



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2020 – 04:26 AM BST

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

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

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

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 : 2.14.2
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) : 2.14.2

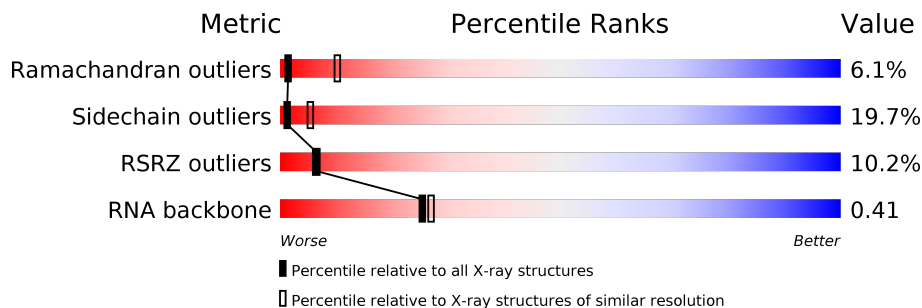
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



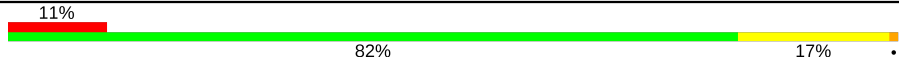



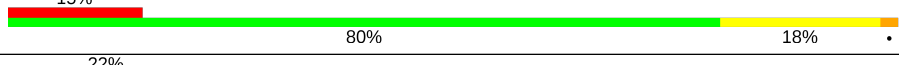
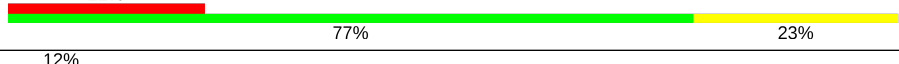
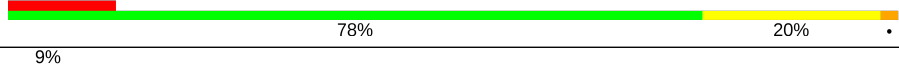

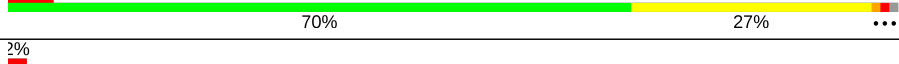


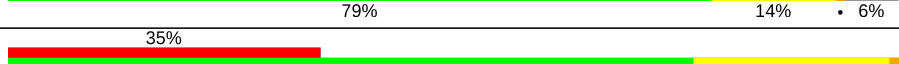

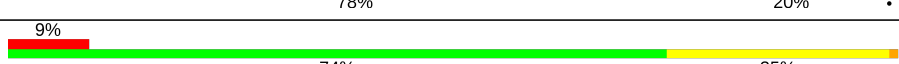

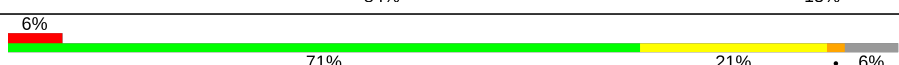
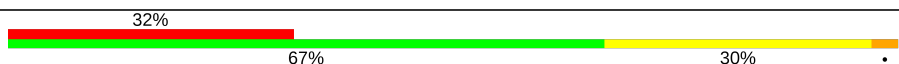

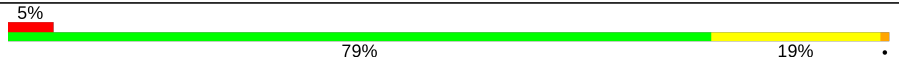


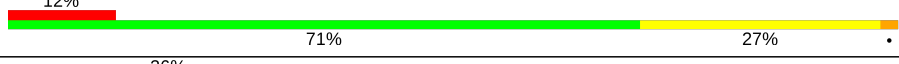
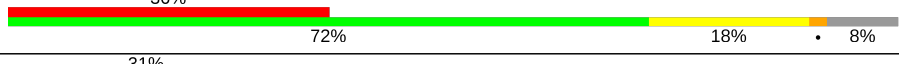


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	1829	
2	S0	206	
2	s0	206	
3	S1	216	
3	s1	216	
4	S2	217	
4	s2	217	

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Mol	Chain	Length	Quality of chain
5	S3	223	
5	s3	223	
6	S4	260	
6	s4	260	
7	S5	206	
7	s5	206	
8	S6	226	
8	s6	226	
9	S7	186	
9	s7	186	
10	S8	199	
10	s8	199	
11	S9	185	
11	s9	185	
12	C0	96	
13	C1	155	
13	c1	155	
14	C2	124	
14	c2	124	
15	C3	150	
15	c3	150	
16	C4	128	
16	c4	128	
17	C5	135	
17	c5	135	

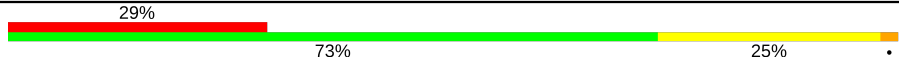
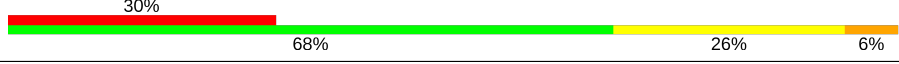
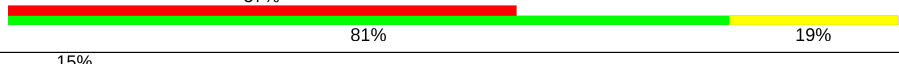



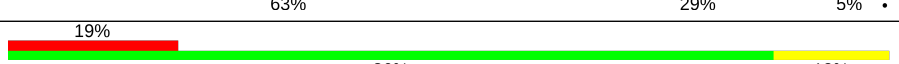
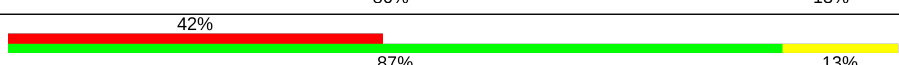
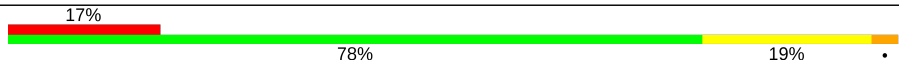

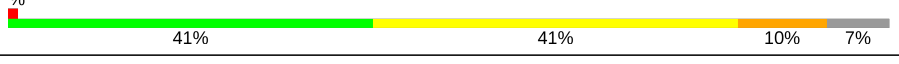
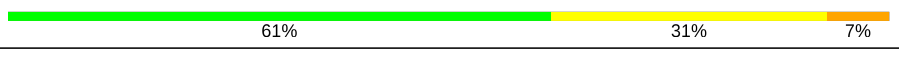


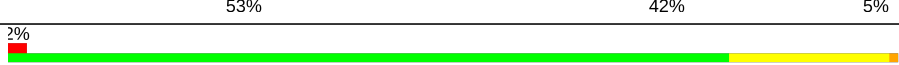










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Mol	Chain	Length	Quality of chain
18	C6	142	54% 79% 19% ..
18	c6	142	39% 77% 20% ..
19	C7	125	31% 74% 18% . .
19	c7	125	20% 70% 22% . 6%
20	C8	145	28% 75% 20% 5%
20	c8	145	27% 79% 19% .
21	C9	143	43% 78% 20% .
21	c9	143	13% 82% 15% .
22	D0	110	34% 71% 26% .
22	d0	110	39% 65% 33% .
23	D1	87	26% 78% 21% .
23	d1	87	8% 76% 22% .
24	D2	129	48% 81% 16% .
24	d2	129	5% 83% 16% .
25	D3	144	2% 79% 18% .
25	d3	144	% 85% 15%
26	D4	134	10% 80% 19% .
26	d4	134	6% 79% 16% .
27	D5	70	7% 64% 33% .
27	d5	70	14% 81% 16% ..
28	D6	97	62% 72% 20% 5% .
28	d6	97	23% 75% 22% .
29	D7	81	40% 84% 16%
29	d7	81	12% 81% 19%
30	D8	63	22% 79% 19% .






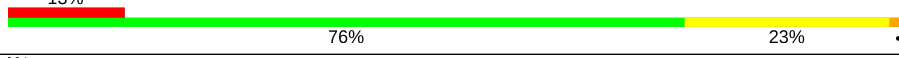

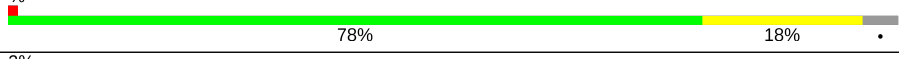



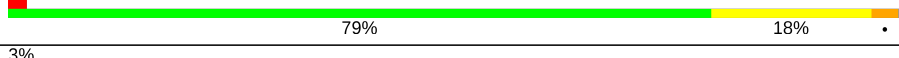








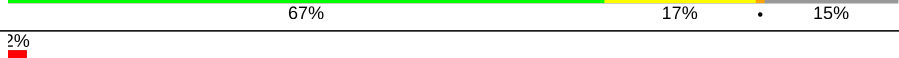
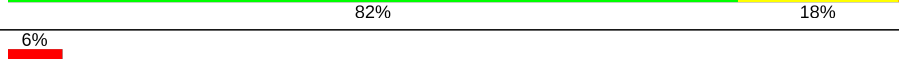

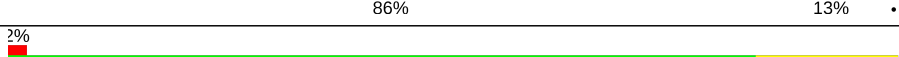

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Mol	Chain	Length	Quality of chain
30	d8	63	
31	D9	53	
31	d9	53	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	159	
36	1	3394	
36	5	3394	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	252	
39	l2	252	
40	L3	386	
40	l3	386	
41	L4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

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Mol	Chain	Length	Quality of chain
43	l6	175	 % 74% 15% 10%
44	L7	223	 83% 15%
44	l7	223	 83% 15%
45	L8	233	 11% 83% 14%
45	l8	233	 10% 78% 20%
46	L9	191	 13% 76% 23%
46	l9	191	 2% 76% 23%
47	M0	220	 % 78% 18%
47	m0	220	 3% 73% 22%
48	M1	169	 45% 75% 22%
48	m1	169	 8% 79% 18%
49	M3	194	 2% 79% 18%
49	m3	194	 3% 78% 20%
50	M4	137	 4% 79% 18%
50	m4	137	 81% 18%
51	M5	203	 14% 80% 19%
51	m5	203	 16% 81% 18%
52	M6	197	 % 86% 13%
52	m6	197	 84% 15%
53	M7	183	 5% 77% 21%
53	m7	183	 % 67% 17% 15%
54	M8	185	 2% 82% 18%
54	m8	185	 6% 75% 24%
55	M9	188	 7% 86% 13%
55	m9	188	 2% 84% 16%


























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Mol	Chain	Length	Quality of chain
56	N0	172	21% 80% 18% •
56	n0	172	% 81% 19%
57	N1	159	12% 78% 19% •
57	n1	159	4% 81% 18% •
58	N2	100	10% 79% 20% •
58	n2	100	21% 78% 20% •
59	N3	136	88% 13%
59	n3	136	% 82% 16% •
60	N4	135	23% 63% 10% 27%
60	n4	135	20% 81% 18% •
61	N5	121	18% 75% 24% •
61	n5	121	7% 77% 21% ••
62	N6	126	4% 75% 23% •
62	n6	126	13% 75% 22% ••
63	N7	135	33% 79% 21% •
63	n7	135	36% 77% 21% •
64	N8	148	% 76% 22% •
64	n8	148	5% 76% 22% •
65	N9	58	9% 81% 17% •
65	n9	58	3% 67% 26% 7%
66	O0	100	9% 82% 15% •
66	o0	100	7% 84% 16%
67	O1	109	4% 76% 21% ••
67	o1	109	11% 74% 26%
68	O2	127	2% 77% 23%

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Mol	Chain	Length	Quality of chain
68	o2	127	 80% 19%
69	O3	106	 83% 16%
69	o3	106	 85% 13%
70	O4	112	 21% 81% 19%
70	o4	112	 9% 86% 13%
71	O5	119	 8% 74% 24%
71	o5	119	 2% 82% 14%
72	O6	99	 8% 70% 28%
72	o6	99	 10% 71% 28%
73	O7	87	 79% 21%
73	o7	87	 5% 78% 21%
74	O8	77	 16% 75% 25%
74	o8	77	 34% 71% 27%
75	O9	50	 82% 14%
75	o9	50	 4% 88% 12%
76	Q0	52	 8% 77% 19%
76	q0	52	 2% 71% 25%
77	Q1	25	 72% 28%
77	q1	25	 64% 36%
78	Q2	105	 8% 73% 23%
78	q2	105	 4% 74% 22%
79	Q3	91	 2% 85% 14%
79	q3	91	 2% 76% 24%
80	6	1800	 3% 54% 37% 9%
81	c0	96	 34% 78% 21%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	2	2030	-	-	-	X
86	OHX	2	2060	-	-	-	X
86	OHX	5	3720	-	-	-	X
86	OHX	5	3739	-	-	-	X
86	OHX	5	3755	-	-	-	X
86	OHX	5	3762	-	-	-	X
86	OHX	5	3768	-	-	-	X
86	OHX	5	3783	-	-	-	X
86	OHX	5	3806	-	-	-	X
86	OHX	6	2052	-	-	-	X
86	OHX	6	2064	-	-	-	X
86	OHX	6	2081	-	-	-	X
86	OHX	6	2087	-	-	-	X
86	OHX	8	218	-	-	-	X
87	MG	1	3834	-	-	-	X
87	MG	1	3848	-	-	-	X
87	MG	1	3853	-	-	-	X
87	MG	1	3856	-	-	-	X
87	MG	1	3879	-	-	-	X
87	MG	1	3884	-	-	-	X
87	MG	1	3964	-	-	-	X
87	MG	1	4014	-	-	-	X
87	MG	1	4067	-	-	-	X
87	MG	1	4084	-	-	-	X
87	MG	1	4087	-	-	-	X
87	MG	1	4095	-	-	-	X
87	MG	1	4112	-	-	-	X
87	MG	1	4126	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	4134	-	-	-	X
87	MG	1	4153	-	-	-	X
87	MG	1	4169	-	-	-	X
87	MG	1	4179	-	-	-	X
87	MG	1	4193	-	-	-	X
87	MG	1	4197	-	-	-	X
87	MG	1	4211	-	-	-	X
87	MG	1	4214	-	-	-	X
87	MG	1	4217	-	-	-	X
87	MG	1	4227	-	-	-	X
87	MG	1	4246	-	-	-	X
87	MG	1	4278	-	-	-	X
87	MG	1	4282	-	-	-	X
87	MG	1	4295	-	-	-	X
87	MG	1	4330	-	-	-	X
87	MG	1	4339	-	-	-	X
87	MG	1	4343	-	-	-	X
87	MG	1	4346	-	-	-	X
87	MG	1	4347	-	-	-	X
87	MG	1	4350	-	-	-	X
87	MG	1	4355	-	-	-	X
87	MG	1	4359	-	-	-	X
87	MG	1	4360	-	-	-	X
87	MG	1	4365	-	-	-	X
87	MG	1	4367	-	-	-	X
87	MG	1	4370	-	-	-	X
87	MG	1	4372	-	-	-	X
87	MG	1	4374	-	-	-	X
87	MG	1	4401	-	-	-	X
87	MG	1	4406	-	-	-	X
87	MG	1	4408	-	-	-	X
87	MG	1	4424	-	-	-	X
87	MG	1	4426	-	-	-	X
87	MG	1	4432	-	-	-	X
87	MG	1	4434	-	-	-	X
87	MG	1	4443	-	-	-	X
87	MG	1	4444	-	-	-	X
87	MG	1	4465	-	-	-	X
87	MG	1	4477	-	-	-	X
87	MG	1	4484	-	-	-	X
87	MG	1	4487	-	-	-	X
87	MG	1	4495	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	2	2093	-	-	-	X
87	MG	2	2113	-	-	-	X
87	MG	2	2139	-	-	-	X
87	MG	2	2150	-	-	-	X
87	MG	2	2154	-	-	-	X
87	MG	2	2156	-	-	-	X
87	MG	2	2162	-	-	-	X
87	MG	2	2173	-	-	-	X
87	MG	2	2180	-	-	-	X
87	MG	2	2185	-	-	-	X
87	MG	2	2194	-	-	-	X
87	MG	2	2196	-	-	-	X
87	MG	2	2198	-	-	-	X
87	MG	2	2201	-	-	-	X
87	MG	2	2205	-	-	-	X
87	MG	2	2208	-	-	-	X
87	MG	2	2214	-	-	-	X
87	MG	2	2217	-	-	-	X
87	MG	2	2224	-	-	-	X
87	MG	2	2225	-	-	-	X
87	MG	2	2239	-	-	-	X
87	MG	2	2245	-	-	-	X
87	MG	2	2249	-	-	-	X
87	MG	2	2257	-	-	-	X
87	MG	2	2259	-	-	-	X
87	MG	3	229	-	-	-	X
87	MG	4	237	-	-	-	X
87	MG	4	241	-	-	-	X
87	MG	4	243	-	-	-	X
87	MG	4	244	-	-	-	X
87	MG	5	3828	-	-	-	X
87	MG	5	3854	-	-	-	X
87	MG	5	3905	-	-	-	X
87	MG	5	3911	-	-	-	X
87	MG	5	3921	-	-	-	X
87	MG	5	3925	-	-	-	X
87	MG	5	4050	-	-	-	X
87	MG	5	4067	-	-	-	X
87	MG	5	4087	-	-	-	X
87	MG	5	4104	-	-	-	X
87	MG	5	4110	-	-	-	X
87	MG	5	4124	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	4129	-	-	-	X
87	MG	5	4131	-	-	-	X
87	MG	5	4135	-	-	-	X
87	MG	5	4137	-	-	-	X
87	MG	5	4141	-	-	-	X
87	MG	5	4156	-	-	-	X
87	MG	5	4172	-	-	-	X
87	MG	5	4178	-	-	-	X
87	MG	5	4186	-	-	-	X
87	MG	5	4203	-	-	-	X
87	MG	5	4222	-	-	-	X
87	MG	5	4252	-	-	-	X
87	MG	5	4262	-	-	-	X
87	MG	5	4265	-	-	-	X
87	MG	5	4281	-	-	-	X
87	MG	5	4322	-	-	-	X
87	MG	5	4324	-	-	-	X
87	MG	5	4327	-	-	-	X
87	MG	5	4336	-	-	-	X
87	MG	5	4338	-	-	-	X
87	MG	5	4347	-	-	-	X
87	MG	5	4349	-	-	-	X
87	MG	5	4354	-	-	-	X
87	MG	5	4355	-	-	-	X
87	MG	5	4360	-	-	-	X
87	MG	5	4397	-	-	-	X
87	MG	5	4408	-	-	-	X
87	MG	5	4423	-	-	-	X
87	MG	5	4426	-	-	-	X
87	MG	5	4448	-	-	-	X
87	MG	5	4455	-	-	-	X
87	MG	5	4457	-	-	-	X
87	MG	5	4479	-	-	-	X
87	MG	5	4492	-	-	-	X
87	MG	5	4516	-	-	-	X
87	MG	5	4529	-	-	-	X
87	MG	5	4543	-	-	-	X
87	MG	5	4553	-	-	-	X
87	MG	5	4556	-	-	-	X
87	MG	5	4563	-	-	-	X
87	MG	6	2124	-	-	-	X
87	MG	6	2162	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	6	2183	-	-	-	X
87	MG	6	2191	-	-	-	X
87	MG	6	2199	-	-	-	X
87	MG	6	2202	-	-	-	X
87	MG	6	2207	-	-	-	X
87	MG	6	2223	-	-	-	X
87	MG	6	2232	-	-	-	X
87	MG	6	2257	-	-	-	X
87	MG	6	2274	-	-	-	X
87	MG	6	2281	-	-	-	X
87	MG	6	2283	-	-	-	X
87	MG	6	2301	-	-	-	X
87	MG	6	2305	-	-	-	X
87	MG	6	2317	-	-	-	X
87	MG	6	2329	-	-	-	X
87	MG	6	2333	-	-	-	X
87	MG	M0	309	-	-	-	X
87	MG	M5	305	-	-	-	X
87	MG	M6	204	-	-	-	X
87	MG	N0	202	-	-	-	X
87	MG	O2	203	-	-	-	X
87	MG	Q0	202	-	-	-	X
87	MG	S4	302	-	-	-	X
87	MG	c9	203	-	-	-	X
87	MG	l7	301	-	-	-	X
87	MG	l8	301	-	-	-	X
87	MG	m7	206	-	-	-	X
87	MG	s8	304	-	-	-	X

2 Entry composition [i](#)

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

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

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

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

- 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	1577	1014	278	283	2	0	0	0
2	s0	206	1583	1017	281	283	2	0	0	0

- 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	1709	1084	310	311	4	0	0	0
3	s1	216	1722	1091	312	315	4	0	0	0

- 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	1635	1047	289	297	2	0	0	0
4	s2	217	1635	1047	289	297	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			
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
			Total	C	N	O	S			
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	C2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

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

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

- Molecule 16 is a protein called 40S ribosomal protein S14-B.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	c4	128	949	582	188	176	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	C5	124	977	622	182	166	7	0	0	0
17	c5	135	1039	658	196	178	7	0	0	0

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O			
27	D5	70	563	360	104	99	0	0	0
27	d5	69	558	357	103	98	0	0	0

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1,Ribosome-bound protein Stm1.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	L5	296	Total 2375	C 1501	N 414	O 458	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	15	294	Total 2359	C 1489	N 412	O 456	S 2	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L8	233	Total 1804	C 1151	N 323	O 327	S 3	0	0	0
45	18	231	Total 1763	C 1130	N 316	O 314	S 3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 81 is a protein called 40S ribosomal protein S10-A,40S ribosomal protein S10-A,40S Ribosomal Protein S10-A.

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

- Molecule 82 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			
82	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 83 is a protein called 60S Ribosomal Protein L12.

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

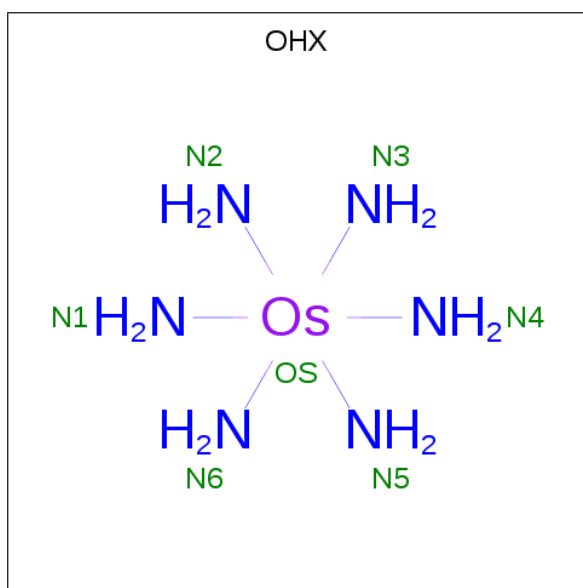
- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

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

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

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	2	1	7	6	1	0	0
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86	2	1	7	6	1	0	0
86	S2	1	7	6	1	0	0
86	S8	1	7	6	1	0	0
86	C3	1	7	6	1	0	0
86	C5	1	7	6	1	0	0
86	C8	1	7	6	1	0	0
86	C8	1	7	6	1	0	0
86	D9	1	7	6	1	0	0
86	SR	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	8	1	7	6	1	0	0
86	12	1	7	6	1	0	0
86	13	1	7	6	1	0	0
86	13	1	7	6	1	0	0
86	14	1	7	6	1	0	0
86	14	1	7	6	1	0	0
86	15	1	7	6	1	0	0
86	15	1	7	6	1	0	0
86	15	1	7	6	1	0	0
86	19	1	7	6	1	0	0
86	m0	1	7	6	1	0	0
86	m0	1	7	6	1	0	0
86	m0	1	7	6	1	0	0
86	m0	1	7	6	1	0	0
86	m1	1	7	6	1	0	0
86	m4	1	7	6	1	0	0
86	m5	1	7	6	1	0	0
86	m5	1	7	6	1	0	0
86	m7	1	7	6	1	0	0
86	m9	1	7	6	1	0	0
86	n1	1	7	6	1	0	0

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	n8	7	Total	Mg	0	0
			7	7		
87	c6	2	Total	Mg	0	0
			2	2		
87	Q0	2	Total	Mg	0	0
			2	2		
87	sM	2	Total	Mg	0	0
			2	2		
87	O3	2	Total	Mg	0	0
			2	2		
87	M9	2	Total	Mg	0	0
			2	2		
87	q0	1	Total	Mg	0	0
			1	1		
87	O2	4	Total	Mg	0	0
			4	4		
87	D9	3	Total	Mg	0	0
			3	3		
87	m9	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	M3	3	Total 3	Mg 3	0	0
87	D4	1	Total 1	Mg 1	0	0
87	S4	2	Total 2	Mg 2	0	0
87	l5	6	Total 6	Mg 6	0	0
87	m6	4	Total 4	Mg 4	0	0
87	o2	3	Total 3	Mg 3	0	0
87	d5	1	Total 1	Mg 1	0	0
87	d9	2	Total 2	Mg 2	0	0
87	m3	1	Total 1	Mg 1	0	0
87	d4	2	Total 2	Mg 2	0	0
87	s4	1	Total 1	Mg 1	0	0
87	M6	4	Total 4	Mg 4	0	0
87	N9	1	Total 1	Mg 1	0	0
87	p0	1	Total 1	Mg 1	0	0
87	n0	5	Total 5	Mg 5	0	0
87	C8	1	Total 1	Mg 1	0	0
87	n9	2	Total 2	Mg 2	0	0
87	M5	4	Total 4	Mg 4	0	0
87	S2	1	Total 1	Mg 1	0	0
87	N6	2	Total 2	Mg 2	0	0
87	D0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	O5	2	Total 2	Mg 2	0	0
87	m5	3	Total 3	Mg 3	0	0
87	n6	1	Total 1	Mg 1	0	0
87	S8	1	Total 1	Mg 1	0	0
87	M8	3	Total 3	Mg 3	0	0
87	q3	1	Total 1	Mg 1	0	0
87	N3	3	Total 3	Mg 3	0	0
87	4	28	Total 28	Mg 28	0	0
87	L2	3	Total 3	Mg 3	0	0
87	o3	4	Total 4	Mg 4	0	0
87	O1	5	Total 5	Mg 5	0	0
87	s8	4	Total 4	Mg 4	0	0
87	m8	4	Total 4	Mg 4	0	0
87	n3	3	Total 3	Mg 3	0	0
87	l2	6	Total 6	Mg 6	0	0
87	N0	2	Total 2	Mg 2	0	0
87	L7	3	Total 3	Mg 3	0	0
87	6	235	Total 235	Mg 235	0	0
87	O4	1	Total 1	Mg 1	0	0
87	C1	2	Total 2	Mg 2	0	0
87	M1	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	D6	1	Total 1	Mg 1	0	0
87	S6	1	Total 1	Mg 1	0	0
87	c9	3	Total 3	Mg 3	0	0
87	l7	7	Total 7	Mg 7	0	0
87	L8	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	o4	1	Total 1	Mg 1	0	0
87	O7	6	Total 6	Mg 6	0	0
87	s6	2	Total 2	Mg 2	0	0
87	M4	1	Total 1	Mg 1	0	0
87	1	698	Total 698	Mg 698	0	0
87	S1	1	Total 1	Mg 1	0	0
87	l8	1	Total 1	Mg 1	0	0
87	Q2	3	Total 3	Mg 3	0	0
87	o7	1	Total 1	Mg 1	0	0
87	m4	1	Total 1	Mg 1	0	0
87	s1	1	Total 1	Mg 1	0	0
87	q2	1	Total 1	Mg 1	0	0
87	c7	1	Total 1	Mg 1	0	0
87	L3	5	Total 5	Mg 5	0	0
87	8	19	Total 19	Mg 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	3	18	Total 18	Mg 18	0	0
87	C5	1	Total 1	Mg 1	0	0
87	q1	2	Total 2	Mg 2	0	0
87	l3	13	Total 13	Mg 13	0	0
87	N1	1	Total 1	Mg 1	0	0
87	2	170	Total 170	Mg 170	0	0
87	L4	7	Total 7	Mg 7	0	0
87	M0	5	Total 5	Mg 5	0	0
87	5	759	Total 759	Mg 759	0	0
87	n1	3	Total 3	Mg 3	0	0
87	c8	4	Total 4	Mg 4	0	0
87	l4	1	Total 1	Mg 1	0	0
87	d2	1	Total 1	Mg 1	0	0
87	d3	2	Total 2	Mg 2	0	0
87	E1	1	Total 1	Mg 1	0	0
87	m0	1	Total 1	Mg 1	0	0
87	M7	10	Total 10	Mg 10	0	0
87	N8	7	Total 7	Mg 7	0	0
87	l9	3	Total 3	Mg 3	0	0
87	7	28	Total 28	Mg 28	0	0
87	o6	1	Total 1	Mg 1	0	0

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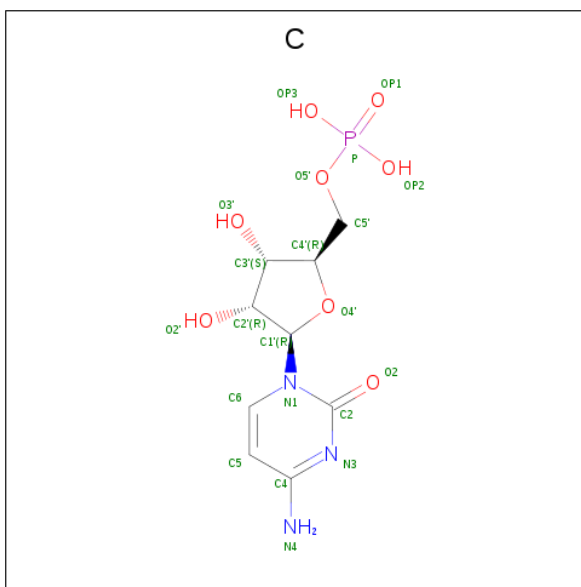
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	m7	8	Total	Mg	0	0
			8	8		

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

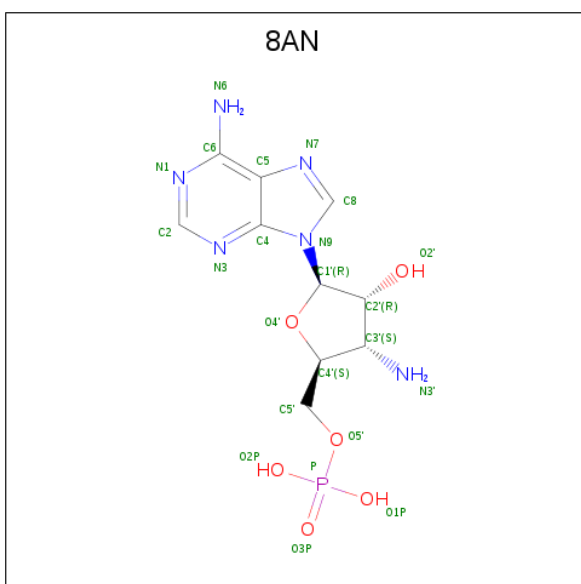
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	Q3	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		
88	Q0	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0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

- Molecule 89 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: C₉H₁₄N₃O₈P).



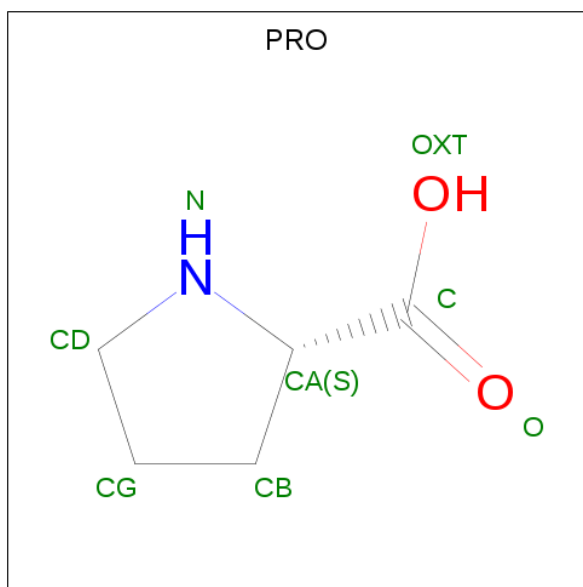
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
89	1	1	20	9	3	7	1	0	0
89	1	1	20	9	3	7	1	0	0
89	5	1	20	9	3	7	1	0	0
89	5	1	20	9	3	7	1	0	0

- Molecule 90 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula: C₁₀H₁₅N₆O₆P).



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

- Molecule 91 is PROLINE (three-letter code: PRO) (formula: C₅H₉NO₂).

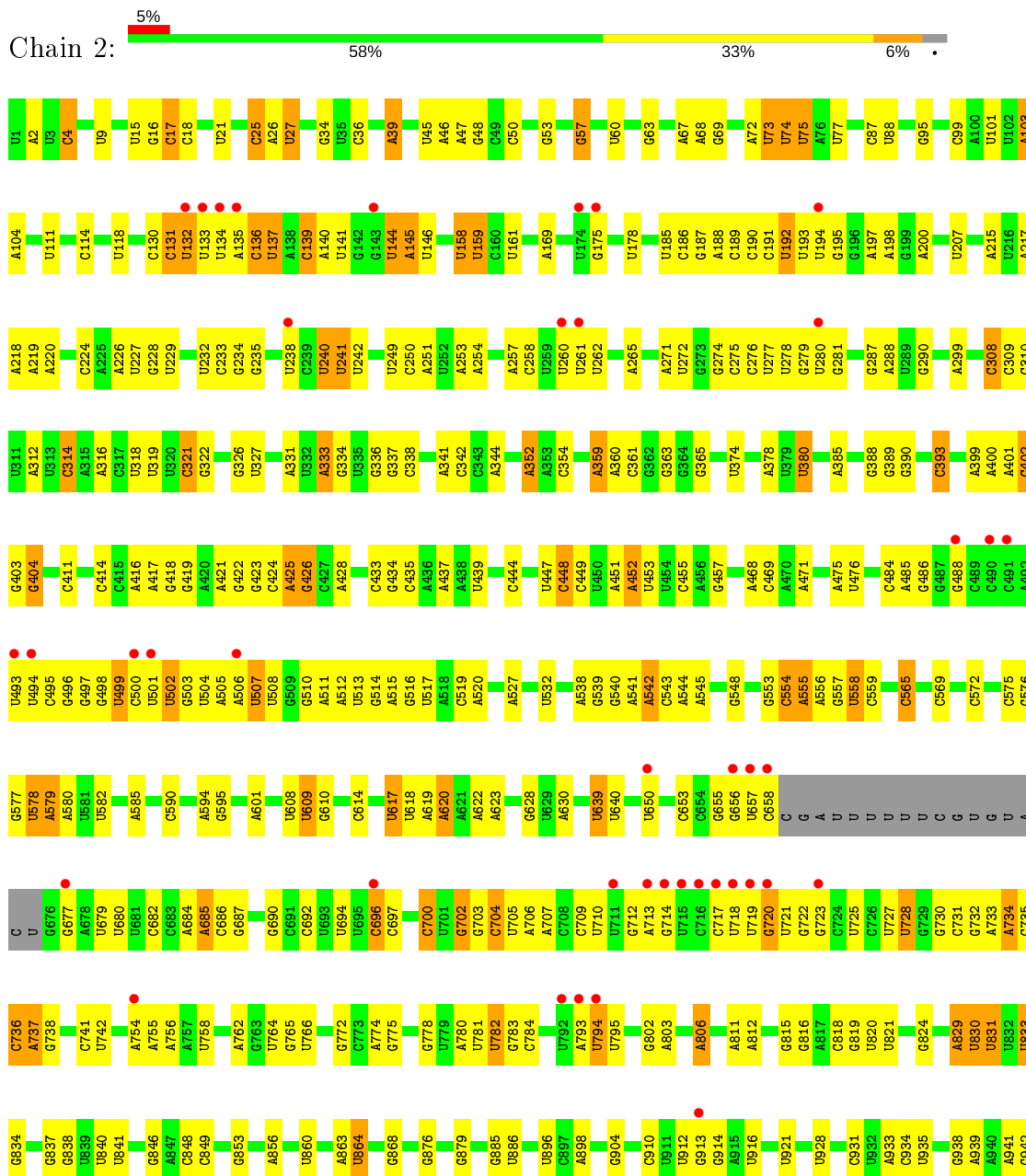


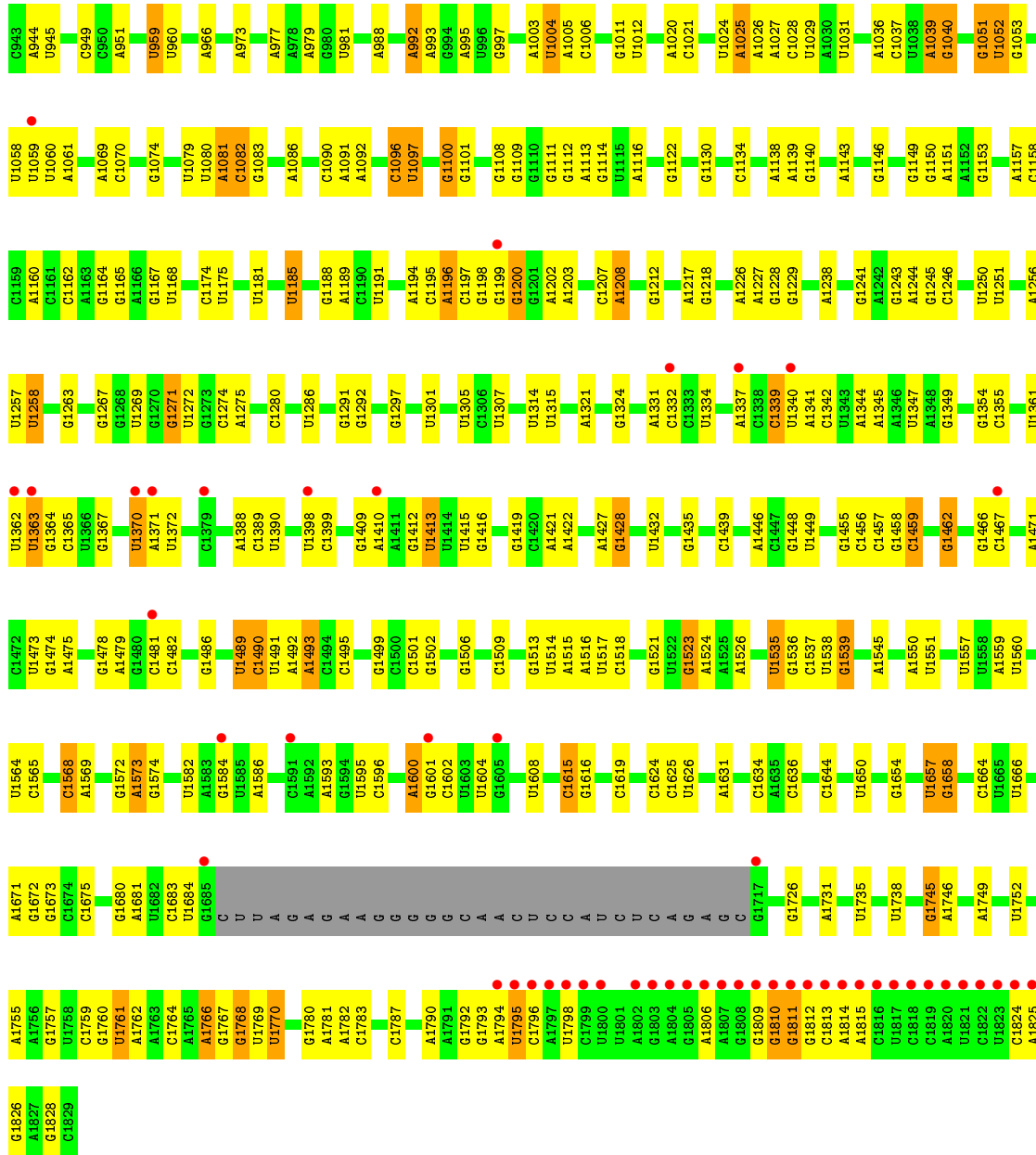
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
91	1	1	Total	C	N	O	0	0
			7	5	1	1		
91	5	1	Total	C	N	O	0	0
			7	5	1	1		

3 Residue-property plots [i](#)

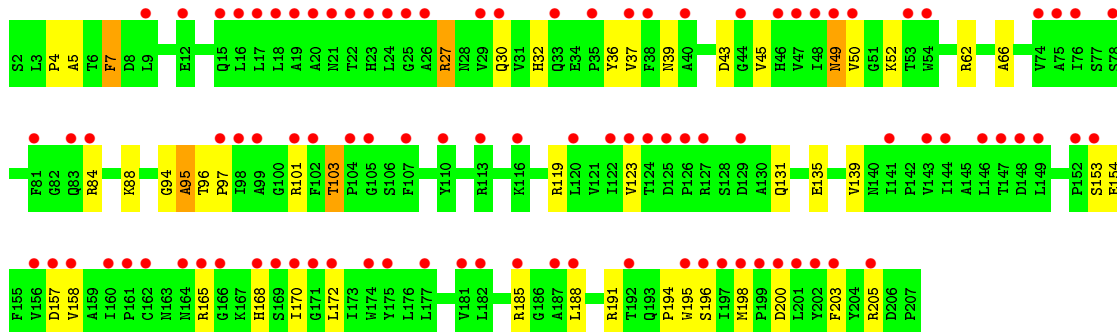
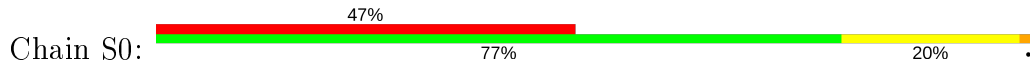
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 18S ribosomal RNA

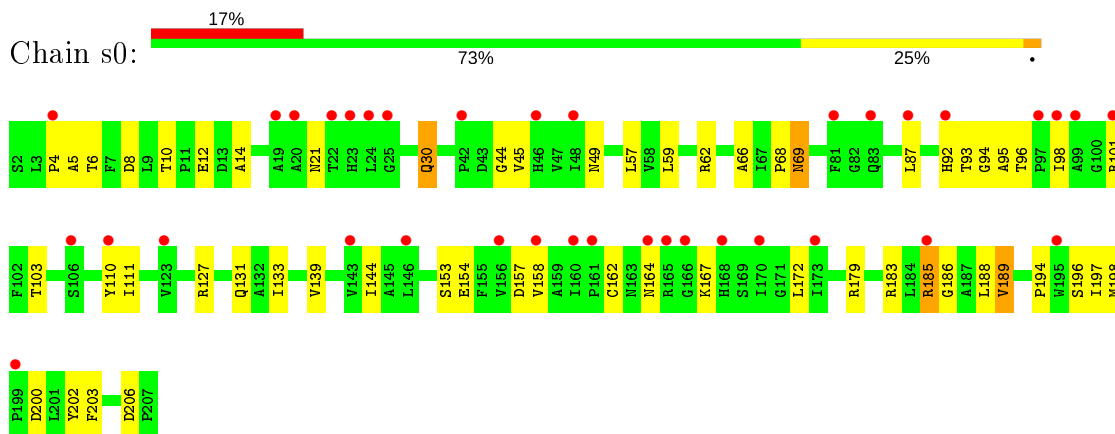




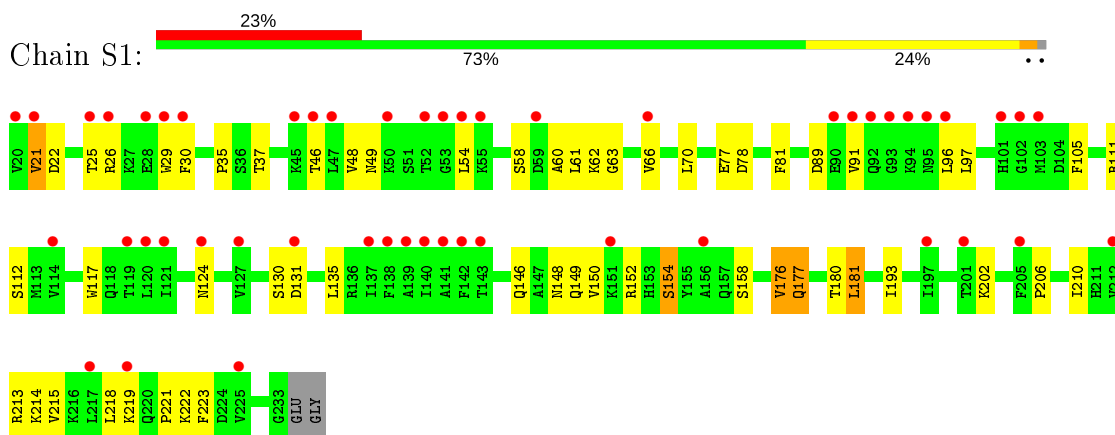
• Molecule 2: 40S ribosomal protein S0-A



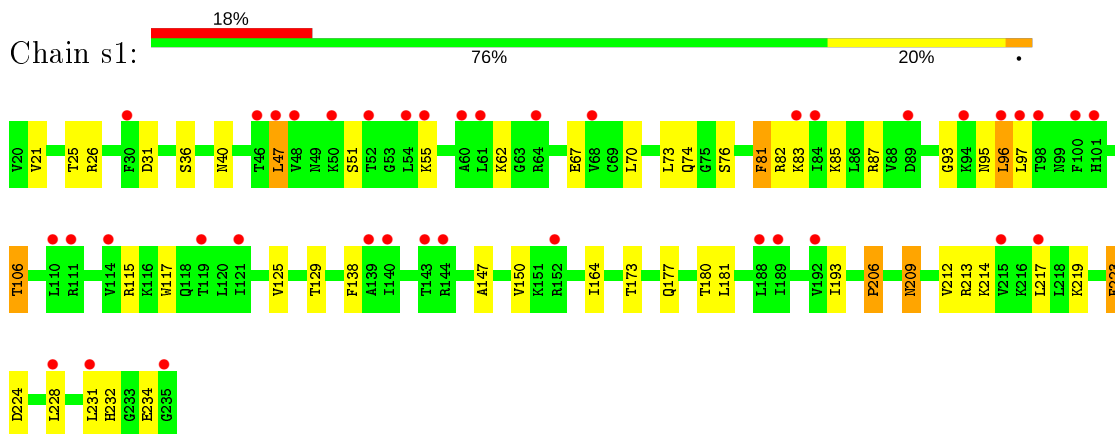
- Molecule 2: 40S ribosomal protein S0-A



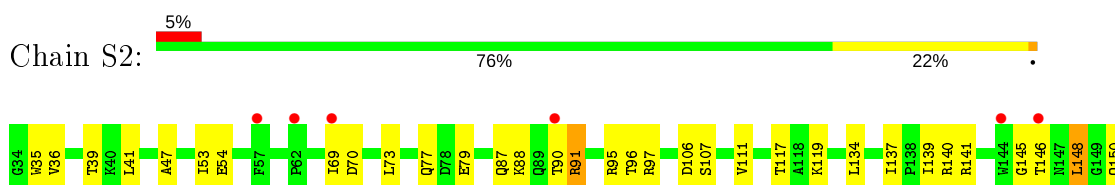
- Molecule 3: 40S ribosomal protein S1-A



- Molecule 3: 40S ribosomal protein S1-A

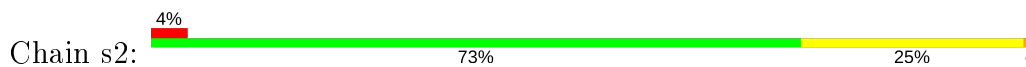


- Molecule 4: 40S ribosomal protein S2

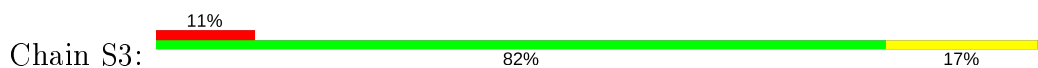




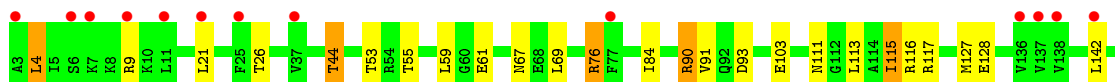
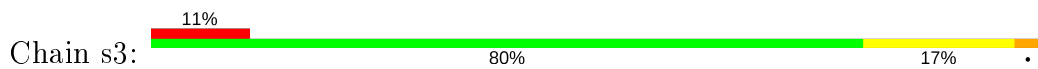
- Molecule 4: 40S ribosomal protein S2



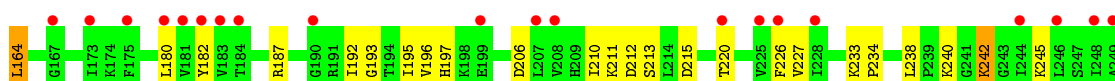
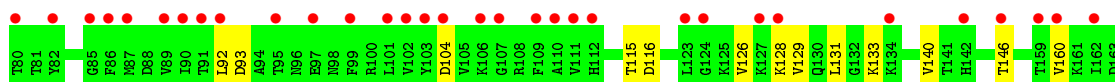
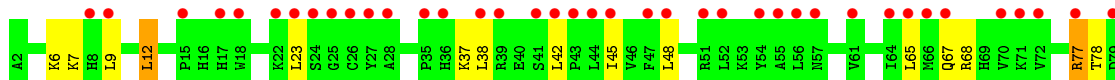
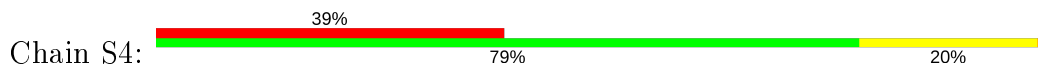
- Molecule 5: 40S ribosomal protein S3

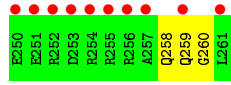


- Molecule 5: 40S ribosomal protein S3

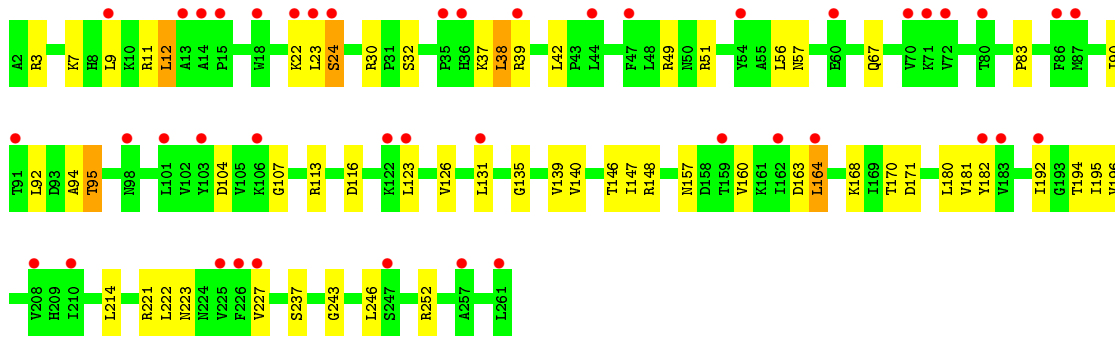
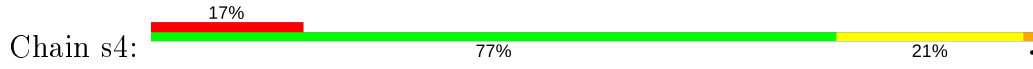


- Molecule 6: 40S ribosomal protein S4-A

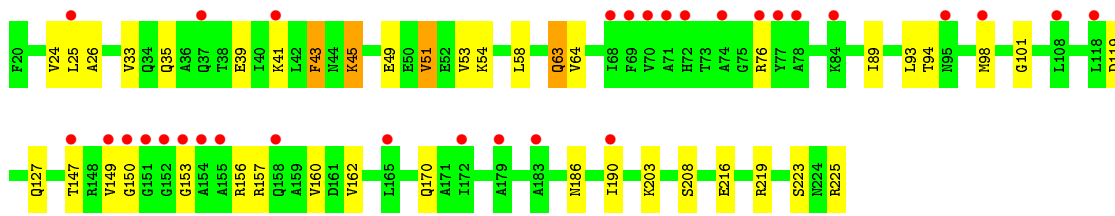
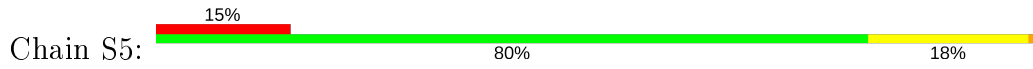




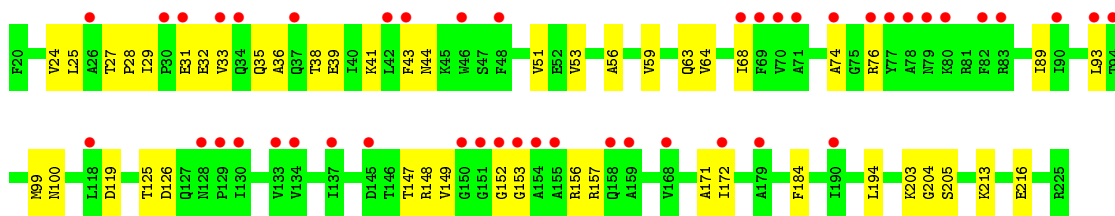
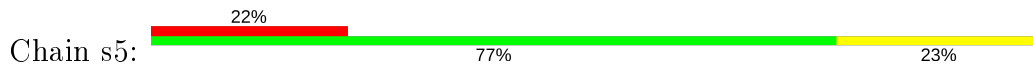
• Molecule 6: 40S ribosomal protein S4-A



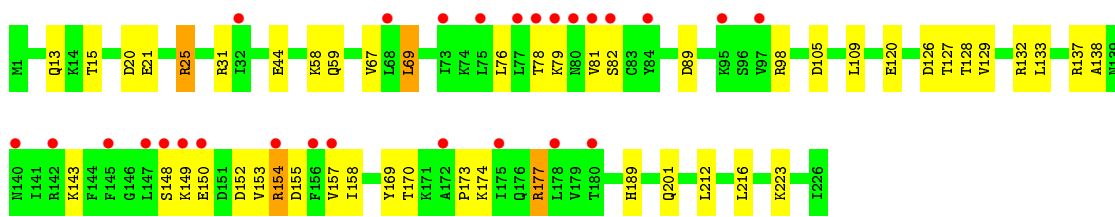
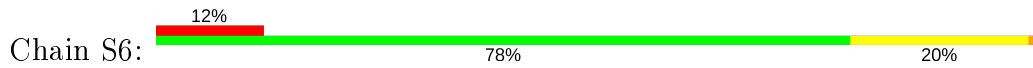
• Molecule 7: 40S ribosomal protein S5

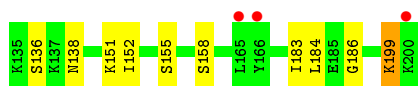


• Molecule 7: 40S ribosomal protein S5

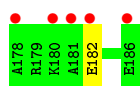
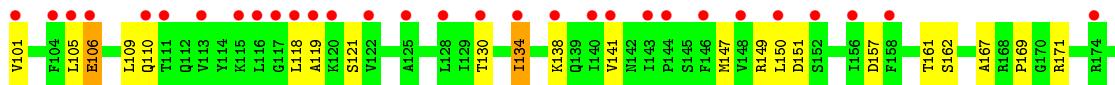
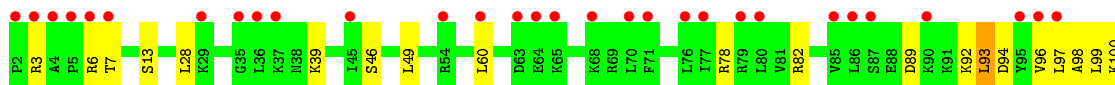
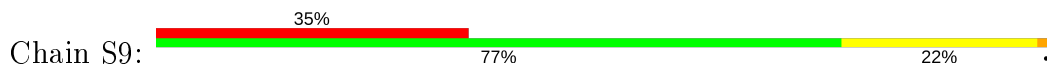


• Molecule 8: 40S ribosomal protein S6-A

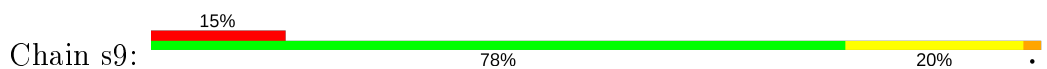




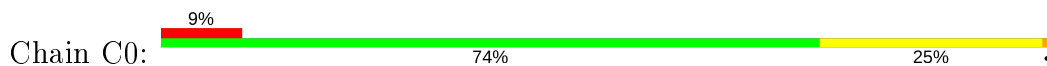
- Molecule 11: 40S ribosomal protein S9-A



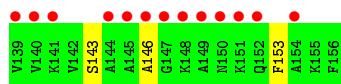
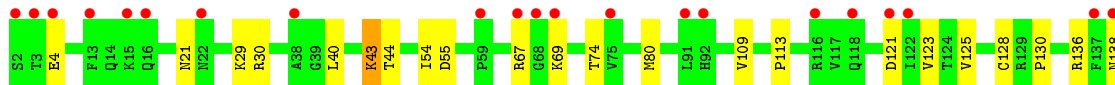
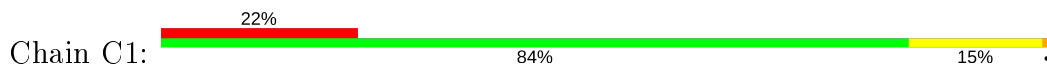
- Molecule 11: 40S ribosomal protein S9-A



- Molecule 12: 40S ribosomal protein S10-A

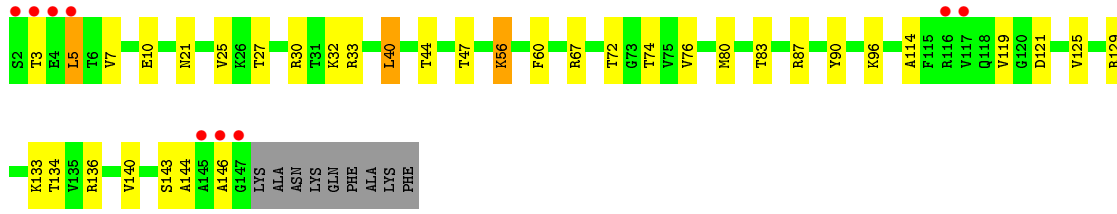


- Molecule 13: 40S ribosomal protein S11-A

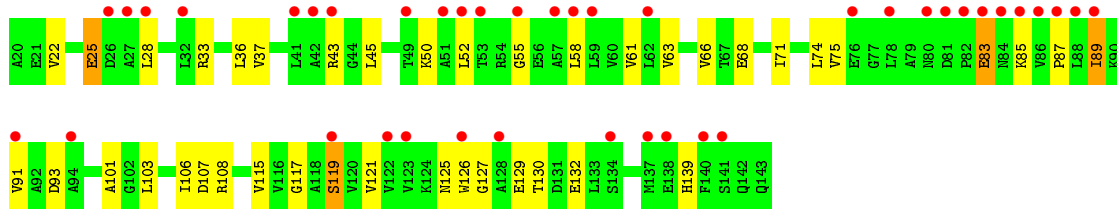


- Molecule 13: 40S ribosomal protein S11-A

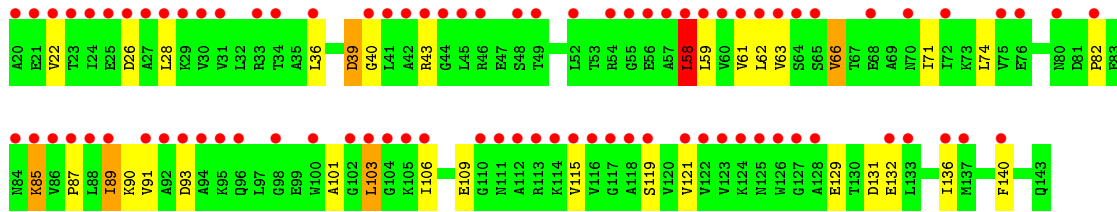
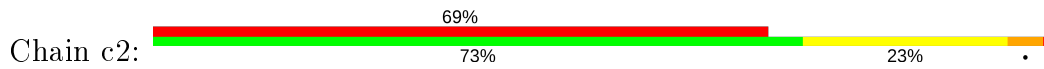




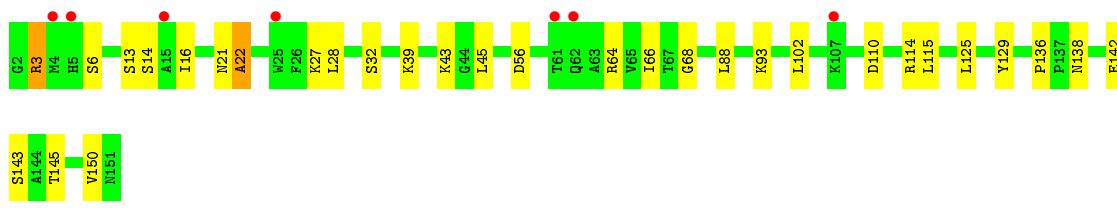
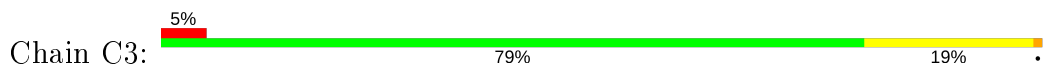
• Molecule 14: 40S ribosomal protein S12



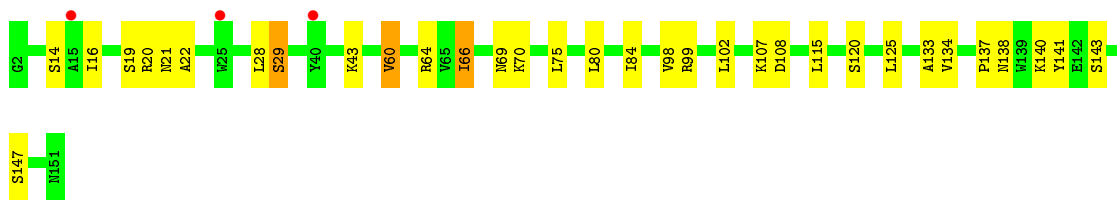
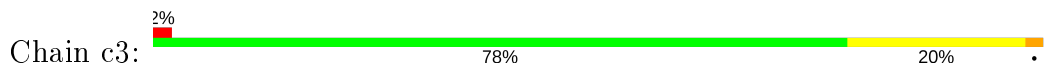
• Molecule 14: 40S ribosomal protein S12



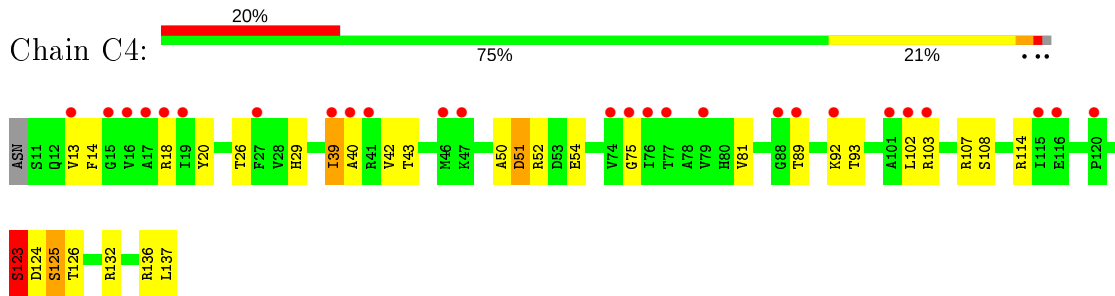
• Molecule 15: 40S ribosomal protein S13



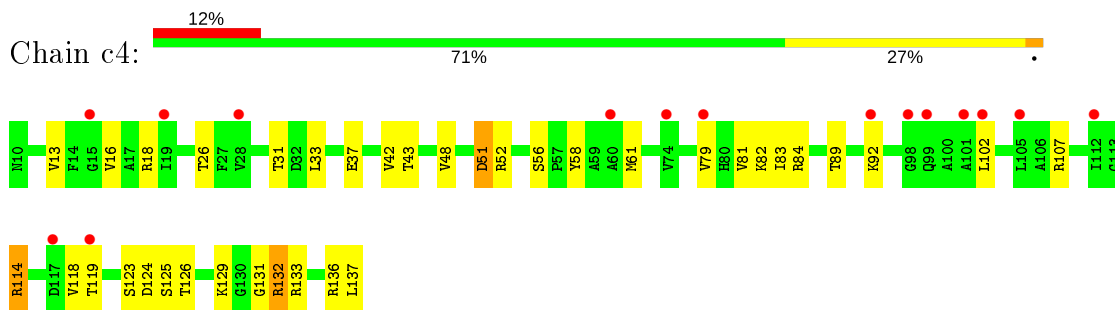
• Molecule 15: 40S ribosomal protein S13



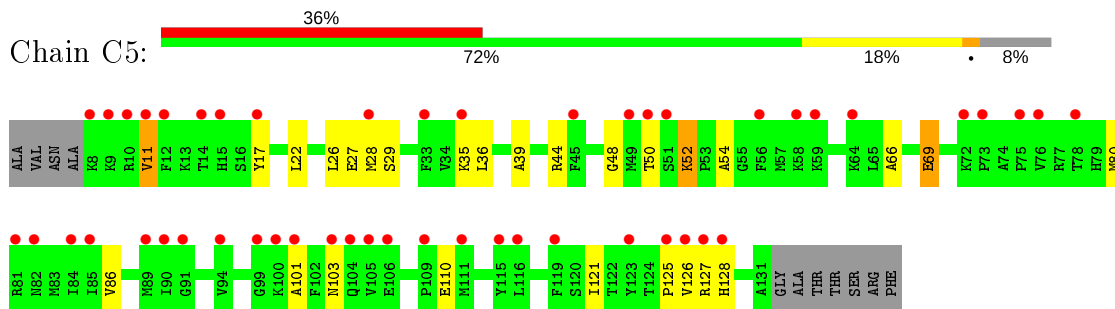
• Molecule 16: 40S ribosomal protein S14-B



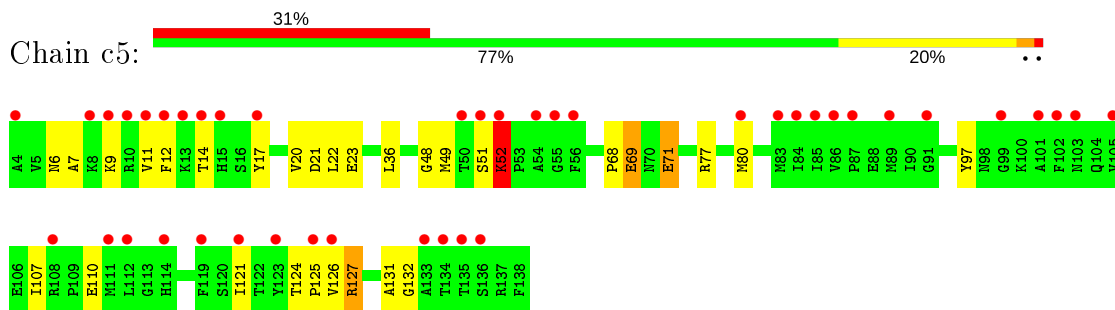
• Molecule 16: 40S ribosomal protein S14-B



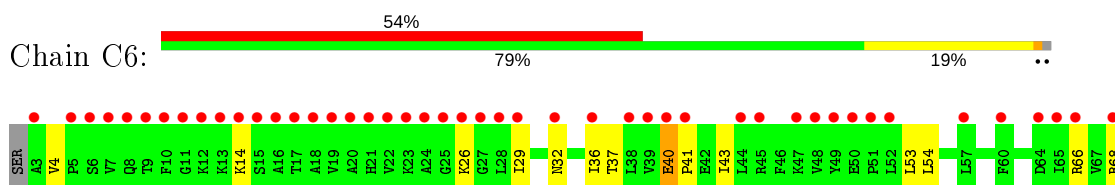
• Molecule 17: 40S ribosomal protein S15

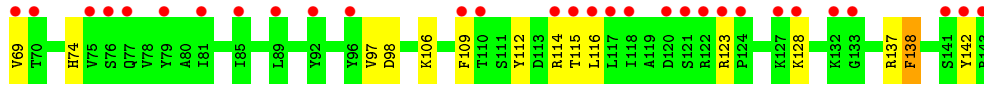


• Molecule 17: 40S ribosomal protein S15

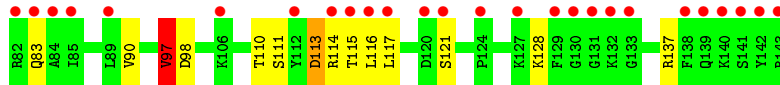
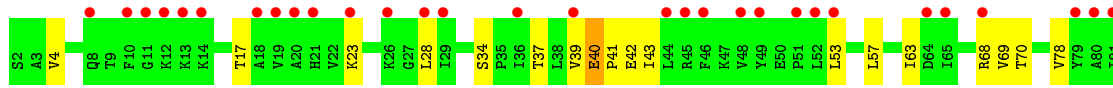
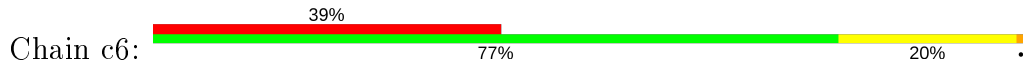


• Molecule 18: 40S ribosomal protein S16-A

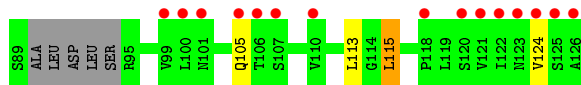
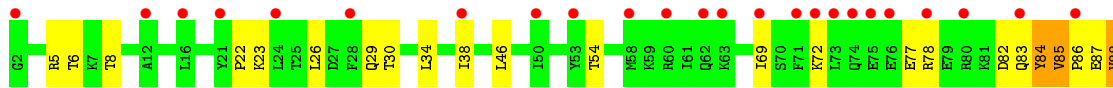
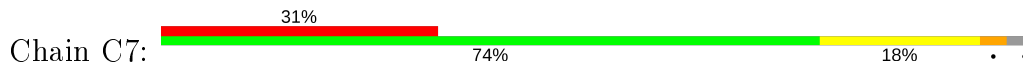




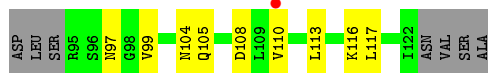
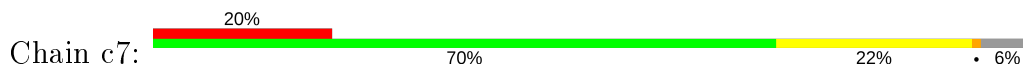
- Molecule 18: 40S ribosomal protein S16-A



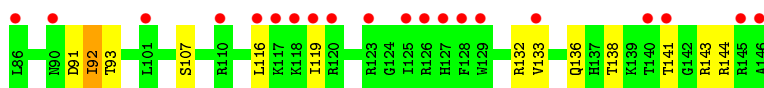
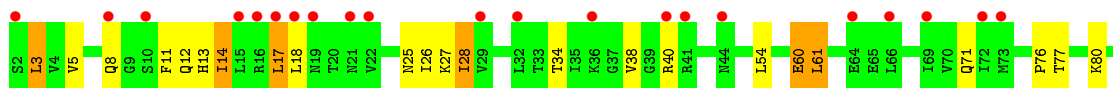
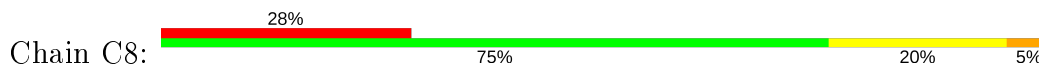
- Molecule 19: 40S ribosomal protein S17-B



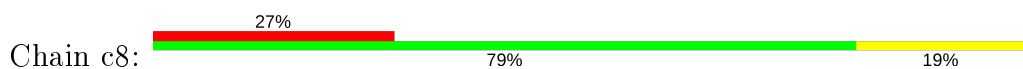
- Molecule 19: 40S ribosomal protein S17-B

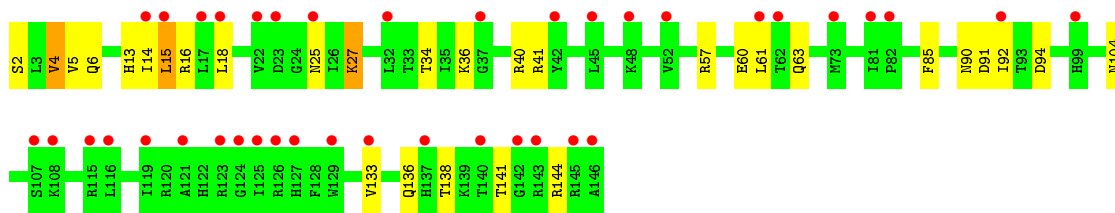


- Molecule 20: 40S ribosomal protein S18-A

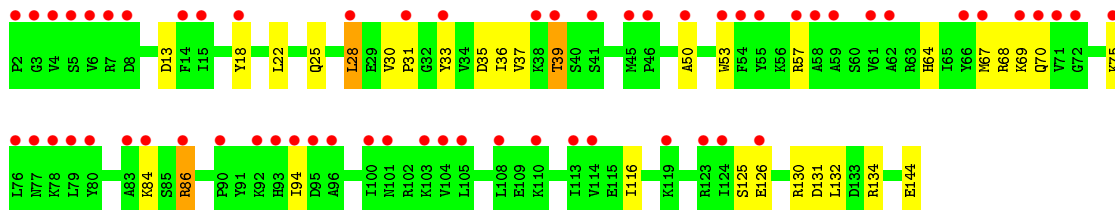
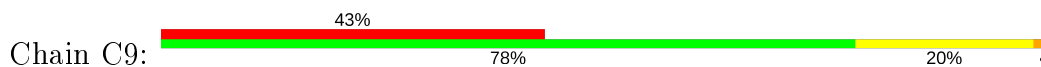


- Molecule 20: 40S ribosomal protein S18-A

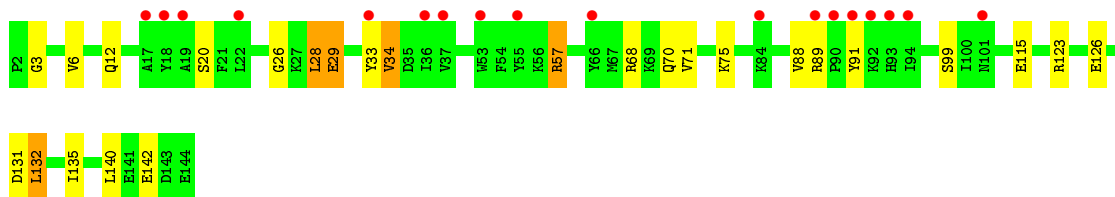
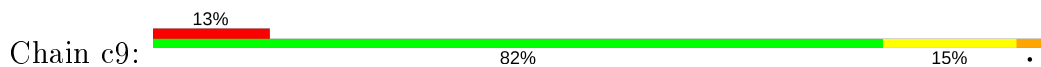




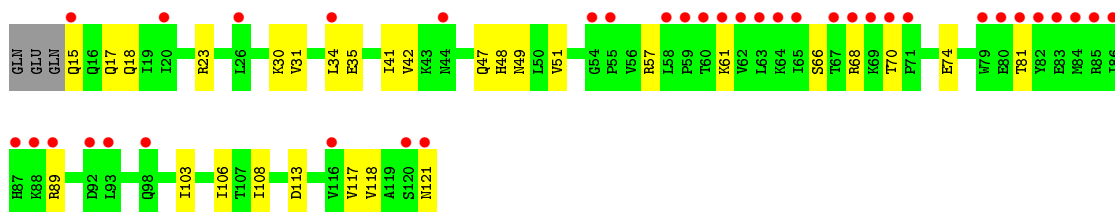
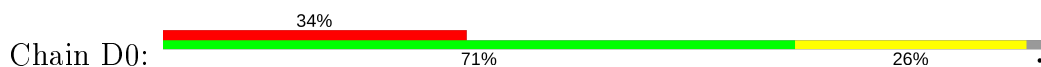
- Molecule 21: 40S ribosomal protein S19-A



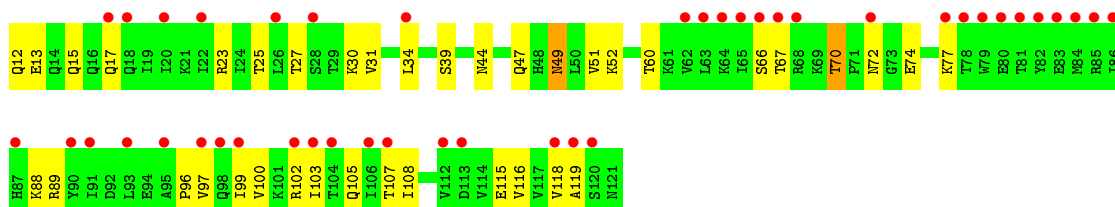
- Molecule 21: 40S ribosomal protein S19-A



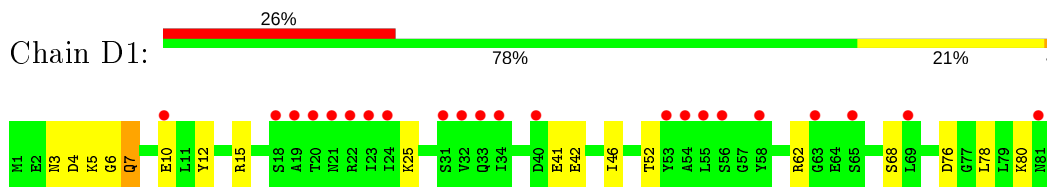
- Molecule 22: 40S ribosomal protein S20



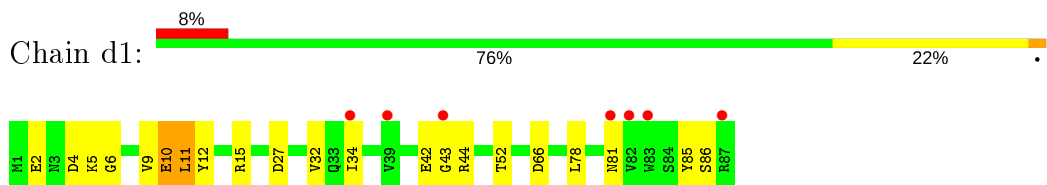
- Molecule 22: 40S ribosomal protein S20



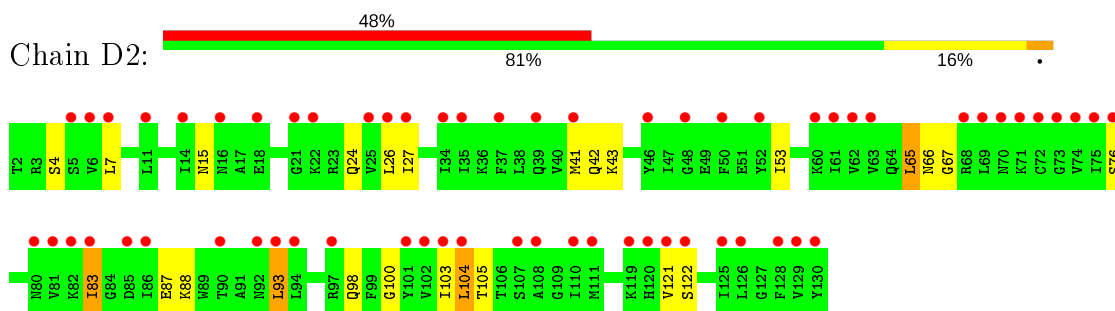
- Molecule 23: 40S ribosomal protein S21-A



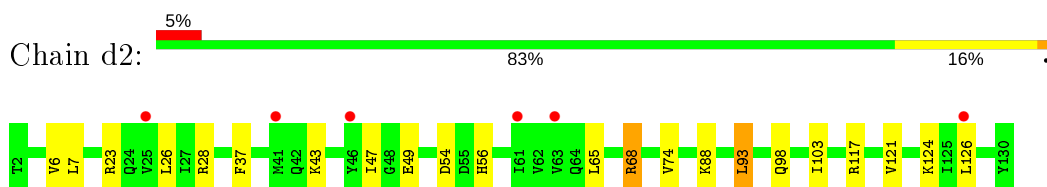
- Molecule 23: 40S ribosomal protein S21-A



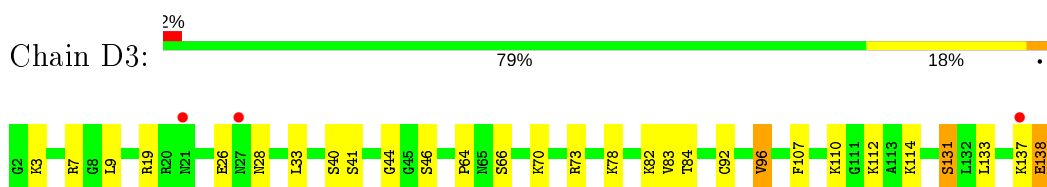
- Molecule 24: 40S ribosomal protein S22-A



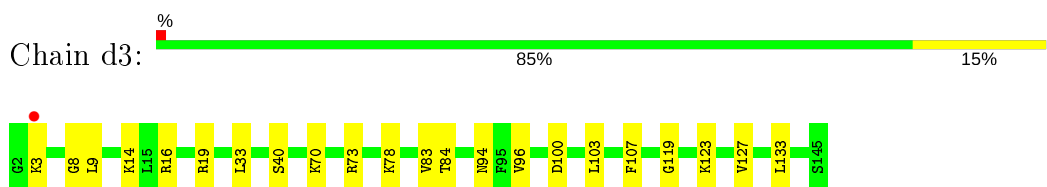
- Molecule 24: 40S ribosomal protein S22-A



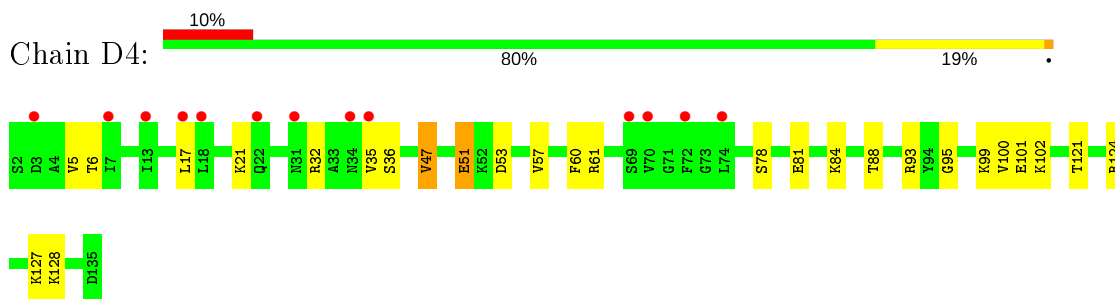
- Molecule 25: 40S ribosomal protein S23-A



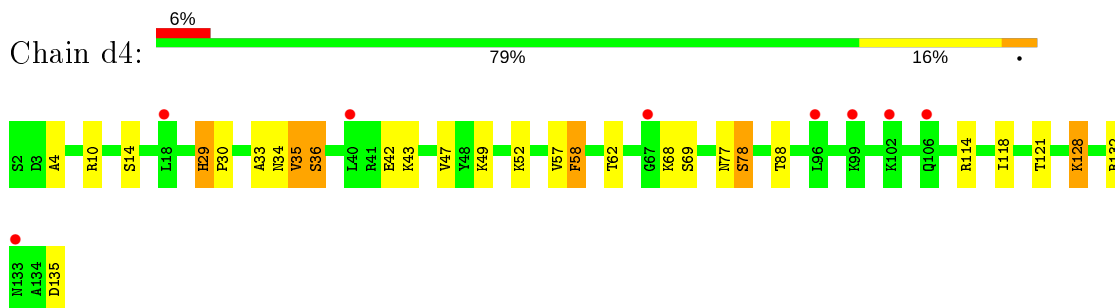
- Molecule 25: 40S ribosomal protein S23-A



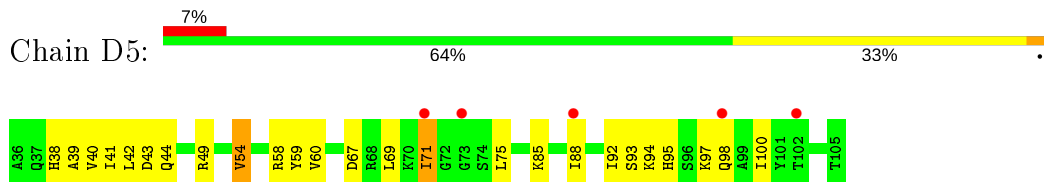
- Molecule 26: 40S ribosomal protein S24-A



