



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:33 am GMT

PDB ID : 5I4L
Title : Crystal structure of Amicoumacin A bound to the yeast 80S ribosome
Authors : Prokhorova, I.V.; Yusupova, G.; Yusupov, M.
Deposited on : 2016-02-12
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

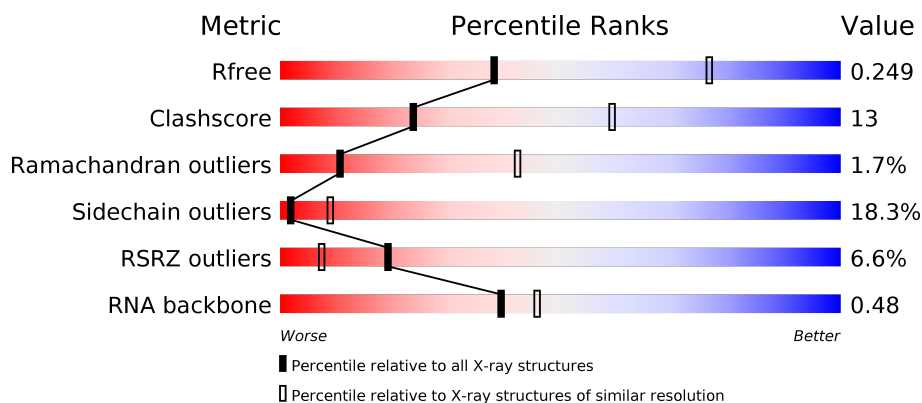
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1800	<div> <div>4%</div> <div>42%</div> <div>40%</div> <div>15%</div> <div>..</div> </div>
1	6	1800	<div> <div>4%</div> <div>46%</div> <div>40%</div> <div>13%</div> <div>.</div> </div>
2	S0	206	<div> <div>13%</div> <div>37%</div> <div>51%</div> <div>12%</div> </div>
2	s0	206	<div> <div>5%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	S1	216	
3	s1	216	
4	S2	217	
4	s2	217	
5	S3	223	
5	s3	223	
6	S4	260	
6	s4	260	
7	S5	206	
7	s5	206	
8	S6	226	
8	s6	226	
9	S7	186	
9	s7	186	
10	S8	200	
10	s8	200	
11	S9	185	
11	s9	185	
12	C0	98	
12	c0	98	
13	C1	156	
13	c1	156	
14	C2	124	
14	c2	124	
15	C3	150	

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Mol	Chain	Length	Quality of chain
15	c3	150	% 80% 19% .
16	C4	128	22% 43% 48% 8% ..
16	c4	128	8% 81% 18% .
17	C5	142	12% 35% 42% 11% 13%
17	c5	142	22% 77% 17% . 5%
18	C6	142	30% 35% 46% 15% ..
18	c6	142	9% 84% 15% .
19	C7	136	10% 32% 45% 10% . 12%
19	c7	136	% 70% 15% . 14%
20	C8	145	18% 39% 46% 13% .
20	c8	145	6% 81% 19% .
21	C9	143	16% 42% 48% 10%
21	c9	143	5% 86% 13% .
22	D0	110	22% 33% 52% 12% ..
22	d0	110	41% 75% 22% .
23	D1	87	7% 37% 51% 13%
23	d1	87	3% 79% 21%
24	D2	129	38% 50% 9% .
24	d2	129	88% 10% .
25	D3	144	% 42% 47% 9% .
25	d3	144	% 85% 15%
26	D4	134	11% 46% 41% 11% .
26	d4	134	8% 88% 10% ..
27	D5	70	31% 21% 63% 14% .
27	d5	70	21% 83% 16% .

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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	63	
30	d8	63	
31	D9	53	
31	d9	53	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	176	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	252	
39	l2	252	
40	L3	386	
40	l3	386	

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Mol	Chain	Length	Quality of chain
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	176	
43	l6	176	
44	L7	223	
44	l7	223	
45	L8	233	
46	L9	191	
46	l9	191	
47	M0	221	
47	m0	221	
48	M1	169	
48	m1	169	
49	M3	194	
49	m3	194	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	197	
52	m6	197	
53	M7	183	
53	m7	183	

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Mol	Chain	Length	Quality of chain
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	100	
58	n2	100	
59	N3	136	
59	n3	136	
60	N4	98	
61	N5	121	
61	n5	121	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	100	
66	o0	100	


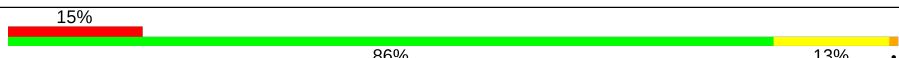
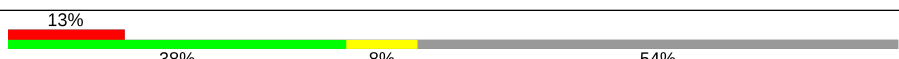
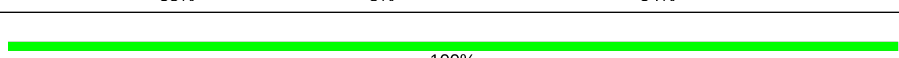
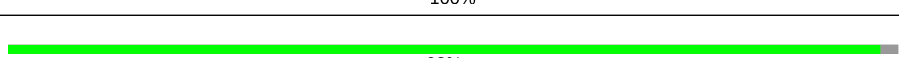
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Mol	Chain	Length	Quality of chain
67	O1	109	
67	o1	109	
68	O2	127	
68	o2	127	
69	O3	106	
69	o3	106	
70	O4	112	
70	o4	112	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	

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Mol	Chain	Length	Quality of chain
79	q3	91	
80	sM	159	
81	l8	231	
82	m2	155	
83	n4	135	
84	p0	312	
85	p1	47	
85	p2	47	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	3416	-	-	-	X
86	OHX	1	3431	-	-	-	X
86	OHX	1	3432	-	-	-	X
86	OHX	1	3447	-	-	-	X
86	OHX	1	3448	-	-	-	X
86	OHX	1	3454	-	-	-	X
86	OHX	1	3475	-	-	-	X
86	OHX	1	3476	-	-	-	X
86	OHX	1	3490	-	-	-	X
86	OHX	1	3491	-	-	-	X
86	OHX	1	3496	-	-	X	-
86	OHX	1	3498	-	-	-	X
86	OHX	1	3501	-	-	-	X
86	OHX	1	3509	-	-	X	-
86	OHX	1	3513	-	-	-	X
86	OHX	1	3514	-	-	-	X
86	OHX	1	3517	-	-	-	X
86	OHX	1	3518	-	-	-	X
86	OHX	1	3521	-	-	-	X
86	OHX	1	3522	-	-	-	X
86	OHX	1	3528	-	-	-	X
86	OHX	1	3533	-	-	-	X
86	OHX	1	3538	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	3540	-	-	-	X
86	OHX	1	3541	-	-	-	X
86	OHX	1	3545	-	-	-	X
86	OHX	1	3547	-	-	-	X
86	OHX	1	3556	-	-	-	X
86	OHX	1	3561	-	-	-	X
86	OHX	1	3564	-	-	-	X
86	OHX	1	3589	-	-	-	X
86	OHX	1	3594	-	-	-	X
86	OHX	1	3596	-	-	-	X
86	OHX	1	3598	-	-	-	X
86	OHX	1	3603	-	-	-	X
86	OHX	1	3606	-	-	-	X
86	OHX	1	3608	-	-	-	X
86	OHX	1	3616	-	-	-	X
86	OHX	1	3620	-	-	-	X
86	OHX	1	3624	-	-	-	X
86	OHX	1	3636	-	-	-	X
86	OHX	1	3641	-	-	-	X
86	OHX	1	3642	-	-	-	X
86	OHX	1	3645	-	-	-	X
86	OHX	1	3646	-	-	-	X
86	OHX	1	3651	-	-	-	X
86	OHX	1	3652	-	-	-	X
86	OHX	1	3657	-	-	-	X
86	OHX	1	3658	-	-	-	X
86	OHX	1	3669	-	-	-	X
86	OHX	1	3676	-	-	-	X
86	OHX	1	3677	-	-	-	X
86	OHX	1	3680	-	-	-	X
86	OHX	1	3681	-	-	X	-
86	OHX	1	3686	-	-	-	X
86	OHX	1	3689	-	-	-	X
86	OHX	1	3691	-	-	-	X
86	OHX	1	3693	-	-	-	X
86	OHX	1	3696	-	-	-	X
86	OHX	1	3701	-	-	X	-
86	OHX	1	3705	-	-	-	X
86	OHX	1	3712	-	-	X	-
86	OHX	2	1922	-	-	-	X
86	OHX	2	1928	-	-	-	X
86	OHX	2	1943	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	2	1960	-	-	-	X
86	OHX	2	1968	-	-	-	X
86	OHX	2	1977	-	-	-	X
86	OHX	2	1997	-	-	-	X
86	OHX	2	1998	-	-	-	X
86	OHX	2	1999	-	-	-	X
86	OHX	2	2005	-	-	-	X
86	OHX	2	2011	-	-	-	X
86	OHX	2	2021	-	-	-	X
86	OHX	2	2026	-	-	-	X
86	OHX	3	202	-	-	-	X
86	OHX	3	203	-	-	-	X
86	OHX	4	211	-	-	-	X
86	OHX	4	214	-	-	-	X
86	OHX	4	217	-	-	-	X
86	OHX	5	3416	-	-	-	X
86	OHX	5	3431	-	-	-	X
86	OHX	5	3437	-	-	-	X
86	OHX	5	3440	-	-	-	X
86	OHX	5	3459	-	-	-	X
86	OHX	5	3464	-	-	-	X
86	OHX	5	3465	-	-	-	X
86	OHX	5	3479	-	-	X	-
86	OHX	5	3480	-	-	-	X
86	OHX	5	3490	-	-	-	X
86	OHX	5	3491	-	-	-	X
86	OHX	5	3494	-	-	-	X
86	OHX	5	3496	-	-	-	X
86	OHX	5	3504	-	-	X	-
86	OHX	5	3511	-	-	-	X
86	OHX	5	3513	-	-	X	-
86	OHX	5	3519	-	-	-	X
86	OHX	5	3523	-	-	-	X
86	OHX	5	3525	-	-	-	X
86	OHX	5	3528	-	-	-	X
86	OHX	5	3529	-	-	-	X
86	OHX	5	3531	-	-	-	X
86	OHX	5	3535	-	-	X	X
86	OHX	5	3536	-	-	-	X
86	OHX	5	3538	-	-	-	X
86	OHX	5	3550	-	-	-	X
86	OHX	5	3558	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	3563	-	-	-	X
86	OHX	5	3564	-	-	-	X
86	OHX	5	3566	-	-	-	X
86	OHX	5	3580	-	-	-	X
86	OHX	5	3586	-	-	-	X
86	OHX	5	3593	-	-	-	X
86	OHX	5	3594	-	-	-	X
86	OHX	5	3600	-	-	-	X
86	OHX	5	3601	-	-	-	X
86	OHX	5	3603	-	-	-	X
86	OHX	5	3608	-	-	-	X
86	OHX	5	3612	-	-	-	X
86	OHX	5	3613	-	-	-	X
86	OHX	5	3618	-	-	-	X
86	OHX	5	3634	-	-	-	X
86	OHX	5	3640	-	-	-	X
86	OHX	5	3641	-	-	-	X
86	OHX	5	3643	-	-	-	X
86	OHX	5	3645	-	-	-	X
86	OHX	5	3650	-	-	-	X
86	OHX	5	3651	-	-	-	X
86	OHX	5	3653	-	-	-	X
86	OHX	5	3658	-	-	-	X
86	OHX	5	3660	-	-	-	X
86	OHX	5	3661	-	-	-	X
86	OHX	5	3665	-	-	-	X
86	OHX	5	3666	-	-	-	X
86	OHX	5	3679	-	-	-	X
86	OHX	5	3681	-	-	-	X
86	OHX	5	3689	-	-	-	X
86	OHX	5	3690	-	-	-	X
86	OHX	5	3691	-	-	X	-
86	OHX	5	3692	-	-	-	X
86	OHX	5	3693	-	-	X	-
86	OHX	5	3698	-	-	-	X
86	OHX	5	3700	-	-	-	X
86	OHX	5	3703	-	-	-	X
86	OHX	5	3706	-	-	-	X
86	OHX	5	3709	-	-	-	X
86	OHX	5	3713	-	-	-	X
86	OHX	5	3715	-	-	-	X
86	OHX	5	3716	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	3719	-	-	-	X
86	OHX	5	3720	-	-	-	X
86	OHX	5	3721	-	-	-	X
86	OHX	6	1922	-	-	X	-
86	OHX	6	1930	-	-	-	X
86	OHX	6	1932	-	-	-	X
86	OHX	6	1946	-	-	-	X
86	OHX	6	1950	-	-	-	X
86	OHX	6	1956	-	-	X	-
86	OHX	6	1958	-	-	-	X
86	OHX	6	1959	-	-	-	X
86	OHX	6	1961	-	-	-	X
86	OHX	6	1966	-	-	-	X
86	OHX	6	1972	-	-	-	X
86	OHX	6	1976	-	-	-	X
86	OHX	6	1986	-	-	-	X
86	OHX	6	1988	-	-	-	X
86	OHX	6	1989	-	-	-	X
86	OHX	6	1999	-	-	-	X
86	OHX	6	2001	-	-	-	X
86	OHX	6	2020	-	-	-	X
86	OHX	6	2023	-	-	-	X
86	OHX	6	2024	-	-	-	X
86	OHX	6	2025	-	-	-	X
86	OHX	6	2034	-	-	-	X
86	OHX	7	203	-	-	-	X
86	OHX	7	205	-	-	-	X
86	OHX	7	208	-	-	-	X
86	OHX	7	211	-	-	-	X
86	OHX	8	209	-	-	-	X
86	OHX	8	210	-	-	-	X
86	OHX	8	212	-	-	-	X
86	OHX	8	213	-	-	-	X
86	OHX	8	214	-	-	-	X
86	OHX	C5	201	-	-	X	-
86	OHX	N9	101	-	-	-	X
86	OHX	O1	201	-	-	X	-
86	OHX	Q2	502	-	-	X	-
86	OHX	S9	201	-	-	X	-
86	OHX	s4	301	-	-	-	X
87	MG	1	3713	-	-	-	X
87	MG	1	3717	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	3718	-	-	-	X
87	MG	1	3719	-	-	-	X
87	MG	1	3721	-	-	-	X
87	MG	1	3725	-	-	-	X
87	MG	1	3726	-	-	-	X
87	MG	1	3727	-	-	-	X
87	MG	1	3731	-	-	-	X
87	MG	1	3742	-	-	-	X
87	MG	1	3746	-	-	-	X
87	MG	1	3750	-	-	-	X
87	MG	1	3753	-	-	-	X
87	MG	1	3762	-	-	-	X
87	MG	1	3769	-	-	-	X
87	MG	1	3778	-	-	-	X
87	MG	1	3779	-	-	-	X
87	MG	1	3780	-	-	-	X
87	MG	1	3786	-	-	-	X
87	MG	1	3789	-	-	-	X
87	MG	1	3790	-	-	-	X
87	MG	1	3793	-	-	-	X
87	MG	1	3796	-	-	-	X
87	MG	1	3800	-	-	-	X
87	MG	1	3802	-	-	-	X
87	MG	1	3805	-	-	-	X
87	MG	1	3808	-	-	-	X
87	MG	1	3809	-	-	-	X
87	MG	1	3811	-	-	-	X
87	MG	1	3813	-	-	-	X
87	MG	1	3817	-	-	-	X
87	MG	1	3818	-	-	-	X
87	MG	1	3819	-	-	-	X
87	MG	1	3821	-	-	-	X
87	MG	1	3823	-	-	-	X
87	MG	1	3827	-	-	-	X
87	MG	1	3828	-	-	-	X
87	MG	1	3829	-	-	-	X
87	MG	1	3835	-	-	-	X
87	MG	1	3839	-	-	-	X
87	MG	1	3840	-	-	-	X
87	MG	1	3841	-	-	-	X
87	MG	1	3842	-	-	-	X
87	MG	1	3848	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	3849	-	-	-	X
87	MG	1	3850	-	-	-	X
87	MG	1	3852	-	-	-	X
87	MG	1	3856	-	-	-	X
87	MG	1	3857	-	-	-	X
87	MG	1	3860	-	-	-	X
87	MG	1	3863	-	-	-	X
87	MG	1	3866	-	-	-	X
87	MG	1	3867	-	-	-	X
87	MG	1	3868	-	-	-	X
87	MG	1	3870	-	-	-	X
87	MG	1	3871	-	-	-	X
87	MG	1	3872	-	-	-	X
87	MG	1	3873	-	-	-	X
87	MG	1	3875	-	-	-	X
87	MG	1	3881	-	-	-	X
87	MG	1	3882	-	-	-	X
87	MG	1	3883	-	-	-	X
87	MG	1	3885	-	-	-	X
87	MG	1	3886	-	-	-	X
87	MG	1	3888	-	-	-	X
87	MG	1	3890	-	-	-	X
87	MG	1	3892	-	-	-	X
87	MG	1	3893	-	-	-	X
87	MG	1	3895	-	-	-	X
87	MG	1	3897	-	-	-	X
87	MG	1	3898	-	-	-	X
87	MG	1	3904	-	-	-	X
87	MG	1	3908	-	-	-	X
87	MG	1	3916	-	-	-	X
87	MG	1	3934	-	-	-	X
87	MG	1	3936	-	-	-	X
87	MG	1	3946	-	-	-	X
87	MG	1	3955	-	-	-	X
87	MG	1	3964	-	-	-	X
87	MG	1	3967	-	-	-	X
87	MG	1	3971	-	-	-	X
87	MG	1	3972	-	-	-	X
87	MG	1	3975	-	-	-	X
87	MG	1	3985	-	-	-	X
87	MG	1	3991	-	-	-	X
87	MG	1	3995	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	3999	-	-	-	X
87	MG	1	4001	-	-	-	X
87	MG	1	4013	-	-	-	X
87	MG	1	4017	-	-	-	X
87	MG	1	4019	-	-	-	X
87	MG	1	4020	-	-	-	X
87	MG	1	4026	-	-	-	X
87	MG	1	4029	-	-	-	X
87	MG	1	4057	-	-	-	X
87	MG	1	4058	-	-	-	X
87	MG	1	4060	-	-	-	X
87	MG	1	4063	-	-	-	X
87	MG	2	2033	-	-	-	X
87	MG	2	2034	-	-	-	X
87	MG	2	2038	-	-	-	X
87	MG	2	2039	-	-	-	X
87	MG	2	2042	-	-	-	X
87	MG	2	2046	-	-	-	X
87	MG	2	2049	-	-	-	X
87	MG	2	2051	-	-	-	X
87	MG	2	2057	-	-	-	X
87	MG	2	2060	-	-	-	X
87	MG	2	2062	-	-	-	X
87	MG	2	2063	-	-	-	X
87	MG	2	2065	-	-	-	X
87	MG	2	2069	-	-	-	X
87	MG	2	2071	-	-	-	X
87	MG	2	2074	-	-	-	X
87	MG	2	2077	-	-	-	X
87	MG	2	2080	-	-	-	X
87	MG	2	2082	-	-	-	X
87	MG	2	2087	-	-	-	X
87	MG	2	2090	-	-	-	X
87	MG	2	2091	-	-	-	X
87	MG	2	2092	-	-	-	X
87	MG	2	2095	-	-	-	X
87	MG	2	2099	-	-	-	X
87	MG	2	2117	-	-	-	X
87	MG	4	221	-	-	-	X
87	MG	4	224	-	-	-	X
87	MG	5	3729	-	-	-	X
87	MG	5	3730	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	3731	-	-	-	X
87	MG	5	3735	-	-	-	X
87	MG	5	3739	-	-	-	X
87	MG	5	3742	-	-	-	X
87	MG	5	3744	-	-	-	X
87	MG	5	3746	-	-	-	X
87	MG	5	3747	-	-	-	X
87	MG	5	3749	-	-	-	X
87	MG	5	3763	-	-	-	X
87	MG	5	3765	-	-	-	X
87	MG	5	3767	-	-	-	X
87	MG	5	3778	-	-	-	X
87	MG	5	3782	-	-	-	X
87	MG	5	3783	-	-	-	X
87	MG	5	3784	-	-	-	X
87	MG	5	3786	-	-	-	X
87	MG	5	3791	-	-	-	X
87	MG	5	3797	-	-	-	X
87	MG	5	3807	-	-	-	X
87	MG	5	3811	-	-	-	X
87	MG	5	3813	-	-	-	X
87	MG	5	3817	-	-	-	X
87	MG	5	3819	-	-	-	X
87	MG	5	3822	-	-	-	X
87	MG	5	3826	-	-	-	X
87	MG	5	3827	-	-	-	X
87	MG	5	3828	-	-	-	X
87	MG	5	3829	-	-	-	X
87	MG	5	3832	-	-	-	X
87	MG	5	3833	-	-	-	X
87	MG	5	3834	-	-	-	X
87	MG	5	3840	-	-	-	X
87	MG	5	3842	-	-	-	X
87	MG	5	3844	-	-	-	X
87	MG	5	3846	-	-	-	X
87	MG	5	3849	-	-	-	X
87	MG	5	3852	-	-	-	X
87	MG	5	3858	-	-	-	X
87	MG	5	3862	-	-	-	X
87	MG	5	3864	-	-	-	X
87	MG	5	3865	-	-	-	X
87	MG	5	3871	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	3874	-	-	-	X
87	MG	5	3875	-	-	-	X
87	MG	5	3876	-	-	-	X
87	MG	5	3881	-	-	-	X
87	MG	5	3882	-	-	-	X
87	MG	5	3884	-	-	-	X
87	MG	5	3885	-	-	-	X
87	MG	5	3886	-	-	-	X
87	MG	5	3887	-	-	-	X
87	MG	5	3890	-	-	-	X
87	MG	5	3891	-	-	-	X
87	MG	5	3897	-	-	-	X
87	MG	5	3901	-	-	-	X
87	MG	5	3902	-	-	-	X
87	MG	5	3904	-	-	-	X
87	MG	5	3905	-	-	-	X
87	MG	5	3906	-	-	-	X
87	MG	5	3908	-	-	-	X
87	MG	5	3909	-	-	-	X
87	MG	5	3910	-	-	-	X
87	MG	5	3911	-	-	-	X
87	MG	5	3912	-	-	-	X
87	MG	5	3913	-	-	-	X
87	MG	5	3914	-	-	-	X
87	MG	5	3920	-	-	-	X
87	MG	5	3922	-	-	-	X
87	MG	5	3924	-	-	-	X
87	MG	5	3925	-	-	-	X
87	MG	5	3928	-	-	-	X
87	MG	5	3936	-	-	-	X
87	MG	5	3938	-	-	-	X
87	MG	5	3944	-	-	-	X
87	MG	5	3945	-	-	-	X
87	MG	5	3952	-	-	-	X
87	MG	5	3955	-	-	-	X
87	MG	5	3962	-	-	-	X
87	MG	5	3967	-	-	-	X
87	MG	5	3969	-	-	-	X
87	MG	5	3981	-	-	-	X
87	MG	5	3984	-	-	-	X
87	MG	5	3994	-	-	-	X
87	MG	5	4006	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	4011	-	-	-	X
87	MG	5	4012	-	-	-	X
87	MG	5	4018	-	-	-	X
87	MG	5	4038	-	-	-	X
87	MG	5	4054	-	-	-	X
87	MG	5	4055	-	-	-	X
87	MG	5	4076	-	-	-	X
87	MG	5	4078	-	-	-	X
87	MG	5	4099	-	-	-	X
87	MG	5	4101	-	-	-	X
87	MG	5	4104	-	-	-	X
87	MG	5	4106	-	-	-	X
87	MG	5	4107	-	-	-	X
87	MG	6	2038	-	-	-	X
87	MG	6	2041	-	-	-	X
87	MG	6	2042	-	-	-	X
87	MG	6	2044	-	-	-	X
87	MG	6	2048	-	-	-	X
87	MG	6	2049	-	-	-	X
87	MG	6	2052	-	-	-	X
87	MG	6	2055	-	-	-	X
87	MG	6	2061	-	-	-	X
87	MG	6	2062	-	-	-	X
87	MG	6	2068	-	-	-	X
87	MG	6	2069	-	-	-	X
87	MG	6	2072	-	-	-	X
87	MG	6	2074	-	-	-	X
87	MG	6	2079	-	-	-	X
87	MG	6	2080	-	-	-	X
87	MG	6	2082	-	-	-	X
87	MG	6	2085	-	-	-	X
87	MG	6	2089	-	-	-	X
87	MG	6	2096	-	-	-	X
87	MG	6	2101	-	-	-	X
87	MG	6	2105	-	-	-	X
87	MG	6	2122	-	-	-	X
87	MG	8	218	-	-	-	X
87	MG	8	222	-	-	-	X
87	MG	L2	301	-	-	-	X
87	MG	L2	302	-	-	-	X
87	MG	L7	302	-	-	-	X
87	MG	M7	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	N3	201	-	-	-	X
87	MG	N8	202	-	-	-	X
87	MG	O2	201	-	-	-	X
87	MG	c1	201	-	-	-	X
87	MG	l2	303	-	-	-	X
87	MG	m5	301	-	-	-	X
87	MG	m7	201	-	-	-	X
87	MG	n3	203	-	-	-	X
87	MG	n8	201	-	-	-	X
88	ZN	D7	101	-	-	-	X
89	UAM	6	2134	-	-	-	X

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 410475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2438	1541	417	472	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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			
74	o8	77	Total	C	N	O	0	0	0
			608	388	114	106			

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
80	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			

- Molecule 81 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 82 is a protein called 60S ribosomal protein L12.

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

- Molecule 83 is a protein called 60S ribosomal protein L24-A.

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

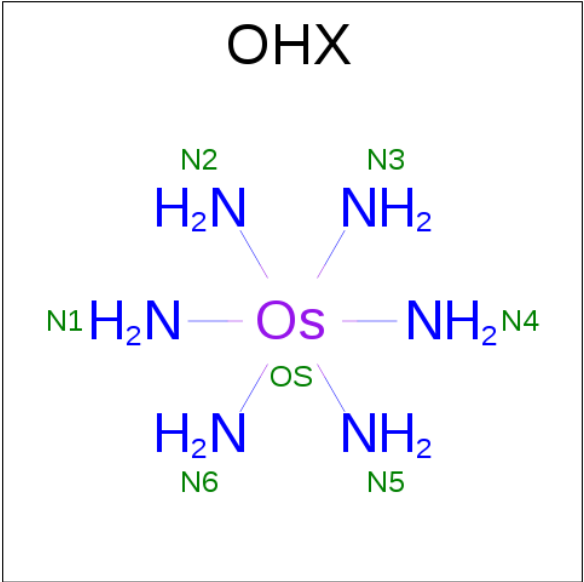
- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called Ribosomal protein P1 alpha, P2 beta.

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

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



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		
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
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		
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
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		
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
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		
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
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		
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
86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
			7	6	1		
86	2	1	Total	N	Os	0	0
			7	6	1		
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86	2	1	Total	N	Os	0	0
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86	2	1	Total	N	Os	0	0
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			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
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
86	S8	1	Total 7	N 6	Os 1	0	0
86	S9	1	Total 7	N 6	Os 1	0	0
86	C1	1	Total 7	N 6	Os 1	0	0
86	C3	1	Total 7	N 6	Os 1	0	0
86	C5	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0
86	SR	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
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		
86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
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86	1	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	M9	1	Total	N	Os	0	0
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86	N9	1	Total	N	Os	0	0
			7	6	1		
86	O1	1	Total	N	Os	0	0
			7	6	1		
86	O3	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	s4	1	Total	N	Os	0	0
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86	s8	1	Total	N	Os	0	0
			7	6	1		
86	s9	1	Total	N	Os	0	0
			7	6	1		
86	c3	1	Total	N	Os	0	0
			7	6	1		
86	c5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	c8	1	Total	N	Os	0	0
			7	6	1		
86	sR	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	7	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		
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	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	L7	3	Total	Mg	0	0
			3	3		
87	n8	2	Total	Mg	0	0
			2	2		
87	c6	1	Total	Mg	0	0
			1	1		
87	6	98	Total	Mg	0	0
			98	98		
87	sM	1	Total	Mg	0	0
			1	1		
87	m5	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	l3	1	Total 1	Mg 1	0	0
87	d6	1	Total 1	Mg 1	0	0
87	2	91	Total 91	Mg 91	0	0
87	L4	1	Total 1	Mg 1	0	0
87	n9	1	Total 1	Mg 1	0	0
87	M5	2	Total 2	Mg 2	0	0
87	S2	1	Total 1	Mg 1	0	0
87	D3	1	Total 1	Mg 1	0	0
87	M9	1	Total 1	Mg 1	0	0
87	q0	1	Total 1	Mg 1	0	0
87	M0	1	Total 1	Mg 1	0	0
87	c1	1	Total 1	Mg 1	0	0
87	5	383	Total 383	Mg 383	0	0
87	O7	1	Total 1	Mg 1	0	0
87	1	353	Total 353	Mg 353	0	0
87	d3	1	Total 1	Mg 1	0	0
87	Q2	1	Total 1	Mg 1	0	0
87	O2	1	Total 1	Mg 1	0	0
87	M3	2	Total 2	Mg 2	0	0
87	N3	1	Total 1	Mg 1	0	0
87	4	17	Total 17	Mg 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	L2	2	Total 2	Mg 2	0	0
87	n6	2	Total 2	Mg 2	0	0
87	o7	2	Total 2	Mg 2	0	0
87	M7	3	Total 3	Mg 3	0	0
87	N8	2	Total 2	Mg 2	0	0
87	q2	1	Total 1	Mg 1	0	0
87	m7	2	Total 2	Mg 2	0	0
87	7	11	Total 11	Mg 11	0	0
87	n3	1	Total 1	Mg 1	0	0
87	q1	1	Total 1	Mg 1	0	0
87	L3	1	Total 1	Mg 1	0	0
87	l2	3	Total 3	Mg 3	0	0
87	8	9	Total 9	Mg 9	0	0
87	3	8	Total 8	Mg 8	0	0

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

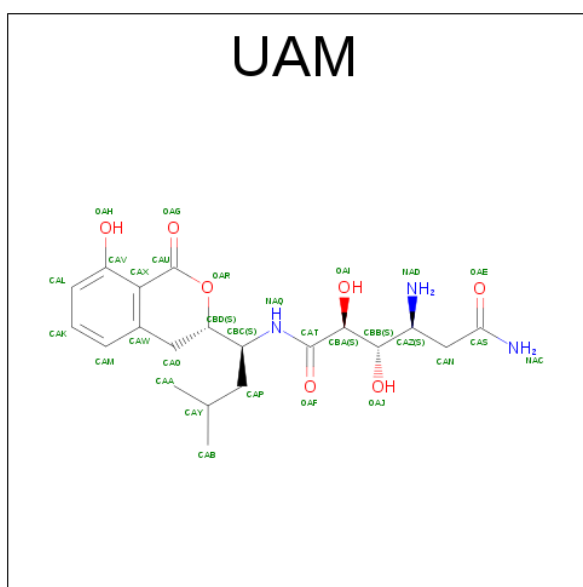
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total 1	Zn 1	0	0
88	D6	1	Total 1	Zn 1	0	0
88	Q2	1	Total 1	Zn 1	0	0
88	e1	1	Total 1	Zn 1	0	0
88	Q3	1	Total 1	Zn 1	0	0

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

- Molecule 89 is Amicoumacin A (three-letter code: UAM) (formula: $C_{20}H_{29}N_3O_7$).

