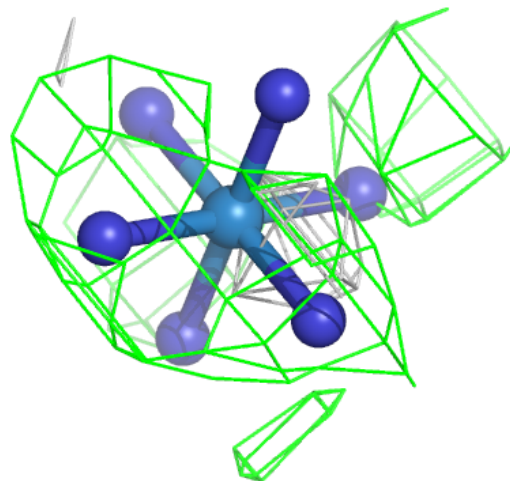
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
92	OHX	1	4108	7/7	0.99	0.18	85,85,85,85	0
92	OHX	5	4194	7/7	0.99	0.21	65,65,65,65	7
93	ZN	q0	201	1/1	1.00	0.17	52,52,52,52	0
91	MG	1	4007	1/1	1.00	0.22	67,67,67,67	0

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.



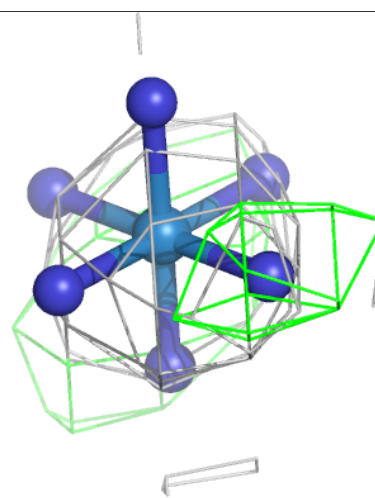
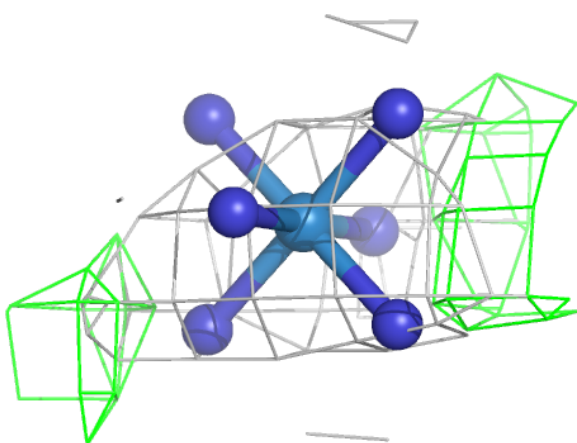
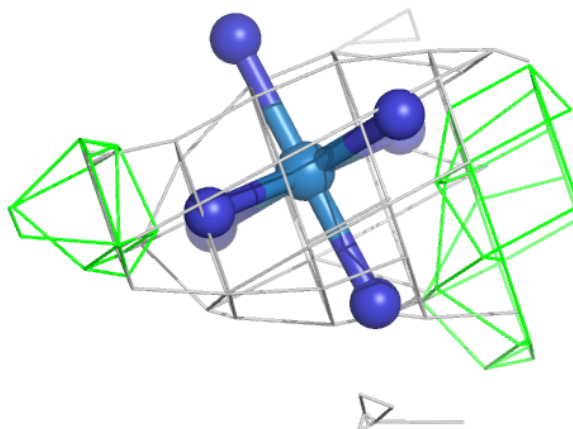
Electron density around OHX 1 4423:

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



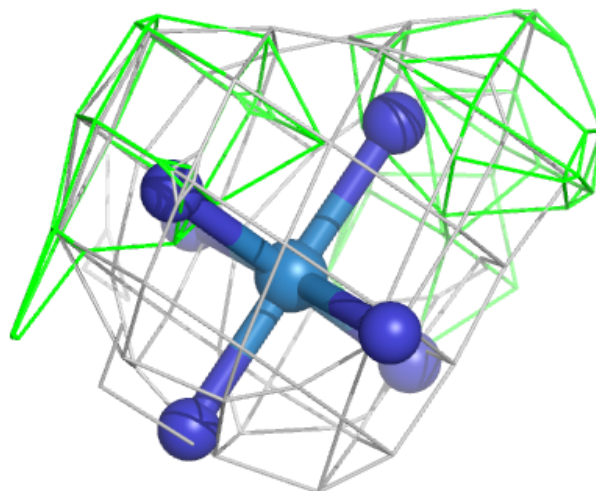
Electron density around OHX 6 2336:

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

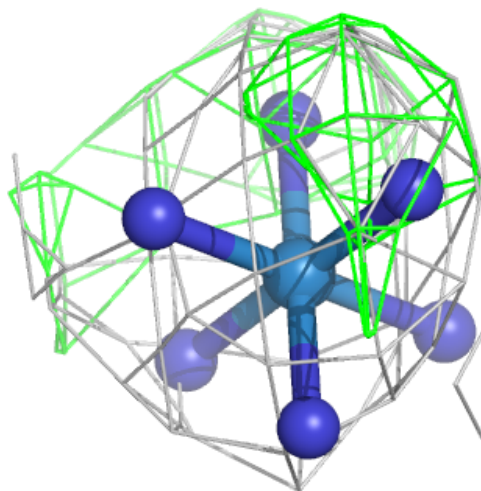
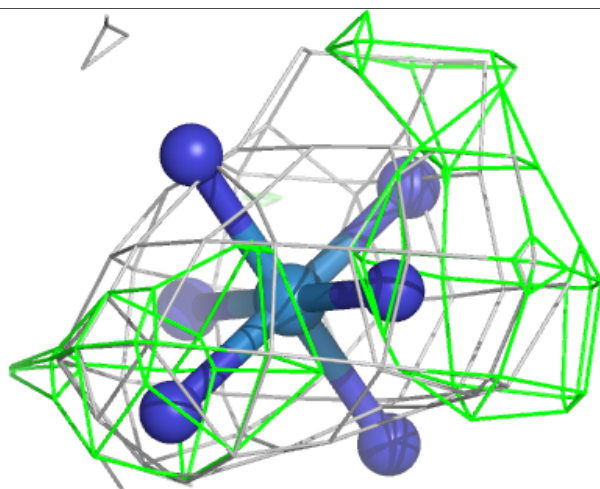


Electron density around OHX 6 2305:

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



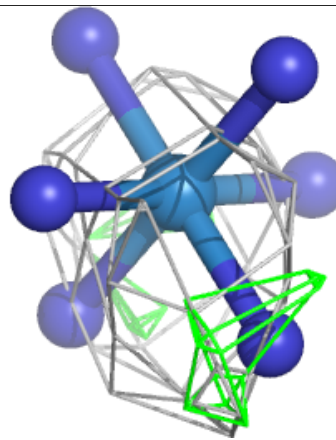
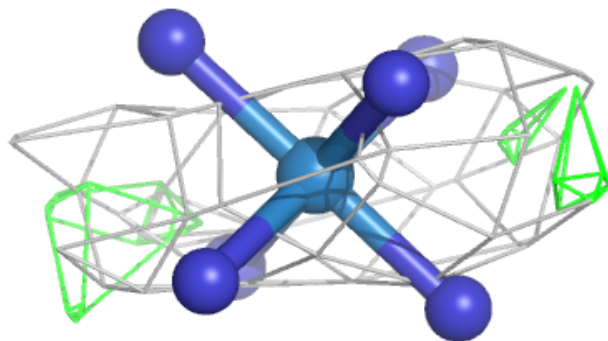
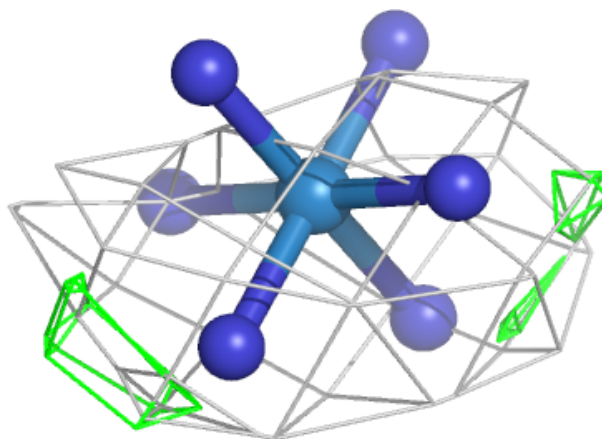
A