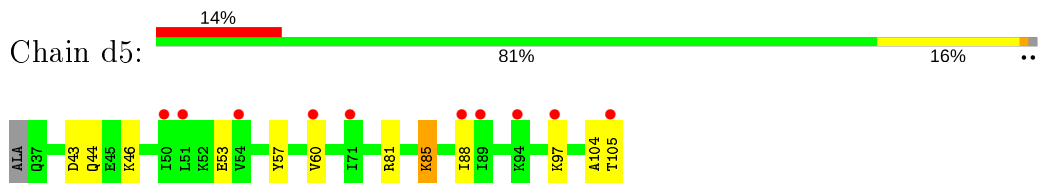
• Molecule 26: 40S ribosomal protein S24-A



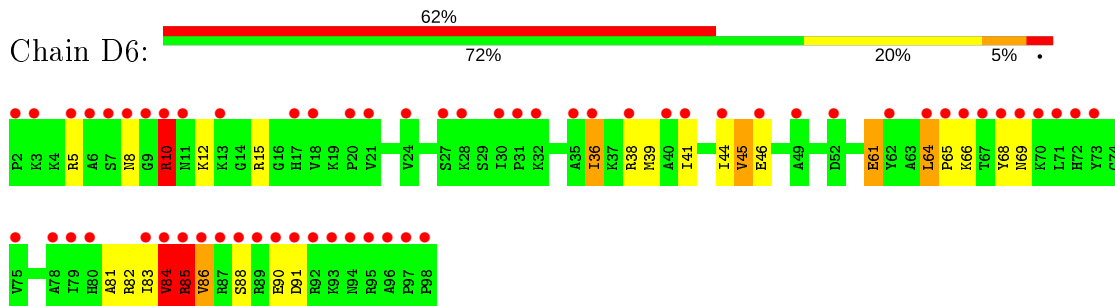
• Molecule 27: 40S ribosomal protein S25-A



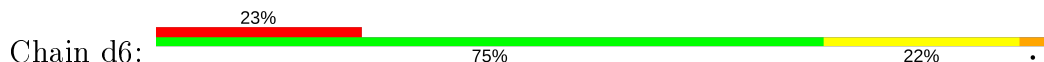
• Molecule 27: 40S ribosomal protein S25-A

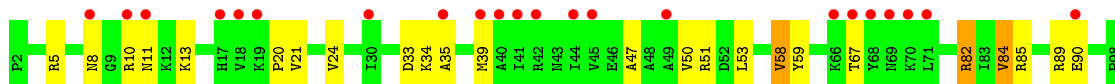


• Molecule 28: 40S ribosomal protein S26-B

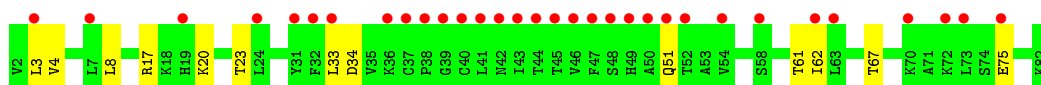
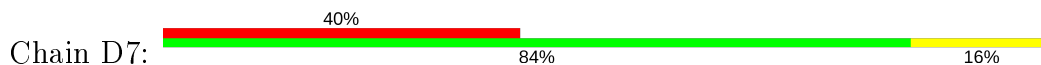


• Molecule 28: 40S ribosomal protein S26-B

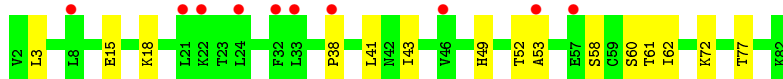
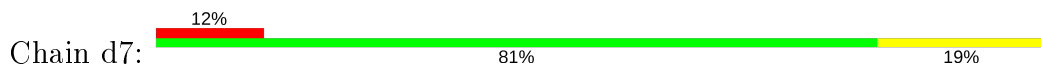




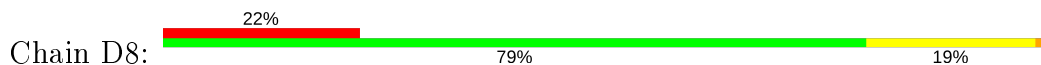
- Molecule 29: 40S ribosomal protein S27-A



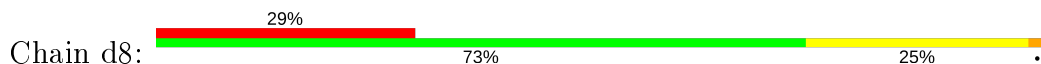
- Molecule 29: 40S ribosomal protein S27-A



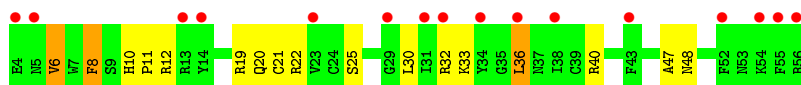
- Molecule 30: 40S ribosomal protein S28-A



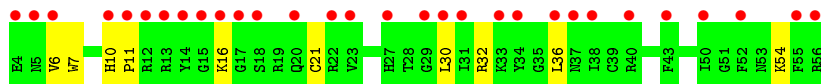
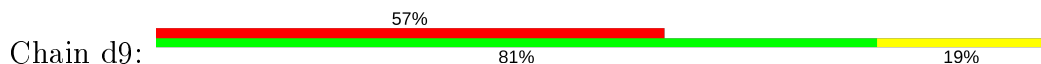
- Molecule 30: 40S ribosomal protein S28-A



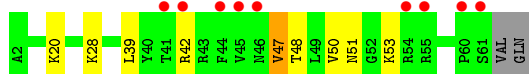
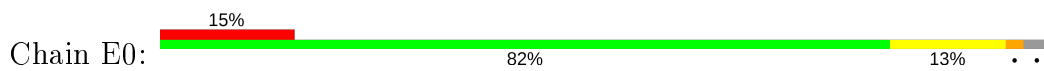
- Molecule 31: 40S ribosomal protein S29-A



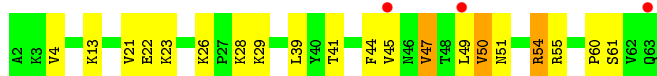
- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A



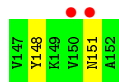
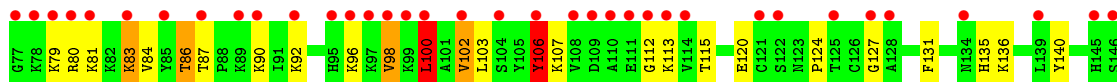
• Molecule 32: 40S ribosomal protein S30-A



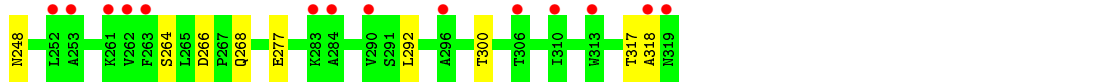
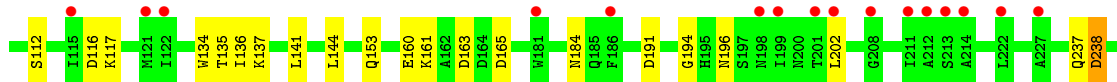
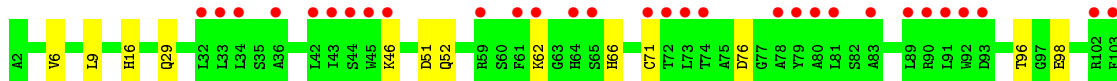
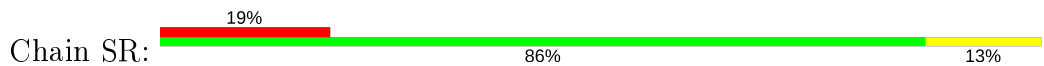
• Molecule 33: Ubiquitin-40S ribosomal protein S31



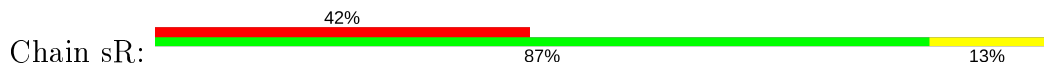
• Molecule 33: Ubiquitin-40S ribosomal protein S31

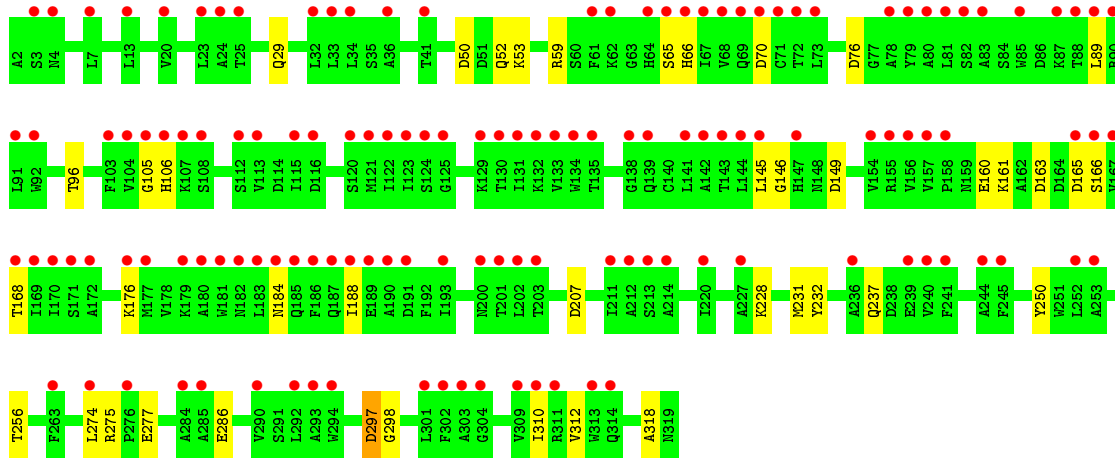


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

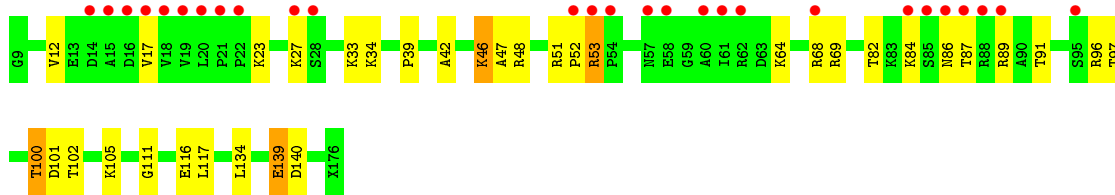
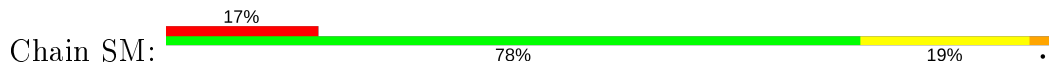


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

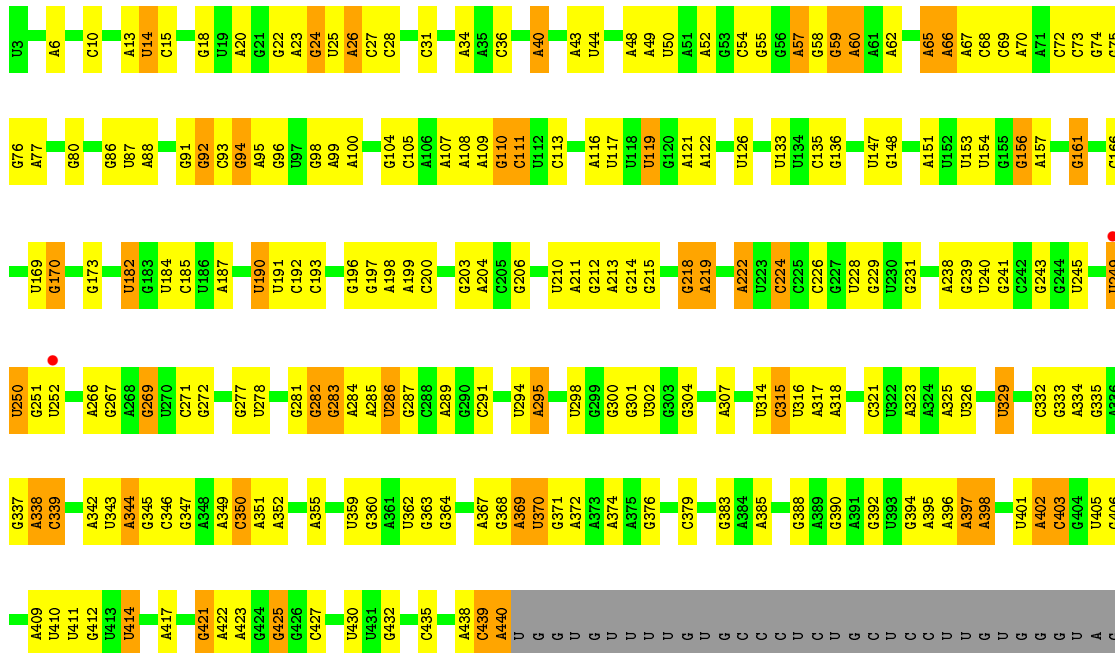
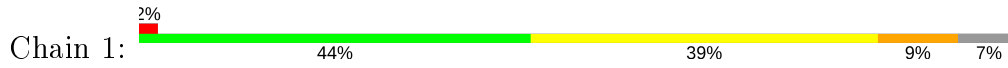


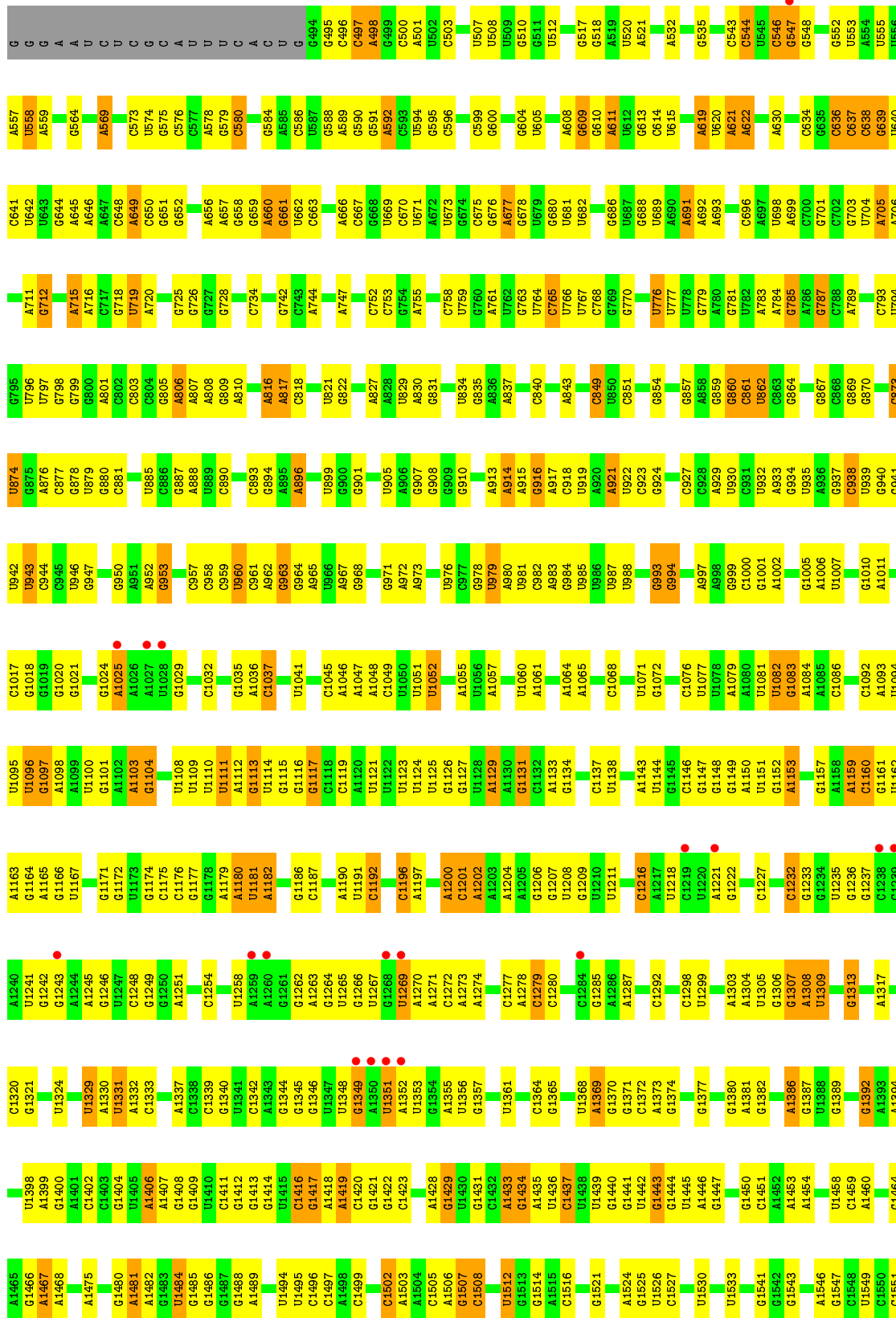


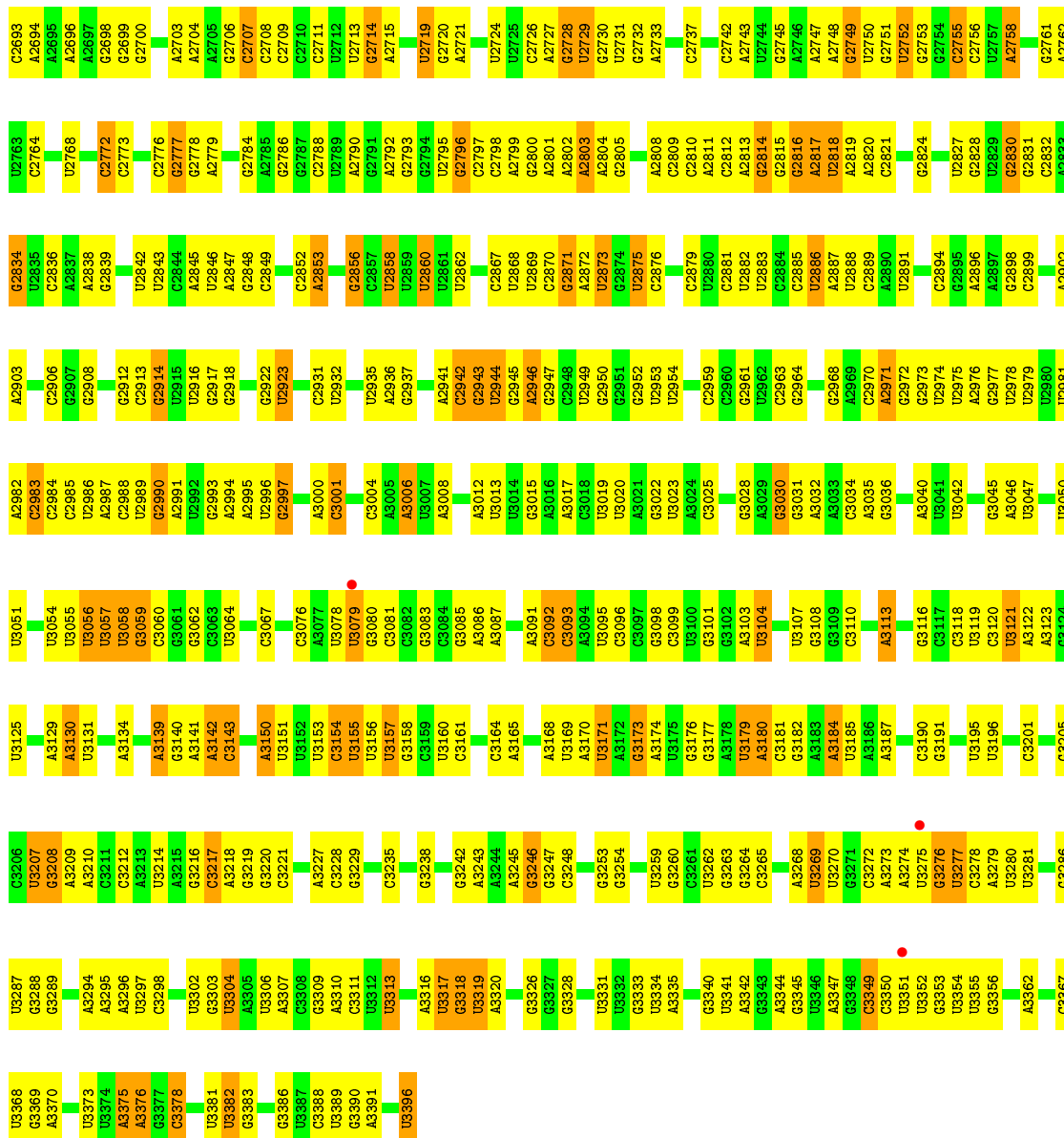
• Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Ribosome-bound protein Stm1



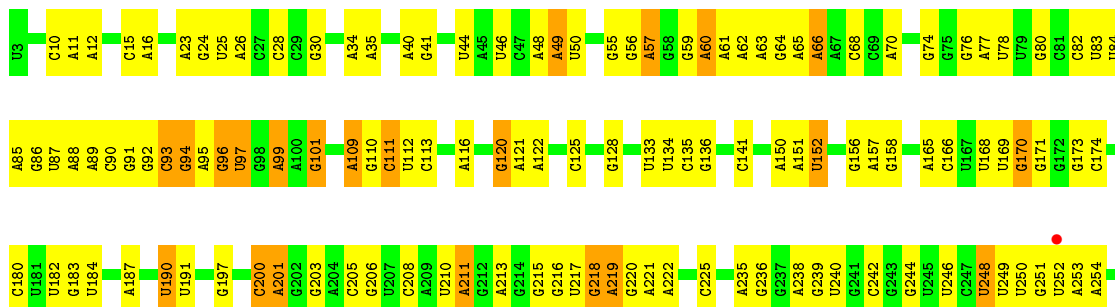
• Molecule 36: 25S ribosomal RNA



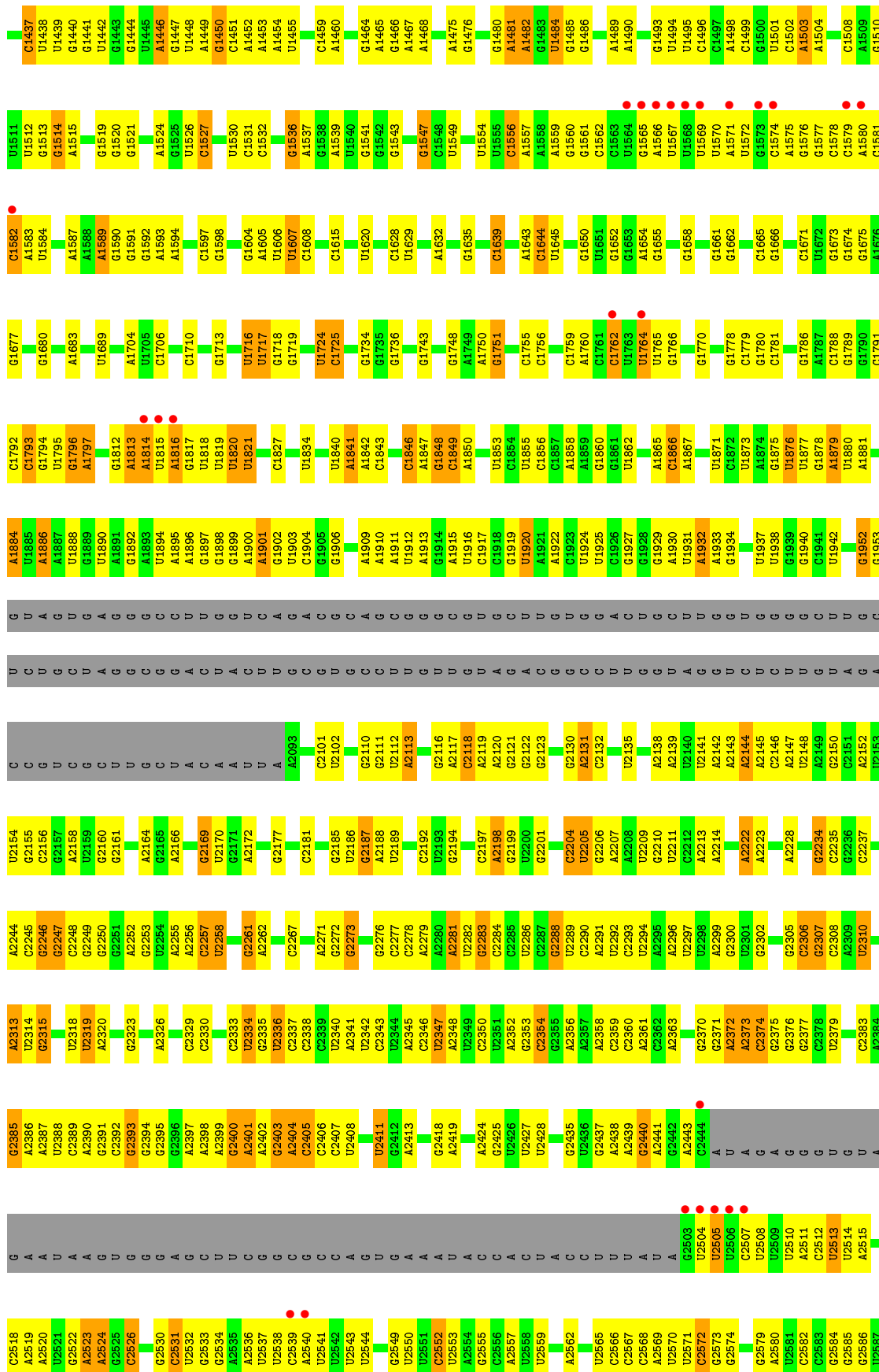


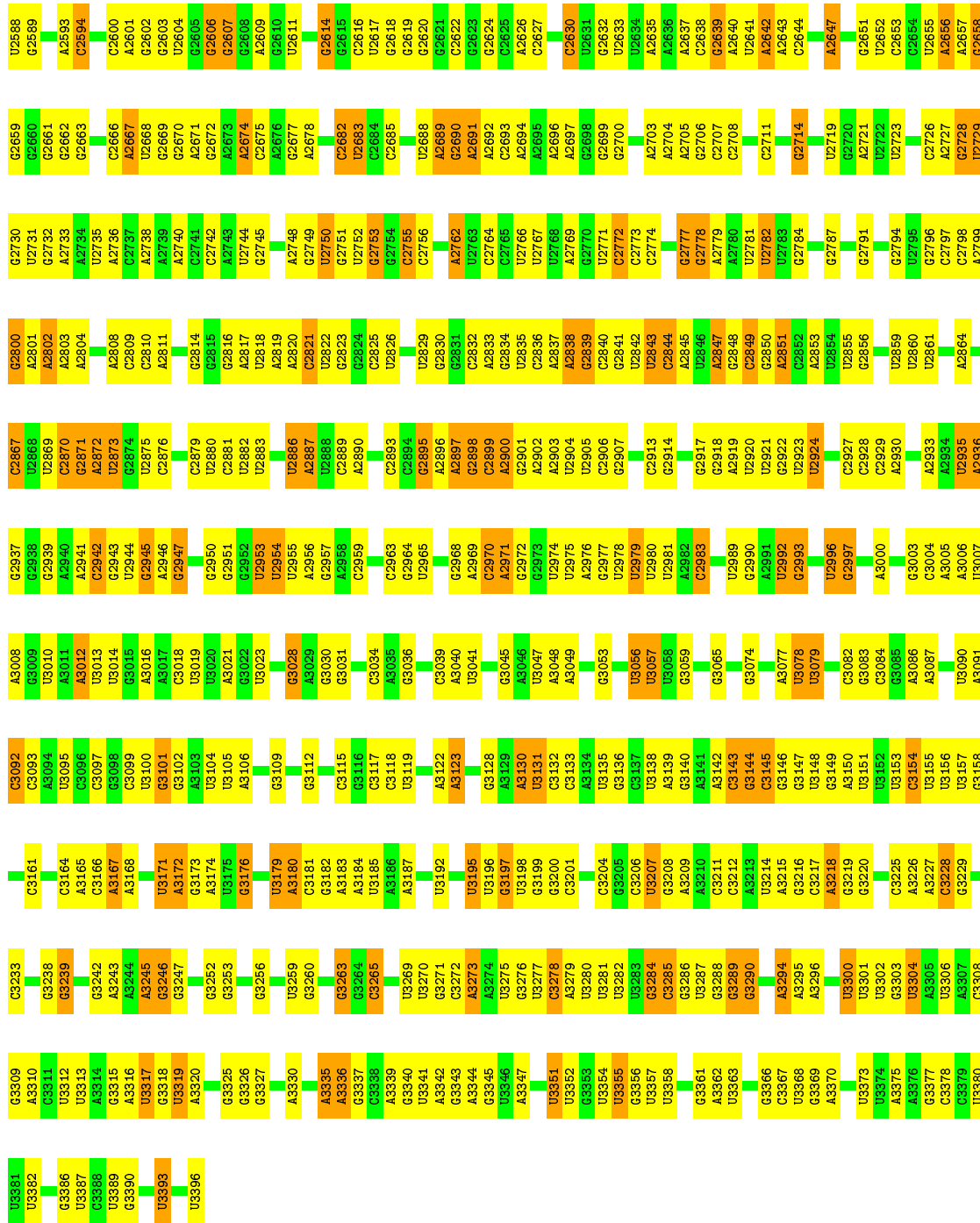


● Molecule 36: 25S ribosomal RNA

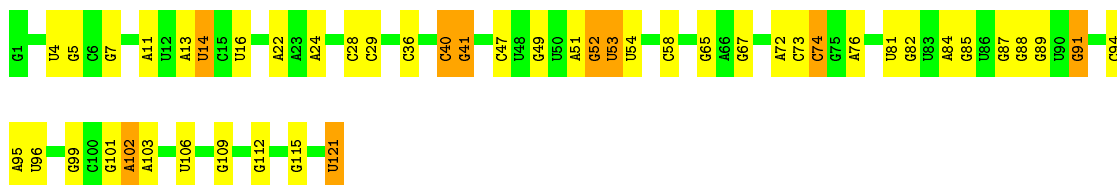


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G1370	A1369	A1193	A1192	G1127	A1046	A973	G902	A820	C654	G582	U492	U	A352	A265
A1373	A1301	A1194	A1194	U1128	A1047	C974	U903	C824	C655	G583	G493	U	G353	A266
G1374	A1302	A1195	C1049	C1049	A1048	C975	A904	C825	A656	G584	G494	U	G358	G267
G1375	A1303	C1196	U1050	U1050	U1049	U976	A904	C826	G658	A585	G495	U	U359	A268
C1376	A1304	A1200	U1051	U1051	U1050	C977	G907	G826	C659	U587	C496	U	G360	G269
G1377	C1306	C1201	U1052	G978	A980	U979	G908	A830	A660	C503	U	U	U271	C270
U1378	G1307	A1202	A1055	U979	U981	U980	C911	G835	G661	A504	U	U	C271	C271
G1379	A1308	A1203	A1056	U981	U981	U980	C911	G836	G662	A504	U	U	G272	G272
G1380	U1309	U1203	A1057	U982	U982	U981	C911	G837	C667	U508	U	U	G273	G273
A1381	G1310	G1139	U1058	U985	U985	U984	A914	A837	G668	G510	U	U	G274	G274
C1385	G1311	G1140	G1059	U985	U985	U984	A915	A838	U669	C593	U	U	U279	U279
A1386	C1312	C1141	U1060	A989	A989	A988	G916	G838	U669	G511	U	U	U280	U280
G1387	G1313	U1142	A1061	U990	U990	U989	A917	C840	U673	U594	U	U	G281	G281
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G1389	U1315	U1144	A1063	A992	C842	U991	U919	C842	G675	C599	U	U	U370	U370
A1390	C1316	U1145	A1064	G993	A842	U992	A920	C842	G676	G600	U	U	A373	A284
C1391	A1317	C1146	A1065	G994	A843	U922	A921	A846	G677	G604	U	U	A374	A285
A1393	G1321	G1147	C1069	U995	A844	U922	A922	A847	G678	U604	U	U	G376	G290
A1394	U1322	U1148	U1070	A996	C851	C923	G924	A847	G679	A607	U	U	G376	G291
G1395	U1323	G1149	U1071	A997	U852	U924	G924	A848	G680	A608	U	U	G383	A295
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A1399	U1241	U1154	A1075	A1002	U776	A933	G934	C852	G685	A614	U	U	A391	G300
G1400	G1242	C1155	U1078	A1003	U777	A934	G934	C853	U688	C614	U	U	A397	G301
A1401	A1245	G1157	A1079	A1004	A780	A935	U935	C854	G689	G617	U	U	A398	G302
C1402	G1246	U1158	A1080	G1006	G781	A936	G937	C855	A691	U620	U	U	A399	G303
A1406	G1246	A1159	U1081	A1006	U882	A937	U938	C856	G694	A621	U	U	G400	G304
A1407	G1250	C1160	U1082	G1010	U883	A938	U939	C857	U698	A622	U	U	U314	U314
G1408	A1251	G1161	G1083	A1011	G941	A939	U940	C858	U704	G546	U	U	C403	C315
G1409	A1252	U1162	A1084	U1014	U942	A940	U941	C859	U705	G547	U	U	G404	U316
C1412	U1253	A1163	A1085	U1015	U943	C944	U943	C860	U706	G548	U	U	U405	A317
G1413	C1254	G1164	C1086	C1016	U944	C945	U944	C861	A707	U549	U	U	A318	A318
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A1419	G1264	G1172	A1098	A1024	U949	U949	A952	C866	A712	U557	U	U	U410	U410
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G1421	G1266	G1174	A1099	A1026	U951	C949	A953	C868	U714	U559	U	U	G412	G412
U1425	A1273	C1175	A1103	A1027	U952	U950	C957	C869	U715	G560	U	U	U414	U414
C1426	G1281	U1176	G1104	U1028	U953	U951	C958	C870	A716	G564	U	U	G415	G415
A1428	G1281	G1177	G1113	G1029	U954	U952	C959	C871	U716	A417	U	U	A416	A416
G1429	U1284	U1178	U1114	C1032	U955	U953	U960	C872	U717	G567	U	U	A417	A417
U1430	C1285	A1179	G1115	C1033	U956	U954	U961	C873	U718	U643	U	U	G420	G420
G1431	A1286	A1180	G1116	U1033	A962	U955	C962	C874	U719	G644	U	U	A336	A336
C1432	U1293	U1181	G1117	U1034	G963	U956	A963	C875	U720	A645	U	U	G337	G337
A1433	A1294	A1182	G1117	G1035	U964	U957	A964	C876	U721	A646	U	U	A422	A422
G1434	A1364	C1183	U1121	A1036	U965	U958	A965	C877	G722	A647	U	U	A423	A423
G1435	A1365	C1187	U1122	U1042	U966	U959	A966	C878	U723	G648	U	U	G340	G340
A1436	A1366	C1187	U1123	C1043	U967	U960	A967	C879	G726	A649	U	U	G341	G341
G1437	A1366	C1187	U1123	C1043	U968	U961	A968	C880	U726	G650	U	U	A426	A426
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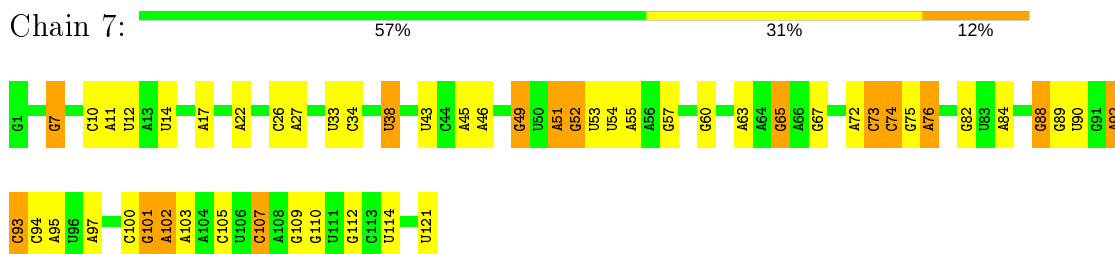




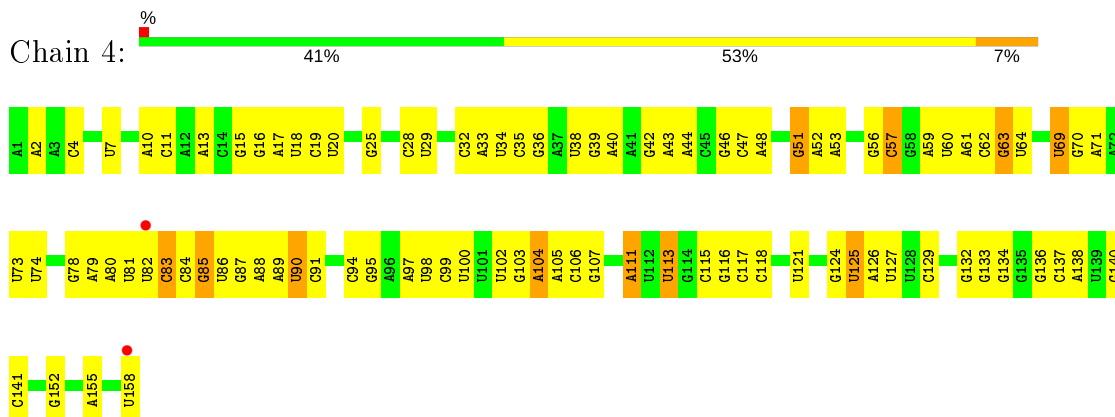
● Molecule 37: 5S ribosomal RNA



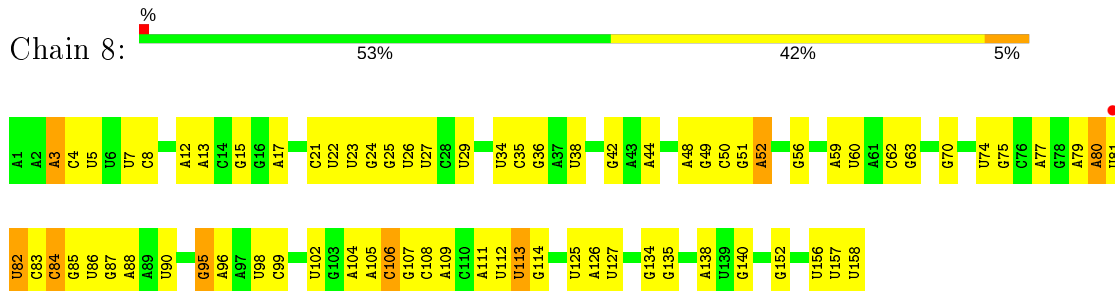
- Molecule 37: 5S ribosomal RNA



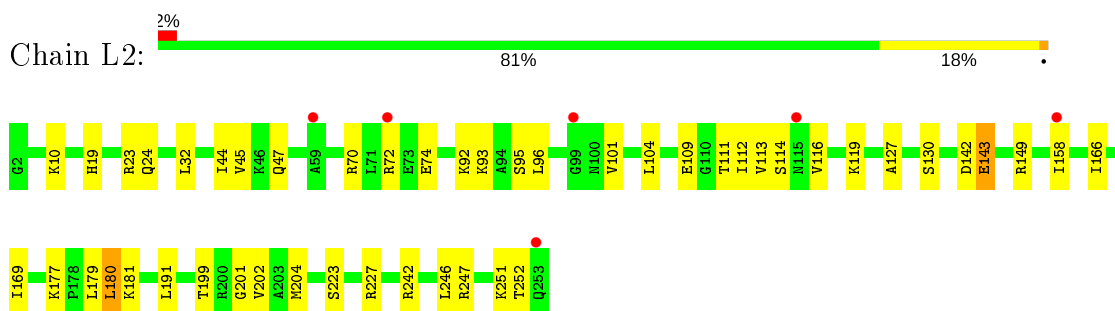
- Molecule 38: 5.8S ribosomal RNA



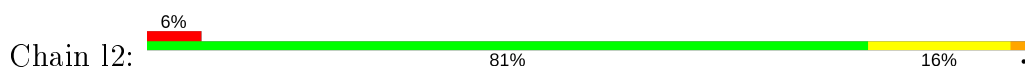
- Molecule 38: 5.8S ribosomal RNA

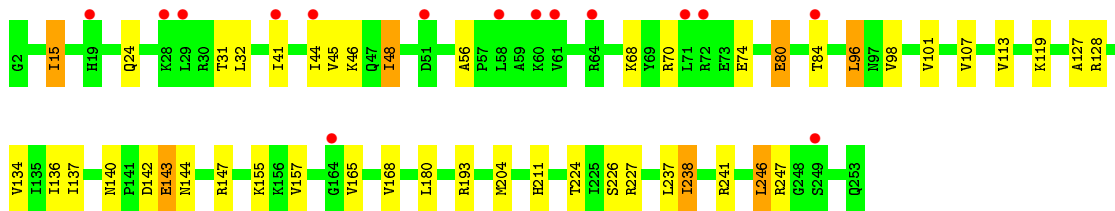


- Molecule 39: 60S ribosomal protein L2-A

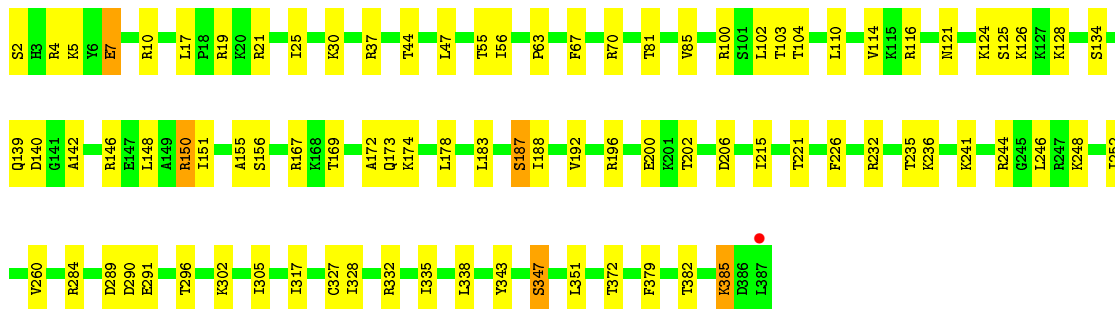
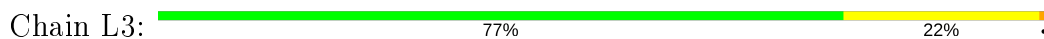


- Molecule 39: 60S ribosomal protein L2-A

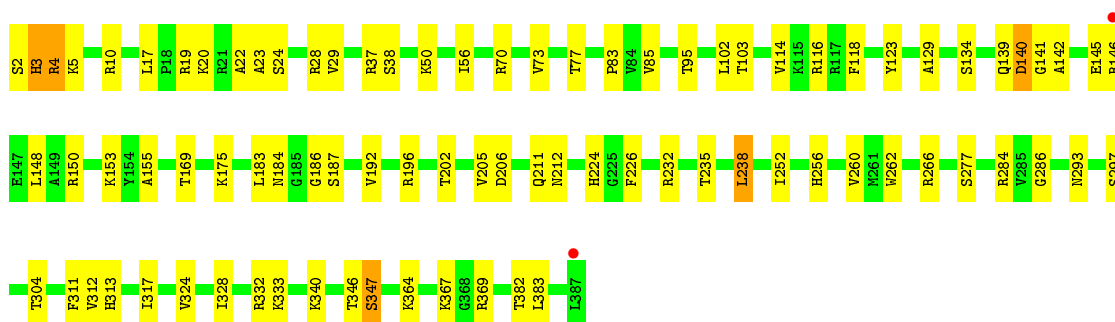
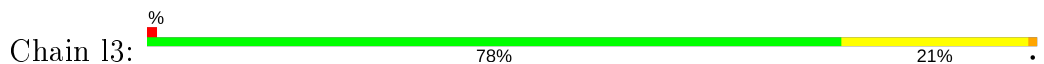




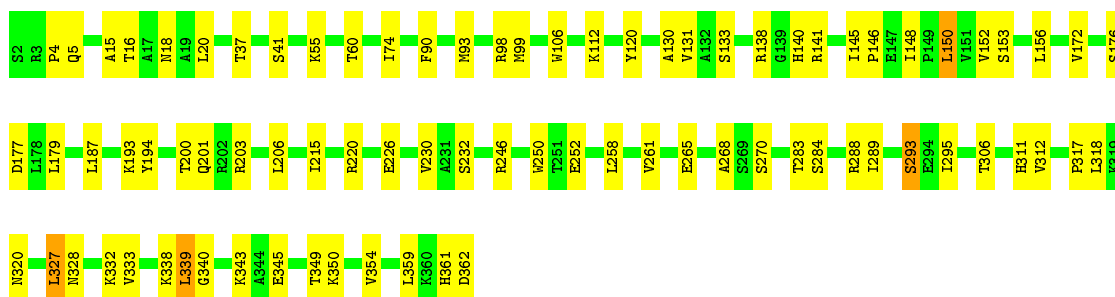
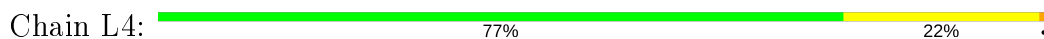
• Molecule 40: 60S ribosomal protein L3




• Molecule 40: 60S ribosomal protein L3

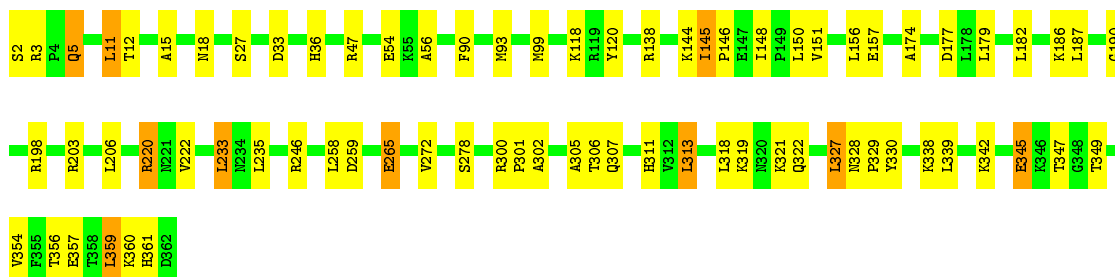


• Molecule 41: 60S ribosomal protein L4-A




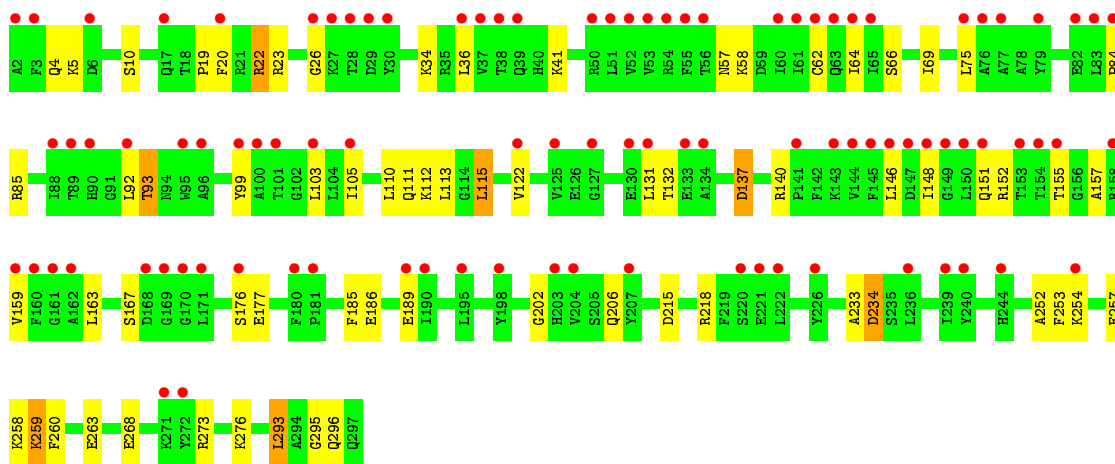
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:  79% 18%




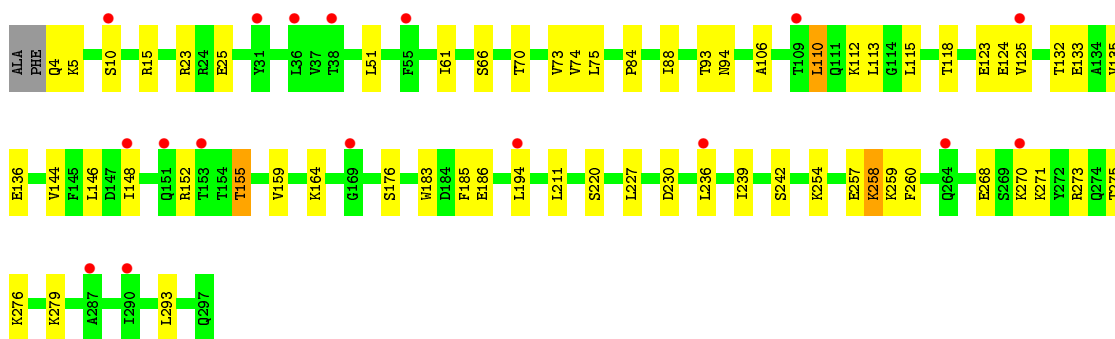
• Molecule 42: 60S ribosomal protein L5

Chain L5:  32% 77% 21%




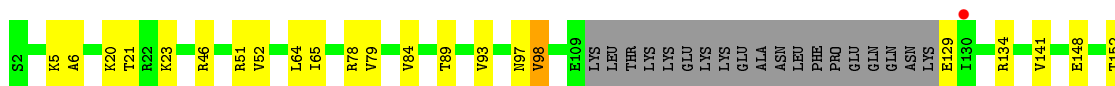
• Molecule 42: 60S ribosomal protein L5

Chain L5:  6% 78% 20%



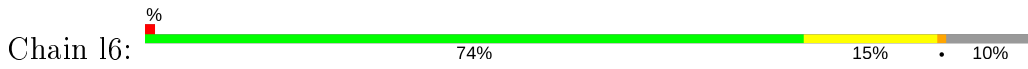
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:  75% 13% 11%

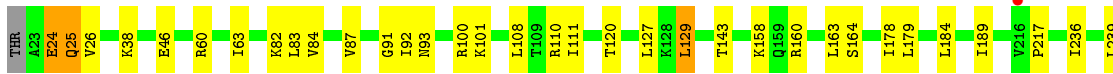
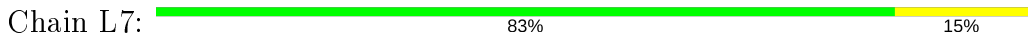




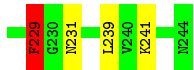
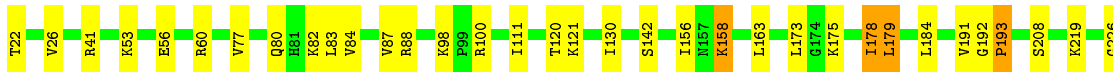
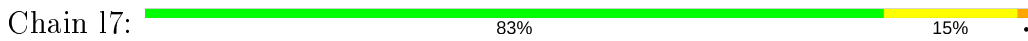
- Molecule 43: 60S ribosomal protein L6-A



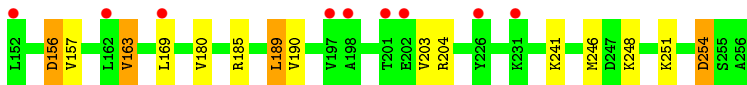
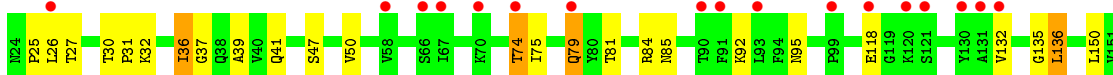
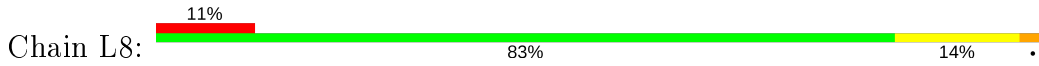
- Molecule 44: 60S ribosomal protein L7-A



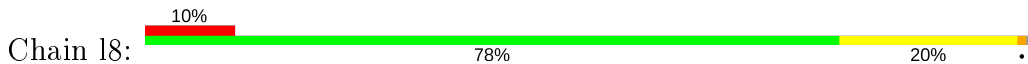
- Molecule 44: 60S ribosomal protein L7-A

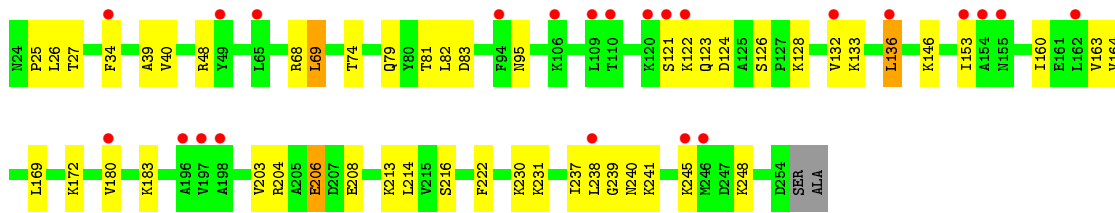


- Molecule 45: 60S ribosomal protein L8-A

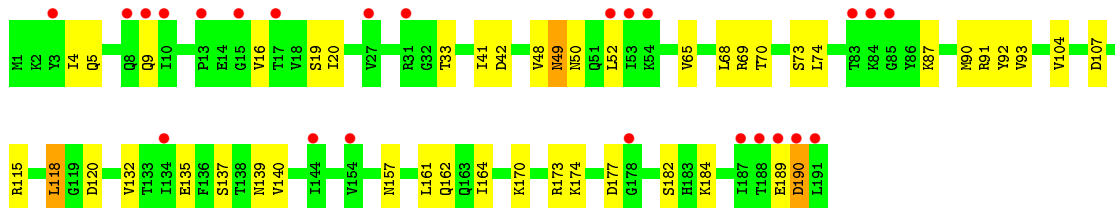
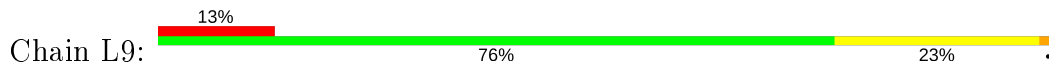


- Molecule 45: 60S ribosomal protein L8-A

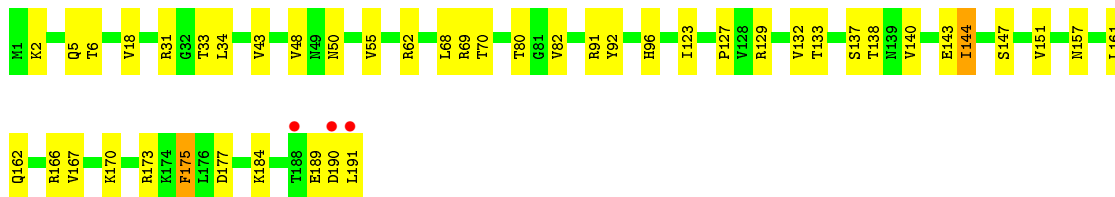
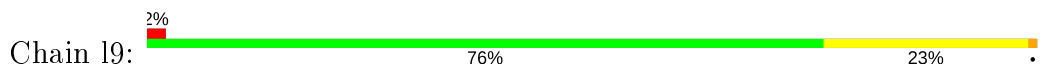




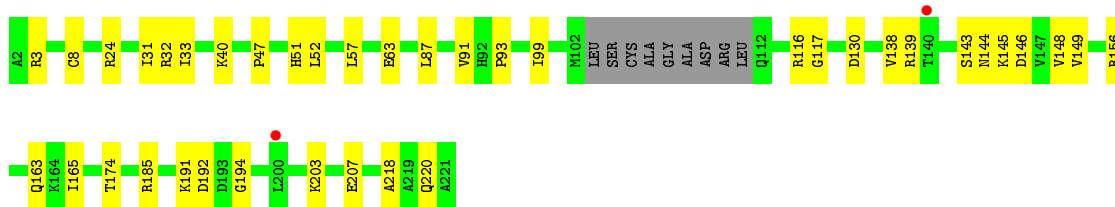
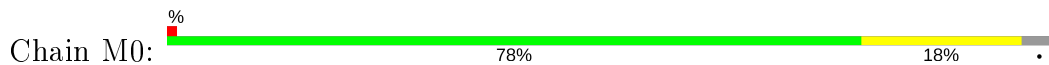
• Molecule 46: 60S ribosomal protein L9-A



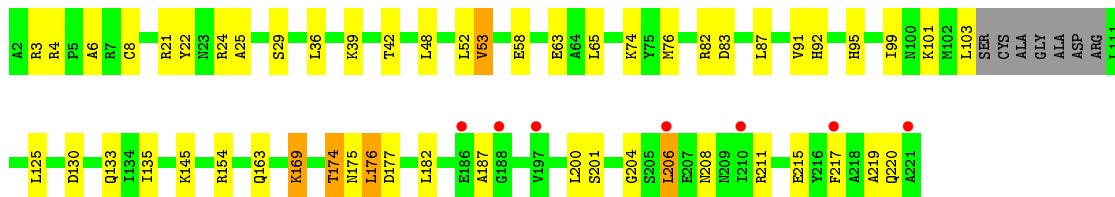
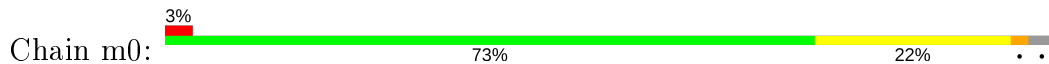
• Molecule 46: 60S ribosomal protein L9-A



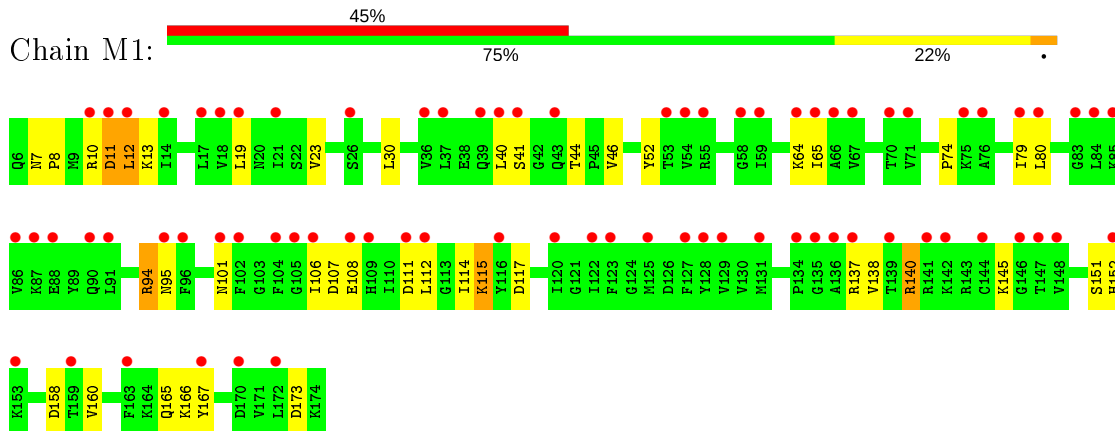
• Molecule 47: 60S ribosomal protein L10



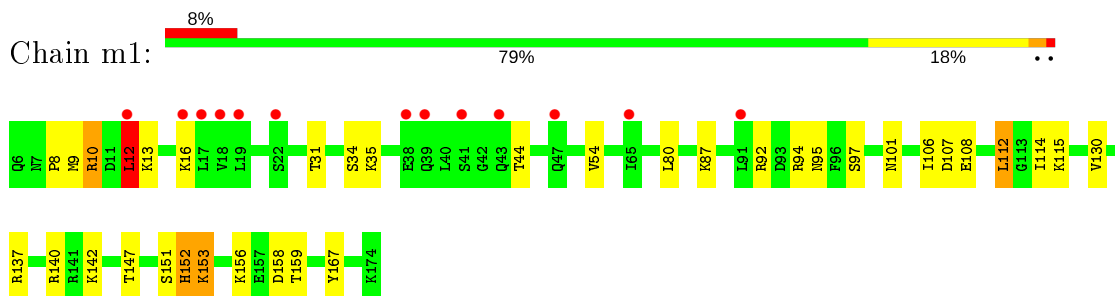
• Molecule 47: 60S ribosomal protein L10



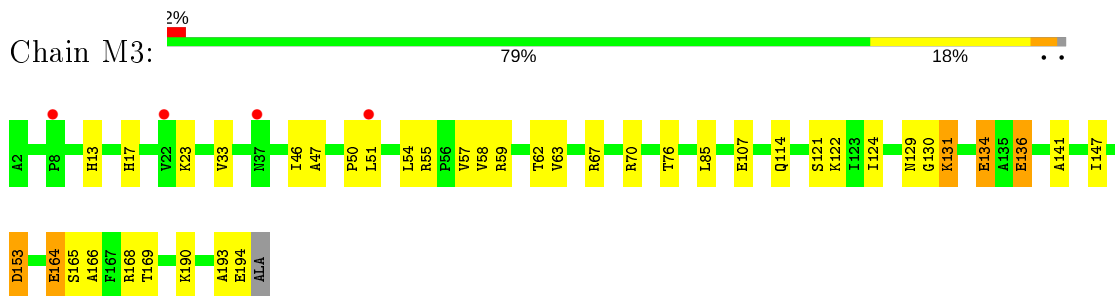
- Molecule 48: 60S ribosomal protein L11-B



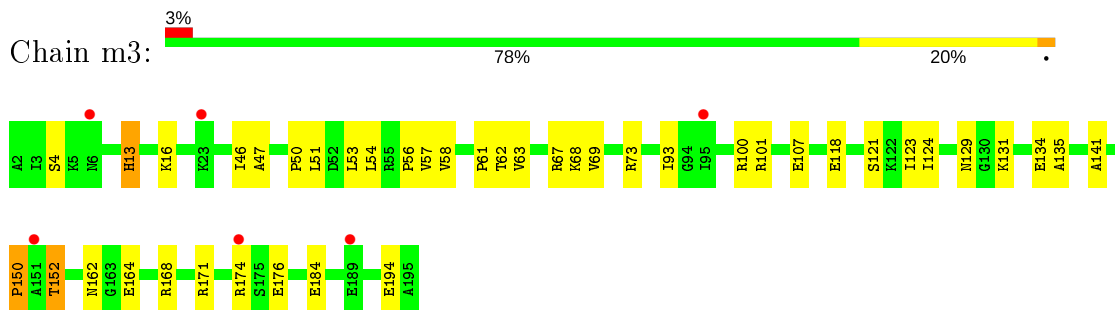
- Molecule 48: 60S ribosomal protein L11-B



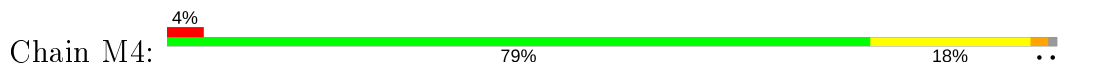
- Molecule 49: 60S ribosomal protein L13-A



- Molecule 49: 60S ribosomal protein L13-A

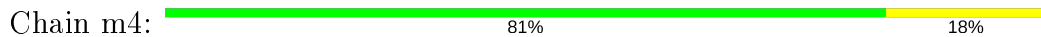


- Molecule 50: 60S ribosomal protein L14-A

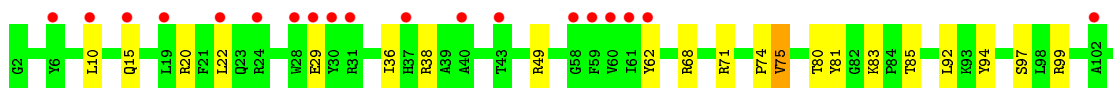
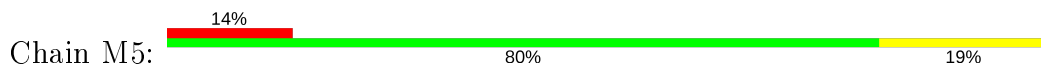




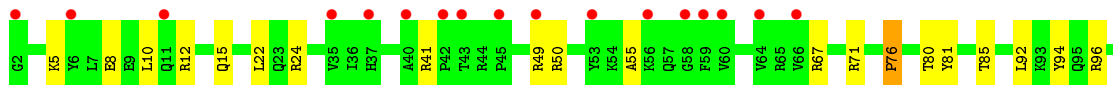
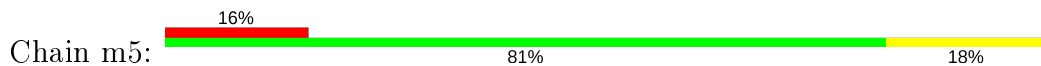
- Molecule 50: 60S ribosomal protein L14-A



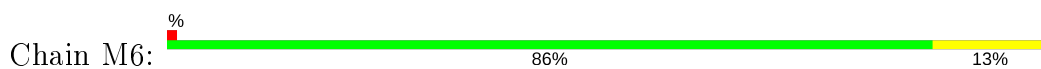
- Molecule 51: 60S ribosomal protein L15-A



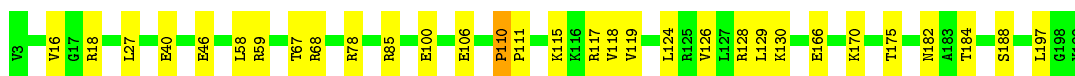
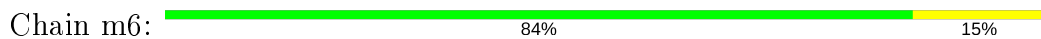
- Molecule 51: 60S ribosomal protein L15-A



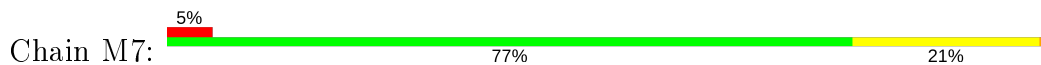
- Molecule 52: 60S ribosomal protein L16-A

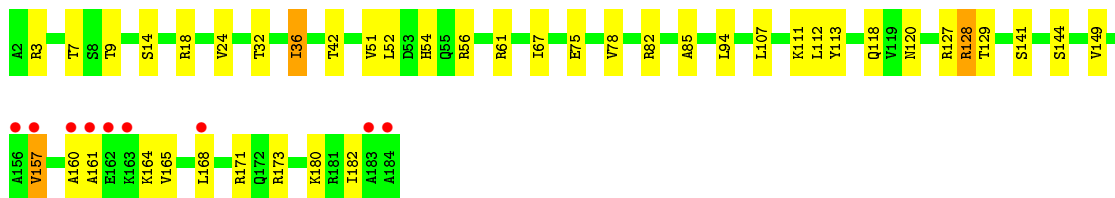


- Molecule 52: 60S ribosomal protein L16-A

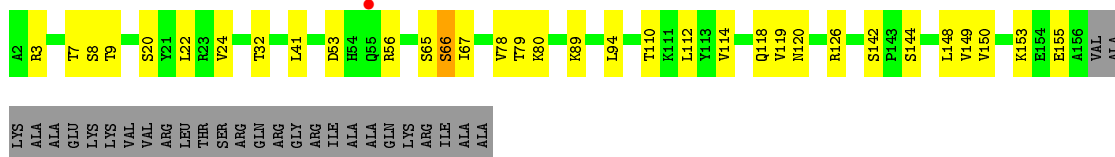


- Molecule 53: 60S ribosomal protein L17-A

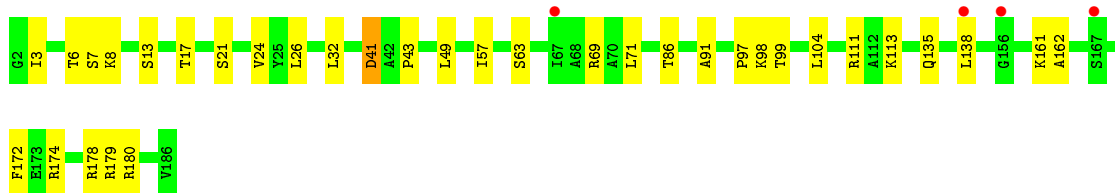
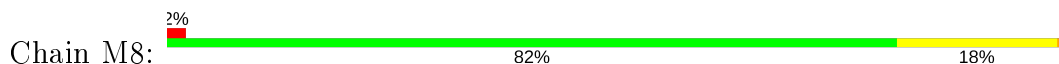




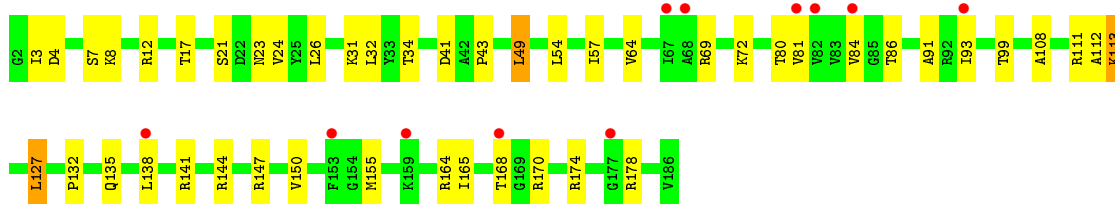
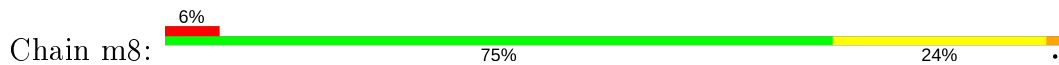
- Molecule 53: 60S ribosomal protein L17-A



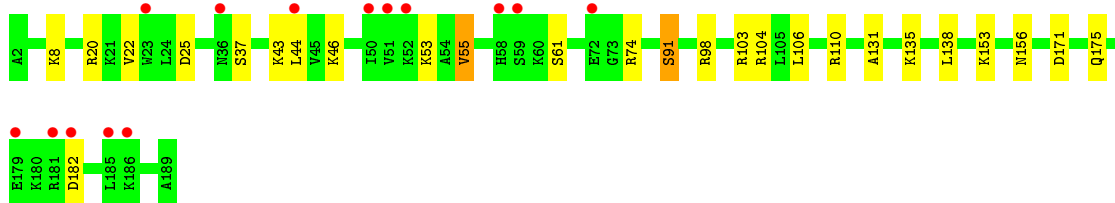
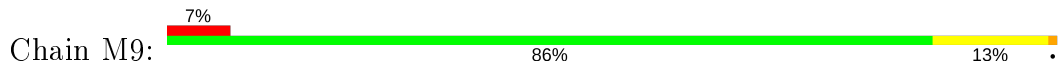
- Molecule 54: 60S ribosomal protein L18-A



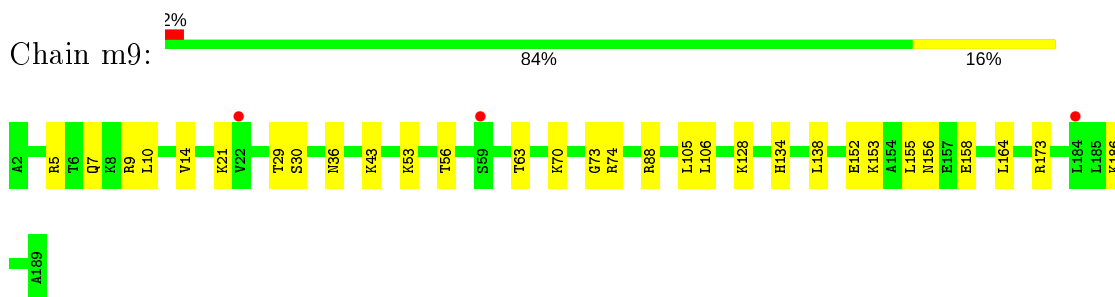
- Molecule 54: 60S ribosomal protein L18-A



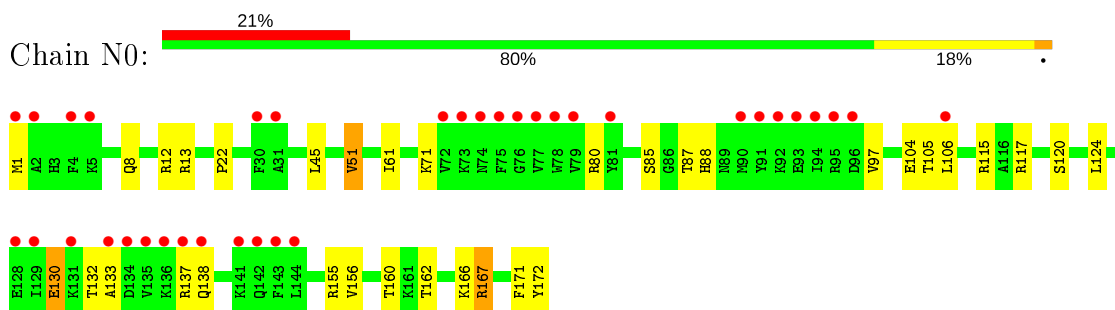
- Molecule 55: 60S ribosomal protein L19-A



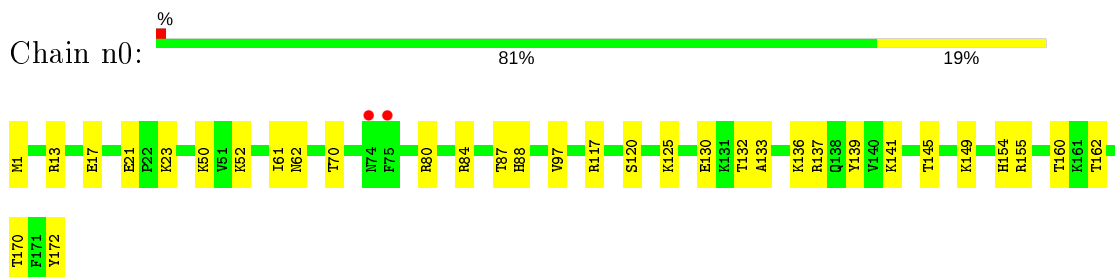
- Molecule 55: 60S ribosomal protein L19-A



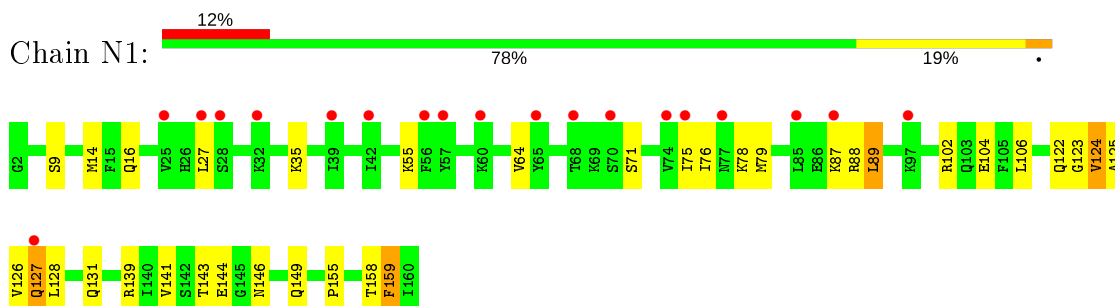
- Molecule 56: 60S ribosomal protein L20-A



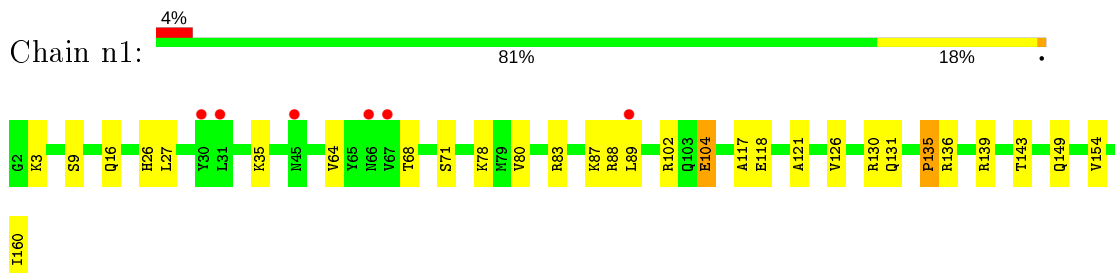
- Molecule 56: 60S ribosomal protein L20-A



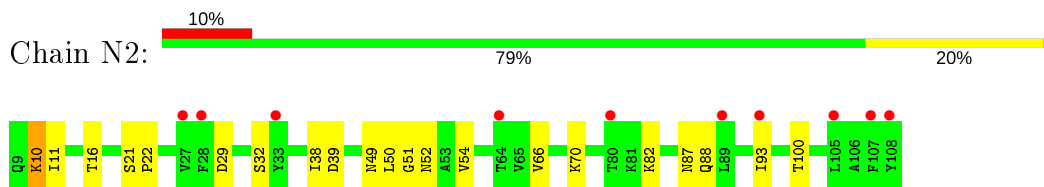
- Molecule 57: 60S ribosomal protein L21-A



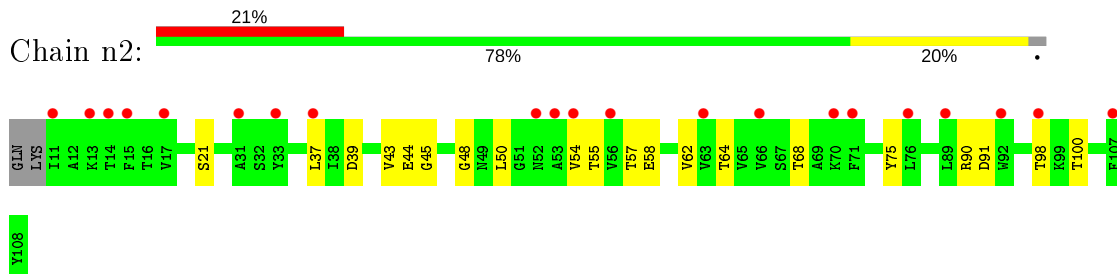
- Molecule 57: 60S ribosomal protein L21-A



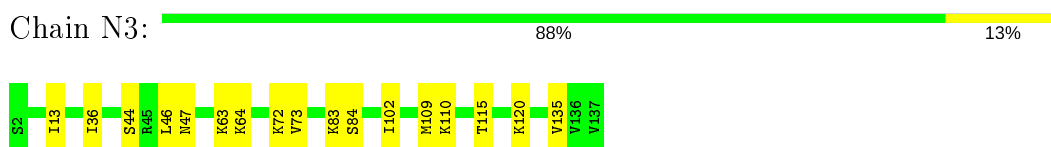
• Molecule 58: 60S ribosomal protein L22-A



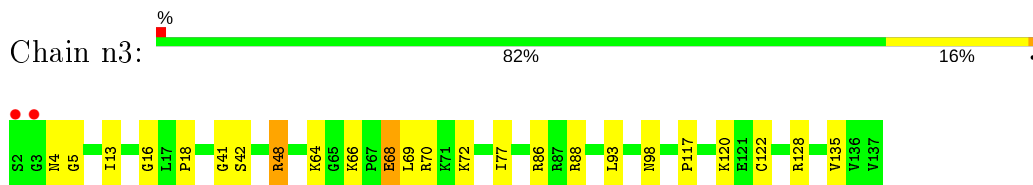
• Molecule 58: 60S ribosomal protein L22-A



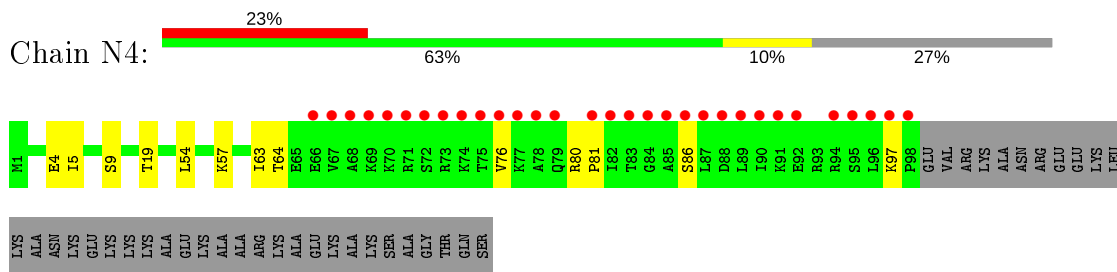
• Molecule 59: 60S ribosomal protein L23-A



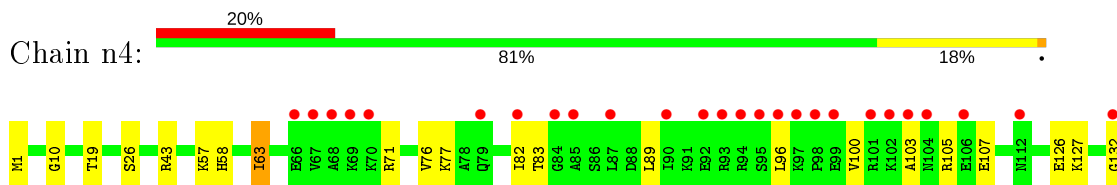
• Molecule 59: 60S ribosomal protein L23-A



• Molecule 60: 60S ribosomal protein L24-A

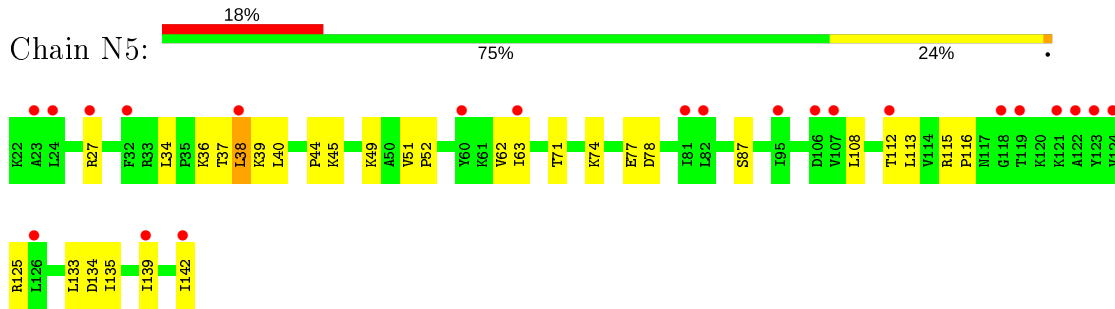


• Molecule 60: 60S ribosomal protein L24-A

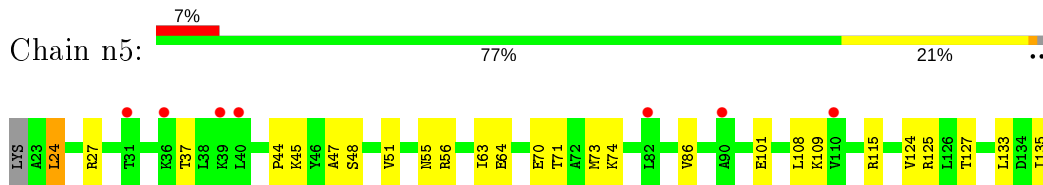


T133
Q134
S135

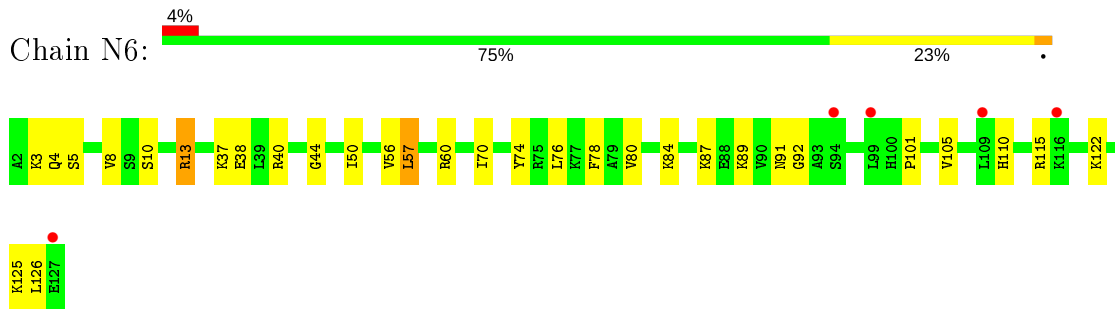
- Molecule 61: 60S ribosomal protein L25