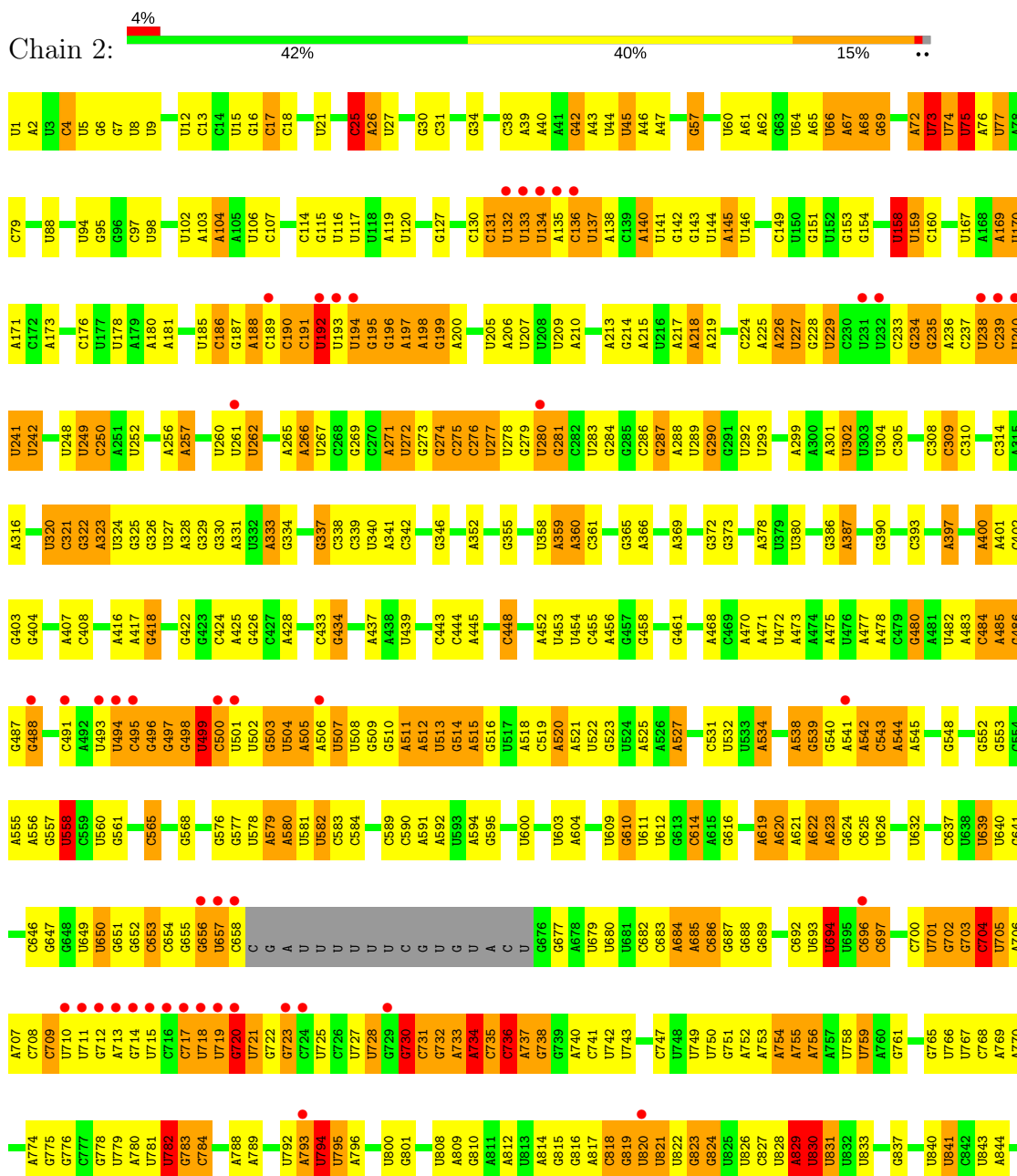


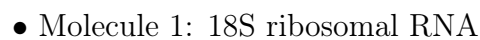
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	6	1	Total	C	N	O	0	0
			30	20	3	7		

3 Residue-property plots

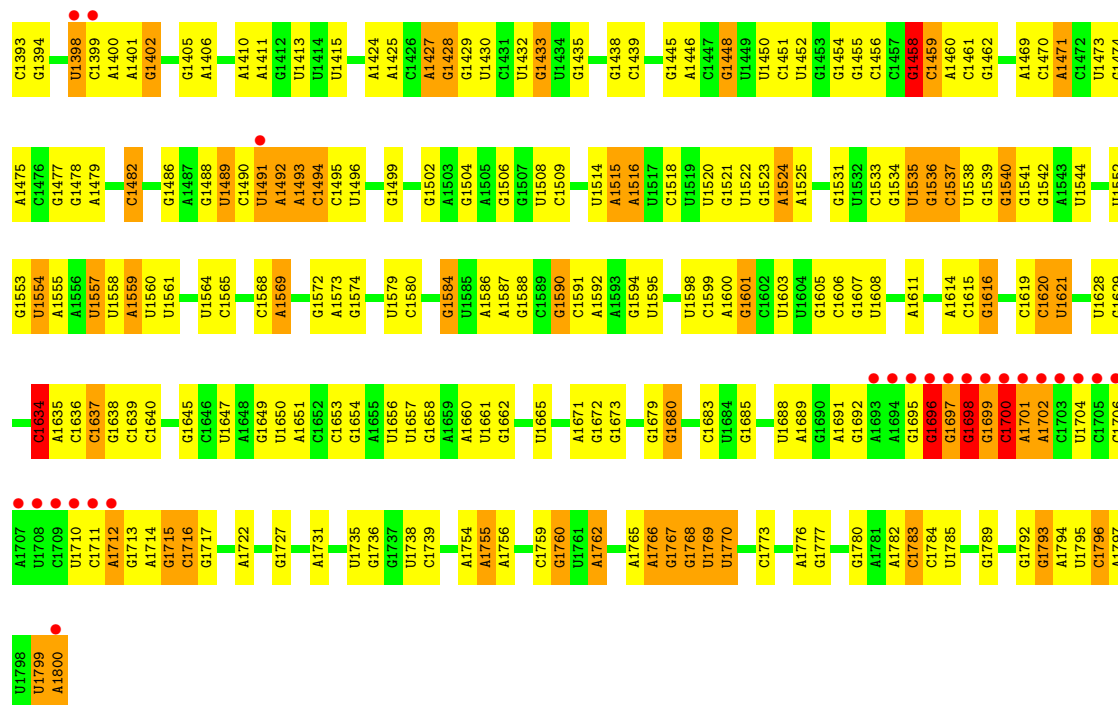
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

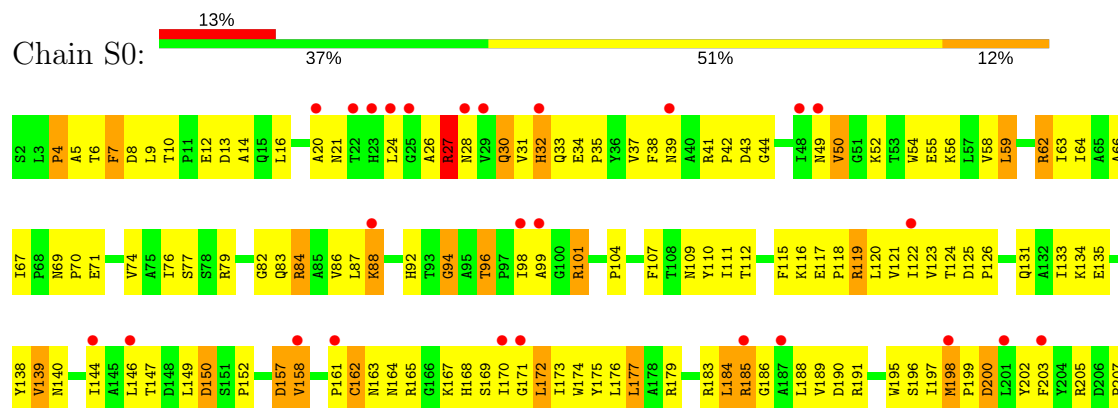




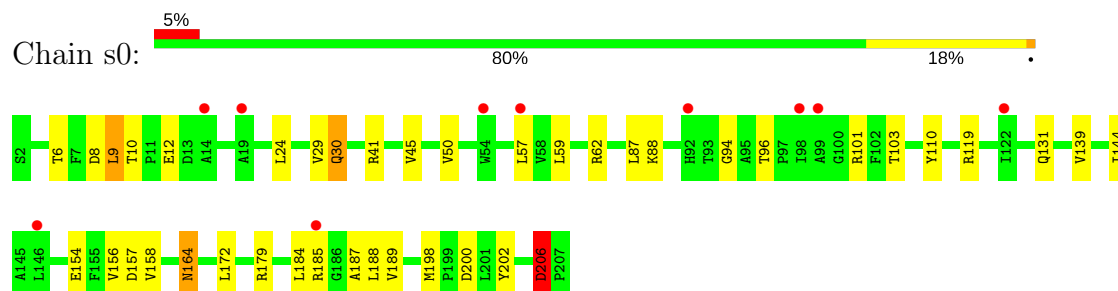




• Molecule 2: 40S ribosomal protein S0-A

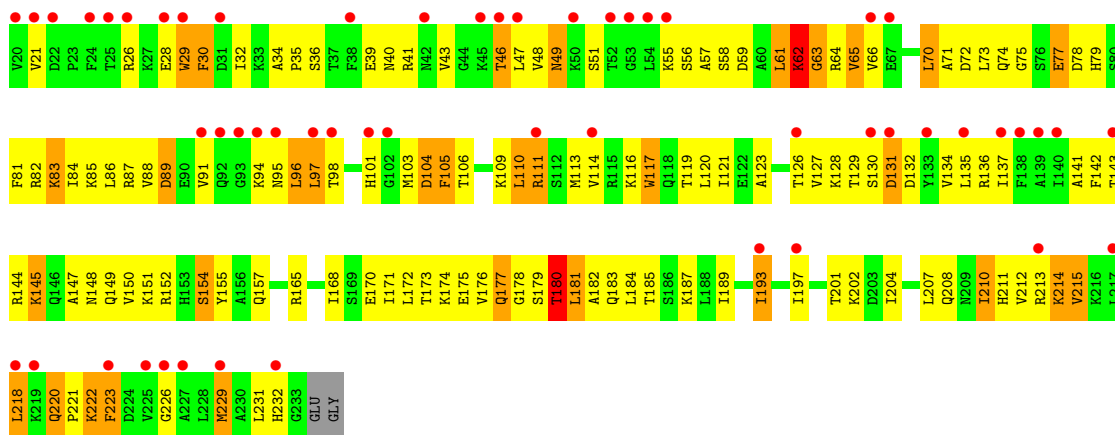


• Molecule 2: 40S ribosomal protein S0-A

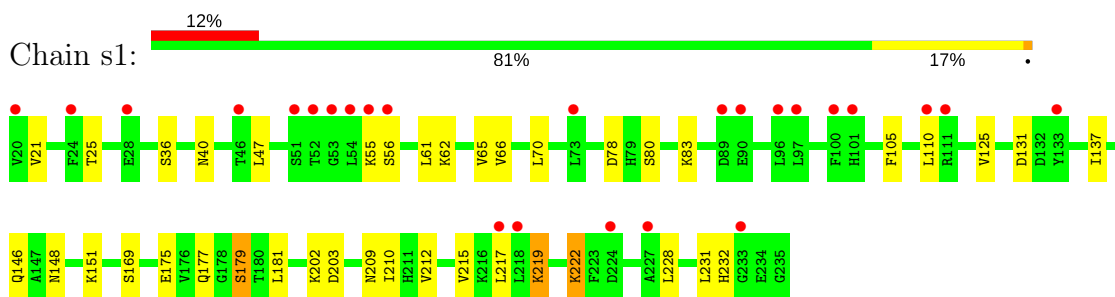


• Molecule 3: 40S ribosomal protein S1-A

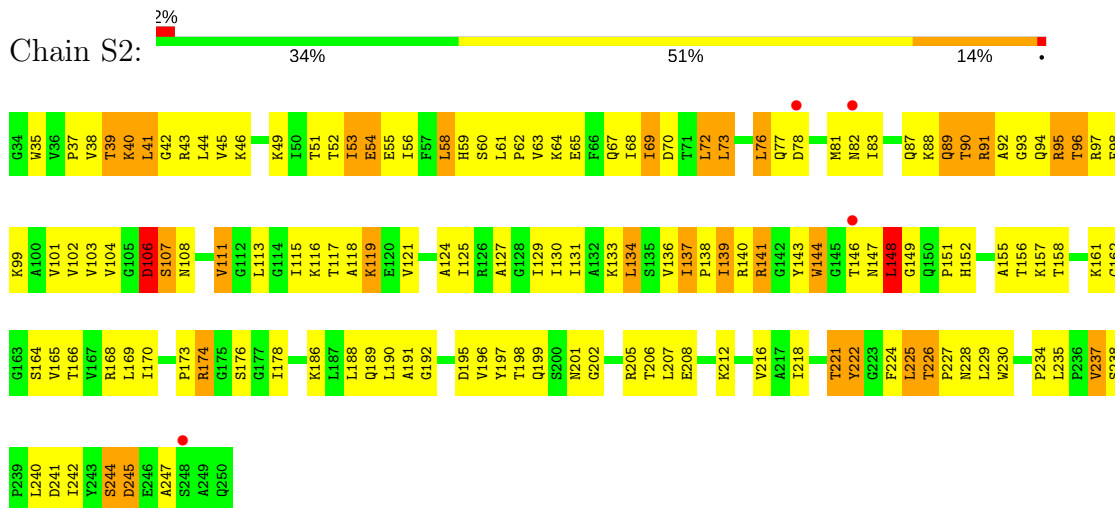




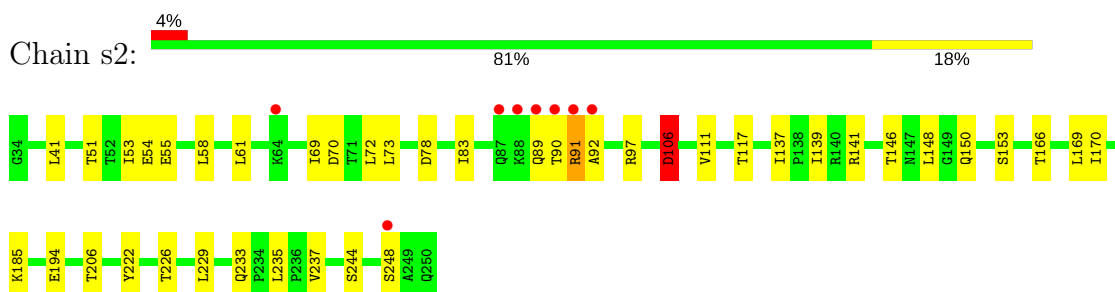
• Molecule 3: 40S ribosomal protein S1-A



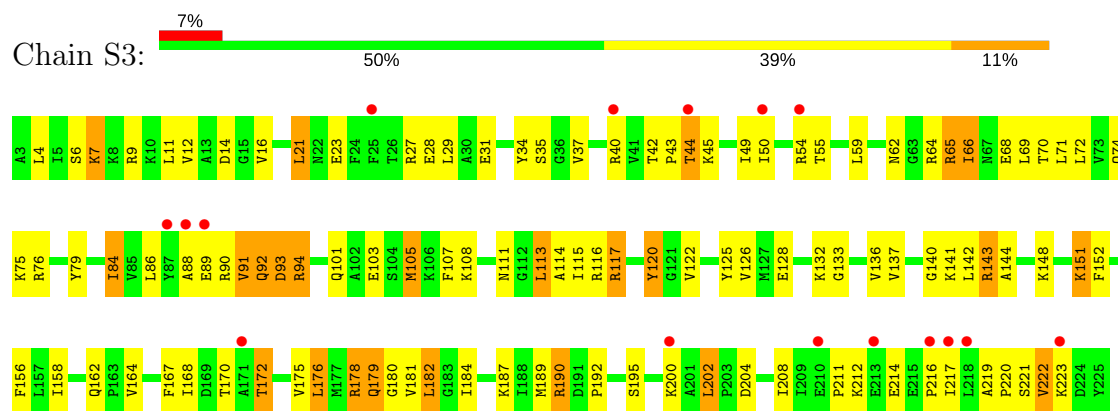
• Molecule 4: 40S ribosomal protein S2



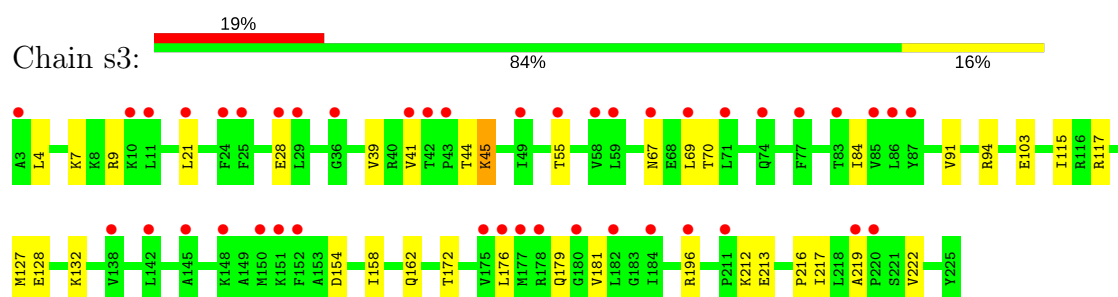
• Molecule 4: 40S ribosomal protein S2



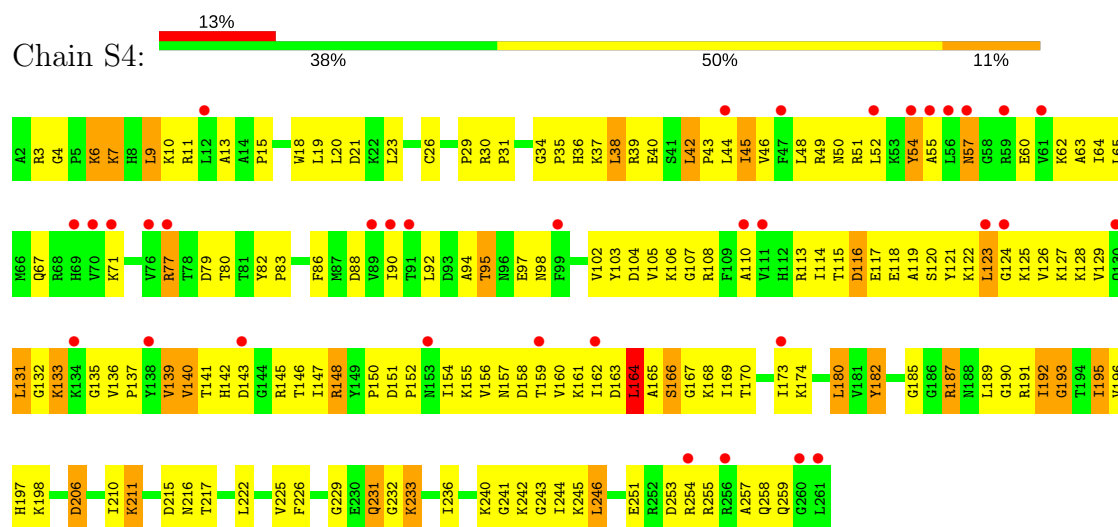
• Molecule 5: 40S ribosomal protein S3



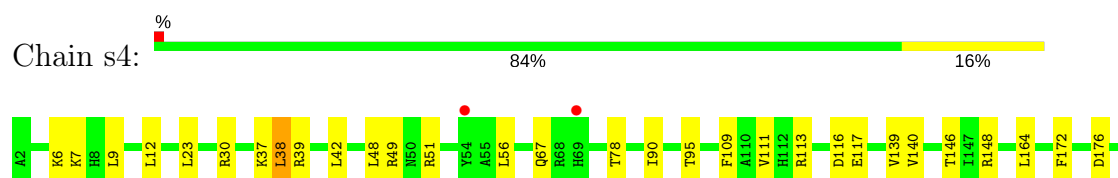
• Molecule 5: 40S ribosomal protein S3



• Molecule 6: 40S ribosomal protein S4-A

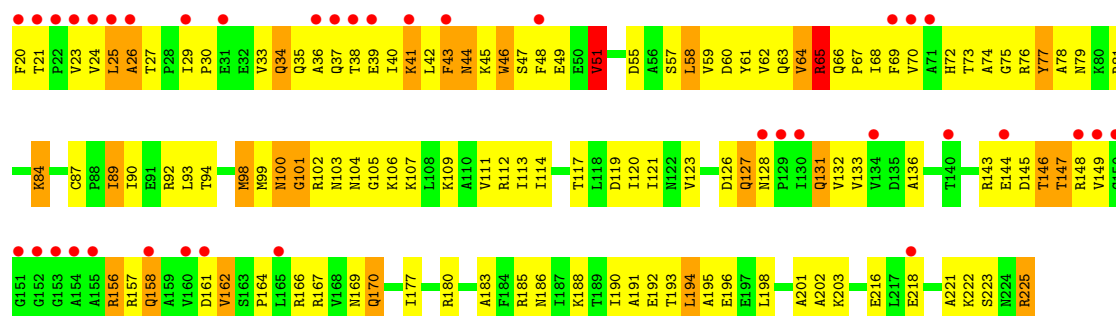
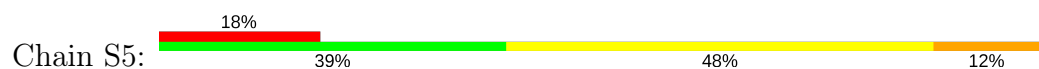


• Molecule 6: 40S ribosomal protein S4-A

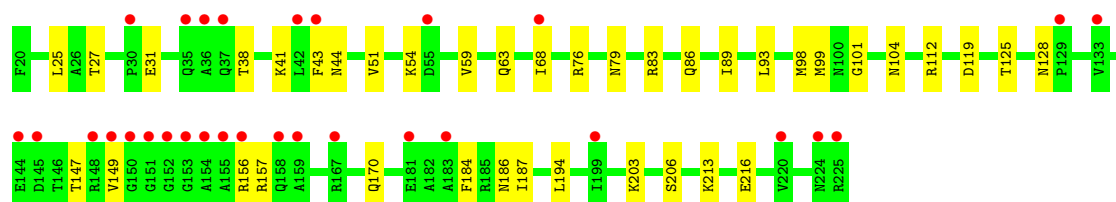
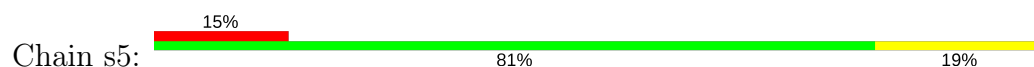




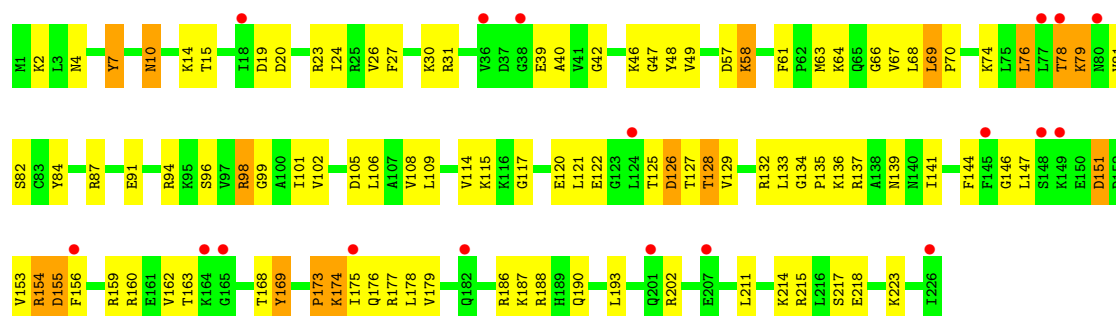
• Molecule 7: 40S ribosomal protein S5



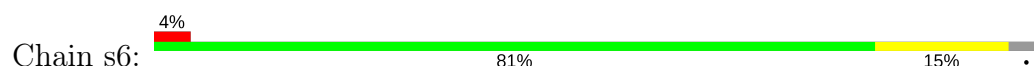
• Molecule 7: 40S ribosomal protein S5

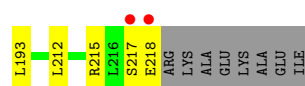


• Molecule 8: 40S ribosomal protein S6-A

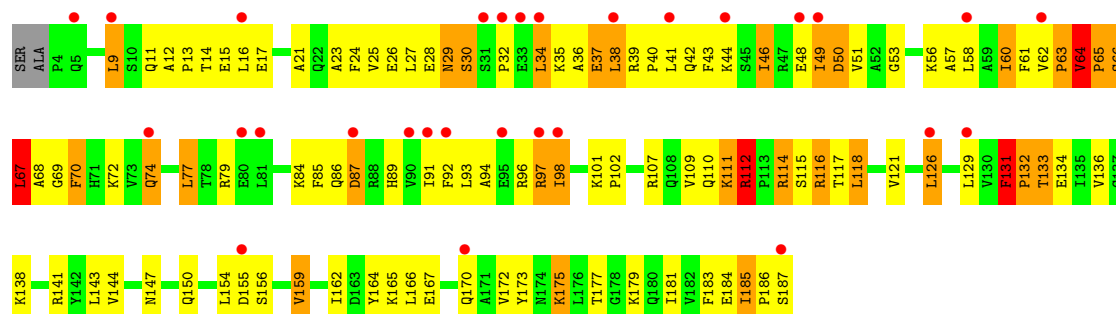
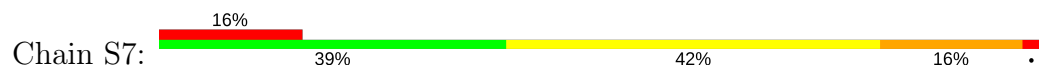


• Molecule 8: 40S ribosomal protein S6-A

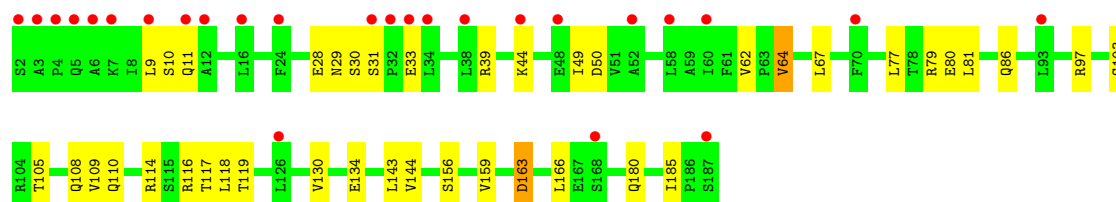
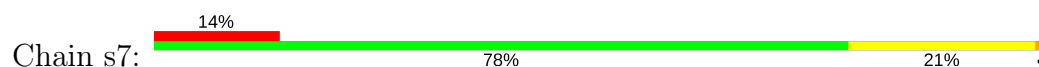




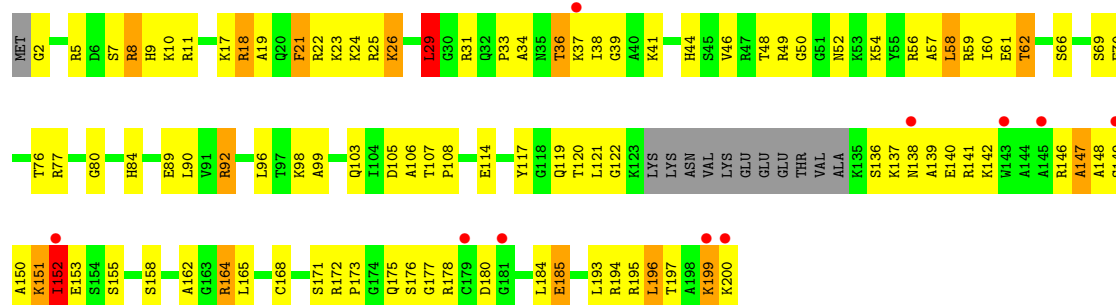
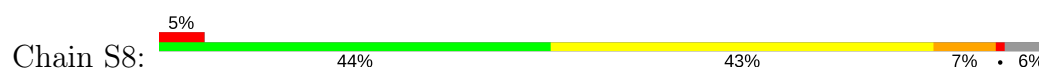
- Molecule 9: 40S ribosomal protein S7-A



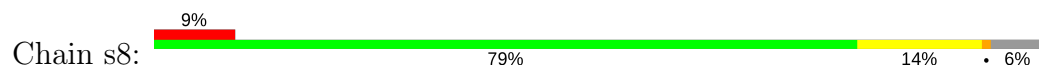
- Molecule 9: 40S ribosomal protein S7-A

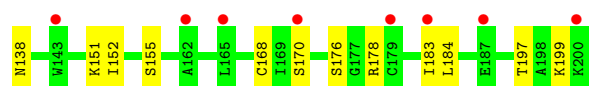


- Molecule 10: 40S ribosomal protein S8-A

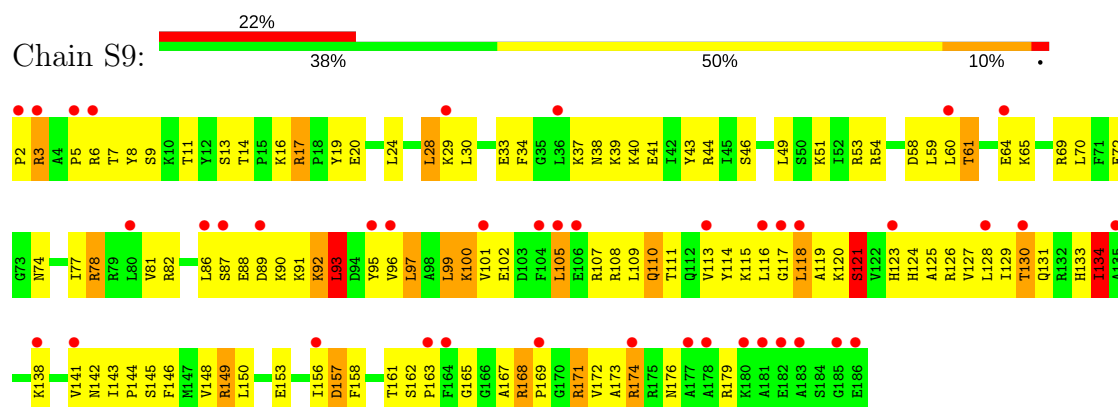


- Molecule 10: 40S ribosomal protein S8-A

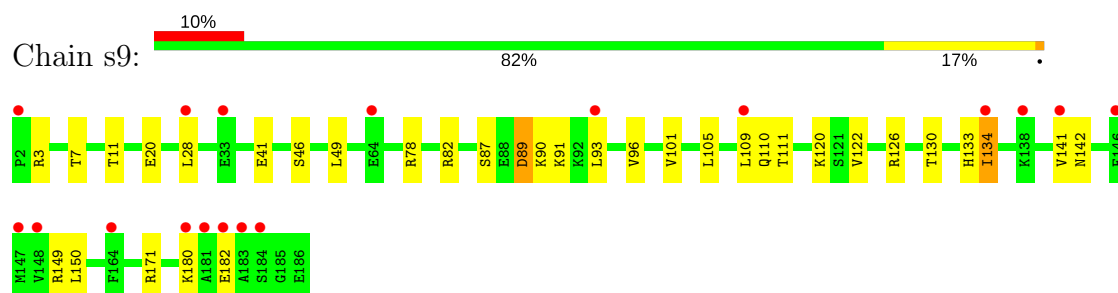




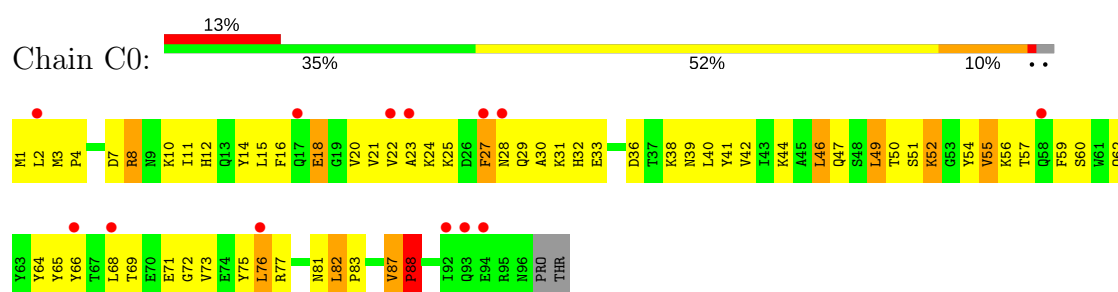
• Molecule 11: 40S ribosomal protein S9-A