A

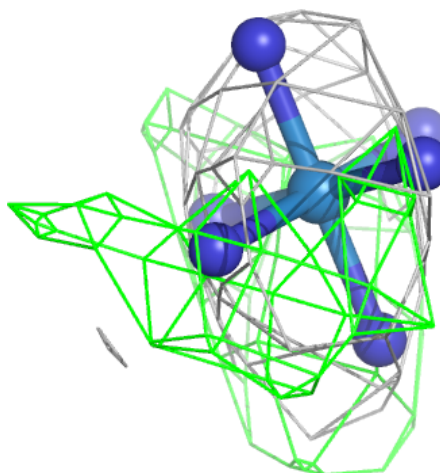
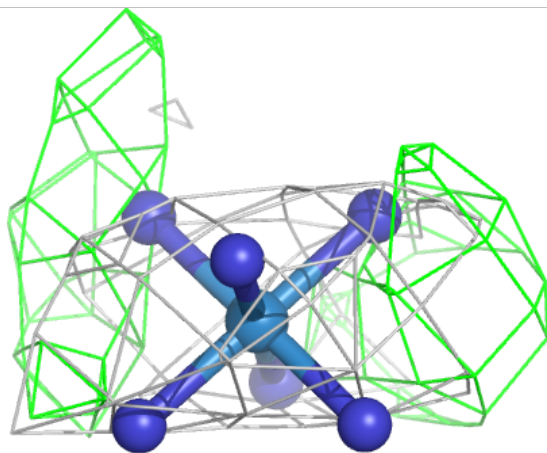
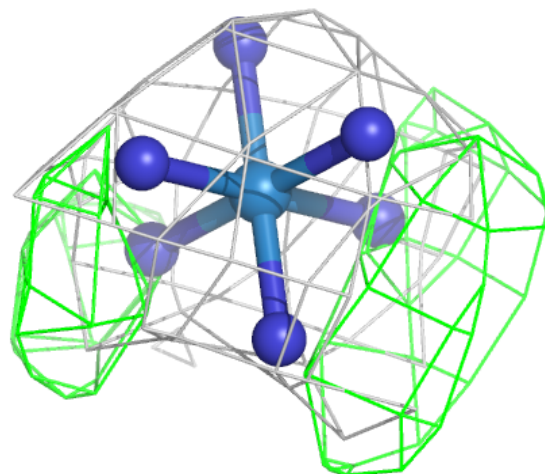
Electron density around OHX 6 2328:

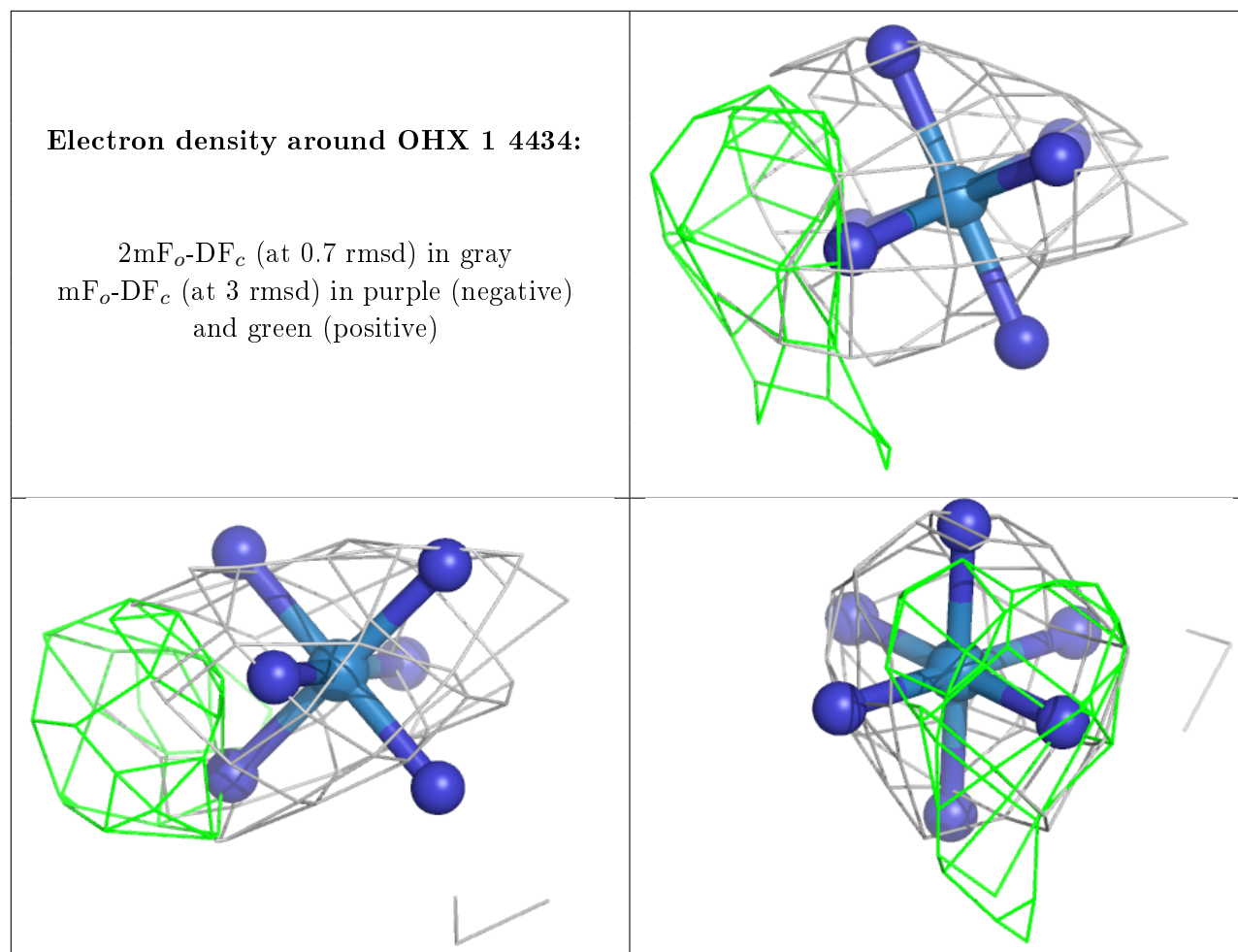
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

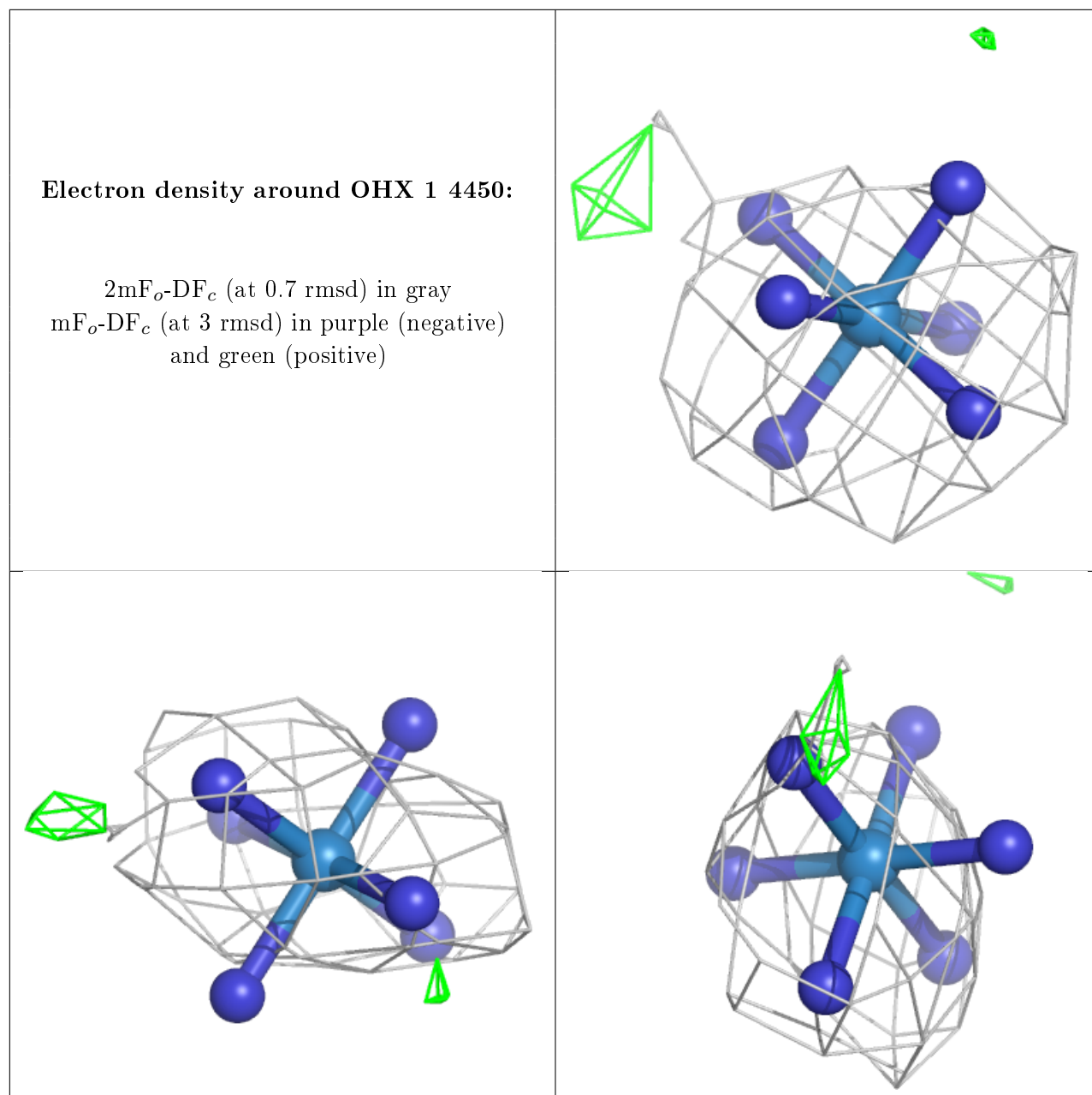


Electron density around OHX 5 4513:

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

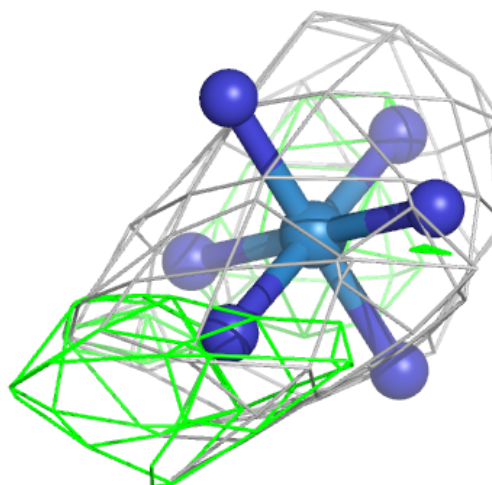
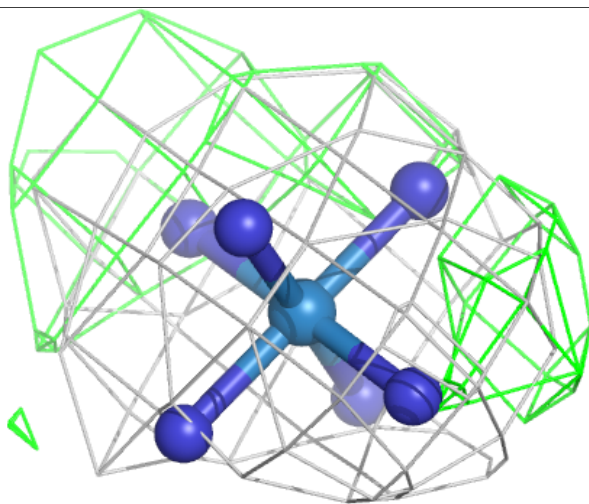
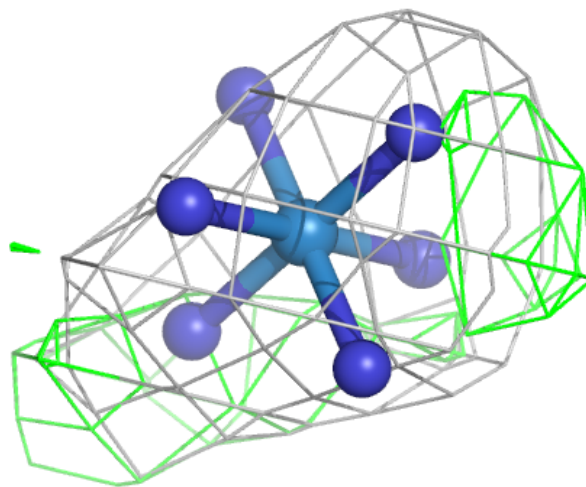






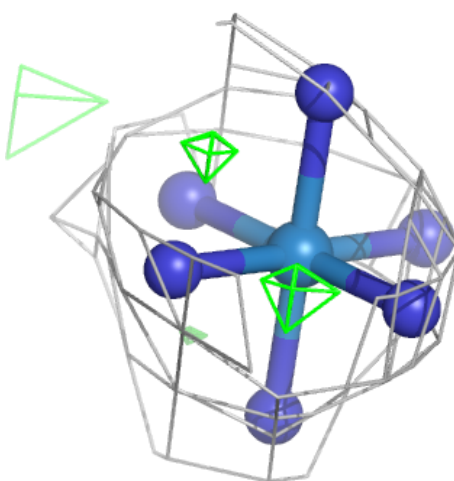
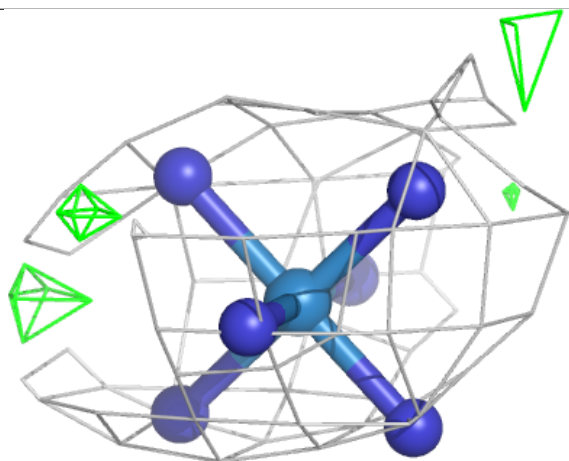
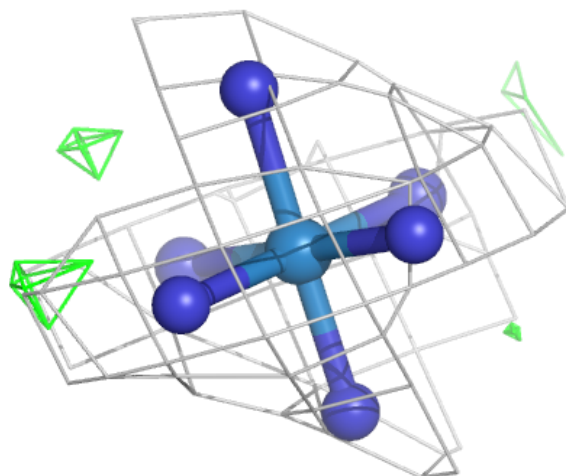
Electron density around OHX 6 2314:

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



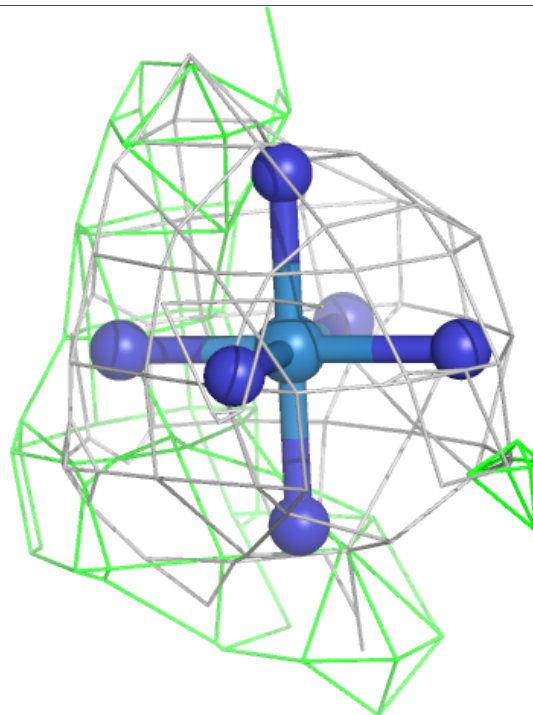
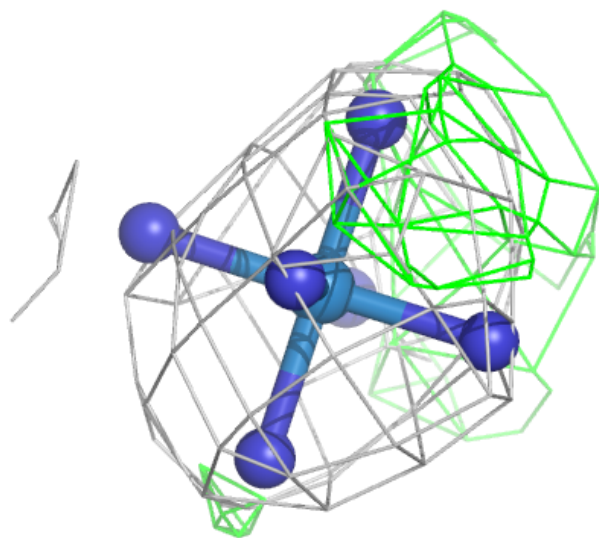
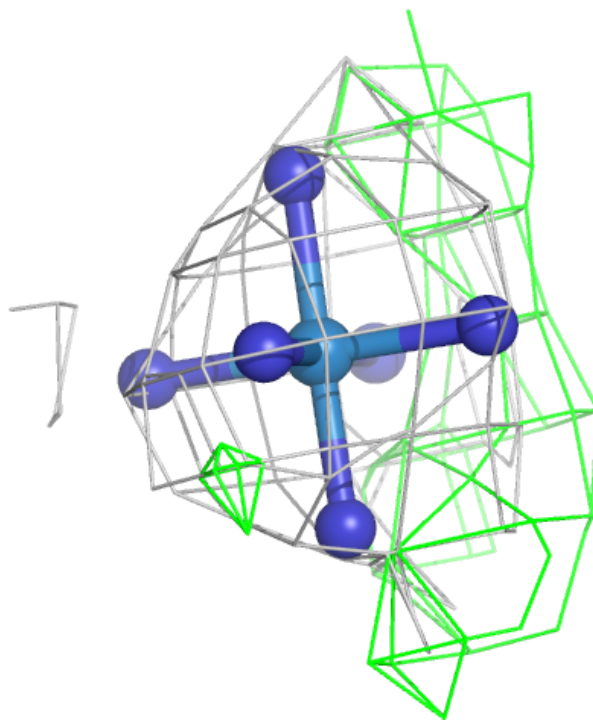
Electron density around OHX 2 2246:

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



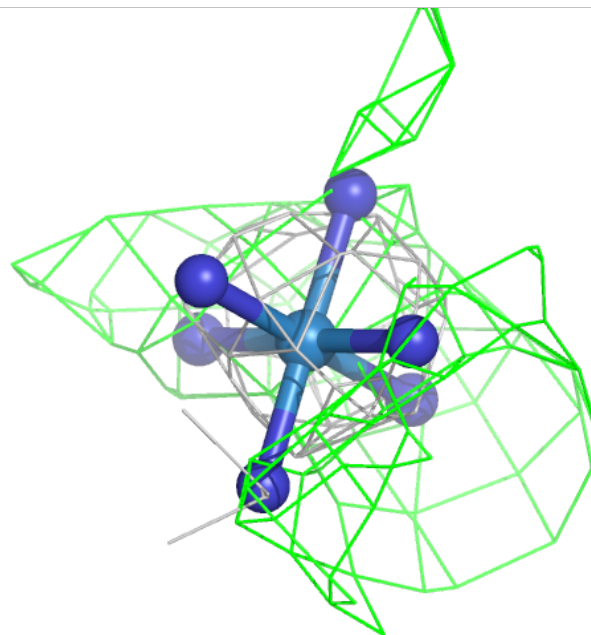
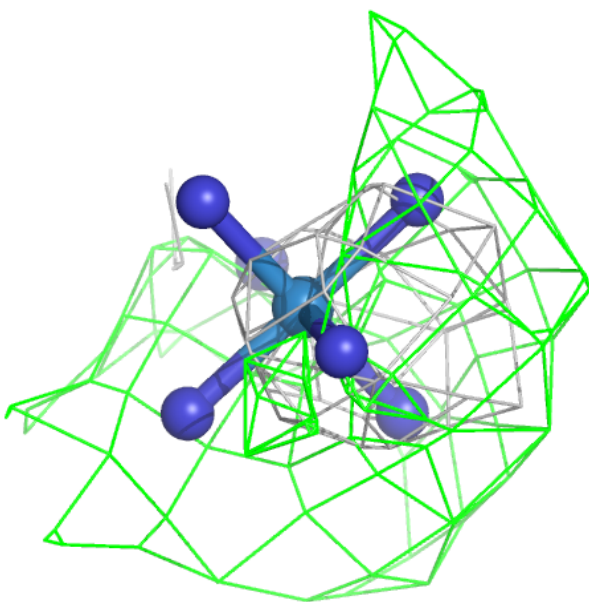
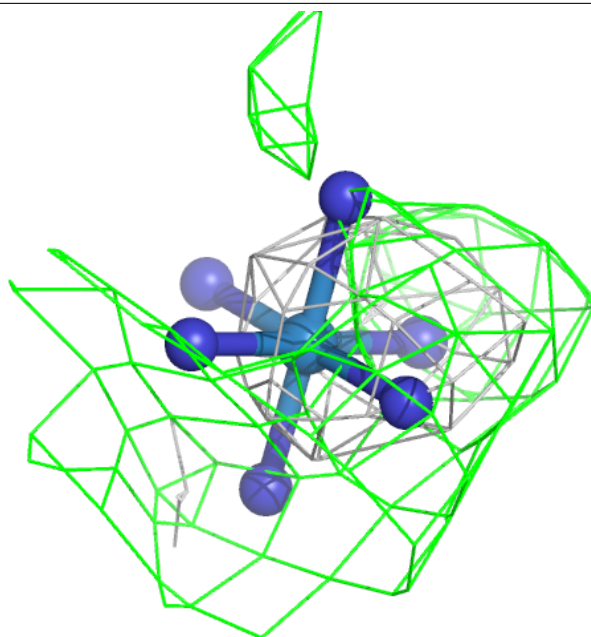
Electron density around OHX 5 4534:

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



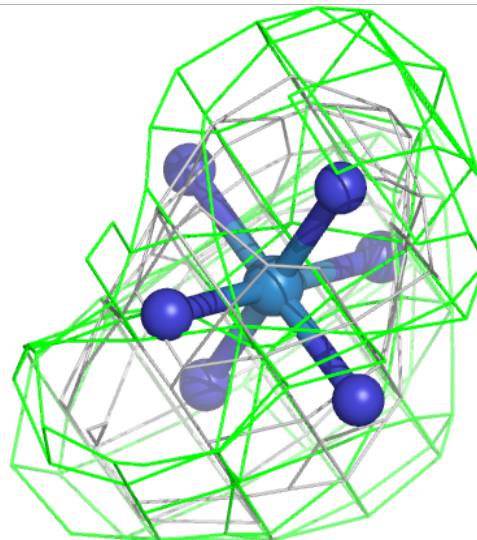
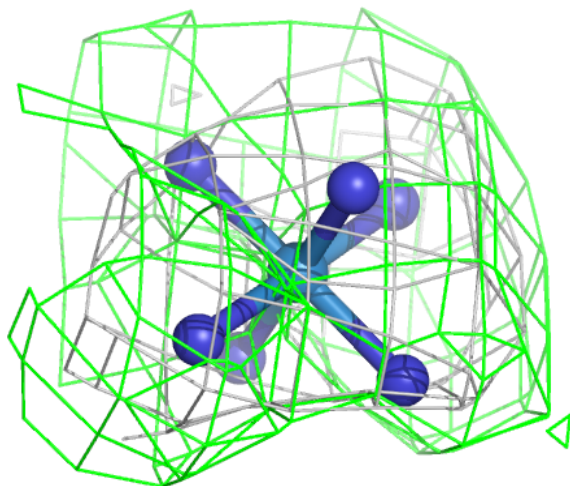
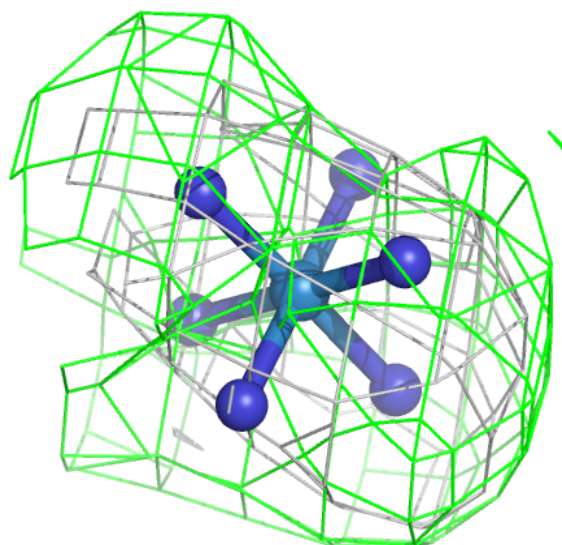
Electron density around OHX 5 4541:

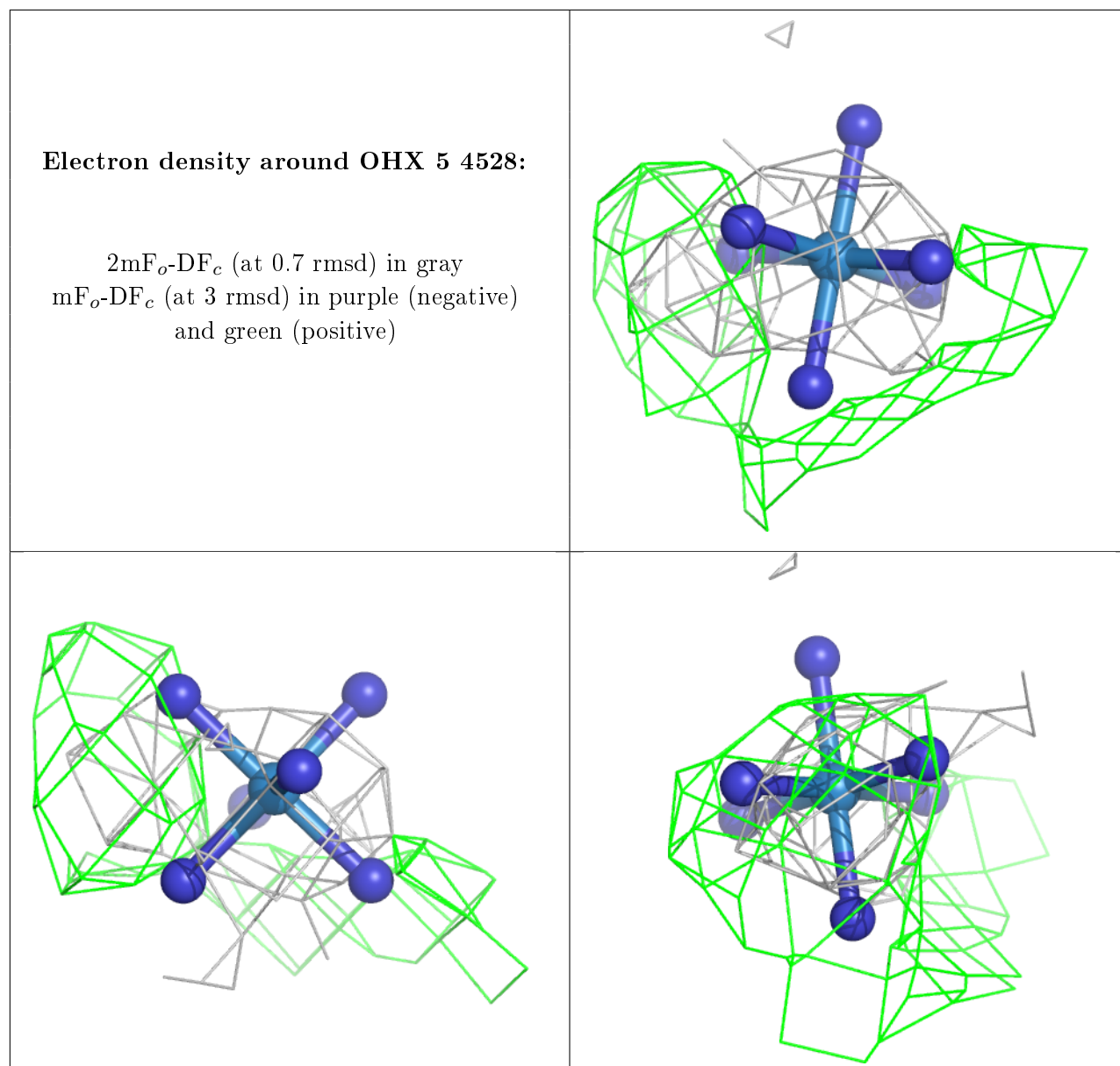
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OHX 5 4495:

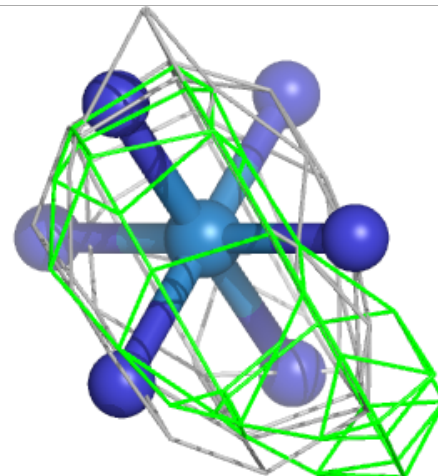
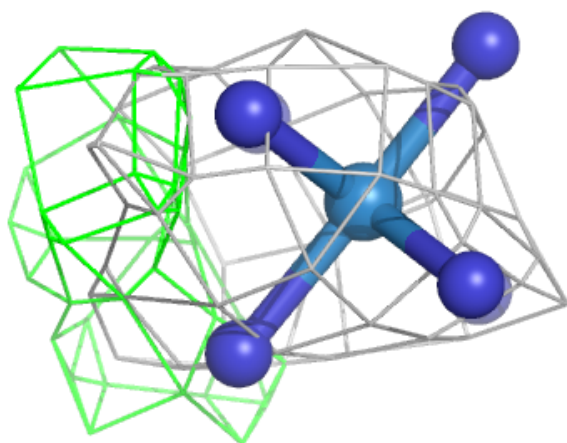
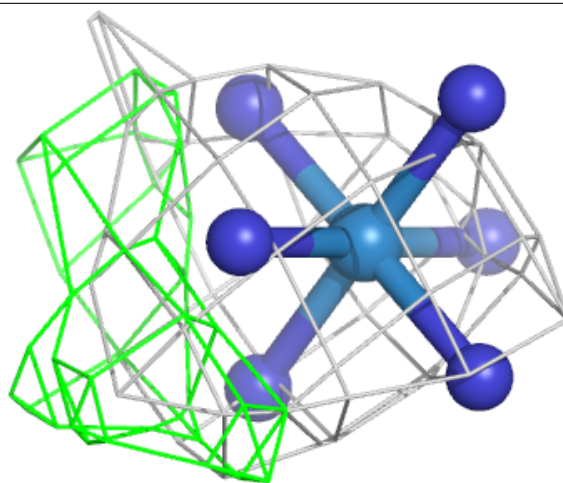
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





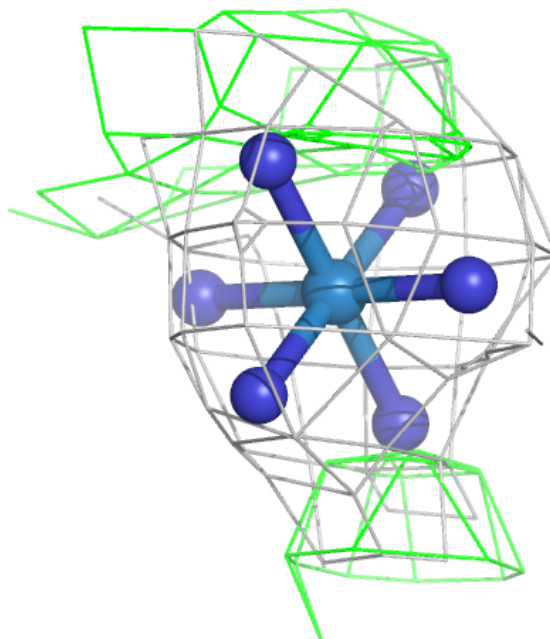
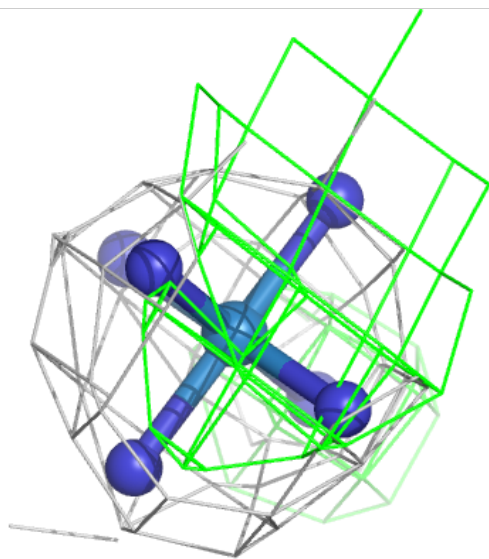
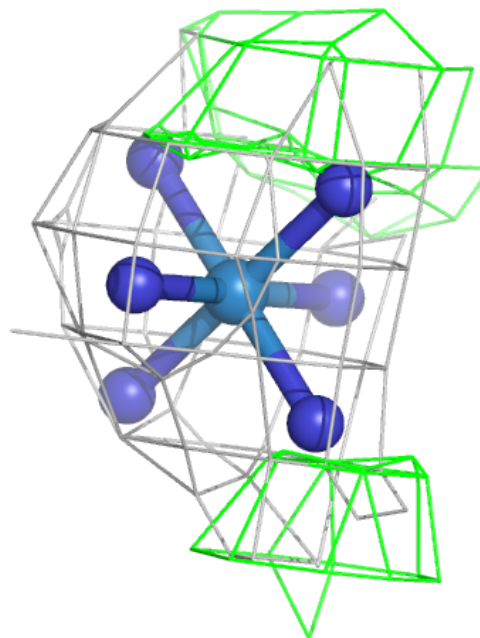
Electron density around OHX 6 2322:

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



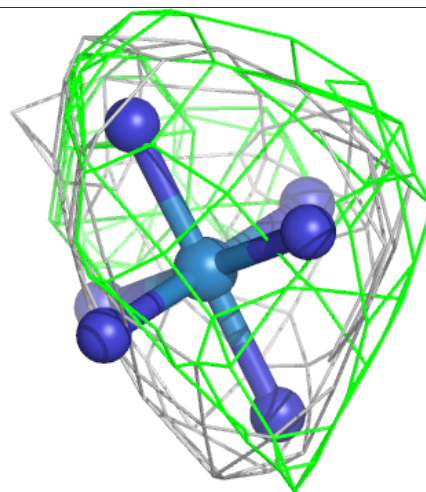
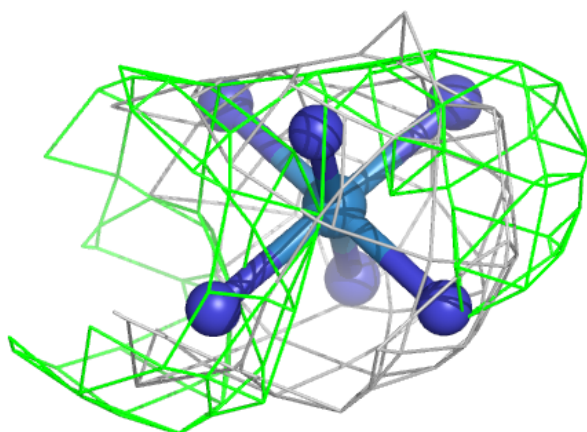
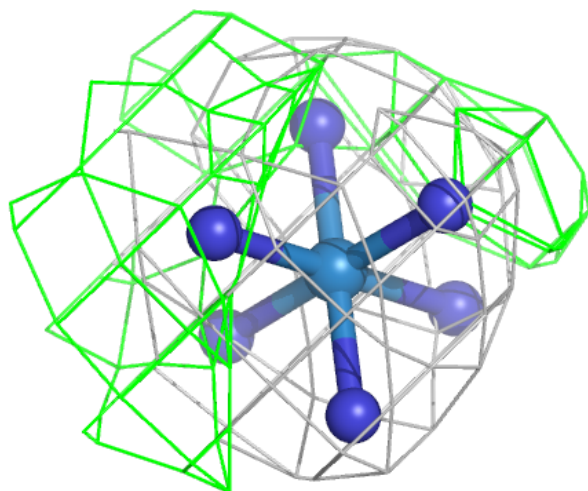
Electron density around OHX 2 2231:

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



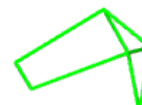
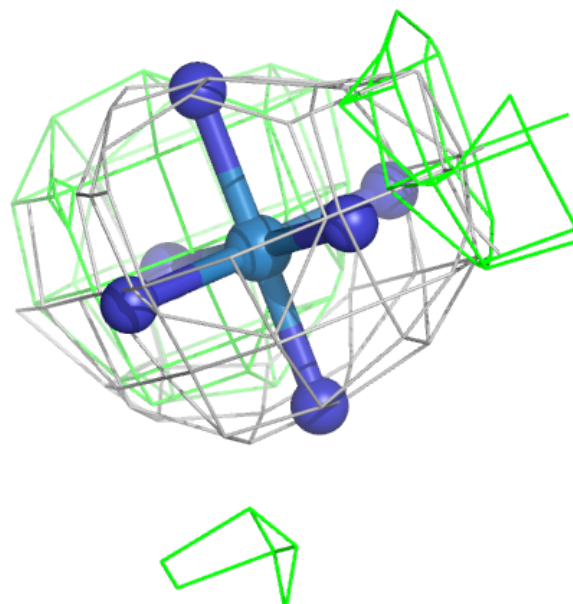
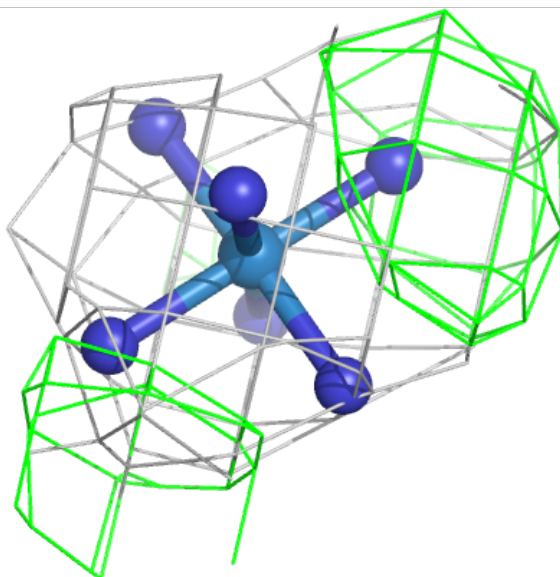
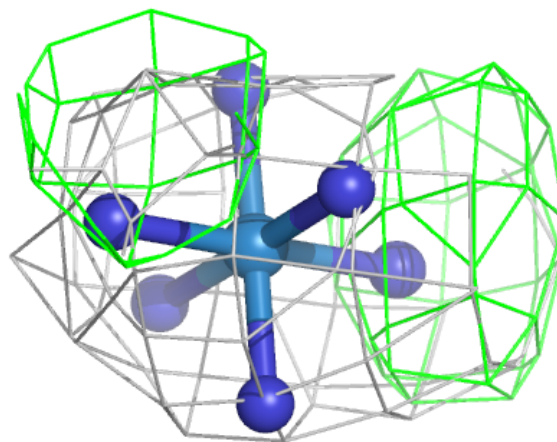
Electron density around OHX 5 4562:

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



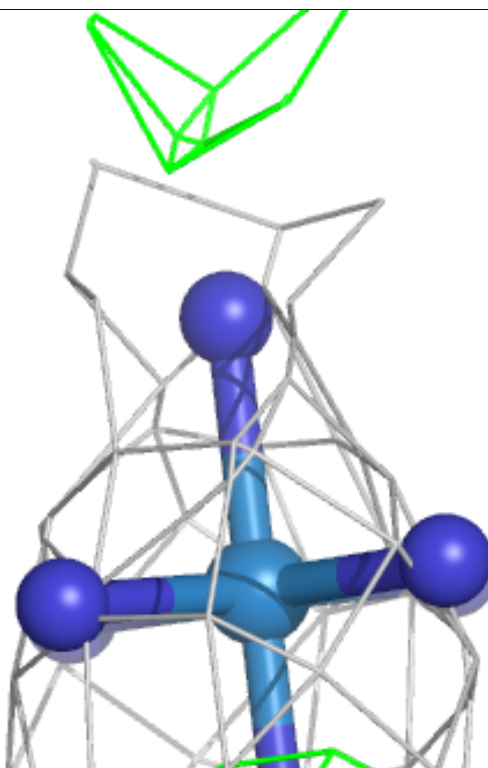
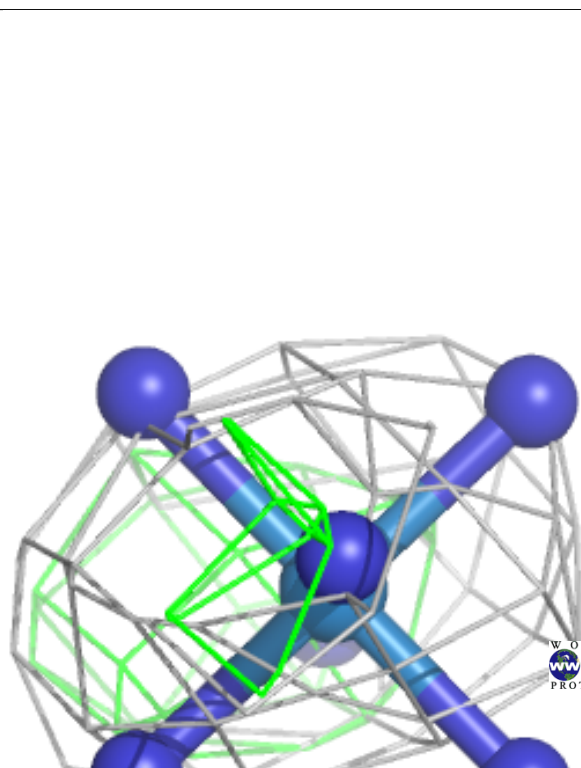
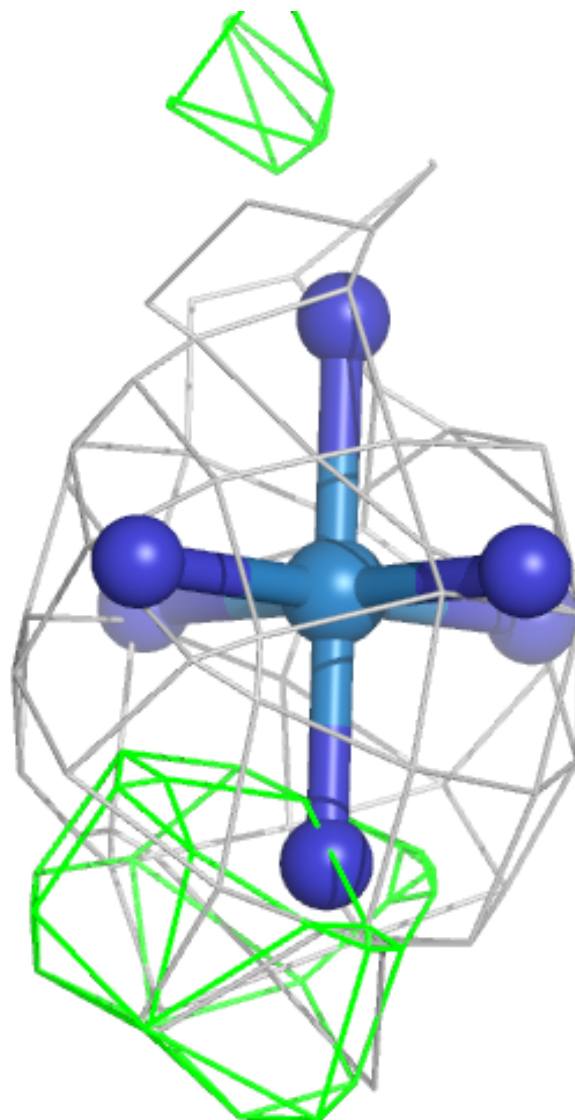
Electron density around OHX 5 4549:

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



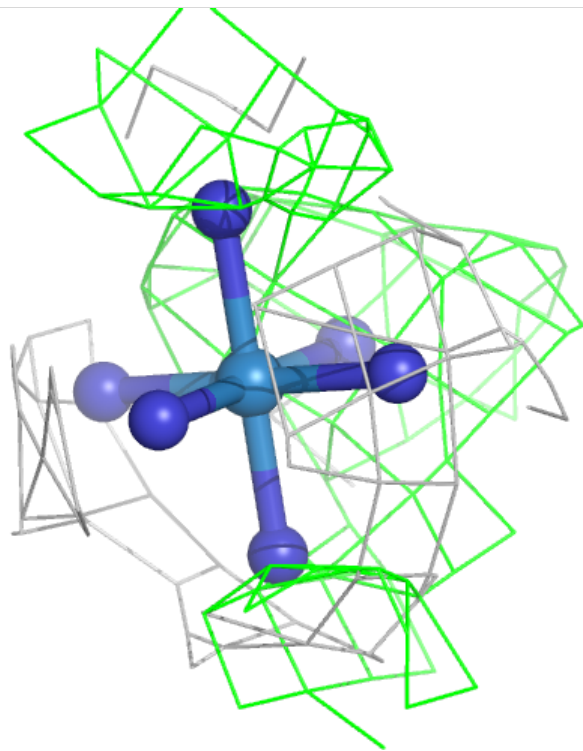
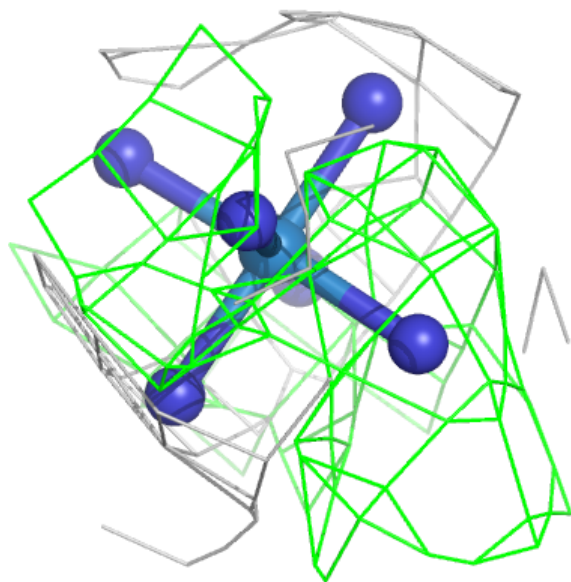
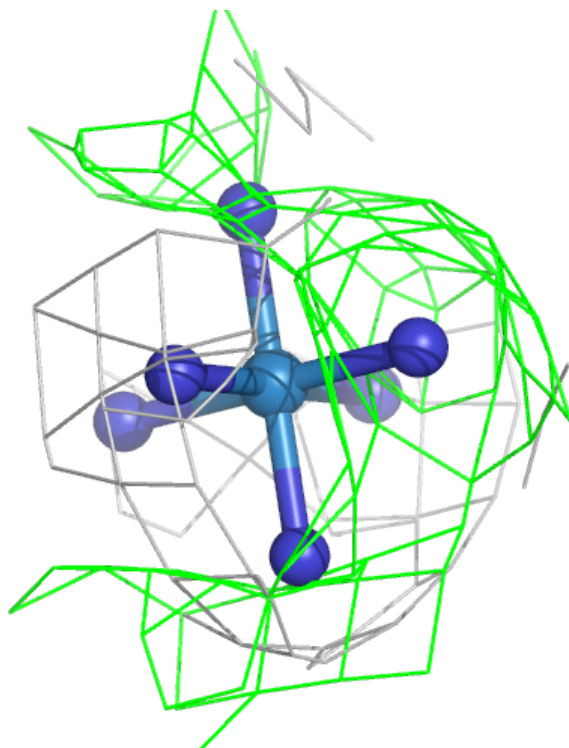
Electron density around OHX 1 4485:

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



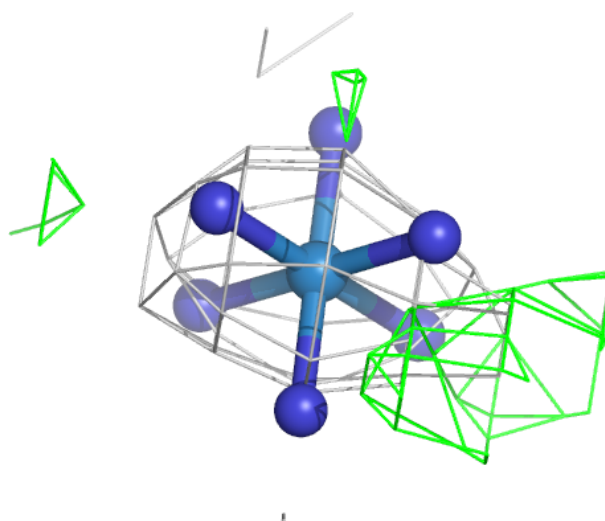
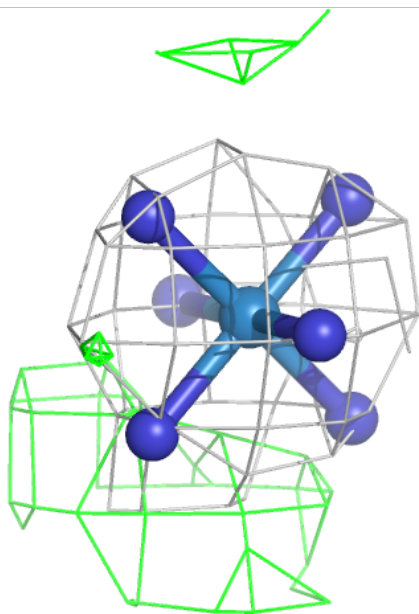
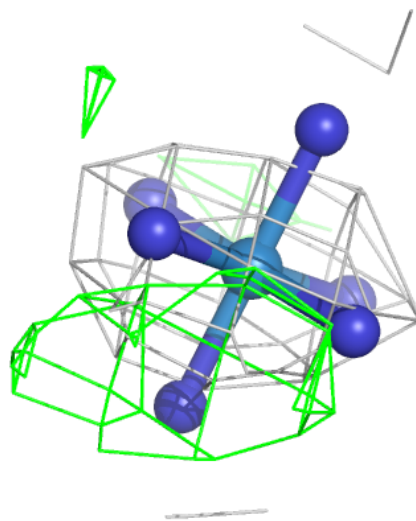
Electron density around OHX 2 2197:

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



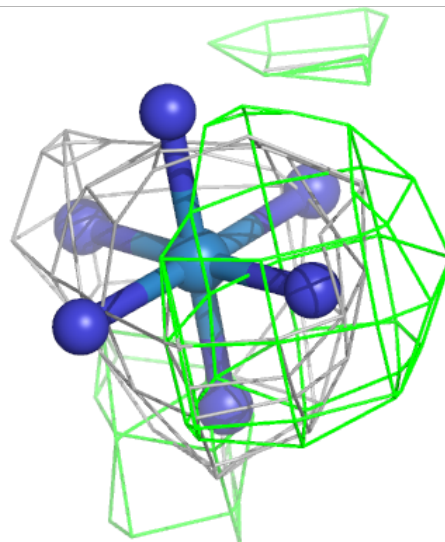
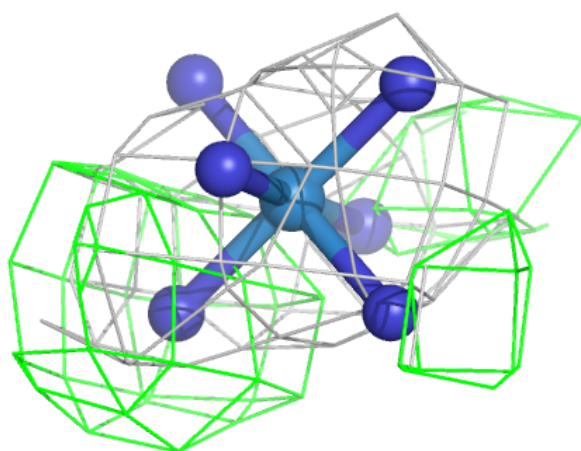
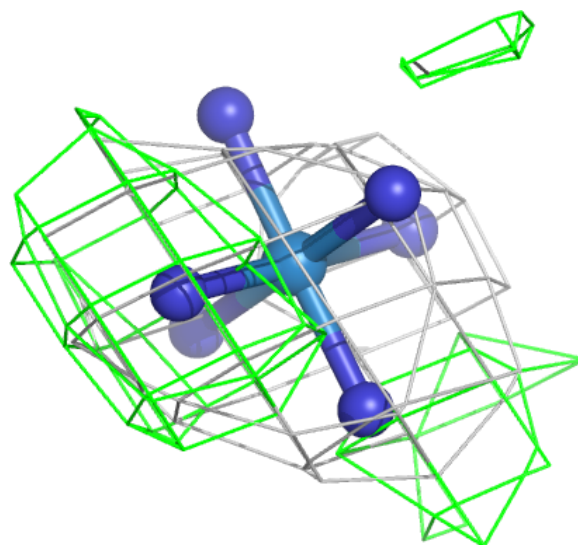
Electron density around OHX 1 4477:

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



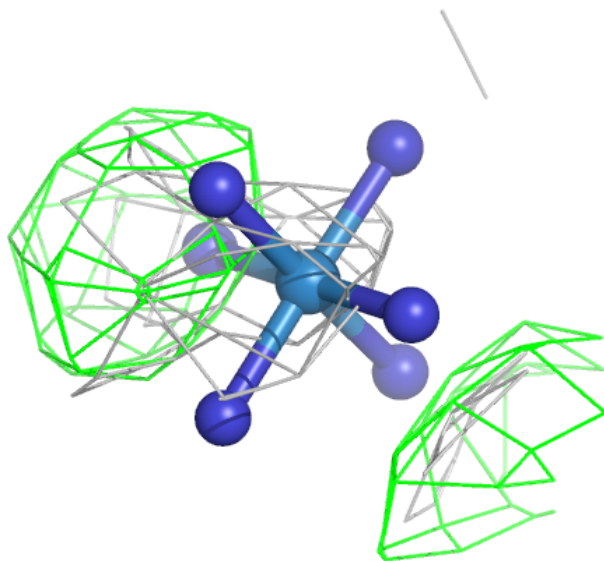
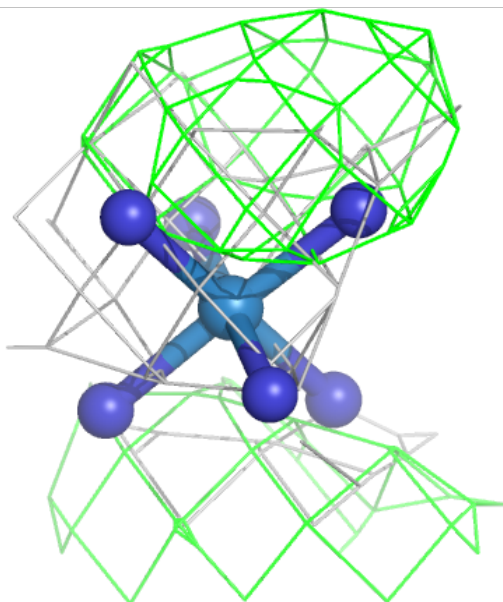
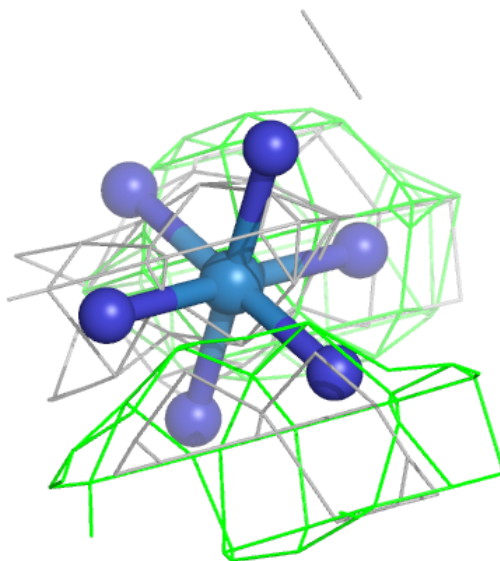
Electron density around OHX 5 4536:

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



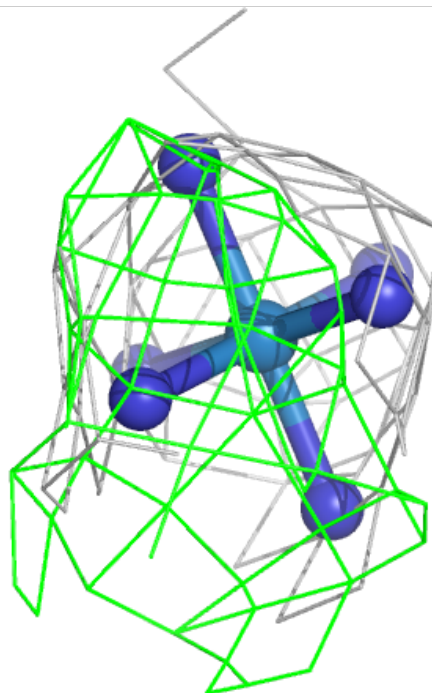
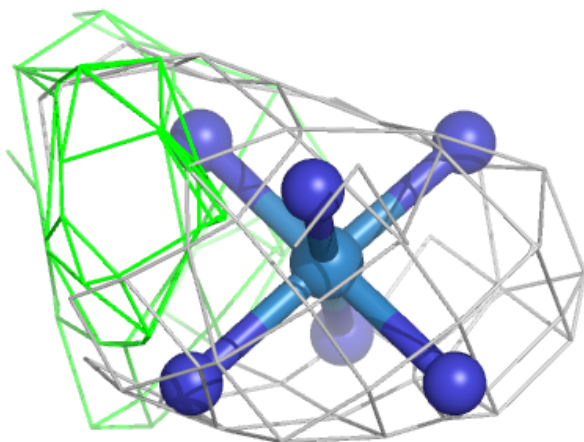
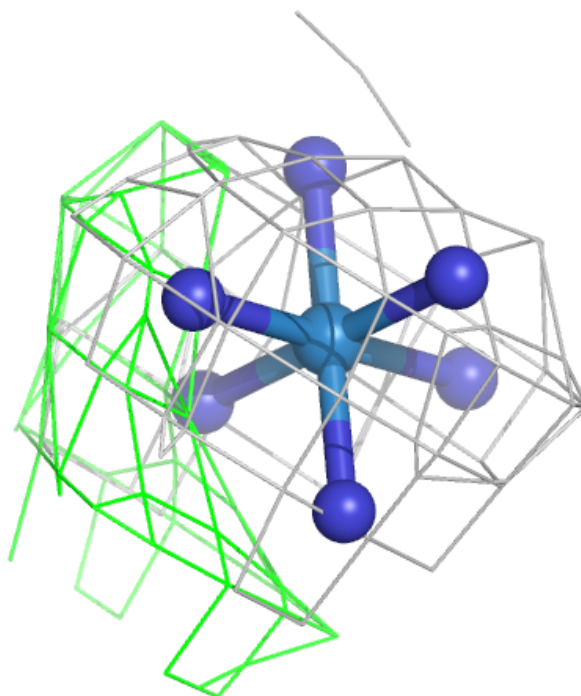
Electron density around OHX 7 239:

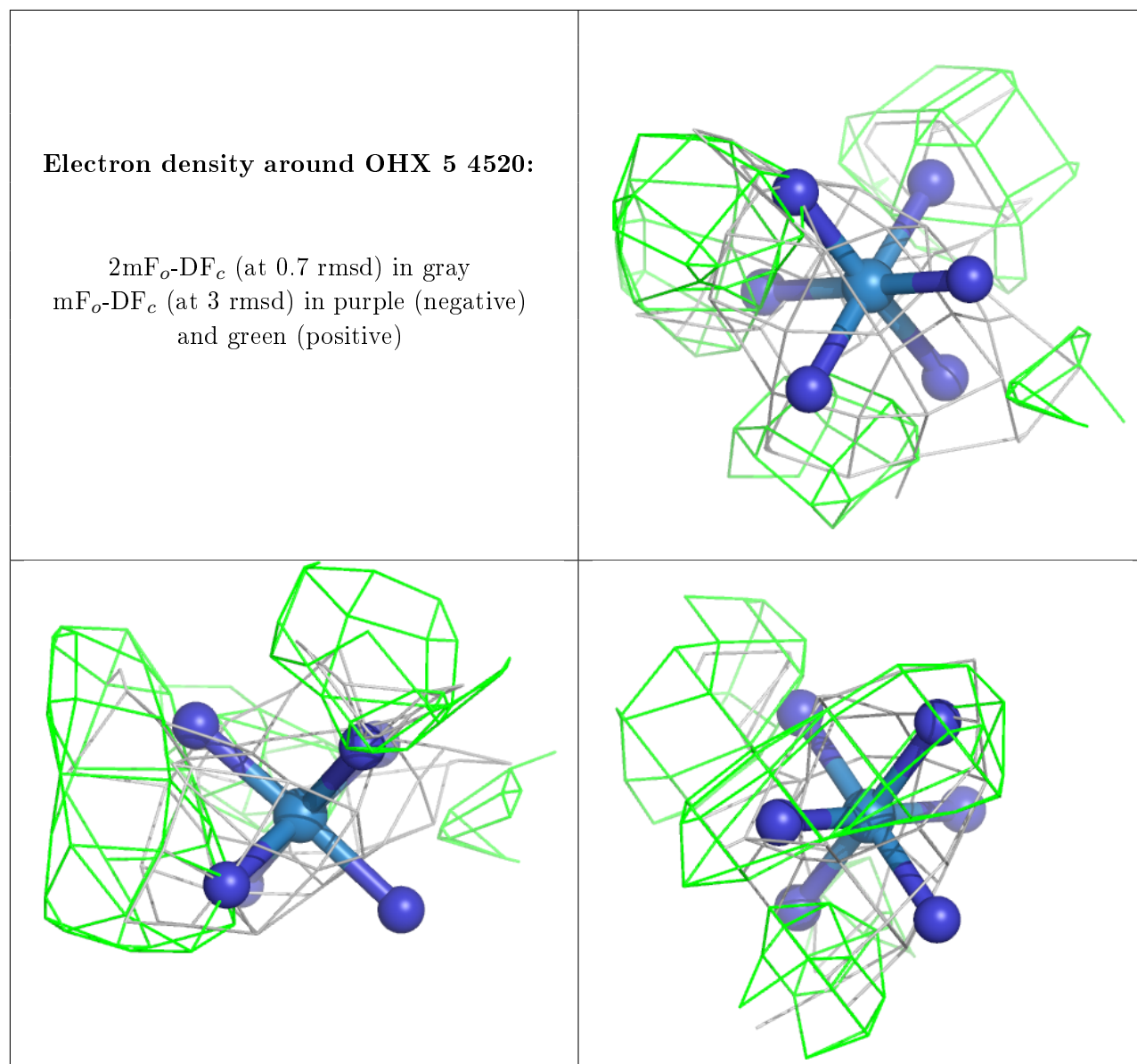
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OHX 1 4463:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.