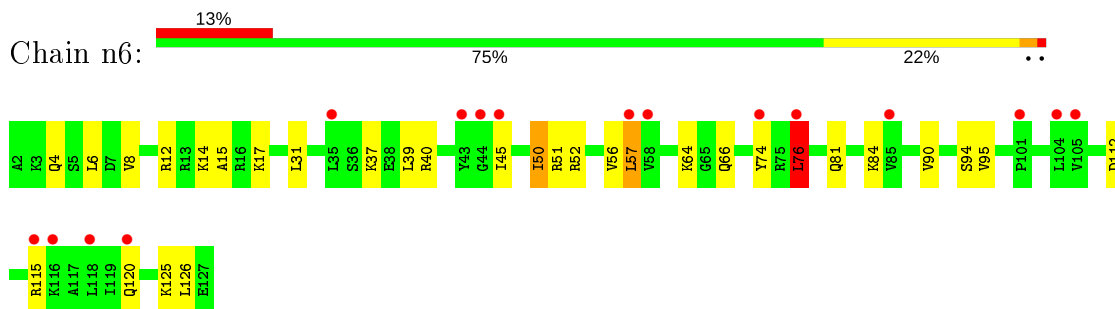
- Molecule 61: 60S ribosomal protein L25



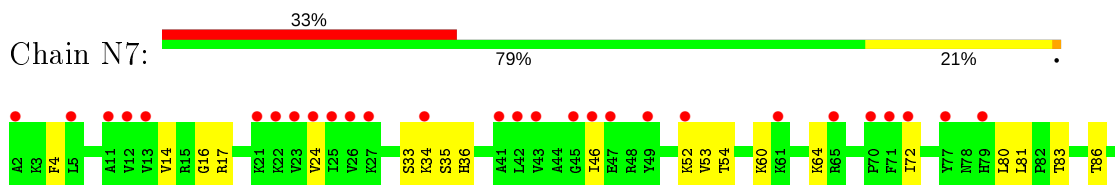
- Molecule 62: 60S ribosomal protein L26-A

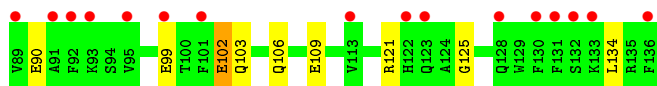


- Molecule 62: 60S ribosomal protein L26-A

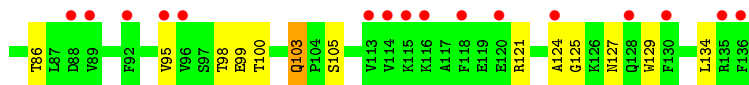
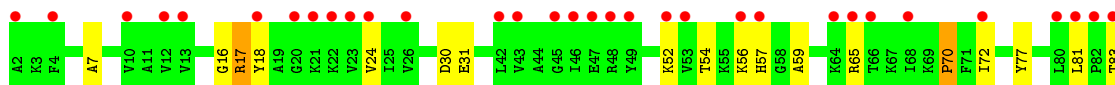
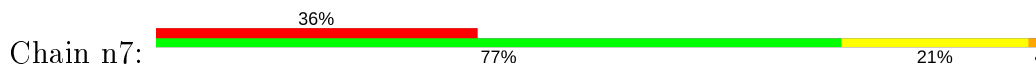


- Molecule 63: 60S ribosomal protein L27-A

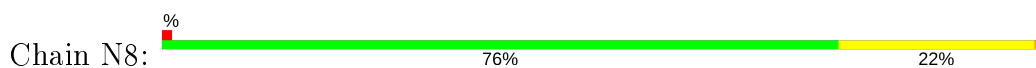




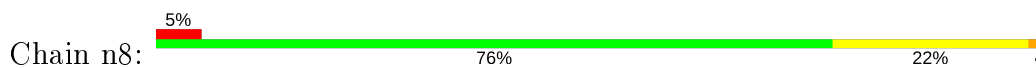
- Molecule 63: 60S ribosomal protein L27-A



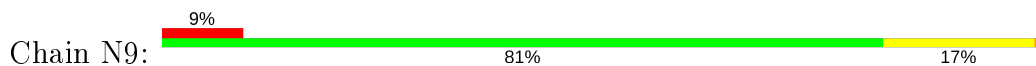
- Molecule 64: 60S ribosomal protein L28



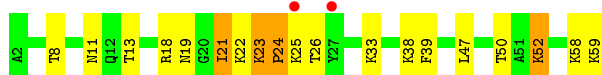
- Molecule 64: 60S ribosomal protein L28



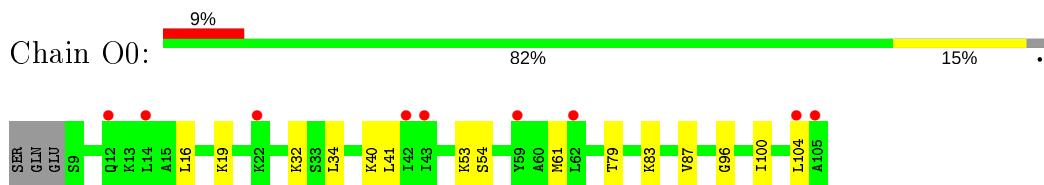
- Molecule 65: 60S ribosomal protein L29



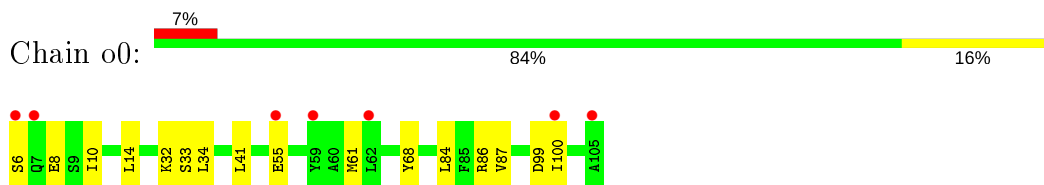
- Molecule 65: 60S ribosomal protein L29



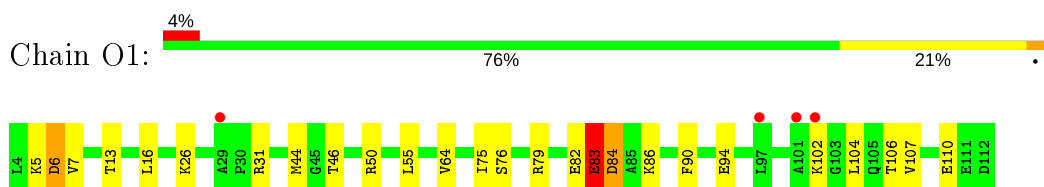
- Molecule 66: 60S ribosomal protein L30



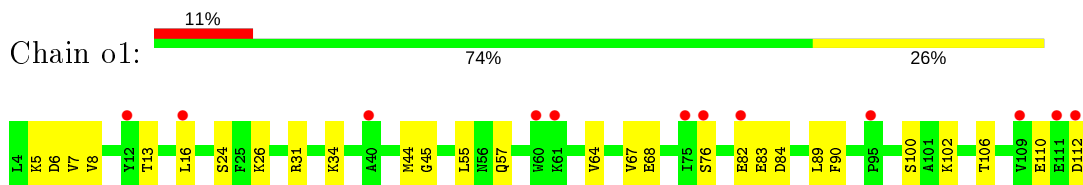
- Molecule 66: 60S ribosomal protein L30



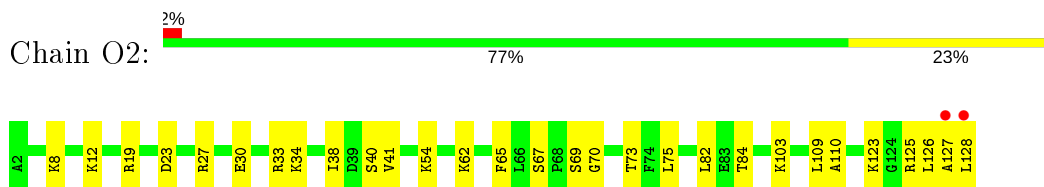
- Molecule 67: 60S ribosomal protein L31-A



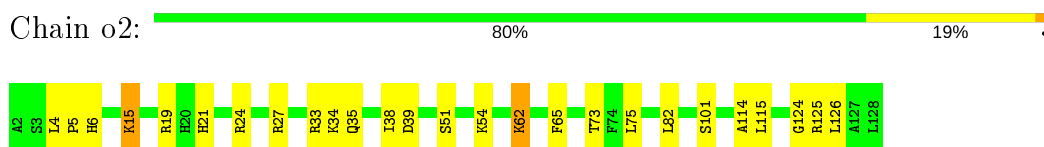
- Molecule 67: 60S ribosomal protein L31-A



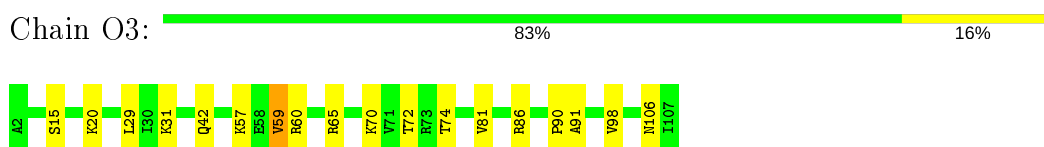
- Molecule 68: 60S ribosomal protein L32




- Molecule 68: 60S ribosomal protein L32

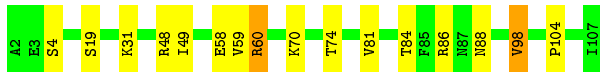


- Molecule 69: 60S ribosomal protein L33-A




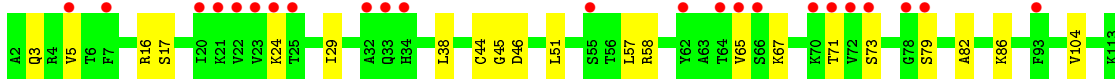
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:  85% 13%




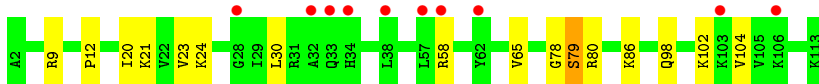
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:  21% 81% 19%




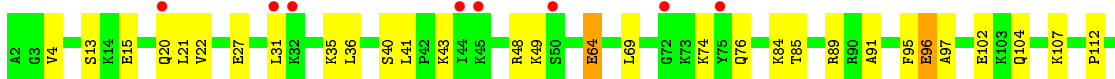
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:  9% 86% 13%




- Molecule 71: 60S ribosomal protein L35-A

Chain O5:  8% 74% 24%




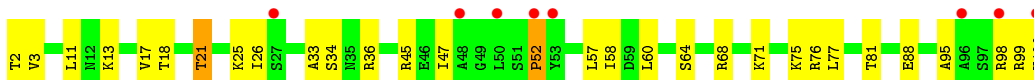
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:  2% 82% 14%

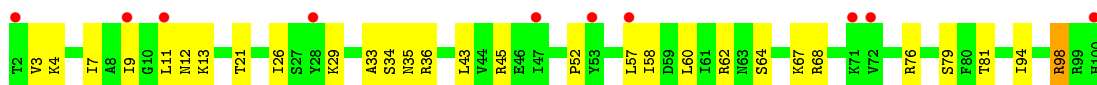


- Molecule 72: 60S ribosomal protein L36-A

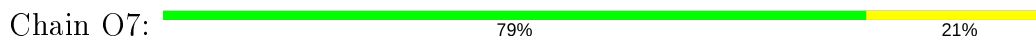
Chain O6:  8% 70% 28%



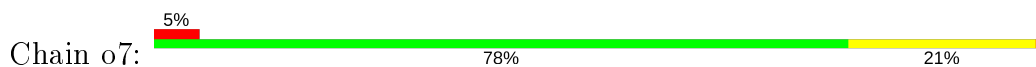
- Molecule 72: 60S ribosomal protein L36-A



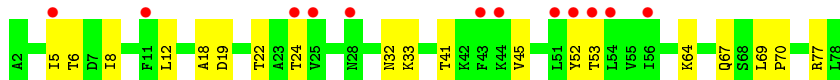
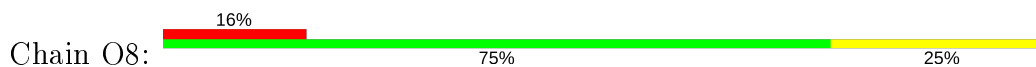
- Molecule 73: 60S ribosomal protein L37-A



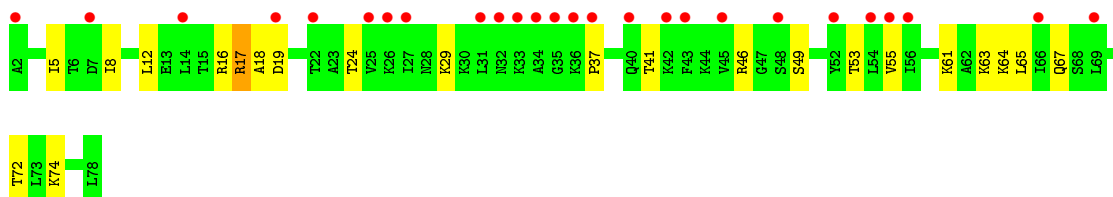
- Molecule 73: 60S ribosomal protein L37-A



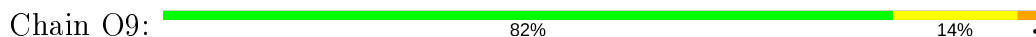
- Molecule 74: 60S ribosomal protein L38



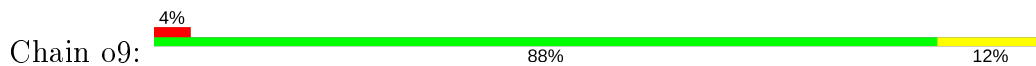
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39

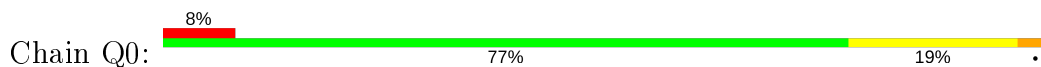


- Molecule 75: 60S ribosomal protein L39

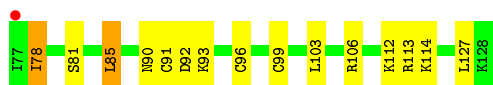




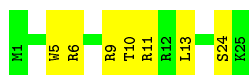
- Molecule 76: Ubiquitin-60S ribosomal protein L40



- Molecule 76: Ubiquitin-60S ribosomal protein L40



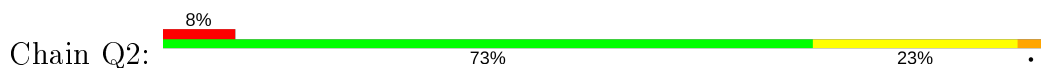
- Molecule 77: 60S ribosomal protein L41-A



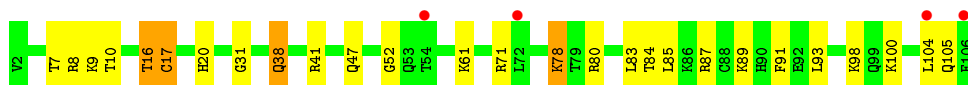
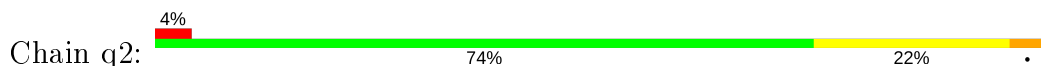
- Molecule 77: 60S ribosomal protein L41-A



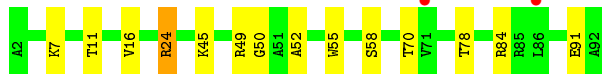
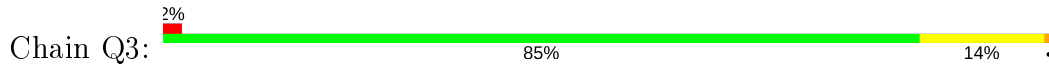
- Molecule 78: 60S ribosomal protein L42-A



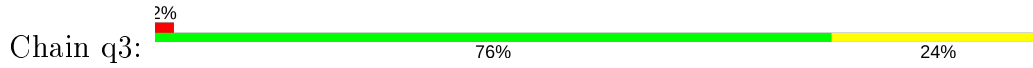
- Molecule 78: 60S ribosomal protein L42-A



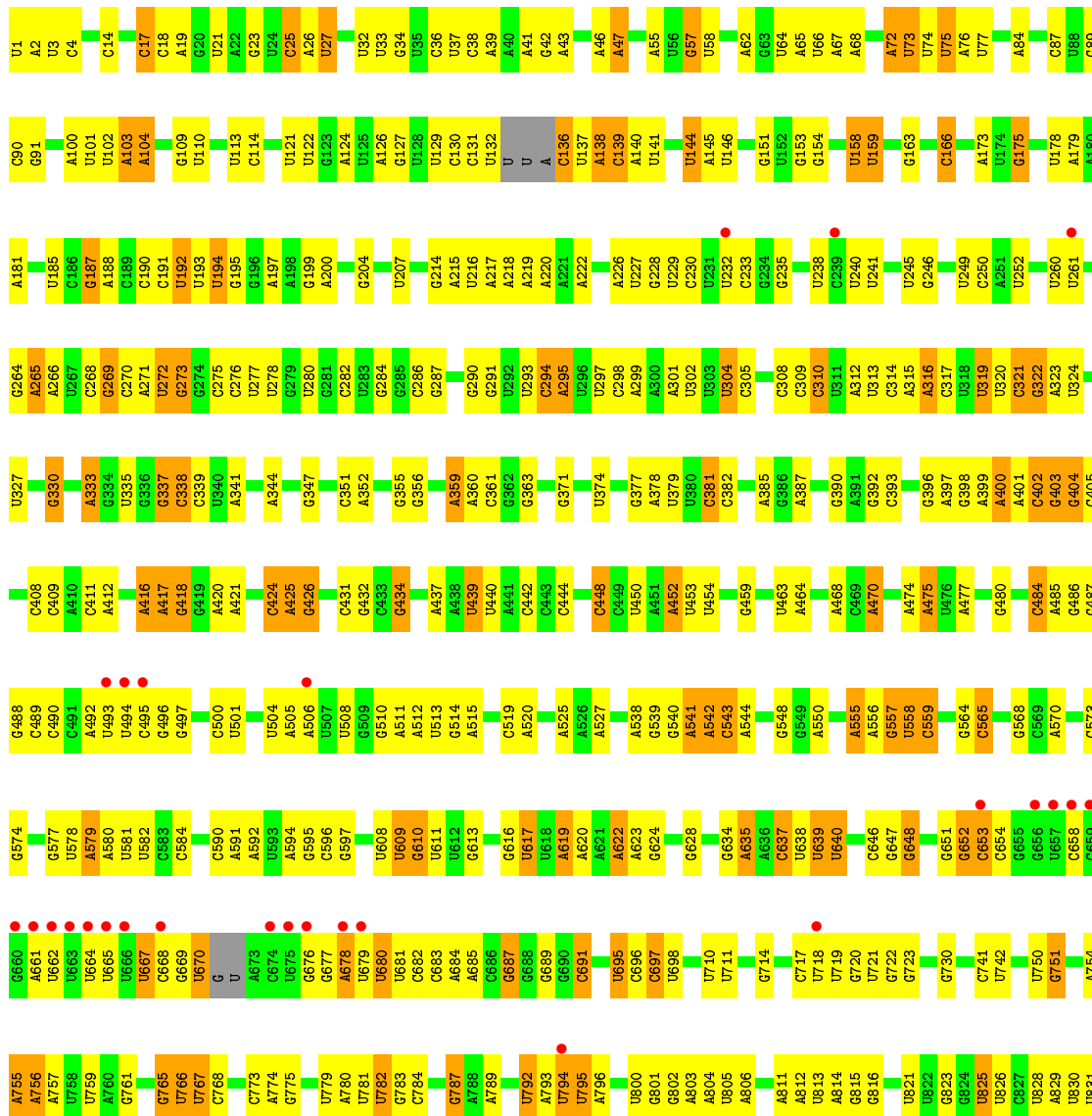
- Molecule 79: 60S ribosomal protein L43-A

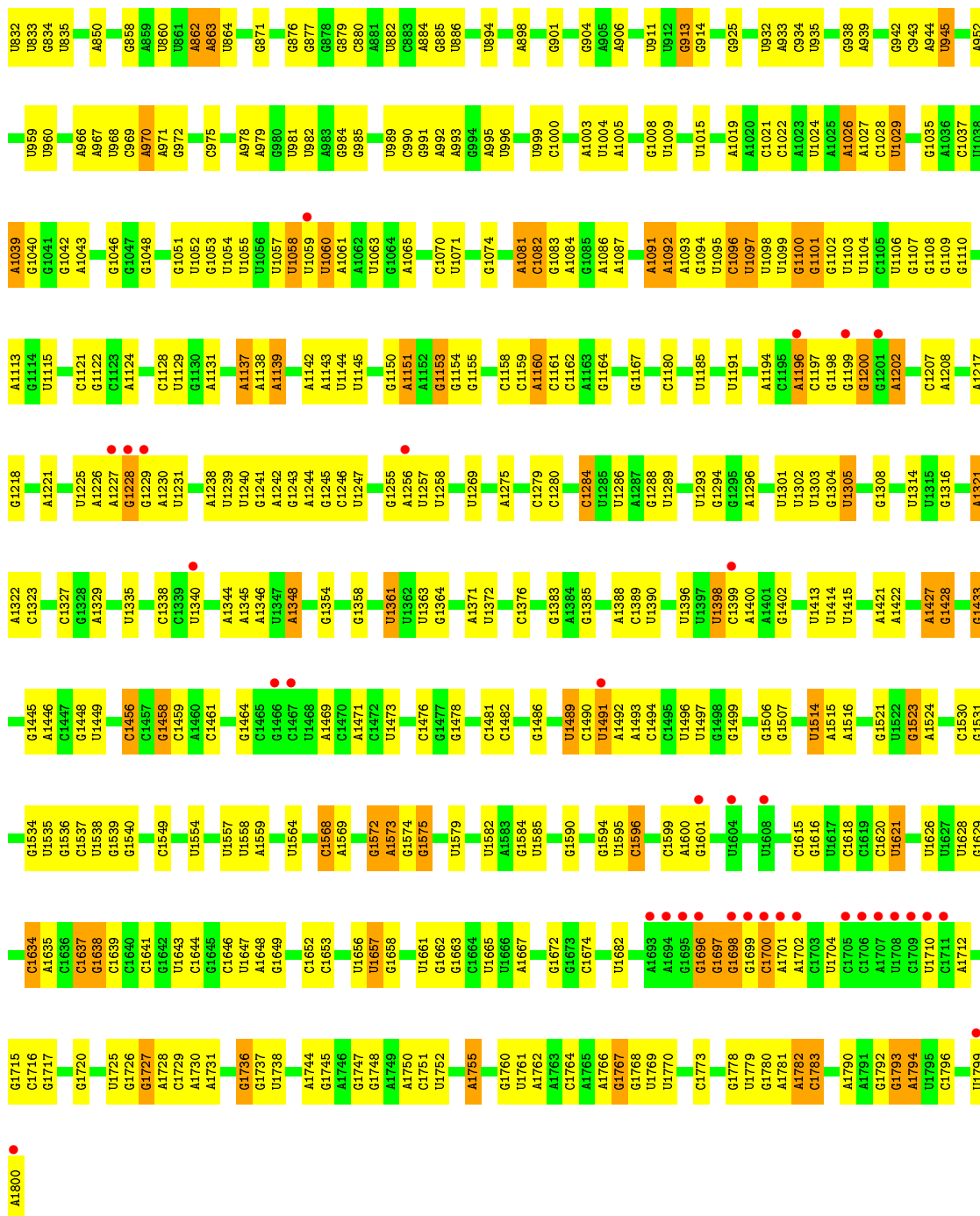


• Molecule 79: 60S ribosomal protein L43-A

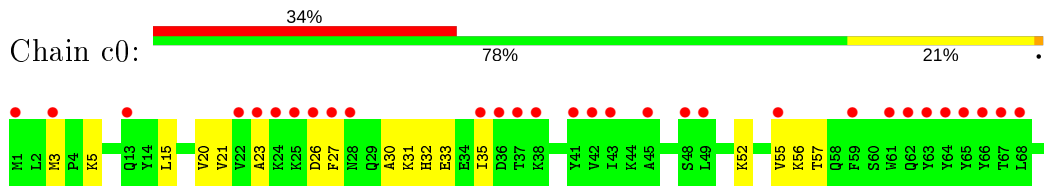


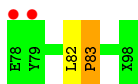
• Molecule 80: 18S ribosomal RNA



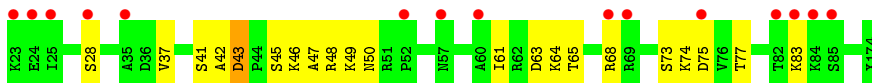
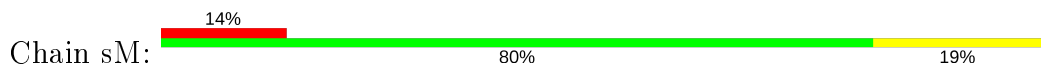


● Molecule 81: 40S ribosomal protein S10-A, 40S ribosomal protein S10-A, 40S Ribosomal Protein S10-A





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

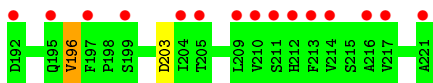
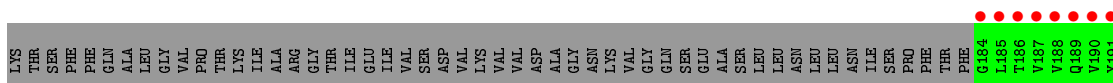
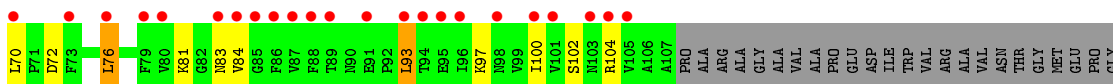
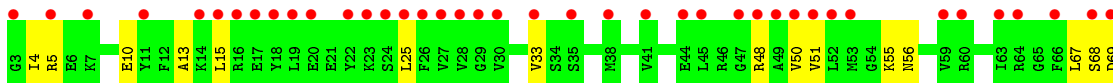
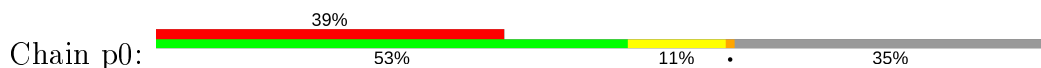


- Molecule 83: 60S Ribosomal Protein L12



There are no outlier residues recorded for this chain.

- Molecule 84: 60S acidic ribosomal protein P0



- Molecule 85: 60S Ribosomal Protein P1/2



There are no outlier residues recorded for this chain.

- Molecule 85: 60S Ribosomal Protein P1/2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.45Å 288.14Å 304.16Å 90.00° 99.11° 90.00°	Depositor
Resolution (Å)	149.31 – 3.30 149.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.3 (149.31-3.30) 92.3 (149.31-3.30)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.211 , 0.265 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	414270	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality 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, 8AN

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

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	S1	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	2
19	C7	0	2
19	c7	0	1
22	d0	0	1
24	d2	0	1
25	D3	0	1
27	D5	0	2
27	d5	0	1
28	D6	0	3
33	E1	0	3
33	e1	0	1
39	L2	0	1
39	l2	0	3
40	L3	0	1
40	l3	0	1
41	l4	0	1
42	L5	0	2
42	l5	0	2
43	L6	0	1
44	l7	0	2
45	L8	0	1
47	M0	0	1
48	m1	0	1
49	m3	0	1
50	m4	0	1
52	M6	0	1
52	m6	0	1
53	M7	0	1
53	m7	0	1
55	m9	0	1
56	N0	0	2
56	n0	0	2
59	n3	0	2

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

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

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

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

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

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
19	C7	22	PRO	Peptide
3	S1	131	ASP	Peptide
9	S7	131	PHE	Peptide
10	S8	8	ARG	Peptide

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	C1	153/155 (99%)	128 (84%)	18 (12%)	7 (5%)	2	15
13	c1	144/155 (93%)	114 (79%)	19 (13%)	11 (8%)	1	6
14	C2	122/124 (98%)	73 (60%)	27 (22%)	22 (18%)	0	1
14	c2	122/124 (98%)	70 (57%)	31 (25%)	21 (17%)	0	1
15	C3	148/150 (99%)	120 (81%)	23 (16%)	5 (3%)	3	22
15	c3	148/150 (99%)	115 (78%)	20 (14%)	13 (9%)	1	5
16	C4	125/128 (98%)	97 (78%)	16 (13%)	12 (10%)	0	4
16	c4	126/128 (98%)	98 (78%)	20 (16%)	8 (6%)	1	9
17	C5	122/135 (90%)	90 (74%)	18 (15%)	14 (12%)	0	2
17	c5	133/135 (98%)	100 (75%)	13 (10%)	20 (15%)	0	1
18	C6	139/142 (98%)	115 (83%)	18 (13%)	6 (4%)	2	16
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	1	11
19	C7	116/125 (93%)	90 (78%)	18 (16%)	8 (7%)	1	8
19	c7	113/125 (90%)	92 (81%)	11 (10%)	10 (9%)	1	5
20	C8	143/145 (99%)	109 (76%)	25 (18%)	9 (6%)	1	9
20	c8	143/145 (99%)	120 (84%)	15 (10%)	8 (6%)	2	11
21	C9	141/143 (99%)	114 (81%)	19 (14%)	8 (6%)	1	11
21	c9	141/143 (99%)	120 (85%)	15 (11%)	6 (4%)	2	16
22	D0	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	14
22	d0	108/110 (98%)	82 (76%)	14 (13%)	12 (11%)	0	2
23	D1	85/87 (98%)	65 (76%)	11 (13%)	9 (11%)	0	3
23	d1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	1	7
24	D2	127/129 (98%)	102 (80%)	21 (16%)	4 (3%)	4	23
24	d2	127/129 (98%)	100 (79%)	25 (20%)	2 (2%)	9	36
25	D3	142/144 (99%)	109 (77%)	22 (16%)	11 (8%)	1	6
25	d3	142/144 (99%)	119 (84%)	20 (14%)	3 (2%)	7	31
26	D4	132/134 (98%)	108 (82%)	16 (12%)	8 (6%)	1	10
26	d4	132/134 (98%)	100 (76%)	19 (14%)	13 (10%)	0	3
27	D5	68/70 (97%)	49 (72%)	11 (16%)	8 (12%)	0	2
27	d5	67/70 (96%)	51 (76%)	13 (19%)	3 (4%)	2	15
28	D6	95/97 (98%)	62 (65%)	18 (19%)	15 (16%)	0	1

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	m0	209/220 (95%)	164 (78%)	30 (14%)	15 (7%)	1	7
48	M1	167/169 (99%)	132 (79%)	16 (10%)	19 (11%)	0	2
48	m1	167/169 (99%)	137 (82%)	18 (11%)	12 (7%)	1	7
49	M3	191/194 (98%)	148 (78%)	28 (15%)	15 (8%)	1	6
49	m3	192/194 (99%)	153 (80%)	26 (14%)	13 (7%)	1	8
50	M4	134/137 (98%)	109 (81%)	14 (10%)	11 (8%)	1	5
50	m4	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	10	38
51	M5	201/203 (99%)	171 (85%)	21 (10%)	9 (4%)	2	15
51	m5	201/203 (99%)	169 (84%)	26 (13%)	6 (3%)	4	24
52	M6	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	15	46
52	m6	195/197 (99%)	179 (92%)	13 (7%)	3 (2%)	10	38
53	M7	181/183 (99%)	144 (80%)	26 (14%)	11 (6%)	1	10
53	m7	153/183 (84%)	127 (83%)	24 (16%)	2 (1%)	12	40
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	4	22
54	m8	183/185 (99%)	151 (82%)	18 (10%)	14 (8%)	1	6
55	M9	186/188 (99%)	159 (86%)	23 (12%)	4 (2%)	6	30
55	m9	186/188 (99%)	165 (89%)	20 (11%)	1 (0%)	29	61
56	N0	170/172 (99%)	149 (88%)	16 (9%)	5 (3%)	4	24
56	n0	170/172 (99%)	150 (88%)	17 (10%)	3 (2%)	8	35
57	N1	157/159 (99%)	133 (85%)	16 (10%)	8 (5%)	2	13
57	n1	157/159 (99%)	132 (84%)	21 (13%)	4 (2%)	5	27
58	N2	98/100 (98%)	70 (71%)	23 (24%)	5 (5%)	2	13
58	n2	96/100 (96%)	82 (85%)	10 (10%)	4 (4%)	3	17
59	N3	134/136 (98%)	118 (88%)	14 (10%)	2 (2%)	10	38
59	n3	134/136 (98%)	120 (90%)	9 (7%)	5 (4%)	3	20
60	N4	96/135 (71%)	73 (76%)	17 (18%)	6 (6%)	1	9
60	n4	133/135 (98%)	103 (77%)	19 (14%)	11 (8%)	1	5
61	N5	119/121 (98%)	99 (83%)	14 (12%)	6 (5%)	2	14
61	n5	118/121 (98%)	103 (87%)	9 (8%)	6 (5%)	2	13
62	N6	124/126 (98%)	100 (81%)	19 (15%)	5 (4%)	3	18
62	n6	124/126 (98%)	108 (87%)	7 (6%)	9 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	N7	133/135 (98%)	109 (82%)	16 (12%)	8 (6%)	1	10
63	n7	133/135 (98%)	105 (79%)	16 (12%)	12 (9%)	1	4
64	N8	146/148 (99%)	109 (75%)	28 (19%)	9 (6%)	1	10
64	n8	146/148 (99%)	114 (78%)	22 (15%)	10 (7%)	1	8
65	N9	56/58 (97%)	44 (79%)	10 (18%)	2 (4%)	3	20
65	n9	56/58 (97%)	37 (66%)	11 (20%)	8 (14%)	0	1
66	O0	95/100 (95%)	85 (90%)	8 (8%)	2 (2%)	7	31
66	o0	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	7	32
67	O1	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	2	14
67	o1	107/109 (98%)	91 (85%)	11 (10%)	5 (5%)	2	14
68	O2	125/127 (98%)	94 (75%)	22 (18%)	9 (7%)	1	7
68	o2	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	14
69	O3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	4	24
69	o3	104/106 (98%)	92 (88%)	6 (6%)	6 (6%)	1	11
70	O4	110/112 (98%)	94 (86%)	12 (11%)	4 (4%)	3	20
70	o4	110/112 (98%)	91 (83%)	16 (14%)	3 (3%)	5	26
71	O5	117/119 (98%)	98 (84%)	11 (9%)	8 (7%)	1	8
71	o5	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	3	22
72	O6	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	0	3
72	o6	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	5
73	O7	85/87 (98%)	67 (79%)	17 (20%)	1 (1%)	13	42
73	o7	85/87 (98%)	70 (82%)	12 (14%)	3 (4%)	3	21
74	O8	75/77 (97%)	61 (81%)	12 (16%)	2 (3%)	5	26
74	o8	75/77 (97%)	60 (80%)	9 (12%)	6 (8%)	1	6
75	O9	48/50 (96%)	39 (81%)	8 (17%)	1 (2%)	7	31
75	o9	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
76	Q0	50/52 (96%)	40 (80%)	8 (16%)	2 (4%)	3	18
76	q0	50/52 (96%)	41 (82%)	8 (16%)	1 (2%)	7	32
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	3 (13%)	1 (4%)	2	16
78	Q2	103/105 (98%)	79 (77%)	19 (18%)	5 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	q2	103/105 (98%)	90 (87%)	8 (8%)	5 (5%)	2	14
79	Q3	89/91 (98%)	76 (85%)	7 (8%)	6 (7%)	1	8
79	q3	89/91 (98%)	78 (88%)	8 (9%)	3 (3%)	3	22
81	c0	82/96 (85%)	63 (77%)	11 (13%)	8 (10%)	0	3
82	sM	61/104 (59%)	38 (62%)	15 (25%)	8 (13%)	0	1
84	p0	139/219 (64%)	115 (83%)	17 (12%)	7 (5%)	2	14
All	All	22262/22948 (97%)	17987 (81%)	2915 (13%)	1360 (6%)	1	10

5 of 1360 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [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%)	133 (81%)	31 (19%)	1	6
2	s0	165/173 (95%)	128 (78%)	37 (22%)	1	3
3	S1	191/192 (100%)	152 (80%)	39 (20%)	1	4
3	s1	192/192 (100%)	148 (77%)	44 (23%)	1	3
4	S2	176/176 (100%)	139 (79%)	37 (21%)	1	4
4	s2	176/176 (100%)	132 (75%)	44 (25%)	0	2
5	S3	182/182 (100%)	149 (82%)	33 (18%)	1	7
5	s3	182/182 (100%)	150 (82%)	32 (18%)	2	8
6	S4	221/221 (100%)	176 (80%)	45 (20%)	1	4
6	s4	221/221 (100%)	179 (81%)	42 (19%)	1	6

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	D1	74/74 (100%)	63 (85%)	11 (15%)	3	13
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	4
24	D2	110/110 (100%)	88 (80%)	22 (20%)	1	5
24	d2	110/110 (100%)	90 (82%)	20 (18%)	1	7
25	D3	119/119 (100%)	98 (82%)	21 (18%)	2	8
25	d3	119/119 (100%)	100 (84%)	19 (16%)	2	11
26	D4	112/112 (100%)	91 (81%)	21 (19%)	1	6
26	d4	112/112 (100%)	91 (81%)	21 (19%)	1	6
27	D5	61/61 (100%)	44 (72%)	17 (28%)	0	1
27	d5	61/61 (100%)	52 (85%)	9 (15%)	3	13
28	D6	83/83 (100%)	63 (76%)	20 (24%)	0	2
28	d6	83/83 (100%)	67 (81%)	16 (19%)	1	6
29	D7	70/70 (100%)	61 (87%)	9 (13%)	4	18
29	d7	70/70 (100%)	61 (87%)	9 (13%)	4	18
30	D8	56/56 (100%)	44 (79%)	12 (21%)	1	4
30	d8	56/56 (100%)	43 (77%)	13 (23%)	1	3
31	D9	47/47 (100%)	35 (74%)	12 (26%)	0	2
31	d9	47/47 (100%)	40 (85%)	7 (15%)	3	13
32	E0	51/53 (96%)	45 (88%)	6 (12%)	5	21
32	e0	53/53 (100%)	37 (70%)	16 (30%)	0	1
33	E1	62/66 (94%)	50 (81%)	12 (19%)	1	5
33	e1	66/66 (100%)	50 (76%)	16 (24%)	0	2
34	SR	259/261 (99%)	226 (87%)	33 (13%)	4	19
34	sR	260/261 (100%)	231 (89%)	29 (11%)	6	23
35	SM	97/107 (91%)	76 (78%)	21 (22%)	1	4
39	L2	193/194 (100%)	155 (80%)	38 (20%)	1	5
39	l2	192/194 (99%)	153 (80%)	39 (20%)	1	5
40	L3	319/322 (99%)	249 (78%)	70 (22%)	1	3
40	l3	321/322 (100%)	252 (78%)	69 (22%)	1	4
41	L4	288/288 (100%)	232 (81%)	56 (19%)	1	5
41	l4	288/288 (100%)	234 (81%)	54 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	L5	244/244 (100%)	198 (81%)	46 (19%)	1	6
42	l5	243/244 (100%)	189 (78%)	54 (22%)	1	3
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	13
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	8
44	L7	186/187 (100%)	160 (86%)	26 (14%)	3	16
44	l7	187/187 (100%)	155 (83%)	32 (17%)	2	9
45	L8	187/191 (98%)	157 (84%)	30 (16%)	2	11
45	l8	177/191 (93%)	142 (80%)	35 (20%)	1	5
46	L9	171/171 (100%)	130 (76%)	41 (24%)	0	2
46	l9	171/171 (100%)	132 (77%)	39 (23%)	1	3
47	M0	177/186 (95%)	151 (85%)	26 (15%)	3	14
47	m0	179/186 (96%)	138 (77%)	41 (23%)	1	3
48	M1	147/147 (100%)	119 (81%)	28 (19%)	1	6
48	m1	147/147 (100%)	120 (82%)	27 (18%)	1	7
49	M3	154/154 (100%)	124 (80%)	30 (20%)	1	5
49	m3	154/154 (100%)	123 (80%)	31 (20%)	1	5
50	M4	107/108 (99%)	87 (81%)	20 (19%)	1	7
50	m4	108/108 (100%)	85 (79%)	23 (21%)	1	4
51	M5	175/175 (100%)	140 (80%)	35 (20%)	1	5
51	m5	175/175 (100%)	140 (80%)	35 (20%)	1	5
52	M6	160/160 (100%)	139 (87%)	21 (13%)	4	17
52	m6	160/160 (100%)	135 (84%)	25 (16%)	2	12
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	3
53	m7	125/145 (86%)	94 (75%)	31 (25%)	0	2
54	M8	150/150 (100%)	124 (83%)	26 (17%)	2	8
54	m8	150/150 (100%)	116 (77%)	34 (23%)	1	3
55	M9	153/153 (100%)	129 (84%)	24 (16%)	2	12
55	m9	153/153 (100%)	125 (82%)	28 (18%)	1	7
56	N0	156/156 (100%)	127 (81%)	29 (19%)	1	7
56	n0	156/156 (100%)	128 (82%)	28 (18%)	2	8
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	3

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

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

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

Mol	Chain	Res	Type
71	O5	4	VAL
8	s6	169	TYR
64	n8	14	HIS
73	O7	16	HIS
3	s1	177	GLN

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

Mol	Chain	Res	Type
47	M0	59	GLN
64	N8	67	HIS
62	n6	120	GLN
47	M0	144	ASN

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Mol	Chain	Res	Type
54	M8	145	ASN

5.3.3 RNA [i](#)

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

5 of 2672 RNA backbone outliers are listed below:

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

5 of 327 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3242	G
80	6	541	A
36	5	2872	A
36	1	3319	U
80	6	75	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3561 ligands modelled in this entry, 2208 are monoatomic - leaving 1353 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2060	-	0,6,6	0.00	-	-		
86	OHX	6	1957	80	0,6,6	0.00	-	-		
86	OHX	1	3502	86,36	0,6,6	0.00	-	-		
86	OHX	2	1928	-	0,6,6	0.00	-	-		
86	OHX	5	3438	36	0,6,6	0.00	-	-		
86	OHX	5	3582	86	0,6,6	0.00	-	-		
86	OHX	1	3657	-	0,6,6	0.00	-	-		
86	OHX	M0	304	86	0,6,6	0.00	-	-		
86	OHX	2	2018	86	0,6,6	0.00	-	-		
86	OHX	1	3785	86	0,6,6	0.00	-	-		
86	OHX	5	3446	-	0,6,6	0.00	-	-		
86	OHX	2	2025	-	0,6,6	0.00	-	-		
86	OHX	6	2086	-	0,6,6	0.00	-	-		
86	OHX	1	3500	-	0,6,6	0.00	-	-		
86	OHX	5	3707	-	0,6,6	0.00	-	-		
86	OHX	6	2083	86	0,6,6	0.00	-	-		
86	OHX	5	3576	-	0,6,6	0.00	-	-		
86	OHX	2	1925	-	0,6,6	0.00	-	-		
86	OHX	5	3468	86	0,6,6	0.00	-	-		
86	OHX	5	3541	86	0,6,6	0.00	-	-		
86	OHX	C5	201	17	0,6,6	0.00	-	-		
86	OHX	6	1928	80	0,6,6	0.00	-	-		
86	OHX	5	3672	-	0,6,6	0.00	-	-		
86	OHX	5	3469	-	0,6,6	0.00	-	-		
86	OHX	m5	501	-	0,6,6	0.00	-	-		
86	OHX	14	401	-	0,6,6	0.00	-	-		
86	OHX	1	3798	-	0,6,6	0.00	-	-		
86	OHX	2	1929	-	0,6,6	0.00	-	-		
86	OHX	2	1946	-	0,6,6	0.00	-	-		
86	OHX	1	3791	86	0,6,6	0.00	-	-		
86	OHX	2	1918	86	0,6,6	0.00	-	-		
86	OHX	5	3427	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3429	36	0,6,6	0.00	-	-	-	
86	OHX	1	3424	-	0,6,6	0.00	-	-	-	
86	OHX	M5	301	-	0,6,6	0.00	-	-	-	
86	OHX	8	212	86	0,6,6	0.00	-	-	-	
86	OHX	5	3638	-	0,6,6	0.00	-	-	-	
86	OHX	6	1968	-	0,6,6	0.00	-	-	-	
86	OHX	2	2009	-	0,6,6	0.00	-	-	-	
86	OHX	5	3483	86	0,6,6	0.00	-	-	-	
86	OHX	6	2073	-	0,6,6	0.00	-	-	-	
86	OHX	7	213	-	0,6,6	0.00	-	-	-	
86	OHX	5	3676	36	0,6,6	0.00	-	-	-	
86	OHX	5	3686	-	0,6,6	0.00	-	-	-	
86	OHX	5	3678	-	0,6,6	0.00	-	-	-	
86	OHX	L4	401	-	0,6,6	0.00	-	-	-	
86	OHX	1	3660	-	0,6,6	0.00	-	-	-	
86	OHX	8	215	-	0,6,6	0.00	-	-	-	
86	OHX	1	3665	-	0,6,6	0.00	-	-	-	
86	OHX	1	3450	86	0,6,6	0.00	-	-	-	
86	OHX	5	3513	36	0,6,6	0.00	-	-	-	
86	OHX	2	1990	1,86	0,6,6	0.00	-	-	-	
86	OHX	2	2017	-	0,6,6	0.00	-	-	-	
86	OHX	1	3781	-	0,6,6	0.00	-	-	-	
86	OHX	6	1943	-	0,6,6	0.00	-	-	-	
86	OHX	1	3491	-	0,6,6	0.00	-	-	-	
86	OHX	5	3531	36	0,6,6	0.00	-	-	-	
86	OHX	5	3542	36	0,6,6	0.00	-	-	-	
86	OHX	5	3437	36	0,6,6	0.00	-	-	-	
86	OHX	2	1912	-	0,6,6	0.00	-	-	-	
86	OHX	5	3432	-	0,6,6	0.00	-	-	-	
86	OHX	5	3409	36	0,6,6	0.00	-	-	-	
86	OHX	2	2034	-	0,6,6	0.00	-	-	-	
86	OHX	L3	403	-	0,6,6	0.00	-	-	-	
86	OHX	1	3739	-	0,6,6	0.00	-	-	-	
86	OHX	4	214	38	0,6,6	0.00	-	-	-	
86	OHX	6	1941	80	0,6,6	0.00	-	-	-	
86	OHX	1	3567	-	0,6,6	0.00	-	-	-	
86	OHX	s8	301	-	0,6,6	0.00	-	-	-	
86	OHX	7	211	86	0,6,6	0.00	-	-	-	
86	OHX	6	2025	-	0,6,6	0.00	-	-	-	
86	OHX	6	2089	80	0,6,6	0.00	-	-	-	
86	OHX	1	3505	86	0,6,6	0.00	-	-	-	
86	OHX	5	3550	-	0,6,6	0.00	-	-	-	
86	OHX	6	1944	80	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3580	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3558	-	0,6,6	0.00	-	-	-	-
86	OHX	M0	301	86	0,6,6	0.00	-	-	-	-
86	OHX	8	205	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3623	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3446	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3758	36	0,6,6	0.00	-	-	-	-
86	OHX	6	2048	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3599	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1994	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3490	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1906	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2030	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3790	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3817	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3607	-	0,6,6	0.00	-	-	-	-
86	OHX	8	202	38	0,6,6	0.00	-	-	-	-
86	OHX	1	3734	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3449	86	0,6,6	0.00	-	-	-	-
86	OHX	2	2071	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1995	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3633	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3639	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1978	80	0,6,6	0.00	-	-	-	-
86	OHX	5	3721	36	0,6,6	0.00	-	-	-	-
86	OHX	2	1901	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3731	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2038	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3448	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3681	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1906	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3736	86	0,6,6	0.00	-	-	-	-
86	OHX	8	214	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3718	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3687	36	0,6,6	0.00	-	-	-	-
86	OHX	2	1924	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3773	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3628	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2019	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3607	36	0,6,6	0.00	-	-	-	-
86	OHX	6	2013	-	0,6,6	0.00	-	-	-	-
86	OHX	4	202	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3688	86	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3621	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3516	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2021	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3543	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3751	86,36	0,6,6	0.00	-	-	-	-
86	OHX	1	3616	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3752	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3421	36	0,6,6	0.00	-	-	-	-
86	OHX	2	1971	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3478	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3650	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2054	80,86	0,6,6	0.00	-	-	-	-
86	OHX	6	2005	86	0,6,6	0.00	-	-	-	-
86	OHX	2	2053	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3777	86	0,6,6	0.00	-	-	-	-
86	OHX	2	2024	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3553	-	0,6,6	0.00	-	-	-	-
86	OHX	8	219	38	0,6,6	0.00	-	-	-	-
86	OHX	5	3811	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3608	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3574	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1987	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3604	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3601	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3631	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3612	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3511	36	0,6,6	0.00	-	-	-	-
86	OHX	2	2064	86	0,6,6	0.00	-	-	-	-
86	OHX	Q2	502	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3696	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3532	-	0,6,6	0.00	-	-	-	-
86	OHX	C3	201	-	0,6,6	0.00	-	-	-	-
86	OHX	3	212	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3657	86	0,6,6	0.00	-	-	-	-
86	OHX	o7	503	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2065	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3711	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3656	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1973	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2088	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2032	80,86	0,6,6	0.00	-	-	-	-
86	OHX	1	3563	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2035	86	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	3	210	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1947	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3503	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3416	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3779	86	0,6,6	0.00	-	-	-	-
86	OHX	2	2022	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3630	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3648	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3706	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3584	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3545	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3672	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3438	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1999	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3683	86,36	0,6,6	0.00	-	-	-	-
86	OHX	1	3700	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3594	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3423	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3626	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3424	36	0,6,6	0.00	-	-	-	-
86	OHX	s1	302	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3772	-	0,6,6	0.00	-	-	-	-
86	OHX	D9	102	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3539	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1935	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3634	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2060	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3422	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3555	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3566	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3729	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3578	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3774	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3479	86	0,6,6	0.00	-	-	-	-
86	OHX	8	213	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3731	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3693	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3699	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3515	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2096	80,86	0,6,6	0.00	-	-	-	-
86	OHX	1	3797	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3411	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3498	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3497	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3533	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3439	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3524	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2002	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3725	86,36	0,6,6	0.00	-	-	-	-
86	OHX	1	3476	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3550	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2047	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3662	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3690	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2058	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3802	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1917	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3461	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3581	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2078	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1908	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3744	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3745	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1907	80	0,6,6	0.00	-	-	-	-
86	OHX	5	3734	86	0,6,6	0.00	-	-	-	-
86	OHX	L3	401	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3448	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3544	-	0,6,6	0.00	-	-	-	-
86	OHX	19	201	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3637	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3455	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3571	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3736	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3586	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3514	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1904	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3559	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3710	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3683	-	0,6,6	0.00	-	-	-	-
86	OHX	sR	401	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3642	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3757	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2011	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3695	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2072	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3596	86	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3678	86	0,6,6	0.00	-	-	-	
86	OHX	6	1970	-	0,6,6	0.00	-	-	-	
86	OHX	6	1977	-	0,6,6	0.00	-	-	-	
86	OHX	2	2056	-	0,6,6	0.00	-	-	-	
86	OHX	1	3458	-	0,6,6	0.00	-	-	-	
86	OHX	6	2041	80	0,6,6	0.00	-	-	-	
86	OHX	6	2031	-	0,6,6	0.00	-	-	-	
86	OHX	1	3461	86	0,6,6	0.00	-	-	-	
86	OHX	5	3472	-	0,6,6	0.00	-	-	-	
86	OHX	5	3684	-	0,6,6	0.00	-	-	-	
86	OHX	5	3522	36	0,6,6	0.00	-	-	-	
86	OHX	1	3490	-	0,6,6	0.00	-	-	-	
86	OHX	2	2011	-	0,6,6	0.00	-	-	-	
86	OHX	2	1934	-	0,6,6	0.00	-	-	-	
86	OHX	6	2026	80	0,6,6	0.00	-	-	-	
86	OHX	1	3810	86	0,6,6	0.00	-	-	-	
86	OHX	6	1934	-	0,6,6	0.00	-	-	-	
86	OHX	1	3444	-	0,6,6	0.00	-	-	-	
86	OHX	6	1910	-	0,6,6	0.00	-	-	-	
86	OHX	5	3644	36	0,6,6	0.00	-	-	-	
86	OHX	1	3786	86	0,6,6	0.00	-	-	-	
86	OHX	6	1963	80	0,6,6	0.00	-	-	-	
86	OHX	2	1982	-	0,6,6	0.00	-	-	-	
86	OHX	5	3663	-	0,6,6	0.00	-	-	-	
86	OHX	2	1960	-	0,6,6	0.00	-	-	-	
86	OHX	6	2052	80	0,6,6	0.00	-	-	-	
86	OHX	2	2059	86	0,6,6	0.00	-	-	-	
86	OHX	1	3809	86,36	0,6,6	0.00	-	-	-	
86	OHX	2	2067	-	0,6,6	0.00	-	-	-	
86	OHX	6	1972	-	0,6,6	0.00	-	-	-	
86	OHX	5	3741	-	0,6,6	0.00	-	-	-	
86	OHX	5	3660	36	0,6,6	0.00	-	-	-	
86	OHX	5	3744	-	0,6,6	0.00	-	-	-	
86	OHX	M0	302	86	0,6,6	0.00	-	-	-	
86	OHX	5	3738	-	0,6,6	0.00	-	-	-	
86	OHX	1	3658	-	0,6,6	0.00	-	-	-	
86	OHX	5	3426	-	0,6,6	0.00	-	-	-	
86	OHX	5	3782	36	0,6,6	0.00	-	-	-	
86	OHX	5	3699	36	0,6,6	0.00	-	-	-	
86	OHX	5	3450	-	0,6,6	0.00	-	-	-	
86	OHX	5	3456	-	0,6,6	0.00	-	-	-	
86	OHX	n1	201	-	0,6,6	0.00	-	-	-	
86	OHX	6	1932	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	1942	80	0,6,6	0.00	-	-	-	
86	OHX	5	3441	-	0,6,6	0.00	-	-	-	
86	OHX	1	3624	36	0,6,6	0.00	-	-	-	
86	OHX	1	3735	-	0,6,6	0.00	-	-	-	
86	OHX	6	1960	-	0,6,6	0.00	-	-	-	
86	OHX	1	3575	86	0,6,6	0.00	-	-	-	
86	OHX	6	2004	-	0,6,6	0.00	-	-	-	
86	OHX	6	1965	86	0,6,6	0.00	-	-	-	
86	OHX	5	3416	-	0,6,6	0.00	-	-	-	
86	OHX	4	203	-	0,6,6	0.00	-	-	-	
86	OHX	1	3482	-	0,6,6	0.00	-	-	-	
86	OHX	1	3488	86	0,6,6	0.00	-	-	-	
86	OHX	2	2028	1	0,6,6	0.00	-	-	-	
86	OHX	5	3408	-	0,6,6	0.00	-	-	-	
86	OHX	1	3483	-	0,6,6	0.00	-	-	-	
86	OHX	6	1909	80,86	0,6,6	0.00	-	-	-	
86	OHX	5	3668	-	0,6,6	0.00	-	-	-	
86	OHX	2	2041	-	0,6,6	0.00	-	-	-	
86	OHX	1	3553	86	0,6,6	0.00	-	-	-	
86	OHX	5	3772	86,36	0,6,6	0.00	-	-	-	
86	OHX	2	1955	-	0,6,6	0.00	-	-	-	
86	OHX	5	3614	-	0,6,6	0.00	-	-	-	
86	OHX	5	3518	36	0,6,6	0.00	-	-	-	
86	OHX	1	3686	-	0,6,6	0.00	-	-	-	
86	OHX	5	3528	-	0,6,6	0.00	-	-	-	
86	OHX	2	1999	-	0,6,6	0.00	-	-	-	
86	OHX	1	3509	-	0,6,6	0.00	-	-	-	
86	OHX	2	1972	1	0,6,6	0.00	-	-	-	
86	OHX	5	3745	-	0,6,6	0.00	-	-	-	
86	OHX	2	2038	-	0,6,6	0.00	-	-	-	
86	OHX	5	3586	86	0,6,6	0.00	-	-	-	
86	OHX	1	3789	86	0,6,6	0.00	-	-	-	
86	OHX	L3	402	-	0,6,6	0.00	-	-	-	
86	OHX	5	3532	-	0,6,6	0.00	-	-	-	
86	OHX	2	2005	-	0,6,6	0.00	-	-	-	
86	OHX	1	3707	-	0,6,6	0.00	-	-	-	
86	OHX	5	3521	-	0,6,6	0.00	-	-	-	
86	OHX	5	3570	36	0,6,6	0.00	-	-	-	
86	OHX	7	201	37	0,6,6	0.00	-	-	-	
86	OHX	1	3743	86	0,6,6	0.00	-	-	-	
86	OHX	5	3485	-	0,6,6	0.00	-	-	-	
86	OHX	1	3776	86	0,6,6	0.00	-	-	-	
86	OHX	2	2037	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	1941	-	0,6,6	0.00	-	-	-	-
86	OHX	8	201	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3569	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3493	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3499	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3717	-	0,6,6	0.00	-	-	-	-
86	OHX	7	202	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3551	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3561	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2000	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1997	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1985	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3788	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3759	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3488	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3520	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2033	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3428	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3481	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3620	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3716	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3548	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3708	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3546	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3522	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3546	86	0,6,6	0.00	-	-	-	-
86	OHX	8	217	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3765	86	0,6,6	0.00	-	-	-	-
86	OHX	m0	302	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3708	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3804	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1919	80,86	0,6,6	0.00	-	-	-	-
86	OHX	1	3597	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3684	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3746	86	0,6,6	0.00	-	-	-	-
86	OHX	3	202	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3455	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1957	-	0,6,6	0.00	-	-	-	-
90	8AN	5	3403	89	19,24,25	8.24	3 (15%)	13,35,38	1.64	3 (23%)
86	OHX	s4	301	-	0,6,6	0.00	-	-	-	-
86	OHX	q1	101	86	0,6,6	0.00	-	-	-	-
86	OHX	3	206	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3437	86	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2034	80,86	0,6,6	0.00	-	-	-	
86	OHX	5	3436	-	0,6,6	0.00	-	-	-	
86	OHX	M0	303	86	0,6,6	0.00	-	-	-	
86	OHX	5	3671	-	0,6,6	0.00	-	-	-	
86	OHX	6	2080	-	0,6,6	0.00	-	-	-	
86	OHX	1	3770	-	0,6,6	0.00	-	-	-	
86	OHX	2	1933	86	0,6,6	0.00	-	-	-	
86	OHX	1	3467	-	0,6,6	0.00	-	-	-	
86	OHX	4	215	86	0,6,6	0.00	-	-	-	
86	OHX	5	3477	36	0,6,6	0.00	-	-	-	
86	OHX	5	3496	-	0,6,6	0.00	-	-	-	
86	OHX	2	2069	86	0,6,6	0.00	-	-	-	
86	OHX	5	3434	86	0,6,6	0.00	-	-	-	
86	OHX	6	1908	-	0,6,6	0.00	-	-	-	
86	OHX	1	3792	86	0,6,6	0.00	-	-	-	
86	OHX	8	204	-	0,6,6	0.00	-	-	-	
86	OHX	1	3534	-	0,6,6	0.00	-	-	-	
86	OHX	5	3766	-	0,6,6	0.00	-	-	-	
86	OHX	1	3680	-	0,6,6	0.00	-	-	-	
86	OHX	5	3615	89,86,36	0,6,6	0.00	-	-	-	
86	OHX	1	3443	-	0,6,6	0.00	-	-	-	
86	OHX	5	3818	86,36	0,6,6	0.00	-	-	-	
86	OHX	M9	201	-	0,6,6	0.00	-	-	-	
86	OHX	6	1931	80,86	0,6,6	0.00	-	-	-	
86	OHX	2	2088	1,86	0,6,6	0.00	-	-	-	
86	OHX	1	3419	-	0,6,6	0.00	-	-	-	
86	OHX	5	3698	-	0,6,6	0.00	-	-	-	
86	OHX	1	3710	-	0,6,6	0.00	-	-	-	
86	OHX	1	3533	-	0,6,6	0.00	-	-	-	
86	OHX	6	2091	86	0,6,6	0.00	-	-	-	
86	OHX	1	3593	-	0,6,6	0.00	-	-	-	
86	OHX	14	402	-	0,6,6	0.00	-	-	-	
86	OHX	5	3423	36	0,6,6	0.00	-	-	-	
86	OHX	2	2003	1	0,6,6	0.00	-	-	-	
86	OHX	1	3547	86	0,6,6	0.00	-	-	-	
86	OHX	2	1975	86	0,6,6	0.00	-	-	-	
86	OHX	2	2045	-	0,6,6	0.00	-	-	-	
86	OHX	1	3495	86	0,6,6	0.00	-	-	-	
86	OHX	1	3592	-	0,6,6	0.00	-	-	-	
86	OHX	5	3447	86	0,6,6	0.00	-	-	-	
86	OHX	6	2001	-	0,6,6	0.00	-	-	-	
86	OHX	5	3538	-	0,6,6	0.00	-	-	-	
86	OHX	2	2001	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	1979	80	0,6,6	0.00	-	-	-	
86	OHX	8	218	38	0,6,6	0.00	-	-	-	
86	OHX	1	3799	86	0,6,6	0.00	-	-	-	
86	OHX	5	3726	36	0,6,6	0.00	-	-	-	
86	OHX	1	3695	86	0,6,6	0.00	-	-	-	
86	OHX	4	211	-	0,6,6	0.00	-	-	-	
86	OHX	5	3687	-	0,6,6	0.00	-	-	-	
86	OHX	2	2026	86	0,6,6	0.00	-	-	-	
86	OHX	5	3689	36	0,6,6	0.00	-	-	-	
86	OHX	5	3598	86,36	0,6,6	0.00	-	-	-	
86	OHX	2	2082	1,86	0,6,6	0.00	-	-	-	
86	OHX	2	2089	86	0,6,6	0.00	-	-	-	
86	OHX	1	3689	86	0,6,6	0.00	-	-	-	
86	OHX	1	3433	-	0,6,6	0.00	-	-	-	
86	OHX	1	3747	36	0,6,6	0.00	-	-	-	
86	OHX	1	3436	-	0,6,6	0.00	-	-	-	
86	OHX	2	2030	86	0,6,6	0.00	-	-	-	
86	OHX	1	3732	-	0,6,6	0.00	-	-	-	
86	OHX	5	3740	-	0,6,6	0.00	-	-	-	
86	OHX	6	2028	80	0,6,6	0.00	-	-	-	
86	OHX	1	3579	36	0,6,6	0.00	-	-	-	
86	OHX	1	3765	-	0,6,6	0.00	-	-	-	
86	OHX	2	2061	-	0,6,6	0.00	-	-	-	
86	OHX	2	2008	86	0,6,6	0.00	-	-	-	
86	OHX	6	2059	86	0,6,6	0.00	-	-	-	
86	OHX	2	1996	-	0,6,6	0.00	-	-	-	
86	OHX	2	2010	-	0,6,6	0.00	-	-	-	
86	OHX	5	3625	36	0,6,6	0.00	-	-	-	
86	OHX	2	2012	-	0,6,6	0.00	-	-	-	
86	OHX	1	3528	-	0,6,6	0.00	-	-	-	
86	OHX	1	3608	-	0,6,6	0.00	-	-	-	
86	OHX	5	3457	86	0,6,6	0.00	-	-	-	
86	OHX	m5	502	-	0,6,6	0.00	-	-	-	
86	OHX	6	2079	-	0,6,6	0.00	-	-	-	
86	OHX	5	3515	-	0,6,6	0.00	-	-	-	
86	OHX	1	3539	86	0,6,6	0.00	-	-	-	
86	OHX	1	3431	86	0,6,6	0.00	-	-	-	
86	OHX	5	3802	86	0,6,6	0.00	-	-	-	
86	OHX	6	2020	80	0,6,6	0.00	-	-	-	
86	OHX	N8	201	-	0,6,6	0.00	-	-	-	
86	OHX	5	3500	-	0,6,6	0.00	-	-	-	
86	OHX	5	3636	86	0,6,6	0.00	-	-	-	
86	OHX	5	3497	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3694	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3519	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3622	-	0,6,6	0.00	-	-	-	-
86	OHX	3	211	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3685	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3776	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1990	80	0,6,6	0.00	-	-	-	-
86	OHX	2	1915	1,86	0,6,6	0.00	-	-	-	-
86	OHX	5	3406	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3620	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2014	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3661	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3773	-	0,6,6	0.00	-	-	-	-
86	OHX	15	303	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3460	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3445	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3754	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3612	36	0,6,6	0.00	-	-	-	-
86	OHX	7	204	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2058	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3454	86,36	0,6,6	0.00	-	-	-	-
86	OHX	6	2012	80	0,6,6	0.00	-	-	-	-
86	OHX	2	2054	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1952	1	0,6,6	0.00	-	-	-	-
86	OHX	q2	502	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3709	86,36	0,6,6	0.00	-	-	-	-
86	OHX	6	1958	80	0,6,6	0.00	-	-	-	-
86	OHX	6	2081	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3602	86	0,6,6	0.00	-	-	-	-
86	OHX	4	207	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3661	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3523	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3517	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2053	80	0,6,6	0.00	-	-	-	-
86	OHX	5	3652	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3492	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3761	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3775	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3778	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3471	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3465	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3526	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3606	36	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2052	1	0,6,6	0.00	-	-	-	
86	OHX	5	3487	-	0,6,6	0.00	-	-	-	
86	OHX	5	3733	86	0,6,6	0.00	-	-	-	
86	OHX	6	2061	86	0,6,6	0.00	-	-	-	
86	OHX	6	1955	80	0,6,6	0.00	-	-	-	
86	OHX	1	3711	86	0,6,6	0.00	-	-	-	
86	OHX	m7	201	-	0,6,6	0.00	-	-	-	
86	OHX	1	3644	-	0,6,6	0.00	-	-	-	
86	OHX	1	3759	-	0,6,6	0.00	-	-	-	
86	OHX	2	1978	-	0,6,6	0.00	-	-	-	
86	OHX	1	3656	86	0,6,6	0.00	-	-	-	
86	OHX	5	3587	86,36	0,6,6	0.00	-	-	-	
86	OHX	6	2022	80,86	0,6,6	0.00	-	-	-	
86	OHX	5	3667	-	0,6,6	0.00	-	-	-	
86	OHX	5	3572	86	0,6,6	0.00	-	-	-	
86	OHX	5	3535	-	0,6,6	0.00	-	-	-	
86	OHX	1	3664	-	0,6,6	0.00	-	-	-	
86	OHX	1	3740	-	0,6,6	0.00	-	-	-	
86	OHX	1	3521	-	0,6,6	0.00	-	-	-	
86	OHX	2	2073	86	0,6,6	0.00	-	-	-	
86	OHX	5	3743	-	0,6,6	0.00	-	-	-	
86	OHX	1	3512	-	0,6,6	0.00	-	-	-	
86	OHX	2	1969	1	0,6,6	0.00	-	-	-	
86	OHX	1	3470	-	0,6,6	0.00	-	-	-	
86	OHX	1	3410	36	0,6,6	0.00	-	-	-	
86	OHX	5	3653	-	0,6,6	0.00	-	-	-	
86	OHX	1	3782	-	0,6,6	0.00	-	-	-	
86	OHX	5	3659	86,36	0,6,6	0.00	-	-	-	
86	OHX	5	3735	86	0,6,6	0.00	-	-	-	
86	OHX	1	3441	86	0,6,6	0.00	-	-	-	
86	OHX	1	3549	-	0,6,6	0.00	-	-	-	
86	OHX	6	2018	86	0,6,6	0.00	-	-	-	
86	OHX	1	3588	86	0,6,6	0.00	-	-	-	
86	OHX	6	2093	80,86	0,6,6	0.00	-	-	-	
86	OHX	1	3748	86	0,6,6	0.00	-	-	-	
86	OHX	1	3697	-	0,6,6	0.00	-	-	-	
86	OHX	6	1905	-	0,6,6	0.00	-	-	-	
86	OHX	1	3696	86	0,6,6	0.00	-	-	-	
86	OHX	5	3780	-	0,6,6	0.00	-	-	-	
86	OHX	1	3531	-	0,6,6	0.00	-	-	-	
86	OHX	6	1971	86	0,6,6	0.00	-	-	-	
86	OHX	2	2023	-	0,6,6	0.00	-	-	-	
86	OHX	6	2036	80	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3467	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1922	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3516	-	0,6,6	0.00	-	-	-	-
86	OHX	m0	303	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1970	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3615	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3566	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2032	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3565	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1980	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3774	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3755	36	0,6,6	0.00	-	-	-	-
86	OHX	15	302	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3526	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3527	86,36	0,6,6	0.00	-	-	-	-
86	OHX	1	3582	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3806	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2074	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3714	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1956	-	0,6,6	0.00	-	-	-	-
86	OHX	8	207	38,86	0,6,6	0.00	-	-	-	-
86	OHX	5	3451	86	0,6,6	0.00	-	-	-	-
86	OHX	4	216	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3685	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3724	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2040	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2029	1	0,6,6	0.00	-	-	-	-
86	OHX	o7	502	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3664	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2010	80,86	0,6,6	0.00	-	-	-	-
86	OHX	6	2044	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1904	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3645	86	0,6,6	0.00	-	-	-	-
86	OHX	M9	202	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1920	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1954	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3496	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3560	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3495	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3666	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3560	36	0,6,6	0.00	-	-	-	-
86	OHX	6	1982	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1988	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	1987	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2015	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3677	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3432	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3536	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1930	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3549	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3529	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3544	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2048	86	0,6,6	0.00	-	-	-	-
86	OHX	3	201	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2068	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3435	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3722	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3625	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2090	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3554	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2056	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3551	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2055	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2009	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3417	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3717	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3792	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1938	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3798	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3487	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1909	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2035	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3793	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1902	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3493	36	0,6,6	0.00	-	-	-	-
86	OHX	6	1980	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3485	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3420	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3597	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3534	36	0,6,6	0.00	-	-	-	-
86	OHX	2	1936	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1992	-	0,6,6	0.00	-	-	-	-
86	OHX	12	301	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3481	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1926	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3552	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3413	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3425	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1959	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3643	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2077	86	0,6,6	0.00	-	-	-	-
86	OHX	c3	201	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3589	-	0,6,6	0.00	-	-	-	-
86	OHX	n3	202	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3720	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3414	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3786	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3530	36	0,6,6	0.00	-	-	-	-
86	OHX	8	221	86	0,6,6	0.00	-	-	-	-
86	OHX	2	2042	-	0,6,6	0.00	-	-	-	-
86	OHX	3	209	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1973	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3413	36	0,6,6	0.00	-	-	-	-
86	OHX	6	1976	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3741	86	0,6,6	0.00	-	-	-	-
86	OHX	7	203	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3778	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1940	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3630	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2077	1,86	0,6,6	0.00	-	-	-	-
86	OHX	6	2027	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3779	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1915	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3479	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3501	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3407	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3593	86,36	0,6,6	0.00	-	-	-	-
86	OHX	6	1966	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1903	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1945	80	0,6,6	0.00	-	-	-	-
86	OHX	5	3547	36	0,6,6	0.00	-	-	-	-
86	OHX	2	1965	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3636	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1935	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3638	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3635	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3728	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3429	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3796	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3509	86	0,6,6	0.00	-	-	-	
86	OHX	6	1962	80	0,6,6	0.00	-	-	-	
86	OHX	1	3805	86	0,6,6	0.00	-	-	-	
86	OHX	1	3676	-	0,6,6	0.00	-	-	-	
86	OHX	1	3651	36	0,6,6	0.00	-	-	-	
86	OHX	1	3511	86	0,6,6	0.00	-	-	-	
86	OHX	6	2023	-	0,6,6	0.00	-	-	-	
86	OHX	2	2020	-	0,6,6	0.00	-	-	-	
86	OHX	1	3614	-	0,6,6	0.00	-	-	-	
86	OHX	5	3475	36	0,6,6	0.00	-	-	-	
86	OHX	6	1937	-	0,6,6	0.00	-	-	-	
86	OHX	1	3812	86	0,6,6	0.00	-	-	-	
86	OHX	6	1917	80	0,6,6	0.00	-	-	-	
86	OHX	6	1918	86	0,6,6	0.00	-	-	-	
86	OHX	5	3806	86,36	0,6,6	0.00	-	-	-	
86	OHX	5	3691	86	0,6,6	0.00	-	-	-	
86	OHX	6	1925	80	0,6,6	0.00	-	-	-	
86	OHX	1	3795	-	0,6,6	0.00	-	-	-	
86	OHX	2	1968	-	0,6,6	0.00	-	-	-	
86	OHX	5	3530	-	0,6,6	0.00	-	-	-	
86	OHX	2	1943	86	0,6,6	0.00	-	-	-	
86	OHX	1	3622	-	0,6,6	0.00	-	-	-	
86	OHX	1	3628	-	0,6,6	0.00	-	-	-	
86	OHX	1	3627	-	0,6,6	0.00	-	-	-	
86	OHX	1	3406	-	0,6,6	0.00	-	-	-	
86	OHX	1	3415	-	0,6,6	0.00	-	-	-	
86	OHX	1	3794	86	0,6,6	0.00	-	-	-	
86	OHX	8	206	-	0,6,6	0.00	-	-	-	
86	OHX	5	3556	-	0,6,6	0.00	-	-	-	
86	OHX	5	3629	36	0,6,6	0.00	-	-	-	
86	OHX	5	3714	-	0,6,6	0.00	-	-	-	
86	OHX	5	3410	36	0,6,6	0.00	-	-	-	
86	OHX	1	3718	86	0,6,6	0.00	-	-	-	
86	OHX	5	3670	36	0,6,6	0.00	-	-	-	
86	OHX	1	3587	36	0,6,6	0.00	-	-	-	
86	OHX	1	3763	86	0,6,6	0.00	-	-	-	
86	OHX	5	3812	-	0,6,6	0.00	-	-	-	
86	OHX	5	3482	86	0,6,6	0.00	-	-	-	
86	OHX	1	3535	86	0,6,6	0.00	-	-	-	
86	OHX	6	1961	-	0,6,6	0.00	-	-	-	
86	OHX	5	3756	36	0,6,6	0.00	-	-	-	
86	OHX	5	3596	86	0,6,6	0.00	-	-	-	
86	OHX	6	2047	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3706	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3721	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3568	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3643	-	0,6,6	0.00	-	-	-	-
86	OHX	N9	101	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2094	80,86	0,6,6	0.00	-	-	-	-
86	OHX	5	3452	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3564	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3610	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3613	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3422	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3645	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3428	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3542	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3796	86,36	0,6,6	0.00	-	-	-	-
86	OHX	2	1911	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2069	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3611	-	0,6,6	0.00	-	-	-	-
86	OHX	SR	401	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3589	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1953	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3494	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3647	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3805	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3463	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1940	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3705	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3452	-	0,6,6	0.00	-	-	-	-
86	OHX	7	207	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3594	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1949	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3674	86,36	0,6,6	0.00	-	-	-	-
86	OHX	2	1942	1	0,6,6	0.00	-	-	-	-
86	OHX	S2	301	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1989	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3442	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1912	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2066	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3616	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2063	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3667	86,36	0,6,6	0.00	-	-	-	-
86	OHX	6	2097	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1983	80	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	4	218	86	0,6,6	0.00	-	-	-	
86	OHX	5	3650	36	0,6,6	0.00	-	-	-	
86	OHX	5	3505	86	0,6,6	0.00	-	-	-	
86	OHX	o3	201	-	0,6,6	0.00	-	-	-	
86	OHX	2	2006	-	0,6,6	0.00	-	-	-	
86	OHX	5	3508	36	0,6,6	0.00	-	-	-	
86	OHX	1	3663	86	0,6,6	0.00	-	-	-	
86	OHX	3	208	-	0,6,6	0.00	-	-	-	
86	OHX	2	1974	-	0,6,6	0.00	-	-	-	
86	OHX	8	216	38	0,6,6	0.00	-	-	-	
86	OHX	1	3760	-	0,6,6	0.00	-	-	-	
86	OHX	5	3666	-	0,6,6	0.00	-	-	-	
86	OHX	1	3668	-	0,6,6	0.00	-	-	-	
86	OHX	1	3518	86	0,6,6	0.00	-	-	-	
86	OHX	2	1931	-	0,6,6	0.00	-	-	-	
86	OHX	1	3454	-	0,6,6	0.00	-	-	-	
86	OHX	5	3420	36	0,6,6	0.00	-	-	-	
86	OHX	1	3653	-	0,6,6	0.00	-	-	-	
86	OHX	1	3641	-	0,6,6	0.00	-	-	-	
86	OHX	5	3697	-	0,6,6	0.00	-	-	-	
86	OHX	5	3658	36	0,6,6	0.00	-	-	-	
86	OHX	1	3473	-	0,6,6	0.00	-	-	-	
86	OHX	4	201	-	0,6,6	0.00	-	-	-	
86	OHX	5	3605	36	0,6,6	0.00	-	-	-	
86	OHX	2	2015	1,86	0,6,6	0.00	-	-	-	
86	OHX	1	3737	36	0,6,6	0.00	-	-	-	
86	OHX	2	2076	1,86	0,6,6	0.00	-	-	-	
86	OHX	6	2002	80,86	0,6,6	0.00	-	-	-	
86	OHX	1	3569	-	0,6,6	0.00	-	-	-	
86	OHX	1	3541	-	0,6,6	0.00	-	-	-	
86	OHX	1	3649	-	0,6,6	0.00	-	-	-	
86	OHX	2	1919	1	0,6,6	0.00	-	-	-	
86	OHX	2	1997	-	0,6,6	0.00	-	-	-	
86	OHX	2	1913	-	0,6,6	0.00	-	-	-	
86	OHX	6	2003	80	0,6,6	0.00	-	-	-	
86	OHX	5	3554	-	0,6,6	0.00	-	-	-	
86	OHX	1	3548	-	0,6,6	0.00	-	-	-	
86	OHX	5	3641	-	0,6,6	0.00	-	-	-	
86	OHX	5	3517	86	0,6,6	0.00	-	-	-	
86	OHX	5	3610	-	0,6,6	0.00	-	-	-	
86	OHX	1	3451	-	0,6,6	0.00	-	-	-	
86	OHX	2	2019	-	0,6,6	0.00	-	-	-	
86	OHX	2	1962	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3761	86	0,6,6	0.00	-	-	-	
86	OHX	1	3506	86	0,6,6	0.00	-	-	-	
86	OHX	5	3679	-	0,6,6	0.00	-	-	-	
86	OHX	1	3618	-	0,6,6	0.00	-	-	-	
86	OHX	1	3788	86	0,6,6	0.00	-	-	-	
86	OHX	5	3800	-	0,6,6	0.00	-	-	-	
86	OHX	1	3730	-	0,6,6	0.00	-	-	-	
86	OHX	3	207	86	0,6,6	0.00	-	-	-	
86	OHX	2	1944	-	0,6,6	0.00	-	-	-	
86	OHX	6	1924	-	0,6,6	0.00	-	-	-	
86	OHX	5	3789	-	0,6,6	0.00	-	-	-	
86	OHX	5	3682	-	0,6,6	0.00	-	-	-	
86	OHX	1	3681	86	0,6,6	0.00	-	-	-	
86	OHX	1	3688	86	0,6,6	0.00	-	-	-	
86	OHX	5	3632	86	0,6,6	0.00	-	-	-	
86	OHX	5	3591	-	0,6,6	0.00	-	-	-	
86	OHX	5	3433	36	0,6,6	0.00	-	-	-	
86	OHX	6	2016	80	0,6,6	0.00	-	-	-	
86	OHX	6	2042	80,86	0,6,6	0.00	-	-	-	
86	OHX	1	3635	-	0,6,6	0.00	-	-	-	
86	OHX	5	3462	36	0,6,6	0.00	-	-	-	
86	OHX	5	3720	36	0,6,6	0.00	-	-	-	
86	OHX	1	3411	86	0,6,6	0.00	-	-	-	
86	OHX	5	3781	-	0,6,6	0.00	-	-	-	
86	OHX	L5	301	-	0,6,6	0.00	-	-	-	
86	OHX	6	1952	80,86	0,6,6	0.00	-	-	-	
86	OHX	5	3633	36	0,6,6	0.00	-	-	-	
86	OHX	5	3768	36	0,6,6	0.00	-	-	-	
86	OHX	7	208	-	0,6,6	0.00	-	-	-	
86	OHX	5	3715	86,36	0,6,6	0.00	-	-	-	
86	OHX	5	3649	36	0,6,6	0.00	-	-	-	
86	OHX	5	3723	-	0,6,6	0.00	-	-	-	
86	OHX	6	1989	80	0,6,6	0.00	-	-	-	
86	OHX	6	2075	80,86	0,6,6	0.00	-	-	-	
86	OHX	7	209	86,37	0,6,6	0.00	-	-	-	
86	OHX	5	3464	86	0,6,6	0.00	-	-	-	
86	OHX	1	3694	-	0,6,6	0.00	-	-	-	
86	OHX	5	3747	36	0,6,6	0.00	-	-	-	
86	OHX	5	3418	-	0,6,6	0.00	-	-	-	
86	OHX	1	3590	86	0,6,6	0.00	-	-	-	
86	OHX	13	402	-	0,6,6	0.00	-	-	-	
86	OHX	1	3408	-	0,6,6	0.00	-	-	-	
86	OHX	1	3764	86	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	1991	80	0,6,6	0.00	-	-	-	
86	OHX	5	3565	-	0,6,6	0.00	-	-	-	
86	OHX	1	3523	-	0,6,6	0.00	-	-	-	
86	OHX	2	2043	-	0,6,6	0.00	-	-	-	
86	OHX	5	3609	86	0,6,6	0.00	-	-	-	
86	OHX	2	1977	86	0,6,6	0.00	-	-	-	
86	OHX	6	1922	-	0,6,6	0.00	-	-	-	
86	OHX	6	1969	-	0,6,6	0.00	-	-	-	
86	OHX	5	3702	36	0,6,6	0.00	-	-	-	
86	OHX	1	3705	86	0,6,6	0.00	-	-	-	
86	OHX	5	3712	-	0,6,6	0.00	-	-	-	
86	OHX	5	3584	-	0,6,6	0.00	-	-	-	
86	OHX	2	2062	1	0,6,6	0.00	-	-	-	
86	OHX	M9	203	-	0,6,6	0.00	-	-	-	
86	OHX	5	3763	-	0,6,6	0.00	-	-	-	
86	OHX	5	3795	-	0,6,6	0.00	-	-	-	
86	OHX	2	1979	86	0,6,6	0.00	-	-	-	
86	OHX	2	2036	-	0,6,6	0.00	-	-	-	
86	OHX	1	3477	86	0,6,6	0.00	-	-	-	
86	OHX	4	212	38	0,6,6	0.00	-	-	-	
86	OHX	6	1938	80,86	0,6,6	0.00	-	-	-	
86	OHX	1	3756	86,36	0,6,6	0.00	-	-	-	
86	OHX	2	1916	1	0,6,6	0.00	-	-	-	
86	OHX	1	3771	-	0,6,6	0.00	-	-	-	
86	OHX	6	2067	86	0,6,6	0.00	-	-	-	
86	OHX	8	208	-	0,6,6	0.00	-	-	-	
86	OHX	2	1927	-	0,6,6	0.00	-	-	-	
86	OHX	5	3573	86	0,6,6	0.00	-	-	-	
86	OHX	1	3691	86,36	0,6,6	0.00	-	-	-	
86	OHX	2	2016	-	0,6,6	0.00	-	-	-	
86	OHX	2	1951	-	0,6,6	0.00	-	-	-	
86	OHX	5	3611	-	0,6,6	0.00	-	-	-	
86	OHX	6	1929	-	0,6,6	0.00	-	-	-	
86	OHX	5	3419	-	0,6,6	0.00	-	-	-	
86	OHX	5	3501	86	0,6,6	0.00	-	-	-	
86	OHX	5	3579	36	0,6,6	0.00	-	-	-	
86	OHX	6	2045	80	0,6,6	0.00	-	-	-	
86	OHX	1	3426	-	0,6,6	0.00	-	-	-	
86	OHX	1	3600	86	0,6,6	0.00	-	-	-	
86	OHX	2	1992	-	0,6,6	0.00	-	-	-	
86	OHX	8	209	-	0,6,6	0.00	-	-	-	
86	OHX	m1	201	-	0,6,6	0.00	-	-	-	
86	OHX	2	2049	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3491	-	0,6,6	0.00	-	-	-	-
86	OHX	m0	301	86	0,6,6	0.00	-	-	-	-
86	OHX	O7	103	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3445	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3415	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3525	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3447	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2050	1	0,6,6	0.00	-	-	-	-
86	OHX	4	204	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3766	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1920	86	0,6,6	0.00	-	-	-	-
86	OHX	4	210	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1903	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3671	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3417	-	0,6,6	0.00	-	-	-	-
86	OHX	O7	102	73	0,6,6	0.00	-	-	-	-
86	OHX	6	2082	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1981	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1936	80	0,6,6	0.00	-	-	-	-
86	OHX	7	206	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3642	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3771	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3693	36	0,6,6	0.00	-	-	-	-
86	OHX	6	2070	80,86	0,6,6	0.00	-	-	-	-
86	OHX	6	2071	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1998	86	0,6,6	0.00	-	-	-	-
86	OHX	c5	202	17	0,6,6	0.00	-	-	-	-
86	OHX	5	3568	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3536	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3767	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3673	86,36	0,6,6	0.00	-	-	-	-
86	OHX	1	3807	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3525	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3440	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3754	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2037	80	0,6,6	0.00	-	-	-	-
86	OHX	5	3442	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3581	36	0,6,6	0.00	-	-	-	-
86	OHX	M7	201	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3750	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3458	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3499	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3588	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3790	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3460	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3567	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1953	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2078	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3713	86,36	0,6,6	0.00	-	-	-	-
86	OHX	M8	201	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2087	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3576	-	0,6,6	0.00	-	-	-	-
86	OHX	3	203	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3475	-	0,6,6	0.00	-	-	-	-
86	OHX	c5	201	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1923	80	0,6,6	0.00	-	-	-	-
86	OHX	6	2064	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3637	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3723	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1914	80,86	0,6,6	0.00	-	-	-	-
86	OHX	1	3701	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3603	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1986	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3724	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1984	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3780	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3431	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3669	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3651	86	0,6,6	0.00	-	-	-	-
86	OHX	2	2074	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2008	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3558	36	0,6,6	0.00	-	-	-	-
86	OHX	7	210	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2080	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3797	36	0,6,6	0.00	-	-	-	-
86	OHX	3	204	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3506	86,36	0,6,6	0.00	-	-	-	-
86	OHX	5	3559	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3682	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3574	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3489	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3462	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2029	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3730	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3809	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2066	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3604	-	0,6,6	0.00	-	-		
86	OHX	1	3504	86	0,6,6	0.00	-	-		
86	OHX	4	206	-	0,6,6	0.00	-	-		
86	OHX	1	3811	86	0,6,6	0.00	-	-		
86	OHX	5	3791	-	0,6,6	0.00	-	-		
86	OHX	2	2087	86	0,6,6	0.00	-	-		
86	OHX	1	3572	-	0,6,6	0.00	-	-		
86	OHX	1	3412	-	0,6,6	0.00	-	-		
86	OHX	1	3659	-	0,6,6	0.00	-	-		
86	OHX	1	3469	86	0,6,6	0.00	-	-		
86	OHX	5	3631	-	0,6,6	0.00	-	-		
90	8AN	1	3403	89	19,24,25	1.05	1 (5%)	13,35,38	1.70	4 (30%)
86	OHX	1	3545	-	0,6,6	0.00	-	-		
86	OHX	5	3634	86	0,6,6	0.00	-	-		
86	OHX	6	1994	-	0,6,6	0.00	-	-		
86	OHX	S8	301	-	0,6,6	0.00	-	-		
86	OHX	2	1993	1	0,6,6	0.00	-	-		
86	OHX	6	1930	80	0,6,6	0.00	-	-		
86	OHX	1	3675	86,36	0,6,6	0.00	-	-		
86	OHX	5	3466	36	0,6,6	0.00	-	-		
86	OHX	5	3803	86	0,6,6	0.00	-	-		
86	OHX	5	3540	86	0,6,6	0.00	-	-		
86	OHX	5	3507	86	0,6,6	0.00	-	-		
86	OHX	1	3557	-	0,6,6	0.00	-	-		
86	OHX	1	3543	-	0,6,6	0.00	-	-		
86	OHX	1	3492	-	0,6,6	0.00	-	-		
86	OHX	2	1988	86	0,6,6	0.00	-	-		
86	OHX	1	3421	-	0,6,6	0.00	-	-		
86	OHX	1	3561	-	0,6,6	0.00	-	-		
86	OHX	6	1996	-	0,6,6	0.00	-	-		
86	OHX	6	2063	-	0,6,6	0.00	-	-		
86	OHX	2	2081	86	0,6,6	0.00	-	-		
86	OHX	1	3762	-	0,6,6	0.00	-	-		
86	OHX	13	401	-	0,6,6	0.00	-	-		
86	OHX	2	1905	-	0,6,6	0.00	-	-		
86	OHX	5	3787	-	0,6,6	0.00	-	-		
86	OHX	5	3562	-	0,6,6	0.00	-	-		
86	OHX	4	217	-	0,6,6	0.00	-	-		
86	OHX	5	3655	86,36	0,6,6	0.00	-	-		
86	OHX	2	2027	86	0,6,6	0.00	-	-		
86	OHX	5	3746	36	0,6,6	0.00	-	-		
86	OHX	1	3449	-	0,6,6	0.00	-	-		
86	OHX	1	3552	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3571	86	0,6,6	0.00	-	-	-	
86	OHX	5	3640	-	0,6,6	0.00	-	-	-	
86	OHX	5	3769	86	0,6,6	0.00	-	-	-	
86	OHX	6	2039	-	0,6,6	0.00	-	-	-	
86	OHX	5	3700	86,36	0,6,6	0.00	-	-	-	
86	OHX	1	3639	86	0,6,6	0.00	-	-	-	
86	OHX	o9	101	-	0,6,6	0.00	-	-	-	
86	OHX	2	1932	-	0,6,6	0.00	-	-	-	
86	OHX	2	1964	-	0,6,6	0.00	-	-	-	
86	OHX	2	1949	-	0,6,6	0.00	-	-	-	
86	OHX	1	3725	36	0,6,6	0.00	-	-	-	
86	OHX	2	1947	-	0,6,6	0.00	-	-	-	
86	OHX	5	3618	-	0,6,6	0.00	-	-	-	
86	OHX	1	3598	86	0,6,6	0.00	-	-	-	
86	OHX	5	3727	86	0,6,6	0.00	-	-	-	
86	OHX	5	3486	86	0,6,6	0.00	-	-	-	
86	OHX	1	3556	-	0,6,6	0.00	-	-	-	
86	OHX	1	3793	-	0,6,6	0.00	-	-	-	
86	OHX	d9	102	86	0,6,6	0.00	-	-	-	
86	OHX	5	3750	36	0,6,6	0.00	-	-	-	
86	OHX	2	2031	86	0,6,6	0.00	-	-	-	
86	OHX	1	3692	-	0,6,6	0.00	-	-	-	
86	OHX	4	213	-	0,6,6	0.00	-	-	-	
86	OHX	1	3619	36	0,6,6	0.00	-	-	-	
86	OHX	2	1914	1	0,6,6	0.00	-	-	-	
86	OHX	1	3585	-	0,6,6	0.00	-	-	-	
86	OHX	2	1961	86	0,6,6	0.00	-	-	-	
86	OHX	1	3727	-	0,6,6	0.00	-	-	-	
86	OHX	1	3580	-	0,6,6	0.00	-	-	-	
86	OHX	2	2021	-	0,6,6	0.00	-	-	-	
86	OHX	5	3600	-	0,6,6	0.00	-	-	-	
86	OHX	5	3690	-	0,6,6	0.00	-	-	-	
86	OHX	5	3512	86	0,6,6	0.00	-	-	-	
86	OHX	6	1948	80,86	0,6,6	0.00	-	-	-	
86	OHX	6	1946	-	0,6,6	0.00	-	-	-	
86	OHX	2	1976	86	0,6,6	0.00	-	-	-	
86	OHX	5	3732	86	0,6,6	0.00	-	-	-	
86	OHX	1	3527	-	0,6,6	0.00	-	-	-	
86	OHX	6	2062	-	0,6,6	0.00	-	-	-	
86	OHX	5	3784	-	0,6,6	0.00	-	-	-	
86	OHX	1	3768	86,36	0,6,6	0.00	-	-	-	
86	OHX	1	3648	-	0,6,6	0.00	-	-	-	
86	OHX	5	3647	36	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3703	36	0,6,6	0.00	-	-	-	
86	OHX	1	3623	-	0,6,6	0.00	-	-	-	
86	OHX	5	3557	36	0,6,6	0.00	-	-	-	
86	OHX	1	3654	-	0,6,6	0.00	-	-	-	
86	OHX	5	3484	-	0,6,6	0.00	-	-	-	
86	OHX	1	3537	-	0,6,6	0.00	-	-	-	
86	OHX	6	2024	80	0,6,6	0.00	-	-	-	
86	OHX	5	3742	-	0,6,6	0.00	-	-	-	
86	OHX	1	3456	86	0,6,6	0.00	-	-	-	
86	OHX	5	3777	-	0,6,6	0.00	-	-	-	
86	OHX	2	1939	-	0,6,6	0.00	-	-	-	
86	OHX	1	3662	-	0,6,6	0.00	-	-	-	
86	OHX	6	1993	80	0,6,6	0.00	-	-	-	
86	OHX	5	3585	-	0,6,6	0.00	-	-	-	
86	OHX	1	3673	-	0,6,6	0.00	-	-	-	
86	OHX	n3	201	-	0,6,6	0.00	-	-	-	
86	OHX	2	2013	1	0,6,6	0.00	-	-	-	
86	OHX	1	3555	-	0,6,6	0.00	-	-	-	
86	OHX	5	3760	86	0,6,6	0.00	-	-	-	
86	OHX	6	1975	80,86	0,6,6	0.00	-	-	-	
86	OHX	5	3808	86	0,6,6	0.00	-	-	-	
86	OHX	5	3753	86,36	0,6,6	0.00	-	-	-	
86	OHX	2	2083	-	0,6,6	0.00	-	-	-	
86	OHX	1	3510	36	0,6,6	0.00	-	-	-	
86	OHX	m4	201	-	0,6,6	0.00	-	-	-	
86	OHX	5	3514	86,36	0,6,6	0.00	-	-	-	
86	OHX	1	3480	86	0,6,6	0.00	-	-	-	
86	OHX	2	1991	1,86	0,6,6	0.00	-	-	-	
86	OHX	8	211	38	0,6,6	0.00	-	-	-	
86	OHX	2	2014	-	0,6,6	0.00	-	-	-	
86	OHX	5	3443	-	0,6,6	0.00	-	-	-	
86	OHX	1	3508	86	0,6,6	0.00	-	-	-	
86	OHX	5	3590	86	0,6,6	0.00	-	-	-	
86	OHX	1	3632	-	0,6,6	0.00	-	-	-	
86	OHX	1	3538	36	0,6,6	0.00	-	-	-	
86	OHX	1	3652	-	0,6,6	0.00	-	-	-	
86	OHX	5	3719	36	0,6,6	0.00	-	-	-	
86	OHX	4	205	-	0,6,6	0.00	-	-	-	
86	OHX	1	3784	-	0,6,6	0.00	-	-	-	
86	OHX	5	3405	36	0,6,6	0.00	-	-	-	
86	OHX	1	3757	86,36	0,6,6	0.00	-	-	-	
86	OHX	1	3749	-	0,6,6	0.00	-	-	-	
86	OHX	2	2065	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3570	-	0,6,6	0.00	-	-	-	-
86	OHX	c8	201	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1907	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3698	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3758	36	0,6,6	0.00	-	-	-	-
86	OHX	15	301	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3617	86,36	0,6,6	0.00	-	-	-	-
86	OHX	6	1933	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3785	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3595	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2046	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3595	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3626	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3453	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3439	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3621	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1902	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3577	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3816	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3414	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3640	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1951	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2084	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3799	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3474	36	0,6,6	0.00	-	-	-	-
86	OHX	2	2007	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3583	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3575	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3425	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3430	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1923	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1959	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3742	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3591	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2046	1	0,6,6	0.00	-	-	-	-
86	OHX	5	3412	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3602	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3692	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1926	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3609	-	0,6,6	0.00	-	-	-	-
86	OHX	8	203	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2092	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3624	86,36	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3430	36	0,6,6	0.00	-	-	-	
86	OHX	5	3603	36	0,6,6	0.00	-	-	-	
86	OHX	1	3787	-	0,6,6	0.00	-	-	-	
86	OHX	5	3537	36	0,6,6	0.00	-	-	-	
86	OHX	5	3675	36	0,6,6	0.00	-	-	-	
86	OHX	6	2085	80	0,6,6	0.00	-	-	-	
86	OHX	5	3564	86	0,6,6	0.00	-	-	-	
86	OHX	6	1901	80	0,6,6	0.00	-	-	-	
86	OHX	1	3427	-	0,6,6	0.00	-	-	-	
86	OHX	1	3814	86,36	0,6,6	0.00	-	-	-	
86	OHX	1	3719	-	0,6,6	0.00	-	-	-	
86	OHX	1	3713	-	0,6,6	0.00	-	-	-	
86	OHX	1	3655	-	0,6,6	0.00	-	-	-	
86	OHX	1	3605	86	0,6,6	0.00	-	-	-	
86	OHX	5	3510	-	0,6,6	0.00	-	-	-	
86	OHX	2	1958	-	0,6,6	0.00	-	-	-	
86	OHX	2	2075	-	0,6,6	0.00	-	-	-	
86	OHX	O1	201	86	0,6,6	0.00	-	-	-	
86	OHX	6	1995	-	0,6,6	0.00	-	-	-	
86	OHX	1	3466	-	0,6,6	0.00	-	-	-	
86	OHX	5	3701	36	0,6,6	0.00	-	-	-	
86	OHX	O3	201	-	0,6,6	0.00	-	-	-	
86	OHX	5	3435	-	0,6,6	0.00	-	-	-	
86	OHX	6	1956	-	0,6,6	0.00	-	-	-	
86	OHX	6	2095	-	0,6,6	0.00	-	-	-	
86	OHX	1	3573	-	0,6,6	0.00	-	-	-	
86	OHX	5	3783	36	0,6,6	0.00	-	-	-	
86	OHX	2	2072	-	0,6,6	0.00	-	-	-	
86	OHX	5	3463	-	0,6,6	0.00	-	-	-	
86	OHX	1	3674	-	0,6,6	0.00	-	-	-	
86	OHX	5	3770	-	0,6,6	0.00	-	-	-	
86	OHX	1	3755	36	0,6,6	0.00	-	-	-	
86	OHX	5	3444	36	0,6,6	0.00	-	-	-	
86	OHX	6	1950	80	0,6,6	0.00	-	-	-	
86	OHX	5	3617	-	0,6,6	0.00	-	-	-	
86	OHX	2	2044	-	0,6,6	0.00	-	-	-	
86	OHX	6	2017	80	0,6,6	0.00	-	-	-	
86	OHX	1	3601	86	0,6,6	0.00	-	-	-	
86	OHX	1	3489	86	0,6,6	0.00	-	-	-	
86	OHX	5	3502	86,36	0,6,6	0.00	-	-	-	
86	OHX	2	1983	-	0,6,6	0.00	-	-	-	
86	OHX	5	3737	36	0,6,6	0.00	-	-	-	
86	OHX	n9	101	-	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3702	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3520	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3619	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1974	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3457	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3407	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3529	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3474	-	0,6,6	0.00	-	-	-	-
86	OHX	m0	304	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3753	86	0,6,6	0.00	-	-	-	-
86	OHX	2	2033	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1984	80	0,6,6	0.00	-	-	-	-
86	OHX	6	2007	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3613	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1985	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3646	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3465	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3468	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3405	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3729	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3775	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3459	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3563	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3453	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3733	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2098	86	0,6,6	0.00	-	-	-	-
86	OHX	2	2000	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1963	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3704	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1964	80	0,6,6	0.00	-	-	-	-
86	OHX	2	2051	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3794	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3513	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3677	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3810	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3680	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3440	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3669	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1921	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3801	86	0,6,6	0.00	-	-	-	-
86	OHX	6	1939	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3813	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3577	36	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	c1	201	86	0,6,6	0.00	-	-	-	
86	OHX	6	1927	80	0,6,6	0.00	-	-	-	
86	OHX	2	1967	-	0,6,6	0.00	-	-	-	
86	OHX	5	3665	-	0,6,6	0.00	-	-	-	
86	OHX	5	3592	-	0,6,6	0.00	-	-	-	
86	OHX	7	212	-	0,6,6	0.00	-	-	-	
86	OHX	6	2006	-	0,6,6	0.00	-	-	-	
86	OHX	2	1950	-	0,6,6	0.00	-	-	-	
86	OHX	5	3751	-	0,6,6	0.00	-	-	-	
86	OHX	5	3704	86	0,6,6	0.00	-	-	-	
86	OHX	5	3504	-	0,6,6	0.00	-	-	-	
86	OHX	1	3670	-	0,6,6	0.00	-	-	-	
86	OHX	5	3476	-	0,6,6	0.00	-	-	-	
86	OHX	1	3464	86	0,6,6	0.00	-	-	-	
86	OHX	8	210	-	0,6,6	0.00	-	-	-	
86	OHX	1	3519	36	0,6,6	0.00	-	-	-	
86	OHX	C8	201	86	0,6,6	0.00	-	-	-	
86	OHX	1	3562	86	0,6,6	0.00	-	-	-	
86	OHX	6	2084	86	0,6,6	0.00	-	-	-	
86	OHX	C8	202	86,36	0,6,6	0.00	-	-	-	
86	OHX	2	2004	-	0,6,6	0.00	-	-	-	
86	OHX	6	2043	86	0,6,6	0.00	-	-	-	
86	OHX	s1	301	-	0,6,6	0.00	-	-	-	
86	OHX	1	3434	-	0,6,6	0.00	-	-	-	
86	OHX	5	3524	86	0,6,6	0.00	-	-	-	
86	OHX	2	2085	86	0,6,6	0.00	-	-	-	
86	OHX	1	3808	86	0,6,6	0.00	-	-	-	
86	OHX	1	3715	86	0,6,6	0.00	-	-	-	
86	OHX	1	3418	-	0,6,6	0.00	-	-	-	
86	OHX	5	3716	86	0,6,6	0.00	-	-	-	
86	OHX	1	3486	-	0,6,6	0.00	-	-	-	
86	OHX	2	2057	-	0,6,6	0.00	-	-	-	
86	OHX	1	3726	-	0,6,6	0.00	-	-	-	
86	OHX	5	3807	86,36	0,6,6	0.00	-	-	-	
86	OHX	5	3801	86	0,6,6	0.00	-	-	-	
86	OHX	6	1998	80	0,6,6	0.00	-	-	-	
86	OHX	5	3459	36	0,6,6	0.00	-	-	-	
86	OHX	4	208	38	0,6,6	0.00	-	-	-	
86	OHX	4	209	-	0,6,6	0.00	-	-	-	
86	OHX	1	3752	-	0,6,6	0.00	-	-	-	
86	OHX	5	3728	-	0,6,6	0.00	-	-	-	
86	OHX	2	1966	-	0,6,6	0.00	-	-	-	
86	OHX	1	3738	86	0,6,6	0.00	-	-	-	