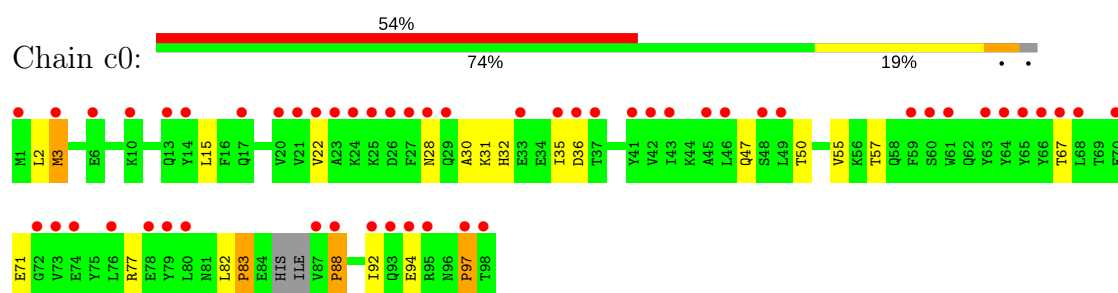
• Molecule 11: 40S ribosomal protein S9-A



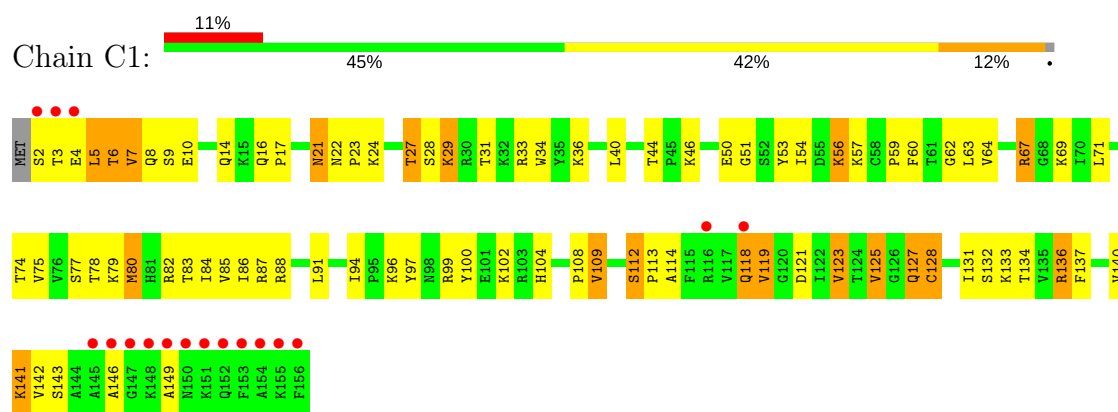
• Molecule 12: 40S ribosomal protein S10-A



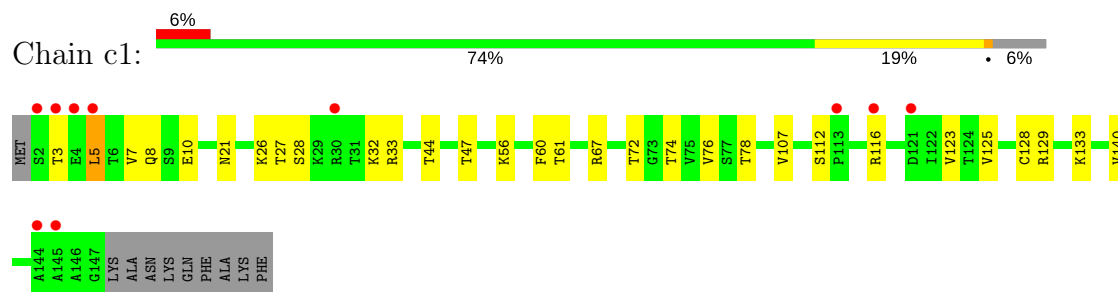
• Molecule 12: 40S ribosomal protein S10-A



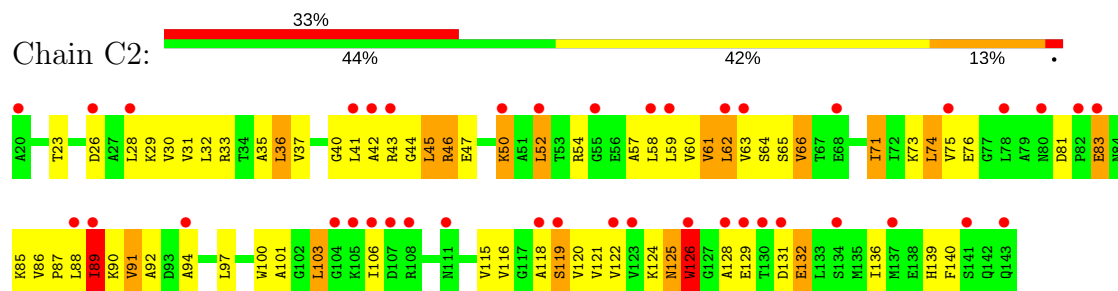
• Molecule 13: 40S ribosomal protein S11-A



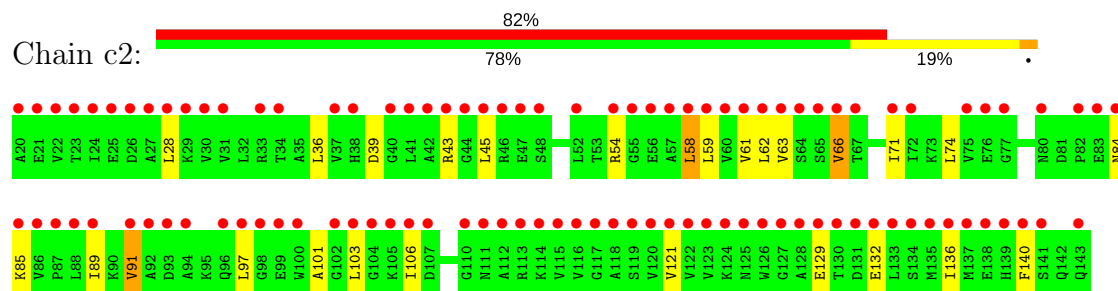
• Molecule 13: 40S ribosomal protein S11-A



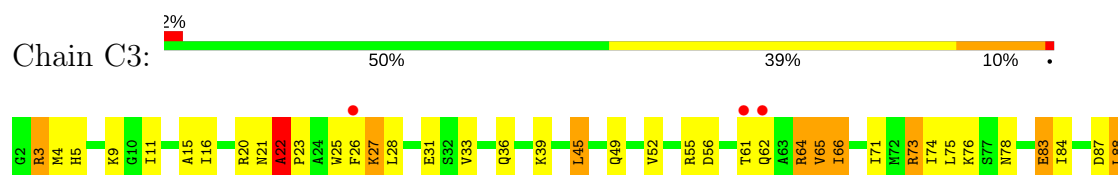
• Molecule 14: 40S ribosomal protein S12



• Molecule 14: 40S ribosomal protein S12

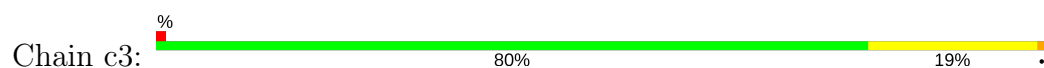


• Molecule 15: 40S ribosomal protein S13

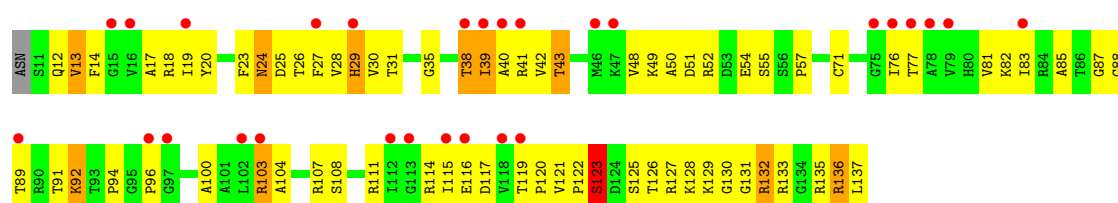
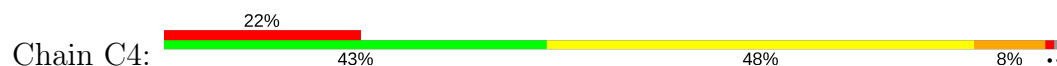




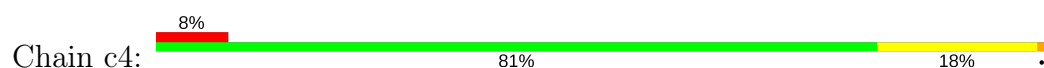
- Molecule 15: 40S ribosomal protein S13



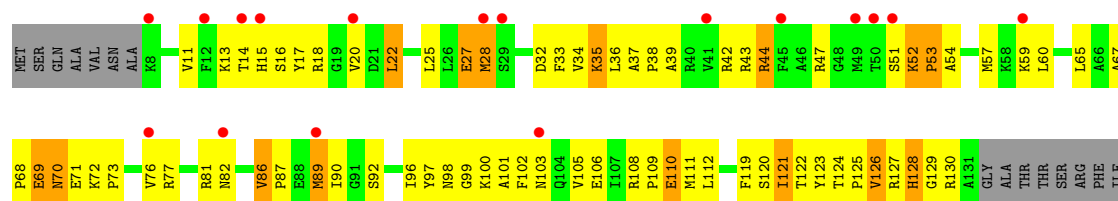
- Molecule 16: 40S ribosomal protein S14-B



- Molecule 16: 40S ribosomal protein S14-B

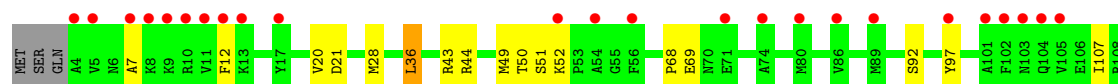
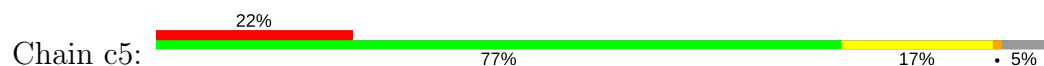


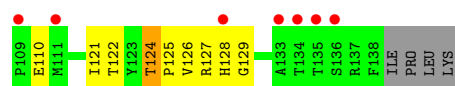
- Molecule 17: 40S ribosomal protein S15



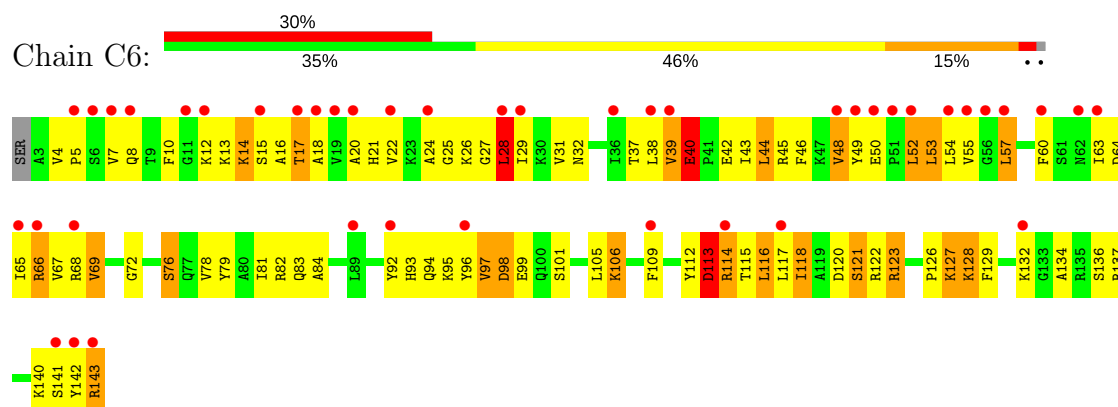
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- Molecule 17: 40S ribosomal protein S15

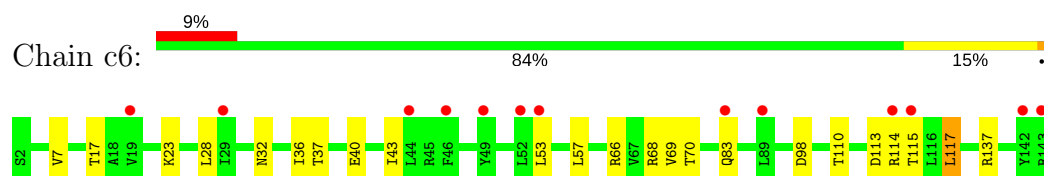




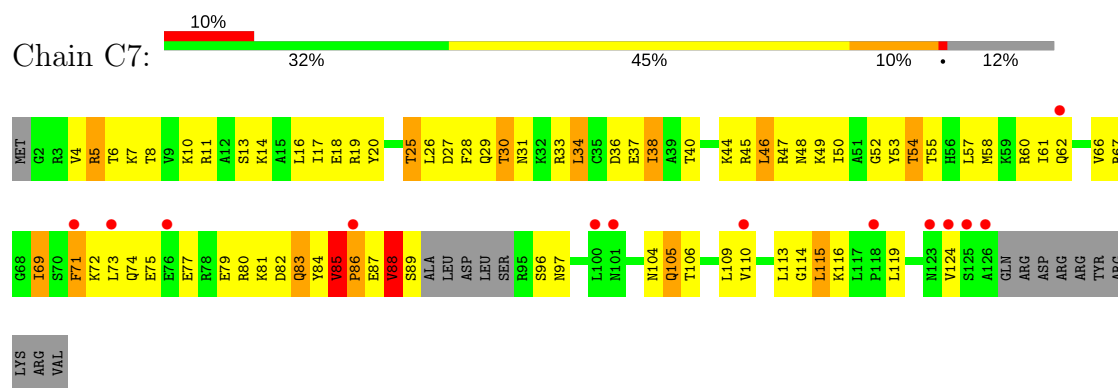
• Molecule 18: 40S ribosomal protein S16-A

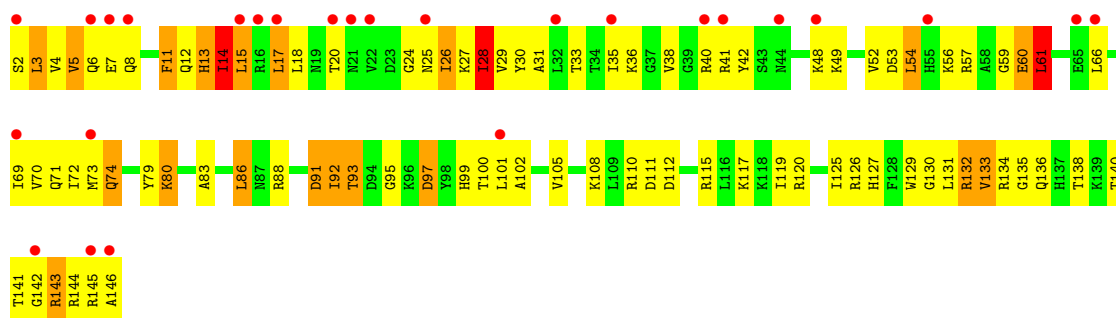


• Molecule 18: 40S ribosomal protein S16-A

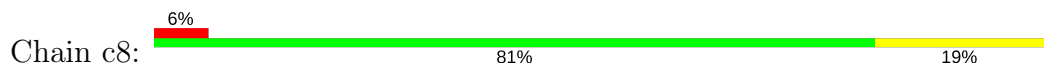


• Molecule 19: 40S ribosomal protein S17-A

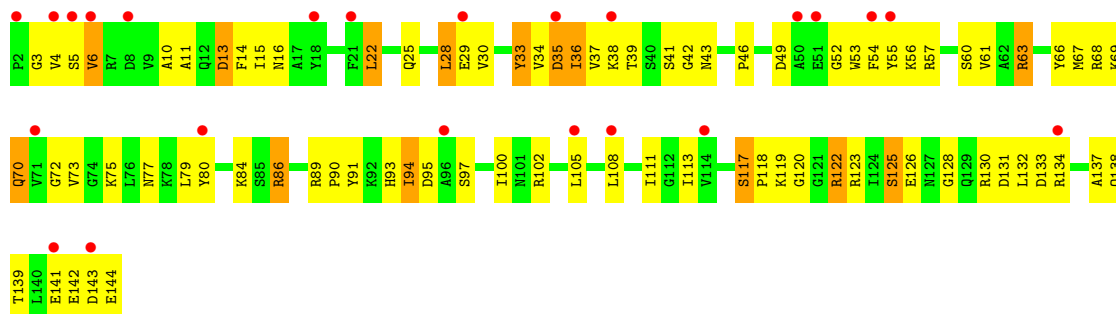
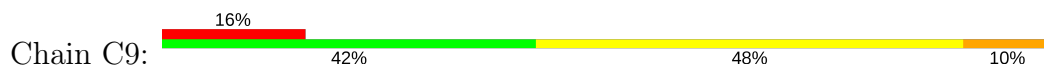




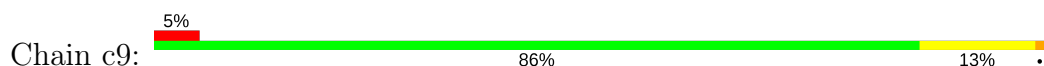
- Molecule 20: 40S ribosomal protein S18-A



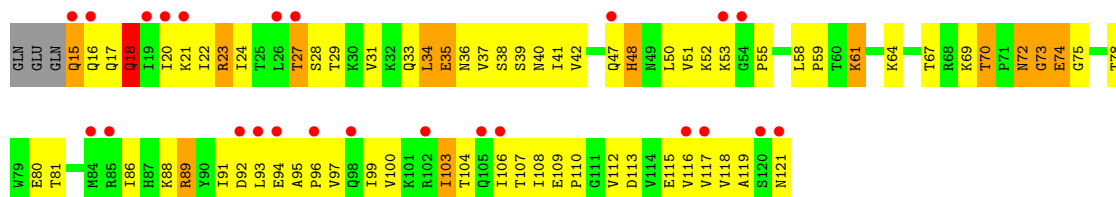
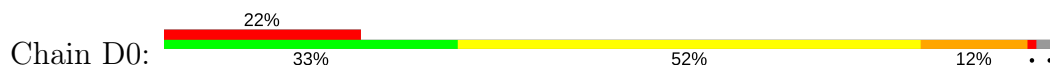
- Molecule 21: 40S ribosomal protein S19-A



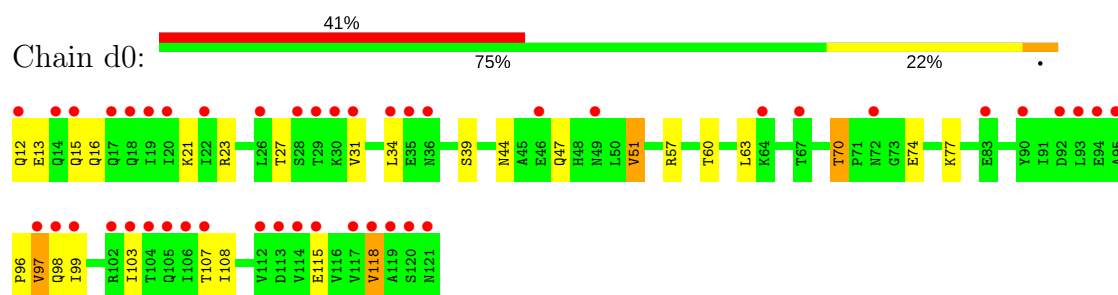
- Molecule 21: 40S ribosomal protein S19-A



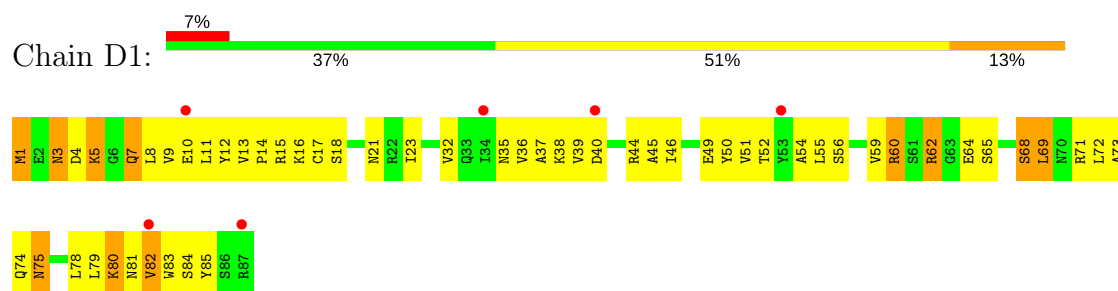
- Molecule 22: 40S ribosomal protein S20



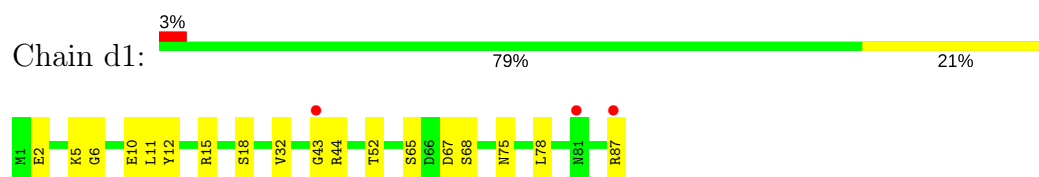
- Molecule 22: 40S ribosomal protein S20



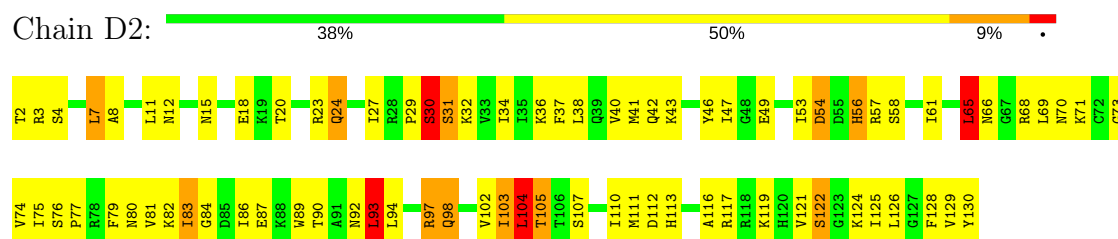
- Molecule 23: 40S ribosomal protein S21-A



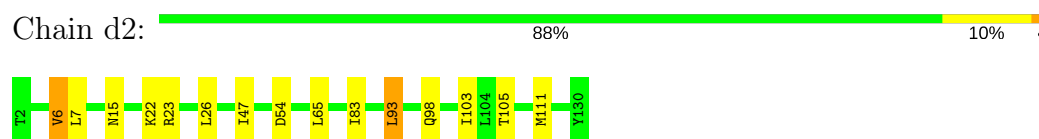
- Molecule 23: 40S ribosomal protein S21-A



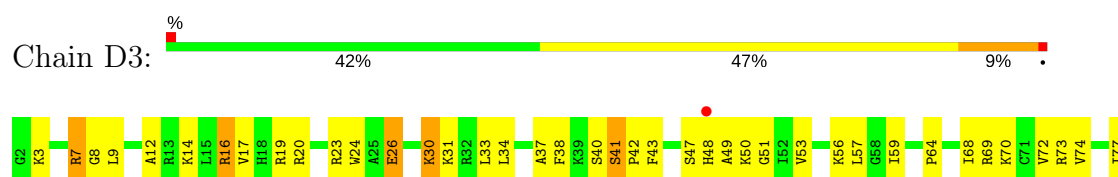
- Molecule 24: 40S ribosomal protein S22-A



- Molecule 24: 40S ribosomal protein S22-A

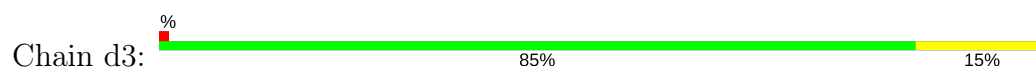


- Molecule 25: 40S ribosomal protein S23-A

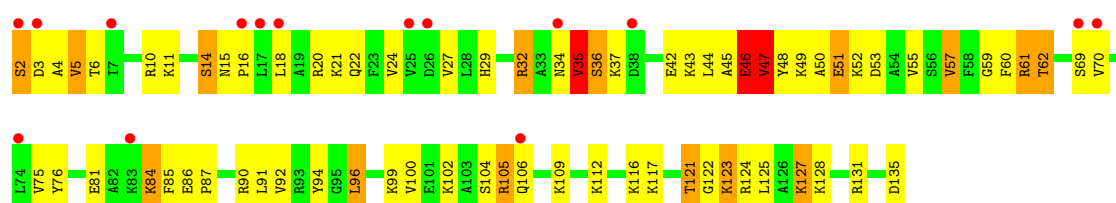




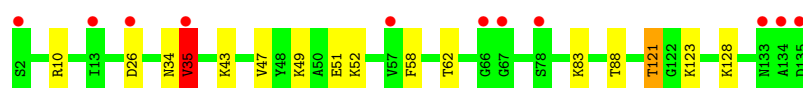
- Molecule 25: 40S ribosomal protein S23-A



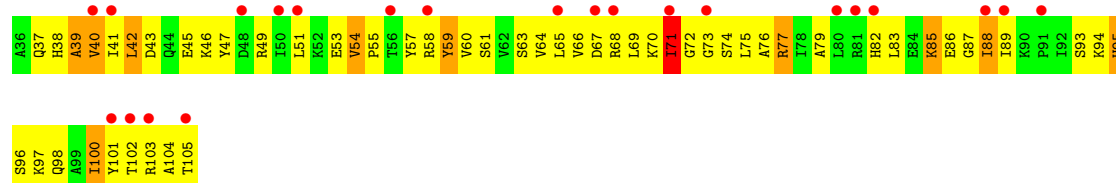
- Molecule 26: 40S ribosomal protein S24-A



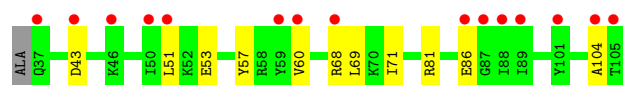
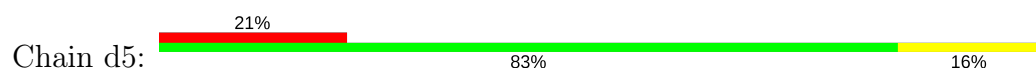
- Molecule 26: 40S ribosomal protein S24-A



- Molecule 27: 40S ribosomal protein S25-A

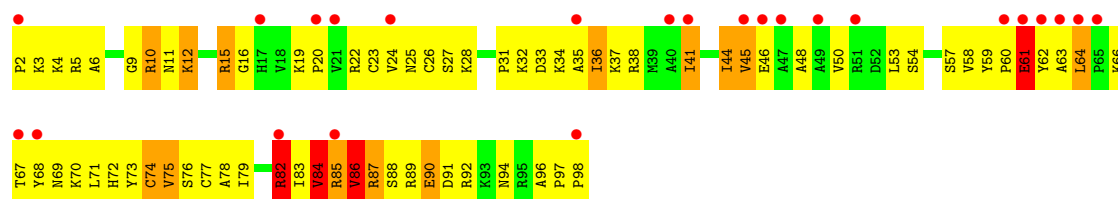


- Molecule 27: 40S ribosomal protein S25-A

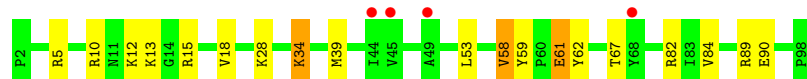
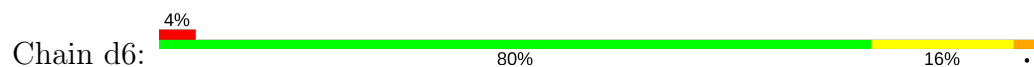


- Molecule 28: 40S ribosomal protein S26-B

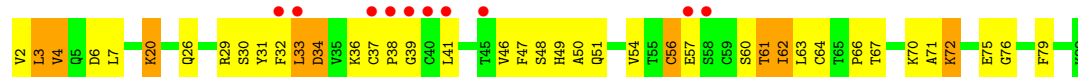




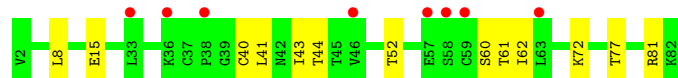
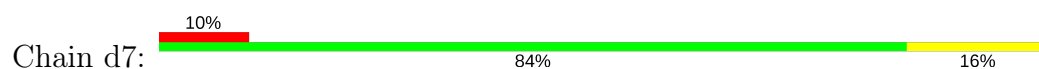
- Molecule 28: 40S ribosomal protein S26-B



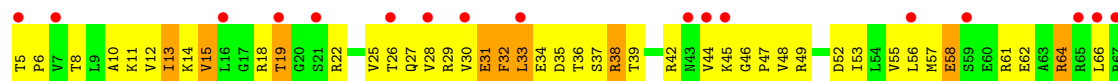
- Molecule 29: 40S ribosomal protein S27-A



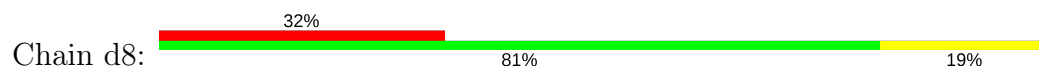
- Molecule 29: 40S ribosomal protein S27-A



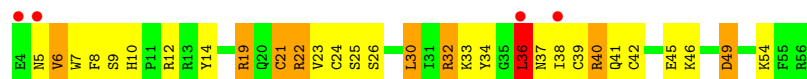
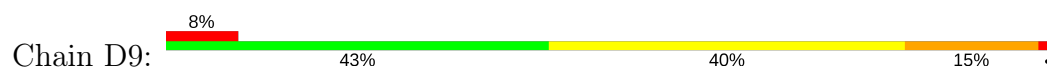
- Molecule 30: 40S ribosomal protein S28-A