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	m9	201	-	0,6,6	0.00	-	-	-	-
86	OHX	2	2040	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3599	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3749	86	0,6,6	0.00	-	-	-	-
86	OHX	3	205	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3540	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3813	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3764	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3769	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3471	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3478	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3480	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3722	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3703	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3498	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3739	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3507	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1913	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3803	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2055	-	0,6,6	0.00	-	-	-	-
86	OHX	6	1916	-	0,6,6	0.00	-	-	-	-
86	OHX	6	2050	80	0,6,6	0.00	-	-	-	-
86	OHX	5	3709	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3627	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3578	-	0,6,6	0.00	-	-	-	-
86	OHX	7	205	-	0,6,6	0.00	-	-	-	-
86	OHX	2	1948	86	0,6,6	0.00	-	-	-	-
86	OHX	5	3654	86	0,6,6	0.00	-	-	-	-
86	OHX	2	1945	86	0,6,6	0.00	-	-	-	-
86	OHX	1	3606	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2049	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3629	36	0,6,6	0.00	-	-	-	-
86	OHX	6	1986	-	0,6,6	0.00	-	-	-	-
86	OHX	1	3472	36	0,6,6	0.00	-	-	-	-
86	OHX	1	3712	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3767	86,36	0,6,6	0.00	-	-	-	-
86	OHX	6	1981	-	0,6,6	0.00	-	-	-	-
86	OHX	5	3762	36	0,6,6	0.00	-	-	-	-
86	OHX	5	3503	36	0,6,6	0.00	-	-	-	-
86	OHX	6	1954	86	0,6,6	0.00	-	-	-	-
86	OHX	6	2076	80	0,6,6	0.00	-	-	-	-
86	OHX	1	3409	36	0,6,6	0.00	-	-	-	-
86	OHX	6	1911	80	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2068	80,86	0,6,6	0.00	-	-	-	
86	OHX	5	3646	-	0,6,6	0.00	-	-	-	
86	OHX	5	3814	86	0,6,6	0.00	-	-	-	
86	OHX	1	3679	-	0,6,6	0.00	-	-	-	
86	OHX	6	2057	80,86	0,6,6	0.00	-	-	-	
86	OHX	2	1937	-	0,6,6	0.00	-	-	-	
86	OHX	6	1967	-	0,6,6	0.00	-	-	-	
86	OHX	2	1910	1	0,6,6	0.00	-	-	-	
86	OHX	8	220	-	0,6,6	0.00	-	-	-	
86	OHX	1	3484	-	0,6,6	0.00	-	-	-	
86	OHX	5	3470	-	0,6,6	0.00	-	-	-	
86	OHX	1	3800	86	0,6,6	0.00	-	-	-	
86	OHX	5	3473	-	0,6,6	0.00	-	-	-	
86	OHX	5	3804	86,36	0,6,6	0.00	-	-	-	
86	OHX	5	3494	-	0,6,6	0.00	-	-	-	
86	OHX	1	3583	-	0,6,6	0.00	-	-	-	
86	OHX	2	2086	-	0,6,6	0.00	-	-	-	
86	OHX	2	2079	-	0,6,6	0.00	-	-	-	
86	OHX	6	2051	-	0,6,6	0.00	-	-	-	
86	OHX	5	3815	86	0,6,6	0.00	-	-	-	
86	OHX	2	2039	86	0,6,6	0.00	-	-	-	
86	OHX	5	3748	-	0,6,6	0.00	-	-	-	
86	OHX	2	2070	86	0,6,6	0.00	-	-	-	
86	OHX	1	3783	86	0,6,6	0.00	-	-	-	
86	OHX	2	1921	86	0,6,6	0.00	-	-	-	

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	8AN	5	3403	89	-	0/3/25/26	0/3/3/3
90	8AN	1	3403	89	-	0/3/25/26	0/3/3/3

All (4) bond length outliers are listed below:

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

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	5	3403	8AN	N3-C2-N1	-3.18	123.70	128.68
90	1	3403	8AN	N3-C2-N1	-3.17	123.72	128.68
90	1	3403	8AN	C4-C5-N7	-2.71	106.58	109.40
90	1	3403	8AN	C2'-C3'-C4'	2.61	106.32	102.68
90	5	3403	8AN	C2'-C3'-C4'	2.57	106.27	102.68

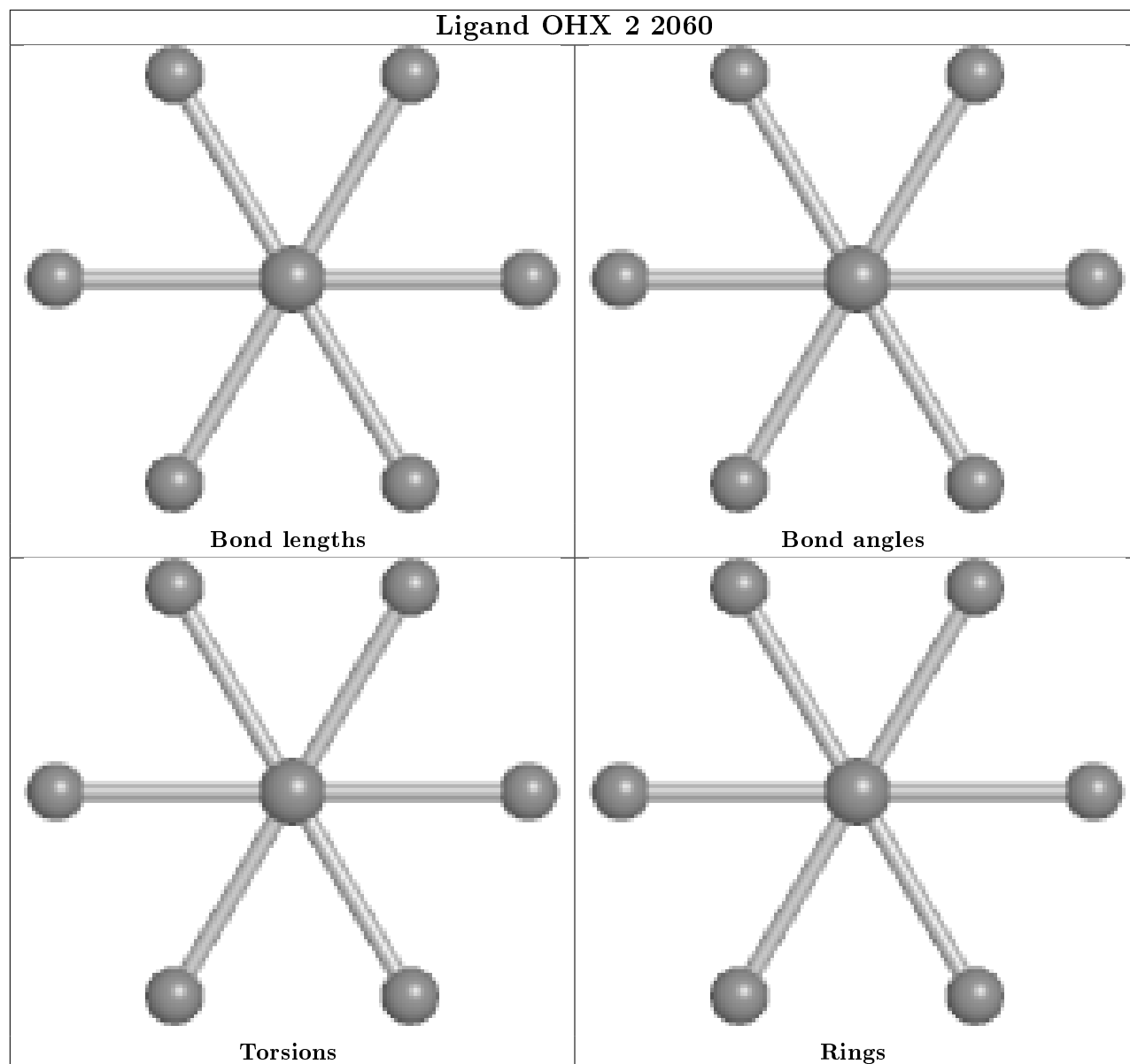
There are no chirality outliers.

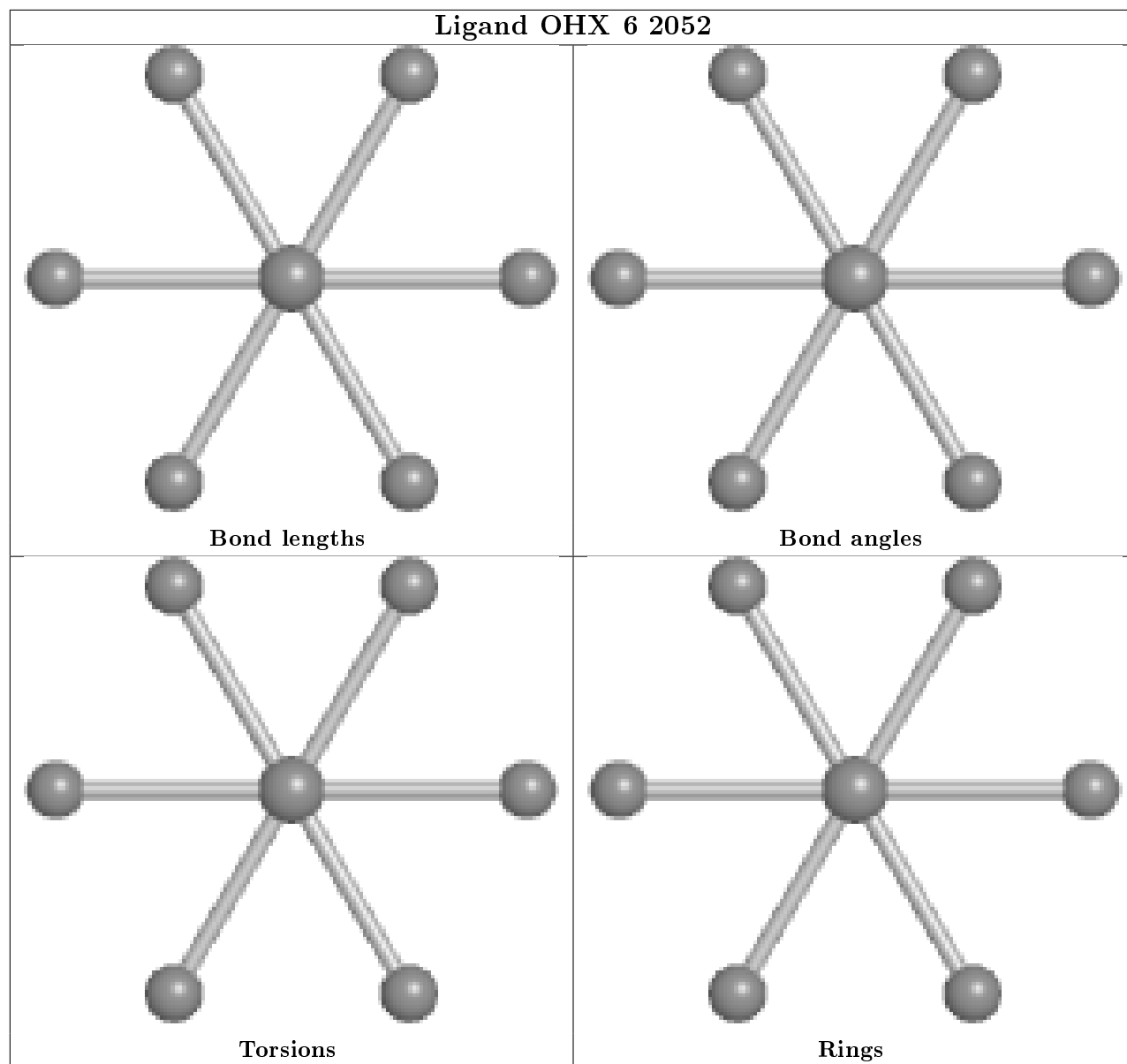
There are no torsion outliers.

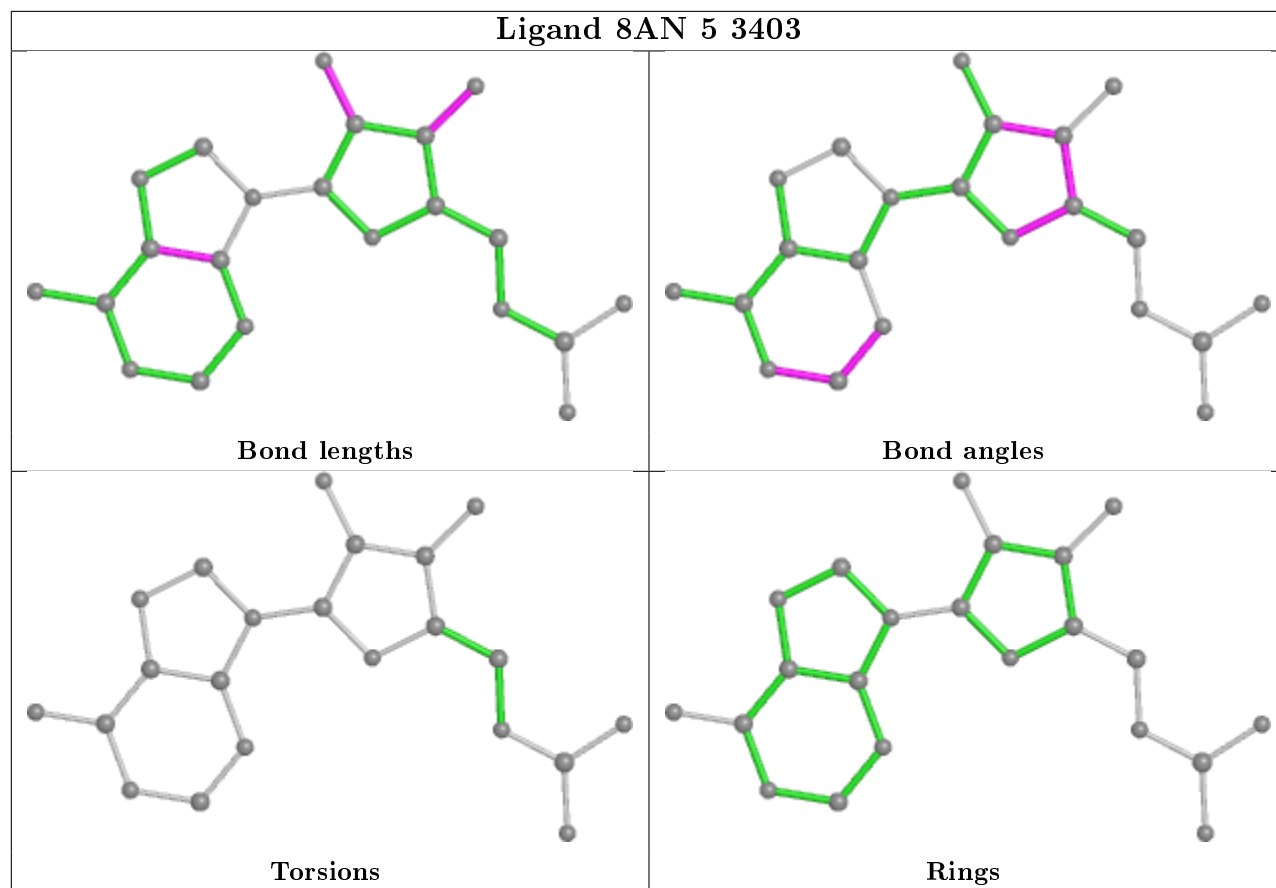
There are no ring outliers.

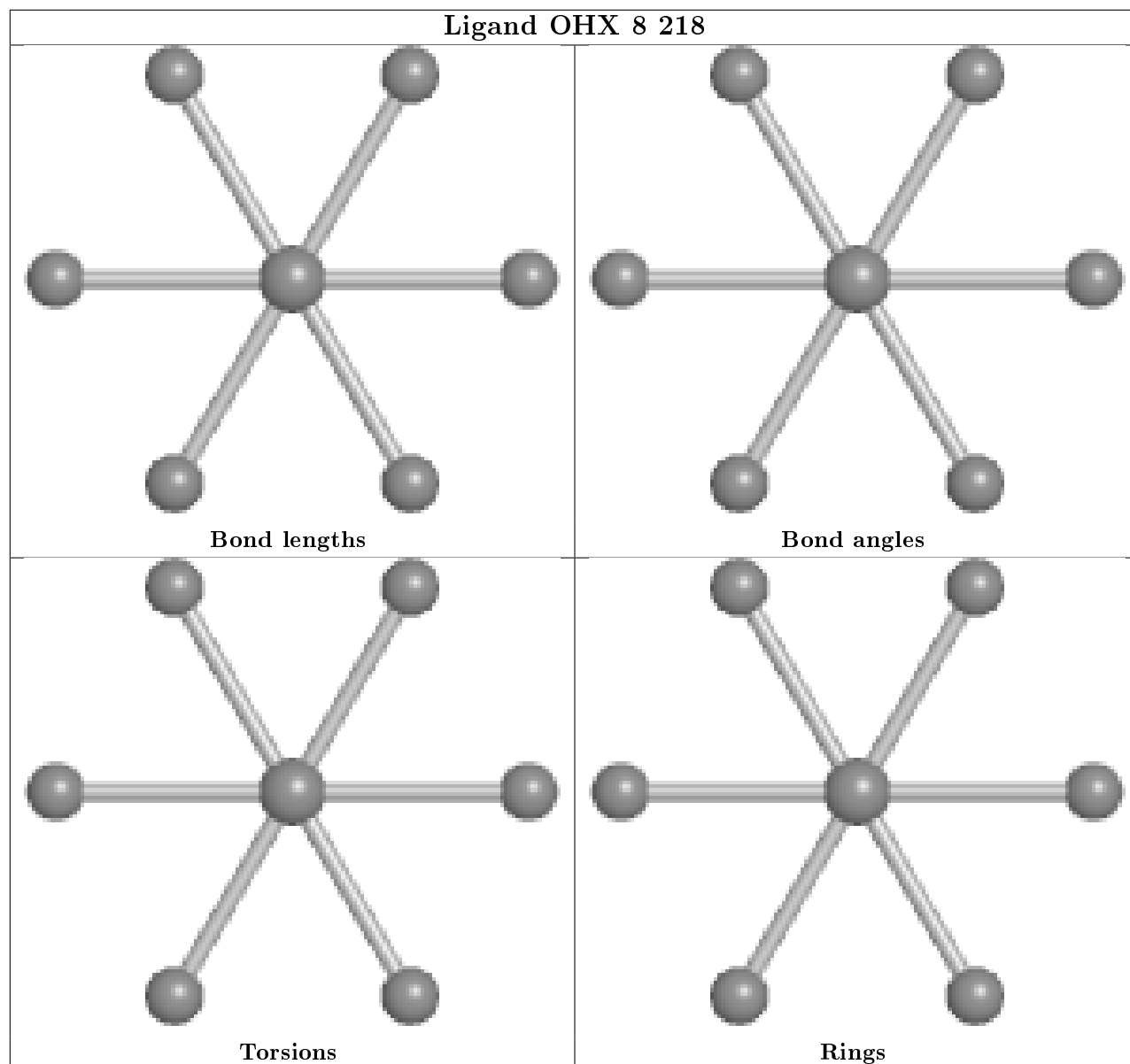
No monomer is involved in short contacts.

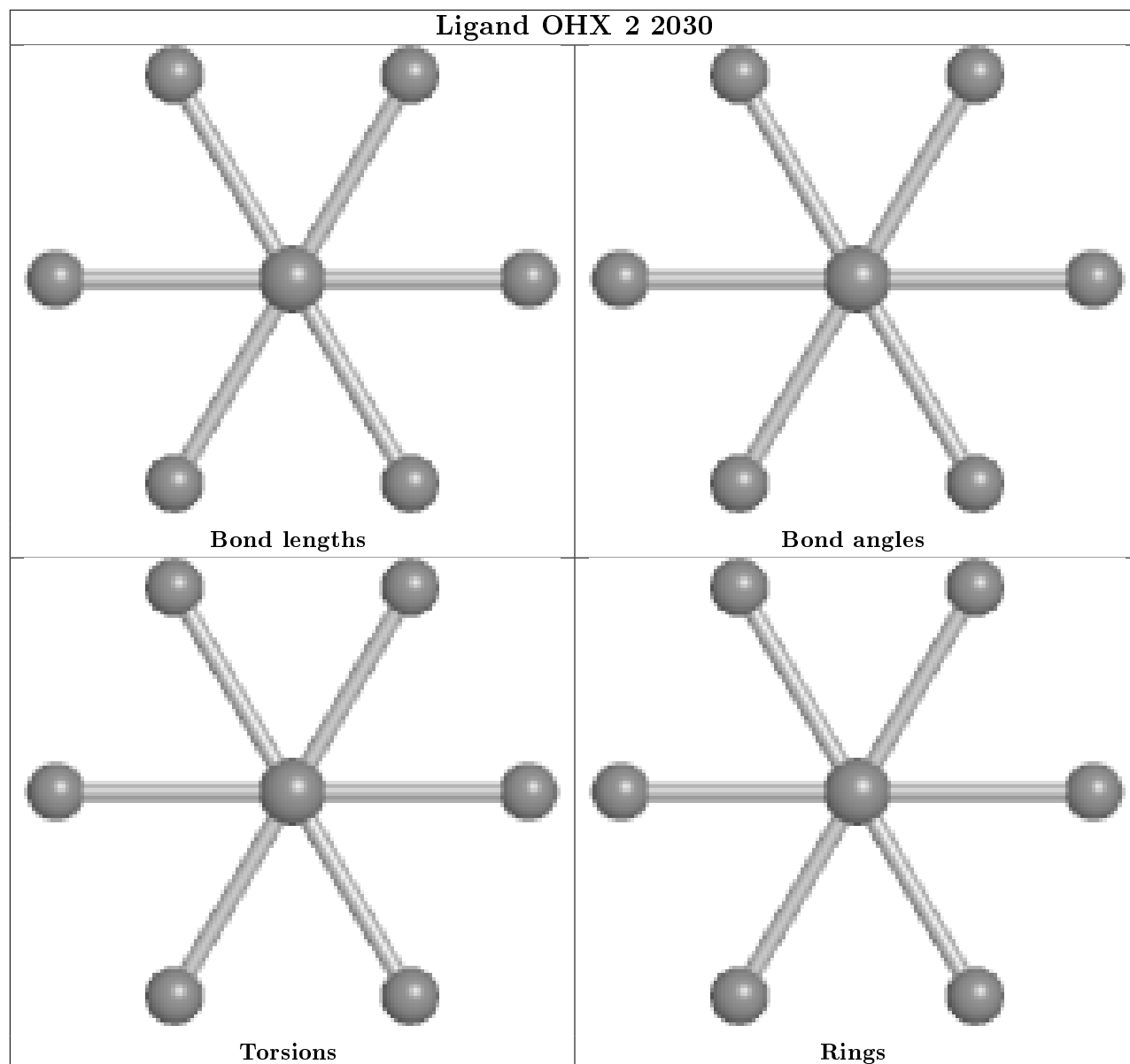
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

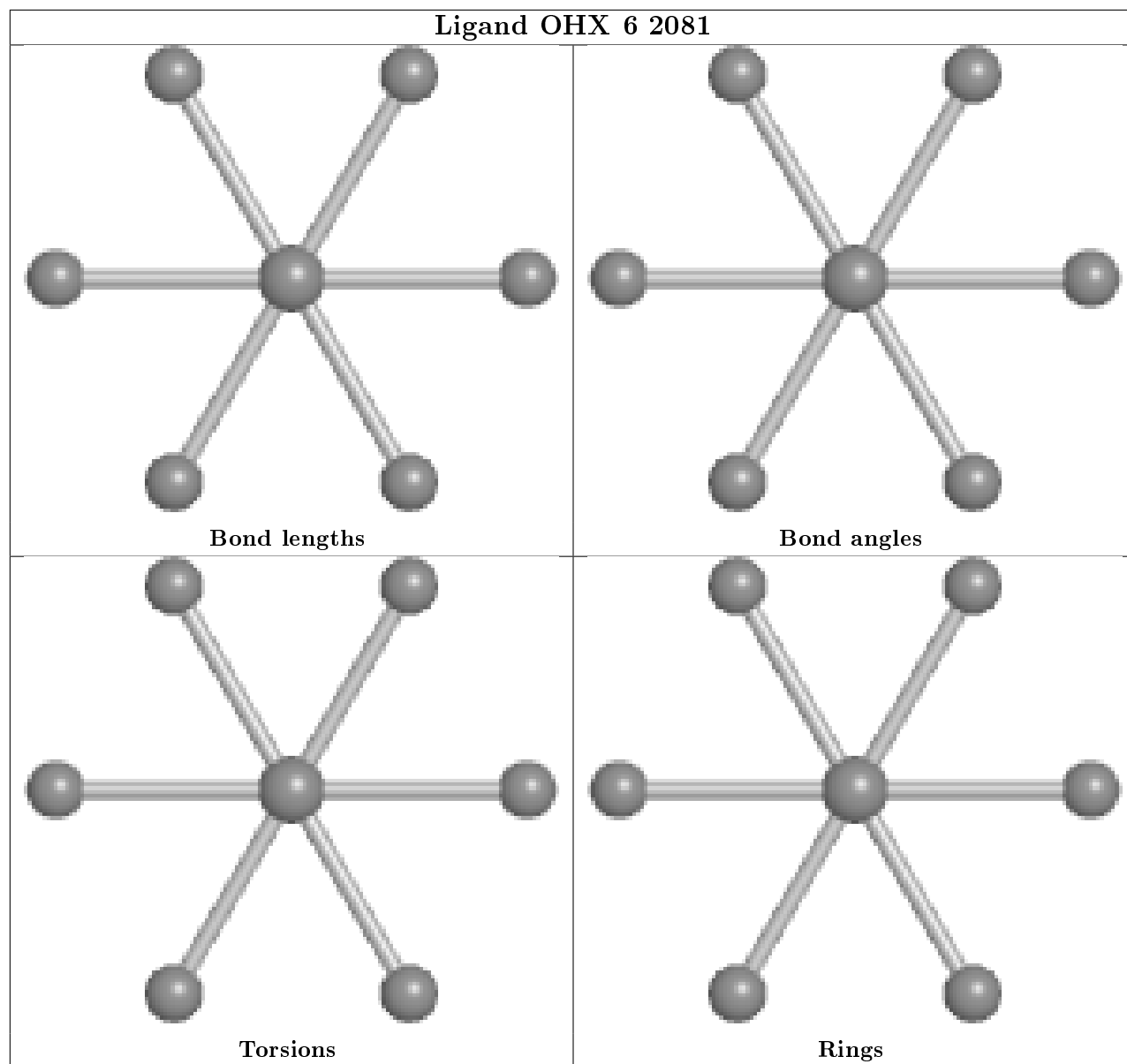


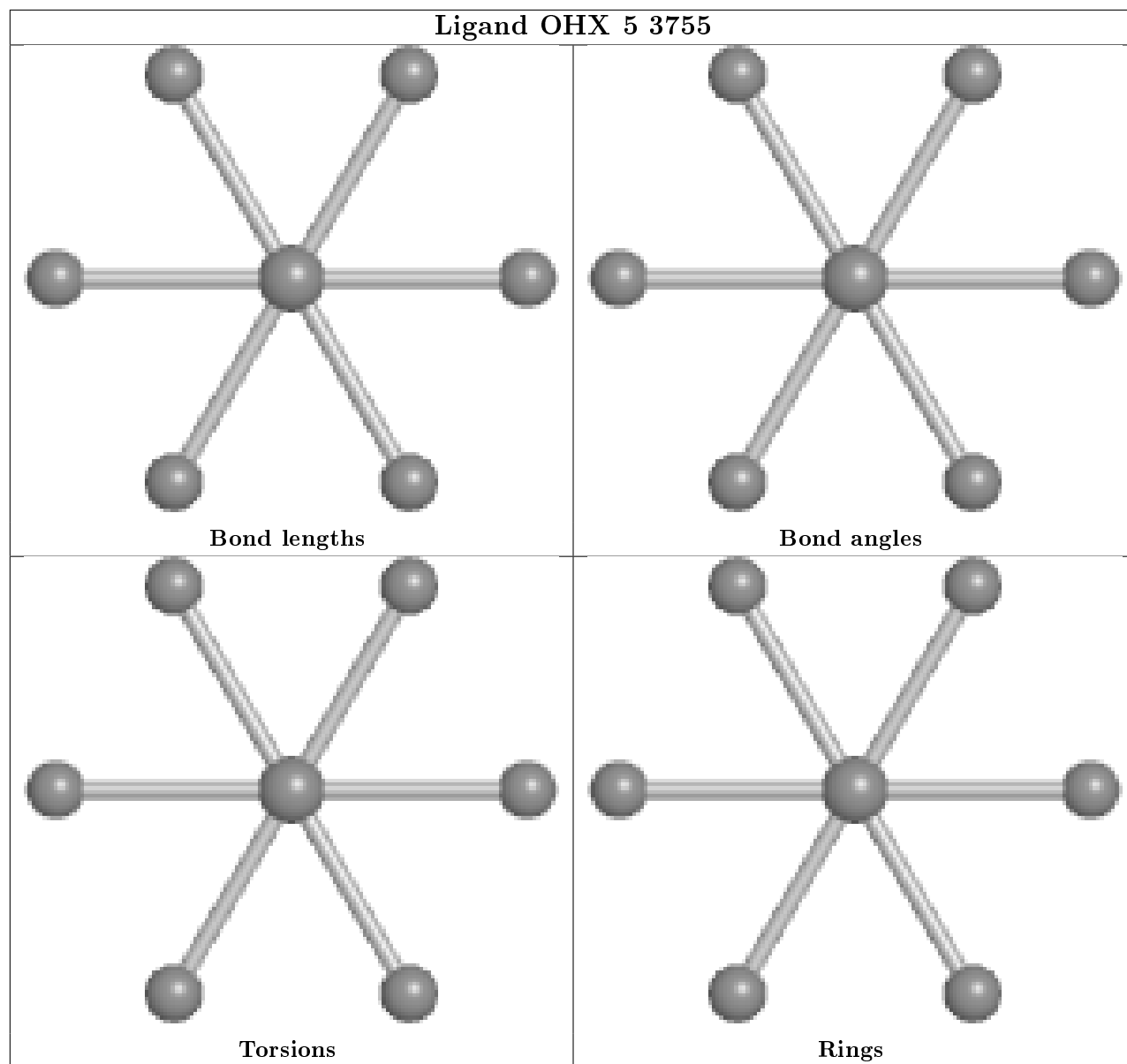


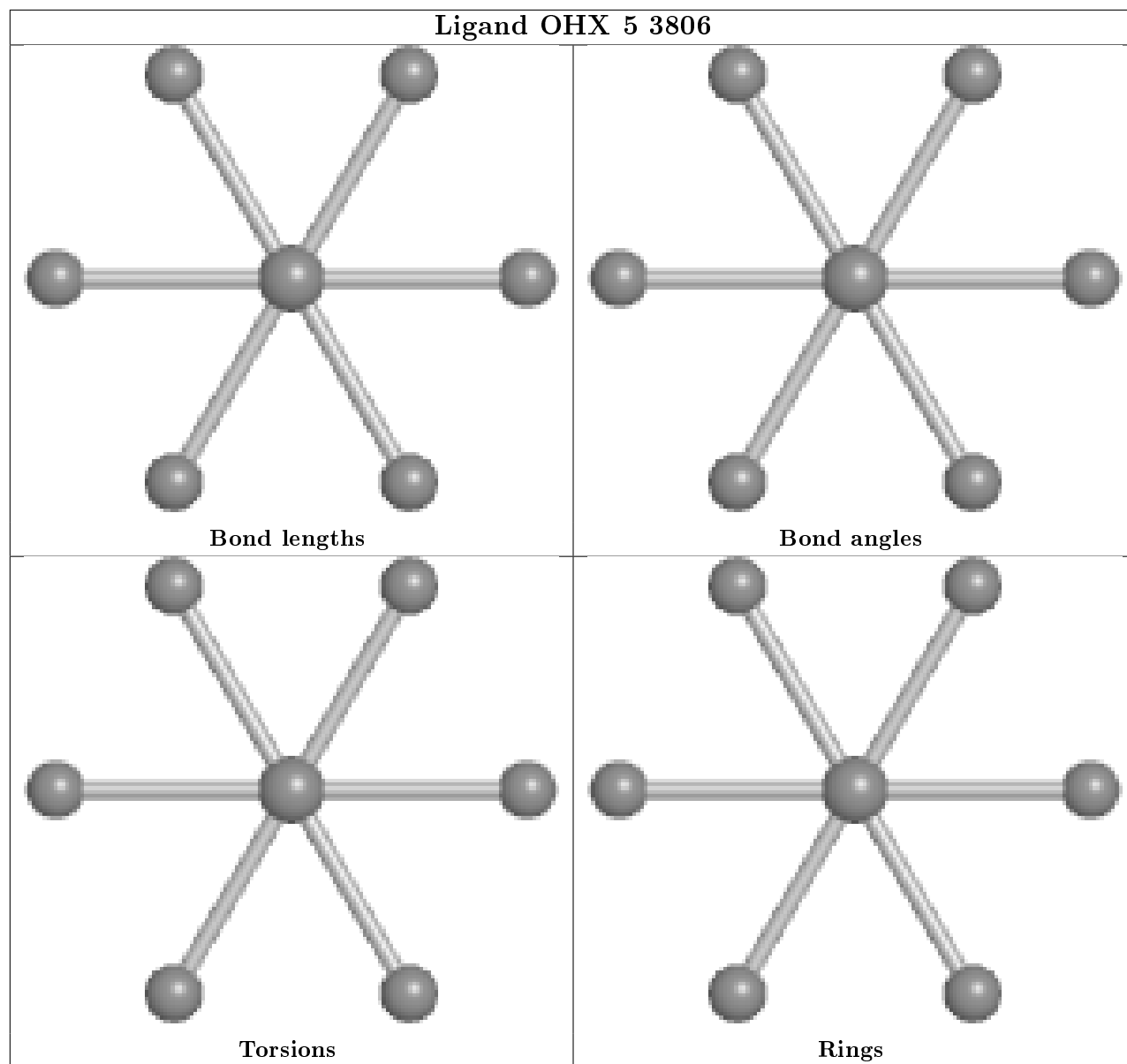


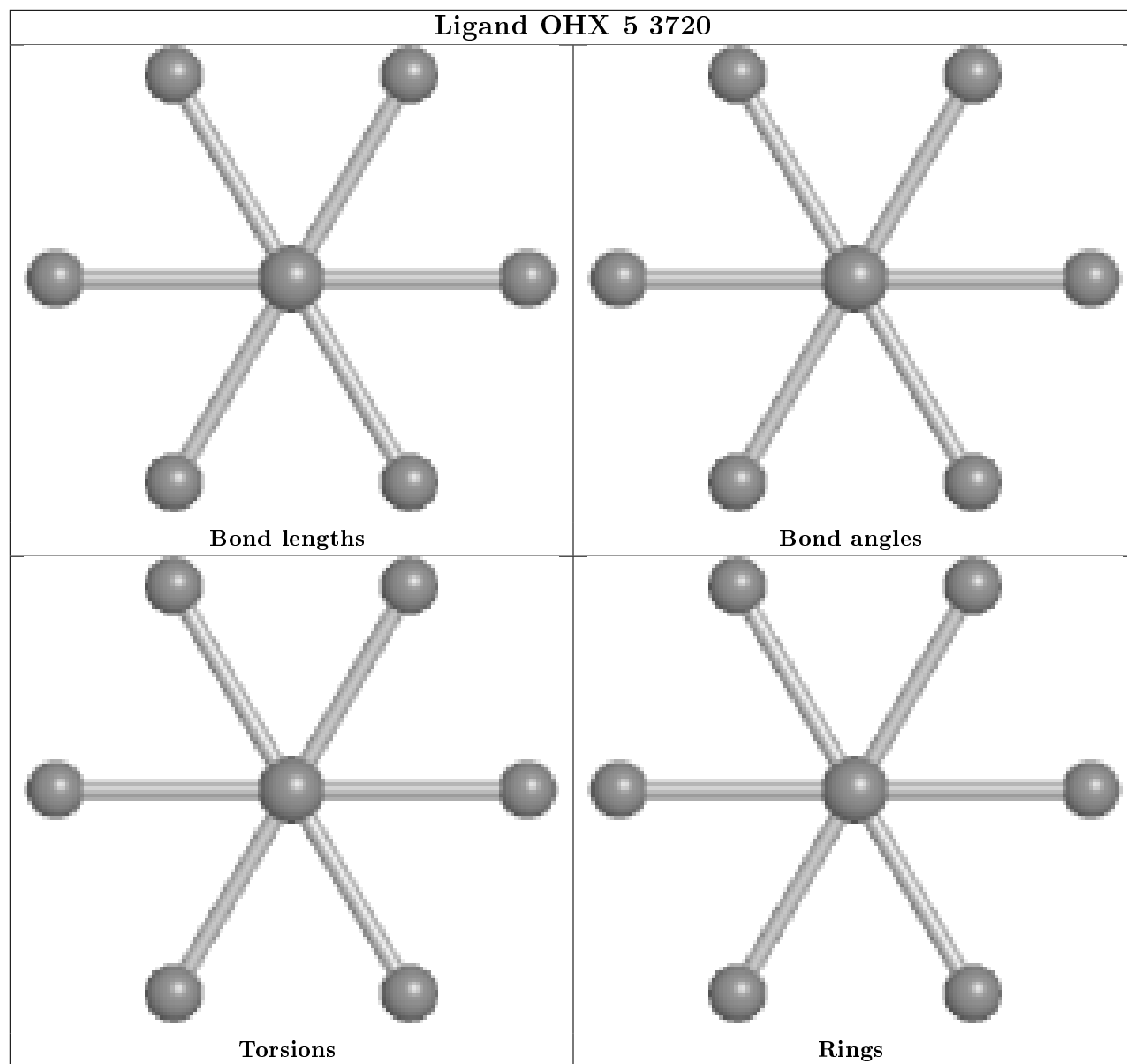


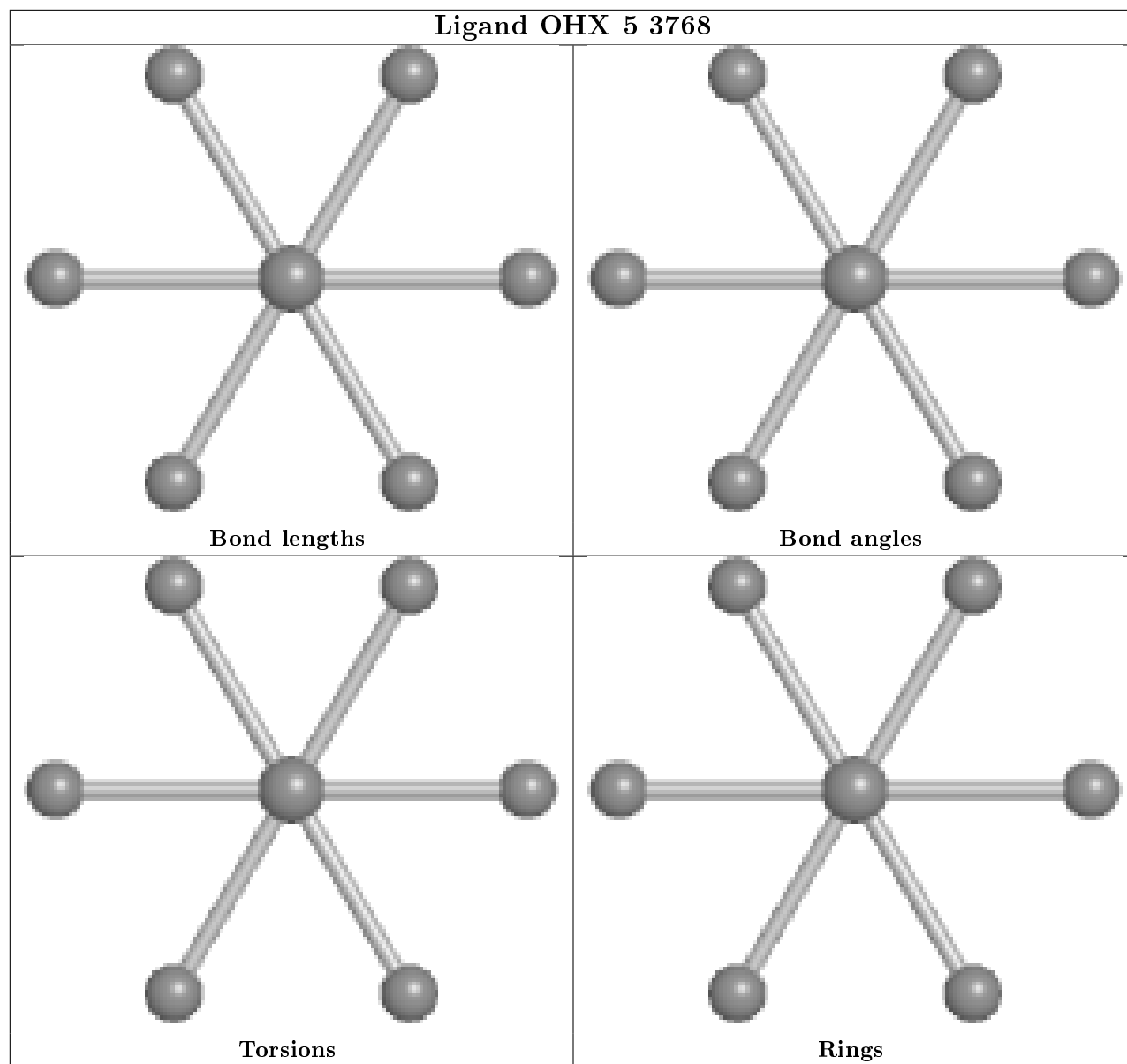


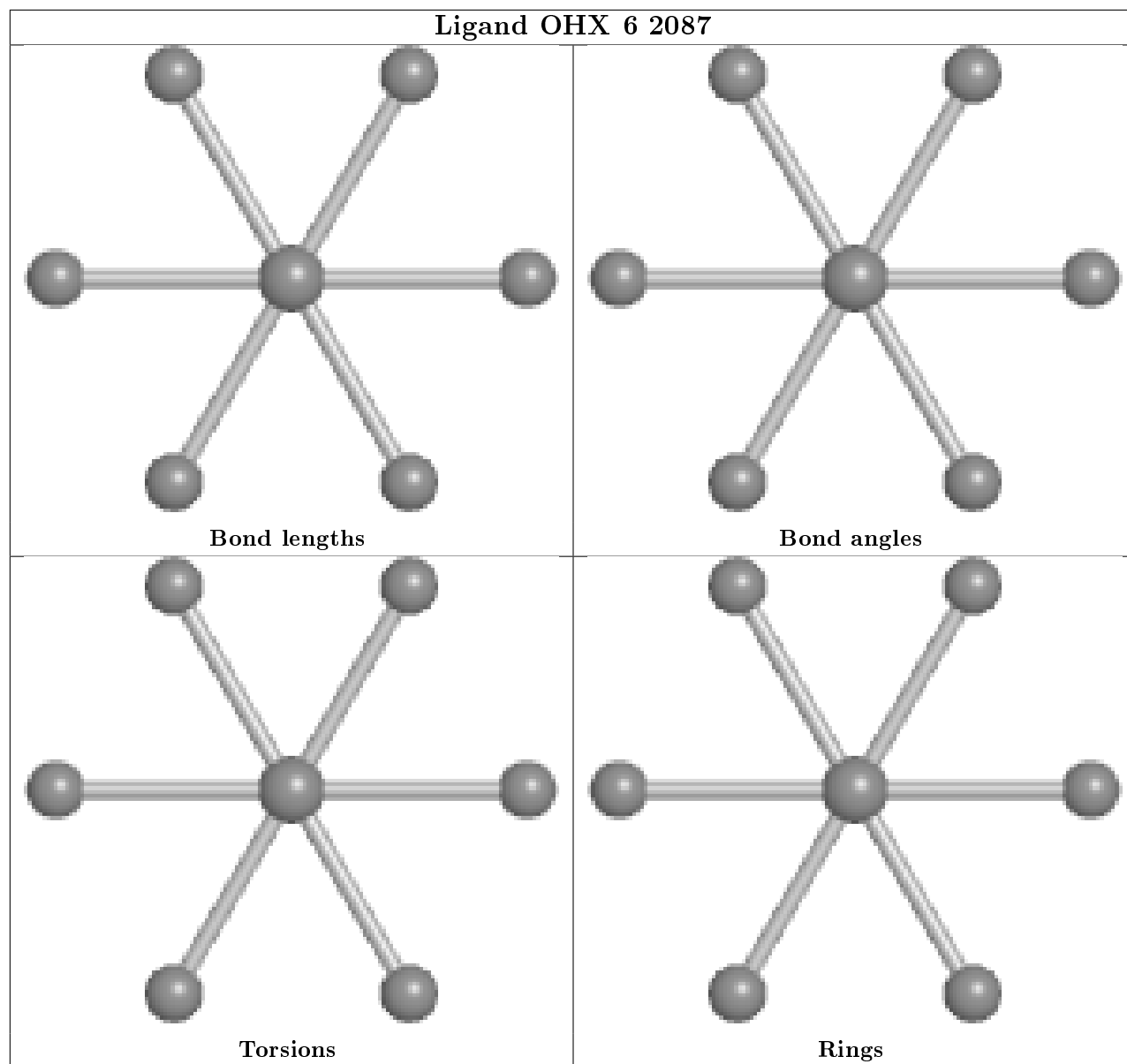


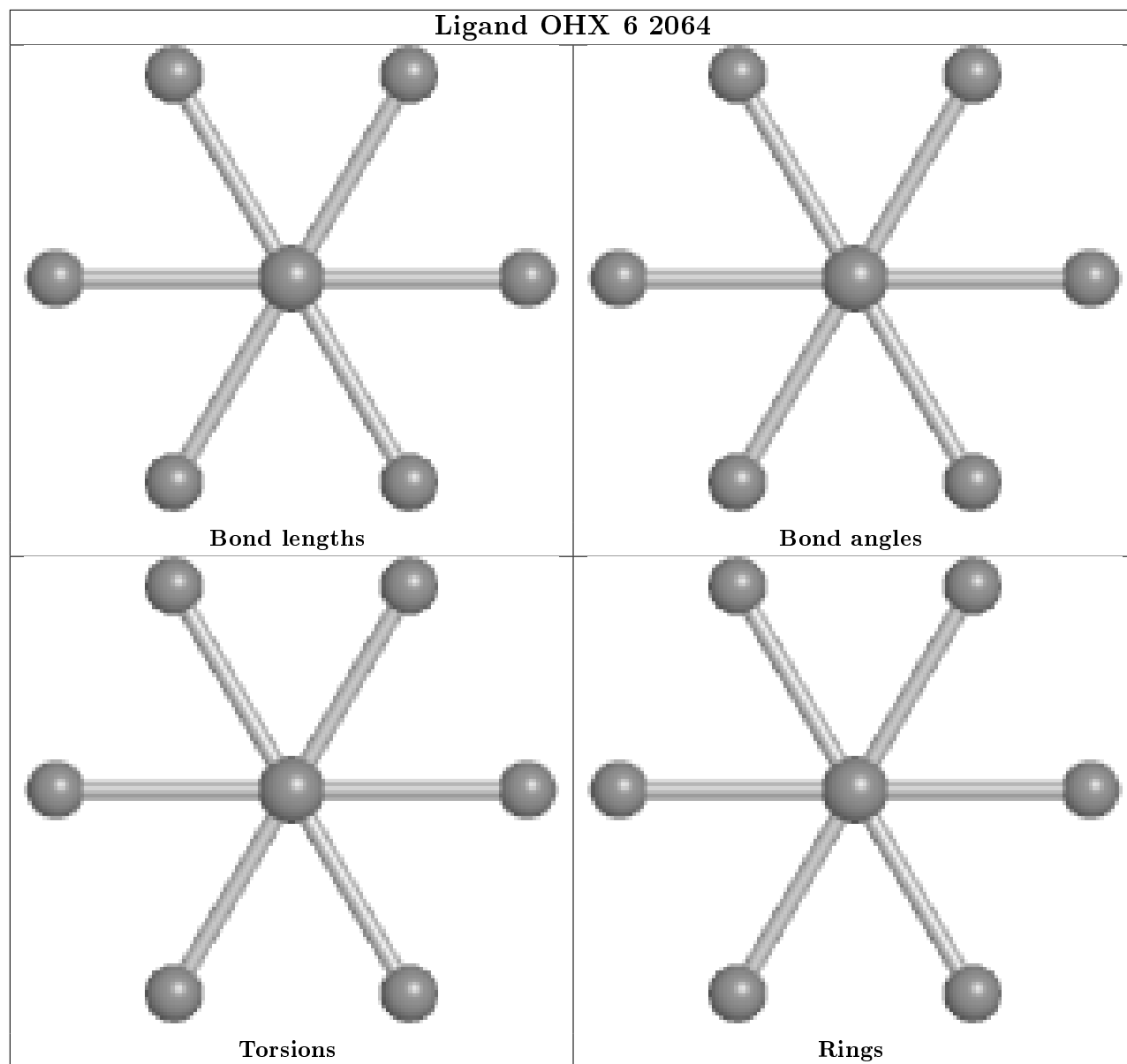


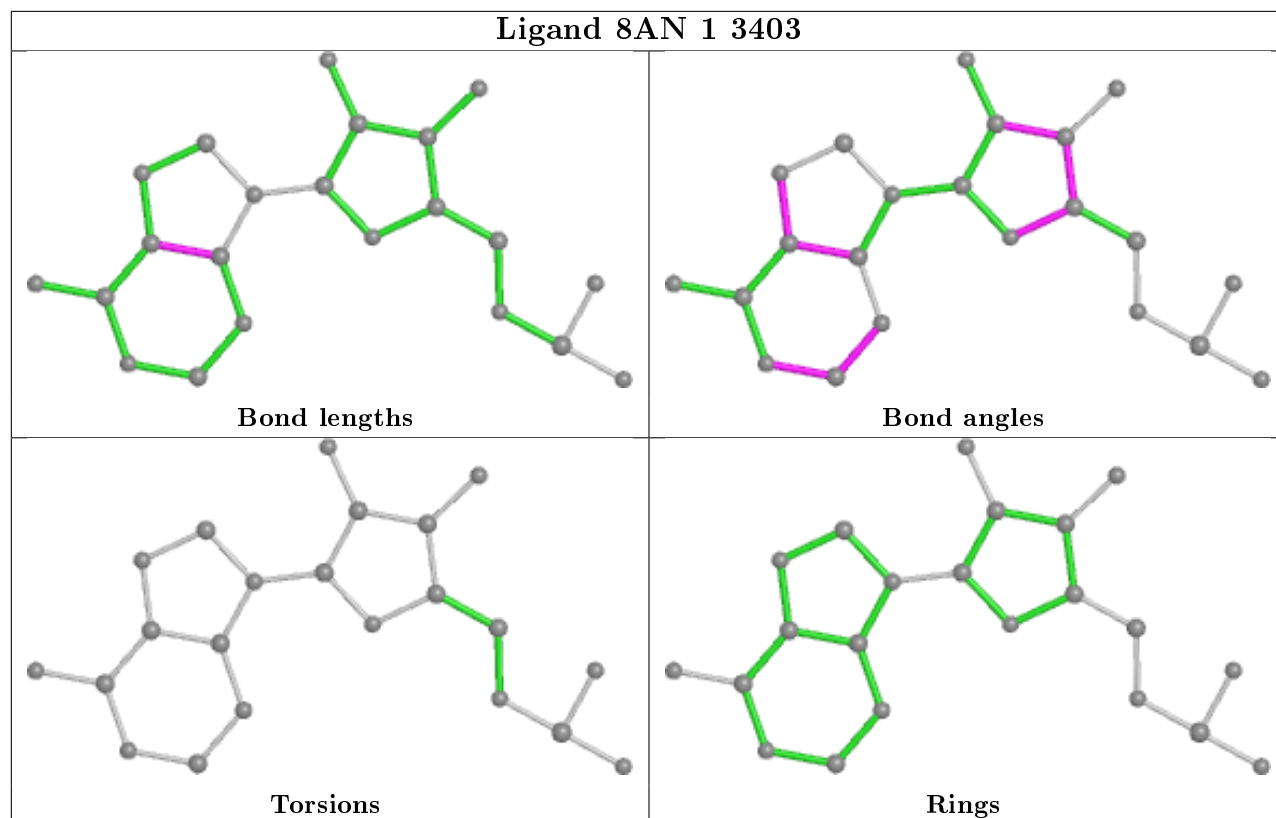


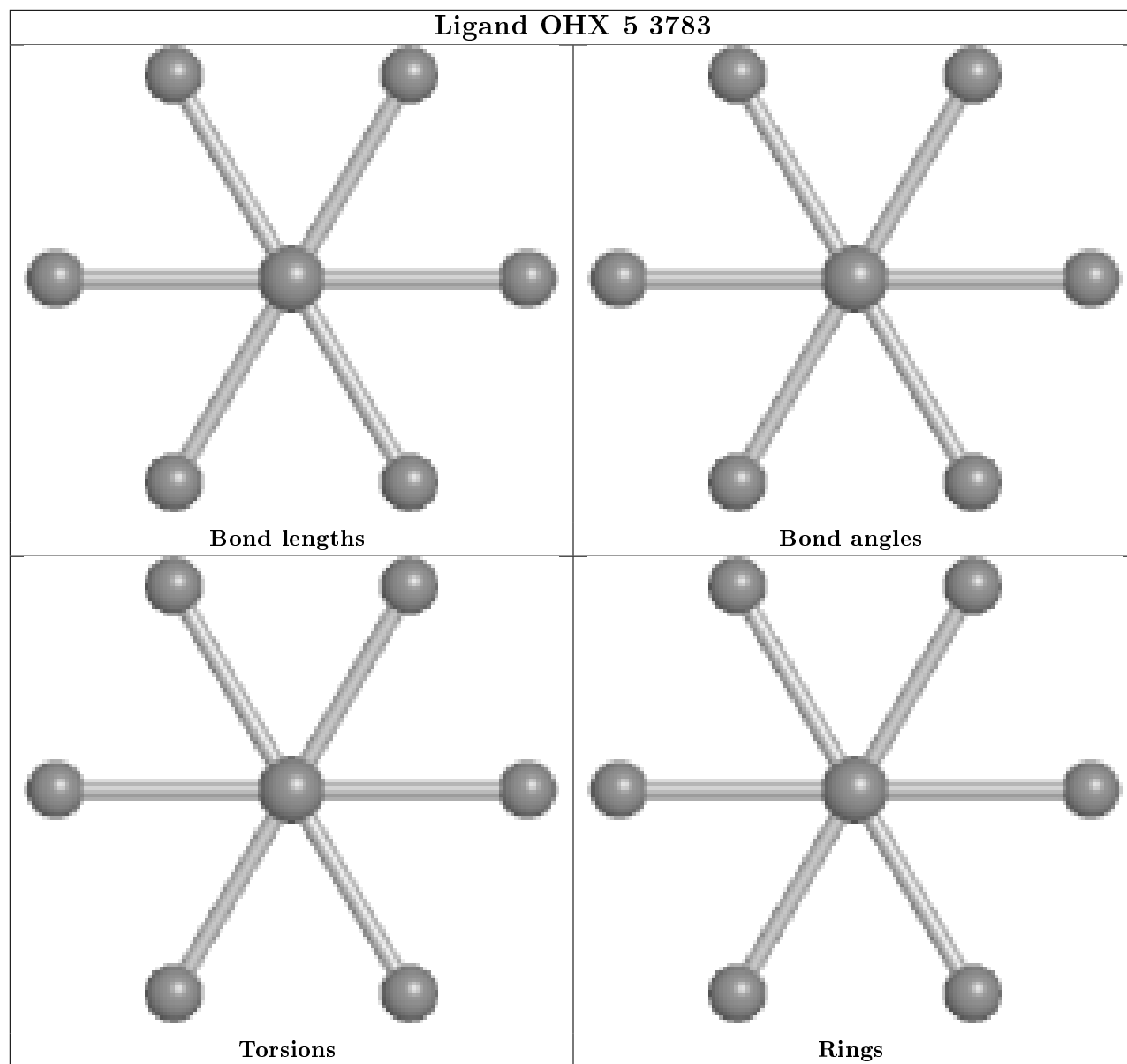


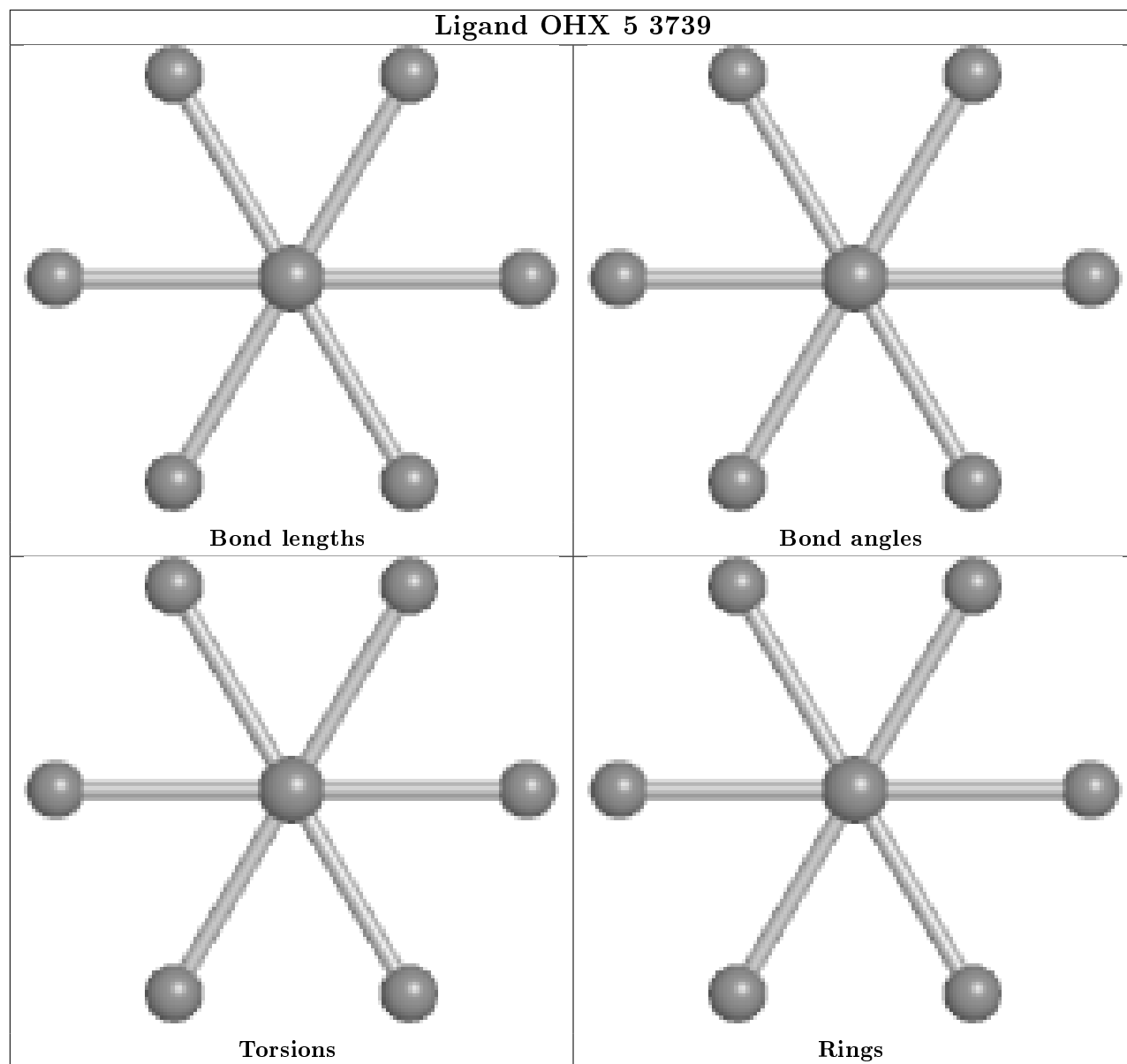


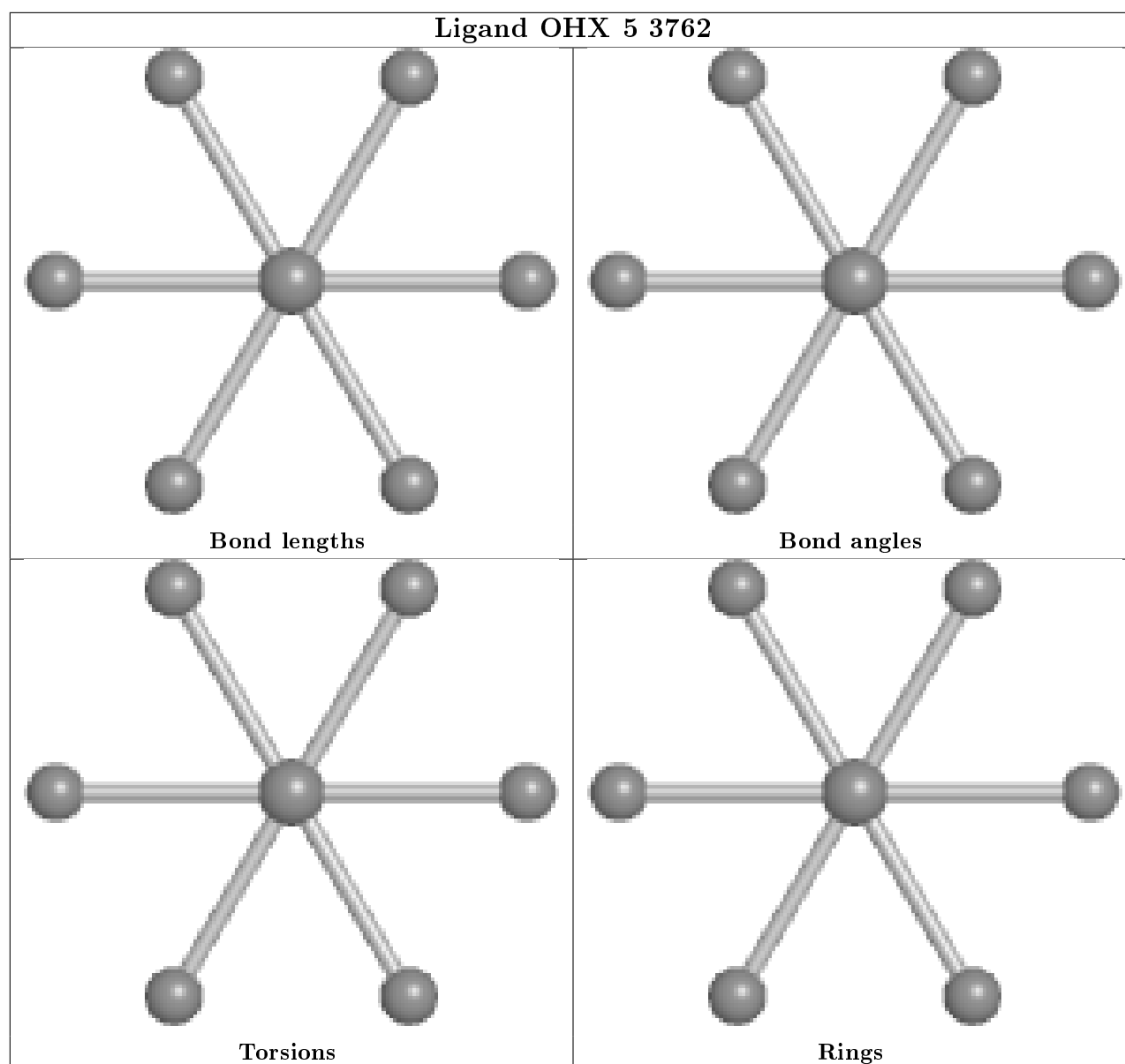












5.7 Other polymers [i](#)

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
83	m2	2
82	sM	2
2	S0	1

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Mol	Chain	Number of breaks
35	SM	1
81	c0	1
47	m0	1
1	2	1

The worst 5 of 9 chain breaks are listed below:

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

6 Fit of model and data 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	1781/1829 (97%)	0.31	92 (5%) 27 25	53, 90, 174, 223	0
2	S0	206/206 (100%)	1.99	97 (47%) 0 0	91, 107, 116, 121	0
2	s0	206/206 (100%)	1.06	36 (17%) 1 1	68, 84, 96, 105	0
3	S1	214/216 (99%)	1.09	50 (23%) 0 1	104, 134, 158, 165	0
3	s1	216/216 (100%)	1.06	39 (18%) 1 1	72, 84, 102, 115	0
4	S2	217/217 (100%)	0.31	11 (5%) 28 26	75, 86, 98, 108	0
4	s2	217/217 (100%)	0.44	8 (3%) 41 38	55, 68, 78, 87	0
5	S3	223/223 (100%)	0.65	24 (10%) 5 5	82, 93, 112, 124	0
5	s3	223/223 (100%)	0.69	25 (11%) 5 5	74, 99, 116, 124	0
6	S4	260/260 (100%)	1.81	101 (38%) 0 0	69, 91, 98, 119	0
6	s4	260/260 (100%)	0.95	43 (16%) 1 2	47, 69, 82, 106	0
7	S5	206/206 (100%)	0.76	31 (15%) 2 2	96, 112, 124, 132	0
7	s5	206/206 (100%)	1.01	45 (21%) 0 1	79, 97, 113, 121	0
8	S6	226/226 (100%)	0.65	27 (11%) 4 4	72, 106, 120, 125	0
8	s6	218/226 (96%)	0.50	21 (9%) 8 8	49, 77, 94, 110	0
9	S7	184/186 (98%)	0.40	10 (5%) 25 24	90, 114, 139, 144	0
9	s7	186/186 (100%)	0.12	4 (2%) 62 60	65, 96, 124, 132	0
10	S8	188/199 (94%)	1.00	30 (15%) 1 2	63, 79, 113, 125	0
10	s8	188/199 (94%)	0.58	17 (9%) 9 9	46, 66, 107, 124	0
11	S9	185/185 (100%)	1.74	65 (35%) 0 0	81, 95, 126, 141	0
11	s9	185/185 (100%)	0.84	27 (14%) 2 2	57, 74, 104, 122	0
12	C0	96/96 (100%)	0.59	9 (9%) 8 9	84, 105, 126, 135	0
13	C1	155/155 (100%)	1.26	34 (21%) 0 1	64, 76, 112, 121	0
13	c1	146/155 (94%)	0.48	9 (6%) 20 20	48, 61, 89, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	C2	124/124 (100%)	1.57	40 (32%) 0 0	133, 139, 151, 157	0
14	c2	124/124 (100%)	3.26	86 (69%) 0 0	167, 183, 195, 200	0
15	C3	150/150 (100%)	0.43	7 (4%) 31 29	75, 88, 104, 108	0
15	c3	150/150 (100%)	0.01	3 (2%) 65 64	57, 70, 86, 88	0
16	C4	127/128 (99%)	0.88	26 (20%) 1 1	75, 129, 142, 144	0
16	c4	128/128 (100%)	0.98	15 (11%) 4 4	54, 86, 94, 104	0
17	C5	124/135 (91%)	1.87	49 (39%) 0 0	79, 94, 110, 126	0
17	c5	135/135 (100%)	1.63	42 (31%) 0 0	67, 97, 112, 115	0
18	C6	141/142 (99%)	2.45	76 (53%) 0 0	82, 102, 107, 110	0
18	c6	142/142 (100%)	1.89	56 (39%) 0 0	73, 91, 104, 121	0
19	C7	120/125 (96%)	1.61	39 (32%) 0 0	91, 105, 124, 126	0
19	c7	117/125 (93%)	0.98	25 (21%) 0 1	78, 91, 105, 112	0
20	C8	145/145 (100%)	1.39	41 (28%) 0 0	77, 97, 120, 127	0
20	c8	145/145 (100%)	1.34	39 (26%) 0 0	73, 89, 109, 114	0
21	C9	143/143 (100%)	1.80	61 (42%) 0 0	85, 99, 111, 120	0
21	c9	143/143 (100%)	0.77	18 (12%) 3 3	76, 85, 99, 107	0
22	D0	107/110 (97%)	1.57	37 (34%) 0 0	77, 105, 124, 127	0
22	d0	110/110 (100%)	1.86	43 (39%) 0 0	74, 102, 127, 134	0
23	D1	87/87 (100%)	1.42	23 (26%) 0 0	87, 95, 109, 115	0
23	d1	87/87 (100%)	0.52	7 (8%) 12 11	65, 73, 93, 100	0
24	D2	129/129 (100%)	2.07	62 (48%) 0 0	73, 84, 90, 100	0
24	d2	129/129 (100%)	0.71	6 (4%) 31 29	53, 61, 68, 76	0
25	D3	144/144 (100%)	0.27	3 (2%) 63 62	64, 71, 83, 97	0
25	d3	144/144 (100%)	0.03	1 (0%) 87 88	45, 52, 62, 77	0
26	D4	134/134 (100%)	0.76	13 (9%) 7 8	81, 102, 113, 118	0
26	d4	134/134 (100%)	0.43	8 (5%) 21 21	56, 76, 87, 91	0
27	D5	70/70 (100%)	0.61	5 (7%) 16 16	108, 118, 124, 125	0
27	d5	69/70 (98%)	1.11	10 (14%) 2 2	89, 104, 111, 113	0
28	D6	97/97 (100%)	2.36	60 (61%) 0 0	79, 94, 142, 143	0
28	d6	97/97 (100%)	1.19	22 (22%) 0 1	58, 72, 97, 100	0
29	D7	81/81 (100%)	1.68	32 (39%) 0 0	90, 106, 133, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	d7	81/81 (100%)	0.88	10 (12%) 4 3	66, 83, 117, 120	0
30	D8	63/63 (100%)	1.13	14 (22%) 0 1	106, 122, 129, 131	0
30	d8	63/63 (100%)	1.39	18 (28%) 0 0	96, 110, 117, 119	0
31	D9	53/53 (100%)	1.39	16 (30%) 0 0	75, 80, 100, 104	0
31	d9	53/53 (100%)	2.42	30 (56%) 0 0	71, 83, 117, 130	0
32	E0	60/62 (96%)	0.83	9 (15%) 2 2	70, 100, 125, 128	0
32	e0	62/62 (100%)	0.03	3 (4%) 30 28	55, 79, 104, 105	0
33	E1	71/76 (93%)	1.28	15 (21%) 1 1	96, 129, 140, 142	0
33	e1	76/76 (100%)	2.21	38 (50%) 0 0	100, 155, 176, 179	0
34	SR	318/318 (100%)	1.04	60 (18%) 1 1	100, 111, 126, 148	0
34	sR	318/318 (100%)	1.80	134 (42%) 0 0	96, 110, 122, 137	0
35	SM	133/159 (83%)	1.20	27 (20%) 1 1	54, 86, 117, 122	0
36	1	3149/3394 (92%)	0.13	52 (1%) 70 68	30, 54, 125, 221	0
36	5	3150/3394 (92%)	0.12	30 (0%) 82 82	31, 50, 117, 193	0
37	3	121/121 (100%)	0.03	0 100 100	40, 70, 86, 94	0
37	7	121/121 (100%)	-0.13	0 100 100	35, 53, 64, 71	0
38	4	158/158 (100%)	0.00	2 (1%) 77 77	40, 60, 96, 129	0
38	8	158/158 (100%)	-0.02	1 (0%) 89 90	42, 64, 97, 126	0
39	L2	252/252 (100%)	0.45	6 (2%) 59 56	40, 57, 74, 83	0
39	12	252/252 (100%)	0.58	15 (5%) 21 21	38, 56, 74, 87	0
40	L3	386/386 (100%)	0.04	1 (0%) 94 94	38, 57, 69, 83	0
40	l3	386/386 (100%)	-0.12	2 (0%) 91 91	30, 42, 56, 76	0
41	L4	361/361 (100%)	-0.16	0 100 100	34, 48, 63, 70	0
41	14	361/361 (100%)	-0.10	0 100 100	37, 52, 70, 76	0
42	L5	296/296 (100%)	1.36	95 (32%) 0 0	51, 76, 94, 108	0
42	15	294/296 (99%)	0.72	17 (5%) 23 22	42, 54, 75, 94	0
43	L6	156/175 (89%)	0.23	1 (0%) 89 90	44, 53, 66, 77	0
43	16	157/175 (89%)	-0.01	1 (0%) 89 90	44, 54, 71, 83	0
44	L7	222/223 (99%)	0.11	1 (0%) 91 91	35, 45, 70, 99	0
44	17	223/223 (100%)	-0.03	0 100 100	35, 43, 74, 102	0
45	L8	233/233 (100%)	0.83	26 (11%) 5 5	65, 83, 108, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	l8	231/233 (99%)	0.75	23 (9%) 7 7	72, 87, 109, 112	0
46	L9	191/191 (100%)	0.66	24 (12%) 3 3	57, 65, 74, 85	0
46	l9	191/191 (100%)	0.16	3 (1%) 72 70	39, 48, 63, 72	0
47	M0	211/220 (95%)	0.05	2 (0%) 84 84	41, 54, 88, 102	0
47	m0	213/220 (96%)	0.17	7 (3%) 46 44	36, 50, 74, 87	0
48	M1	169/169 (100%)	1.89	76 (44%) 0 0	62, 77, 87, 93	0
48	m1	169/169 (100%)	0.76	13 (7%) 13 12	45, 61, 68, 72	0
49	M3	193/194 (99%)	0.35	4 (2%) 63 62	35, 58, 94, 119	0
49	m3	194/194 (100%)	0.48	6 (3%) 49 48	38, 67, 100, 109	0
50	M4	136/137 (99%)	0.06	5 (3%) 41 38	50, 59, 70, 74	0
50	m4	137/137 (100%)	-0.23	0 100 100	44, 50, 66, 72	0
51	M5	203/203 (100%)	0.86	28 (13%) 2 2	38, 55, 66, 68	0
51	m5	203/203 (100%)	0.99	33 (16%) 1 2	42, 61, 73, 76	0
52	M6	197/197 (100%)	-0.02	2 (1%) 82 82	38, 45, 63, 65	0
52	m6	197/197 (100%)	-0.04	0 100 100	31, 37, 63, 68	0
53	M7	183/183 (100%)	0.26	9 (4%) 29 27	41, 47, 96, 121	0
53	m7	155/183 (84%)	-0.03	1 (0%) 89 90	37, 42, 52, 70	0
54	M8	185/185 (100%)	0.36	4 (2%) 62 60	37, 48, 61, 75	0
54	m8	185/185 (100%)	0.60	11 (5%) 22 22	37, 52, 62, 69	0
55	M9	188/188 (100%)	0.40	14 (7%) 14 14	61, 73, 137, 144	0
55	m9	188/188 (100%)	0.13	3 (1%) 72 70	49, 63, 121, 132	0
56	N0	172/172 (100%)	1.01	36 (20%) 1 1	46, 54, 65, 73	0
56	n0	172/172 (100%)	0.10	2 (1%) 79 78	38, 45, 55, 63	0
57	N1	159/159 (100%)	0.79	19 (11%) 4 4	37, 51, 92, 98	0
57	n1	159/159 (100%)	0.34	6 (3%) 40 37	36, 44, 78, 83	0
58	N2	100/100 (100%)	0.60	10 (10%) 7 7	92, 102, 107, 115	0
58	n2	98/100 (98%)	1.07	21 (21%) 0 1	74, 85, 91, 93	0
59	N3	136/136 (100%)	0.41	0 100 100	44, 54, 64, 69	0
59	n3	136/136 (100%)	0.25	2 (1%) 73 72	31, 38, 47, 50	0
60	N4	98/135 (72%)	2.13	31 (31%) 0 0	55, 67, 134, 136	0
60	n4	135/135 (100%)	1.02	27 (20%) 1 1	39, 83, 109, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	N5	121/121 (100%)	1.07	22 (18%) 1 1	57, 69, 85, 107	0
61	n5	120/121 (99%)	0.58	8 (6%) 17 17	56, 69, 87, 93	0
62	N6	126/126 (100%)	0.53	5 (3%) 38 36	44, 61, 70, 79	0
62	n6	126/126 (100%)	1.06	16 (12%) 3 3	50, 66, 80, 83	0
63	N7	135/135 (100%)	1.56	44 (32%) 0 0	83, 96, 107, 111	0
63	n7	135/135 (100%)	1.52	48 (35%) 0 0	82, 96, 113, 117	0
64	N8	148/148 (100%)	0.45	1 (0%) 87 88	31, 49, 67, 75	0
64	n8	148/148 (100%)	0.66	7 (4%) 31 29	33, 54, 68, 71	0
65	N9	58/58 (100%)	0.78	5 (8%) 10 10	34, 54, 89, 101	0
65	n9	58/58 (100%)	0.18	2 (3%) 45 43	35, 52, 73, 77	0
66	O0	97/100 (97%)	0.56	9 (9%) 8 9	80, 88, 103, 106	0
66	o0	100/100 (100%)	0.34	7 (7%) 16 16	72, 83, 100, 103	0
67	O1	109/109 (100%)	0.49	4 (3%) 41 38	55, 65, 88, 92	0
67	o1	109/109 (100%)	0.96	12 (11%) 5 5	43, 53, 80, 96	0
68	O2	127/127 (100%)	-0.06	2 (1%) 72 70	33, 44, 55, 67	0
68	o2	127/127 (100%)	-0.12	0 100 100	34, 49, 59, 64	0
69	O3	106/106 (100%)	0.19	0 100 100	37, 45, 66, 74	0
69	o3	106/106 (100%)	0.25	0 100 100	36, 42, 65, 74	0
70	O4	112/112 (100%)	1.19	23 (20%) 1 1	54, 74, 103, 109	0
70	o4	112/112 (100%)	0.79	10 (8%) 9 10	51, 73, 105, 111	0
71	O5	119/119 (100%)	0.70	9 (7%) 13 13	55, 70, 77, 80	0
71	o5	119/119 (100%)	0.30	2 (1%) 70 68	63, 71, 86, 95	0
72	O6	99/99 (100%)	0.64	8 (8%) 12 11	55, 67, 92, 100	0
72	o6	99/99 (100%)	0.71	10 (10%) 7 6	61, 72, 86, 99	0
73	O7	87/87 (100%)	0.30	0 100 100	41, 46, 67, 75	0
73	o7	87/87 (100%)	0.42	4 (4%) 32 30	37, 49, 77, 91	0
74	O8	77/77 (100%)	0.92	12 (15%) 2 2	82, 92, 103, 106	0
74	o8	77/77 (100%)	1.76	26 (33%) 0 0	81, 89, 97, 99	0
75	O9	50/50 (100%)	0.42	0 100 100	47, 55, 57, 57	0
75	o9	50/50 (100%)	0.47	2 (4%) 38 36	48, 55, 60, 62	0
76	Q0	52/52 (100%)	0.50	4 (7%) 13 12	49, 53, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	q0	52/52 (100%)	-0.01	1 (1%) 66 65	36, 40, 49, 54	0
77	Q1	25/25 (100%)	0.30	0 100 100	57, 62, 66, 66	0
77	q1	25/25 (100%)	0.05	0 100 100	45, 47, 48, 50	0
78	Q2	105/105 (100%)	0.51	8 (7%) 13 13	41, 51, 72, 93	0
78	q2	105/105 (100%)	0.40	4 (3%) 40 37	42, 50, 64, 85	0
79	Q3	91/91 (100%)	0.20	2 (2%) 62 60	46, 59, 74, 81	0
79	q3	91/91 (100%)	0.28	2 (2%) 62 60	42, 55, 67, 73	0
80	6	1795/1800 (99%)	0.17	61 (3%) 45 43	38, 75, 157, 227	0
81	c0	84/96 (87%)	1.66	33 (39%) 0 0	94, 126, 139, 141	0
82	sM	63/104 (60%)	1.32	15 (23%) 0 0	47, 97, 105, 110	0
83	m2	0/150	-	-	-	-
84	p0	143/219 (65%)	2.45	86 (60%) 0 0	88, 109, 177, 181	0
85	p1	0/47	-	-	-	-
85	p2	0/47	-	-	-	-
All	All	33015/34167 (96%)	0.57	3370 (10%) 6 6	30, 69, 125, 227	0

The worst 5 of 3370 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	86	SER	15.4
60	N4	75	THR	13.0
60	N4	84	GLY	12.7
1	2	1807	A	12.6
1	2	1806	A	11.7