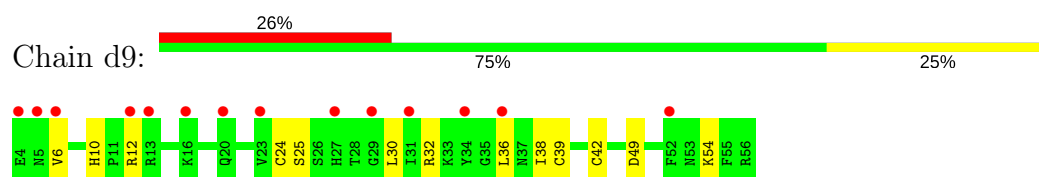
- Molecule 30: 40S ribosomal protein S28-A



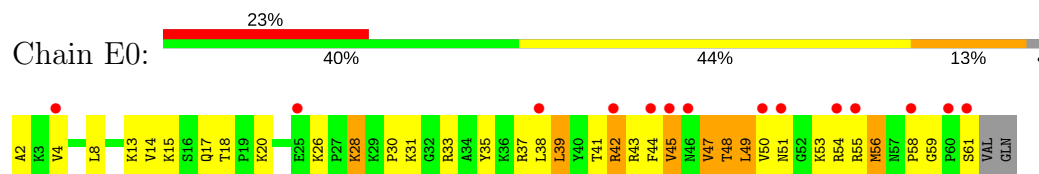
- Molecule 31: 40S ribosomal protein S29-A



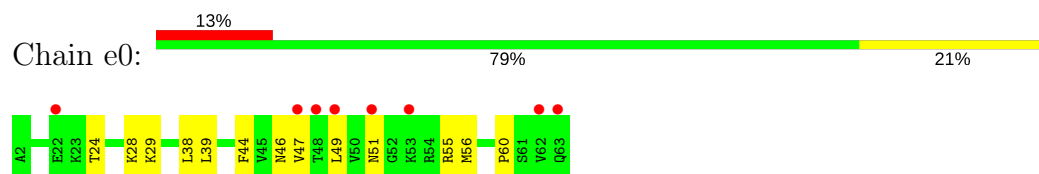
- Molecule 31: 40S ribosomal protein S29-A



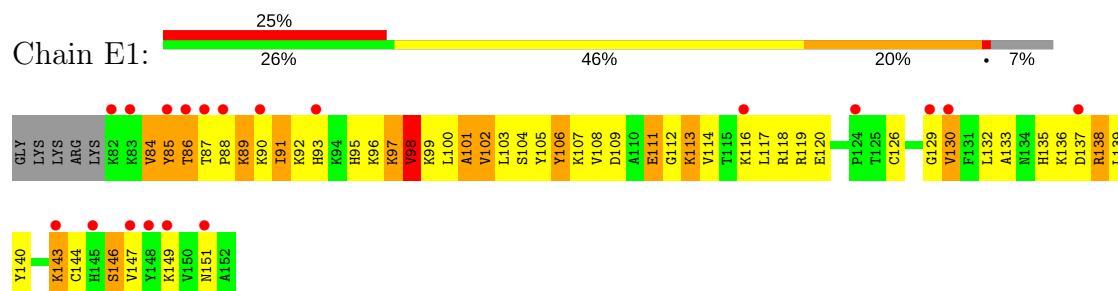
- Molecule 32: 40S ribosomal protein S30-A



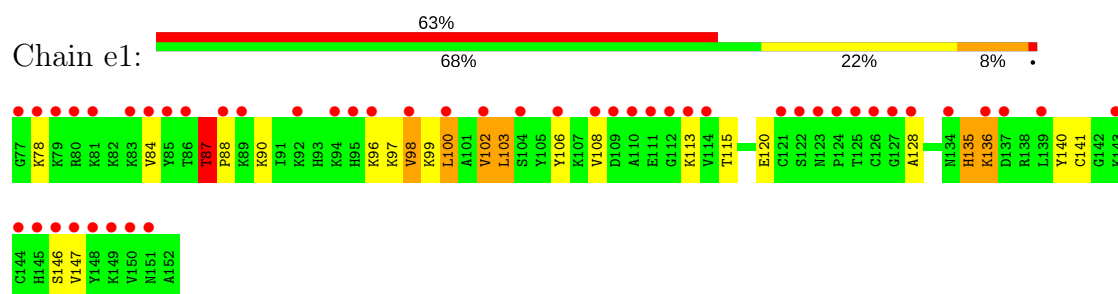
- Molecule 32: 40S ribosomal protein S30-A



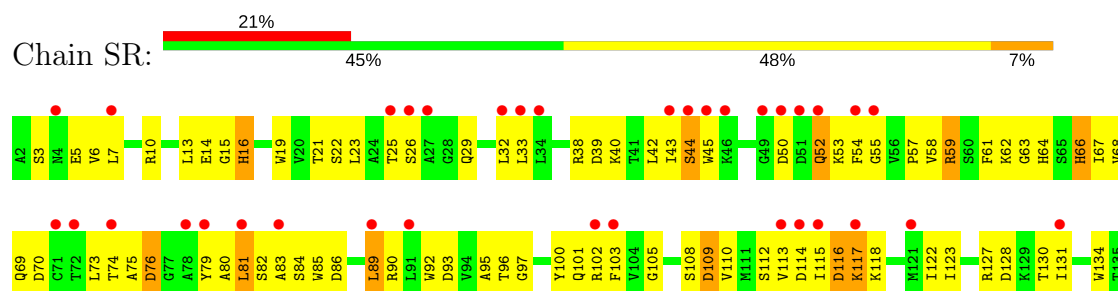
- Molecule 33: Ubiquitin-40S ribosomal protein S31

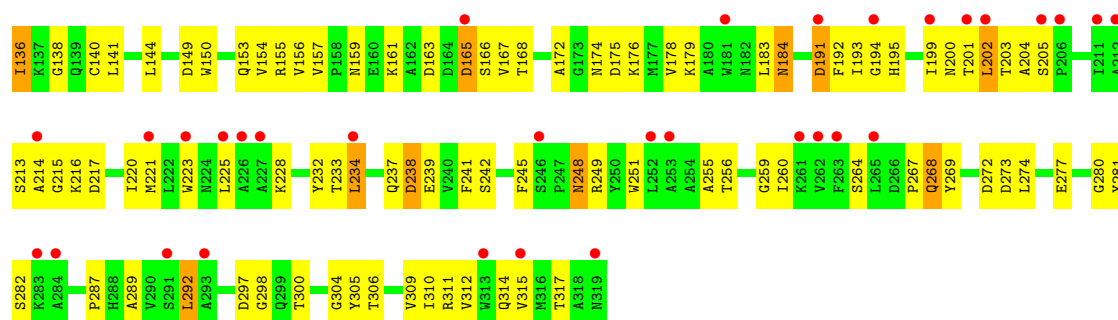


- Molecule 33: Ubiquitin-40S ribosomal protein S31

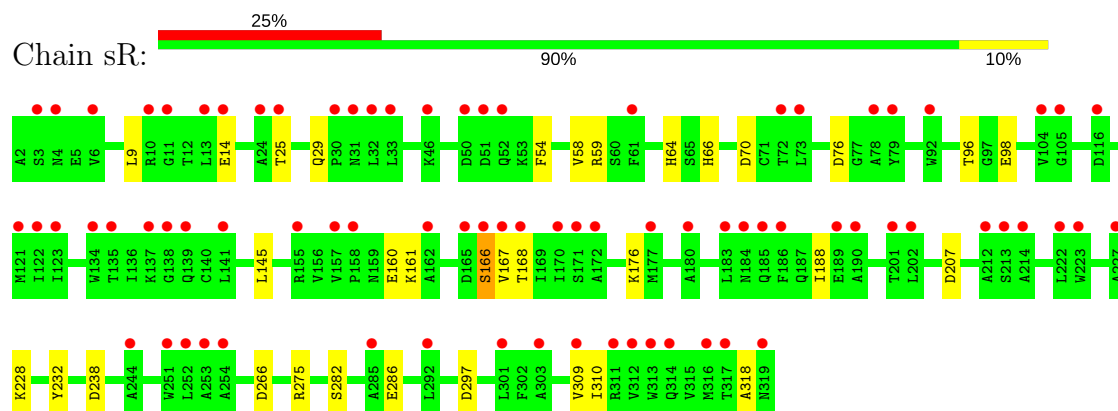


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

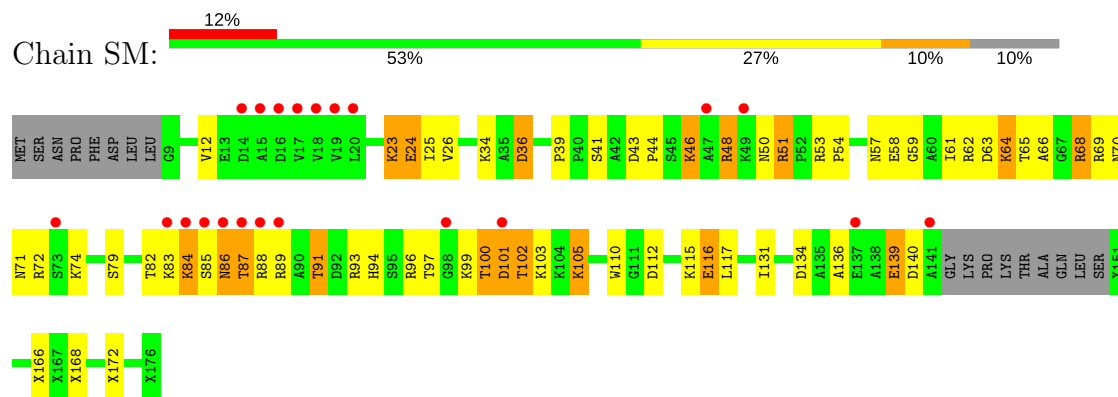




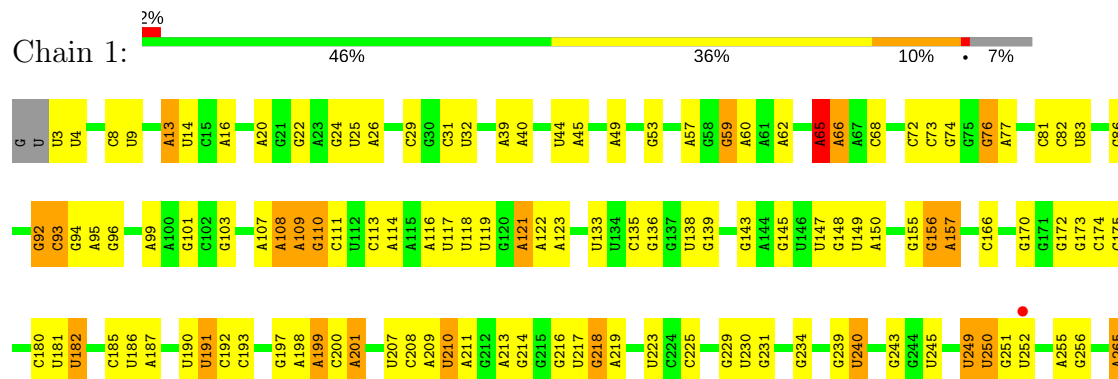
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

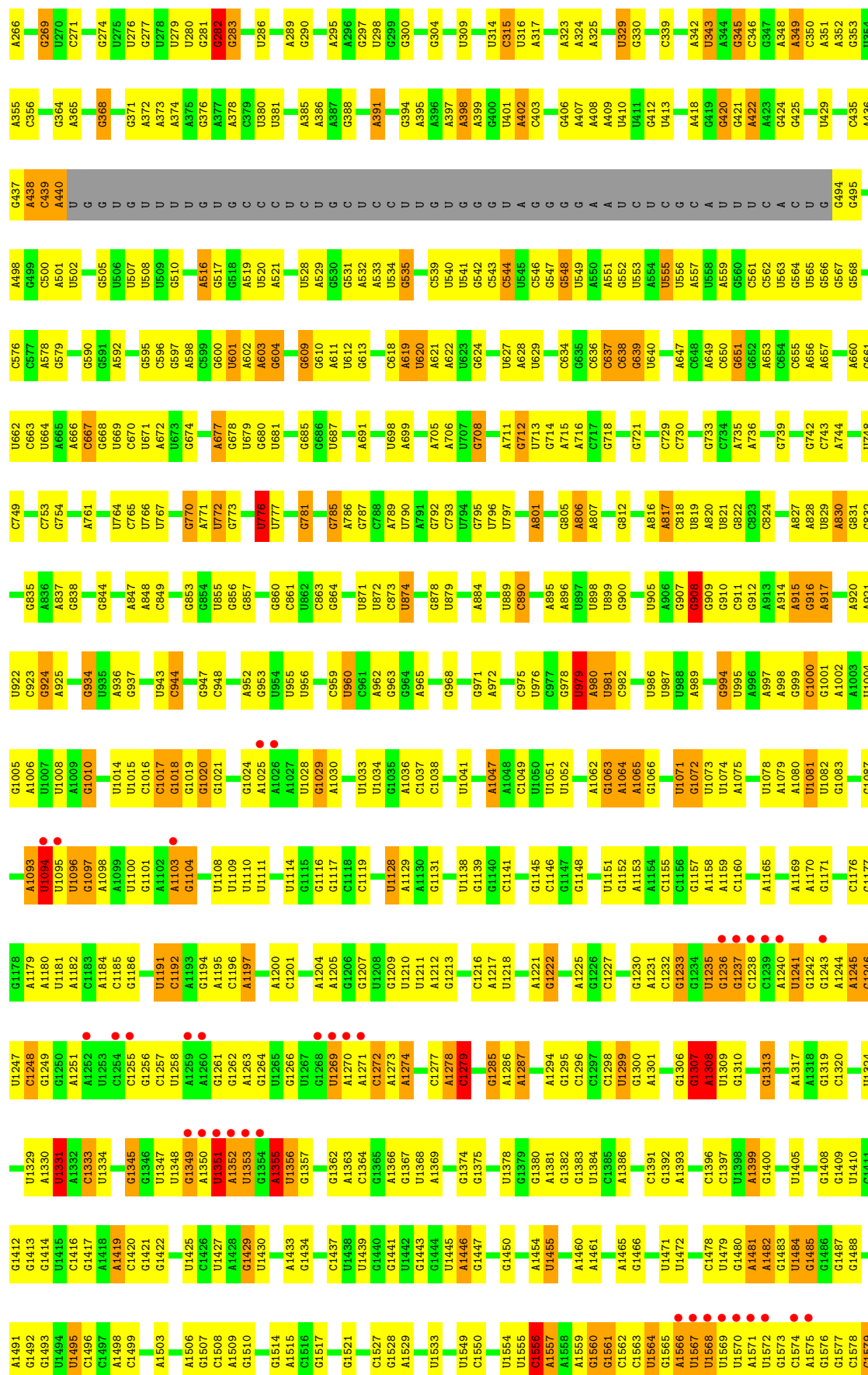


- Molecule 35: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1

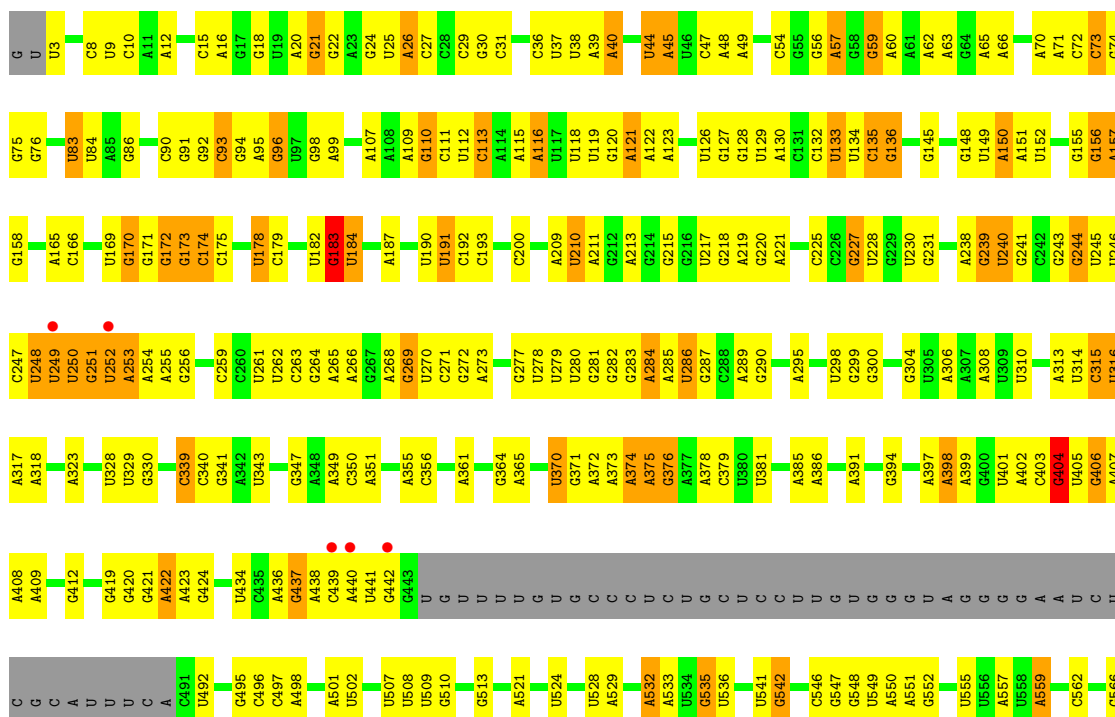


- Molecule 36: 25S ribosomal RNA



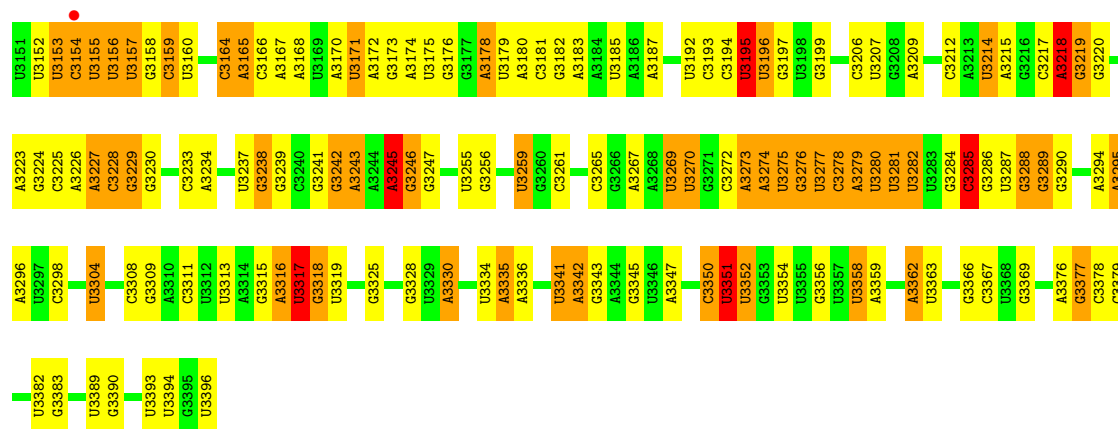






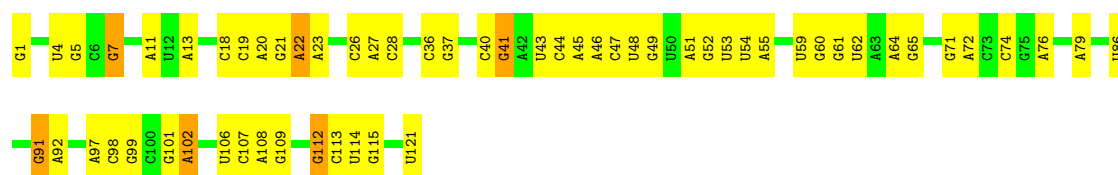






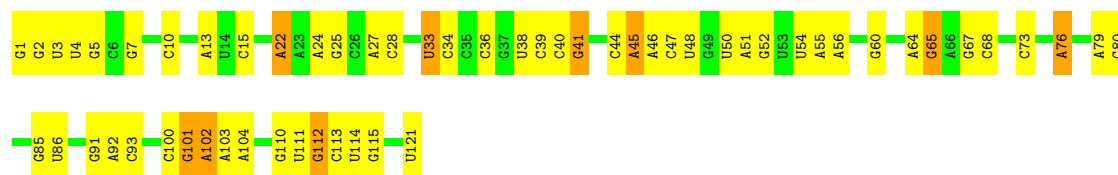
• Molecule 37: 5S ribosomal RNA

Chain 3: 51% 44% 5%



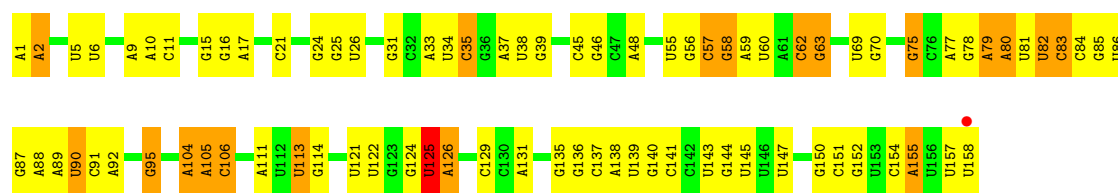
• Molecule 37: 5S ribosomal RNA

Chain 7: 52% 40% 7%



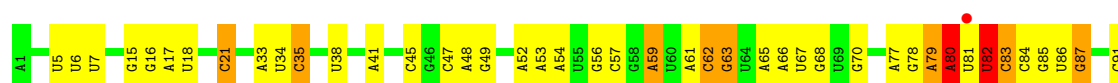
• Molecule 38: 5.8S ribosomal RNA

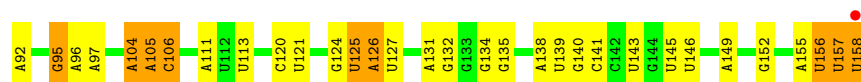
Chain 4: 47% 40% 12%



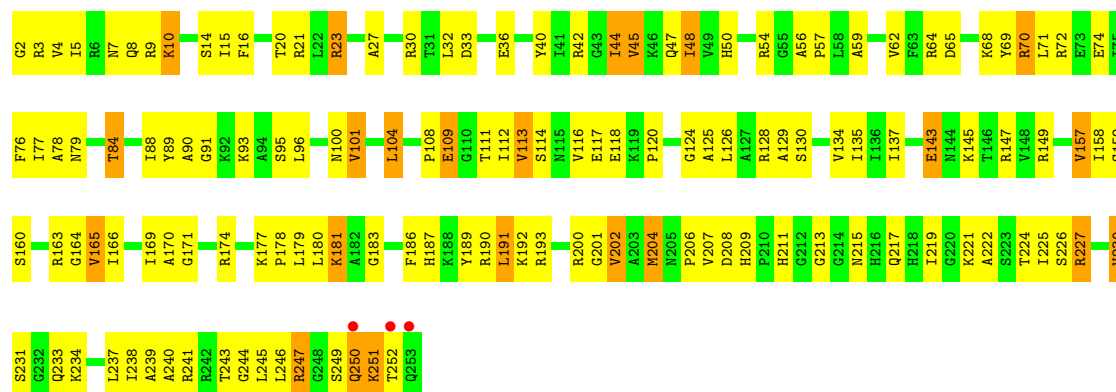
• Molecule 38: 5.8S ribosomal RNA

Chain 8: 53% 35% 11%

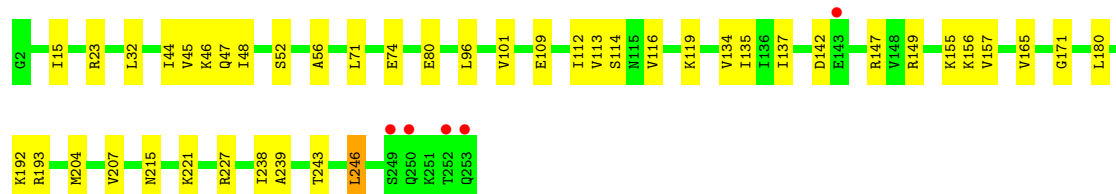
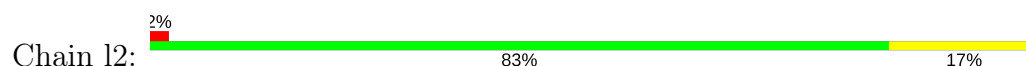




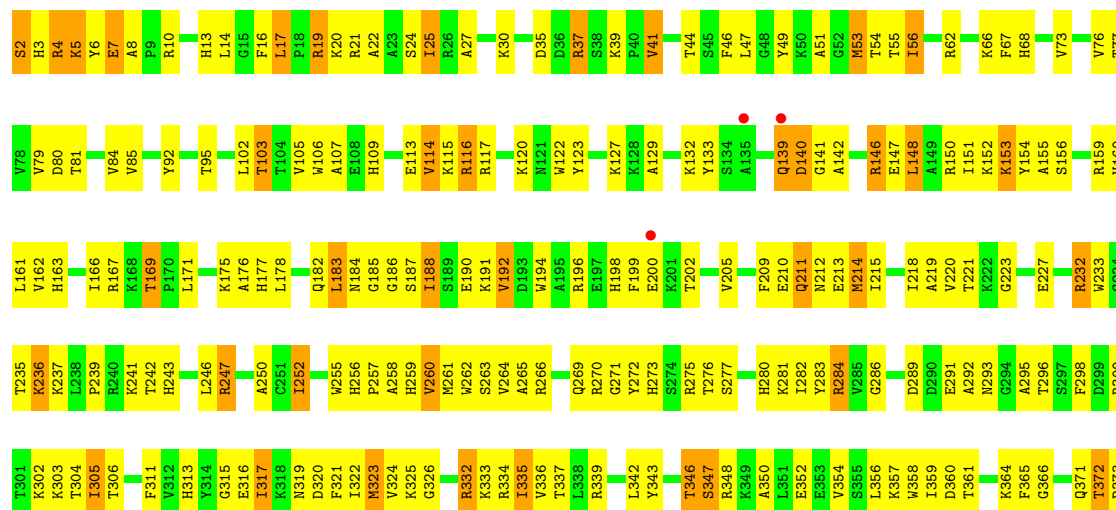
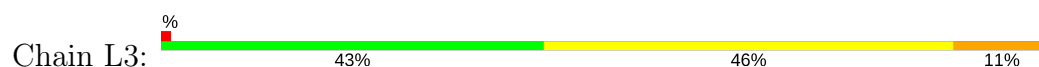
• Molecule 39: 60S ribosomal protein L2-A



• Molecule 39: 60S ribosomal protein L2-A

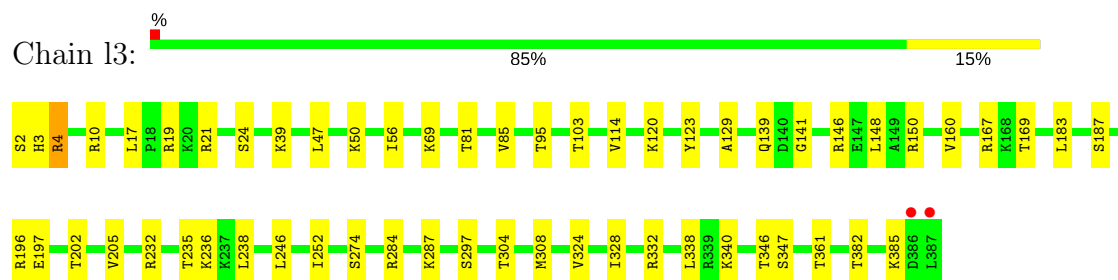


• Molecule 40: 60S ribosomal protein L3

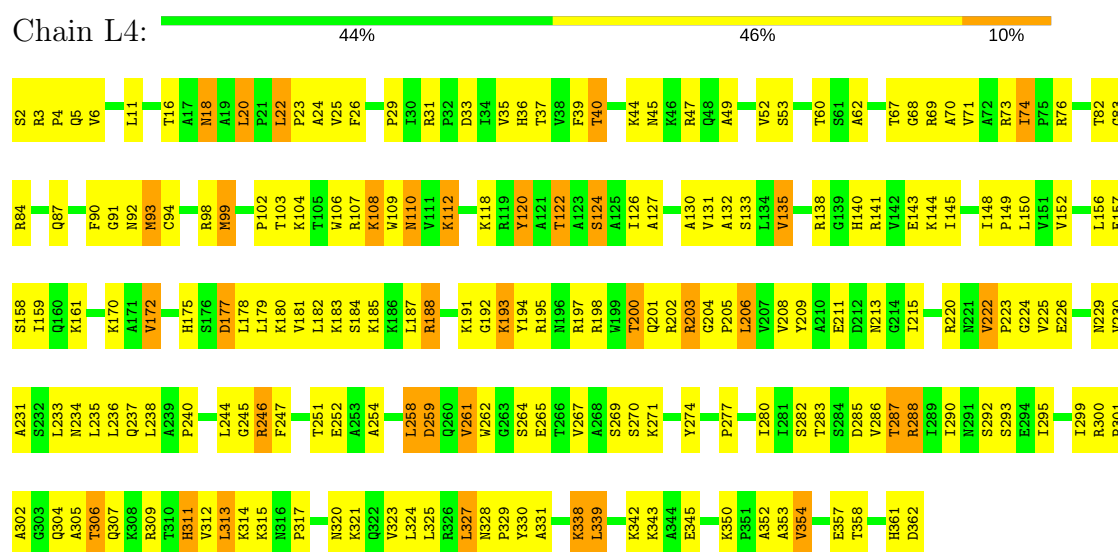




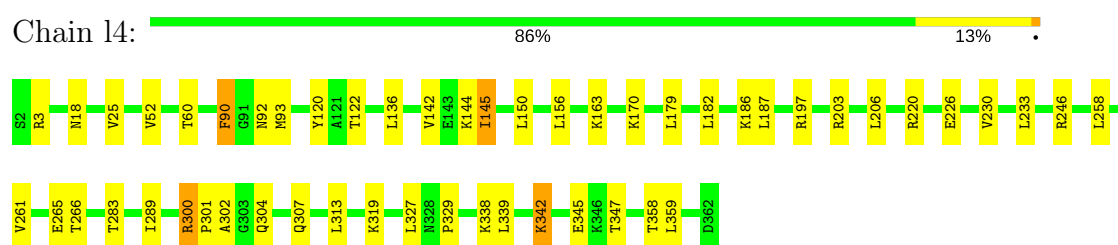
• Molecule 40: 60S ribosomal protein L3



• Molecule 41: 60S ribosomal protein L4-A

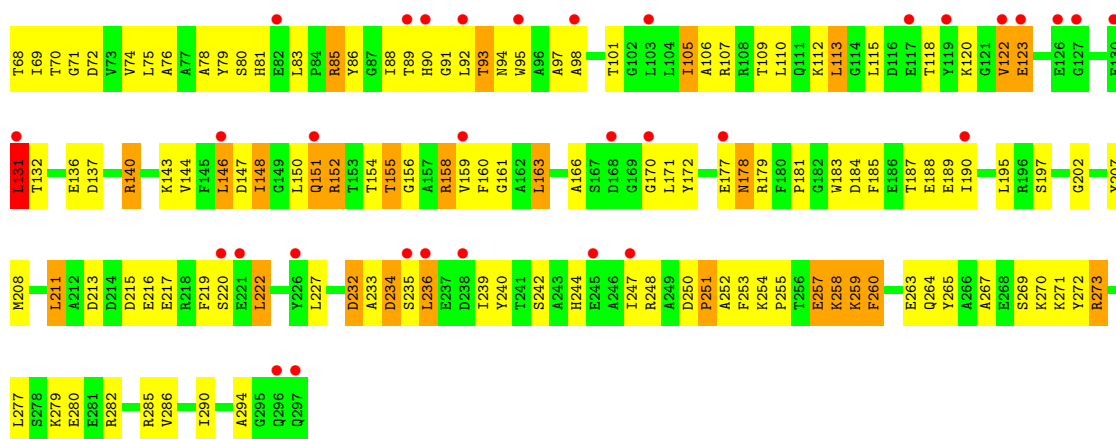


• Molecule 41: 60S ribosomal protein L4-A

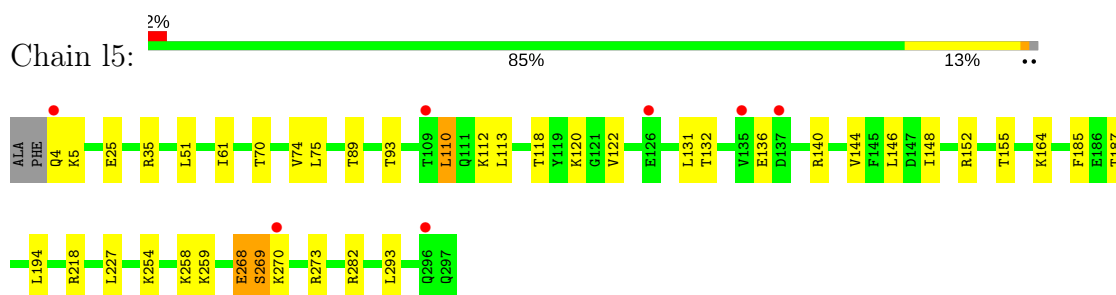


• Molecule 42: 60S ribosomal protein L5

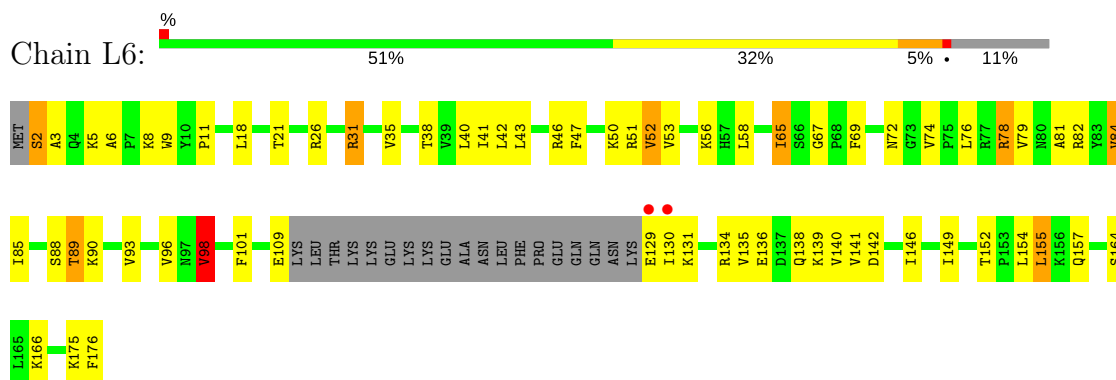




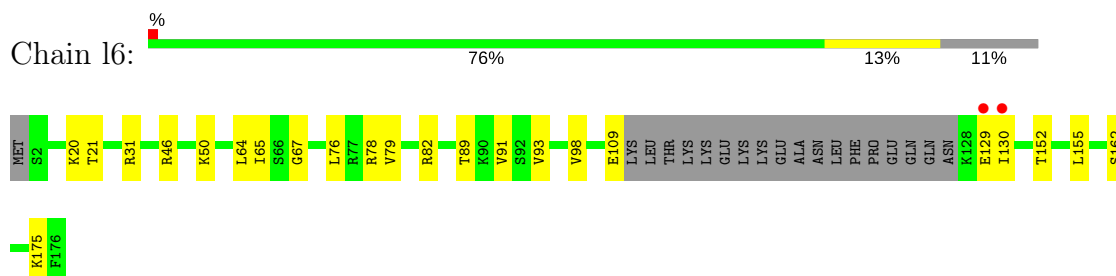
• Molecule 42: 60S ribosomal protein L5



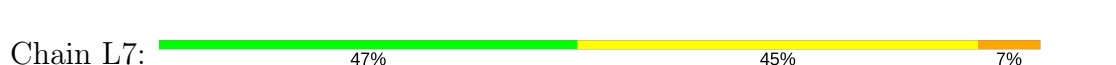
• Molecule 43: 60S ribosomal protein L6-A

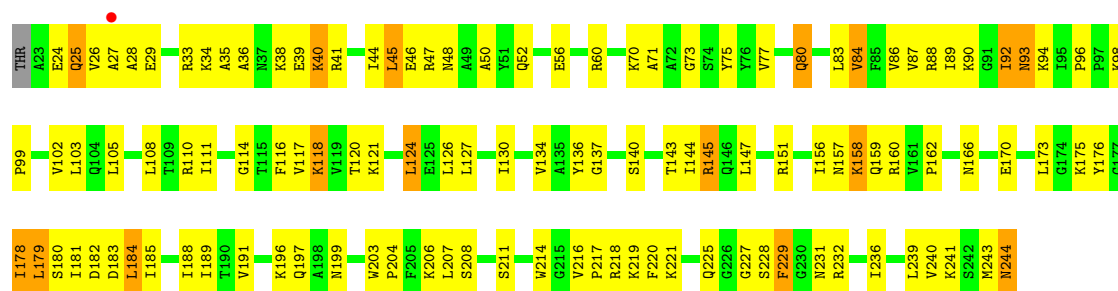


• Molecule 43: 60S ribosomal protein L6-A

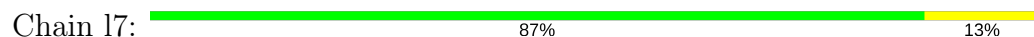


• Molecule 44: 60S ribosomal protein L7-A





• Molecule 44: 60S ribosomal protein L7-A



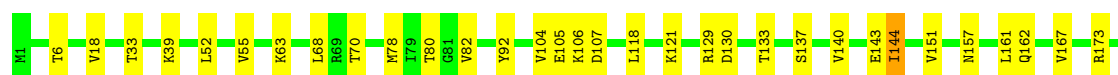
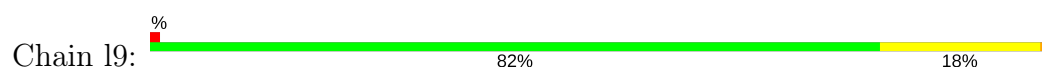
• Molecule 45: 60S ribosomal protein L8-A

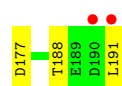


• Molecule 46: 60S ribosomal protein L9-A

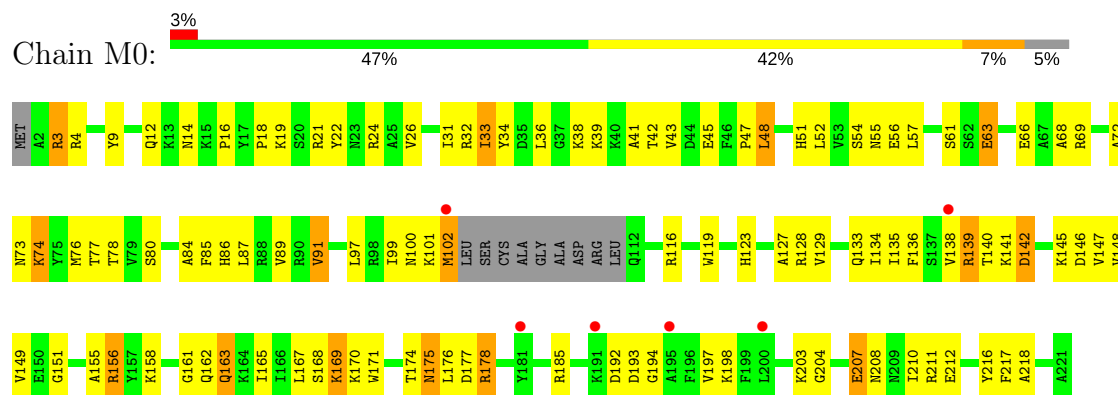


• Molecule 46: 60S ribosomal protein L9-A

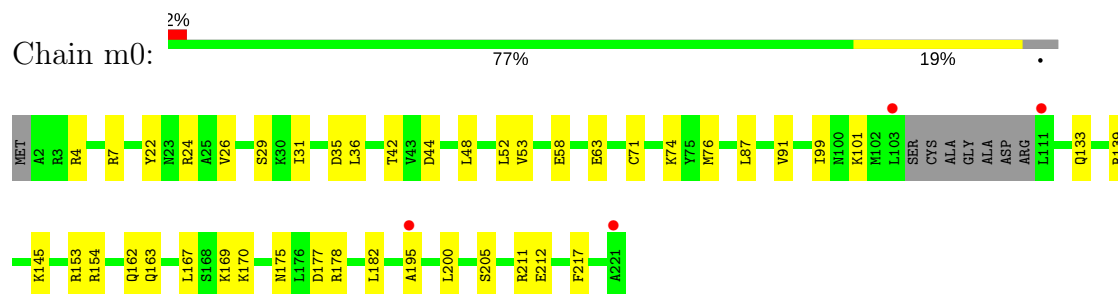




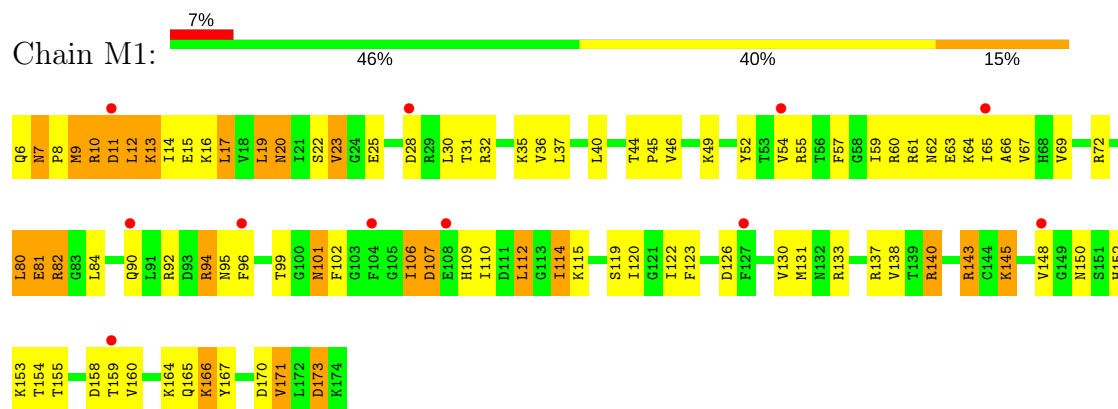
- Molecule 47: 60S ribosomal protein L10



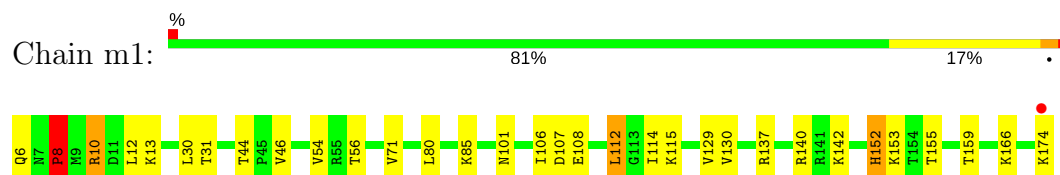
- Molecule 47: 60S ribosomal protein L10



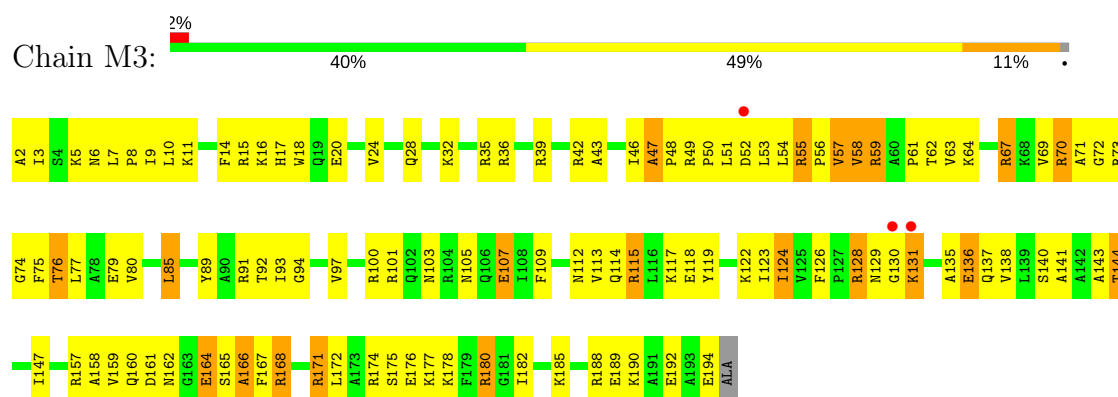
- Molecule 48: 60S ribosomal protein L11-B



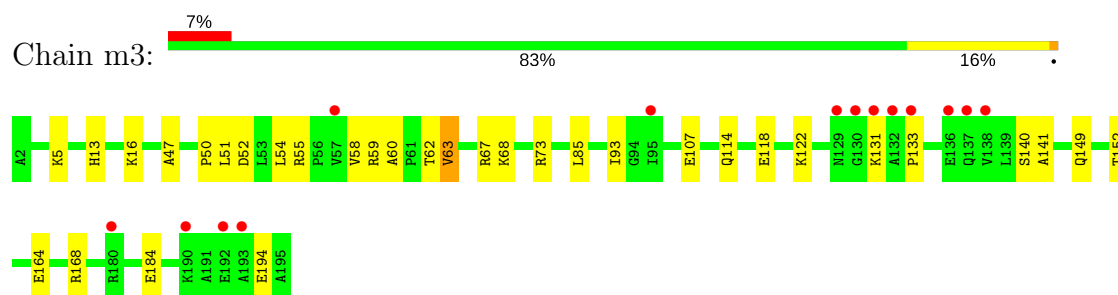
- Molecule 48: 60S ribosomal protein L11-B



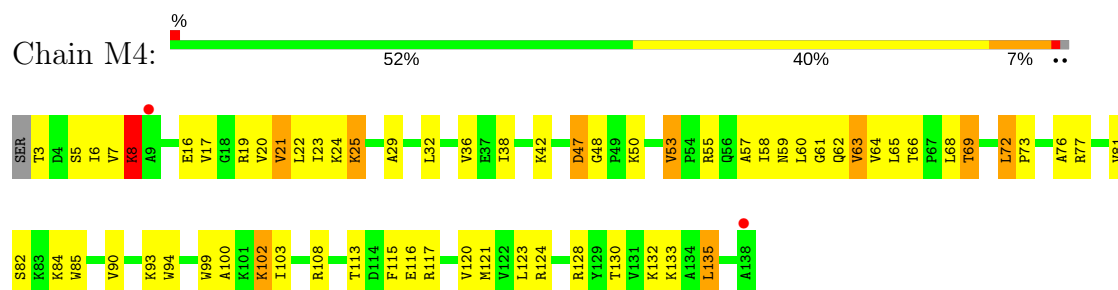
- Molecule 49: 60S ribosomal protein L13-A



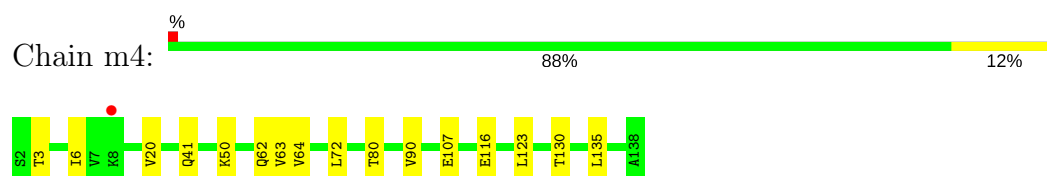
• Molecule 49: 60S ribosomal protein L13-A



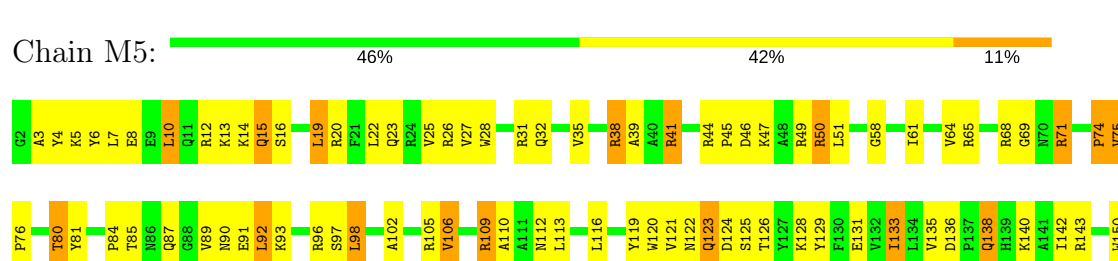
• Molecule 50: 60S ribosomal protein L14-A

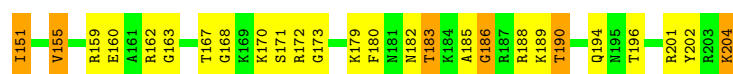


• Molecule 50: 60S ribosomal protein L14-A



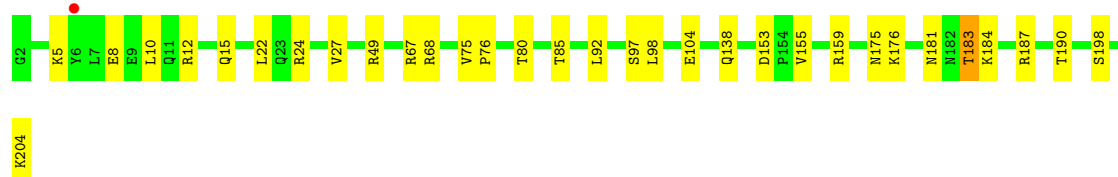
• Molecule 51: 60S ribosomal protein L15-A





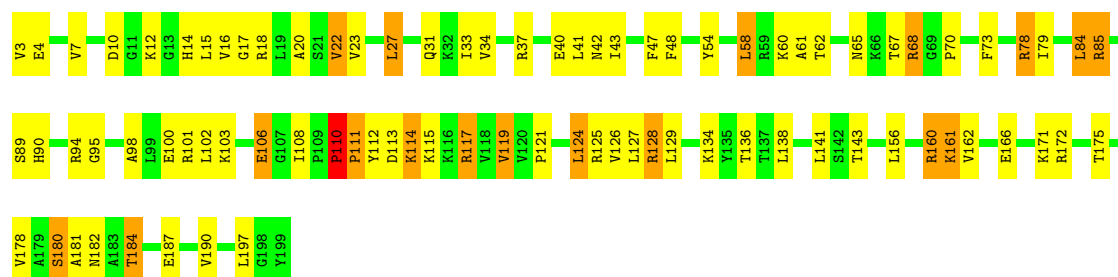
- Molecule 51: 60S ribosomal protein L15-A

Chain m5: 84% 15%



- Molecule 52: 60S ribosomal protein L16-A

Chain M6: 57% 34% 9%



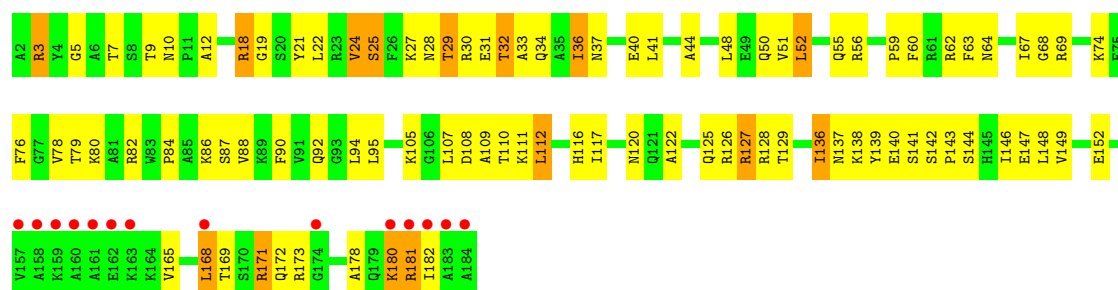
- Molecule 52: 60S ribosomal protein L16-A

Chain m6: 85% 15%



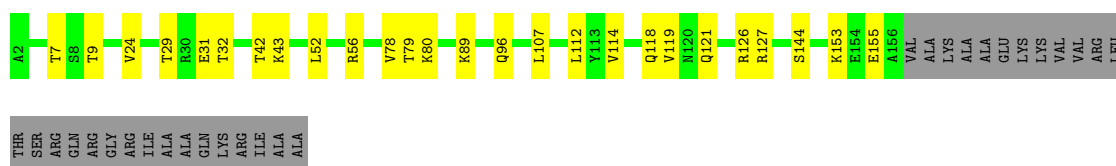
- Molecule 53: 60S ribosomal protein L17-A

Chain M7: 8% 49% 43% 8%



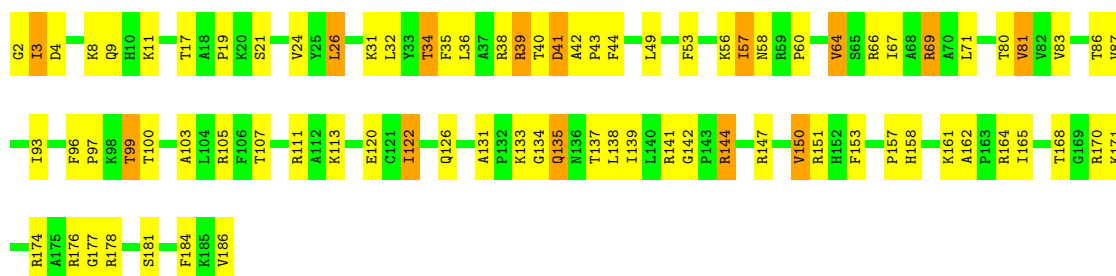
- Molecule 53: 60S ribosomal protein L17-A

Chain m7: 70% 14% 15%



- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 56% 37% 8%



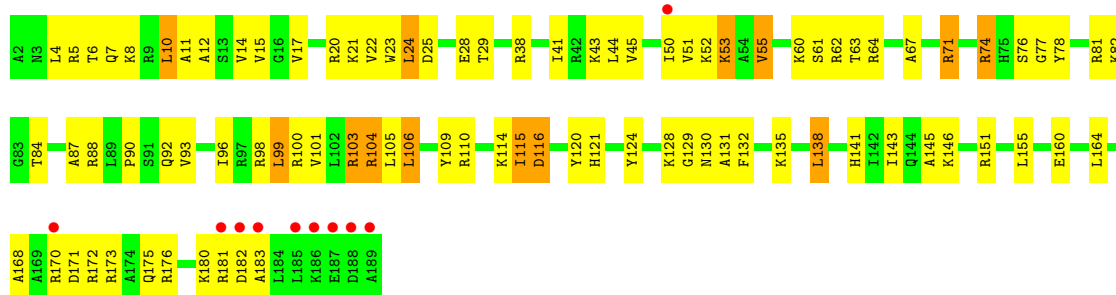
- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 85% 15%



- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 5% 52% 41% 7%



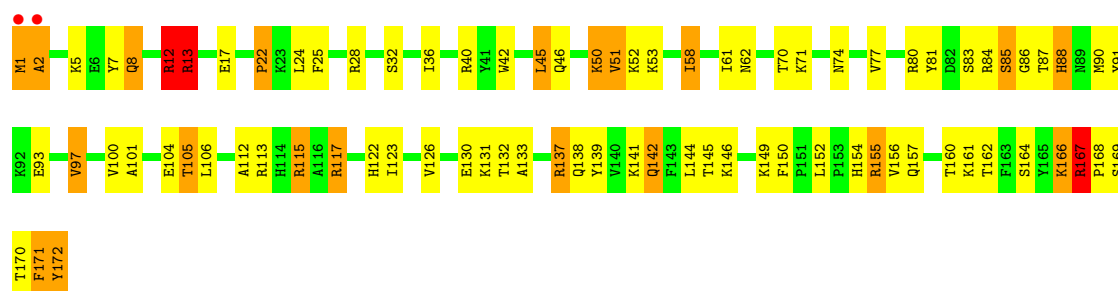
- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 3% 88% 12%



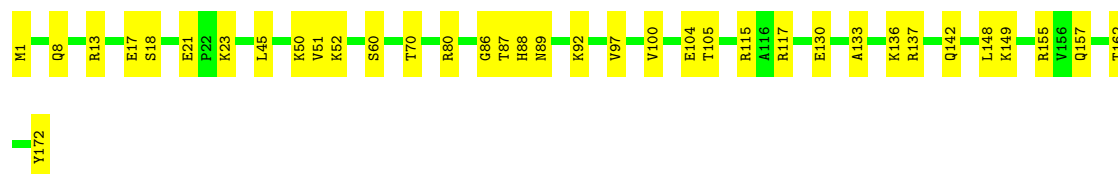
- Molecule 56: 60S ribosomal protein L20-A

Chain N0: 52% 35% 12%



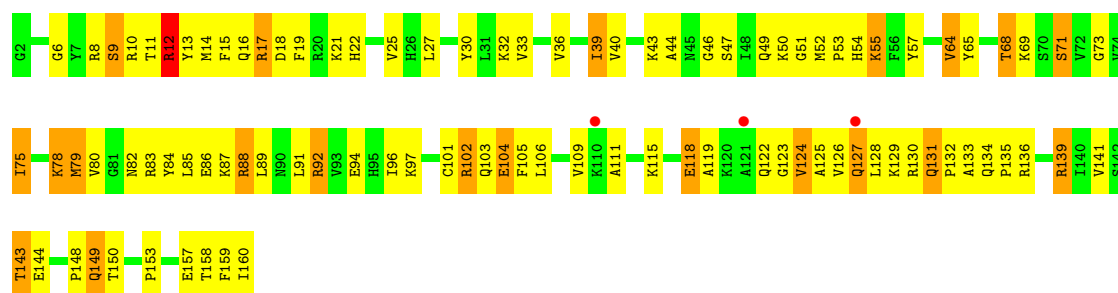
- Molecule 56: 60S ribosomal protein L20-A

Chain n0: 79% 21%



- Molecule 57: 60S ribosomal protein L21-A

Chain N1: 2% 40% 47% 13%



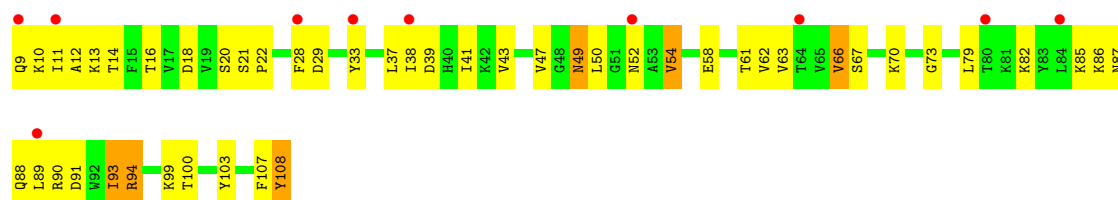
- Molecule 57: 60S ribosomal protein L21-A

Chain n1: 2% 84% 16%

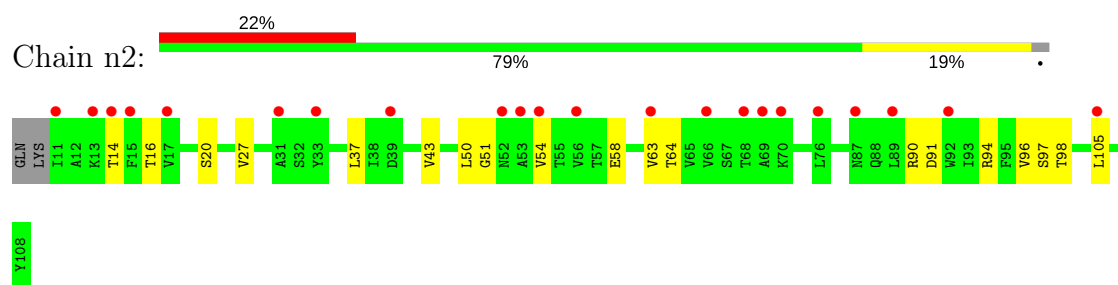


- Molecule 58: 60S ribosomal protein L22-A

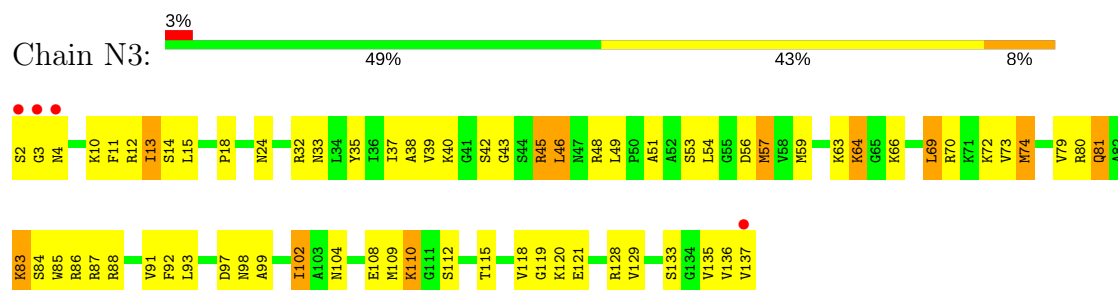
Chain N2: 10% 52% 42% 6%



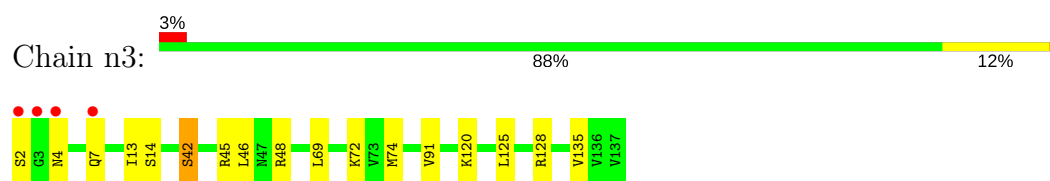
- Molecule 58: 60S ribosomal protein L22-A



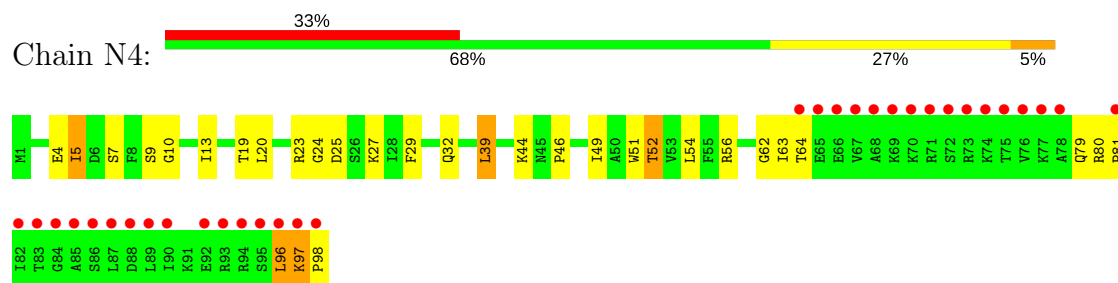
- Molecule 59: 60S ribosomal protein L23-A