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

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

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
87	MG	1	4465	1/1	0.01	1.10	109,109,109,109	0
87	MG	5	3911	1/1	0.01	1.38	53,53,53,53	1
87	MG	5	4349	1/1	0.03	0.67	41,41,41,41	1
87	MG	d5	201	1/1	0.05	0.31	124,124,124,124	0
87	MG	2	2230	1/1	0.06	0.31	124,124,124,124	0
87	MG	1	4054	1/1	0.09	0.33	105,105,105,105	0
87	MG	1	4197	1/1	0.12	0.43	56,56,56,56	0
87	MG	17	301	1/1	0.23	0.74	36,36,36,36	1
87	MG	6	2332	1/1	0.30	0.25	213,213,213,213	0
87	MG	2	2156	1/1	0.30	0.47	86,86,86,86	0
87	MG	1	4401	1/1	0.36	0.40	36,36,36,36	1
87	MG	1	4126	1/1	0.37	0.42	66,66,66,66	0
87	MG	6	2333	1/1	0.37	0.49	59,59,59,59	1
87	MG	1	4087	1/1	0.39	0.66	101,101,101,101	0
87	MG	1	4134	1/1	0.39	1.23	49,49,49,49	1
87	MG	1	4318	1/1	0.41	0.17	115,115,115,115	0
87	MG	5	3921	1/1	0.42	0.55	51,51,51,51	0
87	MG	5	4413	1/1	0.44	0.31	72,72,72,72	0
87	MG	2	2198	1/1	0.46	0.55	120,120,120,120	0
87	MG	5	3905	1/1	0.46	0.73	71,71,71,71	0
87	MG	2	2196	1/1	0.47	0.99	82,82,82,82	0
87	MG	2	2135	1/1	0.48	0.40	72,72,72,72	0
87	MG	M1	201	1/1	0.49	0.28	73,73,73,73	0
87	MG	6	2300	1/1	0.49	0.31	82,82,82,82	0
87	MG	2	2154	1/1	0.49	0.99	68,68,68,68	0
87	MG	2	2217	1/1	0.49	0.52	103,103,103,103	0
87	MG	5	4107	1/1	0.50	0.33	59,59,59,59	0
87	MG	3	226	1/1	0.50	0.23	65,65,65,65	0
87	MG	6	2278	1/1	0.50	0.24	83,83,83,83	0
87	MG	2	2247	1/1	0.50	0.38	115,115,115,115	0
87	MG	6	2317	1/1	0.50	0.45	59,59,59,59	0
87	MG	5	4397	1/1	0.51	0.47	38,38,38,38	1
87	MG	6	2323	1/1	0.52	0.34	70,70,70,70	0
87	MG	6	2231	1/1	0.53	0.29	86,86,86,86	0
87	MG	1	4367	1/1	0.54	0.73	92,92,92,92	0
87	MG	2	2117	1/1	0.54	0.33	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4214	1/1	0.54	0.41	36,36,36,36	0
87	MG	1	4095	1/1	0.54	0.70	41,41,41,41	0
87	MG	2	2147	1/1	0.54	0.20	100,100,100,100	0
87	MG	M9	204	1/1	0.55	0.20	70,70,70,70	0
87	MG	1	4293	1/1	0.55	0.22	127,127,127,127	0
87	MG	5	3901	1/1	0.55	0.36	67,67,67,67	0
86	OHX	6	2064	7/7	0.56	0.59	68,68,68,68	7
87	MG	5	4408	1/1	0.56	0.57	57,57,57,57	0
87	MG	5	4322	1/1	0.56	0.45	62,62,62,62	0
87	MG	2	2257	1/1	0.56	0.42	121,121,121,121	0
87	MG	5	4135	1/1	0.57	0.67	69,69,69,69	0
87	MG	5	4543	1/1	0.57	0.70	41,41,41,41	1
87	MG	6	2223	1/1	0.57	0.66	52,52,52,52	0
87	MG	5	4423	1/1	0.57	0.51	59,59,59,59	0
88	ZN	D7	101	1/1	0.57	0.38	147,147,147,147	0
87	MG	5	4572	1/1	0.57	0.39	69,69,69,69	0
87	MG	2	2169	1/1	0.57	0.25	101,101,101,101	0
87	MG	5	4104	1/1	0.58	0.54	45,45,45,45	1
87	MG	6	2274	1/1	0.59	0.60	42,42,42,42	1
87	MG	5	4354	1/1	0.59	0.91	61,61,61,61	0
87	MG	c9	202	1/1	0.59	0.35	80,80,80,80	0
87	MG	2	2173	1/1	0.59	0.64	116,116,116,116	0
87	MG	1	4343	1/1	0.59	0.58	62,62,62,62	0
87	MG	1	4224	1/1	0.60	0.28	74,74,74,74	0
86	OHX	5	3720	7/7	0.60	0.43	73,73,73,73	7
87	MG	5	4376	1/1	0.60	0.28	72,72,72,72	0
87	MG	1	4484	1/1	0.60	0.73	49,49,49,49	1
87	MG	2	2201	1/1	0.60	0.51	61,61,61,61	0
87	MG	1	4295	1/1	0.61	0.45	41,41,41,41	1
87	MG	6	2281	1/1	0.61	0.41	124,124,124,124	0
87	MG	5	4479	1/1	0.61	0.62	56,56,56,56	1
87	MG	4	243	1/1	0.61	0.76	57,57,57,57	1
87	MG	N8	206	1/1	0.62	0.39	39,39,39,39	0
87	MG	1	4148	1/1	0.62	0.38	69,69,69,69	0
87	MG	c9	203	1/1	0.62	0.40	87,87,87,87	0
87	MG	1	4477	1/1	0.62	0.77	47,47,47,47	0
87	MG	2	2102	1/1	0.62	0.39	84,84,84,84	0
87	MG	s8	304	1/1	0.62	0.50	56,56,56,56	0
87	MG	1	4217	1/1	0.62	0.98	39,39,39,39	1
87	MG	5	4494	1/1	0.62	0.33	69,69,69,69	0
87	MG	6	2304	1/1	0.62	0.37	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	5	4492	1/1	0.63	0.43	41,41,41,41	1
87	MG	1	3916	1/1	0.63	0.20	86,86,86,86	0
87	MG	1	4282	1/1	0.63	0.54	47,47,47,47	1
87	MG	2	2225	1/1	0.63	0.52	58,58,58,58	1
87	MG	D9	103	1/1	0.64	0.15	94,94,94,94	0
87	MG	6	2207	1/1	0.64	0.43	93,93,93,93	0
87	MG	2	2216	1/1	0.64	0.28	69,69,69,69	0
87	MG	n9	102	1/1	0.64	0.32	37,37,37,37	0
87	MG	2	2252	1/1	0.64	0.29	126,126,126,126	0
87	MG	6	2199	1/1	0.64	0.53	83,83,83,83	0
87	MG	Q2	503	1/1	0.64	0.26	62,62,62,62	0
87	MG	p0	301	1/1	0.64	0.31	93,93,93,93	0
87	MG	6	2124	1/1	0.65	0.41	71,71,71,71	0
87	MG	M0	309	1/1	0.65	0.48	46,46,46,46	1
87	MG	5	4316	1/1	0.65	0.37	74,74,74,74	0
87	MG	6	2305	1/1	0.65	0.78	98,98,98,98	0
87	MG	2	2239	1/1	0.65	1.31	86,86,86,86	0
87	MG	5	4462	1/1	0.65	0.34	54,54,54,54	0
87	MG	1	3900	1/1	0.65	0.17	104,104,104,104	0
87	MG	1	4374	1/1	0.65	0.71	44,44,44,44	0
87	MG	5	4576	1/1	0.66	0.37	53,53,53,53	0
87	MG	5	4373	1/1	0.66	0.23	38,38,38,38	1
87	MG	2	2136	1/1	0.66	0.29	71,71,71,71	0
87	MG	2	2175	1/1	0.66	0.27	87,87,87,87	0
87	MG	5	4265	1/1	0.66	0.67	61,61,61,61	0
87	MG	N0	202	1/1	0.66	0.75	51,51,51,51	1
87	MG	4	220	1/1	0.66	0.34	64,64,64,64	0
87	MG	1	4193	1/1	0.66	0.54	40,40,40,40	1
86	OHX	5	3813	7/7	0.66	0.23	173,173,173,173	7
87	MG	5	4155	1/1	0.66	0.29	80,80,80,80	0
87	MG	5	4079	1/1	0.66	0.37	44,44,44,44	0
87	MG	2	2150	1/1	0.66	0.67	74,74,74,74	0
87	MG	5	4074	1/1	0.67	0.24	86,86,86,86	0
87	MG	1	4370	1/1	0.67	0.42	41,41,41,41	1
87	MG	6	2128	1/1	0.67	0.28	68,68,68,68	0
87	MG	5	4338	1/1	0.67	0.66	39,39,39,39	1
87	MG	5	3925	1/1	0.67	0.48	43,43,43,43	1
87	MG	M6	204	1/1	0.67	0.51	39,39,39,39	1
87	MG	1	4426	1/1	0.67	1.07	63,63,63,63	0
87	MG	1	4408	1/1	0.67	1.03	56,56,56,56	1
87	MG	6	2285	1/1	0.67	0.21	68,68,68,68	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4495	1/1	0.67	0.41	71,71,71,71	0
87	MG	M7	211	1/1	0.68	0.22	75,75,75,75	0
86	OHX	2	2060	7/7	0.68	0.45	98,98,98,98	7
87	MG	SM	201	1/1	0.68	0.31	55,55,55,55	0
87	MG	1	4211	1/1	0.68	0.48	58,58,58,58	0
87	MG	5	4264	1/1	0.68	0.35	63,63,63,63	0
87	MG	5	4553	1/1	0.68	0.42	50,50,50,50	1
87	MG	M5	305	1/1	0.68	2.52	69,69,69,69	0
87	MG	5	4067	1/1	0.68	0.49	54,54,54,54	0
87	MG	O2	203	1/1	0.68	0.86	44,44,44,44	1
87	MG	1	4047	1/1	0.68	0.21	83,83,83,83	0
87	MG	1	4227	1/1	0.68	0.88	45,45,45,45	0
87	MG	1	4404	1/1	0.68	0.25	57,57,57,57	0
86	OHX	5	3806	7/7	0.68	0.49	76,76,76,76	7
87	MG	5	4360	1/1	0.68	0.43	50,50,50,50	0
87	MG	6	2329	1/1	0.69	0.43	48,48,48,48	0
87	MG	6	2222	1/1	0.69	0.18	81,81,81,81	0
87	MG	1	4306	1/1	0.69	0.12	126,126,126,126	0
87	MG	3	227	1/1	0.69	0.38	78,78,78,78	0
87	MG	6	2272	1/1	0.69	0.18	98,98,98,98	0
87	MG	n0	201	1/1	0.69	0.31	49,49,49,49	1
87	MG	1	4462	1/1	0.69	0.35	53,53,53,53	0
87	MG	1	3884	1/1	0.69	0.44	50,50,50,50	0
87	MG	2	2194	1/1	0.69	0.60	72,72,72,72	0
87	MG	1	4347	1/1	0.69	0.57	41,41,41,41	1
87	MG	1	4444	1/1	0.70	0.73	41,41,41,41	1
87	MG	6	2240	1/1	0.70	0.15	74,74,74,74	0
87	MG	5	3854	1/1	0.70	0.50	72,72,72,72	0
87	MG	1	4459	1/1	0.70	0.35	46,46,46,46	1
87	MG	l2	305	1/1	0.70	0.34	71,71,71,71	0
87	MG	5	4516	1/1	0.70	0.49	62,62,62,62	1
87	MG	5	4203	1/1	0.70	0.42	36,36,36,36	1
87	MG	1	4055	1/1	0.70	0.36	51,51,51,51	0
86	OHX	5	3762	7/7	0.70	0.44	53,53,53,53	7
87	MG	2	2185	1/1	0.70	0.54	74,74,74,74	0
87	MG	2	2113	1/1	0.70	0.62	68,68,68,68	0
87	MG	1	4365	1/1	0.70	0.60	38,38,38,38	1
87	MG	6	2238	1/1	0.70	0.26	66,66,66,66	0
87	MG	2	2259	1/1	0.71	1.54	74,74,74,74	1
87	MG	1	4179	1/1	0.71	1.31	53,53,53,53	1
87	MG	l5	306	1/1	0.71	0.31	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	4434	1/1	0.71	0.29	93,93,93,93	0
87	MG	1	4088	1/1	0.71	0.29	52,52,52,52	0
87	MG	5	4222	1/1	0.71	0.41	49,49,49,49	0
87	MG	5	4181	1/1	0.71	0.35	55,55,55,55	0
87	MG	1	4469	1/1	0.71	0.36	55,55,55,55	0
87	MG	1	4506	1/1	0.71	0.23	94,94,94,94	0
87	MG	1	4372	1/1	0.71	0.41	76,76,76,76	0
87	MG	5	3886	1/1	0.71	0.17	97,97,97,97	0
87	MG	1	4322	1/1	0.71	0.35	65,65,65,65	0
87	MG	2	2093	1/1	0.71	0.45	74,74,74,74	0
87	MG	1	4339	1/1	0.71	0.87	73,73,73,73	1
87	MG	2	2253	1/1	0.72	0.28	76,76,76,76	0
87	MG	4	237	1/1	0.72	0.47	67,67,67,67	0
87	MG	4	238	1/1	0.72	0.31	59,59,59,59	0
87	MG	7	237	1/1	0.72	0.36	53,53,53,53	1
87	MG	2	2221	1/1	0.72	0.39	61,61,61,61	0
87	MG	5	4137	1/1	0.72	0.55	63,63,63,63	0
87	MG	6	2184	1/1	0.72	0.18	69,69,69,69	0
87	MG	5	4041	1/1	0.72	0.34	51,51,51,51	0
87	MG	5	4172	1/1	0.72	0.42	40,40,40,40	0
87	MG	1	4066	1/1	0.72	0.36	55,55,55,55	0
87	MG	5	4183	1/1	0.72	0.40	54,54,54,54	0
87	MG	4	241	1/1	0.73	0.56	53,53,53,53	0
87	MG	15	304	1/1	0.73	0.16	61,61,61,61	0
87	MG	5	4324	1/1	0.73	0.61	42,42,42,42	1
87	MG	1	4246	1/1	0.73	0.76	41,41,41,41	1
87	MG	1	4067	1/1	0.73	0.46	71,71,71,71	0
87	MG	1	4350	1/1	0.73	0.45	40,40,40,40	1
87	MG	6	2202	1/1	0.73	0.57	81,81,81,81	0
87	MG	4	232	1/1	0.73	0.34	42,42,42,42	0
87	MG	1	4294	1/1	0.73	0.29	58,58,58,58	0
87	MG	2	2204	1/1	0.73	0.19	106,106,106,106	0
87	MG	5	4101	1/1	0.73	0.32	49,49,49,49	0
87	MG	2	2249	1/1	0.73	0.63	97,97,97,97	0
87	MG	1	4169	1/1	0.73	0.46	72,72,72,72	0
87	MG	1	4328	1/1	0.74	0.35	70,70,70,70	0
87	MG	c8	205	1/1	0.74	0.31	93,93,93,93	0
86	OHX	5	3768	7/7	0.74	0.63	47,47,47,47	7
87	MG	m7	205	1/1	0.74	0.36	50,50,50,50	0
87	MG	1	4355	1/1	0.74	0.64	67,67,67,67	0
87	MG	1	4361	1/1	0.74	0.30	67,67,67,67	0
87	MG	2	2167	1/1	0.74	0.26	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	6	2183	1/1	0.74	1.15	54,54,54,54	1
87	MG	1	4346	1/1	0.74	0.72	48,48,48,48	1
87	MG	1	3848	1/1	0.74	0.63	46,46,46,46	0
87	MG	1	3853	1/1	0.74	0.96	41,41,41,41	0
86	OHX	6	2081	7/7	0.74	0.42	91,91,91,91	7
87	MG	1	3899	1/1	0.74	0.23	40,40,40,40	0
87	MG	1	4434	1/1	0.74	0.42	38,38,38,38	1
87	MG	2	2159	1/1	0.74	0.22	75,75,75,75	0
87	MG	5	4347	1/1	0.74	0.73	60,60,60,60	0
87	MG	12	303	1/1	0.75	0.29	55,55,55,55	1
87	MG	2	2208	1/1	0.75	0.43	72,72,72,72	0
87	MG	5	4129	1/1	0.75	0.58	82,82,82,82	0
87	MG	5	4562	1/1	0.75	0.38	68,68,68,68	0
87	MG	1	4178	1/1	0.75	0.38	93,93,93,93	0
87	MG	6	2257	1/1	0.75	0.73	72,72,72,72	0
87	MG	1	3856	1/1	0.75	0.45	63,63,63,63	0
87	MG	5	4165	1/1	0.75	0.19	54,54,54,54	0
87	MG	1	4487	1/1	0.75	0.55	62,62,62,62	0
87	MG	1	4300	1/1	0.75	0.37	46,46,46,46	0
87	MG	2	2205	1/1	0.75	0.68	76,76,76,76	0
87	MG	6	2256	1/1	0.75	0.38	73,73,73,73	0
86	OHX	6	1984	7/7	0.75	0.29	82,82,82,82	7
87	MG	5	4262	1/1	0.75	0.48	39,39,39,39	0
87	MG	6	2244	1/1	0.75	0.29	53,53,53,53	0
87	MG	2	2138	1/1	0.75	0.14	76,76,76,76	0
87	MG	5	4529	1/1	0.75	0.47	37,37,37,37	1
86	OHX	6	2036	7/7	0.75	0.40	48,48,48,48	7
87	MG	5	4082	1/1	0.76	0.19	62,62,62,62	0
87	MG	c8	202	1/1	0.76	0.29	81,81,81,81	0
87	MG	1	4155	1/1	0.76	0.18	54,54,54,54	0
87	MG	5	4336	1/1	0.76	0.43	69,69,69,69	0
87	MG	5	3896	1/1	0.76	0.24	50,50,50,50	0
87	MG	5	4309	1/1	0.76	0.30	74,74,74,74	0
87	MG	1	4278	1/1	0.76	0.65	46,46,46,46	1
87	MG	3	221	1/1	0.76	0.16	70,70,70,70	0
87	MG	1	4359	1/1	0.76	0.45	51,51,51,51	1
87	MG	3	229	1/1	0.76	0.52	52,52,52,52	1
86	OHX	6	2087	7/7	0.76	0.45	71,71,71,71	7
86	OHX	5	3703	7/7	0.76	0.31	86,86,86,86	7
87	MG	1	4084	1/1	0.76	0.52	49,49,49,49	0
86	OHX	6	2022	7/7	0.76	0.22	139,139,139,139	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	3910	1/1	0.76	0.18	88,88,88,88	0
87	MG	5	4050	1/1	0.76	0.53	42,42,42,42	0
87	MG	5	4131	1/1	0.76	0.79	35,35,35,35	1
87	MG	6	2168	1/1	0.76	0.33	59,59,59,59	0
87	MG	5	4087	1/1	0.76	0.48	36,36,36,36	0
87	MG	5	4211	1/1	0.76	0.25	46,46,46,46	0
87	MG	5	4448	1/1	0.76	0.61	42,42,42,42	1
87	MG	6	2283	1/1	0.76	1.35	69,69,69,69	1
87	MG	3	214	1/1	0.76	0.34	46,46,46,46	0
87	MG	5	4481	1/1	0.76	0.40	44,44,44,44	1
87	MG	5	4381	1/1	0.76	0.19	79,79,79,79	0
87	MG	5	4464	1/1	0.76	0.38	66,66,66,66	0
87	MG	5	4244	1/1	0.76	0.28	58,58,58,58	0
87	MG	5	4281	1/1	0.76	0.54	44,44,44,44	1
87	MG	1	4512	1/1	0.76	0.39	41,41,41,41	0
87	MG	5	4252	1/1	0.76	0.69	58,58,58,58	0
87	MG	1	4345	1/1	0.76	0.29	44,44,44,44	1
87	MG	1	4406	1/1	0.76	0.41	46,46,46,46	1
86	OHX	5	3783	7/7	0.76	0.59	56,56,56,56	7
87	MG	2	2203	1/1	0.77	0.14	85,85,85,85	0
87	MG	2	2180	1/1	0.77	0.50	68,68,68,68	0
87	MG	5	4133	1/1	0.77	0.23	57,57,57,57	0
87	MG	6	2197	1/1	0.77	0.25	60,60,60,60	0
87	MG	1	3834	1/1	0.77	0.62	71,71,71,71	0
87	MG	5	4556	1/1	0.77	0.44	43,43,43,43	0
87	MG	6	2301	1/1	0.77	0.49	57,57,57,57	0
87	MG	5	4085	1/1	0.77	0.26	57,57,57,57	0
87	MG	5	4419	1/1	0.77	0.23	39,39,39,39	1
87	MG	5	4457	1/1	0.77	0.64	54,54,54,54	0
87	MG	6	2198	1/1	0.77	0.19	90,90,90,90	0
87	MG	5	4156	1/1	0.77	0.63	41,41,41,41	0
87	MG	5	3864	1/1	0.77	0.32	35,35,35,35	0
87	MG	1	4260	1/1	0.77	0.34	40,40,40,40	0
87	MG	1	4244	1/1	0.77	0.22	72,72,72,72	0
87	MG	5	4455	1/1	0.77	0.50	37,37,37,37	1
86	OHX	6	2080	7/7	0.77	0.21	126,126,126,126	7
87	MG	1	4200	1/1	0.77	0.40	51,51,51,51	0
87	MG	m7	206	1/1	0.77	0.48	35,35,35,35	0
87	MG	1	4486	1/1	0.77	0.23	53,53,53,53	0
86	OHX	1	3660	7/7	0.77	0.34	127,127,127,127	7
87	MG	5	4141	1/1	0.77	0.42	54,54,54,54	0
87	MG	6	2192	1/1	0.77	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	2	2162	1/1	0.77	0.69	85,85,85,85	0
87	MG	2	2149	1/1	0.77	0.25	92,92,92,92	0
87	MG	1	4014	1/1	0.77	0.50	49,49,49,49	0
87	MG	5	4327	1/1	0.77	0.66	82,82,82,82	0
87	MG	5	4488	1/1	0.77	0.35	46,46,46,46	0
87	MG	1	3879	1/1	0.77	0.62	61,61,61,61	0
87	MG	5	4150	1/1	0.77	0.39	41,41,41,41	1
86	OHX	5	3739	7/7	0.78	0.44	72,72,72,72	7
87	MG	2	2214	1/1	0.78	0.60	78,78,78,78	0
90	8AN	1	3403	22/23	0.78	0.34	48,103,107,107	0
87	MG	5	4563	1/1	0.78	0.43	85,85,85,85	0
87	MG	5	4048	1/1	0.78	0.37	34,34,34,34	0
87	MG	6	2191	1/1	0.78	0.41	86,86,86,86	0
87	MG	1	4218	1/1	0.78	0.29	50,50,50,50	0
87	MG	1	4035	1/1	0.78	0.34	44,44,44,44	0
86	OHX	2	2030	7/7	0.78	0.43	112,112,112,112	7
87	MG	6	2212	1/1	0.78	0.28	84,84,84,84	0
87	MG	5	4426	1/1	0.78	0.44	62,62,62,62	0
87	MG	5	4099	1/1	0.78	0.31	61,61,61,61	0
86	OHX	8	218	7/7	0.78	0.56	48,48,48,48	7
87	MG	5	4474	1/1	0.78	0.31	62,62,62,62	0
87	MG	N6	201	1/1	0.78	0.29	63,63,63,63	0
87	MG	D4	201	1/1	0.78	0.28	83,83,83,83	0
87	MG	2	2098	1/1	0.78	0.23	80,80,80,80	0
87	MG	2	2222	1/1	0.78	0.20	80,80,80,80	0
86	OHX	2	2081	7/7	0.78	0.23	120,120,120,120	7
87	MG	1	4348	1/1	0.78	0.15	191,191,191,191	0
87	MG	5	4214	1/1	0.78	0.31	52,52,52,52	0
87	MG	6	2164	1/1	0.78	0.37	87,87,87,87	0
87	MG	6	2162	1/1	0.78	0.46	53,53,53,53	0
87	MG	1	4065	1/1	0.78	0.27	50,50,50,50	0
87	MG	2	2255	1/1	0.78	0.18	88,88,88,88	0
87	MG	2	2177	1/1	0.78	0.40	69,69,69,69	0
87	MG	2	2224	1/1	0.78	0.46	99,99,99,99	0
87	MG	1	4360	1/1	0.78	0.68	55,55,55,55	1
87	MG	5	3850	1/1	0.78	0.37	65,65,65,65	0
87	MG	5	4223	1/1	0.78	0.25	53,53,53,53	0
87	MG	5	4513	1/1	0.78	0.18	97,97,97,97	0
87	MG	2	2245	1/1	0.78	0.46	71,71,71,71	0
87	MG	Q0	202	1/1	0.79	0.90	54,54,54,54	0
87	MG	1	4439	1/1	0.79	0.09	200,200,200,200	0
87	MG	1	4497	1/1	0.79	0.23	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	5	4221	1/1	0.79	0.24	54,54,54,54	0
86	OHX	1	3774	7/7	0.79	0.39	53,53,53,53	7
87	MG	O7	108	1/1	0.79	0.30	69,69,69,69	0
87	MG	5	4090	1/1	0.79	0.13	52,52,52,52	0
87	MG	5	4213	1/1	0.79	0.20	59,59,59,59	0
87	MG	6	2232	1/1	0.79	0.53	53,53,53,53	0
87	MG	5	4186	1/1	0.79	0.76	123,123,123,123	0
87	MG	1	3964	1/1	0.79	0.60	51,51,51,51	0
87	MG	S4	302	1/1	0.79	1.58	87,87,87,87	0
87	MG	5	4355	1/1	0.79	0.60	53,53,53,53	0
87	MG	1	4180	1/1	0.79	0.27	58,58,58,58	0
87	MG	6	2273	1/1	0.79	0.25	80,80,80,80	0
86	OHX	6	2076	7/7	0.79	0.40	74,74,74,74	7
87	MG	5	3828	1/1	0.79	0.46	54,54,54,54	0
87	MG	1	4112	1/1	0.79	0.90	48,48,48,48	0
86	OHX	6	2074	7/7	0.79	0.19	108,108,108,108	7
87	MG	1	4150	1/1	0.79	0.22	73,73,73,73	0
87	MG	1	4153	1/1	0.79	0.64	101,101,101,101	0
87	MG	1	4330	1/1	0.79	0.44	59,59,59,59	0
87	MG	6	2113	1/1	0.79	0.18	75,75,75,75	0
87	MG	6	2115	1/1	0.79	0.25	75,75,75,75	0
87	MG	1	4432	1/1	0.79	1.18	47,47,47,47	1
86	OHX	5	3755	7/7	0.79	0.65	49,49,49,49	7
87	MG	6	2309	1/1	0.79	0.25	65,65,65,65	0
87	MG	1	4443	1/1	0.79	0.52	41,41,41,41	1
87	MG	5	4110	1/1	0.79	0.42	50,50,50,50	0
87	MG	5	4124	1/1	0.79	0.49	57,57,57,57	0
87	MG	1	4424	1/1	0.79	0.46	54,54,54,54	0
87	MG	s8	303	1/1	0.79	0.39	46,46,46,46	0
86	OHX	5	3756	7/7	0.79	0.36	42,42,42,42	7
87	MG	5	4245	1/1	0.79	0.29	65,65,65,65	0
86	OHX	6	2049	7/7	0.79	0.40	70,70,70,70	7
87	MG	6	2107	1/1	0.80	0.23	47,47,47,47	0
87	MG	5	4196	1/1	0.80	0.17	52,52,52,52	0
86	OHX	1	3737	7/7	0.80	0.38	42,42,42,42	7
87	MG	1	4464	1/1	0.80	1.88	60,60,60,60	0
87	MG	1	4501	1/1	0.80	0.37	66,66,66,66	0
86	OHX	6	2077	7/7	0.80	0.28	85,85,85,85	7
87	MG	2	2242	1/1	0.80	0.20	85,85,85,85	0
87	MG	8	232	1/1	0.80	0.44	64,64,64,64	0
87	MG	5	4400	1/1	0.80	0.44	43,43,43,43	1
87	MG	5	4568	1/1	0.80	0.34	38,38,38,38	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	1	4468	1/1	0.80	0.20	70,70,70,70	1
87	MG	1	4215	1/1	0.80	0.34	37,37,37,37	0
87	MG	5	4233	1/1	0.80	0.34	58,58,58,58	1
87	MG	18	301	1/1	0.80	0.51	70,70,70,70	0
86	OHX	6	2096	7/7	0.80	0.29	78,78,78,78	7
86	OHX	6	2052	7/7	0.80	0.47	127,127,127,127	7
87	MG	4	244	1/1	0.80	0.43	41,41,41,41	1
87	MG	5	4142	1/1	0.80	0.33	40,40,40,40	0
87	MG	1	3868	1/1	0.80	0.22	70,70,70,70	0
87	MG	2	2139	1/1	0.80	0.44	70,70,70,70	0
87	MG	1	4216	1/1	0.80	0.26	52,52,52,52	1
87	MG	1	4241	1/1	0.80	0.30	57,57,57,57	0
87	MG	2	2244	1/1	0.80	0.15	78,78,78,78	0
87	MG	6	2271	1/1	0.80	0.36	42,42,42,42	0
87	MG	5	4178	1/1	0.80	0.53	38,38,38,38	1
87	MG	6	2262	1/1	0.80	0.63	114,114,114,114	0
86	OHX	6	1993	7/7	0.80	0.34	78,78,78,78	7
87	MG	6	2277	1/1	0.80	0.37	48,48,48,48	0
87	MG	1	4428	1/1	0.80	0.14	67,67,67,67	0
87	MG	7	235	1/1	0.81	0.30	60,60,60,60	0
87	MG	6	2284	1/1	0.81	0.35	59,59,59,59	0
87	MG	5	4549	1/1	0.81	0.20	77,77,77,77	0
87	MG	6	2138	1/1	0.81	0.68	73,73,73,73	0
87	MG	1	3922	1/1	0.81	0.45	58,58,58,58	0
87	MG	6	2200	1/1	0.81	1.16	74,74,74,74	0
87	MG	N3	202	1/1	0.81	0.45	67,67,67,67	0
87	MG	1	3872	1/1	0.81	0.78	54,54,54,54	0
87	MG	1	4143	1/1	0.81	0.43	54,54,54,54	0
87	MG	5	4176	1/1	0.81	0.42	45,45,45,45	0
87	MG	5	4432	1/1	0.81	0.34	36,36,36,36	1
87	MG	5	3825	1/1	0.81	0.32	48,48,48,48	0
87	MG	5	4535	1/1	0.81	0.77	56,56,56,56	0
87	MG	5	4473	1/1	0.81	0.30	49,49,49,49	0
87	MG	1	4114	1/1	0.81	0.25	67,67,67,67	0
87	MG	1	4132	1/1	0.81	0.29	51,51,51,51	0
86	OHX	2	2086	7/7	0.81	0.30	105,105,105,105	7
87	MG	5	4555	1/1	0.81	0.21	53,53,53,53	0
87	MG	5	4260	1/1	0.81	0.17	59,59,59,59	0
87	MG	2	2191	1/1	0.81	0.58	99,99,99,99	0
87	MG	6	2287	1/1	0.81	0.15	62,62,62,62	0
87	MG	5	4368	1/1	0.81	0.33	53,53,53,53	1
87	MG	1	4335	1/1	0.81	0.67	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	4198	1/1	0.81	0.57	43,43,43,43	0
87	MG	5	4098	1/1	0.81	0.39	50,50,50,50	0
87	MG	5	4566	1/1	0.81	0.32	40,40,40,40	0
87	MG	6	2320	1/1	0.81	0.32	62,62,62,62	0
87	MG	2	2209	1/1	0.81	0.29	71,71,71,71	0
87	MG	5	4318	1/1	0.81	0.30	64,64,64,64	0
87	MG	5	4130	1/1	0.81	0.37	35,35,35,35	1
87	MG	1	3820	1/1	0.81	0.51	44,44,44,44	0
87	MG	2	2254	1/1	0.81	0.26	97,97,97,97	0
87	MG	7	229	1/1	0.81	0.31	38,38,38,38	0
87	MG	d9	104	1/1	0.81	0.19	109,109,109,109	0
86	OHX	6	2056	7/7	0.81	0.18	97,97,97,97	7
87	MG	1	4470	1/1	0.81	0.44	35,35,35,35	1
87	MG	5	4389	1/1	0.81	0.41	63,63,63,63	0
87	MG	c6	201	1/1	0.81	0.41	97,97,97,97	0
87	MG	5	4315	1/1	0.81	0.44	31,31,31,31	1
87	MG	1	4378	1/1	0.81	0.39	41,41,41,41	1
87	MG	2	2126	1/1	0.81	0.64	69,69,69,69	0
86	OHX	5	3629	7/7	0.81	0.49	67,67,67,67	7
87	MG	6	2229	1/1	0.81	0.38	45,45,45,45	0
87	MG	5	4071	1/1	0.82	0.71	89,89,89,89	0
87	MG	6	2195	1/1	0.82	0.24	46,46,46,46	0
87	MG	5	4289	1/1	0.82	0.43	57,57,57,57	1
87	MG	n8	202	1/1	0.82	0.17	51,51,51,51	0
87	MG	c6	202	1/1	0.82	0.25	87,87,87,87	0
87	MG	1	3840	1/1	0.82	0.21	43,43,43,43	0
87	MG	5	4505	1/1	0.82	0.22	49,49,49,49	0
86	OHX	5	3785	7/7	0.82	0.37	53,53,53,53	7
86	OHX	5	3658	7/7	0.82	0.48	51,51,51,51	7
87	MG	5	4439	1/1	0.82	0.34	40,40,40,40	0
86	OHX	2	2072	7/7	0.82	0.33	104,104,104,104	7
87	MG	5	4541	1/1	0.82	0.25	56,56,56,56	0
87	MG	1	4128	1/1	0.82	0.34	55,55,55,55	0
87	MG	l5	305	1/1	0.82	0.14	62,62,62,62	0
87	MG	4	234	1/1	0.82	0.26	67,67,67,67	0
87	MG	2	2110	1/1	0.82	0.57	66,66,66,66	0
87	MG	1	4248	1/1	0.82	0.17	55,55,55,55	0
87	MG	6	2150	1/1	0.82	0.50	59,59,59,59	0
87	MG	1	4138	1/1	0.82	0.34	46,46,46,46	0
87	MG	1	4473	1/1	0.82	0.34	51,51,51,51	0
87	MG	5	4414	1/1	0.82	0.34	38,38,38,38	1
87	MG	5	4524	1/1	0.82	0.30	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	4449	1/1	0.82	0.33	48,48,48,48	0
87	MG	4	224	1/1	0.82	0.35	37,37,37,37	0
87	MG	2	2243	1/1	0.82	0.36	61,61,61,61	0
87	MG	5	4392	1/1	0.82	0.51	134,134,134,134	0
87	MG	6	2324	1/1	0.82	0.52	47,47,47,47	1
86	OHX	M9	203	7/7	0.82	0.25	78,78,78,78	7
87	MG	1	4141	1/1	0.82	0.27	51,51,51,51	0
87	MG	5	4299	1/1	0.82	0.51	47,47,47,47	0
87	MG	6	2201	1/1	0.82	0.09	83,83,83,83	0
86	OHX	6	2028	7/7	0.82	0.38	58,58,58,58	7
87	MG	6	2321	1/1	0.82	0.36	72,72,72,72	0
86	OHX	1	3772	7/7	0.82	0.41	61,61,61,61	7
87	MG	D0	201	1/1	0.82	0.47	71,71,71,71	0
86	OHX	5	3772	7/7	0.82	0.39	115,115,115,115	7
91	PRO	5	3404	7/8	0.82	0.31	71,71,71,71	0
86	OHX	6	2034	7/7	0.82	0.23	134,134,134,134	7
87	MG	1	4508	1/1	0.82	0.32	37,37,37,37	1
87	MG	2	2103	1/1	0.82	0.24	65,65,65,65	0
87	MG	1	4466	1/1	0.82	0.51	43,43,43,43	0
87	MG	2	2165	1/1	0.82	0.18	98,98,98,98	0
87	MG	1	3923	1/1	0.82	0.71	75,75,75,75	0
87	MG	1	4052	1/1	0.82	0.40	49,49,49,49	0
87	MG	5	3916	1/1	0.82	0.32	57,57,57,57	0
86	OHX	2	2041	7/7	0.82	0.39	83,83,83,83	7
87	MG	5	3856	1/1	0.82	0.45	35,35,35,35	0
87	MG	m6	203	1/1	0.82	0.24	41,41,41,41	1
87	MG	2	2146	1/1	0.82	0.24	86,86,86,86	0
87	MG	2	2122	1/1	0.82	0.37	68,68,68,68	0
86	OHX	6	2060	7/7	0.82	0.42	58,58,58,58	7
87	MG	2	2120	1/1	0.83	0.21	70,70,70,70	0
87	MG	7	223	1/1	0.83	0.21	52,52,52,52	0
89	C	1	3402	20/21	0.83	0.30	50,107,109,109	0
87	MG	c9	201	1/1	0.83	0.10	78,78,78,78	0
87	MG	6	2306	1/1	0.83	0.49	79,79,79,79	0
87	MG	8	233	1/1	0.83	0.13	88,88,88,88	0
87	MG	1	4105	1/1	0.83	0.56	47,47,47,47	0
87	MG	5	4140	1/1	0.83	0.20	82,82,82,82	0
87	MG	m4	202	1/1	0.83	0.56	53,53,53,53	1
87	MG	1	4342	1/1	0.83	0.32	58,58,58,58	0
87	MG	6	2225	1/1	0.83	0.52	55,55,55,55	0
87	MG	6	2234	1/1	0.83	0.22	79,79,79,79	0
89	C	5	3401	20/21	0.83	0.25	48,105,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4281	1/1	0.83	0.30	40,40,40,40	0
87	MG	1	4510	1/1	0.83	0.26	50,50,50,50	0
87	MG	5	4438	1/1	0.83	0.51	40,40,40,40	0
87	MG	1	4146	1/1	0.83	0.22	50,50,50,50	0
86	OHX	1	3754	7/7	0.83	0.28	99,99,99,99	7
87	MG	2	2133	1/1	0.83	0.29	76,76,76,76	0
87	MG	5	4503	1/1	0.83	0.23	46,46,46,46	0
87	MG	5	3984	1/1	0.83	0.30	50,50,50,50	0
87	MG	5	4493	1/1	0.83	0.37	38,38,38,38	0
87	MG	6	2210	1/1	0.83	0.24	79,79,79,79	0
87	MG	5	4218	1/1	0.83	0.24	41,41,41,41	0
87	MG	8	231	1/1	0.83	0.54	50,50,50,50	0
87	MG	l3	414	1/1	0.83	0.57	32,32,32,32	1
87	MG	5	3982	1/1	0.83	0.32	57,57,57,57	0
87	MG	O1	203	1/1	0.83	1.06	57,57,57,57	0
87	MG	l3	415	1/1	0.83	0.35	36,36,36,36	1
87	MG	8	237	1/1	0.83	0.21	71,71,71,71	0
87	MG	2	2118	1/1	0.83	0.95	46,46,46,46	0
87	MG	M7	202	1/1	0.83	0.63	52,52,52,52	0
87	MG	6	2249	1/1	0.83	0.24	53,53,53,53	0
86	OHX	1	3739	7/7	0.83	0.44	52,52,52,52	7
87	MG	1	4042	1/1	0.83	0.21	50,50,50,50	0
87	MG	5	3869	1/1	0.83	0.21	62,62,62,62	0
86	OHX	5	3746	7/7	0.83	0.21	149,149,149,149	7
87	MG	5	4231	1/1	0.83	0.67	35,35,35,35	1
86	OHX	2	2034	7/7	0.83	0.42	86,86,86,86	7
87	MG	1	4398	1/1	0.83	0.23	72,72,72,72	0
87	MG	5	4164	1/1	0.83	0.12	83,83,83,83	0
86	OHX	5	3782	7/7	0.83	0.58	45,45,45,45	7
87	MG	6	2311	1/1	0.83	0.91	60,60,60,60	1
87	MG	1	4058	1/1	0.83	0.65	44,44,44,44	0
87	MG	6	2260	1/1	0.83	0.29	55,55,55,55	0
87	MG	1	4301	1/1	0.83	0.68	52,52,52,52	0
87	MG	1	4349	1/1	0.83	0.20	69,69,69,69	0
87	MG	1	4147	1/1	0.83	0.39	48,48,48,48	0
86	OHX	1	3733	7/7	0.83	0.41	46,46,46,46	7
86	OHX	5	3709	7/7	0.83	0.27	41,41,41,41	7
87	MG	2	2164	1/1	0.83	0.28	122,122,122,122	0
87	MG	5	3835	1/1	0.83	0.46	37,37,37,37	0
87	MG	5	4545	1/1	0.83	0.42	34,34,34,34	1
86	OHX	2	2052	7/7	0.83	0.20	189,189,189,189	7
87	MG	5	4412	1/1	0.83	0.40	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	6	2156	1/1	0.83	0.62	66,66,66,66	0
86	OHX	5	3769	7/7	0.83	0.54	78,78,78,78	7
87	MG	7	222	1/1	0.83	0.19	61,61,61,61	0
86	OHX	1	3757	7/7	0.83	0.26	49,49,49,49	7
86	OHX	2	2049	7/7	0.83	0.32	84,84,84,84	7
87	MG	O2	202	1/1	0.84	0.41	32,32,32,32	0
87	MG	1	4173	1/1	0.84	0.46	52,52,52,52	0
87	MG	2	2200	1/1	0.84	0.57	65,65,65,65	0
87	MG	2	2148	1/1	0.84	0.48	130,130,130,130	0
87	MG	5	4544	1/1	0.84	0.76	37,37,37,37	0
86	OHX	6	2073	7/7	0.84	0.35	64,64,64,64	7
87	MG	6	2290	1/1	0.84	0.29	52,52,52,52	0
87	MG	6	2169	1/1	0.84	0.16	85,85,85,85	0
87	MG	5	4121	1/1	0.84	0.20	52,52,52,52	0
87	MG	1	4064	1/1	0.84	0.51	56,56,56,56	0
87	MG	1	4081	1/1	0.84	0.72	46,46,46,46	0
87	MG	5	4550	1/1	0.84	0.98	49,49,49,49	1
87	MG	1	4144	1/1	0.84	0.43	41,41,41,41	0
87	MG	17	306	1/1	0.84	1.64	37,37,37,37	1
87	MG	5	4415	1/1	0.84	0.50	33,33,33,33	1
87	MG	5	4319	1/1	0.84	0.34	59,59,59,59	0
87	MG	5	4437	1/1	0.84	0.40	37,37,37,37	1
90	8AN	5	3403	22/23	0.84	0.29	42,97,101,102	0
87	MG	1	4039	1/1	0.84	0.53	32,32,32,32	0
87	MG	1	4457	1/1	0.84	0.56	43,43,43,43	0
87	MG	2	2197	1/1	0.84	0.40	76,76,76,76	0
86	OHX	5	3767	7/7	0.84	0.53	39,39,39,39	7
87	MG	5	3834	1/1	0.84	0.33	46,46,46,46	0
87	MG	1	4236	1/1	0.84	0.28	52,52,52,52	0
86	OHX	6	2089	7/7	0.84	0.30	74,74,74,74	7
87	MG	1	4226	1/1	0.84	0.12	72,72,72,72	0
87	MG	5	4120	1/1	0.84	0.68	39,39,39,39	0
87	MG	5	4238	1/1	0.84	0.30	33,33,33,33	1
87	MG	2	2163	1/1	0.84	0.60	70,70,70,70	0
87	MG	5	4149	1/1	0.84	0.43	50,50,50,50	0
87	MG	5	4088	1/1	0.84	0.30	42,42,42,42	1
87	MG	1	4228	1/1	0.84	0.19	62,62,62,62	0
86	OHX	6	2024	7/7	0.84	0.23	86,86,86,86	7
86	OHX	7	213	7/7	0.84	0.28	56,56,56,56	7
87	MG	5	4442	1/1	0.84	0.29	34,34,34,34	1
86	OHX	m1	201	7/7	0.84	0.38	73,73,73,73	7
87	MG	6	2208	1/1	0.84	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	M0	306	1/1	0.84	0.29	53,53,53,53	0
86	OHX	5	3790	7/7	0.84	0.38	40,40,40,40	7
86	OHX	2	2084	7/7	0.84	0.16	183,183,183,183	7
87	MG	6	2259	1/1	0.84	0.32	48,48,48,48	0
87	MG	4	230	1/1	0.84	0.29	47,47,47,47	0
87	MG	17	307	1/1	0.84	0.39	38,38,38,38	1
87	MG	m7	202	1/1	0.84	0.53	36,36,36,36	0
87	MG	1	4106	1/1	0.84	0.28	45,45,45,45	0
87	MG	5	4051	1/1	0.84	0.42	33,33,33,33	0
87	MG	2	2095	1/1	0.84	0.38	63,63,63,63	0
87	MG	D9	104	1/1	0.84	0.10	85,85,85,85	0
87	MG	5	4386	1/1	0.84	0.42	37,37,37,37	1
87	MG	5	4293	1/1	0.84	0.62	43,43,43,43	0
87	MG	1	3951	1/1	0.84	0.76	35,35,35,35	0
87	MG	1	4034	1/1	0.84	0.20	54,54,54,54	0
87	MG	2	2192	1/1	0.84	0.43	64,64,64,64	0
86	OHX	7	212	7/7	0.84	0.44	61,61,61,61	7
87	MG	5	4217	1/1	0.84	0.54	66,66,66,66	0
86	OHX	2	2077	7/7	0.84	0.27	139,139,139,139	7
87	MG	1	4157	1/1	0.84	0.34	42,42,42,42	0
87	MG	5	3851	1/1	0.84	0.47	36,36,36,36	0
87	MG	5	3966	1/1	0.84	0.50	39,39,39,39	0
86	OHX	5	3660	7/7	0.84	0.21	42,42,42,42	7
87	MG	5	4401	1/1	0.84	0.34	48,48,48,48	0
87	MG	5	4369	1/1	0.84	0.84	52,52,52,52	1
87	MG	5	4103	1/1	0.84	0.68	35,35,35,35	0
87	MG	1	4357	1/1	0.85	0.20	49,49,49,49	0
86	OHX	5	3812	7/7	0.85	0.59	54,54,54,54	7
87	MG	6	2214	1/1	0.85	0.57	79,79,79,79	0
87	MG	1	4206	1/1	0.85	0.20	48,48,48,48	0
86	OHX	6	2094	7/7	0.85	0.32	102,102,102,102	7
87	MG	5	4179	1/1	0.85	0.29	44,44,44,44	0
86	OHX	1	3747	7/7	0.85	0.33	46,46,46,46	7
87	MG	2	2124	1/1	0.85	0.51	77,77,77,77	0
87	MG	7	228	1/1	0.85	0.29	41,41,41,41	1
87	MG	2	2101	1/1	0.85	0.26	73,73,73,73	0
87	MG	5	4115	1/1	0.85	0.36	35,35,35,35	0
87	MG	1	4124	1/1	0.85	0.35	46,46,46,46	0
87	MG	1	3837	1/1	0.85	0.30	41,41,41,41	0
87	MG	5	4482	1/1	0.85	0.42	45,45,45,45	1
87	MG	2	2211	1/1	0.85	0.16	106,106,106,106	0
87	MG	2	2108	1/1	0.85	0.64	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	6	2206	1/1	0.85	0.23	67,67,67,67	0
87	MG	5	4487	1/1	0.85	0.35	37,37,37,37	0
87	MG	1	4324	1/1	0.85	0.24	54,54,54,54	0
87	MG	2	2182	1/1	0.85	0.38	87,87,87,87	0
87	MG	1	4183	1/1	0.85	0.39	37,37,37,37	0
87	MG	1	3958	1/1	0.85	0.63	32,32,32,32	0
87	MG	1	4184	1/1	0.85	0.16	63,63,63,63	0
86	OHX	6	2053	7/7	0.85	0.22	85,85,85,85	7
87	MG	6	2251	1/1	0.85	0.42	74,74,74,74	0
87	MG	2	2190	1/1	0.85	0.25	78,78,78,78	0
87	MG	5	3880	1/1	0.85	0.48	34,34,34,34	0
86	OHX	6	2095	7/7	0.85	0.38	73,73,73,73	7
87	MG	6	2189	1/1	0.85	0.45	47,47,47,47	0
86	OHX	5	3635	7/7	0.85	0.23	81,81,81,81	7
86	OHX	1	3735	7/7	0.85	0.49	71,71,71,71	7
87	MG	1	3925	1/1	0.85	0.75	49,49,49,49	0
87	MG	1	4258	1/1	0.85	0.55	77,77,77,77	0
87	MG	1	4162	1/1	0.85	0.23	42,42,42,42	0
86	OHX	2	2079	7/7	0.85	0.32	103,103,103,103	7
87	MG	2	2137	1/1	0.85	0.46	126,126,126,126	0
87	MG	5	3935	1/1	0.85	0.37	54,54,54,54	0
87	MG	5	3893	1/1	0.85	0.36	47,47,47,47	0
87	MG	5	3956	1/1	0.85	0.35	47,47,47,47	0
87	MG	1	3907	1/1	0.85	0.20	59,59,59,59	0
87	MG	6	2220	1/1	0.85	0.31	47,47,47,47	0
87	MG	1	4252	1/1	0.85	0.28	58,58,58,58	0
86	OHX	6	2027	7/7	0.85	0.34	83,83,83,83	7
87	MG	5	4323	1/1	0.85	0.68	36,36,36,36	1
86	OHX	5	3758	7/7	0.85	0.32	42,42,42,42	7
87	MG	4	235	1/1	0.85	0.43	90,90,90,90	1
87	MG	2	2210	1/1	0.85	0.34	69,69,69,69	0
87	MG	6	2267	1/1	0.85	0.31	54,54,54,54	0
87	MG	1	4264	1/1	0.85	0.53	53,53,53,53	0
87	MG	5	3860	1/1	0.85	0.42	39,39,39,39	0
86	OHX	6	2085	7/7	0.85	0.41	128,128,128,128	7
87	MG	1	4259	1/1	0.85	0.16	61,61,61,61	0
91	PRO	1	3404	7/8	0.85	0.29	75,75,75,75	0
86	OHX	2	1984	7/7	0.85	0.14	177,177,177,177	7
87	MG	2	2107	1/1	0.85	0.37	60,60,60,60	0
87	MG	2	2202	1/1	0.85	0.22	69,69,69,69	0
87	MG	6	2130	1/1	0.85	0.19	55,55,55,55	0
87	MG	6	2313	1/1	0.85	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	5	3953	1/1	0.85	0.62	45,45,45,45	0
87	MG	5	4229	1/1	0.85	0.46	43,43,43,43	0
86	OHX	2	2071	7/7	0.85	0.34	94,94,94,94	7
87	MG	5	4569	1/1	0.85	0.36	117,117,117,117	0
87	MG	5	4391	1/1	0.85	0.42	52,52,52,52	0
86	OHX	2	2089	7/7	0.85	0.28	121,121,121,121	7
87	MG	M7	204	1/1	0.86	0.51	40,40,40,40	0
87	MG	5	3885	1/1	0.86	0.34	58,58,58,58	0
87	MG	2	2227	1/1	0.86	0.34	63,63,63,63	0
87	MG	n1	204	1/1	0.86	0.33	56,56,56,56	0
86	OHX	6	2012	7/7	0.86	0.30	64,64,64,64	7
87	MG	1	3821	1/1	0.86	0.19	55,55,55,55	0
87	MG	1	4070	1/1	0.86	0.14	70,70,70,70	0
87	MG	5	4204	1/1	0.86	0.55	60,60,60,60	0
87	MG	5	4528	1/1	0.86	0.36	83,83,83,83	1
86	OHX	5	3702	7/7	0.86	0.27	86,86,86,86	7
87	MG	M1	202	1/1	0.86	0.16	72,72,72,72	0
86	OHX	2	2080	7/7	0.86	0.32	66,66,66,66	7
87	MG	1	4182	1/1	0.86	0.21	55,55,55,55	0
86	OHX	5	3797	7/7	0.86	0.50	42,42,42,42	7
87	MG	1	4060	1/1	0.86	0.31	44,44,44,44	0
89	C	1	3401	20/21	0.86	0.26	54,111,113,113	0
87	MG	5	4375	1/1	0.86	0.26	61,61,61,61	0
86	OHX	6	2068	7/7	0.86	0.37	83,83,83,83	7
86	OHX	5	3750	7/7	0.86	0.14	131,131,131,131	7
86	OHX	2	2066	7/7	0.86	0.35	80,80,80,80	7
86	OHX	2	2063	7/7	0.86	0.33	81,81,81,81	7
87	MG	1	4480	1/1	0.86	0.66	48,48,48,48	0
87	MG	1	4393	1/1	0.86	0.24	49,49,49,49	0
87	MG	1	4391	1/1	0.86	0.54	37,37,37,37	1
87	MG	6	2119	1/1	0.86	0.55	59,59,59,59	0
87	MG	5	4304	1/1	0.86	0.14	70,70,70,70	0
87	MG	5	4476	1/1	0.86	0.55	46,46,46,46	0
86	OHX	5	3792	7/7	0.86	0.51	51,51,51,51	7
87	MG	1	4118	1/1	0.86	0.74	42,42,42,42	0
87	MG	5	4290	1/1	0.86	0.42	72,72,72,72	0
87	MG	1	4274	1/1	0.86	0.85	43,43,43,43	1
87	MG	5	4348	1/1	0.86	1.51	46,46,46,46	1
87	MG	1	4036	1/1	0.86	0.35	41,41,41,41	0
87	MG	1	4493	1/1	0.86	0.25	46,46,46,46	0
87	MG	1	4505	1/1	0.86	0.47	51,51,51,51	0
87	MG	5	4250	1/1	0.86	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	3959	1/1	0.86	0.37	55,55,55,55	0
87	MG	5	4574	1/1	0.86	0.34	49,49,49,49	0
87	MG	6	2215	1/1	0.86	0.16	52,52,52,52	0
86	OHX	5	3649	7/7	0.86	0.37	41,41,41,41	7
86	OHX	1	3756	7/7	0.86	0.34	59,59,59,59	7
87	MG	1	4325	1/1	0.86	0.55	52,52,52,52	0
87	MG	5	4440	1/1	0.86	0.40	33,33,33,33	0
86	OHX	5	3763	7/7	0.86	0.32	56,56,56,56	7
87	MG	1	3936	1/1	0.86	0.75	31,31,31,31	0
86	OHX	2	2058	7/7	0.86	0.23	193,193,193,193	7
87	MG	6	2114	1/1	0.86	0.81	49,49,49,49	0
87	MG	o3	204	1/1	0.86	0.55	37,37,37,37	1
87	MG	5	4046	1/1	0.86	0.42	51,51,51,51	0
87	MG	1	3945	1/1	0.86	0.40	43,43,43,43	0
86	OHX	1	3795	7/7	0.86	0.29	79,79,79,79	7
87	MG	1	4498	1/1	0.86	0.31	41,41,41,41	0
87	MG	5	3937	1/1	0.86	0.78	33,33,33,33	0
87	MG	5	4388	1/1	0.86	0.27	40,40,40,40	0
87	MG	5	3951	1/1	0.86	0.98	39,39,39,39	0
87	MG	5	4228	1/1	0.86	0.28	44,44,44,44	0
87	MG	6	2248	1/1	0.86	0.36	53,53,53,53	0
87	MG	5	4317	1/1	0.86	0.18	102,102,102,102	0
87	MG	1	4472	1/1	0.86	0.46	61,61,61,61	0
87	MG	1	3988	1/1	0.86	0.27	42,42,42,42	0
86	OHX	1	3755	7/7	0.86	0.25	79,79,79,79	7
88	ZN	d7	101	1/1	0.86	0.27	135,135,135,135	0
87	MG	C5	202	1/1	0.86	0.60	76,76,76,76	0
87	MG	S8	302	1/1	0.86	1.00	69,69,69,69	1
87	MG	5	4123	1/1	0.86	0.28	42,42,42,42	0
86	OHX	1	3770	7/7	0.86	0.25	141,141,141,141	7
87	MG	1	4297	1/1	0.86	0.32	46,46,46,46	0
87	MG	5	4561	1/1	0.86	0.29	41,41,41,41	0
87	MG	5	3949	1/1	0.86	0.45	28,28,28,28	0
86	OHX	5	3742	7/7	0.86	0.33	49,49,49,49	7
87	MG	5	3884	1/1	0.86	0.44	40,40,40,40	0
87	MG	6	2219	1/1	0.86	0.34	60,60,60,60	0
87	MG	5	4539	1/1	0.86	0.61	56,56,56,56	0
87	MG	5	4330	1/1	0.86	0.19	79,79,79,79	0
87	MG	E1	502	1/1	0.86	0.25	125,125,125,125	0
86	OHX	6	2086	7/7	0.86	0.26	147,147,147,147	7
86	OHX	2	2010	7/7	0.86	0.22	101,101,101,101	7
87	MG	5	4043	1/1	0.86	0.38	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	o3	202	1/1	0.86	0.38	53,53,53,53	0
87	MG	5	4249	1/1	0.86	0.33	60,60,60,60	0
87	MG	2	2235	1/1	0.86	0.27	102,102,102,102	1
87	MG	1	3895	1/1	0.86	0.50	44,44,44,44	0
87	MG	6	2166	1/1	0.86	0.30	88,88,88,88	0
87	MG	5	4199	1/1	0.86	0.19	41,41,41,41	0
87	MG	1	3970	1/1	0.86	0.32	66,66,66,66	0
87	MG	1	4230	1/1	0.86	0.36	41,41,41,41	1
87	MG	5	4520	1/1	0.86	0.39	43,43,43,43	0
87	MG	s4	302	1/1	0.86	0.19	55,55,55,55	0
87	MG	5	4114	1/1	0.86	0.41	43,43,43,43	0
87	MG	1	4352	1/1	0.86	0.27	52,52,52,52	0
86	OHX	8	219	7/7	0.86	0.26	92,92,92,92	7
87	MG	5	4170	1/1	0.86	0.57	36,36,36,36	1
87	MG	2	2090	1/1	0.86	0.36	83,83,83,83	0
87	MG	2	2119	1/1	0.86	0.45	92,92,92,92	0
86	OHX	5	3789	7/7	0.86	0.37	90,90,90,90	7
87	MG	5	4536	1/1	0.86	0.31	42,42,42,42	1
87	MG	5	3871	1/1	0.86	0.39	36,36,36,36	0
87	MG	6	2295	1/1	0.86	0.35	58,58,58,58	1
87	MG	6	2315	1/1	0.86	0.30	54,54,54,54	0
87	MG	1	4503	1/1	0.86	0.28	47,47,47,47	0
86	OHX	m4	201	7/7	0.86	0.52	101,101,101,101	7
86	OHX	1	3783	7/7	0.86	0.33	48,48,48,48	7
86	OHX	1	3781	7/7	0.87	0.28	63,63,63,63	7
86	OHX	6	2093	7/7	0.87	0.30	83,83,83,83	7
87	MG	1	3892	1/1	0.87	0.42	41,41,41,41	0
87	MG	19	204	1/1	0.87	0.33	41,41,41,41	1
87	MG	5	3917	1/1	0.87	0.21	39,39,39,39	0
87	MG	1	4454	1/1	0.87	0.33	50,50,50,50	0
87	MG	5	4163	1/1	0.87	0.40	59,59,59,59	0
87	MG	5	4018	1/1	0.87	0.36	34,34,34,34	0
87	MG	2	2256	1/1	0.87	0.26	66,66,66,66	0
89	C	5	3402	20/21	0.87	0.28	43,100,102,102	0
86	OHX	6	2066	7/7	0.87	0.28	70,70,70,70	7
87	MG	6	2255	1/1	0.87	0.37	54,54,54,54	0
87	MG	1	4122	1/1	0.87	0.34	45,45,45,45	0
87	MG	6	2203	1/1	0.87	0.21	68,68,68,68	0
87	MG	o2	201	1/1	0.87	0.54	35,35,35,35	1
87	MG	5	4158	1/1	0.87	0.35	45,45,45,45	0
87	MG	5	4342	1/1	0.87	0.64	34,34,34,34	0
87	MG	5	3822	1/1	0.87	0.33	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	2	2020	7/7	0.87	0.25	84,84,84,84	7
87	MG	1	3987	1/1	0.87	0.58	40,40,40,40	0
87	MG	1	4073	1/1	0.87	0.22	37,37,37,37	0
87	MG	5	4380	1/1	0.87	0.27	45,45,45,45	0
87	MG	5	3978	1/1	0.87	0.38	40,40,40,40	0
87	MG	d4	202	1/1	0.87	0.27	55,55,55,55	0
87	MG	1	4440	1/1	0.87	0.32	43,43,43,43	0
87	MG	6	2151	1/1	0.87	0.56	47,47,47,47	0
87	MG	5	4421	1/1	0.87	0.17	46,46,46,46	0
87	MG	1	4172	1/1	0.87	0.14	53,53,53,53	0
87	MG	6	2237	1/1	0.87	0.25	55,55,55,55	0
86	OHX	2	2067	7/7	0.87	0.29	92,92,92,92	7
87	MG	5	4180	1/1	0.87	0.32	51,51,51,51	0
87	MG	5	3942	1/1	0.87	0.38	40,40,40,40	0
87	MG	N3	203	1/1	0.87	0.53	51,51,51,51	0
87	MG	1	4395	1/1	0.87	0.66	34,34,34,34	1
86	OHX	6	2037	7/7	0.87	0.25	75,75,75,75	7
86	OHX	5	3647	7/7	0.87	0.28	35,35,35,35	7
87	MG	M7	206	1/1	0.87	0.30	43,43,43,43	0
87	MG	1	4220	1/1	0.87	0.55	39,39,39,39	0
87	MG	1	4461	1/1	0.87	1.07	54,54,54,54	1
87	MG	1	4170	1/1	0.87	0.24	45,45,45,45	0
87	MG	2	2091	1/1	0.87	0.79	44,44,44,44	0
87	MG	1	4446	1/1	0.87	0.52	45,45,45,45	1
87	MG	L8	301	1/1	0.87	0.54	82,82,82,82	0
87	MG	6	2205	1/1	0.87	0.14	84,84,84,84	0
87	MG	5	4132	1/1	0.87	0.27	33,33,33,33	1
87	MG	2	2251	1/1	0.87	0.44	59,59,59,59	1
87	MG	1	3867	1/1	0.87	0.55	42,42,42,42	0
86	OHX	5	3730	7/7	0.87	0.40	42,42,42,42	7
86	OHX	8	213	7/7	0.87	0.27	77,77,77,77	7
87	MG	1	4076	1/1	0.87	0.21	76,76,76,76	0
87	MG	1	4329	1/1	0.87	0.34	60,60,60,60	0
87	MG	5	3853	1/1	0.87	0.47	43,43,43,43	0
87	MG	1	4363	1/1	0.87	0.31	45,45,45,45	1
87	MG	l3	404	1/1	0.87	0.38	33,33,33,33	0
87	MG	1	4110	1/1	0.87	0.71	51,51,51,51	0
87	MG	5	4086	1/1	0.87	0.43	48,48,48,48	0
87	MG	1	4104	1/1	0.87	0.51	52,52,52,52	0
87	MG	7	220	1/1	0.87	0.21	58,58,58,58	0
87	MG	d3	201	1/1	0.87	0.53	47,47,47,47	0
87	MG	1	3857	1/1	0.87	0.28	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	O3	203	1/1	0.87	0.60	47,47,47,47	1
86	OHX	6	2045	7/7	0.87	0.29	61,61,61,61	7
86	OHX	2	2044	7/7	0.87	0.17	134,134,134,134	7
87	MG	5	4039	1/1	0.87	0.45	57,57,57,57	0
86	OHX	5	3779	7/7	0.87	0.26	122,122,122,122	7
87	MG	6	2139	1/1	0.87	0.64	63,63,63,63	0
86	OHX	8	220	7/7	0.87	0.28	77,77,77,77	7
87	MG	l3	409	1/1	0.87	0.42	41,41,41,41	1
87	MG	2	2096	1/1	0.87	0.45	61,61,61,61	0
87	MG	5	4055	1/1	0.87	0.27	33,33,33,33	0
86	OHX	o9	101	7/7	0.87	0.45	52,52,52,52	7
87	MG	6	2178	1/1	0.87	0.32	54,54,54,54	0
86	OHX	6	2072	7/7	0.87	0.32	66,66,66,66	7
87	MG	5	4282	1/1	0.87	0.35	39,39,39,39	0
86	OHX	5	3728	7/7	0.87	0.37	57,57,57,57	7
87	MG	M0	307	1/1	0.87	0.16	45,45,45,45	0
87	MG	1	3849	1/1	0.87	0.63	44,44,44,44	0
86	OHX	1	3624	7/7	0.88	0.26	63,63,63,63	7
87	MG	5	3866	1/1	0.88	0.33	34,34,34,34	0
87	MG	1	4286	1/1	0.88	0.41	40,40,40,40	0
87	MG	m6	202	1/1	0.88	0.65	36,36,36,36	1
87	MG	1	4435	1/1	0.88	0.28	41,41,41,41	1
87	MG	1	3972	1/1	0.88	0.48	41,41,41,41	0
87	MG	2	2132	1/1	0.88	0.48	70,70,70,70	0
86	OHX	5	3781	7/7	0.88	0.26	53,53,53,53	7
87	MG	4	242	1/1	0.88	0.46	45,45,45,45	0
86	OHX	2	2055	7/7	0.88	0.35	72,72,72,72	7
87	MG	5	3865	1/1	0.88	0.52	44,44,44,44	0
87	MG	6	2194	1/1	0.88	0.57	52,52,52,52	0
87	MG	5	4145	1/1	0.88	0.33	49,49,49,49	0
87	MG	5	4365	1/1	0.88	0.33	45,45,45,45	0
87	MG	5	4452	1/1	0.88	1.04	38,38,38,38	1
87	MG	4	222	1/1	0.88	0.56	46,46,46,46	0
86	OHX	5	3754	7/7	0.88	0.16	161,161,161,161	7
87	MG	1	4107	1/1	0.88	0.23	69,69,69,69	0
87	MG	5	4530	1/1	0.88	0.35	43,43,43,43	0
87	MG	1	4485	1/1	0.88	0.46	63,63,63,63	0
87	MG	6	2175	1/1	0.88	0.22	56,56,56,56	0
87	MG	7	232	1/1	0.88	0.25	50,50,50,50	0
87	MG	2	2195	1/1	0.88	0.56	65,65,65,65	0
86	OHX	1	3708	7/7	0.88	0.28	103,103,103,103	7
86	OHX	1	3684	7/7	0.88	0.30	81,81,81,81	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4240	1/1	0.88	0.27	46,46,46,46	0
87	MG	5	4047	1/1	0.88	0.47	40,40,40,40	1
86	OHX	c5	202	7/7	0.88	0.26	98,98,98,98	7
87	MG	5	4251	1/1	0.88	0.28	51,51,51,51	0
86	OHX	6	2007	7/7	0.88	0.37	62,62,62,62	7
87	MG	1	3882	1/1	0.88	0.21	49,49,49,49	0
87	MG	6	2299	1/1	0.88	0.39	59,59,59,59	0
87	MG	5	4267	1/1	0.88	0.37	38,38,38,38	0
86	OHX	1	3759	7/7	0.88	0.27	45,45,45,45	7
86	OHX	2	2065	7/7	0.88	0.15	110,110,110,110	7
87	MG	6	2132	1/1	0.88	0.35	69,69,69,69	0
87	MG	5	4312	1/1	0.88	0.32	29,29,29,29	0
86	OHX	M0	303	7/7	0.88	0.16	96,96,96,96	7
86	OHX	6	2023	7/7	0.88	0.23	80,80,80,80	7
87	MG	1	4234	1/1	0.88	0.45	51,51,51,51	0
86	OHX	5	3605	7/7	0.88	0.44	44,44,44,44	7
87	MG	5	4275	1/1	0.88	0.46	36,36,36,36	1
86	OHX	5	3648	7/7	0.88	0.40	69,69,69,69	7
87	MG	5	4484	1/1	0.88	0.28	39,39,39,39	1
87	MG	5	4261	1/1	0.88	0.30	44,44,44,44	0
87	MG	7	231	1/1	0.88	0.70	43,43,43,43	0
86	OHX	6	2013	7/7	0.88	0.31	82,82,82,82	7
87	MG	5	4154	1/1	0.88	0.28	44,44,44,44	0
87	MG	5	4078	1/1	0.88	0.61	41,41,41,41	0
86	OHX	5	3700	7/7	0.88	0.48	43,43,43,43	7
87	MG	1	3860	1/1	0.88	0.36	49,49,49,49	0
87	MG	1	4499	1/1	0.88	0.17	60,60,60,60	0
86	OHX	2	2046	7/7	0.88	0.16	114,114,114,114	7
86	OHX	6	2041	7/7	0.88	0.27	62,62,62,62	7
87	MG	8	227	1/1	0.88	0.32	61,61,61,61	0
87	MG	2	2223	1/1	0.88	0.40	69,69,69,69	0
87	MG	5	4187	1/1	0.88	0.58	53,53,53,53	0
87	MG	5	4521	1/1	0.88	0.57	59,59,59,59	0
87	MG	5	4560	1/1	0.88	0.27	40,40,40,40	0
87	MG	7	217	1/1	0.88	0.64	43,43,43,43	0
87	MG	7	230	1/1	0.88	0.42	37,37,37,37	1
87	MG	1	3883	1/1	0.88	0.41	48,48,48,48	0
87	MG	5	4219	1/1	0.88	0.54	39,39,39,39	0
87	MG	6	2286	1/1	0.88	0.12	65,65,65,65	0
87	MG	1	4043	1/1	0.88	0.15	66,66,66,66	0
87	MG	1	4195	1/1	0.88	0.44	52,52,52,52	0
87	MG	5	4552	1/1	0.88	0.30	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	O5	201	1/1	0.88	0.23	58,58,58,58	0
87	MG	1	3862	1/1	0.88	0.41	41,41,41,41	0
87	MG	5	4027	1/1	0.88	0.41	41,41,41,41	0
86	OHX	1	3761	7/7	0.88	0.29	117,117,117,117	7
86	OHX	8	216	7/7	0.88	0.26	67,67,67,67	7
86	OHX	2	2048	7/7	0.88	0.30	83,83,83,83	7
87	MG	1	3980	1/1	0.88	0.34	54,54,54,54	0
87	MG	12	302	1/1	0.88	0.45	36,36,36,36	0
87	MG	5	4332	1/1	0.88	0.15	106,106,106,106	0
86	OHX	6	2050	7/7	0.88	0.12	132,132,132,132	7
86	OHX	5	3759	7/7	0.88	0.13	110,110,110,110	7
86	OHX	5	3701	7/7	0.88	0.14	120,120,120,120	7
87	MG	1	4390	1/1	0.88	0.24	36,36,36,36	1
86	OHX	5	3678	7/7	0.88	0.29	51,51,51,51	7
87	MG	5	4128	1/1	0.88	0.27	40,40,40,40	0
87	MG	1	4483	1/1	0.88	0.37	59,59,59,59	0
87	MG	2	2219	1/1	0.88	0.38	62,62,62,62	0
87	MG	6	2293	1/1	0.88	0.85	46,46,46,46	1
87	MG	2	2171	1/1	0.89	0.37	90,90,90,90	0
87	MG	1	4032	1/1	0.89	0.59	49,49,49,49	0
87	MG	1	3832	1/1	0.89	0.69	39,39,39,39	0
87	MG	1	3993	1/1	0.89	0.29	28,28,28,28	0
87	MG	1	4010	1/1	0.89	0.56	41,41,41,41	0
87	MG	1	4018	1/1	0.89	0.58	30,30,30,30	0
86	OHX	1	3790	7/7	0.89	0.32	69,69,69,69	7
87	MG	1	4145	1/1	0.89	0.26	47,47,47,47	0
87	MG	5	4495	1/1	0.89	0.23	53,53,53,53	0
87	MG	1	4005	1/1	0.89	0.42	29,29,29,29	0
87	MG	6	2239	1/1	0.89	0.30	56,56,56,56	1
87	MG	2	2213	1/1	0.89	0.38	55,55,55,55	0
86	OHX	1	3806	7/7	0.89	0.29	54,54,54,54	7
86	OHX	3	212	7/7	0.89	0.28	79,79,79,79	7
87	MG	N8	204	1/1	0.89	0.28	48,48,48,48	0
86	OHX	2	2029	7/7	0.89	0.33	95,95,95,95	7
87	MG	1	4130	1/1	0.89	0.45	58,58,58,58	0
87	MG	2	2158	1/1	0.89	0.40	68,68,68,68	0
86	OHX	m5	502	7/7	0.89	0.29	78,78,78,78	7
87	MG	5	3868	1/1	0.89	0.36	36,36,36,36	0
86	OHX	5	3798	7/7	0.89	0.30	73,73,73,73	7
86	OHX	1	3802	7/7	0.89	0.42	63,63,63,63	7
87	MG	2	2166	1/1	0.89	0.68	55,55,55,55	0
87	MG	5	4436	1/1	0.89	0.33	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	8	238	1/1	0.89	0.47	45,45,45,45	0
87	MG	1	3869	1/1	0.89	0.37	62,62,62,62	0
87	MG	1	4029	1/1	0.89	0.16	62,62,62,62	0
87	MG	C8	203	1/1	0.89	0.06	96,96,96,96	0
87	MG	5	4280	1/1	0.89	0.18	39,39,39,39	0
86	OHX	1	3662	7/7	0.89	0.23	60,60,60,60	7
87	MG	5	4253	1/1	0.89	0.34	44,44,44,44	0
87	MG	2	2193	1/1	0.89	0.21	71,71,71,71	0
86	OHX	5	3787	7/7	0.89	0.22	111,111,111,111	7
87	MG	1	4277	1/1	0.89	0.35	37,37,37,37	0
87	MG	5	4310	1/1	0.89	0.17	50,50,50,50	0
87	MG	5	4361	1/1	0.89	0.70	37,37,37,37	1
87	MG	1	4158	1/1	0.89	0.40	42,42,42,42	1
87	MG	5	4331	1/1	0.89	0.21	62,62,62,62	0
87	MG	1	4140	1/1	0.89	0.35	39,39,39,39	0
87	MG	1	4449	1/1	0.89	0.35	49,49,49,49	1
87	MG	5	3845	1/1	0.89	0.30	46,46,46,46	0
87	MG	6	2193	1/1	0.89	0.31	57,57,57,57	0
87	MG	1	3876	1/1	0.89	0.35	30,30,30,30	0
87	MG	n0	204	1/1	0.89	0.33	45,45,45,45	0
87	MG	5	3918	1/1	0.89	0.58	50,50,50,50	0
86	OHX	6	2065	7/7	0.89	0.17	129,129,129,129	7
87	MG	1	4320	1/1	0.89	0.68	36,36,36,36	1
86	OHX	5	3818	7/7	0.89	0.33	63,63,63,63	7
87	MG	5	4500	1/1	0.89	0.23	54,54,54,54	0
87	MG	1	4185	1/1	0.89	0.79	40,40,40,40	1
87	MG	5	4136	1/1	0.89	0.33	48,48,48,48	0
87	MG	m7	204	1/1	0.89	0.58	40,40,40,40	1
87	MG	5	3830	1/1	0.89	0.33	31,31,31,31	0
87	MG	5	4185	1/1	0.89	0.22	50,50,50,50	0
87	MG	7	234	1/1	0.89	0.34	45,45,45,45	0
86	OHX	6	2017	7/7	0.89	0.34	50,50,50,50	7
87	MG	O7	106	1/1	0.89	1.39	59,59,59,59	0
87	MG	5	3923	1/1	0.89	0.23	35,35,35,35	0
87	MG	m6	201	1/1	0.89	1.03	38,38,38,38	1
87	MG	2	2170	1/1	0.89	0.21	78,78,78,78	0
86	OHX	n3	202	7/7	0.89	0.44	44,44,44,44	7
87	MG	2	2145	1/1	0.89	0.57	97,97,97,97	0
87	MG	5	4301	1/1	0.89	0.38	37,37,37,37	0
87	MG	1	4364	1/1	0.89	0.78	70,70,70,70	0
86	OHX	6	2079	7/7	0.89	0.31	60,60,60,60	7
87	MG	1	4086	1/1	0.89	0.29	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	3	219	1/1	0.89	0.32	63,63,63,63	0
86	OHX	1	3785	7/7	0.89	0.25	47,47,47,47	7
86	OHX	6	2092	7/7	0.89	0.13	104,104,104,104	7
87	MG	5	3963	1/1	0.89	1.02	43,43,43,43	0
87	MG	1	4238	1/1	0.89	0.29	46,46,46,46	0
87	MG	N9	102	1/1	0.89	0.32	38,38,38,38	0
86	OHX	O1	201	7/7	0.89	0.32	77,77,77,77	7
87	MG	5	4255	1/1	0.89	0.39	37,37,37,37	0
87	MG	1	4417	1/1	0.89	0.47	44,44,44,44	1
86	OHX	1	3780	7/7	0.89	0.31	45,45,45,45	7
87	MG	c8	203	1/1	0.89	0.12	86,86,86,86	0
87	MG	8	223	1/1	0.89	0.14	60,60,60,60	0
87	MG	5	3888	1/1	0.89	0.26	37,37,37,37	0
87	MG	5	4076	1/1	0.89	0.19	56,56,56,56	0
87	MG	5	4151	1/1	0.89	0.39	52,52,52,52	0
87	MG	5	4416	1/1	0.89	0.44	38,38,38,38	0
87	MG	1	4115	1/1	0.89	0.49	49,49,49,49	0
87	MG	1	4351	1/1	0.89	0.26	43,43,43,43	0
87	MG	1	4229	1/1	0.89	0.16	64,64,64,64	0
86	OHX	1	3728	7/7	0.89	0.32	37,37,37,37	7
87	MG	5	4507	1/1	0.89	0.48	46,46,46,46	1
87	MG	6	2325	1/1	0.89	0.40	59,59,59,59	0
87	MG	7	236	1/1	0.89	0.12	44,44,44,44	0
87	MG	6	2111	1/1	0.89	0.55	49,49,49,49	0
87	MG	M6	201	1/1	0.89	0.80	40,40,40,40	1
87	MG	L7	302	1/1	0.89	0.62	44,44,44,44	0
87	MG	1	4492	1/1	0.89	0.31	65,65,65,65	0
86	OHX	2	2062	7/7	0.89	0.30	85,85,85,85	7
86	OHX	1	3745	7/7	0.89	0.25	72,72,72,72	7
87	MG	6	2326	1/1	0.89	0.16	79,79,79,79	0
87	MG	2	2232	1/1	0.89	0.08	90,90,90,90	0
87	MG	S2	302	1/1	0.89	0.35	75,75,75,75	0
87	MG	5	4021	1/1	0.89	0.63	36,36,36,36	0
87	MG	1	4100	1/1	0.89	0.40	44,44,44,44	1
87	MG	5	4049	1/1	0.89	0.17	48,48,48,48	0
87	MG	o3	203	1/1	0.89	0.38	40,40,40,40	1
87	MG	7	225	1/1	0.89	0.17	39,39,39,39	0
87	MG	5	4385	1/1	0.89	0.34	34,34,34,34	1
86	OHX	1	3775	7/7	0.90	0.23	84,84,84,84	7
86	OHX	5	3741	7/7	0.90	0.51	53,53,53,53	7
87	MG	1	4373	1/1	0.90	0.33	69,69,69,69	0
87	MG	1	4296	1/1	0.90	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4222	1/1	0.90	0.26	45,45,45,45	0
87	MG	1	4219	1/1	0.90	0.10	54,54,54,54	0
86	OHX	5	3655	7/7	0.90	0.31	47,47,47,47	7
86	OHX	1	3725	7/7	0.90	0.31	68,68,68,68	7
87	MG	5	3981	1/1	0.90	0.47	50,50,50,50	0
86	OHX	2	2019	7/7	0.90	0.28	105,105,105,105	7
87	MG	1	3896	1/1	0.90	0.49	66,66,66,66	0
87	MG	5	3975	1/1	0.90	0.16	74,74,74,74	0
87	MG	1	4482	1/1	0.90	0.49	46,46,46,46	0
86	OHX	1	3727	7/7	0.90	0.15	141,141,141,141	7
87	MG	5	4371	1/1	0.90	0.37	38,38,38,38	1
87	MG	1	4163	1/1	0.90	0.48	52,52,52,52	0
87	MG	1	4287	1/1	0.90	0.24	40,40,40,40	1
87	MG	1	4280	1/1	0.90	0.22	76,76,76,76	0
87	MG	1	4151	1/1	0.90	0.40	50,50,50,50	0
87	MG	1	4190	1/1	0.90	0.32	65,65,65,65	0
86	OHX	5	3737	7/7	0.90	0.25	73,73,73,73	7
87	MG	1	4175	1/1	0.90	0.77	46,46,46,46	0
86	OHX	N8	201	7/7	0.90	0.27	94,94,94,94	7
87	MG	2	2161	1/1	0.90	0.38	63,63,63,63	0
87	MG	5	3904	1/1	0.90	0.34	44,44,44,44	0
87	MG	1	3844	1/1	0.90	0.71	39,39,39,39	0
87	MG	5	4070	1/1	0.90	0.23	49,49,49,49	0
86	OHX	5	3637	7/7	0.90	0.20	109,109,109,109	7
87	MG	5	3962	1/1	0.90	0.55	44,44,44,44	0
87	MG	n6	201	1/1	0.90	0.23	54,54,54,54	0
87	MG	6	2282	1/1	0.90	0.34	55,55,55,55	0
87	MG	1	4251	1/1	0.90	0.39	45,45,45,45	1
86	OHX	6	1989	7/7	0.90	0.30	84,84,84,84	7
86	OHX	1	3736	7/7	0.90	0.16	113,113,113,113	7
86	OHX	s1	302	7/7	0.90	0.25	93,93,93,93	7
87	MG	1	4074	1/1	0.90	0.49	50,50,50,50	0
87	MG	5	3827	1/1	0.90	0.71	46,46,46,46	0
87	MG	5	4346	1/1	0.90	0.19	68,68,68,68	1
87	MG	6	2233	1/1	0.90	0.47	83,83,83,83	0
86	OHX	2	2056	7/7	0.90	0.09	155,155,155,155	7
86	OHX	2	2075	7/7	0.90	0.37	87,87,87,87	7
87	MG	1	4399	1/1	0.90	0.30	54,54,54,54	0
87	MG	5	4542	1/1	0.90	0.24	45,45,45,45	0
87	MG	5	4106	1/1	0.90	0.40	35,35,35,35	0
87	MG	1	4269	1/1	0.90	0.27	68,68,68,68	0
87	MG	5	4053	1/1	0.90	0.47	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	3980	1/1	0.90	0.46	58,58,58,58	0
87	MG	5	3877	1/1	0.90	0.59	38,38,38,38	0
87	MG	1	3822	1/1	0.90	0.38	34,34,34,34	0
87	MG	5	4033	1/1	0.90	0.19	43,43,43,43	0
87	MG	5	4073	1/1	0.90	0.25	36,36,36,36	0
86	OHX	1	3766	7/7	0.90	0.23	59,59,59,59	7
87	MG	5	4007	1/1	0.90	0.52	28,28,28,28	0
87	MG	1	4511	1/1	0.90	0.53	52,52,52,52	0
87	MG	1	3891	1/1	0.90	0.30	45,45,45,45	0
87	MG	1	4488	1/1	0.90	0.16	55,55,55,55	0
87	MG	1	4221	1/1	0.90	0.35	43,43,43,43	0
87	MG	7	219	1/1	0.90	0.28	39,39,39,39	0
87	MG	2	2212	1/1	0.90	0.74	86,86,86,86	0
87	MG	5	3903	1/1	0.90	0.38	61,61,61,61	0
86	OHX	2	2059	7/7	0.90	0.25	66,66,66,66	7
87	MG	2	2144	1/1	0.90	0.31	66,66,66,66	0
86	OHX	5	3650	7/7	0.90	0.28	46,46,46,46	7
87	MG	5	3900	1/1	0.90	0.20	41,41,41,41	0
87	MG	5	4173	1/1	0.90	0.21	82,82,82,82	0
87	MG	1	3894	1/1	0.90	0.47	53,53,53,53	0
87	MG	1	4307	1/1	0.90	0.74	58,58,58,58	1
87	MG	1	4302	1/1	0.90	0.45	48,48,48,48	0
87	MG	5	3974	1/1	0.90	0.33	36,36,36,36	0
87	MG	1	4199	1/1	0.90	0.34	46,46,46,46	0
87	MG	1	4239	1/1	0.90	0.21	45,45,45,45	0
87	MG	5	3907	1/1	0.90	0.69	28,28,28,28	0
87	MG	s8	305	1/1	0.90	0.17	56,56,56,56	0
87	MG	6	2135	1/1	0.90	0.60	50,50,50,50	0
86	OHX	2	2024	7/7	0.90	0.28	91,91,91,91	7
87	MG	2	2099	1/1	0.90	0.48	63,63,63,63	0
87	MG	1	3933	1/1	0.90	0.52	49,49,49,49	0
86	OHX	6	2043	7/7	0.90	0.24	86,86,86,86	7
86	OHX	6	1990	7/7	0.90	0.28	65,65,65,65	7
86	OHX	2	2085	7/7	0.90	0.32	93,93,93,93	7
87	MG	1	4072	1/1	0.90	0.46	40,40,40,40	0
86	OHX	1	3808	7/7	0.90	0.29	60,60,60,60	7
87	MG	6	2153	1/1	0.90	0.46	44,44,44,44	0
87	MG	1	3997	1/1	0.90	0.57	43,43,43,43	0
87	MG	5	4109	1/1	0.90	0.35	40,40,40,40	0
87	MG	1	4050	1/1	0.90	0.39	35,35,35,35	0
87	MG	6	2228	1/1	0.90	0.89	59,59,59,59	1
87	MG	1	3968	1/1	0.90	0.29	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	8	224	1/1	0.90	0.36	52,52,52,52	0
87	MG	5	4344	1/1	0.90	0.46	35,35,35,35	1
87	MG	5	4190	1/1	0.90	0.40	44,44,44,44	1
86	OHX	6	2063	7/7	0.90	0.54	77,77,77,77	7
87	MG	1	4369	1/1	0.90	0.23	43,43,43,43	0
86	OHX	1	3767	7/7	0.90	0.28	45,45,45,45	7
86	OHX	1	3675	7/7	0.90	0.31	49,49,49,49	7
87	MG	5	4358	1/1	0.90	0.21	54,54,54,54	0
87	MG	1	4089	1/1	0.90	0.26	44,44,44,44	0
87	MG	n8	205	1/1	0.90	0.27	39,39,39,39	0
86	OHX	6	2051	7/7	0.90	0.36	82,82,82,82	7
87	MG	1	4125	1/1	0.90	0.43	35,35,35,35	0
86	OHX	2	1989	7/7	0.90	0.24	104,104,104,104	7
86	OHX	5	3726	7/7	0.90	0.23	62,62,62,62	7
87	MG	4	223	1/1	0.90	0.50	32,32,32,32	0
87	MG	1	4136	1/1	0.90	0.63	58,58,58,58	0
87	MG	6	2330	1/1	0.90	0.27	55,55,55,55	1
87	MG	1	4080	1/1	0.90	0.45	51,51,51,51	0
86	OHX	5	3745	7/7	0.90	0.47	37,37,37,37	7
87	MG	3	224	1/1	0.90	0.72	47,47,47,47	0
87	MG	N8	202	1/1	0.90	1.02	37,37,37,37	0
87	MG	5	4570	1/1	0.90	0.44	50,50,50,50	0
87	MG	2	2094	1/1	0.90	0.50	62,62,62,62	0
86	OHX	5	3770	7/7	0.90	0.31	96,96,96,96	7
87	MG	o2	202	1/1	0.90	0.26	49,49,49,49	0
87	MG	6	2152	1/1	0.90	0.45	50,50,50,50	0
86	OHX	1	3777	7/7	0.90	0.31	68,68,68,68	7
87	MG	5	4057	1/1	0.90	0.23	45,45,45,45	0
87	MG	1	4502	1/1	0.90	0.24	46,46,46,46	0
87	MG	5	4126	1/1	0.90	0.18	55,55,55,55	0
87	MG	1	4075	1/1	0.90	0.28	43,43,43,43	0
86	OHX	2	2074	7/7	0.90	0.37	92,92,92,92	7
87	MG	2	2105	1/1	0.90	0.33	72,72,72,72	0
87	MG	4	229	1/1	0.90	0.39	66,66,66,66	0
87	MG	5	4208	1/1	0.90	0.49	32,32,32,32	0
87	MG	L2	303	1/1	0.90	0.69	53,53,53,53	0
86	OHX	5	3676	7/7	0.90	0.41	42,42,42,42	7
87	MG	5	4519	1/1	0.90	0.84	42,42,42,42	1
87	MG	5	3971	1/1	0.90	0.47	27,27,27,27	0
86	OHX	8	217	7/7	0.90	0.24	82,82,82,82	7
86	OHX	5	3689	7/7	0.90	0.12	116,116,116,116	7
87	MG	1	4494	1/1	0.90	0.47	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	6	2308	1/1	0.90	0.68	51,51,51,51	1
87	MG	1	4082	1/1	0.90	0.49	52,52,52,52	1
87	MG	1	4309	1/1	0.90	0.36	44,44,44,44	1
87	MG	1	4225	1/1	0.90	0.43	37,37,37,37	1
87	MG	5	4518	1/1	0.90	0.80	41,41,41,41	0
87	MG	5	4235	1/1	0.90	0.50	38,38,38,38	0
87	MG	8	230	1/1	0.90	0.19	72,72,72,72	0
87	MG	1	3960	1/1	0.91	0.61	43,43,43,43	0
87	MG	1	4171	1/1	0.91	0.34	46,46,46,46	0
87	MG	5	4383	1/1	0.91	0.26	53,53,53,53	0
87	MG	8	228	1/1	0.91	0.31	46,46,46,46	1
87	MG	2	2240	1/1	0.91	0.31	66,66,66,66	0
87	MG	5	3824	1/1	0.91	0.44	39,39,39,39	0
87	MG	1	3912	1/1	0.91	0.24	52,52,52,52	0
86	OHX	1	3688	7/7	0.91	0.27	54,54,54,54	7
86	OHX	M0	304	7/7	0.91	0.15	96,96,96,96	7
87	MG	O1	204	1/1	0.91	0.35	63,63,63,63	0
86	OHX	6	2042	7/7	0.91	0.48	54,54,54,54	7
87	MG	1	4103	1/1	0.91	0.21	88,88,88,88	0
87	MG	3	228	1/1	0.91	0.12	78,78,78,78	0
87	MG	1	4137	1/1	0.91	0.25	38,38,38,38	0
87	MG	1	4384	1/1	0.91	0.28	64,64,64,64	0
86	OHX	1	3730	7/7	0.91	0.29	59,59,59,59	7
87	MG	5	4466	1/1	0.91	0.33	39,39,39,39	0
87	MG	5	4485	1/1	0.91	0.25	95,95,95,95	0
87	MG	6	2179	1/1	0.91	0.12	67,67,67,67	0
87	MG	1	4135	1/1	0.91	0.38	41,41,41,41	0
87	MG	1	4003	1/1	0.91	0.46	44,44,44,44	0
86	OHX	6	2044	7/7	0.91	0.27	78,78,78,78	7
87	MG	6	2235	1/1	0.91	0.20	76,76,76,76	0
86	OHX	6	2025	7/7	0.91	0.17	113,113,113,113	7
86	OHX	1	3707	7/7	0.91	0.15	106,106,106,106	7
87	MG	1	4061	1/1	0.91	0.31	32,32,32,32	0
87	MG	5	4091	1/1	0.91	0.60	53,53,53,53	0
86	OHX	5	3712	7/7	0.91	0.66	36,36,36,36	7
87	MG	1	3829	1/1	0.91	0.32	58,58,58,58	0
87	MG	6	2268	1/1	0.91	0.31	84,84,84,84	0
87	MG	5	4063	1/1	0.91	0.19	37,37,37,37	0
87	MG	5	4062	1/1	0.91	0.45	39,39,39,39	0
87	MG	5	4313	1/1	0.91	0.21	57,57,57,57	0
87	MG	1	4062	1/1	0.91	0.29	33,33,33,33	1
86	OHX	1	3752	7/7	0.91	0.11	180,180,180,180	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	2	2130	1/1	0.91	0.36	75,75,75,75	0
87	MG	1	4402	1/1	0.91	0.19	48,48,48,48	0
87	MG	5	4256	1/1	0.91	0.44	44,44,44,44	0
87	MG	5	4254	1/1	0.91	0.32	38,38,38,38	1
86	OHX	m9	201	7/7	0.91	0.19	70,70,70,70	7
87	MG	5	4167	1/1	0.91	0.76	39,39,39,39	0
87	MG	2	2143	1/1	0.91	0.08	91,91,91,91	0
87	MG	5	4527	1/1	0.91	0.22	55,55,55,55	0
87	MG	5	4239	1/1	0.91	0.28	34,34,34,34	1
87	MG	5	4547	1/1	0.91	0.24	46,46,46,46	0
86	OHX	1	3710	7/7	0.91	0.26	55,55,55,55	7
87	MG	1	4271	1/1	0.91	0.34	48,48,48,48	0
87	MG	5	4523	1/1	0.91	0.26	43,43,43,43	1
87	MG	5	3989	1/1	0.91	0.51	32,32,32,32	0
87	MG	5	4052	1/1	0.91	0.40	39,39,39,39	0
87	MG	1	3969	1/1	0.91	0.32	41,41,41,41	0
87	MG	1	4083	1/1	0.91	0.46	29,29,29,29	0
87	MG	5	4517	1/1	0.91	0.19	54,54,54,54	0
87	MG	5	4258	1/1	0.91	0.23	57,57,57,57	0
87	MG	17	304	1/1	0.91	0.14	49,49,49,49	1
86	OHX	L3	403	7/7	0.91	0.23	85,85,85,85	7
86	OHX	S8	301	7/7	0.91	0.16	108,108,108,108	7
87	MG	1	4188	1/1	0.91	0.31	47,47,47,47	0
87	MG	4	225	1/1	0.91	0.33	55,55,55,55	0
88	ZN	e1	501	1/1	0.91	0.04	163,163,163,163	0
86	OHX	1	3804	7/7	0.91	0.29	67,67,67,67	7
86	OHX	1	3731	7/7	0.91	0.19	100,100,100,100	7
87	MG	1	3877	1/1	0.91	0.65	39,39,39,39	0
86	OHX	5	3776	7/7	0.91	0.32	80,80,80,80	7
87	MG	6	2211	1/1	0.91	0.38	50,50,50,50	0
87	MG	5	4169	1/1	0.91	0.57	43,43,43,43	0
87	MG	2	2157	1/1	0.91	0.37	103,103,103,103	0
87	MG	5	4402	1/1	0.91	0.26	42,42,42,42	1
87	MG	5	3990	1/1	0.91	0.21	57,57,57,57	0
86	OHX	1	3773	7/7	0.91	0.28	71,71,71,71	7
87	MG	5	4359	1/1	0.91	0.39	73,73,73,73	0
86	OHX	1	3729	7/7	0.91	0.39	57,57,57,57	7
87	MG	1	4233	1/1	0.91	0.15	63,63,63,63	0
87	MG	2	2152	1/1	0.91	0.35	88,88,88,88	0
87	MG	1	4090	1/1	0.91	0.31	50,50,50,50	0
87	MG	5	3852	1/1	0.91	0.35	40,40,40,40	0
87	MG	1	4305	1/1	0.91	0.38	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3523	7/7	0.91	0.20	120,120,120,120	7
87	MG	5	3947	1/1	0.91	0.35	43,43,43,43	0
87	MG	2	2134	1/1	0.91	0.61	76,76,76,76	0
87	MG	1	4207	1/1	0.91	0.19	58,58,58,58	0
86	OHX	1	3769	7/7	0.91	0.58	49,49,49,49	7
86	OHX	1	3605	7/7	0.91	0.14	107,107,107,107	7
86	OHX	5	3577	7/7	0.91	0.34	53,53,53,53	7
87	MG	2	2178	1/1	0.91	0.36	79,79,79,79	0
87	MG	1	4093	1/1	0.91	0.87	43,43,43,43	0
87	MG	5	4489	1/1	0.91	0.17	57,57,57,57	0
86	OHX	2	2043	7/7	0.91	0.14	119,119,119,119	7
87	MG	6	2106	1/1	0.91	0.26	68,68,68,68	0
87	MG	4	240	1/1	0.91	0.19	57,57,57,57	0
86	OHX	5	3800	7/7	0.91	0.22	87,87,87,87	7
87	MG	1	3915	1/1	0.91	0.40	48,48,48,48	0
87	MG	6	2270	1/1	0.91	0.55	61,61,61,61	0
86	OHX	2	2078	7/7	0.91	0.17	102,102,102,102	7
87	MG	1	4405	1/1	0.91	0.19	44,44,44,44	0
86	OHX	4	212	7/7	0.91	0.34	42,42,42,42	7
87	MG	1	4256	1/1	0.91	0.21	58,58,58,58	0
87	MG	1	3825	1/1	0.91	0.50	38,38,38,38	0
87	MG	6	2141	1/1	0.91	0.39	40,40,40,40	0
87	MG	5	4378	1/1	0.91	0.20	55,55,55,55	0
87	MG	5	3838	1/1	0.91	0.26	40,40,40,40	0
86	OHX	2	2032	7/7	0.91	0.26	82,82,82,82	7
87	MG	1	4288	1/1	0.91	0.31	52,52,52,52	0
87	MG	1	4191	1/1	0.91	0.17	90,90,90,90	0
86	OHX	1	3787	7/7	0.91	0.24	69,69,69,69	7
87	MG	Q2	505	1/1	0.91	0.20	45,45,45,45	1
87	MG	5	4427	1/1	0.91	0.51	39,39,39,39	1
86	OHX	4	216	7/7	0.91	0.25	73,73,73,73	7
87	MG	1	4453	1/1	0.91	0.29	82,82,82,82	0
87	MG	5	4072	1/1	0.91	0.43	55,55,55,55	0
87	MG	1	3827	1/1	0.91	0.20	67,67,67,67	0
87	MG	s6	302	1/1	0.91	0.35	75,75,75,75	0
87	MG	1	3903	1/1	0.91	0.49	51,51,51,51	0
87	MG	5	4510	1/1	0.91	0.25	33,33,33,33	0
87	MG	1	4139	1/1	0.91	0.60	44,44,44,44	0
87	MG	14	403	1/1	0.91	0.36	39,39,39,39	0
87	MG	1	3845	1/1	0.91	0.41	44,44,44,44	0
87	MG	8	239	1/1	0.91	0.29	71,71,71,71	0
87	MG	5	3889	1/1	0.91	0.08	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	4367	1/1	0.91	0.19	44,44,44,44	0
87	MG	L3	407	1/1	0.91	0.32	51,51,51,51	1
87	MG	5	4069	1/1	0.91	0.27	50,50,50,50	0
87	MG	6	2289	1/1	0.91	0.14	57,57,57,57	0
87	MG	5	4459	1/1	0.91	0.34	36,36,36,36	1
86	OHX	5	3624	7/7	0.91	0.26	51,51,51,51	7
87	MG	1	4425	1/1	0.91	0.25	46,46,46,46	1
87	MG	6	2265	1/1	0.91	0.46	48,48,48,48	0
87	MG	5	3873	1/1	0.91	0.52	45,45,45,45	0
86	OHX	6	2054	7/7	0.91	0.28	65,65,65,65	7
87	MG	8	236	1/1	0.91	0.30	57,57,57,57	0
86	OHX	2	2018	7/7	0.91	0.20	102,102,102,102	7
87	MG	1	4332	1/1	0.91	0.48	37,37,37,37	1
86	OHX	4	208	7/7	0.91	0.22	85,85,85,85	7
86	OHX	1	3762	7/7	0.91	0.16	63,63,63,63	7
86	OHX	1	3622	7/7	0.91	0.29	56,56,56,56	7
86	OHX	2	2083	7/7	0.91	0.20	106,106,106,106	7
86	OHX	5	3661	7/7	0.91	0.29	50,50,50,50	7
87	MG	5	3999	1/1	0.91	0.78	32,32,32,32	0
87	MG	5	3931	1/1	0.91	0.46	42,42,42,42	0
86	OHX	1	3763	7/7	0.91	0.26	64,64,64,64	7
87	MG	Q2	504	1/1	0.91	0.30	50,50,50,50	0
86	OHX	5	3686	7/7	0.91	0.27	56,56,56,56	7
87	MG	6	2221	1/1	0.91	0.31	53,53,53,53	1
87	MG	1	3815	1/1	0.91	0.28	44,44,44,44	0
87	MG	5	3857	1/1	0.91	0.30	47,47,47,47	0
87	MG	1	4235	1/1	0.91	0.31	49,49,49,49	1
87	MG	5	4171	1/1	0.91	0.22	115,115,115,115	0
87	MG	1	4380	1/1	0.91	0.36	30,30,30,30	0
87	MG	5	4112	1/1	0.91	0.34	28,28,28,28	0
87	MG	1	4500	1/1	0.91	0.13	49,49,49,49	0
86	OHX	5	3587	7/7	0.92	0.30	53,53,53,53	7
87	MG	1	3897	1/1	0.92	0.40	43,43,43,43	0
87	MG	15	307	1/1	0.92	0.77	46,46,46,46	1
87	MG	1	4285	1/1	0.92	0.63	52,52,52,52	0
87	MG	5	4468	1/1	0.92	0.20	43,43,43,43	0
87	MG	5	4263	1/1	0.92	0.78	32,32,32,32	1
86	OHX	5	3799	7/7	0.92	0.34	72,72,72,72	7
86	OHX	1	3697	7/7	0.92	0.10	169,169,169,169	7
86	OHX	5	3690	7/7	0.92	0.28	90,90,90,90	7
87	MG	5	4100	1/1	0.92	0.43	32,32,32,32	0
86	OHX	2	2045	7/7	0.92	0.38	73,73,73,73	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	1	4111	1/1	0.92	0.36	40,40,40,40	1
86	OHX	1	3749	7/7	0.92	0.41	62,62,62,62	7
87	MG	5	4060	1/1	0.92	0.33	45,45,45,45	0
86	OHX	1	3699	7/7	0.92	0.24	44,44,44,44	7
87	MG	5	3979	1/1	0.92	0.35	48,48,48,48	0
87	MG	5	4564	1/1	0.92	0.43	34,34,34,34	1
87	MG	5	4506	1/1	0.92	0.25	38,38,38,38	1
87	MG	1	4354	1/1	0.92	0.15	62,62,62,62	0
86	OHX	1	3782	7/7	0.92	0.48	55,55,55,55	7
87	MG	1	4192	1/1	0.92	0.36	38,38,38,38	0
87	MG	1	4121	1/1	0.92	0.42	37,37,37,37	0
87	MG	5	4083	1/1	0.92	0.22	36,36,36,36	1
87	MG	1	4481	1/1	0.92	0.10	82,82,82,82	0
87	MG	5	3821	1/1	0.92	0.58	54,54,54,54	0
87	MG	1	4340	1/1	0.92	0.35	49,49,49,49	1
87	MG	1	3878	1/1	0.92	0.56	46,46,46,46	0
87	MG	1	4108	1/1	0.92	0.35	56,56,56,56	0
87	MG	5	3968	1/1	0.92	0.64	27,27,27,27	0
87	MG	5	4467	1/1	0.92	0.37	37,37,37,37	0
87	MG	1	4142	1/1	0.92	0.35	45,45,45,45	1
87	MG	6	2302	1/1	0.92	0.11	106,106,106,106	0
87	MG	1	4331	1/1	0.92	0.15	86,86,86,86	0
87	MG	M0	305	1/1	0.92	0.22	62,62,62,62	0
86	OHX	1	3742	7/7	0.92	0.39	41,41,41,41	7
87	MG	5	4225	1/1	0.92	0.37	71,71,71,71	0
87	MG	5	4362	1/1	0.92	0.50	49,49,49,49	1
87	MG	1	4247	1/1	0.92	0.89	44,44,44,44	1
87	MG	1	4209	1/1	0.92	0.24	67,67,67,67	1
87	MG	2	2140	1/1	0.92	0.55	81,81,81,81	0
87	MG	5	3882	1/1	0.92	0.41	37,37,37,37	0
87	MG	1	4079	1/1	0.92	0.27	43,43,43,43	0
87	MG	1	4400	1/1	0.92	0.35	59,59,59,59	0
86	OHX	1	3666	7/7	0.92	0.43	62,62,62,62	7
86	OHX	5	3710	7/7	0.92	0.32	79,79,79,79	7
87	MG	6	2154	1/1	0.92	0.26	76,76,76,76	0
87	MG	3	217	1/1	0.92	0.49	36,36,36,36	0
86	OHX	1	3768	7/7	0.92	0.18	50,50,50,50	7
87	MG	5	4174	1/1	0.92	0.22	41,41,41,41	0
87	MG	5	4227	1/1	0.92	0.17	48,48,48,48	0
86	OHX	5	3675	7/7	0.92	0.26	49,49,49,49	7
87	MG	2	2215	1/1	0.92	0.27	78,78,78,78	0
87	MG	5	3832	1/1	0.92	0.53	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	3	209	7/7	0.92	0.22	82,82,82,82	7
87	MG	2	2123	1/1	0.92	0.37	68,68,68,68	0
86	OHX	1	3584	7/7	0.92	0.14	106,106,106,106	7
87	MG	1	4386	1/1	0.92	0.33	53,53,53,53	0
86	OHX	15	301	7/7	0.92	0.17	90,90,90,90	7
87	MG	6	2101	1/1	0.92	0.61	39,39,39,39	0
87	MG	1	4102	1/1	0.92	0.56	44,44,44,44	0
87	MG	1	3886	1/1	0.92	0.34	39,39,39,39	0
86	OHX	5	3793	7/7	0.92	0.32	58,58,58,58	7
87	MG	1	4423	1/1	0.92	0.16	40,40,40,40	1
87	MG	5	3998	1/1	0.92	0.58	41,41,41,41	0
87	MG	1	4031	1/1	0.92	0.52	44,44,44,44	0
87	MG	6	2137	1/1	0.92	0.12	83,83,83,83	0
87	MG	5	3977	1/1	0.92	0.56	55,55,55,55	0
86	OHX	1	3721	7/7	0.92	0.21	96,96,96,96	7
87	MG	sM	201	1/1	0.92	0.15	48,48,48,48	0
87	MG	O7	104	1/1	0.92	0.22	81,81,81,81	0
86	OHX	5	3796	7/7	0.92	0.29	63,63,63,63	7
87	MG	5	3847	1/1	0.92	0.65	38,38,38,38	0
86	OHX	2	2021	7/7	0.92	0.30	72,72,72,72	7
87	MG	l3	407	1/1	0.92	0.40	38,38,38,38	1
87	MG	8	225	1/1	0.92	0.25	55,55,55,55	0
87	MG	1	4119	1/1	0.92	0.23	52,52,52,52	0
87	MG	5	3948	1/1	0.92	0.60	24,24,24,24	0
87	MG	2	2181	1/1	0.92	0.42	80,80,80,80	0
87	MG	1	4232	1/1	0.92	0.55	61,61,61,61	0
87	MG	8	240	1/1	0.92	0.13	72,72,72,72	0
87	MG	6	2217	1/1	0.92	0.64	66,66,66,66	0
87	MG	1	4006	1/1	0.92	0.46	39,39,39,39	0
86	OHX	1	3686	7/7	0.92	0.23	117,117,117,117	7
86	OHX	M7	201	7/7	0.92	0.26	42,42,42,42	7
86	OHX	5	3747	7/7	0.92	0.21	66,66,66,66	7
87	MG	1	3913	1/1	0.92	0.26	49,49,49,49	0
86	OHX	2	1980	7/7	0.92	0.25	93,93,93,93	7
87	MG	6	2161	1/1	0.92	0.47	59,59,59,59	0
87	MG	5	4206	1/1	0.92	0.49	40,40,40,40	0
87	MG	1	4476	1/1	0.92	0.37	81,81,81,81	0
87	MG	1	4063	1/1	0.92	0.33	53,53,53,53	0
87	MG	1	3937	1/1	0.92	0.56	33,33,33,33	0
87	MG	2	2142	1/1	0.92	0.60	61,61,61,61	0
87	MG	6	2253	1/1	0.92	0.46	47,47,47,47	0
87	MG	1	4057	1/1	0.92	0.51	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	19	202	1/1	0.92	0.30	38,38,38,38	0
87	MG	1	4336	1/1	0.92	0.42	43,43,43,43	0
87	MG	2	2188	1/1	0.92	0.17	84,84,84,84	0
87	MG	1	3885	1/1	0.92	0.23	41,41,41,41	0
86	OHX	5	3808	7/7	0.92	0.34	83,83,83,83	7
87	MG	6	2159	1/1	0.92	0.53	45,45,45,45	0
87	MG	8	234	1/1	0.92	0.23	41,41,41,41	1
87	MG	m0	305	1/1	0.92	0.35	32,32,32,32	0
86	OHX	5	3795	7/7	0.92	0.26	54,54,54,54	7
86	OHX	1	3695	7/7	0.92	0.48	56,56,56,56	7
87	MG	2	2114	1/1	0.92	0.32	79,79,79,79	0
87	MG	3	223	1/1	0.92	0.11	62,62,62,62	0
87	MG	1	4261	1/1	0.92	0.55	41,41,41,41	1
87	MG	5	4351	1/1	0.92	0.31	59,59,59,59	0
87	MG	5	4420	1/1	0.92	0.31	40,40,40,40	1
87	MG	1	4023	1/1	0.92	0.32	45,45,45,45	0
87	MG	5	4040	1/1	0.92	0.32	35,35,35,35	0
87	MG	5	3820	1/1	0.92	0.27	32,32,32,32	0
86	OHX	19	201	7/7	0.92	0.31	62,62,62,62	7
86	OHX	sR	401	7/7	0.92	0.20	122,122,122,122	7
87	MG	5	4010	1/1	0.92	0.52	46,46,46,46	0
86	OHX	4	215	7/7	0.92	0.23	74,74,74,74	7
87	MG	1	3996	1/1	0.92	0.53	32,32,32,32	0
87	MG	5	3952	1/1	0.92	0.53	34,34,34,34	0
86	OHX	1	3560	7/7	0.92	0.46	72,72,72,72	7
86	OHX	5	3542	7/7	0.92	0.35	84,84,84,84	7
86	OHX	2	2042	7/7	0.92	0.16	113,113,113,113	7
86	OHX	1	3722	7/7	0.92	0.29	69,69,69,69	7
87	MG	5	4168	1/1	0.92	0.23	45,45,45,45	0
87	MG	5	4240	1/1	0.92	0.38	37,37,37,37	1
87	MG	5	3936	1/1	0.92	0.55	28,28,28,28	0
87	MG	6	2187	1/1	0.92	0.28	77,77,77,77	0
87	MG	1	4123	1/1	0.92	0.91	56,56,56,56	0
87	MG	l3	412	1/1	0.92	0.42	34,34,34,34	0
87	MG	1	4479	1/1	0.92	0.20	41,41,41,41	1
87	MG	5	3943	1/1	0.92	0.21	48,48,48,48	0
87	MG	1	4196	1/1	0.92	0.23	55,55,55,55	0
86	OHX	1	3724	7/7	0.92	0.31	100,100,100,100	7
87	MG	1	4243	1/1	0.92	0.28	45,45,45,45	0
87	MG	5	4080	1/1	0.92	0.43	37,37,37,37	0
88	ZN	E1	501	1/1	0.92	0.08	132,132,132,132	0
87	MG	5	4411	1/1	0.92	0.38	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	l5	303	7/7	0.92	0.25	69,69,69,69	7
87	MG	6	2263	1/1	0.92	0.77	40,40,40,40	0
87	MG	5	4418	1/1	0.92	0.32	64,64,64,64	0
87	MG	d2	201	1/1	0.92	0.30	46,46,46,46	0
86	OHX	c5	201	7/7	0.92	0.20	118,118,118,118	7
87	MG	7	227	1/1	0.92	1.30	50,50,50,50	1
87	MG	5	4045	1/1	0.92	0.26	40,40,40,40	0
87	MG	3	216	1/1	0.92	0.36	55,55,55,55	0
87	MG	1	3943	1/1	0.92	0.61	38,38,38,38	0
87	MG	1	3841	1/1	0.92	0.25	55,55,55,55	0
87	MG	5	4387	1/1	0.92	0.31	45,45,45,45	0
86	OHX	c3	201	7/7	0.92	0.32	79,79,79,79	7
87	MG	5	4286	1/1	0.92	0.63	34,34,34,34	1
87	MG	5	4417	1/1	0.92	0.31	56,56,56,56	0
86	OHX	1	3687	7/7	0.92	0.23	61,61,61,61	7
87	MG	1	4116	1/1	0.92	0.37	36,36,36,36	0
87	MG	1	4203	1/1	0.92	0.93	42,42,42,42	1
87	MG	1	4096	1/1	0.92	0.59	76,76,76,76	0
87	MG	1	4152	1/1	0.92	0.18	75,75,75,75	0
86	OHX	5	3639	7/7	0.92	0.27	138,138,138,138	7
87	MG	1	3826	1/1	0.92	0.33	43,43,43,43	0
86	OHX	1	3796	7/7	0.92	0.46	71,71,71,71	7
87	MG	1	3976	1/1	0.92	0.45	44,44,44,44	0
87	MG	5	4066	1/1	0.92	0.33	53,53,53,53	0
87	MG	7	221	1/1	0.92	0.20	41,41,41,41	0
87	MG	5	4243	1/1	0.92	0.28	58,58,58,58	0
87	MG	2	2097	1/1	0.92	0.24	82,82,82,82	0
86	OHX	5	3778	7/7	0.92	0.19	109,109,109,109	7
87	MG	1	4069	1/1	0.92	0.16	56,56,56,56	0
87	MG	1	4099	1/1	0.92	0.20	59,59,59,59	0
86	OHX	5	3607	7/7	0.92	0.24	112,112,112,112	7
87	MG	1	4413	1/1	0.92	0.34	52,52,52,52	1
87	MG	5	4031	1/1	0.92	0.66	30,30,30,30	0
87	MG	5	4259	1/1	0.92	0.15	54,54,54,54	0
86	OHX	m7	201	7/7	0.92	0.22	49,49,49,49	7
86	OHX	1	3784	7/7	0.93	0.20	66,66,66,66	7
87	MG	1	4131	1/1	0.93	0.23	63,63,63,63	0
87	MG	O3	202	1/1	0.93	0.86	38,38,38,38	1
87	MG	6	2250	1/1	0.93	0.70	47,47,47,47	0
86	OHX	2	2025	7/7	0.93	0.19	94,94,94,94	7
87	MG	5	4202	1/1	0.93	0.35	32,32,32,32	1
87	MG	6	2209	1/1	0.93	0.29	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	6	2314	1/1	0.93	0.38	48,48,48,48	0
87	MG	1	4237	1/1	0.93	0.41	54,54,54,54	0
87	MG	5	4037	1/1	0.93	0.49	35,35,35,35	0
87	MG	6	2252	1/1	0.93	0.39	47,47,47,47	0
87	MG	6	2116	1/1	0.93	0.37	61,61,61,61	0
87	MG	5	4188	1/1	0.93	0.44	45,45,45,45	0
87	MG	1	4041	1/1	0.93	0.43	33,33,33,33	0
87	MG	5	4014	1/1	0.93	0.30	30,30,30,30	0
87	MG	1	4371	1/1	0.93	0.26	43,43,43,43	1
86	OHX	5	3744	7/7	0.93	0.30	56,56,56,56	7
86	OHX	5	3738	7/7	0.93	0.22	53,53,53,53	7
86	OHX	5	3612	7/7	0.93	0.42	39,39,39,39	7
87	MG	6	2143	1/1	0.93	0.72	86,86,86,86	0
87	MG	1	4012	1/1	0.93	0.41	35,35,35,35	0
87	MG	L2	301	1/1	0.93	0.28	39,39,39,39	0
87	MG	5	4054	1/1	0.93	0.50	50,50,50,50	0
87	MG	5	4509	1/1	0.93	0.22	33,33,33,33	0
87	MG	5	4081	1/1	0.93	0.18	48,48,48,48	0
87	MG	l3	405	1/1	0.93	0.31	35,35,35,35	0
87	MG	1	3846	1/1	0.93	0.18	35,35,35,35	0
87	MG	5	4191	1/1	0.93	0.37	44,44,44,44	1
87	MG	5	4395	1/1	0.93	0.26	41,41,41,41	0
86	OHX	5	3614	7/7	0.93	0.43	60,60,60,60	7
87	MG	1	3981	1/1	0.93	0.62	51,51,51,51	0
86	OHX	6	2003	7/7	0.93	0.35	61,61,61,61	7
87	MG	2	2206	1/1	0.93	0.27	58,58,58,58	0
87	MG	6	2122	1/1	0.93	0.17	49,49,49,49	0
87	MG	M7	208	1/1	0.93	0.30	40,40,40,40	0
86	OHX	5	3681	7/7	0.93	0.45	80,80,80,80	7
87	MG	1	4094	1/1	0.93	0.52	48,48,48,48	0
86	OHX	5	3751	7/7	0.93	0.23	61,61,61,61	7
87	MG	5	4366	1/1	0.93	0.49	41,41,41,41	0
86	OHX	2	2022	7/7	0.93	0.25	66,66,66,66	7
87	MG	1	4442	1/1	0.93	0.29	51,51,51,51	0
87	MG	5	4068	1/1	0.93	0.43	42,42,42,42	0
87	MG	1	4394	1/1	0.93	0.53	41,41,41,41	1
86	OHX	5	3761	7/7	0.93	0.26	69,69,69,69	7
86	OHX	2	2016	7/7	0.93	0.17	101,101,101,101	7
87	MG	2	2109	1/1	0.93	0.68	73,73,73,73	0
87	MG	1	3880	1/1	0.93	0.24	49,49,49,49	0
87	MG	1	4208	1/1	0.93	0.79	47,47,47,47	1
87	MG	5	4230	1/1	0.93	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	3633	7/7	0.93	0.40	43,43,43,43	7
87	MG	2	2160	1/1	0.93	0.30	67,67,67,67	0
87	MG	6	2117	1/1	0.93	0.38	61,61,61,61	0
86	OHX	1	3803	7/7	0.93	0.30	48,48,48,48	7
87	MG	5	4394	1/1	0.93	0.73	62,62,62,62	0
86	OHX	2	2057	7/7	0.93	0.23	67,67,67,67	7
87	MG	1	3864	1/1	0.93	0.60	55,55,55,55	0
86	OHX	C5	201	7/7	0.93	0.19	112,112,112,112	7
86	OHX	5	3740	7/7	0.93	0.22	62,62,62,62	7
86	OHX	1	3703	7/7	0.93	0.31	101,101,101,101	7
87	MG	1	3989	1/1	0.93	0.65	37,37,37,37	0
87	MG	6	2170	1/1	0.93	0.21	49,49,49,49	0
86	OHX	6	2008	7/7	0.93	0.27	82,82,82,82	7
87	MG	c8	204	1/1	0.93	0.34	81,81,81,81	0
87	MG	5	4119	1/1	0.93	0.32	61,61,61,61	0
87	MG	5	4456	1/1	0.93	0.10	100,100,100,100	0
87	MG	5	4153	1/1	0.93	0.43	41,41,41,41	0
87	MG	6	2173	1/1	0.93	0.42	56,56,56,56	0
87	MG	1	4276	1/1	0.93	0.62	37,37,37,37	0
87	MG	1	3902	1/1	0.93	0.24	43,43,43,43	0
86	OHX	1	3651	7/7	0.93	0.07	199,199,199,199	7
87	MG	1	4101	1/1	0.93	0.16	57,57,57,57	0
87	MG	1	3938	1/1	0.93	0.61	36,36,36,36	0
86	OHX	C3	201	7/7	0.93	0.33	99,99,99,99	7
87	MG	1	4202	1/1	0.93	0.29	59,59,59,59	1
87	MG	7	215	1/1	0.93	0.51	27,27,27,27	0
87	MG	d3	202	1/1	0.93	1.91	49,49,49,49	1
87	MG	7	233	1/1	0.93	0.17	52,52,52,52	0
87	MG	1	3830	1/1	0.93	0.41	40,40,40,40	0
87	MG	6	2110	1/1	0.93	0.26	82,82,82,82	0
87	MG	5	4166	1/1	0.93	0.57	44,44,44,44	0
86	OHX	6	2020	7/7	0.93	0.26	49,49,49,49	7
86	OHX	5	3718	7/7	0.93	0.10	136,136,136,136	7
87	MG	4	228	1/1	0.93	0.13	58,58,58,58	0
86	OHX	4	213	7/7	0.93	0.23	64,64,64,64	7
87	MG	5	4335	1/1	0.93	0.23	35,35,35,35	0
86	OHX	5	3773	7/7	0.93	0.22	145,145,145,145	7
87	MG	1	4327	1/1	0.93	0.45	51,51,51,51	0
87	MG	1	4085	1/1	0.93	0.58	46,46,46,46	0
87	MG	5	4294	1/1	0.93	0.27	39,39,39,39	0
87	MG	5	4220	1/1	0.93	0.21	49,49,49,49	1
87	MG	1	4127	1/1	0.93	0.39	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	N8	205	1/1	0.93	0.57	31,31,31,31	1
87	MG	5	3887	1/1	0.93	0.30	34,34,34,34	0
87	MG	6	2292	1/1	0.93	0.19	50,50,50,50	1
87	MG	1	3818	1/1	0.93	0.51	58,58,58,58	0
86	OHX	1	3723	7/7	0.93	0.50	57,57,57,57	7
87	MG	2	2115	1/1	0.93	0.71	71,71,71,71	0
87	MG	5	4298	1/1	0.93	0.13	106,106,106,106	0
86	OHX	5	3719	7/7	0.93	0.30	64,64,64,64	7
87	MG	1	3975	1/1	0.93	0.54	41,41,41,41	0
87	MG	3	225	1/1	0.93	0.30	68,68,68,68	0
86	OHX	1	3681	7/7	0.93	0.49	56,56,56,56	7
86	OHX	1	3608	7/7	0.93	0.28	51,51,51,51	7
86	OHX	5	3721	7/7	0.93	0.20	50,50,50,50	7
87	MG	5	4405	1/1	0.93	0.80	70,70,70,70	1
86	OHX	2	2047	7/7	0.93	0.17	106,106,106,106	7
86	OHX	1	3738	7/7	0.93	0.27	68,68,68,68	7
86	OHX	6	2046	7/7	0.93	0.14	100,100,100,100	7
87	MG	5	4393	1/1	0.93	0.41	34,34,34,34	0
87	MG	1	4279	1/1	0.93	0.22	58,58,58,58	0
87	MG	5	4095	1/1	0.93	0.77	60,60,60,60	0
87	MG	5	4374	1/1	0.93	0.27	45,45,45,45	1
87	MG	D6	102	1/1	0.93	0.79	77,77,77,77	0
87	MG	5	4407	1/1	0.93	0.31	48,48,48,48	0
86	OHX	2	2039	7/7	0.93	0.18	103,103,103,103	7
87	MG	1	3994	1/1	0.93	0.42	56,56,56,56	0
86	OHX	1	3671	7/7	0.93	0.32	85,85,85,85	7
86	OHX	6	2030	7/7	0.93	0.19	105,105,105,105	7
86	OHX	1	3659	7/7	0.93	0.28	48,48,48,48	7
86	OHX	5	3615	7/7	0.93	0.31	51,51,51,51	7
87	MG	5	4020	1/1	0.93	0.50	30,30,30,30	0
87	MG	O4	201	1/1	0.93	0.14	77,77,77,77	0
87	MG	1	4213	1/1	0.93	0.38	35,35,35,35	0
86	OHX	2	1999	7/7	0.93	0.19	94,94,94,94	7
87	MG	6	2245	1/1	0.93	0.12	60,60,60,60	0
86	OHX	2	2068	7/7	0.93	0.20	66,66,66,66	7
86	OHX	5	3663	7/7	0.93	0.27	57,57,57,57	7
87	MG	5	4577	1/1	0.93	0.53	44,44,44,44	0
86	OHX	5	3685	7/7	0.93	0.26	88,88,88,88	7
87	MG	l3	411	1/1	0.93	0.51	33,33,33,33	1
86	OHX	6	2040	7/7	0.93	0.27	58,58,58,58	7
87	MG	5	4540	1/1	0.93	0.48	39,39,39,39	1
87	MG	2	2111	1/1	0.93	0.46	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	1	4304	1/1	0.93	0.49	44,44,44,44	1
88	ZN	Q2	501	1/1	0.93	0.04	73,73,73,73	0
87	MG	5	4276	1/1	0.93	0.45	33,33,33,33	1
87	MG	5	4125	1/1	0.93	0.36	38,38,38,38	0
87	MG	2	2176	1/1	0.93	0.40	84,84,84,84	0
87	MG	1	3946	1/1	0.93	0.61	39,39,39,39	0
87	MG	d4	201	1/1	0.93	0.16	68,68,68,68	0
87	MG	5	4009	1/1	0.93	0.41	38,38,38,38	0
86	OHX	2	2064	7/7	0.93	0.08	130,130,130,130	7
87	MG	5	3932	1/1	0.93	0.22	39,39,39,39	0
87	MG	S4	301	1/1	0.93	0.21	76,76,76,76	0
87	MG	1	3835	1/1	0.93	0.64	41,41,41,41	0
86	OHX	4	218	7/7	0.93	0.27	51,51,51,51	7
87	MG	d9	103	1/1	0.93	0.93	83,83,83,83	1
86	OHX	2	2000	7/7	0.93	0.36	110,110,110,110	7
87	MG	7	226	1/1	0.93	0.19	64,64,64,64	0
86	OHX	6	2031	7/7	0.93	0.17	81,81,81,81	7
87	MG	5	4499	1/1	0.93	0.32	55,55,55,55	0
87	MG	o3	205	1/1	0.93	0.72	35,35,35,35	1
87	MG	6	2242	1/1	0.93	0.24	55,55,55,55	1
87	MG	5	4146	1/1	0.93	0.34	43,43,43,43	0
86	OHX	1	3614	7/7	0.93	0.39	53,53,53,53	7
87	MG	5	4422	1/1	0.93	0.23	35,35,35,35	0
87	MG	1	3870	1/1	0.93	0.46	34,34,34,34	0
87	MG	1	4000	1/1	0.93	0.24	39,39,39,39	0
86	OHX	6	2062	7/7	0.93	0.24	74,74,74,74	7
86	OHX	m0	303	7/7	0.93	0.21	86,86,86,86	7
87	MG	1	4204	1/1	0.93	0.50	60,60,60,60	0
86	OHX	1	3676	7/7	0.93	0.22	71,71,71,71	7
86	OHX	1	3812	7/7	0.93	0.32	88,88,88,88	7
87	MG	5	4127	1/1	0.93	0.52	44,44,44,44	1
87	MG	5	4044	1/1	0.93	0.50	35,35,35,35	0
86	OHX	5	3714	7/7	0.93	0.22	82,82,82,82	7
86	OHX	14	401	7/7	0.93	0.31	69,69,69,69	7
87	MG	5	4308	1/1	0.93	0.28	58,58,58,58	0
87	MG	7	224	1/1	0.93	0.38	55,55,55,55	0
87	MG	5	4236	1/1	0.93	0.31	42,42,42,42	0
87	MG	1	4181	1/1	0.93	0.25	75,75,75,75	0
87	MG	m5	504	1/1	0.93	0.15	45,45,45,45	0
87	MG	2	2151	1/1	0.93	0.52	58,58,58,58	0
87	MG	1	3979	1/1	0.93	0.63	45,45,45,45	0
87	MG	6	2297	1/1	0.93	0.21	70,70,70,70	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4198	1/1	0.93	0.52	47,47,47,47	0
87	MG	2	2218	1/1	0.93	0.19	82,82,82,82	0
87	MG	1	4338	1/1	0.93	0.63	37,37,37,37	1
87	MG	6	2125	1/1	0.94	0.50	40,40,40,40	0
86	OHX	5	3715	7/7	0.94	0.22	69,69,69,69	7
86	OHX	6	1997	7/7	0.94	0.20	94,94,94,94	7
87	MG	5	4396	1/1	0.94	0.46	52,52,52,52	1
86	OHX	2	1969	7/7	0.94	0.26	62,62,62,62	7
87	MG	5	4192	1/1	0.94	0.13	36,36,36,36	0
87	MG	5	3920	1/1	0.94	0.27	41,41,41,41	0
86	OHX	6	2075	7/7	0.94	0.31	54,54,54,54	7
87	MG	L4	408	1/1	0.94	0.66	34,34,34,34	1
87	MG	2	2220	1/1	0.94	0.29	70,70,70,70	1
86	OHX	1	3589	7/7	0.94	0.25	50,50,50,50	7
87	MG	1	4270	1/1	0.94	0.15	77,77,77,77	0
87	MG	1	4341	1/1	0.94	0.70	38,38,38,38	1
87	MG	8	222	1/1	0.94	0.38	41,41,41,41	0
86	OHX	5	3786	7/7	0.94	0.33	42,42,42,42	7
87	MG	1	3861	1/1	0.94	0.35	40,40,40,40	0
87	MG	5	3927	1/1	0.94	0.37	38,38,38,38	0
87	MG	4	236	1/1	0.94	0.12	98,98,98,98	0
87	MG	5	4077	1/1	0.94	0.26	34,34,34,34	0
86	OHX	5	3671	7/7	0.94	0.19	56,56,56,56	7
87	MG	1	4289	1/1	0.94	0.19	57,57,57,57	0
86	OHX	1	3704	7/7	0.94	0.48	55,55,55,55	7
87	MG	1	4187	1/1	0.94	0.21	47,47,47,47	1
86	OHX	6	2071	7/7	0.94	0.30	55,55,55,55	7
86	OHX	6	2078	7/7	0.94	0.20	93,93,93,93	7
87	MG	5	4279	1/1	0.94	0.57	36,36,36,36	1
87	MG	5	4446	1/1	0.94	0.32	45,45,45,45	0
87	MG	1	4375	1/1	0.94	0.57	43,43,43,43	1
87	MG	5	4363	1/1	0.94	0.34	42,42,42,42	0
86	OHX	2	2070	7/7	0.94	0.24	78,78,78,78	7
87	MG	5	4201	1/1	0.94	0.19	43,43,43,43	0
87	MG	5	4205	1/1	0.94	0.11	60,60,60,60	0
87	MG	5	4382	1/1	0.94	0.53	47,47,47,47	0
86	OHX	5	3735	7/7	0.94	0.26	62,62,62,62	7
87	MG	6	2109	1/1	0.94	0.35	47,47,47,47	0
87	MG	1	3854	1/1	0.94	0.28	48,48,48,48	0
87	MG	1	4266	1/1	0.94	0.62	33,33,33,33	0
86	OHX	5	3651	7/7	0.94	0.24	63,63,63,63	7
87	MG	6	2176	1/1	0.94	0.16	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4161	1/1	0.94	0.40	47,47,47,47	0
87	MG	1	4430	1/1	0.94	0.32	49,49,49,49	0
86	OHX	6	1931	7/7	0.94	0.22	71,71,71,71	7
87	MG	5	4328	1/1	0.94	0.25	53,53,53,53	0
87	MG	6	2276	1/1	0.94	0.52	40,40,40,40	0
86	OHX	5	3760	7/7	0.94	0.17	89,89,89,89	7
87	MG	1	4496	1/1	0.94	0.79	56,56,56,56	1
86	OHX	5	3579	7/7	0.94	0.26	55,55,55,55	7
87	MG	1	4133	1/1	0.94	0.13	83,83,83,83	0
86	OHX	1	3814	7/7	0.94	0.17	149,149,149,149	7
87	MG	1	3929	1/1	0.94	0.56	40,40,40,40	0
87	MG	5	3934	1/1	0.94	0.62	35,35,35,35	0
87	MG	o4	201	1/1	0.94	1.40	70,70,70,70	1
87	MG	1	3956	1/1	0.94	0.55	40,40,40,40	0
87	MG	6	2167	1/1	0.94	0.22	55,55,55,55	0
86	OHX	5	3791	7/7	0.94	0.24	68,68,68,68	7
87	MG	1	3910	1/1	0.94	0.27	44,44,44,44	0
86	OHX	5	3625	7/7	0.94	0.24	52,52,52,52	7
86	OHX	1	3545	7/7	0.94	0.25	91,91,91,91	7
86	OHX	5	3704	7/7	0.94	0.30	67,67,67,67	7
86	OHX	2	2082	7/7	0.94	0.08	137,137,137,137	7
86	OHX	1	3561	7/7	0.94	0.28	76,76,76,76	7
86	OHX	4	214	7/7	0.94	0.41	46,46,46,46	7
86	OHX	s8	301	7/7	0.94	0.18	104,104,104,104	7
87	MG	l2	306	1/1	0.94	0.48	53,53,53,53	1
86	OHX	2	2003	7/7	0.94	0.16	103,103,103,103	7
87	MG	5	4195	1/1	0.94	0.21	35,35,35,35	1
87	MG	5	3842	1/1	0.94	0.15	45,45,45,45	0
87	MG	1	4156	1/1	0.94	0.11	60,60,60,60	0
86	OHX	2	2027	7/7	0.94	0.14	111,111,111,111	7
87	MG	5	3859	1/1	0.94	0.42	32,32,32,32	0
87	MG	1	4292	1/1	0.94	0.19	39,39,39,39	0
86	OHX	6	2038	7/7	0.94	0.14	88,88,88,88	7
87	MG	4	233	1/1	0.94	0.25	43,43,43,43	1
86	OHX	5	3511	7/7	0.94	0.26	61,61,61,61	7
87	MG	2	2231	1/1	0.94	0.30	82,82,82,82	0
86	OHX	6	2048	7/7	0.94	0.29	51,51,51,51	7
87	MG	1	3967	1/1	0.94	0.49	40,40,40,40	0
86	OHX	1	3793	7/7	0.94	0.30	46,46,46,46	7
86	OHX	5	3571	7/7	0.94	0.24	62,62,62,62	7
86	OHX	1	3694	7/7	0.94	0.23	85,85,85,85	7
87	MG	7	214	1/1	0.94	0.22	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4437	1/1	0.94	0.47	39,39,39,39	1
86	OHX	2	2031	7/7	0.94	0.25	90,90,90,90	7
87	MG	2	2128	1/1	0.94	0.47	60,60,60,60	0
87	MG	5	4554	1/1	0.94	0.26	43,43,43,43	0
87	MG	6	2241	1/1	0.94	0.16	70,70,70,70	0
87	MG	1	4467	1/1	0.94	0.51	58,58,58,58	0
87	MG	n3	204	1/1	0.94	0.14	42,42,42,42	0
87	MG	1	4120	1/1	0.94	0.40	51,51,51,51	0
87	MG	n8	203	1/1	0.94	0.21	41,41,41,41	0
87	MG	6	2140	1/1	0.94	0.33	44,44,44,44	0
87	MG	L4	403	1/1	0.94	0.41	34,34,34,34	0
87	MG	1	4298	1/1	0.94	0.28	53,53,53,53	0
87	MG	5	4333	1/1	0.94	0.29	43,43,43,43	0
87	MG	M7	207	1/1	0.94	0.28	43,43,43,43	0
87	MG	2	2184	1/1	0.94	0.32	59,59,59,59	0
87	MG	6	2312	1/1	0.94	0.29	75,75,75,75	0
87	MG	1	3963	1/1	0.94	0.44	31,31,31,31	0
86	OHX	7	210	7/7	0.94	0.26	63,63,63,63	7
86	OHX	1	3807	7/7	0.94	0.11	112,112,112,112	7
87	MG	5	4024	1/1	0.94	0.74	37,37,37,37	0
87	MG	2	2248	1/1	0.94	0.12	78,78,78,78	0
87	MG	5	3912	1/1	0.94	0.69	40,40,40,40	0
87	MG	6	2131	1/1	0.94	0.35	53,53,53,53	0
87	MG	4	219	1/1	0.94	0.58	54,54,54,54	0
87	MG	5	3909	1/1	0.94	0.18	49,49,49,49	0
87	MG	1	3817	1/1	0.94	0.40	40,40,40,40	0
86	OHX	3	210	7/7	0.94	0.26	53,53,53,53	7
86	OHX	1	3683	7/7	0.94	0.34	61,61,61,61	7
87	MG	1	3887	1/1	0.94	0.62	31,31,31,31	0
87	MG	O7	107	1/1	0.94	0.60	42,42,42,42	1
87	MG	1	3819	1/1	0.94	0.39	106,106,106,106	0
87	MG	2	2238	1/1	0.94	0.32	89,89,89,89	0
86	OHX	2	2028	7/7	0.94	0.17	134,134,134,134	7
87	MG	5	4571	1/1	0.94	0.64	34,34,34,34	1
86	OHX	1	3617	7/7	0.94	0.24	36,36,36,36	7
87	MG	M3	201	1/1	0.94	0.23	45,45,45,45	0
86	OHX	2	2007	7/7	0.94	0.18	101,101,101,101	7
86	OHX	2	2053	7/7	0.94	0.32	80,80,80,80	7
86	OHX	3	211	7/7	0.94	0.24	81,81,81,81	7
87	MG	6	2216	1/1	0.94	0.18	86,86,86,86	0
87	MG	1	3851	1/1	0.94	0.27	53,53,53,53	0
86	OHX	2	2038	7/7	0.94	0.21	85,85,85,85	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	3894	1/1	0.94	0.35	40,40,40,40	1
87	MG	5	4030	1/1	0.94	0.48	34,34,34,34	0
87	MG	C1	202	1/1	0.94	1.17	72,72,72,72	1
87	MG	5	4056	1/1	0.94	0.40	40,40,40,40	0
87	MG	5	4012	1/1	0.94	0.47	33,33,33,33	0
87	MG	5	3986	1/1	0.94	0.40	35,35,35,35	0
86	OHX	4	217	7/7	0.94	0.23	70,70,70,70	7
86	OHX	2	1961	7/7	0.94	0.15	112,112,112,112	7
87	MG	5	3890	1/1	0.94	0.40	46,46,46,46	0
86	OHX	5	3708	7/7	0.94	0.20	43,43,43,43	7
86	OHX	2	1960	7/7	0.94	0.21	97,97,97,97	7
87	MG	5	3914	1/1	0.94	0.56	33,33,33,33	0
87	MG	1	4392	1/1	0.94	1.03	37,37,37,37	1
87	MG	O2	201	1/1	0.94	0.44	30,30,30,30	0
86	OHX	6	1950	7/7	0.94	0.14	100,100,100,100	7
87	MG	2	2129	1/1	0.94	0.26	66,66,66,66	0
87	MG	6	2102	1/1	0.94	0.12	81,81,81,81	0
87	MG	5	4559	1/1	0.94	0.37	73,73,73,73	1
87	MG	5	3863	1/1	0.94	0.34	35,35,35,35	0
86	OHX	2	2002	7/7	0.94	0.29	86,86,86,86	7
87	MG	6	2218	1/1	0.94	0.13	81,81,81,81	0
86	OHX	1	3760	7/7	0.94	0.34	52,52,52,52	7
87	MG	6	2266	1/1	0.94	0.20	71,71,71,71	0
87	MG	1	4303	1/1	0.94	0.82	41,41,41,41	1
87	MG	5	4337	1/1	0.94	0.16	47,47,47,47	0
86	OHX	6	2058	7/7	0.94	0.18	148,148,148,148	7
86	OHX	1	3673	7/7	0.94	0.23	47,47,47,47	7
87	MG	M4	201	1/1	0.94	0.19	53,53,53,53	0
86	OHX	1	3674	7/7	0.94	0.42	64,64,64,64	7
87	MG	Q0	203	1/1	0.94	0.15	52,52,52,52	0
86	OHX	6	1944	7/7	0.94	0.19	60,60,60,60	7
87	MG	5	4209	1/1	0.94	0.12	50,50,50,50	0
86	OHX	1	3530	7/7	0.94	0.24	67,67,67,67	7
87	MG	5	3958	1/1	0.94	0.32	61,61,61,61	0
87	MG	1	4317	1/1	0.94	0.84	38,38,38,38	1
86	OHX	5	3766	7/7	0.94	0.29	66,66,66,66	7
86	OHX	1	3778	7/7	0.94	0.32	56,56,56,56	7
87	MG	4	246	1/1	0.94	0.39	51,51,51,51	0
87	MG	5	3993	1/1	0.94	0.46	29,29,29,29	0
87	MG	1	3871	1/1	0.94	0.35	46,46,46,46	0
87	MG	1	4129	1/1	0.94	0.26	36,36,36,36	0
87	MG	5	4159	1/1	0.94	0.37	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	3844	1/1	0.94	0.25	36,36,36,36	0
87	MG	6	2133	1/1	0.94	0.26	39,39,39,39	0
87	MG	1	4016	1/1	0.94	0.89	38,38,38,38	0
86	OHX	2	2015	7/7	0.94	0.21	87,87,87,87	7
87	MG	6	2103	1/1	0.94	0.22	66,66,66,66	0
87	MG	17	303	1/1	0.94	0.26	34,34,34,34	1
86	OHX	1	3732	7/7	0.94	0.30	55,55,55,55	7
87	MG	1	3990	1/1	0.94	0.69	31,31,31,31	0
86	OHX	5	3645	7/7	0.94	0.25	68,68,68,68	7
87	MG	1	4186	1/1	0.94	0.25	43,43,43,43	0
86	OHX	5	3752	7/7	0.94	0.23	49,49,49,49	7
86	OHX	6	2059	7/7	0.94	0.25	104,104,104,104	7
86	OHX	1	3788	7/7	0.94	0.22	105,105,105,105	7
86	OHX	2	1954	7/7	0.94	0.26	88,88,88,88	7
87	MG	3	230	1/1	0.94	0.13	58,58,58,58	0
87	MG	m7	209	1/1	0.94	0.80	42,42,42,42	1
87	MG	1	4455	1/1	0.94	0.40	43,43,43,43	0
86	OHX	6	2047	7/7	0.94	0.23	67,67,67,67	7
87	MG	2	2172	1/1	0.94	0.25	65,65,65,65	0
87	MG	5	4501	1/1	0.94	0.41	33,33,33,33	1
87	MG	2	2189	1/1	0.94	0.23	94,94,94,94	0
86	OHX	5	3682	7/7	0.94	0.33	75,75,75,75	7
86	OHX	6	2026	7/7	0.94	0.24	151,151,151,151	7
86	OHX	1	3715	7/7	0.94	0.18	77,77,77,77	7
87	MG	1	4009	1/1	0.94	0.61	48,48,48,48	0
87	MG	6	2123	1/1	0.94	0.23	67,67,67,67	0
87	MG	6	2246	1/1	0.94	0.33	50,50,50,50	1
86	OHX	5	3644	7/7	0.94	0.32	47,47,47,47	7
86	OHX	5	3604	7/7	0.94	0.27	70,70,70,70	7
87	MG	1	4046	1/1	0.94	0.27	59,59,59,59	0
87	MG	6	2112	1/1	0.94	0.51	42,42,42,42	0
86	OHX	1	3740	7/7	0.94	0.38	70,70,70,70	7
86	OHX	8	211	7/7	0.94	0.17	105,105,105,105	7
87	MG	1	3823	1/1	0.94	0.43	31,31,31,31	0
87	MG	L7	301	1/1	0.94	0.18	39,39,39,39	0
87	MG	1	4333	1/1	0.94	0.28	49,49,49,49	0
86	OHX	5	3674	7/7	0.94	0.40	39,39,39,39	7
87	MG	2	2168	1/1	0.94	0.41	68,68,68,68	0
86	OHX	5	3696	7/7	0.94	0.27	49,49,49,49	7
86	OHX	l3	402	7/7	0.94	0.23	73,73,73,73	7
87	MG	5	3867	1/1	0.94	0.14	41,41,41,41	0
86	OHX	1	3789	7/7	0.94	0.36	56,56,56,56	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	3961	1/1	0.94	0.57	37,37,37,37	0
87	MG	5	3926	1/1	0.94	0.26	65,65,65,65	0
87	MG	1	4164	1/1	0.94	0.20	62,62,62,62	0
86	OHX	o7	503	7/7	0.94	0.26	53,53,53,53	7
87	MG	5	4458	1/1	0.94	0.25	38,38,38,38	1
87	MG	1	4068	1/1	0.94	0.13	62,62,62,62	0
87	MG	7	238	1/1	0.94	0.82	51,51,51,51	1
86	OHX	6	2010	7/7	0.94	0.33	84,84,84,84	7
87	MG	6	2118	1/1	0.94	0.37	38,38,38,38	0
87	MG	m7	203	1/1	0.94	0.37	33,33,33,33	0
87	MG	5	3879	1/1	0.94	0.42	33,33,33,33	0
86	OHX	2	2061	7/7	0.94	0.22	78,78,78,78	7
87	MG	1	4262	1/1	0.94	0.17	74,74,74,74	0
86	OHX	6	1998	7/7	0.94	0.27	64,64,64,64	7
87	MG	N8	208	1/1	0.94	0.86	45,45,45,45	1
86	OHX	6	2016	7/7	0.94	0.16	91,91,91,91	7
86	OHX	8	215	7/7	0.94	0.51	48,48,48,48	7
86	OHX	1	3764	7/7	0.94	0.42	49,49,49,49	7
87	MG	5	4454	1/1	0.94	0.27	47,47,47,47	0
86	OHX	6	2057	7/7	0.94	0.17	78,78,78,78	7
87	MG	5	4390	1/1	0.94	0.41	39,39,39,39	1
87	MG	1	3831	1/1	0.94	0.23	44,44,44,44	0
87	MG	1	3965	1/1	0.94	0.48	31,31,31,31	0
87	MG	1	4176	1/1	0.94	0.24	72,72,72,72	0
86	OHX	5	3713	7/7	0.94	0.17	70,70,70,70	7
87	MG	5	4058	1/1	0.94	0.42	37,37,37,37	0
87	MG	5	4102	1/1	0.94	0.53	44,44,44,44	0
87	MG	1	4255	1/1	0.94	0.98	48,48,48,48	0
86	OHX	1	3718	7/7	0.94	0.33	73,73,73,73	7
87	MG	1	3906	1/1	0.94	0.39	42,42,42,42	1
87	MG	1	4160	1/1	0.94	0.44	46,46,46,46	0
87	MG	1	3952	1/1	0.94	0.51	48,48,48,48	0
86	OHX	5	3722	7/7	0.94	0.28	76,76,76,76	7
86	OHX	5	3748	7/7	0.94	0.42	54,54,54,54	7
87	MG	2	2186	1/1	0.94	0.29	65,65,65,65	0
87	MG	5	4207	1/1	0.94	0.43	62,62,62,62	0
87	MG	5	4200	1/1	0.94	0.52	43,43,43,43	1
86	OHX	6	2035	7/7	0.94	0.33	82,82,82,82	7
87	MG	1	4313	1/1	0.95	0.44	41,41,41,41	1
86	OHX	1	3648	7/7	0.95	0.30	65,65,65,65	7
87	MG	8	229	1/1	0.95	0.30	52,52,52,52	0
86	OHX	5	3536	7/7	0.95	0.39	53,53,53,53	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	3826	1/1	0.95	0.14	35,35,35,35	0
87	MG	6	2171	1/1	0.95	0.22	79,79,79,79	0
86	OHX	5	3711	7/7	0.95	0.28	83,83,83,83	7
87	MG	1	4267	1/1	0.95	0.28	36,36,36,36	0
86	OHX	5	3549	7/7	0.95	0.50	55,55,55,55	7
87	MG	1	4098	1/1	0.95	0.51	46,46,46,46	0
87	MG	5	4193	1/1	0.95	0.88	39,39,39,39	1
87	MG	q2	503	1/1	0.95	0.74	42,42,42,42	1
86	OHX	1	3682	7/7	0.95	0.17	75,75,75,75	7
86	OHX	5	3664	7/7	0.95	0.24	63,63,63,63	7
87	MG	1	3836	1/1	0.95	0.17	38,38,38,38	1
87	MG	2	2228	1/1	0.95	0.61	56,56,56,56	0
86	OHX	6	1959	7/7	0.95	0.35	57,57,57,57	7
86	OHX	1	3702	7/7	0.95	0.38	42,42,42,42	7
87	MG	5	3883	1/1	0.95	0.34	41,41,41,41	0
86	OHX	1	3607	7/7	0.95	0.19	55,55,55,55	7
87	MG	5	4320	1/1	0.95	0.38	35,35,35,35	1
87	MG	5	4483	1/1	0.95	0.25	34,34,34,34	1
86	OHX	1	3726	7/7	0.95	0.22	54,54,54,54	7
86	OHX	2	2013	7/7	0.95	0.08	158,158,158,158	7
86	OHX	5	3775	7/7	0.95	0.24	59,59,59,59	7
87	MG	4	227	1/1	0.95	0.23	58,58,58,58	0
87	MG	5	4558	1/1	0.95	0.41	50,50,50,50	1
87	MG	m3	201	1/1	0.95	0.48	55,55,55,55	1
87	MG	6	2163	1/1	0.95	0.47	40,40,40,40	0
86	OHX	5	3753	7/7	0.95	0.28	49,49,49,49	7
87	MG	5	4001	1/1	0.95	0.59	36,36,36,36	0
87	MG	5	4157	1/1	0.95	0.30	51,51,51,51	0
87	MG	1	4284	1/1	0.95	0.23	50,50,50,50	0
87	MG	2	2155	1/1	0.95	0.56	60,60,60,60	0
87	MG	5	4160	1/1	0.95	0.34	67,67,67,67	0
87	MG	1	3935	1/1	0.95	0.53	32,32,32,32	0
86	OHX	5	3662	7/7	0.95	0.27	45,45,45,45	7
87	MG	1	4245	1/1	0.95	0.80	47,47,47,47	1
87	MG	1	4344	1/1	0.95	0.22	40,40,40,40	0
87	MG	3	213	1/1	0.95	0.15	78,78,78,78	0
87	MG	5	4064	1/1	0.95	0.22	64,64,64,64	0
87	MG	5	4297	1/1	0.95	0.66	33,33,33,33	1
86	OHX	3	207	7/7	0.95	0.17	85,85,85,85	7
87	MG	n0	203	1/1	0.95	0.20	41,41,41,41	0
87	MG	1	3865	1/1	0.95	0.37	42,42,42,42	0
86	OHX	5	3695	7/7	0.95	0.48	55,55,55,55	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3723	7/7	0.95	0.30	62,62,62,62	7
86	OHX	5	3672	7/7	0.95	0.27	71,71,71,71	7
87	MG	2	2241	1/1	0.95	0.56	60,60,60,60	0
87	MG	5	4117	1/1	0.95	0.71	46,46,46,46	0
87	MG	5	4038	1/1	0.95	0.59	29,29,29,29	0
87	MG	5	4573	1/1	0.95	0.48	30,30,30,30	0
86	OHX	5	3679	7/7	0.95	0.30	47,47,47,47	7
86	OHX	6	1985	7/7	0.95	0.24	90,90,90,90	7
87	MG	5	3954	1/1	0.95	0.41	40,40,40,40	0
87	MG	6	2127	1/1	0.95	0.33	45,45,45,45	0
87	MG	5	4138	1/1	0.95	0.29	100,100,100,100	0
87	MG	6	2147	1/1	0.95	0.43	58,58,58,58	0
86	OHX	1	3670	7/7	0.95	0.28	50,50,50,50	7
87	MG	5	4274	1/1	0.95	0.33	46,46,46,46	0
86	OHX	1	3602	7/7	0.95	0.09	152,152,152,152	7
87	MG	5	4565	1/1	0.95	0.24	37,37,37,37	0
86	OHX	5	3683	7/7	0.95	0.29	60,60,60,60	7
87	MG	1	4166	1/1	0.95	0.60	36,36,36,36	0
86	OHX	5	3736	7/7	0.95	0.18	93,93,93,93	7
87	MG	15	309	1/1	0.95	0.52	54,54,54,54	1
86	OHX	1	3672	7/7	0.95	0.28	46,46,46,46	7
86	OHX	7	209	7/7	0.95	0.27	40,40,40,40	7
87	MG	1	4077	1/1	0.95	0.20	54,54,54,54	0
86	OHX	1	3627	7/7	0.95	0.38	45,45,45,45	7
86	OHX	5	3699	7/7	0.95	0.23	39,39,39,39	7
86	OHX	1	3606	7/7	0.95	0.26	68,68,68,68	7
86	OHX	1	3798	7/7	0.95	0.27	93,93,93,93	7
87	MG	s6	301	1/1	0.95	0.13	71,71,71,71	0
87	MG	5	3945	1/1	0.95	0.42	41,41,41,41	0
86	OHX	O3	201	7/7	0.95	0.31	49,49,49,49	7
86	OHX	5	3688	7/7	0.95	0.53	37,37,37,37	7
87	MG	5	4478	1/1	0.95	0.45	33,33,33,33	0
87	MG	5	3983	1/1	0.95	0.71	35,35,35,35	0
86	OHX	1	3751	7/7	0.95	0.13	146,146,146,146	7
86	OHX	8	206	7/7	0.95	0.23	94,94,94,94	7
87	MG	5	4013	1/1	0.95	0.53	39,39,39,39	0
86	OHX	5	3743	7/7	0.95	0.17	105,105,105,105	7
87	MG	1	4007	1/1	0.95	0.49	46,46,46,46	0
87	MG	1	3966	1/1	0.95	0.40	41,41,41,41	0
86	OHX	1	3535	7/7	0.95	0.30	47,47,47,47	7
87	MG	1	4048	1/1	0.95	0.28	44,44,44,44	0
87	MG	n8	206	1/1	0.95	0.47	37,37,37,37	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	1	3920	1/1	0.95	0.29	52,52,52,52	0
86	OHX	5	3642	7/7	0.95	0.32	39,39,39,39	7
87	MG	1	4109	1/1	0.95	0.24	46,46,46,46	0
86	OHX	6	2005	7/7	0.95	0.21	80,80,80,80	7
87	MG	5	4339	1/1	0.95	0.41	43,43,43,43	0
87	MG	5	3848	1/1	0.95	0.44	33,33,33,33	0
87	MG	1	4422	1/1	0.95	0.25	60,60,60,60	0
87	MG	O1	202	1/1	0.95	0.80	60,60,60,60	1
86	OHX	2	2036	7/7	0.95	0.20	123,123,123,123	7
87	MG	l3	413	1/1	0.95	0.72	32,32,32,32	1
86	OHX	1	3700	7/7	0.95	0.24	47,47,47,47	7
87	MG	1	3850	1/1	0.95	0.27	37,37,37,37	0
87	MG	n0	202	1/1	0.95	0.93	38,38,38,38	1
87	MG	5	4326	1/1	0.95	0.31	53,53,53,53	0
87	MG	5	3915	1/1	0.95	0.21	39,39,39,39	0
87	MG	1	3931	1/1	0.95	0.42	41,41,41,41	0
87	MG	1	3939	1/1	0.95	0.51	37,37,37,37	0
86	OHX	1	3701	7/7	0.95	0.34	68,68,68,68	7
87	MG	5	4194	1/1	0.95	0.34	39,39,39,39	0
87	MG	1	4028	1/1	0.95	0.16	48,48,48,48	0
87	MG	8	235	1/1	0.95	0.68	61,61,61,61	1
87	MG	5	4444	1/1	0.95	0.58	39,39,39,39	0
87	MG	1	4149	1/1	0.95	0.19	82,82,82,82	0
86	OHX	1	3758	7/7	0.95	0.20	55,55,55,55	7
87	MG	6	2145	1/1	0.95	0.51	33,33,33,33	0
86	OHX	1	3716	7/7	0.95	0.35	61,61,61,61	7
87	MG	5	4350	1/1	0.95	0.22	44,44,44,44	1
87	MG	1	4013	1/1	0.95	0.61	47,47,47,47	0
87	MG	1	3824	1/1	0.95	0.32	55,55,55,55	0
87	MG	5	4212	1/1	0.95	0.24	41,41,41,41	0
87	MG	1	4004	1/1	0.95	0.26	44,44,44,44	0
87	MG	5	4134	1/1	0.95	0.48	37,37,37,37	0
87	MG	2	2183	1/1	0.95	0.21	66,66,66,66	0
86	OHX	5	3509	7/7	0.95	0.23	66,66,66,66	7
87	MG	1	4491	1/1	0.95	0.14	36,36,36,36	0
86	OHX	5	3705	7/7	0.95	0.27	46,46,46,46	7
86	OHX	1	3639	7/7	0.95	0.16	85,85,85,85	7
86	OHX	2	1949	7/7	0.95	0.15	108,108,108,108	7
86	OHX	15	302	7/7	0.95	0.16	88,88,88,88	7
87	MG	1	4509	1/1	0.95	0.16	90,90,90,90	0
87	MG	5	4424	1/1	0.95	0.21	63,63,63,63	0
87	MG	5	4372	1/1	0.95	0.39	38,38,38,38	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4263	1/1	0.95	0.20	45,45,45,45	1
86	OHX	d9	102	7/7	0.95	0.27	97,97,97,97	7
86	OHX	2	2005	7/7	0.95	0.34	86,86,86,86	7
87	MG	1	4475	1/1	0.95	0.40	62,62,62,62	0
87	MG	5	3965	1/1	0.95	0.16	55,55,55,55	0
86	OHX	1	3619	7/7	0.95	0.35	70,70,70,70	7
87	MG	1	4078	1/1	0.95	0.37	31,31,31,31	0
87	MG	6	2188	1/1	0.95	0.19	52,52,52,52	0
87	MG	1	4411	1/1	0.95	0.38	42,42,42,42	1
86	OHX	1	3792	7/7	0.95	0.16	147,147,147,147	7
86	OHX	5	3784	7/7	0.95	0.53	55,55,55,55	7
86	OHX	2	2006	7/7	0.95	0.30	72,72,72,72	7
87	MG	1	4419	1/1	0.95	0.45	34,34,34,34	1
87	MG	2	2104	1/1	0.95	0.22	70,70,70,70	0
87	MG	M8	202	1/1	0.95	1.44	39,39,39,39	1
87	MG	6	2129	1/1	0.95	0.24	59,59,59,59	0
87	MG	O7	105	1/1	0.95	0.10	51,51,51,51	0
86	OHX	1	3635	7/7	0.95	0.33	45,45,45,45	7
87	MG	5	4248	1/1	0.95	0.21	39,39,39,39	1
86	OHX	2	2001	7/7	0.95	0.27	82,82,82,82	7
87	MG	3	218	1/1	0.95	0.47	35,35,35,35	0
87	MG	5	3976	1/1	0.95	0.40	41,41,41,41	0
86	OHX	2	1991	7/7	0.95	0.13	104,104,104,104	7
87	MG	1	3924	1/1	0.95	0.51	36,36,36,36	0
86	OHX	2	1962	7/7	0.95	0.20	97,97,97,97	7
87	MG	1	3839	1/1	0.95	0.67	46,46,46,46	0
86	OHX	5	3764	7/7	0.95	0.20	71,71,71,71	7
87	MG	5	4537	1/1	0.95	0.20	38,38,38,38	0
86	OHX	5	3694	7/7	0.95	0.27	55,55,55,55	7
86	OHX	L5	301	7/7	0.95	0.18	78,78,78,78	7
86	OHX	5	3654	7/7	0.95	0.34	55,55,55,55	7
86	OHX	5	3622	7/7	0.95	0.31	74,74,74,74	7
87	MG	1	4291	1/1	0.95	0.53	41,41,41,41	0
87	MG	1	3842	1/1	0.95	0.63	45,45,45,45	0
86	OHX	6	2055	7/7	0.95	0.48	59,59,59,59	7
86	OHX	1	3692	7/7	0.95	0.22	65,65,65,65	7
86	OHX	8	214	7/7	0.95	0.18	100,100,100,100	7
87	MG	5	4032	1/1	0.95	0.12	49,49,49,49	0
86	OHX	1	3629	7/7	0.95	0.09	186,186,186,186	7
87	MG	5	3996	1/1	0.95	0.54	31,31,31,31	0
87	MG	5	4162	1/1	0.95	0.37	49,49,49,49	0
86	OHX	6	2000	7/7	0.95	0.32	63,63,63,63	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	3874	1/1	0.95	0.68	31,31,31,31	0
87	MG	5	4226	1/1	0.95	0.39	36,36,36,36	0
87	MG	1	4049	1/1	0.95	0.24	42,42,42,42	0
87	MG	5	3967	1/1	0.95	0.80	28,28,28,28	0
86	OHX	1	3555	7/7	0.95	0.17	89,89,89,89	7
86	OHX	6	2033	7/7	0.95	0.20	67,67,67,67	7
86	OHX	1	3661	7/7	0.95	0.34	45,45,45,45	7
86	OHX	2	1965	7/7	0.95	0.20	91,91,91,91	7
87	MG	6	2328	1/1	0.95	1.14	54,54,54,54	1
86	OHX	5	3620	7/7	0.95	0.33	42,42,42,42	7
86	OHX	2	2026	7/7	0.95	0.20	93,93,93,93	7
87	MG	5	4352	1/1	0.95	0.62	54,54,54,54	1
87	MG	6	2261	1/1	0.95	0.36	60,60,60,60	0
87	MG	1	4321	1/1	0.95	0.18	44,44,44,44	1
86	OHX	5	3603	7/7	0.95	0.22	43,43,43,43	7
87	MG	5	4345	1/1	0.95	0.10	95,95,95,95	0
87	MG	6	2331	1/1	0.95	0.53	76,76,76,76	0
87	MG	6	2316	1/1	0.95	0.31	60,60,60,60	1
87	MG	5	4292	1/1	0.95	0.40	37,37,37,37	0
87	MG	5	4242	1/1	0.95	0.37	44,44,44,44	0
87	MG	1	3859	1/1	0.95	0.25	89,89,89,89	0
86	OHX	8	212	7/7	0.95	0.18	85,85,85,85	7
86	OHX	5	3638	7/7	0.95	0.34	73,73,73,73	7
86	OHX	1	3631	7/7	0.95	0.37	51,51,51,51	7
87	MG	2	2127	1/1	0.95	0.33	60,60,60,60	0
87	MG	5	4096	1/1	0.95	0.40	34,34,34,34	0
87	MG	M6	203	1/1	0.95	0.87	40,40,40,40	1
87	MG	5	4093	1/1	0.95	0.79	34,34,34,34	0
87	MG	5	4097	1/1	0.95	0.43	40,40,40,40	0
86	OHX	6	2070	7/7	0.95	0.20	71,71,71,71	7
87	MG	1	4456	1/1	0.95	0.64	56,56,56,56	1
86	OHX	M8	201	7/7	0.95	0.20	53,53,53,53	7
87	MG	5	4525	1/1	0.95	0.26	41,41,41,41	0
87	MG	1	3852	1/1	0.95	0.70	30,30,30,30	0
86	OHX	6	2018	7/7	0.95	0.40	54,54,54,54	7
87	MG	1	3978	1/1	0.95	0.66	28,28,28,28	0
87	MG	5	3964	1/1	0.95	0.44	33,33,33,33	0
86	OHX	6	1971	7/7	0.95	0.16	85,85,85,85	7
87	MG	1	3991	1/1	0.95	0.28	36,36,36,36	0
86	OHX	6	1982	7/7	0.95	0.17	98,98,98,98	7
86	OHX	5	3780	7/7	0.95	0.17	110,110,110,110	7
87	MG	L3	404	1/1	0.95	0.42	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3677	7/7	0.95	0.36	74,74,74,74	7
87	MG	1	3974	1/1	0.95	0.31	54,54,54,54	0
86	OHX	6	1999	7/7	0.95	0.18	85,85,85,85	7
87	MG	5	3841	1/1	0.95	0.39	43,43,43,43	0
87	MG	5	4061	1/1	0.95	0.18	51,51,51,51	0
87	MG	1	4445	1/1	0.95	0.25	41,41,41,41	0
87	MG	5	4005	1/1	0.95	0.48	30,30,30,30	0
86	OHX	5	3531	7/7	0.95	0.24	57,57,57,57	7
87	MG	5	4430	1/1	0.95	0.31	45,45,45,45	0
87	MG	1	4421	1/1	0.95	0.21	41,41,41,41	1
86	OHX	6	2029	7/7	0.95	0.23	82,82,82,82	7
87	MG	q1	102	1/1	0.95	0.30	43,43,43,43	0
87	MG	M9	205	1/1	0.95	0.51	68,68,68,68	1
87	MG	L4	404	1/1	0.95	0.62	42,42,42,42	1
87	MG	1	4323	1/1	0.95	0.40	42,42,42,42	1
87	MG	5	4410	1/1	0.95	0.22	47,47,47,47	1
87	MG	5	4379	1/1	0.95	0.34	37,37,37,37	1
87	MG	5	4515	1/1	0.95	0.55	34,34,34,34	0
86	OHX	1	3551	7/7	0.95	0.29	65,65,65,65	7
86	OHX	1	3656	7/7	0.95	0.36	69,69,69,69	7
87	MG	1	4507	1/1	0.95	0.68	36,36,36,36	1
86	OHX	6	1980	7/7	0.95	0.23	61,61,61,61	7
86	OHX	2	2051	7/7	0.95	0.28	86,86,86,86	7
87	MG	1	4415	1/1	0.95	0.23	60,60,60,60	1
87	MG	5	4471	1/1	0.95	0.35	55,55,55,55	0
86	OHX	1	3664	7/7	0.95	0.40	65,65,65,65	7
87	MG	6	2296	1/1	0.95	0.71	54,54,54,54	1
87	MG	6	2120	1/1	0.95	0.32	43,43,43,43	0
87	MG	5	4377	1/1	0.95	0.29	36,36,36,36	1
87	MG	4	226	1/1	0.95	0.36	61,61,61,61	0
87	MG	5	4016	1/1	0.95	0.72	29,29,29,29	0
86	OHX	1	3559	7/7	0.95	0.23	90,90,90,90	7
86	OHX	1	3546	7/7	0.95	0.27	52,52,52,52	7
86	OHX	5	3724	7/7	0.95	0.28	58,58,58,58	7
87	MG	2	2229	1/1	0.95	0.14	84,84,84,84	0
86	OHX	1	3630	7/7	0.95	0.28	57,57,57,57	7
87	MG	1	4412	1/1	0.95	0.49	32,32,32,32	1
86	OHX	5	3749	7/7	0.95	0.37	39,39,39,39	7
86	OHX	1	3451	7/7	0.96	0.31	77,77,77,77	7
87	MG	2	2199	1/1	0.96	0.36	81,81,81,81	0
87	MG	1	4290	1/1	0.96	0.28	40,40,40,40	1
87	MG	L3	408	1/1	0.96	0.81	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	4465	1/1	0.96	0.15	44,44,44,44	0
87	MG	1	4159	1/1	0.96	0.23	45,45,45,45	0
87	MG	D9	105	1/1	0.96	0.50	76,76,76,76	0
86	OHX	5	3601	7/7	0.96	0.18	89,89,89,89	7
86	OHX	5	3606	7/7	0.96	0.16	74,74,74,74	7
87	MG	5	4305	1/1	0.96	0.28	34,34,34,34	1
87	MG	1	3914	1/1	0.96	0.44	34,34,34,34	0
87	MG	1	3898	1/1	0.96	0.38	48,48,48,48	0
86	OHX	1	3511	7/7	0.96	0.23	66,66,66,66	7
87	MG	5	4512	1/1	0.96	0.45	53,53,53,53	1
87	MG	1	4071	1/1	0.96	0.42	40,40,40,40	0
86	OHX	4	210	7/7	0.96	0.14	101,101,101,101	7
87	MG	l3	406	1/1	0.96	0.55	31,31,31,31	1
87	MG	q1	103	1/1	0.96	0.43	46,46,46,46	1
87	MG	1	4044	1/1	0.96	0.22	69,69,69,69	0
86	OHX	5	3687	7/7	0.96	0.28	46,46,46,46	7
86	OHX	2	1943	7/7	0.96	0.15	95,95,95,95	7
86	OHX	1	3626	7/7	0.96	0.35	84,84,84,84	7
87	MG	1	4038	1/1	0.96	0.34	45,45,45,45	0
87	MG	6	2180	1/1	0.96	0.41	52,52,52,52	0
87	MG	5	4325	1/1	0.96	0.17	74,74,74,74	0
86	OHX	1	3566	7/7	0.96	0.20	92,92,92,92	7
87	MG	5	3924	1/1	0.96	0.30	42,42,42,42	0
86	OHX	6	1961	7/7	0.96	0.33	65,65,65,65	7
87	MG	5	3831	1/1	0.96	0.19	43,43,43,43	0
86	OHX	2	1994	7/7	0.96	0.12	111,111,111,111	7
87	MG	5	3881	1/1	0.96	0.25	41,41,41,41	0
86	OHX	1	3579	7/7	0.96	0.24	53,53,53,53	7
86	OHX	2	2040	7/7	0.96	0.16	88,88,88,88	7
86	OHX	5	3626	7/7	0.96	0.27	69,69,69,69	7
87	MG	8	226	1/1	0.96	0.27	63,63,63,63	0
87	MG	M7	205	1/1	0.96	0.42	42,42,42,42	0
87	MG	5	4271	1/1	0.96	0.48	40,40,40,40	1
87	MG	l5	308	1/1	0.96	1.26	49,49,49,49	1
87	MG	6	2126	1/1	0.96	0.46	43,43,43,43	0
87	MG	1	3932	1/1	0.96	0.49	28,28,28,28	0
86	OHX	6	1966	7/7	0.96	0.31	56,56,56,56	7
86	OHX	5	3539	7/7	0.96	0.28	54,54,54,54	7
86	OHX	2	1970	7/7	0.96	0.22	89,89,89,89	7
87	MG	5	3972	1/1	0.96	0.62	31,31,31,31	0
86	OHX	1	3634	7/7	0.96	0.08	121,121,121,121	7
86	OHX	5	3774	7/7	0.96	0.15	66,66,66,66	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4027	1/1	0.96	0.32	43,43,43,43	0
86	OHX	5	3527	7/7	0.96	0.25	49,49,49,49	7
86	OHX	5	3668	7/7	0.96	0.22	39,39,39,39	7
86	OHX	2	1931	7/7	0.96	0.16	116,116,116,116	7
86	OHX	1	3663	7/7	0.96	0.33	48,48,48,48	7
86	OHX	1	3642	7/7	0.96	0.26	52,52,52,52	7
86	OHX	5	3697	7/7	0.96	0.46	44,44,44,44	7
87	MG	6	2108	1/1	0.96	0.23	98,98,98,98	0
87	MG	N6	202	1/1	0.96	0.48	58,58,58,58	1
86	OHX	2	2033	7/7	0.96	0.12	113,113,113,113	7
87	MG	5	4247	1/1	0.96	0.48	37,37,37,37	0
87	MG	1	3904	1/1	0.96	0.28	42,42,42,42	0
87	MG	5	4084	1/1	0.96	0.23	41,41,41,41	0
86	OHX	6	1938	7/7	0.96	0.19	69,69,69,69	7
87	MG	5	4116	1/1	0.96	0.81	36,36,36,36	1
86	OHX	1	3693	7/7	0.96	0.32	81,81,81,81	7
86	OHX	1	3714	7/7	0.96	0.29	45,45,45,45	7
87	MG	sM	202	1/1	0.96	0.47	44,44,44,44	0
87	MG	1	4272	1/1	0.96	0.17	46,46,46,46	1
87	MG	m5	505	1/1	0.96	0.49	58,58,58,58	0
86	OHX	5	3684	7/7	0.96	0.59	43,43,43,43	7
87	MG	5	4340	1/1	0.96	0.56	34,34,34,34	0
87	MG	1	4250	1/1	0.96	0.44	53,53,53,53	1
87	MG	5	4278	1/1	0.96	0.51	35,35,35,35	1
87	MG	5	4182	1/1	0.96	0.28	66,66,66,66	0
86	OHX	6	2015	7/7	0.96	0.32	65,65,65,65	7
86	OHX	1	3655	7/7	0.96	0.21	64,64,64,64	7
87	MG	1	4409	1/1	0.96	0.25	46,46,46,46	0
86	OHX	1	3636	7/7	0.96	0.26	75,75,75,75	7
87	MG	5	4006	1/1	0.96	0.60	37,37,37,37	0
87	MG	5	4161	1/1	0.96	0.47	38,38,38,38	0
87	MG	6	2121	1/1	0.96	0.38	61,61,61,61	0
87	MG	5	4370	1/1	0.96	1.03	47,47,47,47	1
87	MG	5	4241	1/1	0.96	0.40	38,38,38,38	1
86	OHX	1	3720	7/7	0.96	0.15	104,104,104,104	7
87	MG	1	4326	1/1	0.96	0.14	42,42,42,42	0
87	MG	5	4144	1/1	0.96	0.23	44,44,44,44	0
87	MG	6	2149	1/1	0.96	0.29	65,65,65,65	0
87	MG	1	4448	1/1	0.96	0.29	37,37,37,37	1
86	OHX	6	1969	7/7	0.96	0.24	68,68,68,68	7
86	OHX	2	1973	7/7	0.96	0.19	103,103,103,103	7
87	MG	1	3911	1/1	0.96	0.33	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	5	4480	1/1	0.96	0.72	50,50,50,50	1
86	OHX	2	2069	7/7	0.96	0.25	78,78,78,78	7
86	OHX	1	3698	7/7	0.96	0.20	51,51,51,51	7
87	MG	5	4232	1/1	0.96	0.67	35,35,35,35	1
87	MG	1	4429	1/1	0.96	0.42	49,49,49,49	1
87	MG	1	3921	1/1	0.96	0.48	37,37,37,37	0
86	OHX	2	1955	7/7	0.96	0.18	91,91,91,91	7
87	MG	1	4356	1/1	0.96	0.26	88,88,88,88	0
87	MG	5	3843	1/1	0.96	0.23	62,62,62,62	0
87	MG	1	4249	1/1	0.96	0.16	54,54,54,54	0
87	MG	6	2177	1/1	0.96	0.29	80,80,80,80	0
86	OHX	6	2067	7/7	0.96	0.30	70,70,70,70	7
87	MG	5	3861	1/1	0.96	0.35	36,36,36,36	0
86	OHX	2	1993	7/7	0.96	0.18	80,80,80,80	7
87	MG	5	3895	1/1	0.96	0.14	59,59,59,59	0
86	OHX	5	3564	7/7	0.96	0.25	89,89,89,89	7
87	MG	6	2160	1/1	0.96	0.42	59,59,59,59	0
87	MG	5	4017	1/1	0.96	0.65	33,33,33,33	0
87	MG	6	2204	1/1	0.96	0.17	47,47,47,47	0
87	MG	2	2141	1/1	0.96	0.29	67,67,67,67	0
86	OHX	5	3568	7/7	0.96	0.32	53,53,53,53	7
86	OHX	5	3532	7/7	0.96	0.24	38,38,38,38	7
87	MG	7	239	1/1	0.96	0.81	50,50,50,50	1
87	MG	5	3961	1/1	0.96	0.64	29,29,29,29	0
87	MG	L3	405	1/1	0.96	0.25	42,42,42,42	0
87	MG	1	3934	1/1	0.96	0.36	40,40,40,40	0
87	MG	1	3875	1/1	0.96	0.62	35,35,35,35	0
87	MG	1	3995	1/1	0.96	0.71	36,36,36,36	0
87	MG	5	3878	1/1	0.96	0.58	54,54,54,54	0
87	MG	5	4314	1/1	0.96	0.18	33,33,33,33	0
87	MG	5	3973	1/1	0.96	0.49	34,34,34,34	0
86	OHX	1	3517	7/7	0.96	0.26	61,61,61,61	7
86	OHX	1	3583	7/7	0.96	0.34	54,54,54,54	7
86	OHX	5	3670	7/7	0.96	0.18	51,51,51,51	7
87	MG	5	3846	1/1	0.96	0.31	43,43,43,43	0
86	OHX	5	3677	7/7	0.96	0.24	48,48,48,48	7
86	OHX	1	3603	7/7	0.96	0.29	128,128,128,128	7
86	OHX	5	3551	7/7	0.96	0.20	66,66,66,66	7
87	MG	n8	201	1/1	0.96	0.37	33,33,33,33	0
86	OHX	5	3594	7/7	0.96	0.35	42,42,42,42	7
86	OHX	1	3711	7/7	0.96	0.24	67,67,67,67	7
87	MG	1	4174	1/1	0.96	0.36	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	3665	7/7	0.96	0.48	47,47,47,47	7
86	OHX	5	3613	7/7	0.96	0.22	70,70,70,70	7
87	MG	5	4329	1/1	0.96	0.38	47,47,47,47	0
86	OHX	D9	102	7/7	0.96	0.19	83,83,83,83	7
87	MG	1	3917	1/1	0.96	0.19	49,49,49,49	0
86	OHX	5	3692	7/7	0.96	0.30	38,38,38,38	7
87	MG	5	4111	1/1	0.96	0.57	36,36,36,36	0
86	OHX	1	3572	7/7	0.96	0.15	95,95,95,95	7
87	MG	1	4312	1/1	0.96	0.23	41,41,41,41	0
86	OHX	5	3634	7/7	0.96	0.26	42,42,42,42	7
87	MG	2	2233	1/1	0.96	0.20	72,72,72,72	0
86	OHX	5	3557	7/7	0.96	0.24	49,49,49,49	7
86	OHX	2	1988	7/7	0.96	0.20	80,80,80,80	7
87	MG	1	4403	1/1	0.96	0.35	65,65,65,65	0
86	OHX	6	1996	7/7	0.96	0.14	90,90,90,90	7
86	OHX	2	2073	7/7	0.96	0.18	89,89,89,89	7
86	OHX	1	3611	7/7	0.96	0.25	42,42,42,42	7
87	MG	1	3962	1/1	0.96	0.23	46,46,46,46	0
87	MG	2	2250	1/1	0.96	0.22	79,79,79,79	0
86	OHX	2	1933	7/7	0.96	0.28	71,71,71,71	7
87	MG	1	3863	1/1	0.96	0.36	38,38,38,38	0
87	MG	5	4189	1/1	0.96	0.41	35,35,35,35	1
87	MG	5	4461	1/1	0.96	0.86	45,45,45,45	1
86	OHX	5	3596	7/7	0.96	0.26	43,43,43,43	7
86	OHX	5	3555	7/7	0.96	0.27	60,60,60,60	7
86	OHX	1	3706	7/7	0.96	0.69	60,60,60,60	7
86	OHX	5	3698	7/7	0.96	0.16	66,66,66,66	7
87	MG	5	4113	1/1	0.96	0.29	39,39,39,39	0
86	OHX	5	3817	7/7	0.96	0.17	85,85,85,85	7
86	OHX	1	3813	7/7	0.96	0.25	60,60,60,60	7
87	MG	5	4034	1/1	0.96	0.09	45,45,45,45	0
87	MG	1	4011	1/1	0.96	0.61	31,31,31,31	0
86	OHX	5	3717	7/7	0.96	0.18	56,56,56,56	7
86	OHX	5	3631	7/7	0.96	0.32	89,89,89,89	7
87	MG	o7	504	1/1	0.96	0.48	37,37,37,37	1
86	OHX	1	3533	7/7	0.96	0.18	129,129,129,129	7
87	MG	6	2158	1/1	0.96	0.52	40,40,40,40	0
86	OHX	6	2091	7/7	0.96	0.15	96,96,96,96	7
86	OHX	5	3643	7/7	0.96	0.32	53,53,53,53	7
86	OHX	1	3654	7/7	0.96	0.36	65,65,65,65	7
87	MG	5	4291	1/1	0.96	0.22	35,35,35,35	1
87	MG	5	3898	1/1	0.96	0.37	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3811	7/7	0.96	0.61	44,44,44,44	7
86	OHX	5	3610	7/7	0.96	0.50	60,60,60,60	7
86	OHX	6	1925	7/7	0.96	0.20	87,87,87,87	7
86	OHX	1	3669	7/7	0.96	0.40	54,54,54,54	7
86	OHX	6	1992	7/7	0.96	0.18	71,71,71,71	7
87	MG	6	2230	1/1	0.96	0.40	59,59,59,59	0
86	OHX	5	3659	7/7	0.96	0.19	58,58,58,58	7
86	OHX	2	1968	7/7	0.96	0.38	77,77,77,77	7
87	MG	6	2104	1/1	0.96	0.33	52,52,52,52	0
86	OHX	6	2001	7/7	0.96	0.35	68,68,68,68	7
86	OHX	1	3679	7/7	0.96	0.20	42,42,42,42	7
86	OHX	5	3590	7/7	0.96	0.15	83,83,83,83	7
87	MG	2	2112	1/1	0.96	0.59	69,69,69,69	0
86	OHX	1	3543	7/7	0.96	0.17	64,64,64,64	7
87	MG	m8	1504	1/1	0.96	0.94	42,42,42,42	1
87	MG	1	4167	1/1	0.96	0.67	42,42,42,42	1
87	MG	l3	408	1/1	0.96	0.41	31,31,31,31	0
87	MG	1	4268	1/1	0.96	0.41	32,32,32,32	0
86	OHX	5	3809	7/7	0.96	0.33	86,86,86,86	7
86	OHX	8	208	7/7	0.96	0.23	63,63,63,63	7
87	MG	5	3906	1/1	0.96	0.53	48,48,48,48	0
87	MG	1	4033	1/1	0.96	0.34	73,73,73,73	0
86	OHX	1	3604	7/7	0.96	0.37	62,62,62,62	7
87	MG	5	4215	1/1	0.96	0.36	38,38,38,38	0
86	OHX	1	3657	7/7	0.96	0.24	40,40,40,40	7
86	OHX	1	3649	7/7	0.96	0.23	52,52,52,52	7
87	MG	1	4451	1/1	0.96	0.55	58,58,58,58	1
86	OHX	1	3539	7/7	0.96	0.16	147,147,147,147	7
87	MG	5	3913	1/1	0.96	0.26	55,55,55,55	0
86	OHX	1	3665	7/7	0.96	0.36	59,59,59,59	7
87	MG	3	222	1/1	0.96	0.31	45,45,45,45	0
86	OHX	5	3533	7/7	0.96	0.22	47,47,47,47	7
87	MG	1	3947	1/1	0.96	0.50	37,37,37,37	0
86	OHX	1	3534	7/7	0.96	0.29	65,65,65,65	7
86	OHX	6	1991	7/7	0.96	0.15	83,83,83,83	7
87	MG	1	4489	1/1	0.96	0.64	56,56,56,56	1
87	MG	N1	201	1/1	0.96	0.52	42,42,42,42	1
87	MG	N8	203	1/1	0.96	0.62	33,33,33,33	0
87	MG	5	4551	1/1	0.96	0.60	41,41,41,41	1
87	MG	5	4433	1/1	0.96	0.67	45,45,45,45	1
86	OHX	2	1946	7/7	0.96	0.12	110,110,110,110	7
87	MG	5	4404	1/1	0.96	0.93	38,38,38,38	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4353	1/1	0.96	0.30	59,59,59,59	0
87	MG	1	4397	1/1	0.96	0.40	38,38,38,38	1
86	OHX	5	3815	7/7	0.96	0.34	66,66,66,66	7
87	MG	5	3919	1/1	0.96	0.64	44,44,44,44	0
87	MG	1	3940	1/1	0.96	0.66	38,38,38,38	0
87	MG	6	2243	1/1	0.96	0.39	68,68,68,68	0
87	MG	1	3816	1/1	0.96	0.67	49,49,49,49	0
86	OHX	1	3691	7/7	0.96	0.21	67,67,67,67	7
86	OHX	m0	304	7/7	0.96	0.34	43,43,43,43	7
87	MG	1	4436	1/1	0.96	0.20	41,41,41,41	0
86	OHX	1	3685	7/7	0.96	0.17	95,95,95,95	7
87	MG	5	4343	1/1	0.96	0.95	53,53,53,53	1
87	MG	1	4253	1/1	0.96	0.32	66,66,66,66	0
87	MG	1	4015	1/1	0.96	0.54	53,53,53,53	0
87	MG	6	2327	1/1	0.96	0.38	78,78,78,78	0
86	OHX	O7	103	7/7	0.96	0.24	60,60,60,60	7
86	OHX	SR	401	7/7	0.96	0.12	130,130,130,130	7
86	OHX	2	1947	7/7	0.96	0.17	130,130,130,130	7
87	MG	1	4385	1/1	0.96	0.37	32,32,32,32	1
87	MG	1	3927	1/1	0.96	0.87	40,40,40,40	0
86	OHX	5	3707	7/7	0.96	0.16	46,46,46,46	7
86	OHX	5	3506	7/7	0.96	0.25	41,41,41,41	7
86	OHX	1	3771	7/7	0.96	0.52	52,52,52,52	7
87	MG	5	4306	1/1	0.96	0.73	35,35,35,35	1
87	MG	1	4040	1/1	0.96	0.31	47,47,47,47	0
86	OHX	1	3748	7/7	0.96	0.24	89,89,89,89	7
87	MG	5	4036	1/1	0.96	0.54	34,34,34,34	0
87	MG	1	4410	1/1	0.96	0.41	56,56,56,56	0
87	MG	m9	202	1/1	0.96	0.70	54,54,54,54	1
87	MG	6	2100	1/1	0.96	0.13	60,60,60,60	0
86	OHX	2	1998	7/7	0.96	0.14	94,94,94,94	7
86	OHX	2	2023	7/7	0.96	0.24	71,71,71,71	7
87	MG	5	4237	1/1	0.96	0.47	36,36,36,36	1
87	MG	1	4022	1/1	0.96	0.77	22,22,22,22	0
87	MG	5	4025	1/1	0.96	0.44	32,32,32,32	0
87	MG	5	4059	1/1	0.96	0.44	39,39,39,39	0
87	MG	m8	1503	1/1	0.96	0.57	52,52,52,52	0
86	OHX	6	1964	7/7	0.96	0.26	49,49,49,49	7
87	MG	5	4015	1/1	0.96	0.74	38,38,38,38	0
87	MG	o2	203	1/1	0.96	0.36	34,34,34,34	1
87	MG	6	2174	1/1	0.96	0.37	58,58,58,58	0
87	MG	5	3876	1/1	0.96	0.36	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4383	1/1	0.96	0.54	33,33,33,33	1
86	OHX	1	3765	7/7	0.96	0.20	93,93,93,93	7
86	OHX	6	1979	7/7	0.96	0.23	79,79,79,79	7
87	MG	1	4030	1/1	0.96	0.24	46,46,46,46	0
86	OHX	6	1953	7/7	0.96	0.20	137,137,137,137	7
87	MG	5	3985	1/1	0.96	0.64	50,50,50,50	0
87	MG	1	4092	1/1	0.96	0.57	42,42,42,42	0
87	MG	1	3930	1/1	0.96	0.13	41,41,41,41	0
87	MG	1	3918	1/1	0.96	0.23	57,57,57,57	0
86	OHX	1	3505	7/7	0.96	0.29	50,50,50,50	7
87	MG	5	3988	1/1	0.96	0.58	28,28,28,28	0
87	MG	1	4447	1/1	0.96	0.35	44,44,44,44	0
87	MG	1	3948	1/1	0.96	0.18	34,34,34,34	0
87	MG	6	2291	1/1	0.96	0.32	65,65,65,65	0
87	MG	5	3829	1/1	0.96	0.47	39,39,39,39	0
87	MG	5	3872	1/1	0.96	0.41	32,32,32,32	0
87	MG	5	3992	1/1	0.96	0.62	33,33,33,33	0
86	OHX	1	3746	7/7	0.96	0.20	71,71,71,71	7
87	MG	5	4470	1/1	0.96	0.26	36,36,36,36	1
87	MG	12	307	1/1	0.96	0.92	46,46,46,46	1
86	OHX	5	3608	7/7	0.96	0.35	44,44,44,44	7
86	OHX	5	3493	7/7	0.96	0.23	67,67,67,67	7
87	MG	17	302	1/1	0.96	0.61	35,35,35,35	1
87	MG	1	4113	1/1	0.96	0.27	49,49,49,49	0
86	OHX	1	3615	7/7	0.96	0.18	68,68,68,68	7
86	OHX	6	2097	7/7	0.96	0.24	70,70,70,70	7
86	OHX	1	3516	7/7	0.96	0.22	65,65,65,65	7
86	OHX	6	2069	7/7	0.96	0.16	78,78,78,78	7
87	MG	5	4399	1/1	0.96	0.97	46,46,46,46	1
86	OHX	1	3616	7/7	0.96	0.29	60,60,60,60	7
86	OHX	5	3777	7/7	0.96	0.41	38,38,38,38	7
87	MG	1	4020	1/1	0.96	0.49	32,32,32,32	0
87	MG	L4	406	1/1	0.96	0.67	38,38,38,38	1
87	MG	5	3892	1/1	0.96	0.26	46,46,46,46	0
87	MG	5	4028	1/1	0.96	0.29	38,38,38,38	0
87	MG	1	3949	1/1	0.96	0.46	31,31,31,31	0
86	OHX	6	1976	7/7	0.96	0.14	95,95,95,95	7
87	MG	2	2092	1/1	0.96	0.62	40,40,40,40	0
86	OHX	1	3538	7/7	0.96	0.22	62,62,62,62	7
86	OHX	6	1933	7/7	0.97	0.16	82,82,82,82	7
87	MG	5	4004	1/1	0.97	0.59	42,42,42,42	0
86	OHX	6	2090	7/7	0.97	0.18	68,68,68,68	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	6	2269	1/1	0.97	0.12	89,89,89,89	0
86	OHX	6	2009	7/7	0.97	0.30	56,56,56,56	7
87	MG	5	3938	1/1	0.97	0.69	28,28,28,28	0
87	MG	O2	204	1/1	0.97	0.18	33,33,33,33	0
86	OHX	2	1974	7/7	0.97	0.21	137,137,137,137	7
86	OHX	1	3521	7/7	0.97	0.48	59,59,59,59	7
87	MG	1	4314	1/1	0.97	0.28	40,40,40,40	1
86	OHX	5	3534	7/7	0.97	0.23	42,42,42,42	7
86	OHX	5	3537	7/7	0.97	0.13	114,114,114,114	7
87	MG	6	2264	1/1	0.97	0.35	46,46,46,46	1
86	OHX	1	3713	7/7	0.97	0.30	58,58,58,58	7
86	OHX	6	1986	7/7	0.97	0.17	73,73,73,73	7
87	MG	5	3970	1/1	0.97	0.68	38,38,38,38	0
87	MG	6	2280	1/1	0.97	0.18	46,46,46,46	0
86	OHX	2	1959	7/7	0.97	0.17	127,127,127,127	7
86	OHX	2	1990	7/7	0.97	0.13	111,111,111,111	7
87	MG	1	4168	1/1	0.97	0.15	35,35,35,35	1
87	MG	5	4197	1/1	0.97	0.28	36,36,36,36	0
87	MG	L4	407	1/1	0.97	0.46	55,55,55,55	1
87	MG	1	3905	1/1	0.97	0.20	48,48,48,48	0
86	OHX	1	3558	7/7	0.97	0.20	62,62,62,62	7
86	OHX	2	2012	7/7	0.97	0.13	102,102,102,102	7
87	MG	6	2196	1/1	0.97	0.31	45,45,45,45	1
86	OHX	5	3802	7/7	0.97	0.22	55,55,55,55	7
86	OHX	5	3611	7/7	0.97	0.21	52,52,52,52	7
87	MG	1	3873	1/1	0.97	0.73	39,39,39,39	0
87	MG	5	3950	1/1	0.97	0.60	36,36,36,36	0
87	MG	5	4477	1/1	0.97	1.27	38,38,38,38	1
87	MG	5	3870	1/1	0.97	0.49	34,34,34,34	0
87	MG	5	4152	1/1	0.97	0.35	40,40,40,40	0
86	OHX	1	3633	7/7	0.97	0.26	79,79,79,79	7
87	MG	1	3971	1/1	0.97	0.23	43,43,43,43	0
86	OHX	6	2082	7/7	0.97	0.27	54,54,54,54	7
87	MG	1	4471	1/1	0.97	0.26	33,33,33,33	1
86	OHX	2	1981	7/7	0.97	0.26	106,106,106,106	7
86	OHX	8	204	7/7	0.97	0.22	66,66,66,66	7
86	OHX	5	3771	7/7	0.97	0.24	60,60,60,60	7
86	OHX	6	2019	7/7	0.97	0.28	55,55,55,55	7
86	OHX	5	3693	7/7	0.97	0.24	45,45,45,45	7
86	OHX	1	3502	7/7	0.97	0.26	63,63,63,63	7
86	OHX	5	3621	7/7	0.97	0.29	43,43,43,43	7
86	OHX	5	3646	7/7	0.97	0.35	52,52,52,52	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3569	7/7	0.97	0.27	78,78,78,78	7
86	OHX	1	3618	7/7	0.97	0.20	78,78,78,78	7
86	OHX	2	1976	7/7	0.97	0.18	92,92,92,92	7
86	OHX	1	3637	7/7	0.97	0.33	76,76,76,76	7
86	OHX	2	1937	7/7	0.97	0.15	94,94,94,94	7
86	OHX	2	2017	7/7	0.97	0.13	108,108,108,108	7
87	MG	n8	204	1/1	0.97	0.54	55,55,55,55	1
86	OHX	1	3658	7/7	0.97	0.24	49,49,49,49	7
86	OHX	7	207	7/7	0.97	0.20	78,78,78,78	7
86	OHX	6	1970	7/7	0.97	0.13	88,88,88,88	7
87	MG	5	4277	1/1	0.97	0.53	35,35,35,35	1
87	MG	5	4019	1/1	0.97	0.56	30,30,30,30	0
86	OHX	2	2050	7/7	0.97	0.10	96,96,96,96	7
86	OHX	O7	102	7/7	0.97	0.20	73,73,73,73	7
87	MG	6	2099	1/1	0.97	0.54	43,43,43,43	0
87	MG	5	4118	1/1	0.97	0.40	32,32,32,32	1
87	MG	5	4504	1/1	0.97	0.68	39,39,39,39	1
87	MG	q0	202	1/1	0.97	0.14	42,42,42,42	0
86	OHX	5	3640	7/7	0.97	0.14	73,73,73,73	7
87	MG	4	245	1/1	0.97	0.39	95,95,95,95	0
86	OHX	1	3532	7/7	0.97	0.26	59,59,59,59	7
87	MG	6	2318	1/1	0.97	0.38	54,54,54,54	0
87	MG	1	3992	1/1	0.97	0.50	27,27,27,27	0
86	OHX	1	3805	7/7	0.97	0.26	73,73,73,73	7
86	OHX	6	2032	7/7	0.97	0.21	61,61,61,61	7
86	OHX	2	1987	7/7	0.97	0.22	75,75,75,75	7
87	MG	1	4311	1/1	0.97	0.12	57,57,57,57	1
87	MG	1	4097	1/1	0.97	0.19	42,42,42,42	0
87	MG	7	218	1/1	0.97	0.49	30,30,30,30	0
86	OHX	1	3791	7/7	0.97	0.24	68,68,68,68	7
87	MG	1	4025	1/1	0.97	0.45	39,39,39,39	0
87	MG	5	4508	1/1	0.97	0.44	40,40,40,40	1
87	MG	4	221	1/1	0.97	0.35	65,65,65,65	0
87	MG	1	3908	1/1	0.97	0.41	43,43,43,43	0
87	MG	6	2105	1/1	0.97	0.38	49,49,49,49	0
87	MG	2	2125	1/1	0.97	0.46	85,85,85,85	0
86	OHX	2	2087	7/7	0.97	0.25	71,71,71,71	7
86	OHX	5	3474	7/7	0.97	0.20	78,78,78,78	7
86	OHX	2	1935	7/7	0.97	0.15	98,98,98,98	7
87	MG	1	3855	1/1	0.97	0.39	32,32,32,32	0
87	MG	2	2174	1/1	0.97	0.62	68,68,68,68	0
87	MG	5	3987	1/1	0.97	0.49	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	6	1994	7/7	0.97	0.13	76,76,76,76	7
86	OHX	14	402	7/7	0.97	0.19	55,55,55,55	7
86	OHX	1	3570	7/7	0.97	0.28	41,41,41,41	7
87	MG	5	4409	1/1	0.97	0.33	39,39,39,39	0
87	MG	O5	202	1/1	0.97	0.76	54,54,54,54	1
87	MG	5	4272	1/1	0.97	0.33	48,48,48,48	0
86	OHX	1	3547	7/7	0.97	0.34	56,56,56,56	7
86	OHX	5	3517	7/7	0.97	0.23	56,56,56,56	7
86	OHX	5	3540	7/7	0.97	0.24	54,54,54,54	7
87	MG	5	3908	1/1	0.97	0.16	76,76,76,76	0
87	MG	1	3893	1/1	0.97	0.37	51,51,51,51	0
86	OHX	6	1930	7/7	0.97	0.29	59,59,59,59	7
87	MG	1	3999	1/1	0.97	0.50	32,32,32,32	0
86	OHX	1	3492	7/7	0.97	0.18	113,113,113,113	7
86	OHX	6	1937	7/7	0.97	0.18	88,88,88,88	7
86	OHX	5	3565	7/7	0.97	0.35	72,72,72,72	7
87	MG	2	2106	1/1	0.97	0.24	60,60,60,60	0
86	OHX	1	3690	7/7	0.97	0.23	66,66,66,66	7
87	MG	6	2155	1/1	0.97	0.20	72,72,72,72	0
87	MG	1	3998	1/1	0.97	0.55	27,27,27,27	0
86	OHX	2	1964	7/7	0.97	0.15	101,101,101,101	7
86	OHX	c8	201	7/7	0.97	0.16	95,95,95,95	7
86	OHX	5	3462	7/7	0.97	0.20	56,56,56,56	7
86	OHX	L3	401	7/7	0.97	0.22	56,56,56,56	7
87	MG	5	3969	1/1	0.97	0.41	41,41,41,41	0
86	OHX	2	2009	7/7	0.97	0.33	70,70,70,70	7
86	OHX	5	3538	7/7	0.97	0.25	42,42,42,42	7
86	OHX	8	205	7/7	0.97	0.23	64,64,64,64	7
86	OHX	5	3734	7/7	0.97	0.23	70,70,70,70	7
87	MG	O7	109	1/1	0.97	0.59	46,46,46,46	1
86	OHX	5	3580	7/7	0.97	0.23	63,63,63,63	7
87	MG	5	4300	1/1	0.97	0.21	32,32,32,32	0
86	OHX	1	3580	7/7	0.97	0.16	89,89,89,89	7
87	MG	6	2213	1/1	0.97	0.79	68,68,68,68	1
87	MG	1	4460	1/1	0.97	0.35	75,75,75,75	0
86	OHX	1	3705	7/7	0.97	0.23	64,64,64,64	7
86	OHX	1	3689	7/7	0.97	0.26	55,55,55,55	7
87	MG	6	2186	1/1	0.97	0.32	53,53,53,53	0
87	MG	5	4257	1/1	0.97	0.51	29,29,29,29	0
86	OHX	2	1916	7/7	0.97	0.17	89,89,89,89	7
86	OHX	1	3744	7/7	0.97	0.26	60,60,60,60	7
87	MG	5	4496	1/1	0.97	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3667	7/7	0.97	0.28	49,49,49,49	7
87	MG	1	4017	1/1	0.97	0.40	35,35,35,35	0
86	OHX	M9	202	7/7	0.97	0.16	78,78,78,78	7
86	OHX	M0	302	7/7	0.97	0.33	48,48,48,48	7
86	OHX	6	1958	7/7	0.97	0.17	77,77,77,77	7
86	OHX	1	3644	7/7	0.97	0.15	91,91,91,91	7
87	MG	5	4384	1/1	0.97	0.38	34,34,34,34	1
87	MG	5	4075	1/1	0.97	0.29	36,36,36,36	0
86	OHX	5	3513	7/7	0.97	0.10	107,107,107,107	7
86	OHX	1	3585	7/7	0.97	0.24	54,54,54,54	7
86	OHX	1	3613	7/7	0.97	0.25	62,62,62,62	7
86	OHX	5	3561	7/7	0.97	0.31	51,51,51,51	7
86	OHX	2	1996	7/7	0.97	0.29	93,93,93,93	7
87	MG	1	4452	1/1	0.97	0.41	44,44,44,44	0
86	OHX	2	1956	7/7	0.97	0.17	91,91,91,91	7
86	OHX	1	3734	7/7	0.97	0.24	52,52,52,52	7
86	OHX	5	3500	7/7	0.97	0.18	75,75,75,75	7
87	MG	5	4284	1/1	0.97	0.30	44,44,44,44	1
87	MG	5	4548	1/1	0.97	0.24	42,42,42,42	1
87	MG	7	241	1/1	0.97	0.66	47,47,47,47	1
87	MG	1	4358	1/1	0.97	0.45	51,51,51,51	0
86	OHX	1	3598	7/7	0.97	0.31	100,100,100,100	7
87	MG	6	2157	1/1	0.97	0.47	46,46,46,46	0
87	MG	17	305	1/1	0.97	0.44	40,40,40,40	0
86	OHX	5	3574	7/7	0.97	0.22	53,53,53,53	7
86	OHX	5	3653	7/7	0.97	0.28	64,64,64,64	7
87	MG	1	3955	1/1	0.97	0.46	36,36,36,36	0
86	OHX	5	3581	7/7	0.97	0.26	46,46,46,46	7
86	OHX	1	3587	7/7	0.97	0.25	77,77,77,77	7
86	OHX	5	3518	7/7	0.97	0.18	60,60,60,60	7
87	MG	1	3866	1/1	0.97	0.50	49,49,49,49	0
87	MG	5	4011	1/1	0.97	0.53	33,33,33,33	0
86	OHX	7	211	7/7	0.97	0.26	52,52,52,52	7
86	OHX	6	1960	7/7	0.97	0.23	72,72,72,72	7
86	OHX	1	3573	7/7	0.97	0.24	58,58,58,58	7
87	MG	5	4008	1/1	0.97	0.53	48,48,48,48	0
86	OHX	1	3569	7/7	0.97	0.16	79,79,79,79	7
86	OHX	1	3621	7/7	0.97	0.17	73,73,73,73	7
87	MG	6	2307	1/1	0.97	0.19	68,68,68,68	0
87	MG	1	4490	1/1	0.97	0.73	100,100,100,100	0
86	OHX	c1	201	7/7	0.97	0.20	79,79,79,79	7
86	OHX	5	3484	7/7	0.97	0.27	57,57,57,57	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	1	3595	7/7	0.97	0.20	95,95,95,95	7
86	OHX	5	3656	7/7	0.97	0.32	58,58,58,58	7
86	OHX	1	3537	7/7	0.97	0.12	112,112,112,112	7
86	OHX	5	3669	7/7	0.97	0.35	37,37,37,37	7
86	OHX	5	3522	7/7	0.97	0.28	56,56,56,56	7
86	OHX	5	3623	7/7	0.97	0.26	46,46,46,46	7
86	OHX	1	3480	7/7	0.97	0.23	75,75,75,75	7
86	OHX	5	3552	7/7	0.97	0.22	47,47,47,47	7
86	OHX	5	3563	7/7	0.97	0.13	93,93,93,93	7
86	OHX	1	3574	7/7	0.97	0.25	56,56,56,56	7
86	OHX	2	2014	7/7	0.97	0.16	80,80,80,80	7
86	OHX	5	3556	7/7	0.97	0.12	107,107,107,107	7
86	OHX	5	3706	7/7	0.97	0.16	74,74,74,74	7
87	MG	5	3874	1/1	0.97	0.34	43,43,43,43	0
86	OHX	1	3594	7/7	0.97	0.15	74,74,74,74	7
86	OHX	1	3811	7/7	0.97	0.18	89,89,89,89	7
87	MG	5	4532	1/1	0.97	0.17	43,43,43,43	0
86	OHX	6	1975	7/7	0.97	0.20	61,61,61,61	7
86	OHX	2	2037	7/7	0.97	0.16	60,60,60,60	7
86	OHX	2	1941	7/7	0.97	0.19	92,92,92,92	7
87	MG	1	3973	1/1	0.97	0.41	29,29,29,29	0
87	MG	1	3881	1/1	0.97	0.24	47,47,47,47	0
86	OHX	2	1915	7/7	0.97	0.14	122,122,122,122	7
86	OHX	1	3576	7/7	0.97	0.22	53,53,53,53	7
87	MG	5	4567	1/1	0.97	0.31	48,48,48,48	1
87	MG	5	4023	1/1	0.97	0.69	32,32,32,32	0
86	OHX	1	3719	7/7	0.97	0.17	86,86,86,86	7
86	OHX	3	208	7/7	0.97	0.21	85,85,85,85	7
87	MG	13	403	1/1	0.97	0.54	26,26,26,26	0
86	OHX	5	3632	7/7	0.97	0.18	63,63,63,63	7
86	OHX	2	2011	7/7	0.97	0.28	69,69,69,69	7
86	OHX	1	3743	7/7	0.97	0.21	76,76,76,76	7
87	MG	5	4445	1/1	0.97	0.36	32,32,32,32	1
87	MG	5	4526	1/1	0.97	0.27	51,51,51,51	1
87	MG	2	2116	1/1	0.97	0.32	89,89,89,89	0
86	OHX	5	3546	7/7	0.97	0.23	52,52,52,52	7
87	MG	5	4026	1/1	0.97	0.50	37,37,37,37	0
86	OHX	2	1932	7/7	0.97	0.16	92,92,92,92	7
87	MG	5	3902	1/1	0.97	0.26	71,71,71,71	0
86	OHX	2	1952	7/7	0.97	0.10	131,131,131,131	7
87	MG	N0	201	1/1	0.97	1.23	49,49,49,49	1
86	OHX	1	3527	7/7	0.97	0.31	81,81,81,81	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	2	2008	7/7	0.97	0.15	83,83,83,83	7
86	OHX	5	3575	7/7	0.97	0.23	66,66,66,66	7
86	OHX	1	3568	7/7	0.97	0.13	79,79,79,79	7
87	MG	6	2142	1/1	0.97	0.21	73,73,73,73	0
86	OHX	5	3600	7/7	0.97	0.28	57,57,57,57	7
86	OHX	2	1957	7/7	0.97	0.18	79,79,79,79	7
87	MG	1	4242	1/1	0.97	0.38	37,37,37,37	0
87	MG	2	2258	1/1	0.97	0.50	74,74,74,74	1
86	OHX	5	3602	7/7	0.97	0.30	86,86,86,86	7
86	OHX	1	3550	7/7	0.97	0.20	55,55,55,55	7
86	OHX	2	2076	7/7	0.97	0.15	122,122,122,122	7
86	OHX	1	3623	7/7	0.97	0.21	51,51,51,51	7
87	MG	5	4472	1/1	0.97	0.17	42,42,42,42	0
86	OHX	6	2002	7/7	0.97	0.23	52,52,52,52	7
86	OHX	4	207	7/7	0.97	0.19	61,61,61,61	7
86	OHX	1	3593	7/7	0.97	0.27	56,56,56,56	7
86	OHX	5	3725	7/7	0.97	0.20	75,75,75,75	7
86	OHX	5	3554	7/7	0.97	0.23	57,57,57,57	7
86	OHX	1	3779	7/7	0.97	0.25	50,50,50,50	7
86	OHX	6	1956	7/7	0.97	0.16	90,90,90,90	7
86	OHX	6	1973	7/7	0.97	0.19	86,86,86,86	7
88	ZN	q2	501	1/1	0.97	0.09	69,69,69,69	0
86	OHX	1	3501	7/7	0.97	0.28	83,83,83,83	7
86	OHX	5	3461	7/7	0.97	0.32	72,72,72,72	7
87	MG	1	4051	1/1	0.97	0.30	41,41,41,41	0
86	OHX	5	3547	7/7	0.97	0.12	136,136,136,136	7
87	MG	1	3957	1/1	0.97	0.46	34,34,34,34	0
86	OHX	5	3570	7/7	0.97	0.12	98,98,98,98	7
86	OHX	2	2054	7/7	0.97	0.21	87,87,87,87	7
87	MG	2	2131	1/1	0.97	0.15	73,73,73,73	0
87	MG	4	231	1/1	0.97	0.27	56,56,56,56	0
86	OHX	4	211	7/7	0.97	0.13	99,99,99,99	7
87	MG	l2	304	1/1	0.97	0.71	44,44,44,44	1
87	MG	c7	201	1/1	0.97	0.52	81,81,81,81	1
87	MG	5	3891	1/1	0.97	0.53	39,39,39,39	0
87	MG	1	3953	1/1	0.97	0.63	38,38,38,38	0
86	OHX	4	203	7/7	0.97	0.22	61,61,61,61	7
86	OHX	5	3558	7/7	0.97	0.20	45,45,45,45	7
86	OHX	5	3691	7/7	0.97	0.23	54,54,54,54	7
87	MG	5	4498	1/1	0.97	0.52	45,45,45,45	1
86	OHX	2	1944	7/7	0.97	0.22	72,72,72,72	7
86	OHX	2	1992	7/7	0.97	0.23	75,75,75,75	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3571	7/7	0.97	0.25	64,64,64,64	7
86	OHX	6	1968	7/7	0.97	0.30	74,74,74,74	7
87	MG	M8	204	1/1	0.97	0.73	46,46,46,46	1
87	MG	2	2179	1/1	0.97	0.18	85,85,85,85	0
87	MG	1	4002	1/1	0.97	0.53	36,36,36,36	0
86	OHX	s4	301	7/7	0.97	0.27	79,79,79,79	7
86	OHX	5	3492	7/7	0.97	0.27	42,42,42,42	7
86	OHX	2	2004	7/7	0.97	0.13	89,89,89,89	7
86	OHX	1	3470	7/7	0.97	0.30	88,88,88,88	7
87	MG	5	4089	1/1	0.97	0.25	37,37,37,37	0
87	MG	1	3901	1/1	0.97	0.27	66,66,66,66	0
86	OHX	5	3559	7/7	0.97	0.23	53,53,53,53	7
86	OHX	5	3519	7/7	0.97	0.14	132,132,132,132	7
87	MG	5	4486	1/1	0.97	0.34	46,46,46,46	0
87	MG	L7	303	1/1	0.97	0.17	42,42,42,42	0
86	OHX	2	1983	7/7	0.97	0.27	70,70,70,70	7
86	OHX	1	3610	7/7	0.97	0.18	110,110,110,110	7
87	MG	5	4285	1/1	0.97	0.25	38,38,38,38	1
86	OHX	6	2021	7/7	0.97	0.23	53,53,53,53	7
86	OHX	8	203	7/7	0.97	0.17	86,86,86,86	7
86	OHX	5	3543	7/7	0.97	0.37	60,60,60,60	7
86	OHX	2	1953	7/7	0.97	0.15	64,64,64,64	7
86	OHX	5	3801	7/7	0.97	0.23	66,66,66,66	7
86	OHX	1	3620	7/7	0.97	0.26	60,60,60,60	7
86	OHX	6	2014	7/7	0.97	0.28	74,74,74,74	7
86	OHX	1	3645	7/7	0.97	0.22	58,58,58,58	7
86	OHX	2	1945	7/7	0.97	0.13	110,110,110,110	7
86	OHX	1	3696	7/7	0.97	0.30	63,63,63,63	7
87	MG	5	4429	1/1	0.97	0.30	37,37,37,37	1
87	MG	5	4311	1/1	0.97	0.36	37,37,37,37	1
86	OHX	6	1995	7/7	0.97	0.24	113,113,113,113	7
86	OHX	L4	401	7/7	0.97	0.26	59,59,59,59	7
87	MG	1	4337	1/1	0.97	0.34	42,42,42,42	0
87	MG	1	4438	1/1	0.97	0.37	64,64,64,64	0
86	OHX	2	1966	7/7	0.97	0.19	61,61,61,61	7
86	OHX	5	3816	7/7	0.97	0.29	43,43,43,43	7
87	MG	5	3899	1/1	0.97	0.38	32,32,32,32	0
87	MG	q3	502	1/1	0.97	0.41	43,43,43,43	1
86	OHX	1	3647	7/7	0.97	0.26	64,64,64,64	7
86	OHX	1	3709	7/7	0.97	0.17	59,59,59,59	7
87	MG	6	2224	1/1	0.97	0.46	47,47,47,47	0
86	OHX	3	205	7/7	0.97	0.15	80,80,80,80	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	5	4273	1/1	0.97	0.44	34,34,34,34	1
86	OHX	1	3510	7/7	0.97	0.27	93,93,93,93	7
86	OHX	5	3617	7/7	0.97	0.15	74,74,74,74	7
87	MG	s1	303	1/1	0.97	0.17	77,77,77,77	0
86	OHX	6	2061	7/7	0.97	0.21	102,102,102,102	7
87	MG	5	4224	1/1	0.97	0.36	38,38,38,38	0
86	OHX	2	1942	7/7	0.97	0.17	74,74,74,74	7
86	OHX	6	1954	7/7	0.97	0.18	149,149,149,149	7
86	OHX	1	3526	7/7	0.97	0.22	47,47,47,47	7
87	MG	3	215	1/1	0.97	0.39	51,51,51,51	0
86	OHX	1	3646	7/7	0.97	0.32	54,54,54,54	7
86	OHX	1	3553	7/7	0.97	0.22	60,60,60,60	7
86	OHX	6	1981	7/7	0.97	0.42	45,45,45,45	7
86	OHX	6	1983	7/7	0.97	0.19	95,95,95,95	7
86	OHX	5	3729	7/7	0.97	0.33	58,58,58,58	7
86	OHX	5	3582	7/7	0.97	0.19	67,67,67,67	7
87	MG	1	3833	1/1	0.97	0.21	84,84,84,84	0
86	OHX	5	3560	7/7	0.97	0.27	50,50,50,50	7
86	OHX	5	3666	7/7	0.97	0.31	65,65,65,65	7
86	OHX	1	3473	7/7	0.97	0.25	60,60,60,60	7
87	MG	1	3828	1/1	0.97	0.44	40,40,40,40	0
86	OHX	5	3794	7/7	0.97	0.23	57,57,57,57	7
86	OHX	5	3535	7/7	0.97	0.28	42,42,42,42	7
86	OHX	5	3680	7/7	0.97	0.34	38,38,38,38	7
87	MG	1	4377	1/1	0.97	0.44	35,35,35,35	1
87	MG	5	4463	1/1	0.97	0.73	36,36,36,36	1
86	OHX	1	3596	7/7	0.97	0.21	70,70,70,70	7
86	OHX	5	3586	7/7	0.97	0.14	83,83,83,83	7
86	OHX	2	1950	7/7	0.97	0.17	97,97,97,97	7
86	OHX	1	3612	7/7	0.97	0.35	46,46,46,46	7
87	MG	N8	207	1/1	0.97	1.16	39,39,39,39	1
87	MG	1	4368	1/1	0.97	0.20	38,38,38,38	0
87	MG	5	3840	1/1	0.97	0.58	60,60,60,60	0
87	MG	6	2258	1/1	0.97	0.30	84,84,84,84	0
86	OHX	5	3479	7/7	0.97	0.22	79,79,79,79	7
87	MG	5	4122	1/1	0.97	0.21	48,48,48,48	1
86	OHX	5	3488	7/7	0.97	0.27	48,48,48,48	7
87	MG	5	4502	1/1	0.97	0.42	42,42,42,42	1
87	MG	5	4065	1/1	0.97	0.11	39,39,39,39	0
86	OHX	2	1911	7/7	0.97	0.14	109,109,109,109	0
86	OHX	8	209	7/7	0.97	0.20	88,88,88,88	7
87	MG	2	2100	1/1	0.97	0.33	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	1	4474	1/1	0.97	0.67	55,55,55,55	0
86	OHX	1	3638	7/7	0.97	0.17	82,82,82,82	7
86	OHX	2	1967	7/7	0.97	0.20	92,92,92,92	7
86	OHX	5	3657	7/7	0.97	0.26	41,41,41,41	7
86	OHX	5	3585	7/7	0.97	0.53	44,44,44,44	7
86	OHX	2	1978	7/7	0.97	0.12	121,121,121,121	7
86	OHX	5	3438	7/7	0.97	0.27	48,48,48,48	7
86	OHX	1	3582	7/7	0.97	0.18	67,67,67,67	7
87	MG	O1	205	1/1	0.97	0.22	65,65,65,65	0
86	OHX	5	3544	7/7	0.97	0.14	99,99,99,99	7
86	OHX	5	3765	7/7	0.97	0.25	42,42,42,42	7
86	OHX	6	2088	7/7	0.97	0.27	71,71,71,71	7
87	MG	6	2310	1/1	0.97	0.79	48,48,48,48	1
87	MG	1	3986	1/1	0.97	0.21	54,54,54,54	0
86	OHX	6	2083	7/7	0.97	0.24	82,82,82,82	7
87	MG	M3	203	1/1	0.97	0.69	46,46,46,46	1
86	OHX	7	208	7/7	0.97	0.21	54,54,54,54	7
86	OHX	1	3557	7/7	0.97	0.18	87,87,87,87	7
86	OHX	5	3548	7/7	0.97	0.30	48,48,48,48	7
87	MG	s8	302	1/1	0.97	0.28	45,45,45,45	0
87	MG	5	3946	1/1	0.97	0.57	33,33,33,33	0
87	MG	1	4091	1/1	0.97	0.38	39,39,39,39	0
86	OHX	1	3599	7/7	0.97	0.23	42,42,42,42	7
86	OHX	6	1988	7/7	0.97	0.22	57,57,57,57	7
86	OHX	6	1987	7/7	0.97	0.21	70,70,70,70	7
87	MG	5	4210	1/1	0.97	0.56	35,35,35,35	1
86	OHX	2	1938	7/7	0.97	0.28	70,70,70,70	7
86	OHX	1	3564	7/7	0.98	0.20	54,54,54,54	7
86	OHX	2	1925	7/7	0.98	0.12	112,112,112,112	7
87	MG	1	4382	1/1	0.98	0.35	70,70,70,70	0
87	MG	5	3833	1/1	0.98	0.34	59,59,59,59	0
86	OHX	6	1945	7/7	0.98	0.28	58,58,58,58	7
86	OHX	1	3476	7/7	0.98	0.22	70,70,70,70	7
87	MG	1	4433	1/1	0.98	0.32	43,43,43,43	0
87	MG	6	2319	1/1	0.98	0.26	57,57,57,57	0
87	MG	6	2247	1/1	0.98	0.20	50,50,50,50	0
86	OHX	5	3463	7/7	0.98	0.24	58,58,58,58	7
86	OHX	M5	301	7/7	0.98	0.18	75,75,75,75	7
87	MG	n3	203	1/1	0.98	0.46	29,29,29,29	0
86	OHX	1	3503	7/7	0.98	0.28	57,57,57,57	7
86	OHX	1	3741	7/7	0.98	0.20	56,56,56,56	7
86	OHX	1	3490	7/7	0.98	0.35	54,54,54,54	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	2	1940	7/7	0.98	0.15	85,85,85,85	7
86	OHX	2	1939	7/7	0.98	0.16	98,98,98,98	7
87	MG	M8	203	1/1	0.98	0.75	41,41,41,41	0
87	MG	1	4458	1/1	0.98	0.17	47,47,47,47	0
87	MG	6	2303	1/1	0.98	0.45	78,78,78,78	0
86	OHX	5	3434	7/7	0.98	0.31	38,38,38,38	7
86	OHX	5	3598	7/7	0.98	0.17	73,73,73,73	7
87	MG	5	4398	1/1	0.98	0.25	38,38,38,38	1
86	OHX	5	3593	7/7	0.98	0.27	44,44,44,44	7
87	MG	6	2172	1/1	0.98	0.33	76,76,76,76	0
87	MG	6	2146	1/1	0.98	0.49	37,37,37,37	0
87	MG	M7	210	1/1	0.98	0.13	45,45,45,45	1
86	OHX	5	3541	7/7	0.98	0.20	55,55,55,55	7
86	OHX	1	3786	7/7	0.98	0.25	73,73,73,73	7
86	OHX	1	3640	7/7	0.98	0.32	83,83,83,83	7
87	MG	1	4414	1/1	0.98	0.29	50,50,50,50	1
86	OHX	1	3531	7/7	0.98	0.24	49,49,49,49	7
86	OHX	1	3565	7/7	0.98	0.31	84,84,84,84	7
86	OHX	1	3515	7/7	0.98	0.21	98,98,98,98	7
86	OHX	6	1946	7/7	0.98	0.22	71,71,71,71	7
87	MG	5	3939	1/1	0.98	0.26	39,39,39,39	0
86	OHX	1	3653	7/7	0.98	0.14	59,59,59,59	7
87	MG	5	4035	1/1	0.98	0.19	46,46,46,46	0
87	MG	5	4184	1/1	0.98	0.38	40,40,40,40	1
86	OHX	6	1935	7/7	0.98	0.23	56,56,56,56	7
86	OHX	1	3524	7/7	0.98	0.19	55,55,55,55	7
87	MG	M5	303	1/1	0.98	0.73	41,41,41,41	1
86	OHX	5	3641	7/7	0.98	0.22	52,52,52,52	7
86	OHX	1	3507	7/7	0.98	0.29	60,60,60,60	7
86	OHX	2	1971	7/7	0.98	0.32	80,80,80,80	7
86	OHX	6	1949	7/7	0.98	0.22	73,73,73,73	7
87	MG	5	3875	1/1	0.98	0.49	31,31,31,31	0
86	OHX	1	3458	7/7	0.98	0.22	79,79,79,79	7
86	OHX	2	1908	7/7	0.98	0.15	104,104,104,104	0
87	MG	2	2234	1/1	0.98	0.24	76,76,76,76	0
87	MG	3	220	1/1	0.98	0.17	55,55,55,55	0
86	OHX	5	3475	7/7	0.98	0.21	81,81,81,81	7
86	OHX	M9	201	7/7	0.98	0.19	68,68,68,68	7
87	MG	5	3929	1/1	0.98	0.49	39,39,39,39	0
86	OHX	6	1972	7/7	0.98	0.25	59,59,59,59	7
86	OHX	5	3589	7/7	0.98	0.24	46,46,46,46	7
86	OHX	6	1918	7/7	0.98	0.24	56,56,56,56	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	3	203	7/7	0.98	0.26	56,56,56,56	7
87	MG	6	2185	1/1	0.98	0.31	44,44,44,44	0
87	MG	1	4388	1/1	0.98	0.27	35,35,35,35	1
86	OHX	6	1921	7/7	0.98	0.31	51,51,51,51	7
86	OHX	6	1907	7/7	0.98	0.14	76,76,76,76	0
87	MG	M0	308	1/1	0.98	0.80	44,44,44,44	1
86	OHX	3	201	7/7	0.98	0.20	71,71,71,71	7
86	OHX	5	3516	7/7	0.98	0.20	60,60,60,60	7
87	MG	5	4092	1/1	0.98	0.26	36,36,36,36	1
86	OHX	5	3504	7/7	0.98	0.23	75,75,75,75	7
87	MG	5	3855	1/1	0.98	0.42	36,36,36,36	0
86	OHX	5	3465	7/7	0.98	0.38	40,40,40,40	7
86	OHX	1	3541	7/7	0.98	0.26	54,54,54,54	7
86	OHX	1	3652	7/7	0.98	0.32	58,58,58,58	7
86	OHX	6	1977	7/7	0.98	0.23	86,86,86,86	7
86	OHX	6	1942	7/7	0.98	0.19	70,70,70,70	7
86	OHX	2	1928	7/7	0.98	0.27	75,75,75,75	7
87	MG	1	3950	1/1	0.98	0.48	31,31,31,31	0
87	MG	5	4546	1/1	0.98	0.35	34,34,34,34	1
87	MG	1	4201	1/1	0.98	0.28	38,38,38,38	0
86	OHX	1	3810	7/7	0.98	0.24	62,62,62,62	7
86	OHX	1	3487	7/7	0.98	0.26	74,74,74,74	7
86	OHX	1	3586	7/7	0.98	0.20	50,50,50,50	7
87	MG	n1	202	1/1	0.98	0.98	40,40,40,40	1
86	OHX	1	3753	7/7	0.98	0.25	51,51,51,51	7
87	MG	1	4283	1/1	0.98	0.34	38,38,38,38	1
86	OHX	1	3717	7/7	0.98	0.24	50,50,50,50	7
86	OHX	5	3562	7/7	0.98	0.22	51,51,51,51	7
87	MG	5	4356	1/1	0.98	0.69	45,45,45,45	0
86	OHX	5	3491	7/7	0.98	0.32	51,51,51,51	7
86	OHX	6	1963	7/7	0.98	0.24	72,72,72,72	7
87	MG	m8	1502	1/1	0.98	0.17	47,47,47,47	0
86	OHX	5	3550	7/7	0.98	0.26	47,47,47,47	7
86	OHX	5	3524	7/7	0.98	0.17	88,88,88,88	7
87	MG	5	3940	1/1	0.98	0.70	34,34,34,34	0
86	OHX	6	2004	7/7	0.98	0.26	54,54,54,54	7
87	MG	1	4194	1/1	0.98	0.42	47,47,47,47	1
86	OHX	2	1917	7/7	0.98	0.18	85,85,85,85	7
86	OHX	2	1934	7/7	0.98	0.19	103,103,103,103	7
86	OHX	5	3497	7/7	0.98	0.20	62,62,62,62	7
87	MG	5	4425	1/1	0.98	0.30	48,48,48,48	1
87	MG	5	4269	1/1	0.98	0.26	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3591	7/7	0.98	0.12	90,90,90,90	7
86	OHX	5	3487	7/7	0.98	0.34	48,48,48,48	7
86	OHX	5	3591	7/7	0.98	0.27	52,52,52,52	7
87	MG	1	4037	1/1	0.98	0.47	45,45,45,45	0
87	MG	5	3955	1/1	0.98	0.48	32,32,32,32	0
86	OHX	1	3528	7/7	0.98	0.23	68,68,68,68	7
87	MG	5	4022	1/1	0.98	0.52	31,31,31,31	0
86	OHX	1	3609	7/7	0.98	0.29	49,49,49,49	7
86	OHX	7	203	7/7	0.98	0.22	54,54,54,54	7
86	OHX	5	3716	7/7	0.98	0.31	60,60,60,60	7
87	MG	5	3933	1/1	0.98	0.22	46,46,46,46	0
87	MG	1	3928	1/1	0.98	0.39	43,43,43,43	0
86	OHX	2	1927	7/7	0.98	0.18	94,94,94,94	7
86	OHX	5	3459	7/7	0.98	0.17	80,80,80,80	7
87	MG	5	4538	1/1	0.98	0.80	48,48,48,48	1
86	OHX	5	3494	7/7	0.98	0.29	89,89,89,89	7
87	MG	1	4275	1/1	0.98	0.15	46,46,46,46	0
87	MG	M5	304	1/1	0.98	0.58	40,40,40,40	1
87	MG	1	4053	1/1	0.98	0.23	44,44,44,44	0
86	OHX	1	3600	7/7	0.98	0.14	68,68,68,68	7
87	MG	5	4246	1/1	0.98	0.23	45,45,45,45	0
87	MG	5	3957	1/1	0.98	0.45	30,30,30,30	0
86	OHX	2	1972	7/7	0.98	0.16	81,81,81,81	7
87	MG	5	4491	1/1	0.98	0.61	35,35,35,35	1
86	OHX	6	1962	7/7	0.98	0.23	62,62,62,62	7
87	MG	1	3984	1/1	0.98	0.70	37,37,37,37	0
87	MG	m7	208	1/1	0.98	0.57	40,40,40,40	1
87	MG	1	3941	1/1	0.98	0.50	36,36,36,36	0
87	MG	5	3959	1/1	0.98	0.38	35,35,35,35	0
86	OHX	1	3801	7/7	0.98	0.25	57,57,57,57	7
87	MG	1	4210	1/1	0.98	0.53	47,47,47,47	0
86	OHX	5	3456	7/7	0.98	0.14	115,115,115,115	0
86	OHX	1	3577	7/7	0.98	0.25	114,114,114,114	7
87	MG	1	4379	1/1	0.98	0.49	33,33,33,33	0
86	OHX	6	1947	7/7	0.98	0.24	59,59,59,59	7
87	MG	1	3954	1/1	0.98	0.58	47,47,47,47	0
86	OHX	5	3502	7/7	0.98	0.24	46,46,46,46	7
86	OHX	5	3630	7/7	0.98	0.16	75,75,75,75	7
86	OHX	6	1965	7/7	0.98	0.15	83,83,83,83	7
87	MG	5	4042	1/1	0.98	0.50	35,35,35,35	0
86	OHX	1	3536	7/7	0.98	0.25	54,54,54,54	7
86	OHX	5	3673	7/7	0.98	0.23	44,44,44,44	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3520	7/7	0.98	0.24	52,52,52,52	7
86	OHX	7	202	7/7	0.98	0.18	60,60,60,60	7
86	OHX	5	3618	7/7	0.98	0.29	52,52,52,52	7
86	OHX	6	1974	7/7	0.98	0.27	67,67,67,67	7
86	OHX	5	3529	7/7	0.98	0.26	51,51,51,51	7
87	MG	1	4418	1/1	0.98	0.40	60,60,60,60	1
86	OHX	6	1909	7/7	0.98	0.17	79,79,79,79	7
87	MG	1	3890	1/1	0.98	0.38	49,49,49,49	0
86	OHX	1	3628	7/7	0.98	0.14	74,74,74,74	7
86	OHX	6	1934	7/7	0.98	0.30	57,57,57,57	7
86	OHX	1	3794	7/7	0.98	0.22	68,68,68,68	7
86	OHX	5	3584	7/7	0.98	0.23	52,52,52,52	7
87	MG	6	2165	1/1	0.98	0.28	45,45,45,45	0
86	OHX	5	3498	7/7	0.98	0.17	66,66,66,66	7
86	OHX	1	3449	7/7	0.98	0.19	88,88,88,88	7
86	OHX	5	3499	7/7	0.98	0.20	46,46,46,46	7
86	OHX	m0	302	7/7	0.98	0.47	45,45,45,45	7
86	OHX	2	1977	7/7	0.98	0.12	138,138,138,138	7
86	OHX	2	1963	7/7	0.98	0.18	83,83,83,83	7
87	MG	1	4257	1/1	0.98	0.42	44,44,44,44	1
86	OHX	6	1919	7/7	0.98	0.17	68,68,68,68	7
86	OHX	1	3597	7/7	0.98	0.19	37,37,37,37	7
86	OHX	2	1948	7/7	0.98	0.20	67,67,67,67	7
87	MG	1	4212	1/1	0.98	0.31	41,41,41,41	1
87	MG	n8	207	1/1	0.98	0.76	39,39,39,39	1
86	OHX	3	202	7/7	0.98	0.27	48,48,48,48	7
86	OHX	1	3712	7/7	0.98	0.19	62,62,62,62	7
86	OHX	l3	401	7/7	0.98	0.25	52,52,52,52	7
87	MG	1	3942	1/1	0.98	0.60	32,32,32,32	0
86	OHX	5	3583	7/7	0.98	0.15	148,148,148,148	7
86	OHX	3	204	7/7	0.98	0.21	85,85,85,85	7
86	OHX	5	3810	7/7	0.98	0.26	63,63,63,63	7
86	OHX	5	3452	7/7	0.98	0.30	70,70,70,70	7
86	OHX	5	3578	7/7	0.98	0.25	55,55,55,55	7
86	OHX	5	3489	7/7	0.98	0.22	51,51,51,51	7
87	MG	1	4001	1/1	0.98	0.56	28,28,28,28	0
87	MG	5	4296	1/1	0.98	0.28	48,48,48,48	1
87	MG	n9	103	1/1	0.98	0.83	40,40,40,40	1
86	OHX	1	3504	7/7	0.98	0.17	90,90,90,90	7
87	MG	5	3991	1/1	0.98	0.50	34,34,34,34	0
86	OHX	6	2006	7/7	0.98	0.27	54,54,54,54	7
86	OHX	5	3477	7/7	0.98	0.26	44,44,44,44	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	3521	7/7	0.98	0.18	56,56,56,56	7
87	MG	1	4308	1/1	0.98	0.36	55,55,55,55	0
87	MG	5	4428	1/1	0.98	0.09	69,69,69,69	0
86	OHX	6	1911	7/7	0.98	0.19	59,59,59,59	7
87	MG	n3	205	1/1	0.98	0.28	34,34,34,34	1
86	OHX	5	3807	7/7	0.98	0.13	147,147,147,147	7
87	MG	L3	406	1/1	0.98	0.40	39,39,39,39	1
86	OHX	5	3733	7/7	0.98	0.21	57,57,57,57	7
87	MG	5	4094	1/1	0.98	0.28	52,52,52,52	0
87	MG	6	2144	1/1	0.98	0.26	55,55,55,55	0
87	MG	1	3888	1/1	0.98	0.22	66,66,66,66	0
87	MG	1	3838	1/1	0.98	0.23	59,59,59,59	0
86	OHX	6	1948	7/7	0.98	0.18	86,86,86,86	7
87	MG	5	4268	1/1	0.98	0.18	46,46,46,46	0
86	OHX	5	3470	7/7	0.98	0.18	90,90,90,90	7
86	OHX	6	2084	7/7	0.98	0.20	79,79,79,79	7
86	OHX	1	3495	7/7	0.98	0.26	44,44,44,44	7
86	OHX	1	3592	7/7	0.98	0.27	52,52,52,52	7
86	OHX	2	1921	7/7	0.98	0.15	88,88,88,88	7
87	MG	6	2288	1/1	0.98	0.14	65,65,65,65	0
86	OHX	1	3552	7/7	0.98	0.36	60,60,60,60	7
87	MG	N3	201	1/1	0.98	0.59	39,39,39,39	0
86	OHX	6	1955	7/7	0.98	0.17	145,145,145,145	7
87	MG	n0	205	1/1	0.98	0.85	41,41,41,41	1
86	OHX	1	3452	7/7	0.98	0.26	70,70,70,70	7
86	OHX	1	3556	7/7	0.98	0.26	70,70,70,70	7
86	OHX	1	3422	7/7	0.98	0.30	56,56,56,56	7
86	OHX	5	3486	7/7	0.98	0.19	64,64,64,64	7
86	OHX	6	1940	7/7	0.98	0.21	64,64,64,64	7
86	OHX	1	3436	7/7	0.98	0.34	46,46,46,46	7
87	MG	n1	203	1/1	0.98	0.45	37,37,37,37	1
86	OHX	5	3525	7/7	0.98	0.32	42,42,42,42	7
86	OHX	6	1957	7/7	0.98	0.18	63,63,63,63	7
87	MG	2	2237	1/1	0.98	0.16	80,80,80,80	0
86	OHX	S2	301	7/7	0.98	0.27	81,81,81,81	7
87	MG	6	2279	1/1	0.98	0.43	80,80,80,80	0
86	OHX	6	1943	7/7	0.98	0.14	108,108,108,108	7
87	MG	o6	201	1/1	0.98	0.38	69,69,69,69	1
86	OHX	5	3520	7/7	0.98	0.28	42,42,42,42	7
86	OHX	1	3750	7/7	0.98	0.22	46,46,46,46	7
86	OHX	5	3515	7/7	0.98	0.34	40,40,40,40	7
87	MG	6	2254	1/1	0.98	0.21	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	6	2275	1/1	0.98	0.20	67,67,67,67	1
86	OHX	5	3572	7/7	0.98	0.21	66,66,66,66	7
87	MG	5	4270	1/1	0.98	0.07	45,45,45,45	0
86	OHX	5	3636	7/7	0.98	0.39	44,44,44,44	7
86	OHX	5	3508	7/7	0.98	0.21	38,38,38,38	7
87	MG	5	4533	1/1	0.98	0.60	36,36,36,36	1
87	MG	m7	207	1/1	0.98	0.52	41,41,41,41	1
86	OHX	2	1986	7/7	0.98	0.16	80,80,80,80	7
86	OHX	5	3788	7/7	0.98	0.24	58,58,58,58	7
86	OHX	6	1928	7/7	0.98	0.17	118,118,118,118	7
86	OHX	5	3616	7/7	0.98	0.34	46,46,46,46	7
87	MG	L4	405	1/1	0.98	0.36	38,38,38,38	1
87	MG	1	4273	1/1	0.98	0.42	45,45,45,45	1
86	OHX	m5	501	7/7	0.98	0.18	81,81,81,81	7
86	OHX	5	3480	7/7	0.98	0.20	63,63,63,63	7
86	OHX	5	3512	7/7	0.98	0.19	69,69,69,69	7
86	OHX	2	1929	7/7	0.98	0.28	66,66,66,66	7
86	OHX	5	3481	7/7	0.98	0.26	69,69,69,69	7
87	MG	2	2246	1/1	0.98	0.21	77,77,77,77	0
86	OHX	4	205	7/7	0.98	0.21	75,75,75,75	7
86	OHX	1	3508	7/7	0.98	0.15	71,71,71,71	7
86	OHX	1	3548	7/7	0.98	0.19	59,59,59,59	7
87	MG	M7	203	1/1	0.98	0.38	36,36,36,36	0
86	OHX	5	3732	7/7	0.98	0.23	49,49,49,49	7
86	OHX	1	3474	7/7	0.98	0.36	90,90,90,90	7
86	OHX	1	3481	7/7	0.98	0.23	88,88,88,88	7
87	MG	1	4254	1/1	0.98	0.30	51,51,51,51	0
87	MG	5	4143	1/1	0.98	0.19	34,34,34,34	1
86	OHX	m0	301	7/7	0.98	0.13	86,86,86,86	7
86	OHX	4	209	7/7	0.98	0.27	45,45,45,45	7
86	OHX	3	206	7/7	0.98	0.20	81,81,81,81	7
86	OHX	2	1982	7/7	0.98	0.11	100,100,100,100	7
86	OHX	8	210	7/7	0.98	0.31	49,49,49,49	7
86	OHX	1	3563	7/7	0.98	0.30	50,50,50,50	7
86	OHX	6	1941	7/7	0.98	0.14	79,79,79,79	7
87	MG	1	4396	1/1	0.98	0.58	45,45,45,45	1
86	OHX	1	3523	7/7	0.98	0.17	95,95,95,95	7
86	OHX	5	3667	7/7	0.98	0.23	41,41,41,41	7
87	MG	5	4334	1/1	0.98	0.42	37,37,37,37	0
86	OHX	8	207	7/7	0.98	0.14	74,74,74,74	7
87	MG	1	4021	1/1	0.98	0.62	37,37,37,37	0
86	OHX	6	1914	7/7	0.98	0.25	52,52,52,52	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3652	7/7	0.98	0.18	65,65,65,65	7
86	OHX	1	3486	7/7	0.98	0.24	65,65,65,65	7
86	OHX	2	1910	7/7	0.98	0.17	94,94,94,94	7
86	OHX	5	3566	7/7	0.98	0.22	96,96,96,96	7
87	MG	5	4029	1/1	0.98	0.55	26,26,26,26	0
86	OHX	1	3590	7/7	0.98	0.12	91,91,91,91	7
86	OHX	5	3437	7/7	0.98	0.18	100,100,100,100	0
88	ZN	d6	500	1/1	0.98	0.08	67,67,67,67	0
86	OHX	2	1997	7/7	0.98	0.14	88,88,88,88	7
86	OHX	2	1958	7/7	0.98	0.19	75,75,75,75	7
86	OHX	6	1939	7/7	0.98	0.22	103,103,103,103	7
87	MG	1	3983	1/1	0.98	0.36	40,40,40,40	0
87	MG	6	2294	1/1	0.98	0.17	43,43,43,43	0
87	MG	2	2226	1/1	0.98	0.21	76,76,76,76	0
86	OHX	5	3501	7/7	0.98	0.20	57,57,57,57	7
86	OHX	5	3505	7/7	0.98	0.17	59,59,59,59	7
87	MG	5	4431	1/1	0.98	0.39	44,44,44,44	1
86	OHX	1	3485	7/7	0.98	0.24	87,87,87,87	7
86	OHX	1	3643	7/7	0.98	0.24	52,52,52,52	7
87	MG	1	4231	1/1	0.98	0.22	44,44,44,44	0
86	OHX	5	3526	7/7	0.98	0.31	46,46,46,46	7
87	MG	7	240	1/1	0.98	0.56	53,53,53,53	1
86	OHX	5	3731	7/7	0.98	0.28	48,48,48,48	7
87	MG	2	2153	1/1	0.98	0.23	72,72,72,72	0
86	OHX	1	3632	7/7	0.98	0.25	43,43,43,43	7
86	OHX	1	3466	7/7	0.98	0.25	45,45,45,45	7
87	MG	1	4265	1/1	0.98	0.32	56,56,56,56	0
86	OHX	5	3599	7/7	0.98	0.15	56,56,56,56	7
87	MG	1	4376	1/1	0.98	0.64	34,34,34,34	1
86	OHX	C8	202	7/7	0.98	0.14	94,94,94,94	7
87	MG	1	4389	1/1	0.98	0.32	59,59,59,59	1
86	OHX	5	3805	7/7	0.98	0.21	88,88,88,88	7
86	OHX	1	3549	7/7	0.98	0.22	54,54,54,54	7
86	OHX	2	1922	7/7	0.98	0.20	75,75,75,75	7
86	OHX	1	3446	7/7	0.98	0.22	65,65,65,65	7
86	OHX	1	3581	7/7	0.98	0.17	54,54,54,54	7
87	MG	6	2182	1/1	0.98	0.22	51,51,51,51	0
86	OHX	6	1913	7/7	0.98	0.15	85,85,85,85	7
87	MG	5	3819	1/1	0.98	0.46	36,36,36,36	0
87	MG	1	4478	1/1	0.98	1.01	47,47,47,47	1
86	OHX	1	3601	7/7	0.98	0.19	49,49,49,49	7
86	OHX	1	3484	7/7	0.98	0.20	62,62,62,62	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	1	3457	7/7	0.98	0.27	50,50,50,50	7
86	OHX	5	3803	7/7	0.98	0.21	69,69,69,69	7
87	MG	5	4002	1/1	0.98	0.44	37,37,37,37	0
87	MG	1	4315	1/1	0.98	0.46	35,35,35,35	1
86	OHX	5	3485	7/7	0.98	0.27	46,46,46,46	7
87	MG	5	4147	1/1	0.98	0.51	36,36,36,36	0
86	OHX	2	1985	7/7	0.98	0.35	59,59,59,59	7
87	MG	5	3941	1/1	0.98	0.55	30,30,30,30	0
86	OHX	1	3468	7/7	0.98	0.23	65,65,65,65	7
86	OHX	1	3809	7/7	0.98	0.19	83,83,83,83	7
86	OHX	1	3459	7/7	0.98	0.21	81,81,81,81	7
87	MG	5	4177	1/1	0.98	0.31	42,42,42,42	0
87	MG	5	4534	1/1	0.98	0.17	54,54,54,54	0
87	MG	5	4403	1/1	0.98	0.35	40,40,40,40	1
86	OHX	5	3490	7/7	0.98	0.29	50,50,50,50	7
86	OHX	5	3528	7/7	0.98	0.25	62,62,62,62	7
86	OHX	1	3544	7/7	0.98	0.28	52,52,52,52	7
86	OHX	5	3496	7/7	0.98	0.25	48,48,48,48	7
86	OHX	1	3491	7/7	0.98	0.12	118,118,118,118	7
86	OHX	1	3650	7/7	0.98	0.17	96,96,96,96	7
86	OHX	2	1912	7/7	0.98	0.14	109,109,109,109	0
86	OHX	6	1952	7/7	0.98	0.16	84,84,84,84	7
86	OHX	1	3678	7/7	0.98	0.27	44,44,44,44	7
86	OHX	1	3567	7/7	0.98	0.36	48,48,48,48	7
87	MG	5	4175	1/1	0.98	0.23	86,86,86,86	0
87	MG	S6	301	1/1	0.98	0.23	103,103,103,103	0
86	OHX	6	1927	7/7	0.98	0.13	109,109,109,109	7
87	MG	5	3839	1/1	0.98	0.48	55,55,55,55	0
86	OHX	1	3680	7/7	0.98	0.36	60,60,60,60	7
86	OHX	1	3499	7/7	0.98	0.26	54,54,54,54	7
86	OHX	5	3588	7/7	0.98	0.21	43,43,43,43	7
86	OHX	2	1930	7/7	0.98	0.30	77,77,77,77	7
86	OHX	5	3553	7/7	0.98	0.14	84,84,84,84	7
86	OHX	1	3519	7/7	0.98	0.21	50,50,50,50	7
86	OHX	1	3529	7/7	0.98	0.24	66,66,66,66	7
87	MG	5	4514	1/1	0.98	0.37	30,30,30,30	1
86	OHX	1	3641	7/7	0.98	0.15	89,89,89,89	7
86	OHX	5	3453	7/7	0.98	0.30	79,79,79,79	7
86	OHX	6	1951	7/7	0.98	0.13	133,133,133,133	7
87	MG	1	3847	1/1	0.98	0.10	49,49,49,49	0
86	OHX	2	1995	7/7	0.98	0.19	86,86,86,86	7
86	OHX	1	3554	7/7	0.98	0.20	78,78,78,78	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	MG	5	4287	1/1	0.98	0.27	39,39,39,39	1
87	MG	1	3926	1/1	0.98	0.49	34,34,34,34	0
87	MG	5	3823	1/1	0.98	0.36	33,33,33,33	0
86	OHX	1	3625	7/7	0.98	0.15	61,61,61,61	7
86	OHX	1	3540	7/7	0.98	0.10	128,128,128,128	7
87	MG	6	2298	1/1	0.98	0.12	86,86,86,86	0
86	OHX	1	3460	7/7	0.98	0.27	60,60,60,60	7
86	OHX	1	3799	7/7	0.98	0.26	54,54,54,54	7
86	OHX	2	2088	7/7	0.98	0.26	94,94,94,94	7
86	OHX	5	3609	7/7	0.98	0.20	96,96,96,96	7
86	OHX	2	1936	7/7	0.98	0.27	72,72,72,72	7
87	MG	6	2181	1/1	0.98	0.32	55,55,55,55	0
86	OHX	12	301	7/7	0.98	0.22	63,63,63,63	7
86	OHX	5	3431	7/7	0.98	0.23	61,61,61,61	7
86	OHX	5	3627	7/7	0.98	0.14	81,81,81,81	7
86	OHX	2	1924	7/7	0.98	0.15	89,89,89,89	7
86	OHX	6	2011	7/7	0.98	0.21	57,57,57,57	7
87	MG	1	3944	1/1	0.98	0.47	35,35,35,35	0
86	OHX	L3	402	7/7	0.98	0.19	67,67,67,67	7
86	OHX	5	3814	7/7	0.98	0.21	70,70,70,70	7
86	OHX	6	1978	7/7	0.98	0.20	52,52,52,52	7
86	OHX	6	1967	7/7	0.98	0.19	47,47,47,47	7
87	MG	5	4475	1/1	0.98	0.30	39,39,39,39	0
87	MG	5	4003	1/1	0.98	0.62	27,27,27,27	0
87	MG	5	3995	1/1	0.98	0.64	34,34,34,34	0
86	OHX	5	3628	7/7	0.98	0.28	66,66,66,66	7
87	MG	m8	1501	1/1	0.98	0.64	42,42,42,42	1
86	OHX	5	3804	7/7	0.98	0.24	52,52,52,52	7
87	MG	1	3843	1/1	0.98	0.51	43,43,43,43	0
86	OHX	1	3776	7/7	0.98	0.23	59,59,59,59	7
86	OHX	2	1979	7/7	0.98	0.21	75,75,75,75	7
86	OHX	5	3597	7/7	0.98	0.27	46,46,46,46	7
86	OHX	1	3509	7/7	0.98	0.29	42,42,42,42	7
86	OHX	5	3619	7/7	0.98	0.26	38,38,38,38	7
87	MG	2	2187	1/1	0.99	0.13	87,87,87,87	0
86	OHX	1	3438	7/7	0.99	0.23	59,59,59,59	7
86	OHX	5	3458	7/7	0.99	0.30	42,42,42,42	7
86	OHX	5	3507	7/7	0.99	0.32	62,62,62,62	7
86	OHX	1	3434	7/7	0.99	0.19	68,68,68,68	7
86	OHX	6	1929	7/7	0.99	0.29	53,53,53,53	7
86	OHX	5	3447	7/7	0.99	0.21	60,60,60,60	7
86	OHX	5	3418	7/7	0.99	0.24	58,58,58,58	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	1	3441	7/7	0.99	0.21	52,52,52,52	7
86	OHX	1	3408	7/7	0.99	0.19	59,59,59,59	2
86	OHX	4	201	7/7	0.99	0.26	52,52,52,52	2
86	OHX	1	3409	7/7	0.99	0.15	58,58,58,58	1
86	OHX	6	1904	7/7	0.99	0.18	71,71,71,71	7
87	MG	6	2226	1/1	0.99	0.14	107,107,107,107	0
87	MG	1	4026	1/1	0.99	0.23	40,40,40,40	0
86	OHX	5	3424	7/7	0.99	0.19	70,70,70,70	0
87	MG	1	4441	1/1	0.99	0.14	43,43,43,43	1
86	OHX	2	1914	7/7	0.99	0.25	69,69,69,69	7
86	OHX	7	201	7/7	0.99	0.23	70,70,70,70	7
86	OHX	1	3488	7/7	0.99	0.25	49,49,49,49	7
86	OHX	1	3475	7/7	0.99	0.20	49,49,49,49	7
86	OHX	5	3416	7/7	0.99	0.25	46,46,46,46	7
86	OHX	5	3436	7/7	0.99	0.20	54,54,54,54	7
86	OHX	1	3416	7/7	0.99	0.20	69,69,69,69	0
87	MG	1	4117	1/1	0.99	0.34	59,59,59,59	0
87	MG	5	4522	1/1	0.99	0.21	35,35,35,35	1
86	OHX	5	3408	7/7	0.99	0.22	42,42,42,42	2
87	MG	1	4205	1/1	0.99	0.20	52,52,52,52	1
87	MG	5	4341	1/1	0.99	0.67	46,46,46,46	0
87	MG	1	4019	1/1	0.99	0.73	27,27,27,27	0
87	MG	1	4416	1/1	0.99	0.26	60,60,60,60	0
87	MG	5	4575	1/1	0.99	0.39	48,48,48,48	1
86	OHX	5	3457	7/7	0.99	0.23	67,67,67,67	7
87	MG	5	3997	1/1	0.99	0.32	31,31,31,31	0
87	MG	5	3930	1/1	0.99	0.54	34,34,34,34	0
86	OHX	1	3431	7/7	0.99	0.17	86,86,86,86	7
87	MG	1	4154	1/1	0.99	0.23	81,81,81,81	0
86	OHX	1	3513	7/7	0.99	0.23	49,49,49,49	7
86	OHX	5	3573	7/7	0.99	0.31	64,64,64,64	7
86	OHX	1	3439	7/7	0.99	0.24	69,69,69,69	7
87	MG	2	2121	1/1	0.99	0.28	73,73,73,73	0
86	OHX	5	3410	7/7	0.99	0.21	58,58,58,58	2
86	OHX	2	1951	7/7	0.99	0.22	87,87,87,87	7
87	MG	L4	402	1/1	0.99	0.30	43,43,43,43	0
87	MG	1	4165	1/1	0.99	0.28	54,54,54,54	0
86	OHX	7	204	7/7	0.99	0.18	43,43,43,43	7
87	MG	5	3960	1/1	0.99	0.45	37,37,37,37	0
86	OHX	5	3482	7/7	0.99	0.24	54,54,54,54	7
86	OHX	8	221	7/7	0.99	0.16	74,74,74,74	7
86	OHX	2	1919	7/7	0.99	0.20	78,78,78,78	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	2	1918	7/7	0.99	0.19	80,80,80,80	7
86	OHX	1	3479	7/7	0.99	0.26	55,55,55,55	7
86	OHX	2	1913	7/7	0.99	0.27	87,87,87,87	7
86	OHX	1	3426	7/7	0.99	0.19	71,71,71,71	7
87	MG	1	4431	1/1	0.99	0.45	42,42,42,42	1
87	MG	5	4288	1/1	0.99	0.23	39,39,39,39	1
86	OHX	1	3433	7/7	0.99	0.20	53,53,53,53	7
86	OHX	5	3448	7/7	0.99	0.26	46,46,46,46	7
86	OHX	6	2098	7/7	0.99	0.20	113,113,113,113	7
86	OHX	5	3471	7/7	0.99	0.15	76,76,76,76	7
86	OHX	5	3449	7/7	0.99	0.19	72,72,72,72	7
86	OHX	o7	502	7/7	0.99	0.24	64,64,64,64	7
87	MG	5	4307	1/1	0.99	0.23	41,41,41,41	1
86	OHX	5	3445	7/7	0.99	0.23	63,63,63,63	7
86	OHX	5	3460	7/7	0.99	0.19	68,68,68,68	7
87	MG	5	4357	1/1	0.99	0.33	36,36,36,36	1
86	OHX	5	3413	7/7	0.99	0.17	51,51,51,51	7
86	OHX	5	3411	7/7	0.99	0.22	50,50,50,50	7
86	OHX	5	3430	7/7	0.99	0.21	40,40,40,40	7
87	MG	1	4334	1/1	0.99	0.22	56,56,56,56	0
87	MG	1	4450	1/1	0.99	0.12	54,54,54,54	0
86	OHX	5	3422	7/7	0.99	0.20	55,55,55,55	7
86	OHX	4	204	7/7	0.99	0.20	57,57,57,57	7
87	MG	1	3985	1/1	0.99	0.63	28,28,28,28	0
86	OHX	7	205	7/7	0.99	0.22	68,68,68,68	7
86	OHX	2	1904	7/7	0.99	0.18	89,89,89,89	7
87	MG	5	4364	1/1	0.99	0.17	35,35,35,35	1
86	OHX	6	1903	7/7	0.99	0.23	63,63,63,63	3
87	MG	C1	201	1/1	0.99	1.02	69,69,69,69	0
86	OHX	5	3405	7/7	0.99	0.17	48,48,48,48	3
87	MG	L2	302	1/1	0.99	0.61	46,46,46,46	0
87	MG	1	3919	1/1	0.99	0.45	42,42,42,42	0
87	MG	5	4283	1/1	0.99	0.24	41,41,41,41	0
86	OHX	2	1907	7/7	0.99	0.15	93,93,93,93	7
87	MG	5	4497	1/1	0.99	0.22	41,41,41,41	1
86	OHX	1	3417	7/7	0.99	0.20	56,56,56,56	7
86	OHX	5	3414	7/7	0.99	0.23	43,43,43,43	7
87	MG	5	3944	1/1	0.99	0.47	32,32,32,32	0
87	MG	m6	204	1/1	0.99	0.30	40,40,40,40	0
86	OHX	1	3440	7/7	0.99	0.14	75,75,75,75	7
86	OHX	1	3562	7/7	0.99	0.15	71,71,71,71	7
86	OHX	1	3462	7/7	0.99	0.24	59,59,59,59	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	8	201	7/7	0.99	0.22	55,55,55,55	7
86	OHX	2	2035	7/7	0.99	0.16	95,95,95,95	7
87	MG	5	3837	1/1	0.99	0.66	33,33,33,33	0
87	MG	5	3858	1/1	0.99	0.23	58,58,58,58	0
86	OHX	1	3493	7/7	0.99	0.19	56,56,56,56	7
86	OHX	1	3430	7/7	0.99	0.21	55,55,55,55	7
86	OHX	5	3592	7/7	0.99	0.12	63,63,63,63	7
87	MG	1	4177	1/1	0.99	0.28	49,49,49,49	1
86	OHX	5	3443	7/7	0.99	0.15	82,82,82,82	7
86	OHX	5	3514	7/7	0.99	0.24	39,39,39,39	7
86	OHX	5	3412	7/7	0.99	0.19	64,64,64,64	7
86	OHX	1	3525	7/7	0.99	0.31	44,44,44,44	7
87	MG	5	3994	1/1	0.99	0.64	21,21,21,21	0
87	MG	5	3897	1/1	0.99	0.28	52,52,52,52	0
86	OHX	1	3423	7/7	0.99	0.23	62,62,62,62	7
87	MG	6	2136	1/1	0.99	0.27	54,54,54,54	0
87	MG	5	4511	1/1	0.99	0.87	52,52,52,52	1
86	OHX	1	3506	7/7	0.99	0.25	38,38,38,38	7
87	MG	13	410	1/1	0.99	0.58	31,31,31,31	1
86	OHX	1	3494	7/7	0.99	0.17	66,66,66,66	7
86	OHX	1	3588	7/7	0.99	0.22	47,47,47,47	7
86	OHX	1	3454	7/7	0.99	0.31	61,61,61,61	7
86	OHX	2	1905	7/7	0.99	0.26	71,71,71,71	7
86	OHX	6	1906	7/7	0.99	0.25	55,55,55,55	7
86	OHX	1	3463	7/7	0.99	0.24	74,74,74,74	7
87	MG	1	4362	1/1	0.99	0.27	42,42,42,42	0
87	MG	5	4108	1/1	0.99	0.23	49,49,49,49	0
86	OHX	5	3454	7/7	0.99	0.18	77,77,77,77	7
87	MG	5	3836	1/1	0.99	0.23	34,34,34,34	0
87	MG	6	2322	1/1	0.99	0.20	62,62,62,62	0
87	MG	1	4504	1/1	0.99	0.16	60,60,60,60	0
87	MG	5	4450	1/1	0.99	0.21	44,44,44,44	0
86	OHX	1	3797	7/7	0.99	0.18	85,85,85,85	7
87	MG	1	4463	1/1	0.99	0.25	51,51,51,51	0
86	OHX	1	3497	7/7	0.99	0.23	50,50,50,50	7
86	OHX	5	3576	7/7	0.99	0.16	56,56,56,56	7
87	MG	5	4435	1/1	0.99	0.26	50,50,50,50	0
86	OHX	1	3467	7/7	0.99	0.12	113,113,113,113	7
86	OHX	5	3439	7/7	0.99	0.22	57,57,57,57	7
87	MG	6	2148	1/1	0.99	0.57	45,45,45,45	0
86	OHX	5	3483	7/7	0.99	0.31	49,49,49,49	7
86	OHX	5	3444	7/7	0.99	0.27	70,70,70,70	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	3442	7/7	0.99	0.24	56,56,56,56	7
87	MG	5	4139	1/1	0.99	0.18	38,38,38,38	0
86	OHX	1	3469	7/7	0.99	0.20	75,75,75,75	7
86	OHX	5	3441	7/7	0.99	0.18	54,54,54,54	7
86	OHX	5	3446	7/7	0.99	0.22	56,56,56,56	7
87	MG	1	4427	1/1	0.99	0.21	55,55,55,55	1
86	OHX	1	3447	7/7	0.99	0.23	69,69,69,69	7
87	MG	6	2227	1/1	0.99	0.13	52,52,52,52	0
86	OHX	1	3448	7/7	0.99	0.19	59,59,59,59	7
88	ZN	q0	201	1/1	0.99	0.15	40,40,40,40	0
88	ZN	q3	501	1/1	0.99	0.15	64,64,64,64	0
87	MG	5	3928	1/1	0.99	0.29	38,38,38,38	0
86	OHX	6	1912	7/7	0.99	0.18	72,72,72,72	7
87	MG	5	4453	1/1	0.99	0.44	33,33,33,33	1
86	OHX	5	3495	7/7	0.99	0.20	47,47,47,47	7
86	OHX	5	3478	7/7	0.99	0.30	45,45,45,45	7
86	OHX	n3	201	7/7	0.99	0.23	55,55,55,55	7
87	MG	1	4316	1/1	0.99	0.53	51,51,51,51	0
87	MG	2	2236	1/1	0.99	0.25	64,64,64,64	0
86	OHX	5	3417	7/7	0.99	0.20	63,63,63,63	0
87	MG	1	4223	1/1	0.99	0.24	37,37,37,37	1
86	OHX	1	3411	7/7	0.99	0.18	64,64,64,64	0
86	OHX	5	3425	7/7	0.99	0.22	49,49,49,49	7
86	OHX	2	1923	7/7	0.99	0.21	80,80,80,80	7
87	MG	5	4105	1/1	0.99	0.28	38,38,38,38	0
86	OHX	1	3437	7/7	0.99	0.20	61,61,61,61	7
86	OHX	5	3468	7/7	0.99	0.22	63,63,63,63	7
87	MG	M6	202	1/1	0.99	0.78	41,41,41,41	1
88	ZN	D6	101	1/1	0.99	0.07	88,88,88,88	0
86	OHX	2	1920	7/7	0.99	0.21	84,84,84,84	7
86	OHX	1	3435	7/7	0.99	0.24	45,45,45,45	7
86	OHX	n9	101	7/7	0.99	0.22	59,59,59,59	7
86	OHX	5	3450	7/7	0.99	0.23	41,41,41,41	7
86	OHX	6	1902	7/7	0.99	0.17	77,77,77,77	2
86	OHX	2	1909	7/7	0.99	0.17	94,94,94,94	7
86	OHX	1	3424	7/7	0.99	0.22	49,49,49,49	7
86	OHX	5	3426	7/7	0.99	0.20	59,59,59,59	7
86	OHX	5	3435	7/7	0.99	0.21	50,50,50,50	7
86	OHX	1	3461	7/7	0.99	0.14	96,96,96,96	7
86	OHX	5	3757	7/7	0.99	0.17	75,75,75,75	7
86	OHX	5	3455	7/7	0.99	0.25	54,54,54,54	7
87	MG	M5	302	1/1	0.99	0.58	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	3595	7/7	0.99	0.26	46,46,46,46	7
86	OHX	6	1922	7/7	0.99	0.16	58,58,58,58	7
87	MG	O1	206	1/1	0.99	0.61	59,59,59,59	1
86	OHX	1	3514	7/7	0.99	0.21	50,50,50,50	7
86	OHX	6	1905	7/7	0.99	0.18	74,74,74,74	0
86	OHX	5	3469	7/7	0.99	0.23	49,49,49,49	7
86	OHX	1	3413	7/7	0.99	0.22	55,55,55,55	1
86	OHX	1	3456	7/7	0.99	0.18	85,85,85,85	7
88	ZN	D9	101	1/1	0.99	0.09	79,79,79,79	0
86	OHX	Q2	502	7/7	0.99	0.22	45,45,45,45	7
87	MG	5	4303	1/1	0.99	0.16	43,43,43,43	1
86	OHX	1	3445	7/7	0.99	0.26	51,51,51,51	7
86	OHX	1	3472	7/7	0.99	0.23	54,54,54,54	7
86	OHX	1	3482	7/7	0.99	0.20	59,59,59,59	7
87	MG	19	203	1/1	0.99	0.15	46,46,46,46	1
87	MG	5	4406	1/1	0.99	0.31	37,37,37,37	0
86	OHX	5	3530	7/7	0.99	0.14	94,94,94,94	7
86	OHX	2	1975	7/7	0.99	0.11	112,112,112,112	7
86	OHX	1	3406	7/7	0.99	0.20	58,58,58,58	2
87	MG	5	4441	1/1	0.99	0.14	33,33,33,33	0
86	OHX	1	3483	7/7	0.99	0.26	55,55,55,55	7
86	OHX	5	3429	7/7	0.99	0.21	49,49,49,49	7
86	OHX	2	1926	7/7	0.99	0.20	81,81,81,81	7
86	OHX	5	3419	7/7	0.99	0.25	55,55,55,55	7
86	OHX	5	3545	7/7	0.99	0.20	46,46,46,46	7
87	MG	7	216	1/1	0.99	0.33	53,53,53,53	0
87	MG	1	4008	1/1	0.99	0.16	52,52,52,52	0
86	OHX	1	3415	7/7	0.99	0.24	53,53,53,53	7
86	OHX	1	3471	7/7	0.99	0.27	43,43,43,43	7
86	OHX	s1	301	7/7	0.99	0.15	80,80,80,80	0
86	OHX	5	3451	7/7	0.99	0.28	43,43,43,43	7
86	OHX	2	1901	7/7	0.99	0.22	81,81,81,81	0
86	OHX	1	3427	7/7	0.99	0.24	65,65,65,65	7
86	OHX	5	3415	7/7	0.99	0.18	74,74,74,74	1
87	MG	5	4443	1/1	0.99	0.36	32,32,32,32	0
86	OHX	5	3567	7/7	0.99	0.27	39,39,39,39	7
86	OHX	7	206	7/7	0.99	0.21	67,67,67,67	7
86	OHX	6	1920	7/7	0.99	0.16	114,114,114,114	7
86	OHX	5	3421	7/7	0.99	0.21	45,45,45,45	7
87	MG	1	4059	1/1	0.99	0.27	38,38,38,38	0
86	OHX	6	1936	7/7	0.99	0.22	57,57,57,57	7
86	OHX	M0	301	7/7	0.99	0.39	49,49,49,49	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	6	1917	7/7	0.99	0.20	55,55,55,55	7
86	OHX	1	3464	7/7	0.99	0.33	50,50,50,50	7
87	MG	6	2134	1/1	0.99	0.43	42,42,42,42	0
86	OHX	1	3496	7/7	0.99	0.27	45,45,45,45	7
87	MG	5	4353	1/1	0.99	0.33	39,39,39,39	1
87	MG	1	4299	1/1	0.99	0.22	44,44,44,44	1
86	OHX	5	3473	7/7	0.99	0.16	61,61,61,61	7
86	OHX	1	3425	7/7	0.99	0.22	71,71,71,71	7
86	OHX	N9	101	7/7	0.99	0.21	58,58,58,58	7
86	OHX	1	3444	7/7	0.99	0.25	61,61,61,61	7
87	MG	m5	503	1/1	0.99	0.22	48,48,48,48	0
86	OHX	5	3467	7/7	0.99	0.22	66,66,66,66	7
86	OHX	1	3578	7/7	0.99	0.21	40,40,40,40	7
86	OHX	1	3432	7/7	0.99	0.17	64,64,64,64	7
86	OHX	1	3420	7/7	0.99	0.18	59,59,59,59	7
86	OHX	2	1906	7/7	0.99	0.17	82,82,82,82	7
86	OHX	8	202	7/7	0.99	0.24	49,49,49,49	2
86	OHX	1	3407	7/7	0.99	0.24	48,48,48,48	2
87	MG	5	4447	1/1	0.99	0.31	34,34,34,34	1
86	OHX	2	1903	7/7	0.99	0.18	90,90,90,90	0
86	OHX	1	3465	7/7	0.99	0.22	62,62,62,62	7
87	MG	5	4321	1/1	0.99	0.22	66,66,66,66	1
86	OHX	1	3575	7/7	0.99	0.24	47,47,47,47	7
87	MG	5	3862	1/1	0.99	0.53	35,35,35,35	0
86	OHX	1	3428	7/7	0.99	0.16	79,79,79,79	0
87	MG	1	3982	1/1	0.99	0.36	31,31,31,31	0
86	OHX	1	3542	7/7	0.99	0.26	49,49,49,49	7
86	OHX	1	3478	7/7	0.99	0.19	58,58,58,58	7
86	OHX	5	3428	7/7	0.99	0.24	64,64,64,64	0
87	MG	5	4490	1/1	0.99	0.18	46,46,46,46	0
86	OHX	1	3455	7/7	0.99	0.24	70,70,70,70	7
86	OHX	1	3453	7/7	0.99	0.15	74,74,74,74	7
88	ZN	O7	101	1/1	0.99	0.14	47,47,47,47	0
86	OHX	6	1916	7/7	0.99	0.18	65,65,65,65	7
86	OHX	5	3727	7/7	0.99	0.24	53,53,53,53	7
87	MG	5	4451	1/1	0.99	0.23	39,39,39,39	1
86	OHX	6	1923	7/7	0.99	0.16	71,71,71,71	7
86	OHX	1	3800	7/7	0.99	0.23	41,41,41,41	7
86	OHX	1	3442	7/7	0.99	0.21	55,55,55,55	7
87	MG	5	4266	1/1	0.99	0.24	42,42,42,42	1
86	OHX	4	202	7/7	0.99	0.21	55,55,55,55	7
88	ZN	Q3	501	1/1	0.99	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
87	MG	5	4531	1/1	0.99	0.29	39,39,39,39	0
86	OHX	5	3433	7/7	0.99	0.22	47,47,47,47	7
87	MG	5	4295	1/1	0.99	0.41	43,43,43,43	0
86	OHX	5	3420	7/7	0.99	0.22	56,56,56,56	7
86	OHX	5	3476	7/7	0.99	0.24	46,46,46,46	7
86	OHX	o3	201	7/7	0.99	0.31	51,51,51,51	7
86	OHX	6	1908	7/7	0.99	0.21	71,71,71,71	7
86	OHX	1	3668	7/7	0.99	0.21	50,50,50,50	7
87	MG	2	2207	1/1	0.99	0.25	61,61,61,61	0
86	OHX	1	3518	7/7	0.99	0.24	41,41,41,41	7
86	OHX	6	1926	7/7	0.99	0.20	55,55,55,55	7
86	OHX	1	3418	7/7	0.99	0.28	49,49,49,49	7
87	MG	5	4000	1/1	0.99	0.32	34,34,34,34	0
86	OHX	5	3407	7/7	0.99	0.25	44,44,44,44	2
86	OHX	5	3510	7/7	0.99	0.25	48,48,48,48	7
87	MG	5	3849	1/1	0.99	0.44	34,34,34,34	0
87	MG	5	4148	1/1	0.99	0.28	32,32,32,32	1
87	MG	1	4045	1/1	0.99	0.20	35,35,35,35	0
87	MG	1	4056	1/1	0.99	0.54	44,44,44,44	0
86	OHX	1	3522	7/7	0.99	0.27	40,40,40,40	7
86	OHX	1	3443	7/7	0.99	0.26	61,61,61,61	7
86	OHX	4	206	7/7	0.99	0.16	88,88,88,88	7
87	MG	1	3858	1/1	0.99	0.21	51,51,51,51	0
86	OHX	1	3414	7/7	0.99	0.15	67,67,67,67	0
87	MG	1	3909	1/1	0.99	0.32	43,43,43,43	0
86	OHX	C8	201	7/7	0.99	0.14	94,94,94,94	7
86	OHX	5	3432	7/7	0.99	0.25	59,59,59,59	7
86	OHX	5	3472	7/7	0.99	0.25	53,53,53,53	7
86	OHX	1	3498	7/7	0.99	0.24	62,62,62,62	7
86	OHX	5	3423	7/7	0.99	0.16	56,56,56,56	7
86	OHX	q1	101	7/7	0.99	0.24	46,46,46,46	7
86	OHX	5	3464	7/7	0.99	0.19	45,45,45,45	7
87	MG	1	3889	1/1	0.99	0.35	37,37,37,37	0
86	OHX	5	3466	7/7	0.99	0.16	63,63,63,63	7
86	OHX	5	3440	7/7	0.99	0.25	51,51,51,51	7
87	MG	1	3977	1/1	0.99	0.44	41,41,41,41	0
87	MG	5	4216	1/1	0.99	0.17	44,44,44,44	0
87	MG	1	4024	1/1	0.99	0.33	37,37,37,37	0
87	MG	1	4366	1/1	0.99	0.41	42,42,42,42	1
86	OHX	1	3421	7/7	0.99	0.24	48,48,48,48	7
86	OHX	5	3503	7/7	0.99	0.20	104,104,104,104	7
87	MG	4	239	1/1	0.99	0.60	40,40,40,40	1