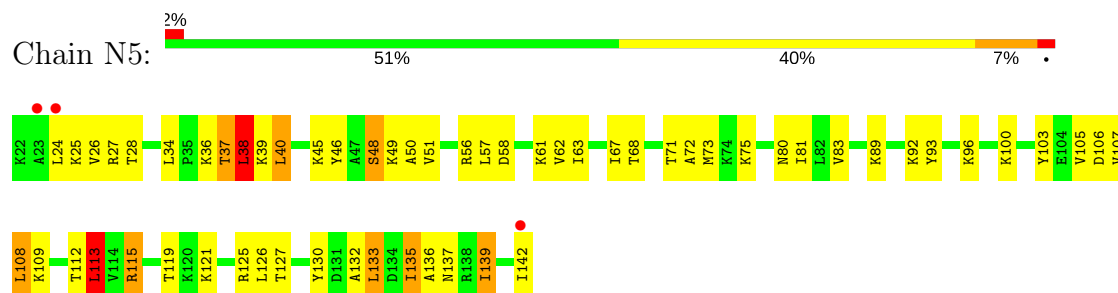
- Molecule 59: 60S ribosomal protein L23-A



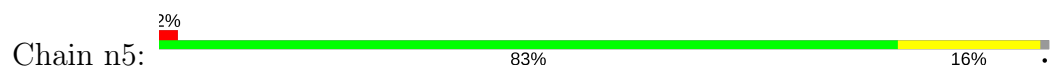
- Molecule 60: 60S ribosomal protein L24-A



- Molecule 61: 60S ribosomal protein L25



- Molecule 61: 60S ribosomal protein L25

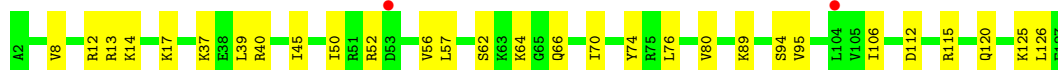
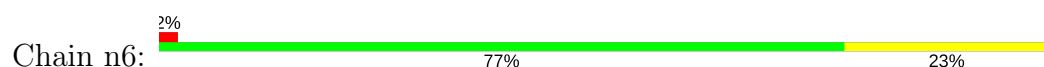




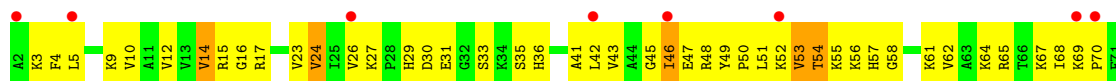
- Molecule 62: 60S ribosomal protein L26-A



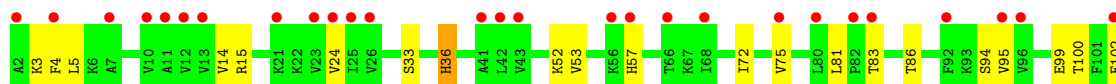
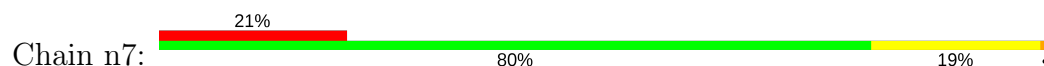
- Molecule 62: 60S ribosomal protein L26-A



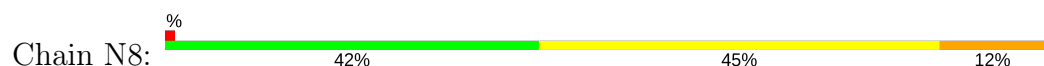
- Molecule 63: 60S ribosomal protein L27-A

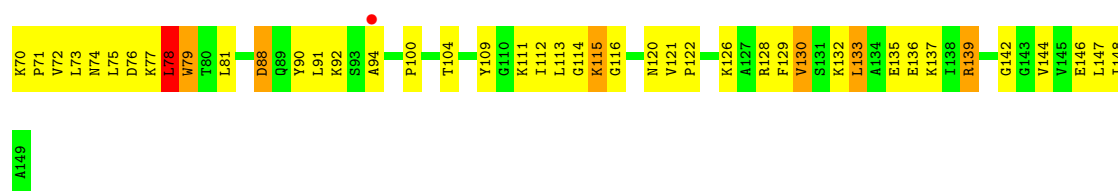


- Molecule 63: 60S ribosomal protein L27-A

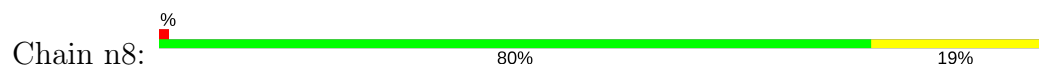


- Molecule 64: 60S ribosomal protein L28

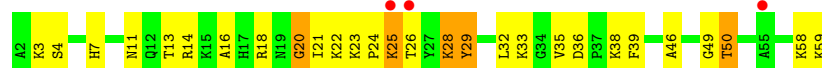




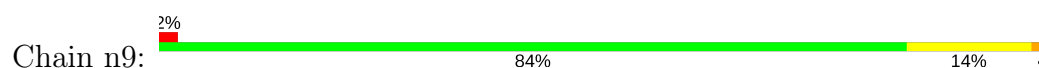
- Molecule 64: 60S ribosomal protein L28



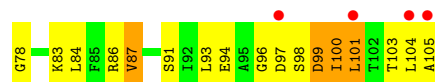
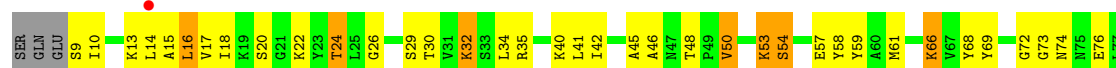
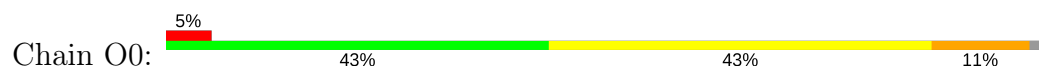
- Molecule 65: 60S ribosomal protein L29



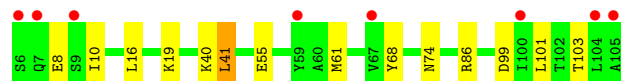
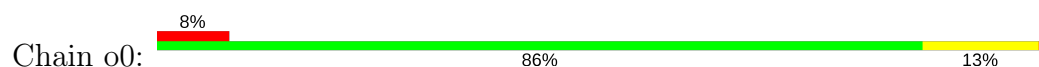
- Molecule 65: 60S ribosomal protein L29



- Molecule 66: 60S ribosomal protein L30

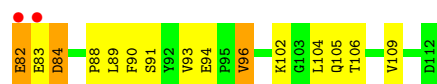


- Molecule 66: 60S ribosomal protein L30

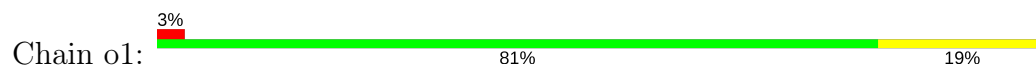


- Molecule 67: 60S ribosomal protein L31-A

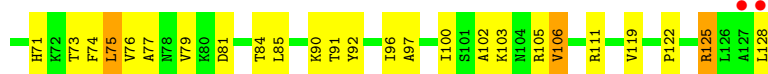




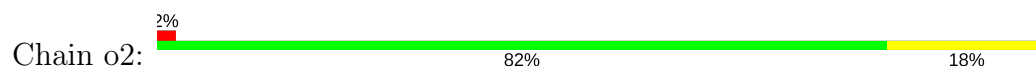
- Molecule 67: 60S ribosomal protein L31-A



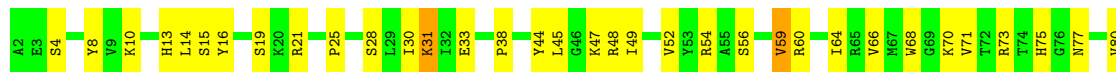
- Molecule 68: 60S ribosomal protein L32



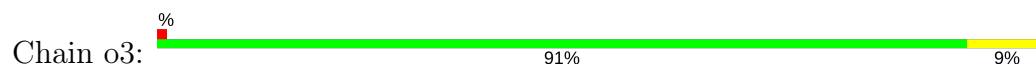
- Molecule 68: 60S ribosomal protein L32



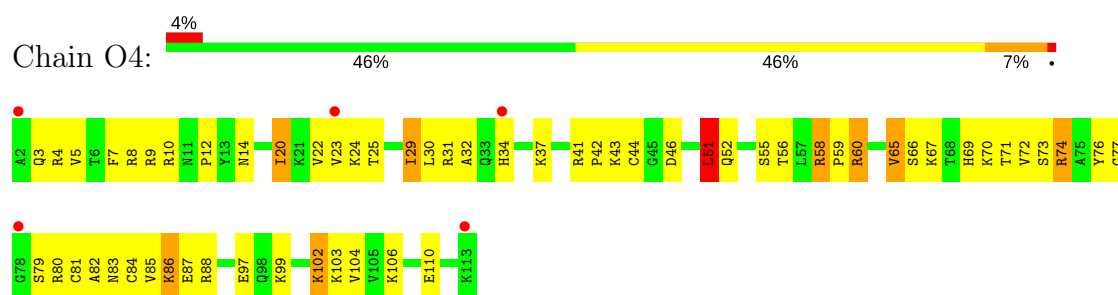
- Molecule 69: 60S ribosomal protein L33-A



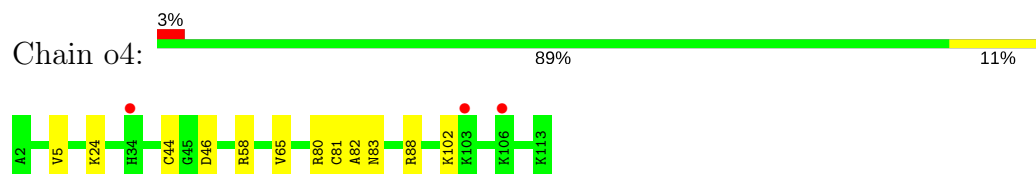
- Molecule 69: 60S ribosomal protein L33-A



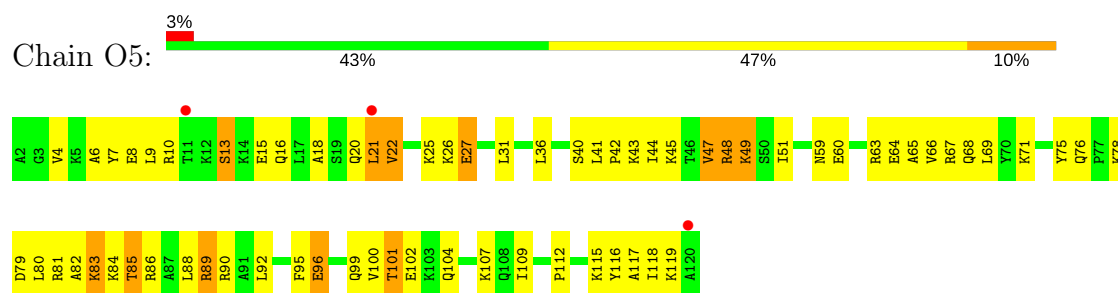
- Molecule 70: 60S ribosomal protein L34-A



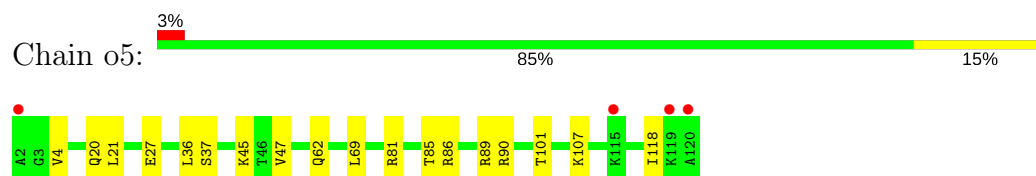
- Molecule 70: 60S ribosomal protein L34-A



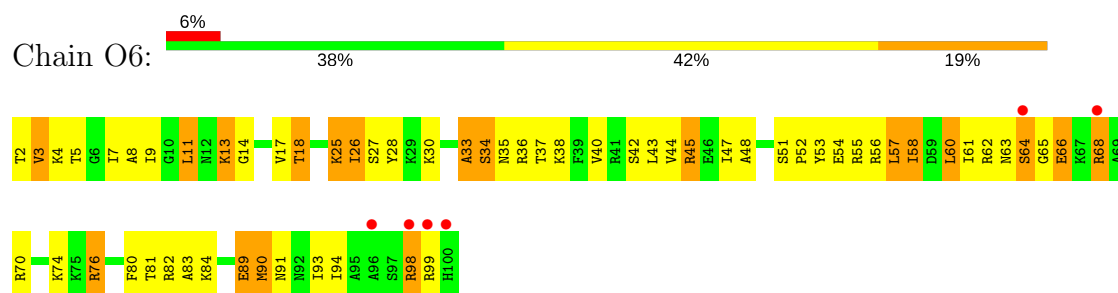
- Molecule 71: 60S ribosomal protein L35-A



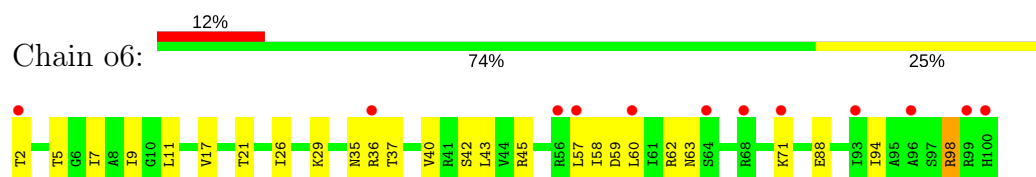
- Molecule 71: 60S ribosomal protein L35-A



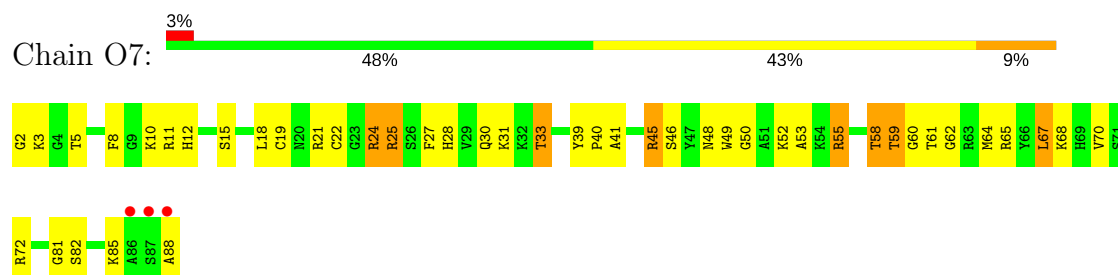
- Molecule 72: 60S ribosomal protein L36-A



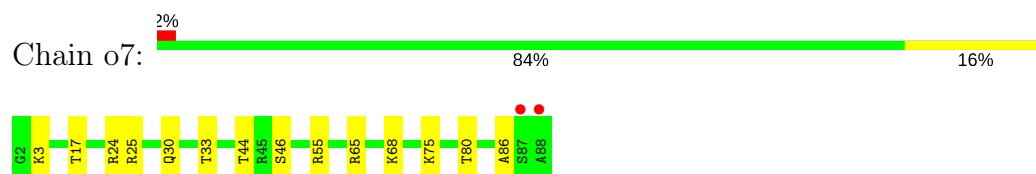
- Molecule 72: 60S ribosomal protein L36-A



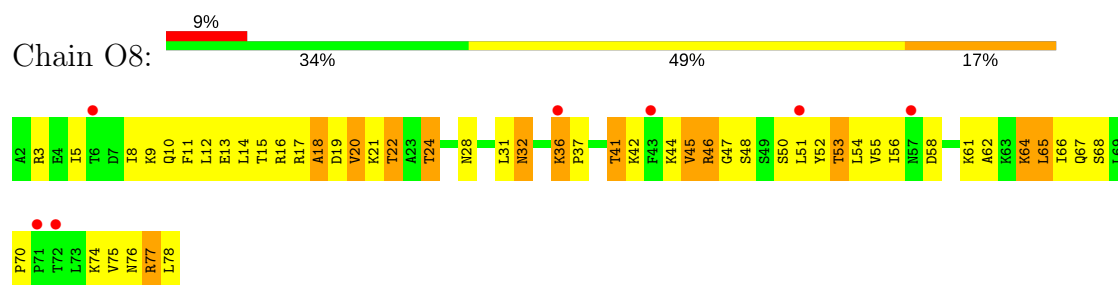
- Molecule 73: 60S ribosomal protein L37-A



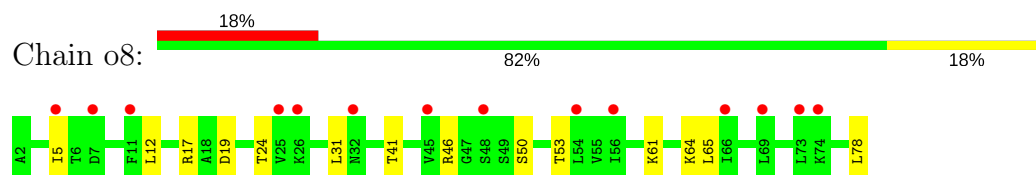
- Molecule 73: 60S ribosomal protein L37-A



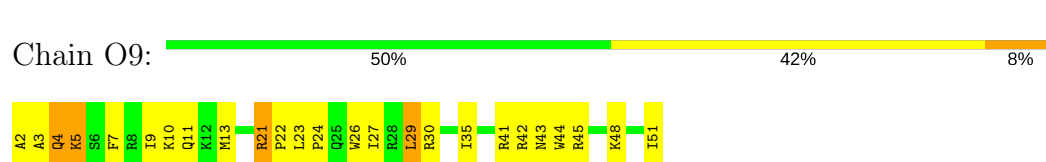
- Molecule 74: 60S ribosomal protein L38



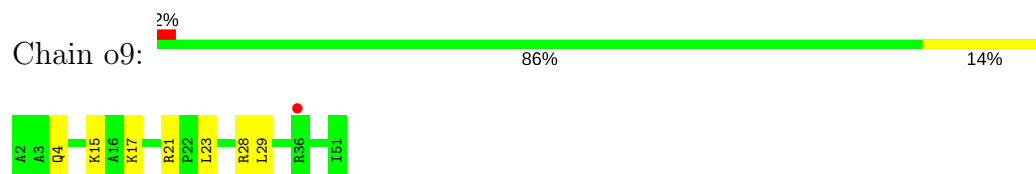
- Molecule 74: 60S ribosomal protein L38



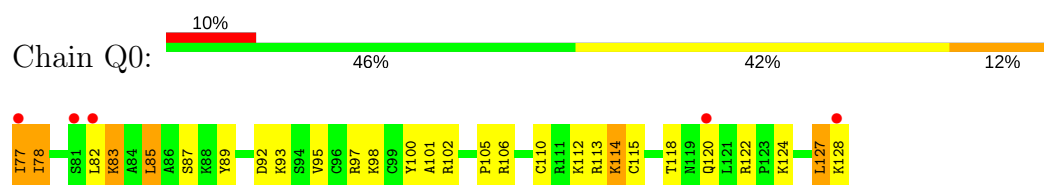
- Molecule 75: 60S ribosomal protein L39



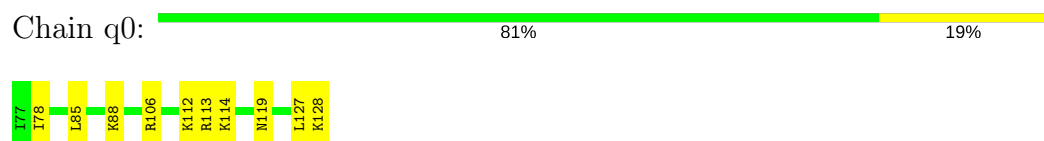
- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40



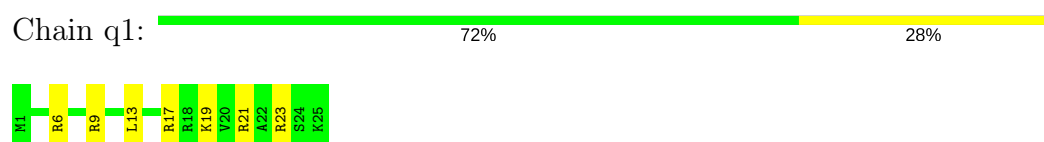
- Molecule 76: Ubiquitin-60S ribosomal protein L40



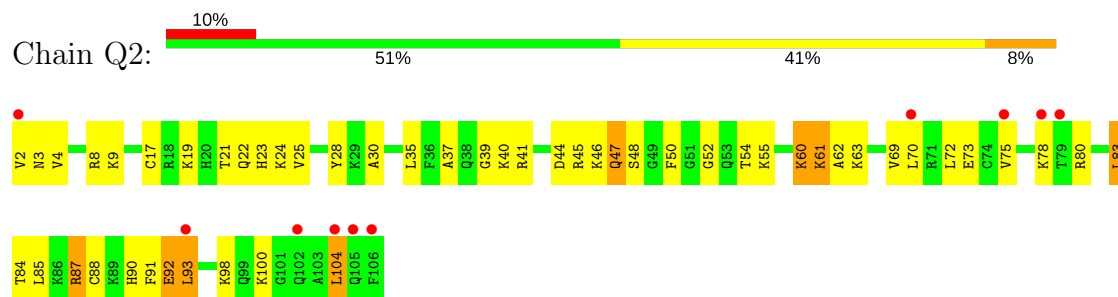
- Molecule 77: 60S ribosomal protein L41-A



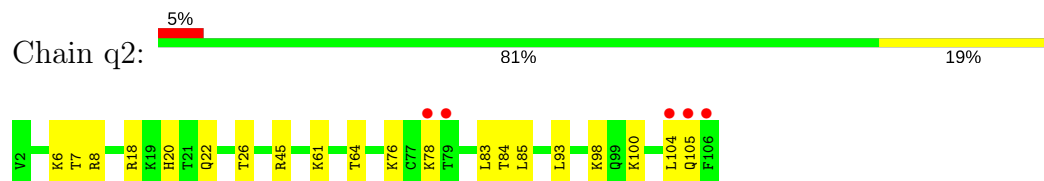
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A

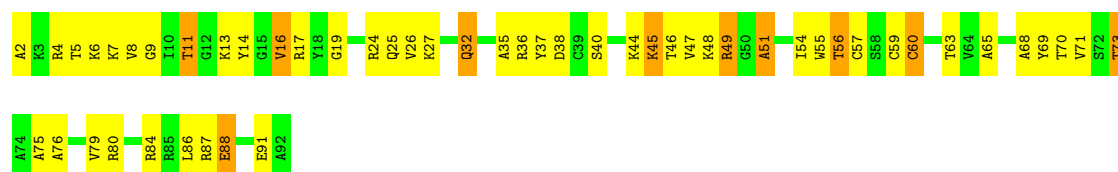


- Molecule 78: 60S ribosomal protein L42-A

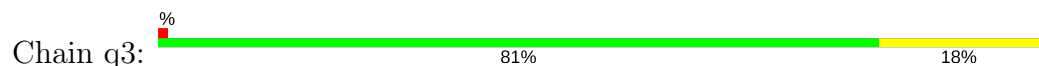


- Molecule 79: 60S ribosomal protein L43-A

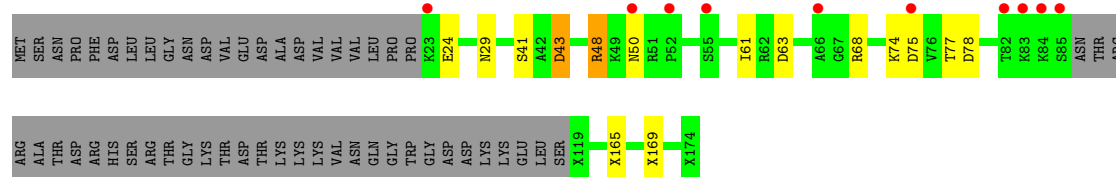




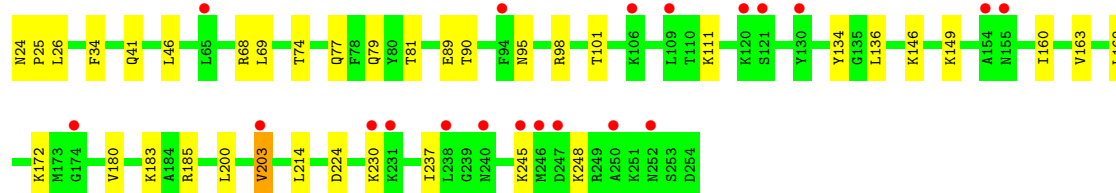
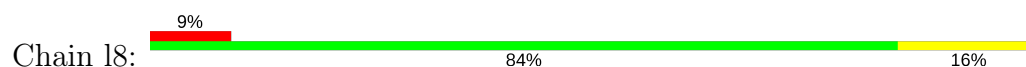
- Molecule 79: 60S ribosomal protein L43-A



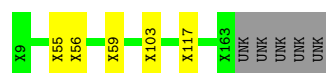
- Molecule 80: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein STM1



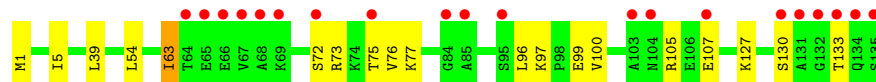
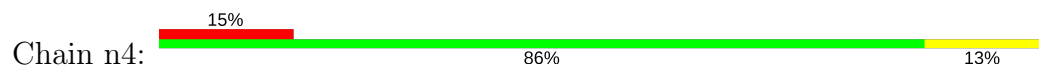
- Molecule 81: 60S ribosomal protein L8-A



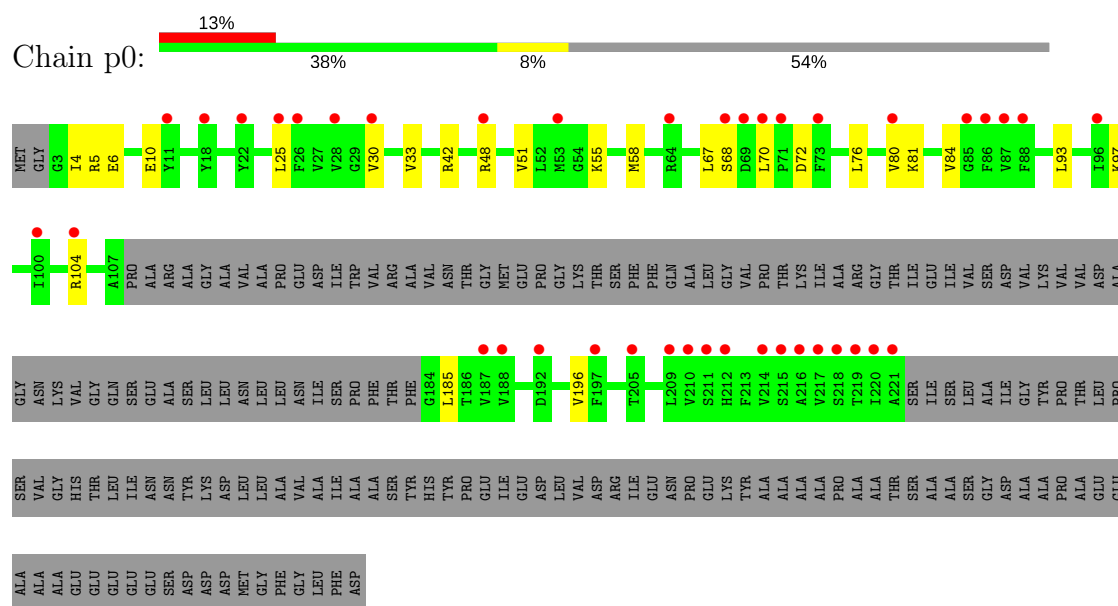
- Molecule 82: 60S ribosomal protein L12



- Molecule 83: 60S ribosomal protein L24-A



- Molecule 84: 60S acidic ribosomal protein P0



- Molecule 85: Ribosomal protein P1 alpha, P2 beta



There are no outlier residues recorded for this chain.