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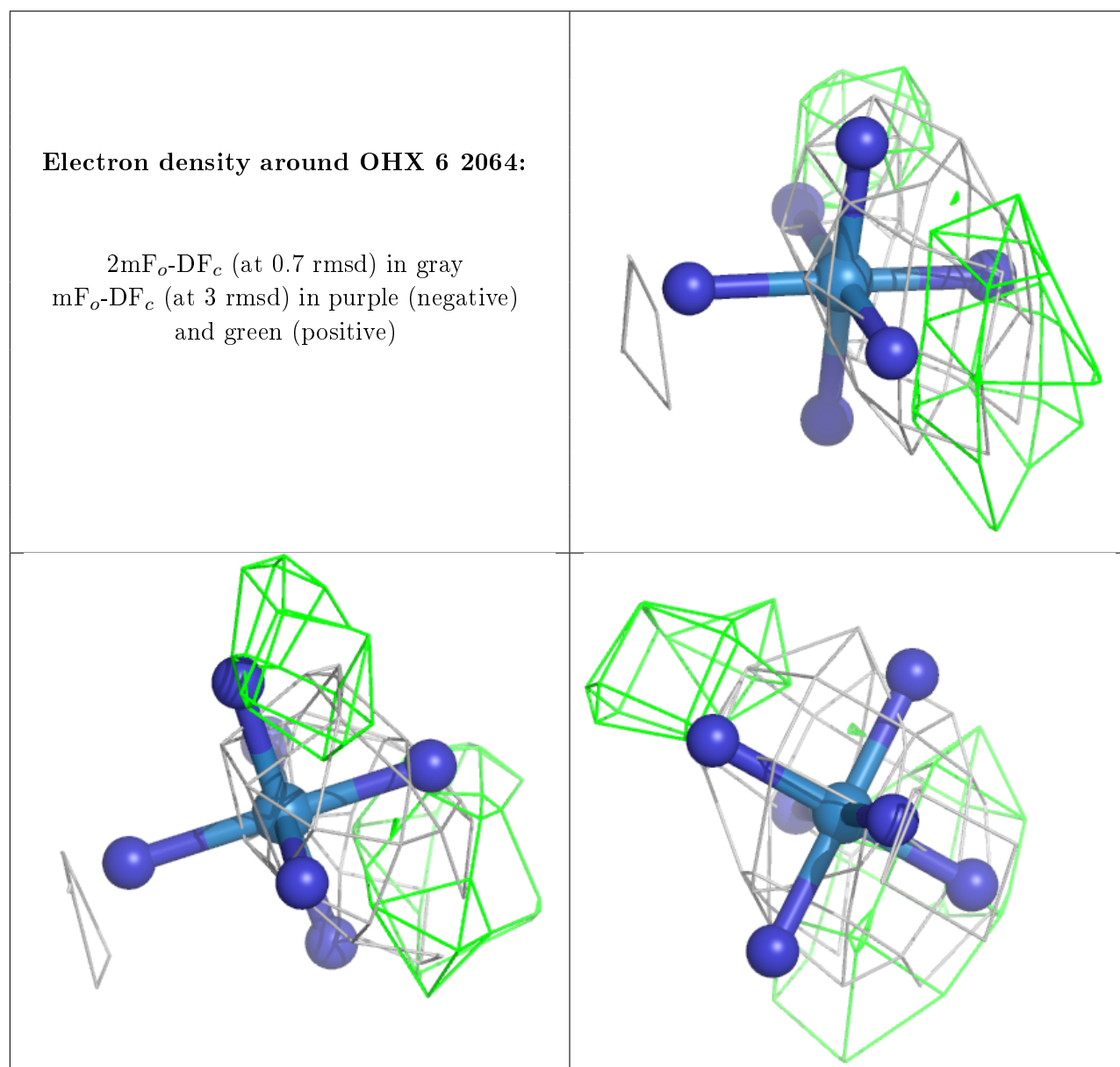
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3512	7/7	0.99	0.15	74,74,74,74	7
86	OHX	q2	502	7/7	0.99	0.20	51,51,51,51	7
86	OHX	6	1924	7/7	0.99	0.20	54,54,54,54	7
87	MG	1	4387	1/1	0.99	0.35	51,51,51,51	1
86	OHX	6	1915	7/7	0.99	0.27	63,63,63,63	7
86	OHX	n1	201	7/7	0.99	0.19	48,48,48,48	7
86	OHX	1	3450	7/7	0.99	0.17	46,46,46,46	7
86	OHX	6	1932	7/7	0.99	0.23	47,47,47,47	7
87	MG	6	2190	1/1	0.99	0.16	44,44,44,44	0
87	MG	1	4319	1/1	0.99	0.19	59,59,59,59	0
86	OHX	1	3500	7/7	0.99	0.19	41,41,41,41	7
86	OHX	1	3477	7/7	0.99	0.23	62,62,62,62	7
86	OHX	1	3419	7/7	0.99	0.19	66,66,66,66	7
86	OHX	6	2039	7/7	0.99	0.22	46,46,46,46	7
87	MG	M7	209	1/1	0.99	0.35	42,42,42,42	0
87	MG	S1	301	1/1	1.00	0.13	105,105,105,105	0
86	OHX	5	3409	7/7	1.00	0.23	57,57,57,57	1
87	MG	5	4302	1/1	1.00	0.19	40,40,40,40	0
87	MG	5	4469	1/1	1.00	0.25	38,38,38,38	0
87	MG	1	4407	1/1	1.00	0.11	47,47,47,47	1
86	OHX	1	3489	7/7	1.00	0.16	89,89,89,89	7
86	OHX	1	3412	7/7	1.00	0.20	47,47,47,47	7
86	OHX	5	3406	7/7	1.00	0.19	48,48,48,48	0
86	OHX	6	1901	7/7	1.00	0.21	62,62,62,62	0
86	OHX	1	3405	7/7	1.00	0.21	48,48,48,48	0
87	MG	5	3922	1/1	1.00	0.43	33,33,33,33	0
87	MG	5	4460	1/1	1.00	0.30	62,62,62,62	0
87	MG	M3	202	1/1	1.00	0.53	49,49,49,49	1
87	MG	1	4420	1/1	1.00	0.22	56,56,56,56	0
88	ZN	Q0	201	1/1	1.00	0.13	53,53,53,53	0
87	MG	1	4310	1/1	1.00	0.13	45,45,45,45	1
87	MG	6	2236	1/1	1.00	0.18	54,54,54,54	0
86	OHX	5	3427	7/7	1.00	0.17	66,66,66,66	7
86	OHX	1	3429	7/7	1.00	0.22	62,62,62,62	7
88	ZN	o7	501	1/1	1.00	0.14	53,53,53,53	0
87	MG	1	4381	1/1	1.00	0.19	60,60,60,60	0
88	ZN	d9	101	1/1	1.00	0.10	81,81,81,81	0
86	OHX	1	3410	7/7	1.00	0.18	53,53,53,53	3
87	MG	5	4557	1/1	1.00	0.17	50,50,50,50	0
87	MG	1	4189	1/1	1.00	0.21	46,46,46,46	0
87	MG	5	4234	1/1	1.00	0.22	44,44,44,44	0
86	OHX	6	1910	7/7	1.00	0.19	60,60,60,60	7