- Molecule 85: Ribosomal protein P1 alpha, P2 beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	434.23Å 287.91Å 304.12Å 90.00° 99.11° 90.00°	Depositor
Resolution (Å)	103.62 – 3.10 103.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (103.62-3.10) 91.8 (103.62-3.10)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.251 0.212 , 0.249	Depositor DCC
R_{free} test set	26600 reflections (2.22%)	DCC
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	410475	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.37	0/42442	0.93	91/66130 (0.1%)
1	6	0.42	1/42765 (0.0%)	0.93	69/66634 (0.1%)
2	S0	0.33	0/1617	0.59	0/2215
2	s0	0.33	0/1623	0.60	1/2222 (0.0%)
3	S1	0.30	0/1735	0.61	0/2335
3	s1	0.32	1/1748 (0.1%)	0.61	0/2352
4	S2	0.32	0/1665	0.59	0/2263
4	s2	0.33	0/1665	0.62	0/2263
5	S3	0.31	0/1759	0.56	0/2368
5	s3	0.31	0/1759	0.57	0/2368
6	S4	0.32	0/2109	0.63	2/2839 (0.1%)
6	s4	0.34	0/2109	0.66	3/2839 (0.1%)
7	S5	0.28	0/1629	0.56	0/2202
7	s5	0.30	0/1629	0.57	0/2202
8	S6	0.31	0/1823	0.53	0/2439
8	s6	0.34	0/1779	0.58	0/2379
9	S7	0.32	0/1506	0.66	1/2028 (0.0%)
9	s7	0.31	0/1516	0.63	1/2043 (0.0%)
10	S8	0.33	0/1514	0.60	1/2021 (0.0%)
10	s8	0.35	0/1514	0.59	1/2021 (0.0%)
11	S9	0.31	0/1519	0.57	1/2035 (0.0%)
11	s9	0.33	0/1519	0.60	0/2035
12	C0	0.30	0/789	0.67	1/1067 (0.1%)
12	c0	0.30	0/776	0.70	3/1047 (0.3%)
13	C1	0.35	0/1239	0.60	0/1673
13	c1	0.39	1/1194 (0.1%)	0.61	1/1610 (0.1%)
14	C2	0.31	0/898	0.69	1/1220 (0.1%)
14	c2	0.28	0/898	0.67	1/1220 (0.1%)
15	C3	0.33	0/1215	0.55	1/1638 (0.1%)
15	c3	0.31	0/1215	0.60	1/1638 (0.1%)
16	C4	0.30	0/901	0.62	0/1217
16	c4	0.32	0/960	0.57	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.33	0/998	0.60	0/1341
17	c5	0.31	0/1060	0.65	1/1426 (0.1%)
18	C6	0.30	0/1125	0.66	2/1510 (0.1%)
18	c6	0.31	0/1131	0.57	1/1518 (0.1%)
19	C7	0.36	0/935	0.72	2/1254 (0.2%)
19	c7	0.31	0/914	0.60	0/1224
20	C8	0.30	0/1211	0.58	0/1628
20	c8	0.31	0/1211	0.59	1/1628 (0.1%)
21	C9	0.30	0/1130	0.52	0/1517
21	c9	0.35	0/1130	0.55	0/1517
22	D0	0.32	0/865	0.60	0/1169
22	d0	0.32	0/892	0.60	0/1205
23	D1	0.31	0/693	0.58	0/935
23	d1	0.31	0/693	0.58	0/935
24	D2	0.32	0/1038	0.62	3/1395 (0.2%)
24	d2	0.35	0/1038	0.61	1/1395 (0.1%)
25	D3	0.37	0/1139	0.61	0/1518
25	d3	0.38	0/1139	0.60	0/1518
26	D4	0.32	0/1087	0.57	0/1449
26	d4	0.34	0/1087	0.64	1/1449 (0.1%)
27	D5	0.31	0/571	0.62	0/768
27	d5	0.31	0/566	0.51	0/761
28	D6	0.32	0/782	0.67	1/1047 (0.1%)
28	d6	0.34	0/782	0.58	0/1047
29	D7	0.28	0/620	0.61	0/838
29	d7	0.30	0/620	0.63	0/838
30	D8	0.27	0/499	0.54	0/670
30	d8	0.31	0/499	0.59	0/670
31	D9	0.40	0/452	0.68	1/600 (0.2%)
31	d9	0.32	0/452	0.57	0/600
32	E0	0.30	0/483	0.55	0/643
32	e0	0.35	0/499	0.66	0/665
33	E1	0.33	0/577	0.87	1/770 (0.1%)
33	e1	0.35	0/619	0.91	3/822 (0.4%)
34	SR	0.29	0/2490	0.55	0/3389
34	sR	0.28	0/2491	0.56	0/3391
35	SM	0.32	0/984	0.60	0/1323
36	1	0.53	0/75394	0.99	140/117545 (0.1%)
36	5	0.54	1/75414 (0.0%)	0.99	107/117575 (0.1%)
37	3	0.41	0/2883	0.86	1/4491 (0.0%)
37	7	0.52	0/2883	0.96	2/4491 (0.0%)
38	4	0.52	0/3746	0.97	3/5832 (0.1%)
38	8	0.44	0/3746	0.90	5/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.38	0/1948	0.63	0/2617
39	l2	0.37	0/1946	0.65	1/2614 (0.0%)
40	L3	0.38	0/3146	0.63	0/4228
40	l3	0.43	0/3146	0.65	1/4228 (0.0%)
41	L4	0.41	0/2800	0.66	3/3790 (0.1%)
41	l4	0.38	0/2800	0.65	1/3790 (0.0%)
42	L5	0.34	0/2425	0.60	1/3271 (0.0%)
42	l5	0.39	0/2408	0.59	1/3248 (0.0%)
43	L6	0.37	0/1260	0.58	0/1694
43	l6	0.40	0/1269	0.62	1/1705 (0.1%)
44	L7	0.38	0/1821	0.58	0/2451
44	l7	0.41	0/1828	0.62	2/2461 (0.1%)
45	L8	0.33	0/1836	0.54	0/2481
46	L9	0.33	0/1539	0.56	0/2073
46	l9	0.39	0/1539	0.58	0/2073
47	M0	0.38	0/1741	0.60	1/2335 (0.0%)
47	m0	0.42	0/1758	0.65	0/2358
48	M1	0.32	0/1374	0.56	0/1842
48	m1	0.36	0/1374	0.67	3/1842 (0.2%)
49	M3	0.39	0/1568	0.65	1/2106 (0.0%)
49	m3	0.36	0/1573	0.62	0/2113
50	M4	0.36	0/1068	0.55	0/1438
50	m4	0.40	0/1074	0.56	0/1446
51	M5	0.38	0/1757	0.60	0/2354
51	m5	0.35	0/1757	0.59	0/2354
52	M6	0.42	0/1585	0.57	0/2128
52	m6	0.52	0/1585	0.61	0/2128
53	M7	0.39	0/1443	0.63	0/1944
53	m7	0.43	0/1250	0.61	0/1683
54	M8	0.39	0/1465	0.63	1/1965 (0.1%)
54	m8	0.38	0/1465	0.61	0/1965
55	M9	0.31	0/1538	0.51	1/2050 (0.0%)
55	m9	0.34	0/1538	0.47	0/2050
56	N0	0.37	0/1481	0.62	0/1990
56	n0	0.42	0/1481	0.58	0/1990
57	N1	0.39	0/1300	0.60	0/1743
57	n1	0.43	0/1300	0.59	0/1743
58	N2	0.33	0/812	0.59	0/1099
58	n2	0.32	0/794	0.56	0/1076
59	N3	0.38	0/1018	0.60	0/1369
59	n3	0.43	0/1018	0.65	0/1369
60	N4	0.34	0/712	0.62	2/958 (0.2%)
61	N5	0.35	0/979	0.62	2/1321 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	n5	0.34	0/974	0.58	0/1314
62	N6	0.38	0/1004	0.65	1/1341 (0.1%)
62	n6	0.36	0/1004	0.63	0/1341
63	N7	0.33	0/1118	0.54	0/1497
63	n7	0.40	1/1118 (0.1%)	0.53	0/1497
64	N8	0.41	0/1204	0.67	1/1612 (0.1%)
64	n8	0.40	0/1204	0.71	1/1612 (0.1%)
65	N9	0.38	0/473	0.57	0/629
65	n9	0.39	0/473	0.64	0/629
66	O0	0.31	0/751	0.52	0/1008
66	o0	0.30	0/775	0.54	1/1040 (0.1%)
67	O1	0.36	0/890	0.55	0/1196
67	o1	0.40	0/897	0.63	0/1205
68	O2	0.46	1/1041 (0.1%)	0.60	0/1394
68	o2	0.42	0/1041	0.65	0/1394
69	O3	0.43	0/868	0.60	0/1168
69	o3	0.46	0/868	0.67	0/1168
70	O4	0.33	0/890	0.59	1/1189 (0.1%)
70	o4	0.33	0/890	0.58	0/1189
71	O5	0.37	0/978	0.60	1/1301 (0.1%)
71	o5	0.33	0/974	0.51	0/1297
72	O6	0.34	0/778	0.57	0/1034
72	o6	0.34	0/777	0.58	0/1033
73	O7	0.41	0/696	0.70	0/923
73	o7	0.38	0/696	0.67	0/923
74	O8	0.33	0/618	0.55	0/826
74	o8	0.31	0/614	0.56	0/822
75	O9	0.41	0/443	0.65	0/588
75	o9	0.38	0/443	0.57	0/588
76	Q0	0.38	0/423	0.62	0/562
76	q0	0.47	0/423	0.66	0/562
77	Q1	0.33	0/234	0.54	0/300
77	q1	0.39	0/234	0.58	0/300
78	Q2	0.39	0/860	0.64	1/1136 (0.1%)
78	q2	0.38	0/860	0.58	0/1136
79	Q3	0.39	0/701	0.62	0/934
79	q3	0.40	0/701	0.63	0/934
80	sM	0.34	0/480	0.64	0/642
81	l8	0.33	0/1795	0.55	0/2429
83	n4	0.37	0/1052	0.63	1/1398 (0.1%)
84	p0	0.33	0/1092	0.55	0/1474
All	All	0.44	6/430471 (0.0%)	0.84	486/632040 (0.1%)

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
2	S0	0	1
2	s0	0	3
3	S1	0	1
3	s1	0	1
4	S2	0	1
4	s2	0	2
5	S3	0	1
5	s3	0	1
6	S4	0	1
7	S5	0	3
7	s5	0	4
9	S7	0	2
9	s7	0	3
10	S8	0	2
10	s8	0	1
11	s9	0	1
14	c2	0	1
15	c3	0	1
16	C4	0	3
16	c4	0	2
17	C5	0	2
17	c5	0	3
18	C6	0	2
18	c6	0	2
19	C7	0	1
19	c7	0	3
20	c8	0	1
22	D0	0	1
22	d0	0	1
23	d1	0	1
24	D2	0	1
24	d2	0	1
25	D3	0	1
25	d3	0	1
26	D4	0	1
26	d4	0	1
27	D5	0	2
27	d5	0	2
28	D6	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	e0	0	1
33	E1	0	3
33	e1	0	3
34	sR	0	1
39	l2	0	1
40	l3	0	2
41	L4	0	1
41	l4	0	1
42	L5	0	3
42	l5	0	3
43	l6	0	1
44	l7	0	1
45	L8	0	2
46	L9	0	1
48	m1	0	1
49	M3	0	1
49	m3	0	1
50	M4	0	1
50	m4	0	1
51	M5	0	1
51	m5	0	1
52	M6	0	1
52	m6	0	1
53	m7	0	1
56	N0	0	3
56	n0	0	2
57	N1	0	1
58	n2	0	1
60	N4	0	2
63	n7	0	2
64	n8	0	1
65	N9	0	1
65	n9	0	1
66	o0	0	1
67	o1	0	1
70	o4	0	1
71	o5	0	1
79	Q3	0	1
79	q3	0	1
80	sM	0	2
81	l8	0	1
82	m2	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	126

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-8.63	1.31	1.38
63	n7	36	HIS	C-N	7.01	1.47	1.34
68	O2	51	SER	C-N	-6.35	1.19	1.34
1	6	163	G	N9-C4	-5.93	1.33	1.38
13	c1	128	CYS	CB-SG	-5.29	1.73	1.81

The worst 5 of 486 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-16.34	116.20	126.00
36	5	1152	G	N3-C4-C5	15.93	136.56	128.60
1	6	163	G	N3-C4-N9	-11.53	119.08	126.00
36	1	1308	A	C8-N9-C4	-11.40	101.24	105.80
36	5	2726	C	C6-N1-C2	-10.77	115.99	120.30

There are no chirality outliers.

5 of 126 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S0	94	GLY	Peptide
3	S1	131	ASP	Peptide
4	S2	106	ASP	Peptide
5	S3	219	ALA	Peptide
6	S4	57	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37948	0	19094	791	1
1	6	38238	0	19240	741	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S0	1577	0	1567	125	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	151	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	132	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	101	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	138	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	145	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1878	95	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	100	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	119	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	121	0
11	s9	1494	0	1573	0	0
12	C0	772	0	727	57	0
12	c0	761	0	697	0	0
13	C1	1213	0	1257	73	0
13	c1	1168	0	1233	0	0
14	C2	890	0	887	65	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	60	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	69	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	83	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	107	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	70	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	110	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	74	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	70	0
22	d0	882	0	939	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	D1	684	0	672	63	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	66	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	66	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	79	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	75	0
27	d5	558	0	598	0	0
28	D6	769	0	814	80	0
28	d6	769	0	814	0	0
29	D7	610	0	633	37	0
29	d7	610	0	633	0	0
30	D8	497	0	535	45	0
30	d8	497	0	535	0	0
31	D9	442	0	428	29	0
31	d9	442	0	430	0	0
32	E0	475	0	525	37	0
32	e0	491	0	542	0	0
33	E1	566	0	602	53	0
33	e1	608	0	658	0	0
34	SR	2437	0	2386	147	0
34	sR	2438	0	2381	0	0
35	SM	1104	0	969	72	0
36	1	67355	0	33847	1180	1
36	5	67376	0	33859	1117	1
37	3	2579	0	1304	50	0
37	7	2579	0	1304	50	0
38	4	3353	0	1695	72	0
38	8	3353	0	1695	61	0
39	L2	1914	0	1981	143	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	209	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	188	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	184	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	59	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	118	0
46	L9	1518	0	1587	114	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	105	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	84	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	121	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	58	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	121	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	82	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	91	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	82	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	84	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	73	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	94	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	29	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	64	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	19	0
61	N5	964	0	1025	54	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	70	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	80	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	96	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	26	0
65	n9	462	0	491	0	0
66	O0	743	0	797	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	o0	767	0	816	0	0
67	O1	876	0	912	43	0
67	o1	883	0	918	0	0
68	O2	1020	0	1089	70	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	49	0
69	o3	850	0	880	0	0
70	O4	880	0	945	65	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	67	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	61	0
72	o6	770	0	846	0	0
73	O7	681	0	682	43	0
73	o7	681	0	683	0	0
74	O8	612	0	682	30	0
74	o8	608	0	671	0	0
75	O9	436	0	475	28	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	30	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	15	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	40	0
78	q2	847	0	918	0	0
79	Q3	694	0	735	45	0
79	q3	694	0	734	0	0
80	sM	680	0	538	0	0
81	l8	1763	0	1819	0	0
82	m2	750	0	167	0	0
83	n4	1038	0	1071	0	0
84	p0	1077	0	1041	0	0
85	p1	235	0	49	0	0
85	p2	230	0	49	0	0
86	1	2184	0	0	187	0
86	2	896	0	0	90	0
86	3	56	0	0	2	0
86	4	105	0	0	9	0
86	5	2268	0	0	208	0
86	6	959	0	0	100	0
86	7	77	0	0	3	0
86	8	105	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	C1	7	0	0	1	0
86	C3	7	0	0	1	0
86	C5	7	0	0	5	0
86	C8	7	0	0	0	1
86	L3	14	0	0	3	0
86	L4	7	0	0	3	0
86	M0	7	0	0	3	0
86	M5	7	0	0	0	0
86	M7	7	0	0	0	0
86	M9	7	0	0	1	0
86	N9	7	0	0	1	0
86	O1	7	0	0	5	0
86	O3	7	0	0	3	0
86	Q2	7	0	0	4	0
86	S8	7	0	0	2	0
86	S9	7	0	0	4	0
86	SR	7	0	0	1	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	l3	14	0	0	0	0
86	l4	7	0	0	0	0
86	l5	14	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	n1	7	0	0	0	0
86	n3	14	0	0	0	0
86	n9	7	0	0	0	0
86	o3	7	0	0	0	0
86	o7	7	0	0	0	0
86	q2	7	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	1	353	0	0	0	0
87	2	91	0	0	0	0
87	3	8	0	0	0	0
87	4	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	5	383	0	0	0	0
87	6	98	0	0	0	0
87	7	11	0	0	0	0
87	8	9	0	0	0	0
87	D3	1	0	0	0	0
87	L2	2	0	0	0	0
87	L3	1	0	0	0	0
87	L4	1	0	0	0	0
87	L7	3	0	0	0	0
87	M0	1	0	0	0	0
87	M3	2	0	0	0	0
87	M5	2	0	0	0	0
87	M7	3	0	0	0	0
87	M9	1	0	0	0	0
87	N3	1	0	0	0	0
87	N8	2	0	0	0	0
87	O2	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q2	1	0	0	0	0
87	S2	1	0	0	0	0
87	c1	1	0	0	0	0
87	c6	1	0	0	0	0
87	d3	1	0	0	0	0
87	d6	1	0	0	0	0
87	l2	3	0	0	0	0
87	l3	1	0	0	0	0
87	m5	3	0	0	0	0
87	m7	2	0	0	0	0
87	n3	1	0	0	0	0
87	n6	2	0	0	0	0
87	n8	2	0	0	0	0
87	n9	1	0	0	0	0
87	o7	2	0	0	0	0
87	q0	1	0	0	0	0
87	q1	1	0	0	0	0
87	q2	1	0	0	0	0
87	sM	1	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	Q0	1	0	0	0	0
88	Q2	1	0	0	0	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
89	6	30	0	28	0	0
All	All	410475	0	297522	8655	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 8655 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S7:64:VAL:HG22	9:S7:94:ALA:HB1	3.28	1.08
50:M4:48:GLY:HA3	50:M4:53:VAL:HB	3.99	1.05
1:2:702:G:HO2'	1:2:703:G:H8	1.00	0.98
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.43	0.98
36:1:2656:A:H4'	78:Q2:98:LYS:HD2	1.45	0.96

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:3195:U:OP1	86:C8:201:OHX:N6[2_555]	2.11	0.09
1:2:1353:U:O2'	36:5:3165:A:OP1[2_546]	2.12	0.08

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%)	173 (85%)	27 (13%)	4 (2%)	9	37
2	s0	204/206 (99%)	175 (86%)	21 (10%)	8 (4%)	3	21
3	S1	212/216 (98%)	167 (79%)	40 (19%)	5 (2%)	7	32
3	s1	214/216 (99%)	182 (85%)	29 (14%)	3 (1%)	13	47
4	S2	215/217 (99%)	200 (93%)	11 (5%)	4 (2%)	9	39
4	s2	215/217 (99%)	195 (91%)	17 (8%)	3 (1%)	13	47
5	S3	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	10	40
5	s3	221/223 (99%)	185 (84%)	31 (14%)	5 (2%)	7	33
6	S4	258/260 (99%)	232 (90%)	24 (9%)	2 (1%)	22	62
6	s4	258/260 (99%)	230 (89%)	25 (10%)	3 (1%)	15	51
7	S5	204/206 (99%)	181 (89%)	15 (7%)	8 (4%)	3	21
7	s5	204/206 (99%)	182 (89%)	19 (9%)	3 (2%)	12	45
8	S6	224/226 (99%)	207 (92%)	14 (6%)	3 (1%)	14	48
8	s6	216/226 (96%)	198 (92%)	14 (6%)	4 (2%)	9	39
9	S7	182/186 (98%)	148 (81%)	20 (11%)	14 (8%)	1	6
9	s7	184/186 (99%)	154 (84%)	27 (15%)	3 (2%)	11	43
10	S8	184/200 (92%)	161 (88%)	21 (11%)	2 (1%)	17	54
10	s8	184/200 (92%)	170 (92%)	11 (6%)	3 (2%)	11	43
11	S9	183/185 (99%)	163 (89%)	16 (9%)	4 (2%)	8	35
11	s9	183/185 (99%)	164 (90%)	18 (10%)	1 (0%)	32	71
12	C0	94/98 (96%)	75 (80%)	17 (18%)	2 (2%)	8	36
12	c0	92/98 (94%)	67 (73%)	14 (15%)	11 (12%)	0	2
13	C1	153/156 (98%)	131 (86%)	20 (13%)	2 (1%)	14	48
13	c1	144/156 (92%)	124 (86%)	15 (10%)	5 (4%)	4	23
14	C2	122/124 (98%)	89 (73%)	27 (22%)	6 (5%)	2	16
14	c2	122/124 (98%)	85 (70%)	33 (27%)	4 (3%)	4	25
15	C3	148/150 (99%)	138 (93%)	9 (6%)	1 (1%)	25	64
15	c3	148/150 (99%)	130 (88%)	15 (10%)	3 (2%)	9	37
16	C4	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	c4	126/128 (98%)	111 (88%)	14 (11%)	1 (1%)	22	62
17	C5	122/142 (86%)	102 (84%)	14 (12%)	6 (5%)	2	16
17	c5	133/142 (94%)	109 (82%)	17 (13%)	7 (5%)	2	14
18	C6	139/142 (98%)	124 (89%)	13 (9%)	2 (1%)	13	47
18	c6	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
19	C7	116/136 (85%)	100 (86%)	11 (10%)	5 (4%)	3	18
19	c7	113/136 (83%)	99 (88%)	11 (10%)	3 (3%)	6	30
20	C8	143/145 (99%)	120 (84%)	18 (13%)	5 (4%)	4	23
20	c8	143/145 (99%)	121 (85%)	17 (12%)	5 (4%)	4	23
21	C9	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
21	c9	141/143 (99%)	125 (89%)	14 (10%)	2 (1%)	13	47
22	D0	105/110 (96%)	91 (87%)	13 (12%)	1 (1%)	18	57
22	d0	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	3	17
23	D1	85/87 (98%)	71 (84%)	13 (15%)	1 (1%)	15	51
23	d1	85/87 (98%)	75 (88%)	9 (11%)	1 (1%)	15	51
24	D2	127/129 (98%)	118 (93%)	6 (5%)	3 (2%)	7	32
24	d2	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	22	62
25	D3	142/144 (99%)	118 (83%)	19 (13%)	5 (4%)	4	23
25	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
26	D4	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	3	17
26	d4	132/134 (98%)	111 (84%)	18 (14%)	3 (2%)	7	33
27	D5	68/70 (97%)	51 (75%)	14 (21%)	3 (4%)	3	18
27	d5	67/70 (96%)	58 (87%)	8 (12%)	1 (2%)	12	45
28	D6	95/97 (98%)	70 (74%)	19 (20%)	6 (6%)	1	10
28	d6	95/97 (98%)	76 (80%)	12 (13%)	7 (7%)	1	7
29	D7	79/81 (98%)	69 (87%)	8 (10%)	2 (2%)	6	31
29	d7	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	14	48
30	D8	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
30	d8	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
31	D9	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
31	d9	51/53 (96%)	48 (94%)	2 (4%)	1 (2%)	9	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	E0	58/62 (94%)	49 (84%)	7 (12%)	2 (3%)	4	24
32	e0	60/62 (97%)	51 (85%)	7 (12%)	2 (3%)	4	25
33	E1	69/76 (91%)	45 (65%)	18 (26%)	6 (9%)	1	5
33	e1	74/76 (97%)	49 (66%)	18 (24%)	7 (10%)	1	4
34	SR	316/318 (99%)	288 (91%)	28 (9%)	0	100	100
34	sR	316/318 (99%)	286 (90%)	26 (8%)	4 (1%)	14	48
35	SM	131/176 (74%)	108 (82%)	17 (13%)	6 (5%)	3	17
39	L2	250/252 (99%)	234 (94%)	15 (6%)	1 (0%)	38	75
39	l2	250/252 (99%)	225 (90%)	22 (9%)	3 (1%)	15	51
40	L3	384/386 (100%)	356 (93%)	24 (6%)	4 (1%)	18	57
40	l3	384/386 (100%)	362 (94%)	20 (5%)	2 (0%)	32	71
41	L4	359/361 (99%)	327 (91%)	32 (9%)	0	100	100
41	l4	359/361 (99%)	327 (91%)	25 (7%)	7 (2%)	9	39
42	L5	294/296 (99%)	257 (87%)	33 (11%)	4 (1%)	13	47
42	l5	292/296 (99%)	275 (94%)	17 (6%)	0	100	100
43	L6	152/176 (86%)	145 (95%)	6 (4%)	1 (1%)	25	64
43	l6	153/176 (87%)	139 (91%)	12 (8%)	2 (1%)	14	48
44	L7	220/223 (99%)	208 (94%)	11 (5%)	1 (0%)	32	71
44	l7	221/223 (99%)	208 (94%)	11 (5%)	2 (1%)	20	60
45	L8	231/233 (99%)	203 (88%)	22 (10%)	6 (3%)	6	31
46	L9	189/191 (99%)	171 (90%)	17 (9%)	1 (0%)	32	71
46	l9	189/191 (99%)	175 (93%)	12 (6%)	2 (1%)	17	54
47	M0	207/221 (94%)	188 (91%)	19 (9%)	0	100	100
47	m0	209/221 (95%)	188 (90%)	18 (9%)	3 (1%)	13	47
48	M1	167/169 (99%)	141 (84%)	20 (12%)	6 (4%)	4	23
48	m1	167/169 (99%)	143 (86%)	18 (11%)	6 (4%)	4	23
49	M3	191/194 (98%)	171 (90%)	14 (7%)	6 (3%)	5	26
49	m3	192/194 (99%)	166 (86%)	17 (9%)	9 (5%)	3	17
50	M4	134/137 (98%)	125 (93%)	7 (5%)	2 (2%)	12	45
50	m4	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
51	M5	201/203 (99%)	191 (95%)	8 (4%)	2 (1%)	18	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	m5	201/203 (99%)	186 (92%)	12 (6%)	3 (2%)	12	45
52	M6	195/197 (99%)	189 (97%)	4 (2%)	2 (1%)	18	57
52	m6	195/197 (99%)	184 (94%)	11 (6%)	0	100	100
53	M7	181/183 (99%)	169 (93%)	12 (7%)	0	100	100
53	m7	153/183 (84%)	146 (95%)	7 (5%)	0	100	100
54	M8	183/185 (99%)	169 (92%)	12 (7%)	2 (1%)	17	54
54	m8	183/185 (99%)	169 (92%)	13 (7%)	1 (0%)	32	71
55	M9	186/188 (99%)	175 (94%)	9 (5%)	2 (1%)	17	54
55	m9	186/188 (99%)	173 (93%)	13 (7%)	0	100	100
56	N0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	10	40
56	n0	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
57	N1	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	14	48
57	n1	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	14	48
58	N2	98/100 (98%)	85 (87%)	12 (12%)	1 (1%)	18	57
58	n2	96/100 (96%)	91 (95%)	4 (4%)	1 (1%)	18	57
59	N3	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
59	n3	134/136 (98%)	130 (97%)	3 (2%)	1 (1%)	25	64
60	N4	96/98 (98%)	84 (88%)	10 (10%)	2 (2%)	8	36
61	N5	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
61	n5	118/121 (98%)	104 (88%)	14 (12%)	0	100	100
62	N6	124/126 (98%)	115 (93%)	9 (7%)	0	100	100
62	n6	124/126 (98%)	119 (96%)	3 (2%)	2 (2%)	11	43
63	N7	133/135 (98%)	124 (93%)	6 (4%)	3 (2%)	7	33
63	n7	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	7	33
64	N8	146/148 (99%)	131 (90%)	12 (8%)	3 (2%)	8	36
64	n8	146/148 (99%)	131 (90%)	13 (9%)	2 (1%)	13	47
65	N9	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
65	n9	56/58 (97%)	46 (82%)	9 (16%)	1 (2%)	10	40
66	O0	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
66	o0	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
67	O1	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	20	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	o1	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	20	60
68	O2	125/127 (98%)	121 (97%)	4 (3%)	0	100	100
68	o2	125/127 (98%)	116 (93%)	6 (5%)	3 (2%)	7	32
69	O3	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
69	o3	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
70	O4	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
70	o4	110/112 (98%)	102 (93%)	7 (6%)	1 (1%)	20	60
71	O5	117/119 (98%)	108 (92%)	9 (8%)	0	100	100
71	o5	117/119 (98%)	106 (91%)	11 (9%)	0	100	100
72	O6	97/99 (98%)	79 (81%)	15 (16%)	3 (3%)	5	26
72	o6	97/99 (98%)	87 (90%)	8 (8%)	2 (2%)	8	36
73	O7	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
73	o7	85/87 (98%)	78 (92%)	6 (7%)	1 (1%)	15	51
74	O8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	3	20
74	o8	75/77 (97%)	67 (89%)	7 (9%)	1 (1%)	14	48
75	O9	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
76	Q0	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
76	q0	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	9	37
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	89 (86%)	14 (14%)	0	100	100
78	q2	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	18	57
79	Q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	17	54
79	q3	89/91 (98%)	85 (96%)	3 (3%)	1 (1%)	17	54
80	sM	61/159 (38%)	50 (82%)	8 (13%)	3 (5%)	2	16
81	l8	229/231 (99%)	197 (86%)	28 (12%)	4 (2%)	11	42
83	n4	133/135 (98%)	111 (84%)	16 (12%)	6 (4%)	3	17
84	p0	139/312 (45%)	126 (91%)	12 (9%)	1 (1%)	25	64
All	All	22272/23122 (96%)	19937 (90%)	1963 (9%)	372 (2%)	11	42