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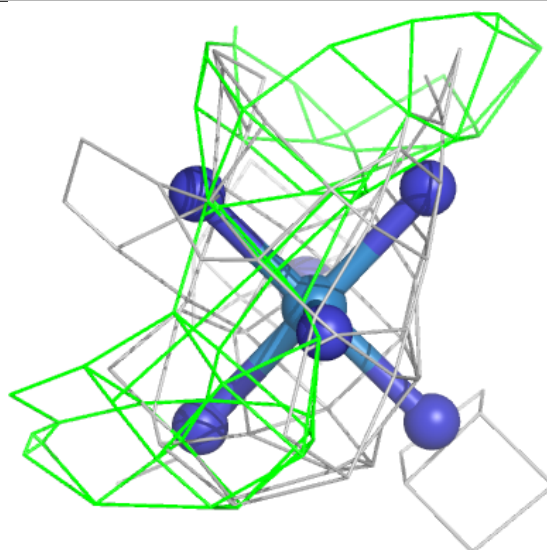
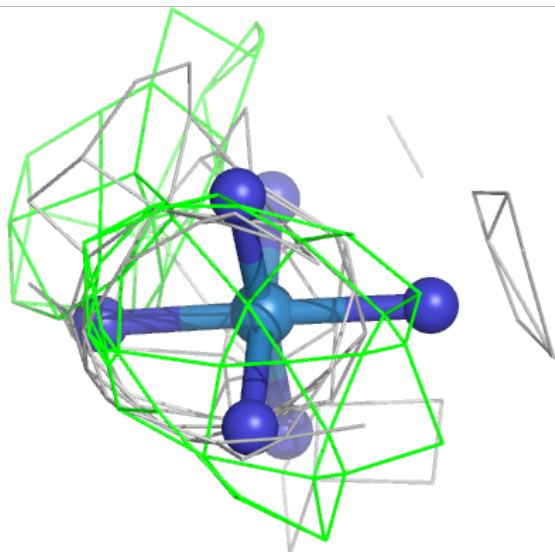
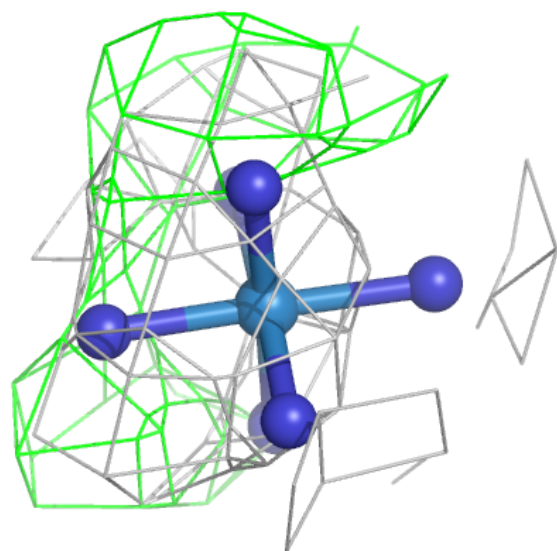
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	2	1902	7/7	1.00	0.18	86,86,86,86	0

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.



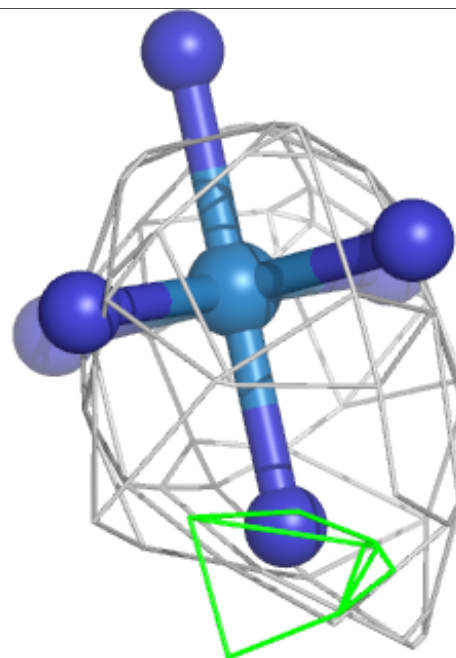
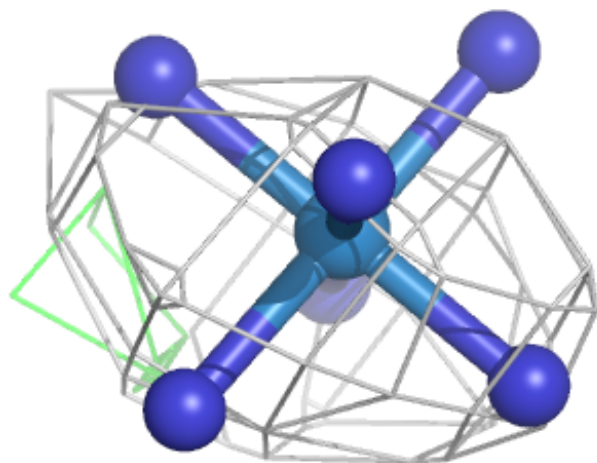
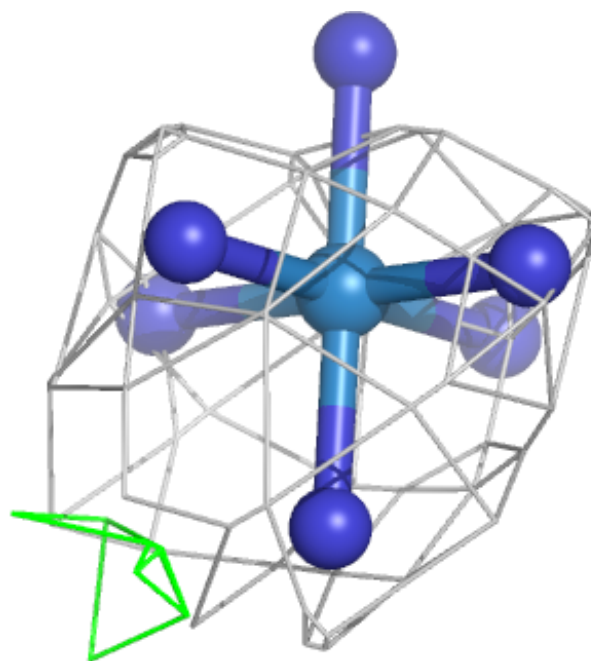
Electron density around OHX 5 3720:

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



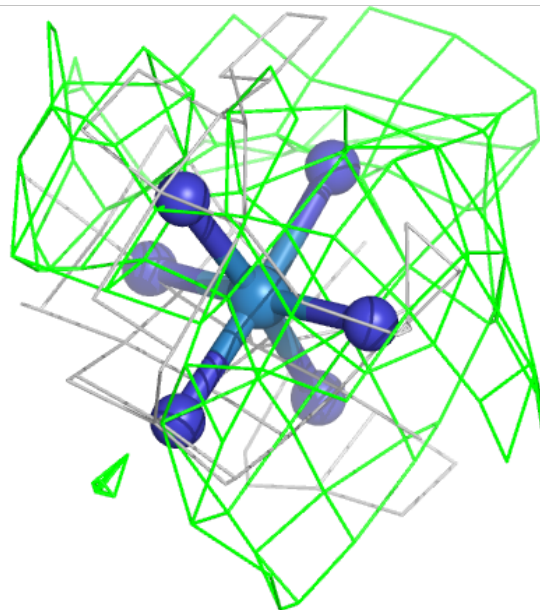
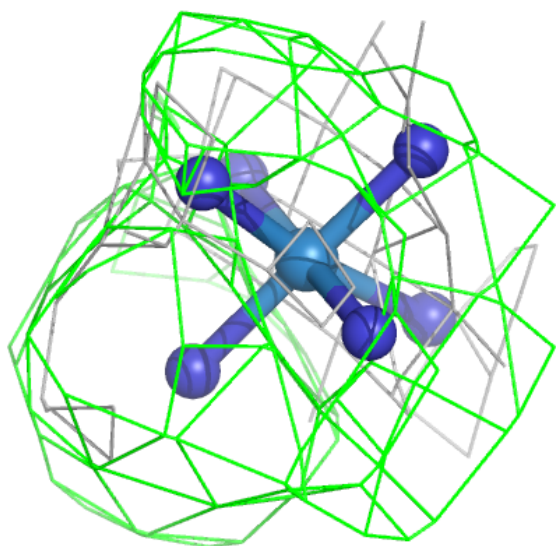
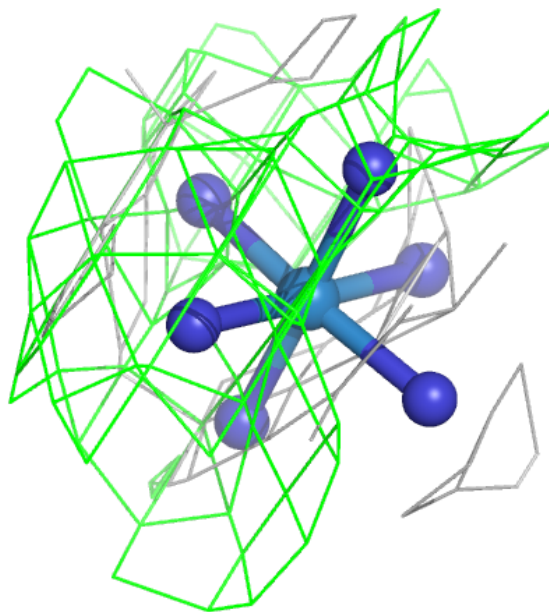
Electron density around OHX 2 2060:

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



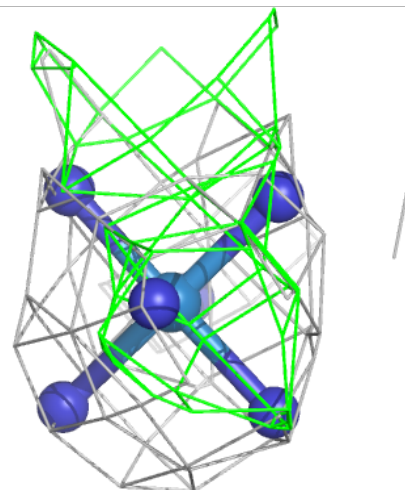
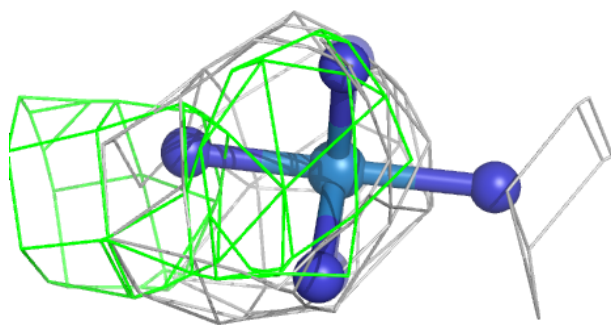
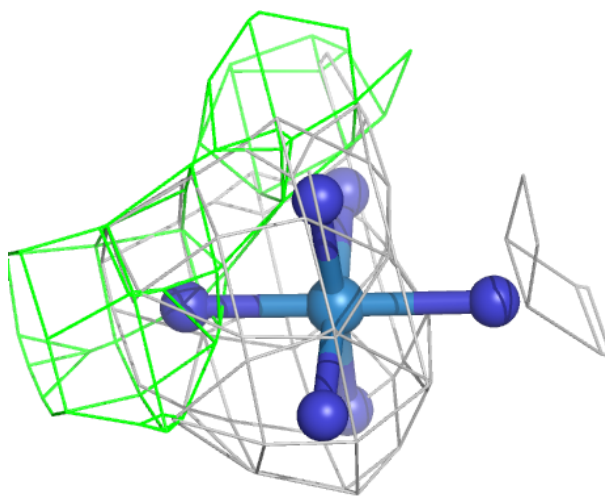
Electron density around OHX 5 3806:

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



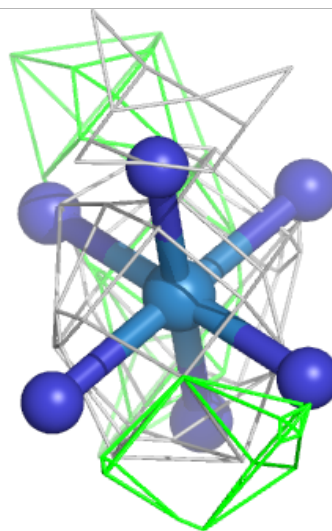
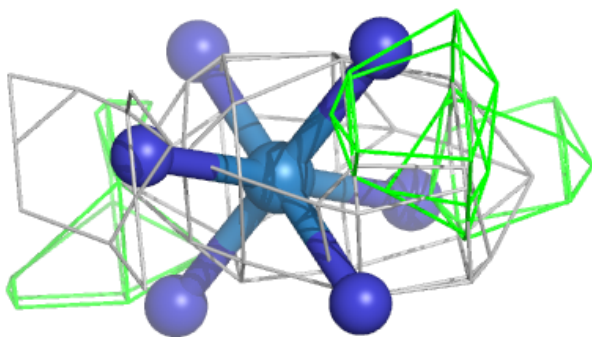
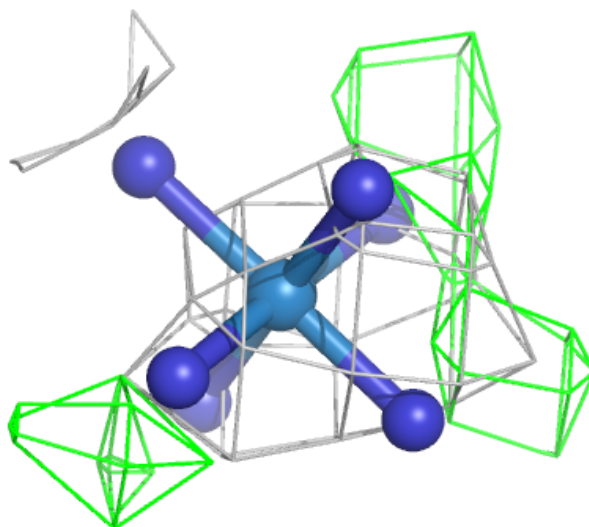
Electron density around OHX 5 3762:

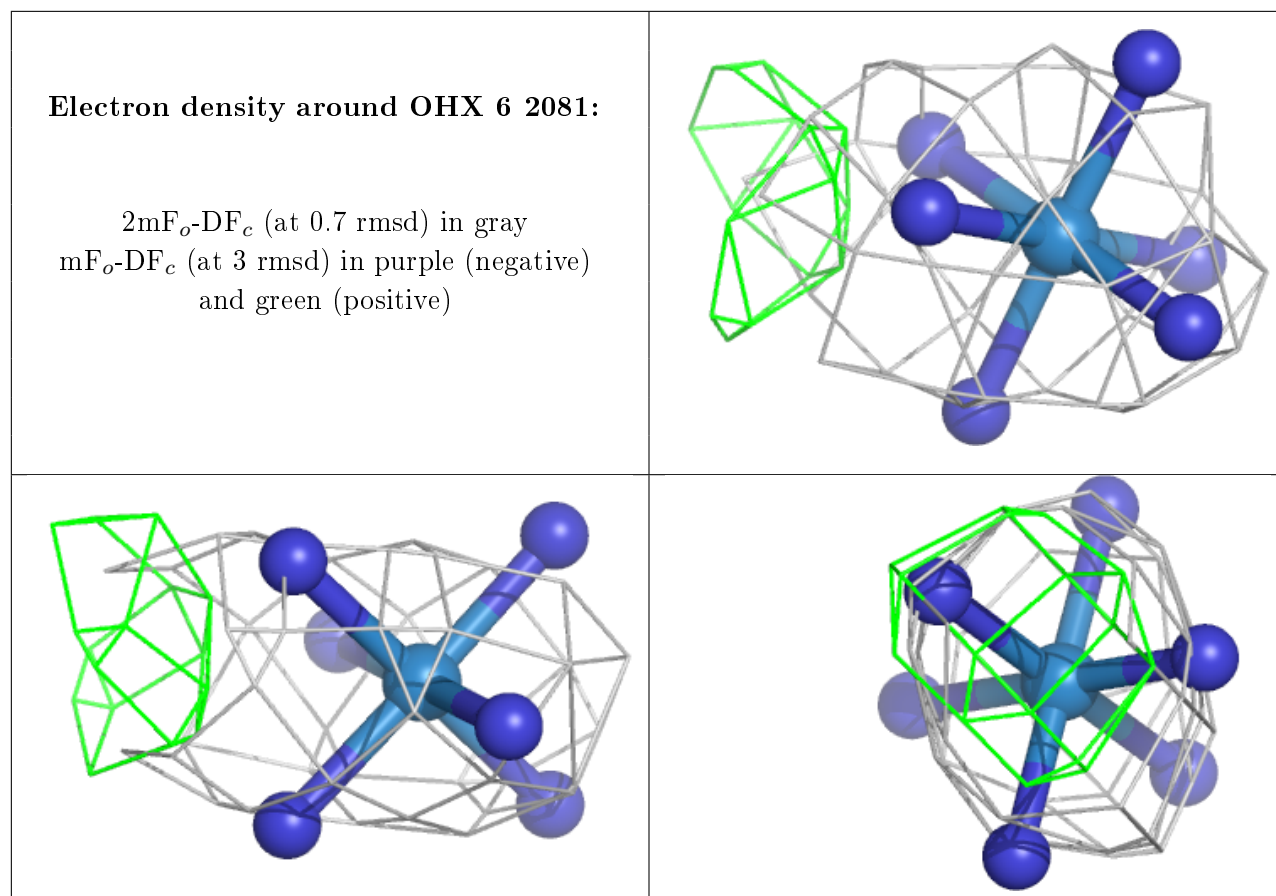
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

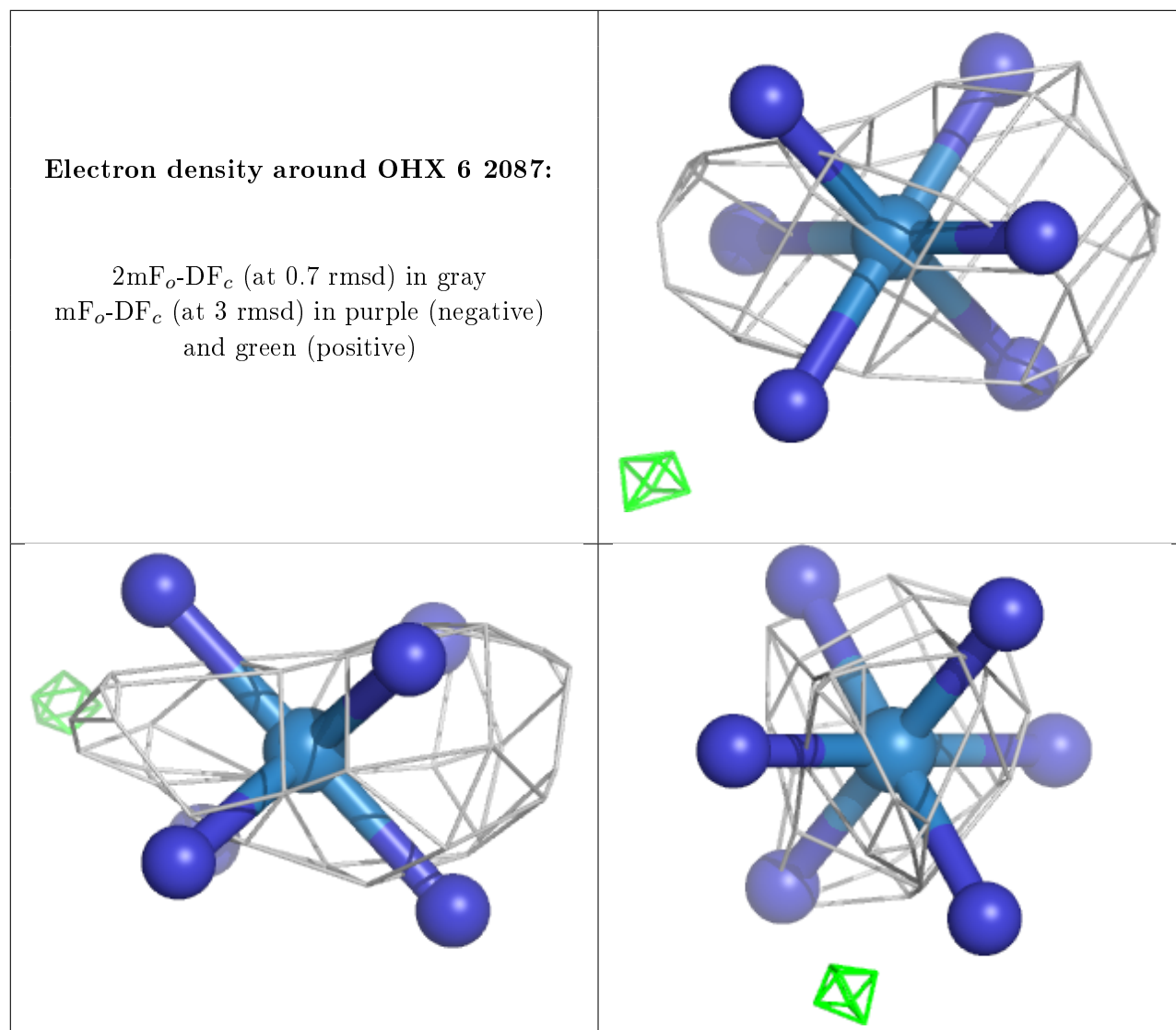


Electron density around OHX 5 3768:

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

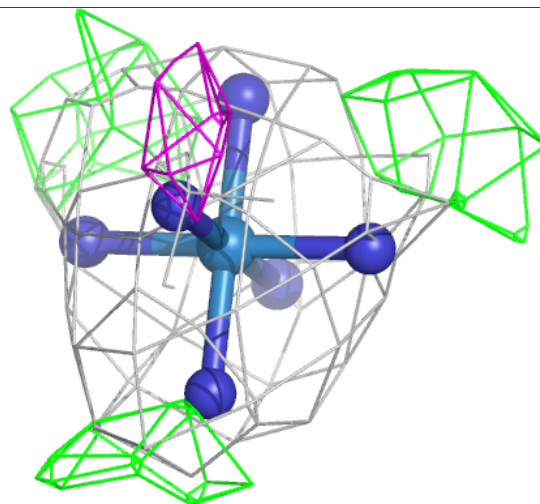
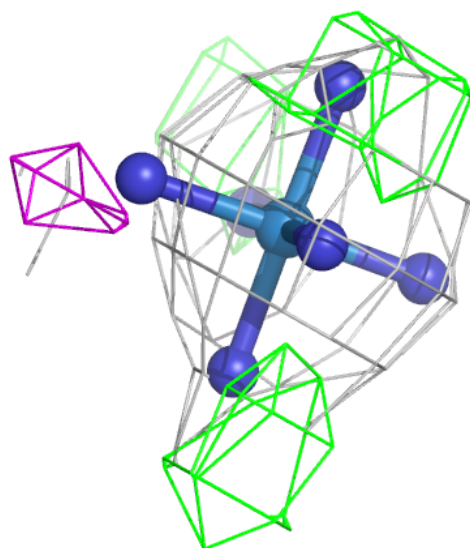
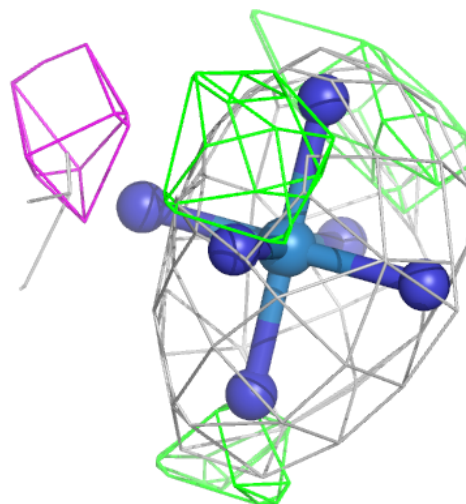






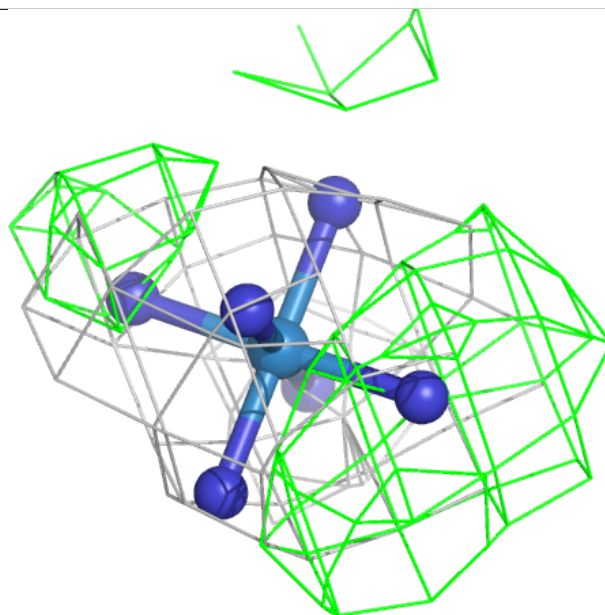
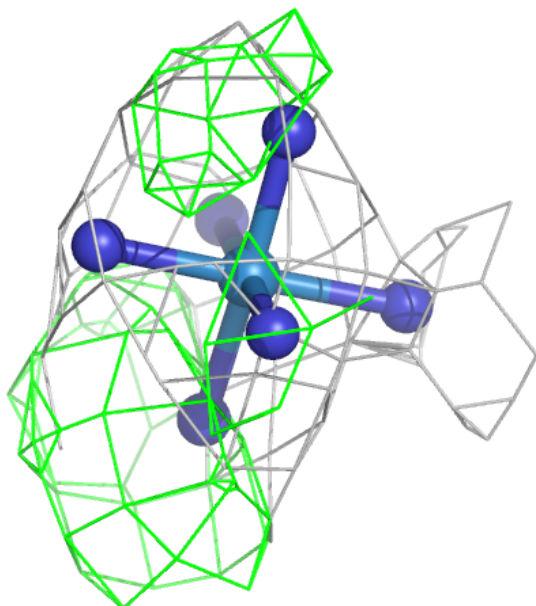
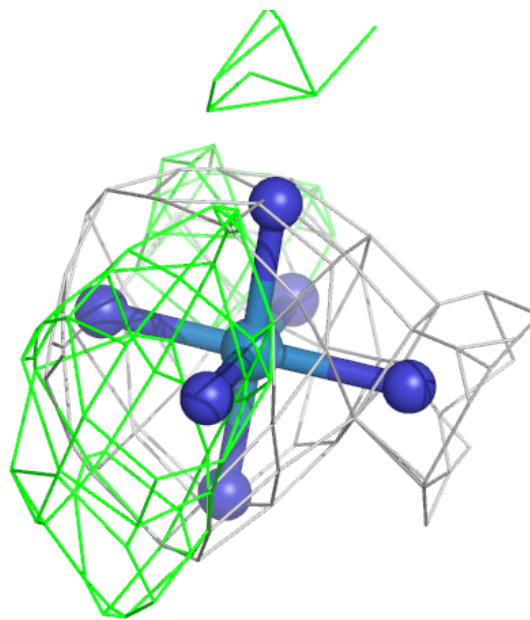
Electron density around OHX 5 3783:

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



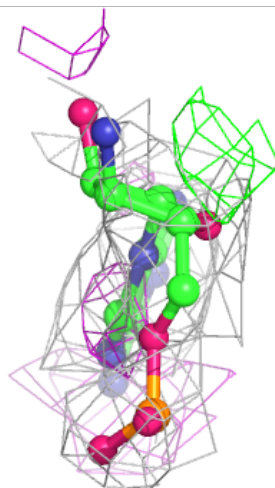
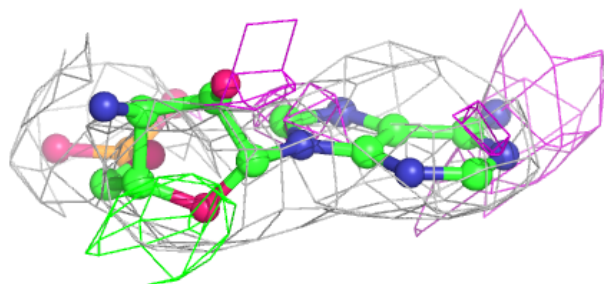
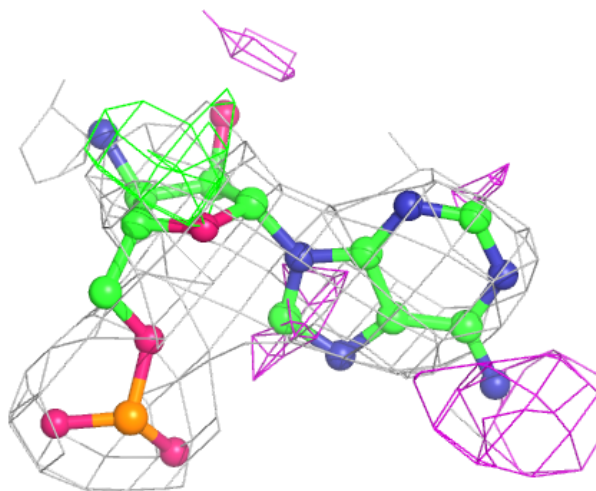
Electron density around OHX 5 3739:

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



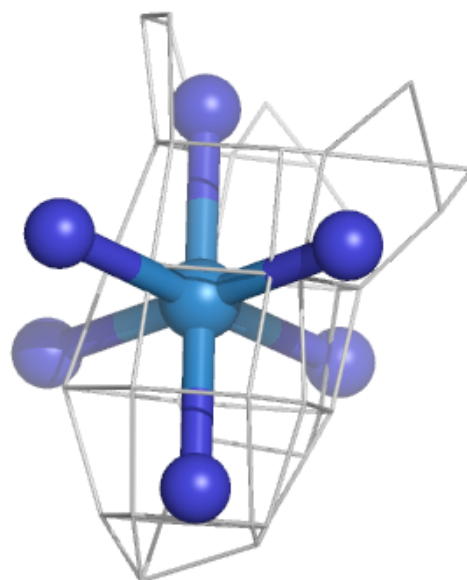
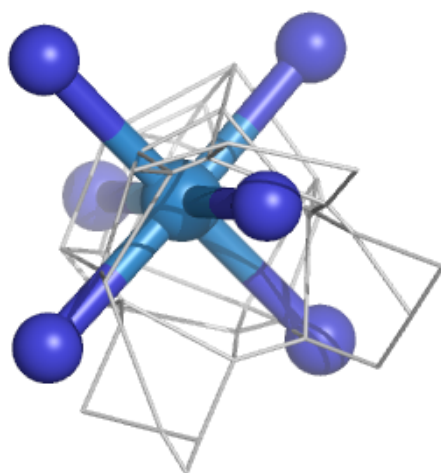
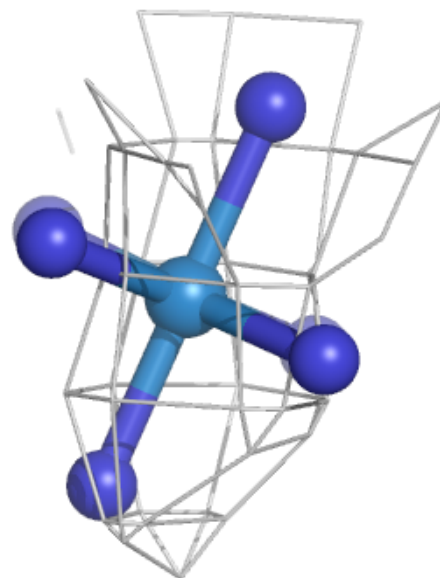
Electron density around 8AN 1 3403:

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



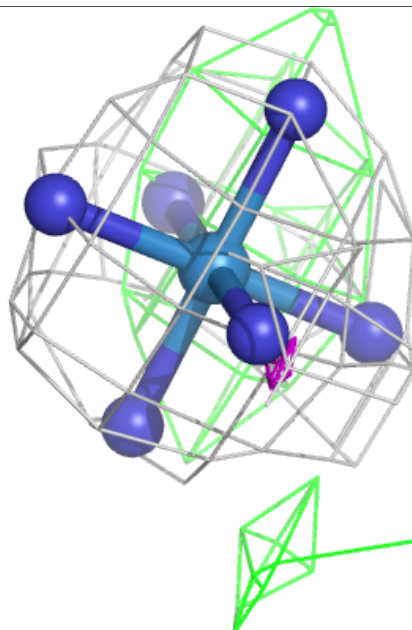
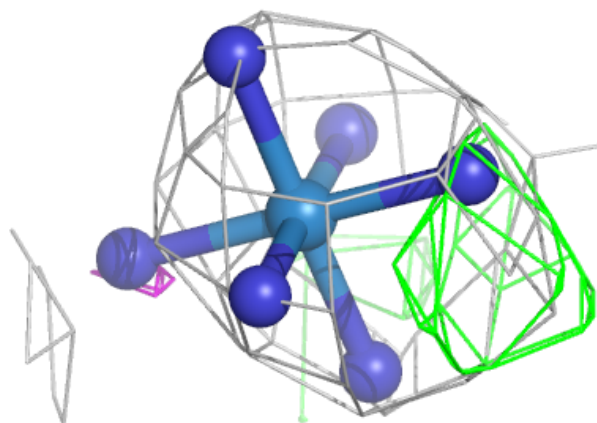
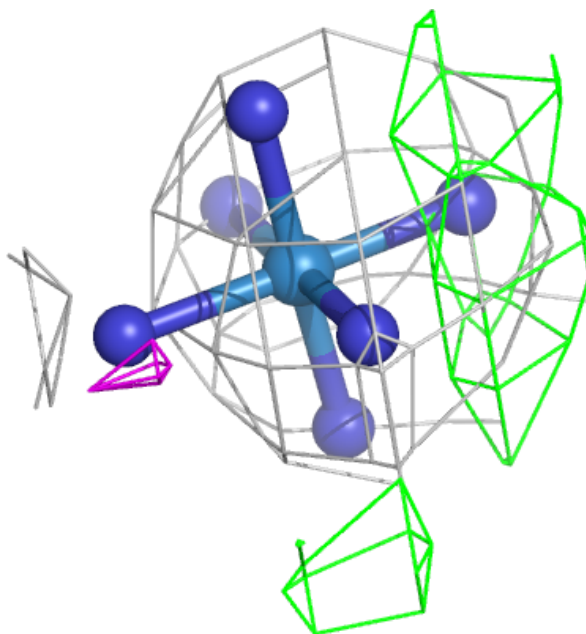
Electron density around OHX 2 2030:

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



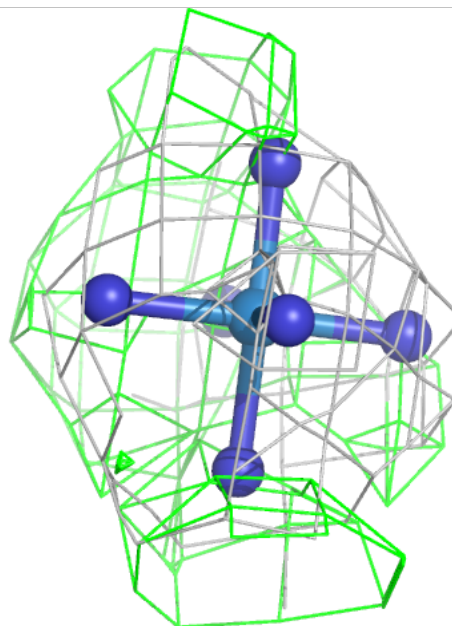
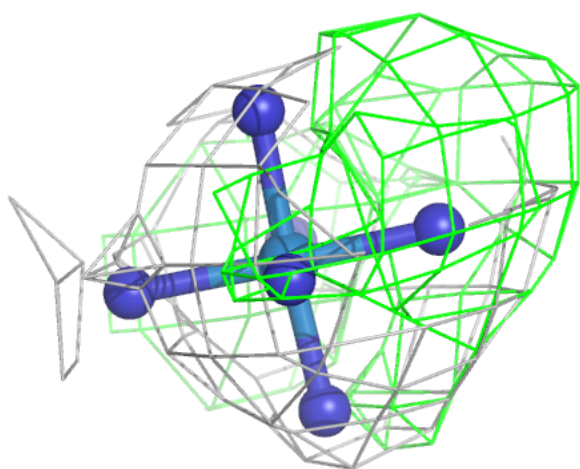
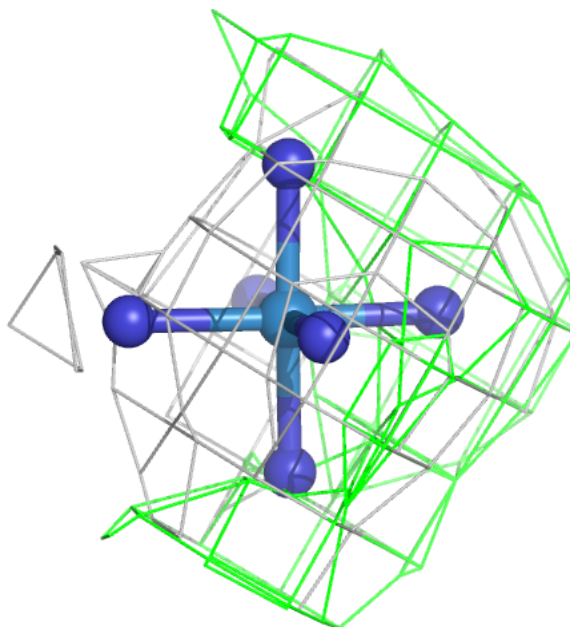
Electron density around OHX 8 218:

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



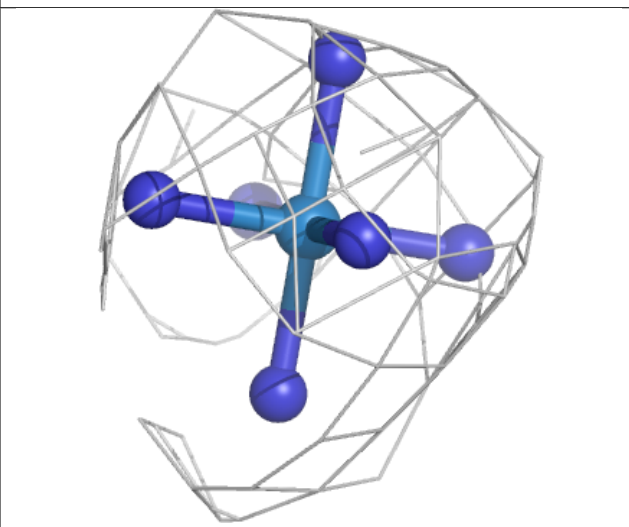
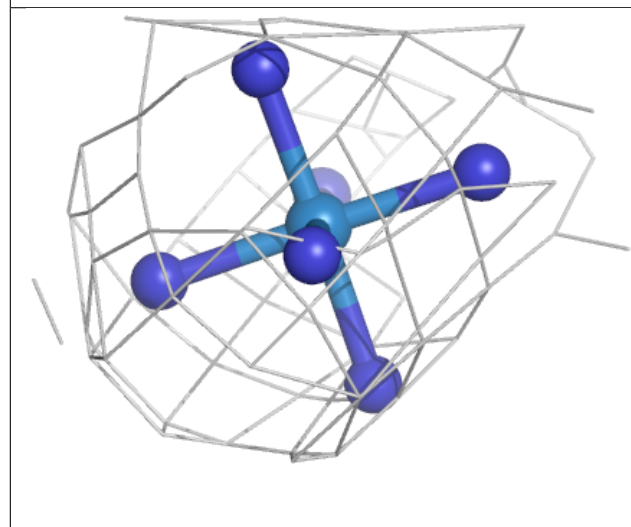
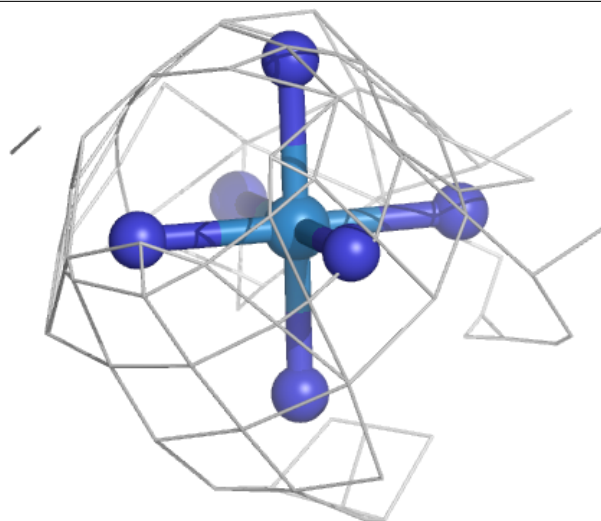
Electron density around OHX 5 3755:

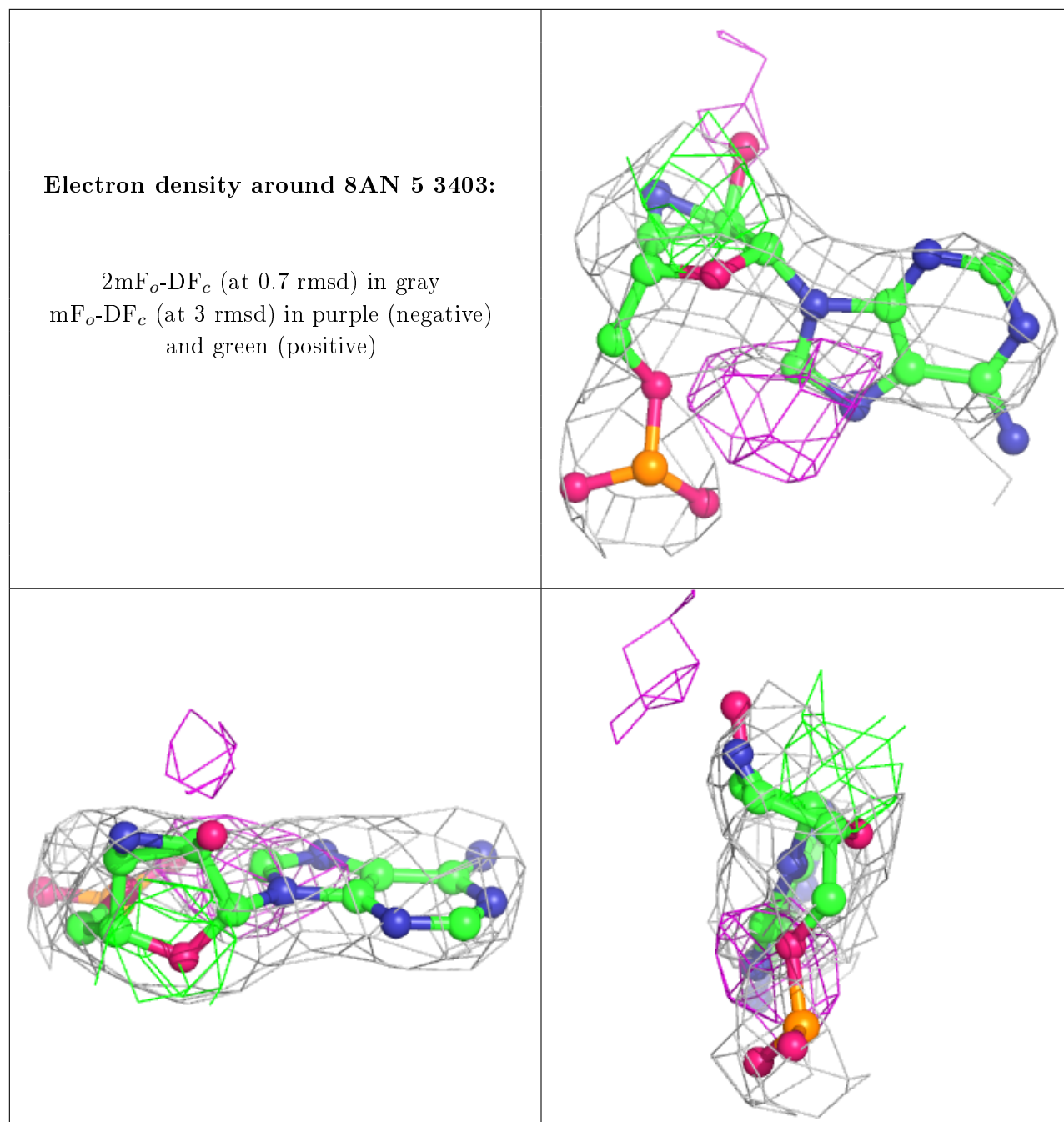
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OHX 6 2052:

$2mF_o-DF_c$ (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.