5 of 372 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	S7	64	VAL
9	S7	111	LYS
9	S7	131	PHE
9	S7	133	THR
12	C0	87	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/173 (95%)	134 (82%)	30 (18%)	2	9
2	s0	165/173 (95%)	131 (79%)	34 (21%)	1	6
3	S1	191/192 (100%)	152 (80%)	39 (20%)	1	6
3	s1	192/192 (100%)	154 (80%)	38 (20%)	1	6
4	S2	176/176 (100%)	141 (80%)	35 (20%)	1	6
4	s2	176/176 (100%)	136 (77%)	40 (23%)	1	4
5	S3	182/182 (100%)	147 (81%)	35 (19%)	1	7
5	s3	182/182 (100%)	151 (83%)	31 (17%)	2	11
6	S4	221/221 (100%)	180 (81%)	41 (19%)	2	8
6	s4	221/221 (100%)	184 (83%)	37 (17%)	2	11
7	S5	173/173 (100%)	145 (84%)	28 (16%)	3	12
7	s5	173/173 (100%)	141 (82%)	32 (18%)	2	8
8	S6	188/193 (97%)	162 (86%)	26 (14%)	4	19
8	s6	187/193 (97%)	155 (83%)	32 (17%)	2	11
9	S7	165/166 (99%)	135 (82%)	30 (18%)	2	9
9	s7	165/166 (99%)	129 (78%)	36 (22%)	1	5
10	S8	150/161 (93%)	127 (85%)	23 (15%)	3	14
10	s8	150/161 (93%)	123 (82%)	27 (18%)	2	9
11	S9	158/158 (100%)	126 (80%)	32 (20%)	1	6
11	s9	158/158 (100%)	124 (78%)	34 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	C0	77/91 (85%)	61 (79%)	16 (21%)	1	6
12	c0	73/91 (80%)	60 (82%)	13 (18%)	2	9
13	C1	129/137 (94%)	105 (81%)	24 (19%)	2	8
13	c1	129/137 (94%)	105 (81%)	24 (19%)	2	8
14	C2	88/100 (88%)	65 (74%)	23 (26%)	0	2
14	c2	88/100 (88%)	64 (73%)	24 (27%)	0	1
15	C3	127/127 (100%)	102 (80%)	25 (20%)	1	6
15	c3	127/127 (100%)	101 (80%)	26 (20%)	1	6
16	C4	81/97 (84%)	65 (80%)	16 (20%)	1	6
16	c4	97/97 (100%)	75 (77%)	22 (23%)	1	4
17	C5	101/118 (86%)	87 (86%)	14 (14%)	4	18
17	c5	103/118 (87%)	86 (84%)	17 (16%)	2	12
18	C6	117/118 (99%)	89 (76%)	28 (24%)	1	3
18	c6	118/118 (100%)	97 (82%)	21 (18%)	2	9
19	C7	94/124 (76%)	72 (77%)	22 (23%)	1	3
19	c7	92/124 (74%)	75 (82%)	17 (18%)	2	8
20	C8	128/128 (100%)	104 (81%)	24 (19%)	2	8
20	c8	128/128 (100%)	106 (83%)	22 (17%)	2	11
21	C9	115/115 (100%)	92 (80%)	23 (20%)	1	6
21	c9	115/115 (100%)	96 (84%)	19 (16%)	2	12
22	D0	100/103 (97%)	80 (80%)	20 (20%)	1	6
22	d0	103/103 (100%)	77 (75%)	26 (25%)	0	2
23	D1	74/74 (100%)	63 (85%)	11 (15%)	3	15
23	d1	74/74 (100%)	58 (78%)	16 (22%)	1	5
24	D2	110/110 (100%)	89 (81%)	21 (19%)	2	7
24	d2	110/110 (100%)	96 (87%)	14 (13%)	5	21
25	D3	119/119 (100%)	95 (80%)	24 (20%)	1	6
25	d3	119/119 (100%)	99 (83%)	20 (17%)	2	11
26	D4	112/112 (100%)	91 (81%)	21 (19%)	2	8
26	d4	112/112 (100%)	98 (88%)	14 (12%)	5	22
27	D5	61/61 (100%)	47 (77%)	14 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	d5	61/61 (100%)	53 (87%)	8 (13%)	5	20
28	D6	83/83 (100%)	63 (76%)	20 (24%)	1	3
28	d6	83/83 (100%)	68 (82%)	15 (18%)	2	9
29	D7	70/70 (100%)	60 (86%)	10 (14%)	4	17
29	d7	70/70 (100%)	58 (83%)	12 (17%)	2	11
30	D8	56/56 (100%)	42 (75%)	14 (25%)	1	2
30	d8	56/56 (100%)	44 (79%)	12 (21%)	1	5
31	D9	47/47 (100%)	33 (70%)	14 (30%)	0	1
31	d9	47/47 (100%)	35 (74%)	12 (26%)	0	2
32	E0	51/53 (96%)	43 (84%)	8 (16%)	3	13
32	e0	53/53 (100%)	43 (81%)	10 (19%)	2	7
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	3
33	e1	66/66 (100%)	47 (71%)	19 (29%)	0	1
34	SR	259/261 (99%)	228 (88%)	31 (12%)	6	24
34	sR	259/261 (99%)	230 (89%)	29 (11%)	7	29
35	SM	97/122 (80%)	75 (77%)	22 (23%)	1	4
39	L2	193/194 (100%)	163 (84%)	30 (16%)	3	14
39	l2	192/194 (99%)	152 (79%)	40 (21%)	1	6
40	L3	320/322 (99%)	256 (80%)	64 (20%)	1	6
40	l3	319/322 (99%)	266 (83%)	53 (17%)	2	11
41	L4	288/288 (100%)	238 (83%)	50 (17%)	2	10
41	l4	288/288 (100%)	241 (84%)	47 (16%)	3	12
42	L5	244/244 (100%)	194 (80%)	50 (20%)	1	6
42	l5	243/244 (100%)	203 (84%)	40 (16%)	2	12
43	L6	134/153 (88%)	117 (87%)	17 (13%)	5	21
43	l6	135/153 (88%)	116 (86%)	19 (14%)	4	18
44	L7	186/187 (100%)	160 (86%)	26 (14%)	4	18
44	l7	187/187 (100%)	159 (85%)	28 (15%)	3	15
45	L8	187/191 (98%)	159 (85%)	28 (15%)	3	15
46	L9	171/171 (100%)	136 (80%)	35 (20%)	1	6
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	M0	177/187 (95%)	151 (85%)	26 (15%)	3	16
47	m0	179/187 (96%)	139 (78%)	40 (22%)	1	4
48	M1	147/147 (100%)	117 (80%)	30 (20%)	1	6
48	m1	147/147 (100%)	120 (82%)	27 (18%)	2	9
49	M3	154/154 (100%)	126 (82%)	28 (18%)	2	9
49	m3	154/154 (100%)	130 (84%)	24 (16%)	3	13
50	M4	107/108 (99%)	90 (84%)	17 (16%)	3	13
50	m4	108/108 (100%)	93 (86%)	15 (14%)	4	18
51	M5	175/175 (100%)	146 (83%)	29 (17%)	2	11
51	m5	175/175 (100%)	146 (83%)	29 (17%)	2	11
52	M6	160/160 (100%)	132 (82%)	28 (18%)	2	10
52	m6	160/160 (100%)	132 (82%)	28 (18%)	2	10
53	M7	140/145 (97%)	115 (82%)	25 (18%)	2	9
53	m7	125/145 (86%)	100 (80%)	25 (20%)	1	6
54	M8	150/150 (100%)	126 (84%)	24 (16%)	3	12
54	m8	150/150 (100%)	124 (83%)	26 (17%)	2	10
55	M9	153/153 (100%)	134 (88%)	19 (12%)	5	23
55	m9	153/153 (100%)	130 (85%)	23 (15%)	3	15
56	N0	156/156 (100%)	116 (74%)	40 (26%)	0	2
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	5
57	N1	136/136 (100%)	105 (77%)	31 (23%)	1	4
57	n1	136/136 (100%)	112 (82%)	24 (18%)	2	10
58	N2	87/87 (100%)	70 (80%)	17 (20%)	1	7
58	n2	85/87 (98%)	68 (80%)	17 (20%)	1	6
59	N3	104/104 (100%)	83 (80%)	21 (20%)	1	6
59	n3	104/104 (100%)	87 (84%)	17 (16%)	3	12
60	N4	57/86 (66%)	50 (88%)	7 (12%)	5	23
61	N5	104/105 (99%)	78 (75%)	26 (25%)	1	2
61	n5	104/105 (99%)	85 (82%)	19 (18%)	2	9
62	N6	109/109 (100%)	87 (80%)	22 (20%)	1	6
62	n6	109/109 (100%)	82 (75%)	27 (25%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	N7	115/115 (100%)	95 (83%)	20 (17%)	2	10
63	n7	115/115 (100%)	92 (80%)	23 (20%)	1	6
64	N8	118/118 (100%)	96 (81%)	22 (19%)	2	8
64	n8	118/118 (100%)	90 (76%)	28 (24%)	1	3
65	N9	46/46 (100%)	38 (83%)	8 (17%)	2	10
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	10
66	O0	81/84 (96%)	65 (80%)	16 (20%)	1	6
66	o0	84/84 (100%)	71 (84%)	13 (16%)	3	14
67	O1	92/96 (96%)	77 (84%)	15 (16%)	3	12
67	o1	94/96 (98%)	75 (80%)	19 (20%)	1	6
68	O2	109/109 (100%)	96 (88%)	13 (12%)	6	25
68	o2	109/109 (100%)	89 (82%)	20 (18%)	2	9
69	O3	90/90 (100%)	78 (87%)	12 (13%)	4	20
69	o3	90/90 (100%)	80 (89%)	10 (11%)	7	29
70	O4	95/95 (100%)	81 (85%)	14 (15%)	3	16
70	o4	95/95 (100%)	85 (90%)	10 (10%)	8	31
71	O5	104/104 (100%)	84 (81%)	20 (19%)	1	7
71	o5	103/104 (99%)	86 (84%)	17 (16%)	2	12
72	O6	81/81 (100%)	60 (74%)	21 (26%)	0	2
72	o6	80/81 (99%)	55 (69%)	25 (31%)	0	1
73	O7	70/70 (100%)	61 (87%)	9 (13%)	5	21
73	o7	70/70 (100%)	57 (81%)	13 (19%)	2	8
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0	1
74	o8	67/68 (98%)	54 (81%)	13 (19%)	1	7
75	O9	45/45 (100%)	40 (89%)	5 (11%)	7	29
75	o9	45/45 (100%)	38 (84%)	7 (16%)	3	13
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	3	15
76	q0	47/47 (100%)	38 (81%)	9 (19%)	2	7
77	Q1	23/23 (100%)	18 (78%)	5 (22%)	1	5
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	72 (80%)	18 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1	5
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	11
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	4
80	sM	54/103 (52%)	42 (78%)	12 (22%)	1	4
81	l8	177/190 (93%)	144 (81%)	33 (19%)	2	8
83	n4	100/114 (88%)	87 (87%)	13 (13%)	5	21
84	p0	105/254 (41%)	81 (77%)	24 (23%)	1	4
All	All	18725/19364 (97%)	15293 (82%)	3432 (18%)	2	9

5 of 3432 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	O2	33	ARG
8	s6	78	THR
63	n7	103	GLN
71	O5	49	LYS
3	s1	47	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
78	Q2	47	GLN
11	s9	123	HIS
70	o4	3	GLN
3	s1	149	GLN
11	s9	124	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	480 (27%)	0
1	6	1792/1800 (99%)	466 (26%)	0
36	1	3145/3396 (92%)	667 (21%)	0
36	5	3145/3396 (92%)	677 (21%)	0
37	3	120/121 (99%)	15 (12%)	0
37	7	120/121 (99%)	19 (15%)	0
38	4	157/158 (99%)	35 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
38	8	157/158 (99%)	34 (21%)	0
All	All	10413/10950 (95%)	2393 (22%)	0

5 of 2393 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	21	U
1	2	25	C

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2029 ligands modelled in this entry, 1035 are monoatomic - leaving 994 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	1	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3429	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3577	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3583	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3662	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3663	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3696	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3706	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1909	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1937	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1980	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3415	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3458	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3463	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3501	36	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3504	36	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3544	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3587	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3630	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3673	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3696	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3716	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3722	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3723	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1927	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1935	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1978	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2021	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2027	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
89	UAM	6	2134	-	31,31,31	0.17	0	39,44,44	0.64	2 (5%)
86	OHX	7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	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
86	OHX	1	3401	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3402	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3403	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3404	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3405	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3406	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3407	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3408	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3409	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3410	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3411	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3412	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3413	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3414	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3415	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3416	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3417	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3418	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3419	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3420	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3421	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3422	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3423	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3424	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3425	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3426	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3427	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3428	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3429	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3430	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3431	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3432	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3433	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3434	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3435	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3436	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3437	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3438	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3439	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3440	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3441	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3442	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3443	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3444	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3445	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3446	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3447	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3448	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3449	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3450	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3451	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3452	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3453	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3454	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3455	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3456	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3457	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3458	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3459	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3460	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3461	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3462	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3463	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3464	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3465	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3466	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3467	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3468	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3469	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3470	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3471	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3472	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3473	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3474	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3475	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3476	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3477	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3478	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3479	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3480	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3481	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3482	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3483	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3484	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3485	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3486	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3487	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3488	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3489	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3490	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3491	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3492	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3493	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3494	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3495	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3496	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3497	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3498	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3499	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3500	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3501	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3502	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3503	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3504	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3505	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3506	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3507	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3508	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3509	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3510	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3511	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3512	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3513	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3514	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3515	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3516	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3517	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3518	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3519	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3520	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3521	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3522	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3523	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3524	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3525	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3526	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3527	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3528	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3529	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3530	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3531	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3532	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3533	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3534	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3535	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3536	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3537	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3538	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3539	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3540	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3541	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3542	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3543	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3544	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3545	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3546	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3547	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3548	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3549	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3550	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3551	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3552	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3553	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3554	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3555	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3556	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3557	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3558	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3559	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3560	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3561	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3562	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3563	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3564	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3565	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3566	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3567	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3568	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3569	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3570	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3571	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3572	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3573	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3574	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3575	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3576	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3577	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3578	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3579	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3580	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3581	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3582	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3583	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3584	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3585	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3586	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3587	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3588	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3589	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3590	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3591	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3592	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3593	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3594	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3595	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3596	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3597	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3598	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3599	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3600	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3601	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3602	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3603	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3604	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3605	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3606	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3607	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3608	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3609	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3610	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3611	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3612	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3613	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3614	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3615	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3616	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3617	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3618	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3619	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3620	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3621	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3622	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3623	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3624	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3625	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3626	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3627	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3628	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3629	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3630	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3631	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3632	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3633	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3634	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3635	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3636	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3637	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3638	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3639	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3640	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3641	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3642	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3643	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3644	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3645	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3646	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3647	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3648	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3649	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3650	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3651	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3652	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3653	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3654	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3655	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3656	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3657	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3658	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3659	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3660	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3661	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3662	36	-	0/0/0/0	0/0/0/0
86	OHX	1	3663	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3664	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3665	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3666	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3667	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3668	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3669	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3670	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3671	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3672	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3673	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3674	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3675	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3676	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3677	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3678	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3679	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3680	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3681	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3682	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3683	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3684	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3685	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3686	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3687	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3688	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3689	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3690	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3691	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3692	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3693	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3694	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3695	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3696	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3697	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3698	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3699	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3700	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3701	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3702	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3703	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3704	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3705	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3706	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3707	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3708	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3709	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3710	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3711	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3712	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1901	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1902	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1903	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1904	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1905	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1906	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1907	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1908	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1909	1	-	0/0/0/0	0/0/0/0
86	OHX	2	1910	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1911	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1912	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1913	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1914	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1915	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1916	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1917	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1918	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1919	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1920	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1921	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	1922	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1923	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1924	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1925	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1926	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1927	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1928	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1929	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1930	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1931	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1932	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1933	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1934	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1935	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1936	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1937	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1938	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1939	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1940	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1941	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1942	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1943	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1944	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1945	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1946	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1947	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1948	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1949	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1950	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1951	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1952	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1953	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1954	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1955	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1956	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1957	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1958	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1959	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1960	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1961	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1962	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1963	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	1964	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1965	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1966	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1967	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1968	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1969	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1970	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1971	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1972	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1973	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1974	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1975	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1976	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1977	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1978	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1979	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1980	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1981	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1982	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1983	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1984	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1985	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1986	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1987	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1988	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1989	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1990	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1991	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1992	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1993	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1994	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1995	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1996	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1997	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1998	-	-	0/0/0/0	0/0/0/0
86	OHX	2	1999	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2000	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2001	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2002	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2003	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2004	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2005	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2006	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2007	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2008	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2009	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2010	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2011	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2012	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2013	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2014	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2015	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2016	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2017	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2018	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2019	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2020	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2021	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	3	204	-	-	0/0/0/0	0/0/0/0
86	OHX	3	205	-	-	0/0/0/0	0/0/0/0
86	OHX	3	206	-	-	0/0/0/0	0/0/0/0
86	OHX	3	207	-	-	0/0/0/0	0/0/0/0
86	OHX	3	208	-	-	0/0/0/0	0/0/0/0
86	OHX	4	203	-	-	0/0/0/0	0/0/0/0
86	OHX	4	204	-	-	0/0/0/0	0/0/0/0
86	OHX	4	205	-	-	0/0/0/0	0/0/0/0
86	OHX	4	206	-	-	0/0/0/0	0/0/0/0
86	OHX	4	207	-	-	0/0/0/0	0/0/0/0
86	OHX	4	208	-	-	0/0/0/0	0/0/0/0
86	OHX	4	209	-	-	0/0/0/0	0/0/0/0
86	OHX	4	210	-	-	0/0/0/0	0/0/0/0
86	OHX	4	211	-	-	0/0/0/0	0/0/0/0
86	OHX	4	212	-	-	0/0/0/0	0/0/0/0
86	OHX	4	213	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	4	214	-	-	0/0/0/0	0/0/0/0
86	OHX	4	215	-	-	0/0/0/0	0/0/0/0
86	OHX	4	216	-	-	0/0/0/0	0/0/0/0
86	OHX	4	217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3401	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3402	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3403	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3404	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3405	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3406	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3407	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3408	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3409	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3410	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3411	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3412	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3413	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3414	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3415	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3416	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3417	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3418	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3419	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3420	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3421	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3422	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3423	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3424	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3425	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3426	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3427	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3428	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3429	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3430	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3431	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3432	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3433	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3434	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3435	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3436	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3437	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3438	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3439	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3440	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3441	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3442	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3443	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3444	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3445	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3446	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3447	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3448	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3449	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3450	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3451	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3452	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3453	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3454	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3455	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3456	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3457	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3458	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3459	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3460	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3461	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3462	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3463	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3464	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3465	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3466	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3467	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3468	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3469	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3470	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3471	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3472	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3473	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3474	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3475	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3476	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3477	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3478	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3479	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3480	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3481	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3482	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3483	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3484	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3485	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3486	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3487	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3488	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3489	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3490	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3491	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3492	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3493	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3494	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3495	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3496	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3497	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3498	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3499	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3500	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3501	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3502	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3503	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3504	36	-	0/0/0/0	0/0/0/0
86	OHX	5	3505	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3506	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3507	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3508	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3509	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3510	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3511	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3512	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3513	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3514	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3515	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3516	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3517	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3518	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3519	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3520	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3521	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3522	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3523	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3524	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3525	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3526	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3527	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3528	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3529	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3530	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3531	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3532	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3533	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3534	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3535	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3536	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3537	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3538	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3539	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3540	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3541	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3542	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3543	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3544	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3545	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3546	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3547	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3548	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3549	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3550	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3551	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3552	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3553	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3554	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3555	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3556	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3557	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3558	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3559	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3560	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3561	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3562	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3563	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3564	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3565	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3566	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3567	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3568	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3569	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3570	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3571	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3572	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3573	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3574	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3575	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3576	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3577	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3578	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3579	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3580	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3581	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3582	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3583	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3584	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3585	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3586	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3587	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3588	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3589	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3590	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3591	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3592	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3593	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3594	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3595	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3596	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3597	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3598	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3599	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3600	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3601	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3602	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3603	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3604	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3605	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3606	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3607	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3608	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3609	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3610	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3611	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3612	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3613	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3614	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3615	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3616	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3617	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3618	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3619	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3620	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3621	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3622	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3623	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3624	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3625	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3626	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3627	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3628	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3629	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3630	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3631	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3632	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3633	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3634	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3635	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3636	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3637	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3638	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3639	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3640	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3641	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3642	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3643	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3644	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3645	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3646	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3647	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3648	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3649	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3650	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3651	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3652	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3653	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3654	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3655	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3656	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3657	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3658	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3659	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3660	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3661	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3662	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3663	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3664	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3665	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3666	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3667	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3668	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3669	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3670	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3671	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3672	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3673	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3674	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3675	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3676	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3677	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3678	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3679	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3680	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3681	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3682	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3683	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3684	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3685	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3686	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3687	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3688	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3689	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3690	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3691	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3692	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3693	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3694	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3695	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3696	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3697	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3698	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3699	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3700	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3701	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3702	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3703	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3704	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3705	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3706	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3707	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3708	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3709	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3710	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3711	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3712	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3713	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3714	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3715	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3716	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3717	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3718	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3719	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3720	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3721	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3722	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3723	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3724	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1901	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1902	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1903	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1904	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1905	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1906	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1907	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1908	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	1909	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1910	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1911	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1912	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1913	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1914	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1915	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1916	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1917	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1918	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1919	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1920	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1921	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1922	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1923	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1924	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1925	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1926	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1927	1	-	0/0/0/0	0/0/0/0
86	OHX	6	1928	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1929	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1930	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1931	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1932	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1933	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1934	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1935	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1936	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1937	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1938	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1939	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1940	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1941	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1942	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1943	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1944	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1945	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1946	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1947	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1948	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1949	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1950	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	1951	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1952	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1953	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1954	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1955	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1956	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1957	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1958	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1959	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1960	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1961	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1962	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1963	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1964	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1965	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1966	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1967	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1968	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1969	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1970	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1971	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1972	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1973	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1974	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1975	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1976	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1977	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1978	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1979	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1980	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1981	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1982	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1983	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1984	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1985	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1986	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1987	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1988	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1989	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1990	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1991	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1992	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	1993	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1994	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1995	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1996	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1997	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1998	-	-	0/0/0/0	0/0/0/0
86	OHX	6	1999	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2000	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2001	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2002	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2003	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2004	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2005	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2006	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2007	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2008	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2009	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2010	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2011	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2012	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2013	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2014	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2015	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2016	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2017	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2018	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2019	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2020	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2021	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2022	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2023	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2027	1	-	0/0/0/0	0/0/0/0
86	OHX	6	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2032	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2034	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2037	-	-	0/0/0/0	0/0/0/0
89	UAM	6	2134	-	-	0/28/40/40	0/2/2/2
86	OHX	7	201	-	-	0/0/0/0	0/0/0/0
86	OHX	7	202	-	-	0/0/0/0	0/0/0/0
86	OHX	7	203	-	-	0/0/0/0	0/0/0/0
86	OHX	7	204	-	-	0/0/0/0	0/0/0/0
86	OHX	7	205	-	-	0/0/0/0	0/0/0/0
86	OHX	7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	7	208	-	-	0/0/0/0	0/0/0/0
86	OHX	7	209	-	-	0/0/0/0	0/0/0/0
86	OHX	7	210	-	-	0/0/0/0	0/0/0/0
86	OHX	7	211	-	-	0/0/0/0	0/0/0/0
86	OHX	8	202	-	-	0/0/0/0	0/0/0/0
86	OHX	8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	8	204	-	-	0/0/0/0	0/0/0/0
86	OHX	8	205	-	-	0/0/0/0	0/0/0/0
86	OHX	8	206	-	-	0/0/0/0	0/0/0/0
86	OHX	8	207	-	-	0/0/0/0	0/0/0/0
86	OHX	8	208	-	-	0/0/0/0	0/0/0/0
86	OHX	8	209	-	-	0/0/0/0	0/0/0/0
86	OHX	8	210	-	-	0/0/0/0	0/0/0/0
86	OHX	8	211	-	-	0/0/0/0	0/0/0/0
86	OHX	8	212	-	-	0/0/0/0	0/0/0/0
86	OHX	8	213	-	-	0/0/0/0	0/0/0/0
86	OHX	8	214	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	401	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	401	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	301	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	O1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	301	-	-	0/0/0/0	0/0/0/0
86	OHX	S9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	401	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	401	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	301	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	6	2134	UAM	OAR-CBD-CBC	-2.31	103.52	106.72
89	6	2134	UAM	CAZ-CAN-CAS	2.15	115.82	112.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

455 monomers are involved in 642 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3403	OHX	1	0
86	1	3405	OHX	3	0
86	1	3406	OHX	2	0
86	1	3409	OHX	2	0
86	1	3411	OHX	1	0
86	1	3413	OHX	1	0
86	1	3415	OHX	1	0
86	1	3416	OHX	1	0
86	1	3418	OHX	2	0
86	1	3420	OHX	1	0
86	1	3421	OHX	2	0
86	1	3425	OHX	1	0
86	1	3426	OHX	1	0
86	1	3429	OHX	1	0
86	1	3430	OHX	1	0
86	1	3438	OHX	1	0
86	1	3441	OHX	1	0
86	1	3444	OHX	1	0
86	1	3446	OHX	1	0
86	1	3450	OHX	2	0
86	1	3456	OHX	1	0
86	1	3460	OHX	1	0
86	1	3466	OHX	1	0
86	1	3469	OHX	1	0
86	1	3471	OHX	1	0
86	1	3472	OHX	2	0
86	1	3478	OHX	2	0
86	1	3479	OHX	1	0
86	1	3480	OHX	1	0
86	1	3485	OHX	1	0
86	1	3486	OHX	1	0
86	1	3491	OHX	1	0
86	1	3492	OHX	1	0
86	1	3495	OHX	1	0
86	1	3496	OHX	6	0
86	1	3498	OHX	3	0
86	1	3501	OHX	1	0
86	1	3504	OHX	1	0
86	1	3508	OHX	1	0
86	1	3509	OHX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3510	OHX	2	0
86	1	3512	OHX	1	0
86	1	3513	OHX	1	0
86	1	3514	OHX	1	0
86	1	3515	OHX	2	0
86	1	3517	OHX	1	0
86	1	3518	OHX	1	0
86	1	3519	OHX	2	0
86	1	3520	OHX	2	0
86	1	3521	OHX	1	0
86	1	3523	OHX	1	0
86	1	3526	OHX	3	0
86	1	3528	OHX	2	0
86	1	3529	OHX	1	0
86	1	3531	OHX	2	0
86	1	3534	OHX	1	0
86	1	3535	OHX	1	0
86	1	3538	OHX	1	0
86	1	3539	OHX	3	0
86	1	3543	OHX	1	0
86	1	3544	OHX	1	0
86	1	3545	OHX	1	0
86	1	3550	OHX	2	0
86	1	3551	OHX	1	0
86	1	3554	OHX	1	0
86	1	3561	OHX	1	0
86	1	3563	OHX	2	0
86	1	3564	OHX	1	0
86	1	3567	OHX	1	0
86	1	3569	OHX	1	0
86	1	3570	OHX	1	0
86	1	3573	OHX	1	0
86	1	3575	OHX	1	0
86	1	3576	OHX	3	0
86	1	3577	OHX	1	0
86	1	3578	OHX	1	0
86	1	3579	OHX	1	0
86	1	3580	OHX	2	0
86	1	3581	OHX	3	0
86	1	3583	OHX	1	0
86	1	3587	OHX	1	0
86	1	3591	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3592	OHX	3	0
86	1	3595	OHX	1	0
86	1	3596	OHX	1	0
86	1	3597	OHX	1	0
86	1	3600	OHX	1	0
86	1	3601	OHX	1	0
86	1	3608	OHX	1	0
86	1	3610	OHX	1	0
86	1	3612	OHX	1	0
86	1	3614	OHX	1	0
86	1	3618	OHX	3	0
86	1	3621	OHX	1	0
86	1	3623	OHX	2	0
86	1	3627	OHX	1	0
86	1	3628	OHX	1	0
86	1	3630	OHX	1	0
86	1	3631	OHX	1	0
86	1	3641	OHX	2	0
86	1	3646	OHX	1	0
86	1	3649	OHX	1	0
86	1	3651	OHX	1	0
86	1	3653	OHX	2	0
86	1	3657	OHX	2	0
86	1	3659	OHX	1	0
86	1	3662	OHX	1	0
86	1	3665	OHX	3	0
86	1	3666	OHX	2	0
86	1	3669	OHX	2	0
86	1	3670	OHX	1	0
86	1	3675	OHX	2	0
86	1	3679	OHX	1	0
86	1	3681	OHX	4	0
86	1	3684	OHX	1	0
86	1	3685	OHX	1	0
86	1	3686	OHX	1	0
86	1	3689	OHX	1	0
86	1	3690	OHX	2	0
86	1	3691	OHX	3	0
86	1	3693	OHX	1	0
86	1	3695	OHX	1	0
86	1	3696	OHX	2	0
86	1	3697	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3699	OHX	2	0
86	1	3700	OHX	1	0
86	1	3701	OHX	5	0
86	1	3708	OHX	2	0
86	1	3709	OHX	1	0
86	1	3712	OHX	4	0
86	2	1904	OHX	1	0
86	2	1910	OHX	1	0
86	2	1911	OHX	1	0
86	2	1913	OHX	2	0
86	2	1914	OHX	2	0
86	2	1917	OHX	1	0
86	2	1918	OHX	1	0
86	2	1919	OHX	1	0
86	2	1920	OHX	1	0
86	2	1921	OHX	1	0
86	2	1923	OHX	1	0
86	2	1924	OHX	1	0
86	2	1925	OHX	2	0
86	2	1926	OHX	1	0
86	2	1929	OHX	1	0
86	2	1930	OHX	2	0
86	2	1931	OHX	1	0
86	2	1936	OHX	1	0
86	2	1937	OHX	2	0
86	2	1938	OHX	1	0
86	2	1939	OHX	1	0
86	2	1942	OHX	1	0
86	2	1943	OHX	1	0
86	2	1944	OHX	1	0
86	2	1945	OHX	1	0
86	2	1947	OHX	1	0
86	2	1948	OHX	2	0
86	2	1949	OHX	2	0
86	2	1951	OHX	1	0
86	2	1952	OHX	2	0
86	2	1953	OHX	2	0
86	2	1960	OHX	3	0
86	2	1962	OHX	1	0
86	2	1964	OHX	3	0
86	2	1965	OHX	1	0
86	2	1966	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	1967	OHX	1	0
86	2	1971	OHX	1	0
86	2	1978	OHX	1	0
86	2	1980	OHX	1	0
86	2	1982	OHX	1	0
86	2	1983	OHX	2	0
86	2	1984	OHX	3	0
86	2	1988	OHX	1	0
86	2	1989	OHX	1	0
86	2	1992	OHX	1	0
86	2	1993	OHX	1	0
86	2	1995	OHX	2	0
86	2	1997	OHX	1	0
86	2	2000	OHX	1	0
86	2	2002	OHX	1	0
86	2	2003	OHX	2	0
86	2	2004	OHX	1	0
86	2	2005	OHX	1	0
86	2	2006	OHX	1	0
86	2	2007	OHX	1	0
86	2	2011	OHX	1	0
86	2	2012	OHX	1	0
86	2	2014	OHX	1	0
86	2	2015	OHX	1	0
86	2	2017	OHX	2	0
86	2	2018	OHX	1	0
86	2	2019	OHX	3	0
86	2	2020	OHX	1	0
86	2	2021	OHX	2	0
86	2	2023	OHX	1	0
86	2	2024	OHX	1	0
86	2	2027	OHX	1	0
86	3	205	OHX	1	0
86	3	206	OHX	1	0
86	4	205	OHX	1	0
86	4	206	OHX	2	0
86	4	208	OHX	1	0
86	4	209	OHX	2	0
86	4	212	OHX	1	0
86	4	214	OHX	2	0
86	5	3401	OHX	3	0
86	5	3403	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3406	OHX	2	0
86	5	3407	OHX	1	0
86	5	3409	OHX	1	0
86	5	3411	OHX	1	0
86	5	3413	OHX	1	0
86	5	3414	OHX	1	0
86	5	3415	OHX	1	0
86	5	3418	OHX	2	0
86	5	3420	OHX	1	0
86	5	3423	OHX	2	0
86	5	3426	OHX	1	0
86	5	3427	OHX	1	0
86	5	3432	OHX	1	0
86	5	3434	OHX	1	0
86	5	3435	OHX	1	0
86	5	3436	OHX	1	0
86	5	3438	OHX	1	0
86	5	3449	OHX	2	0
86	5	3454	OHX	1	0
86	5	3455	OHX	3	0
86	5	3457	OHX	2	0
86	5	3460	OHX	1	0
86	5	3461	OHX	1	0
86	5	3463	OHX	3	0
86	5	3464	OHX	2	0
86	5	3467	OHX	1	0
86	5	3473	OHX	2	0
86	5	3477	OHX	1	0
86	5	3479	OHX	5	0
86	5	3480	OHX	1	0
86	5	3483	OHX	1	0
86	5	3484	OHX	1	0
86	5	3485	OHX	2	0
86	5	3486	OHX	1	0
86	5	3487	OHX	1	0
86	5	3496	OHX	1	0
86	5	3498	OHX	1	0
86	5	3499	OHX	1	0
86	5	3500	OHX	1	0
86	5	3501	OHX	1	0
86	5	3503	OHX	1	0
86	5	3504	OHX	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3505	OHX	1	0
86	5	3507	OHX	1	0
86	5	3508	OHX	1	0
86	5	3509	OHX	2	0
86	5	3513	OHX	5	0
86	5	3515	OHX	1	0
86	5	3517	OHX	1	0
86	5	3518	OHX	1	0
86	5	3520	OHX	1	0
86	5	3521	OHX	1	0
86	5	3523	OHX	1	0
86	5	3525	OHX	2	0
86	5	3526	OHX	1	0
86	5	3528	OHX	1	0
86	5	3529	OHX	1	0
86	5	3532	OHX	2	0
86	5	3534	OHX	2	0
86	5	3535	OHX	4	0
86	5	3539	OHX	1	0
86	5	3540	OHX	1	0
86	5	3542	OHX	1	0
86	5	3546	OHX	1	0
86	5	3547	OHX	1	0
86	5	3548	OHX	1	0
86	5	3550	OHX	1	0
86	5	3551	OHX	1	0
86	5	3552	OHX	1	0
86	5	3554	OHX	1	0
86	5	3556	OHX	3	0
86	5	3566	OHX	2	0
86	5	3567	OHX	2	0
86	5	3569	OHX	1	0
86	5	3572	OHX	1	0
86	5	3575	OHX	2	0
86	5	3577	OHX	2	0
86	5	3578	OHX	1	0
86	5	3581	OHX	2	0
86	5	3582	OHX	1	0
86	5	3583	OHX	1	0
86	5	3585	OHX	1	0
86	5	3586	OHX	1	0
86	5	3587	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3589	OHX	1	0
86	5	3590	OHX	1	0
86	5	3591	OHX	2	0
86	5	3592	OHX	1	0
86	5	3593	OHX	2	0
86	5	3595	OHX	1	0
86	5	3597	OHX	1	0
86	5	3600	OHX	2	0
86	5	3602	OHX	1	0
86	5	3603	OHX	1	0
86	5	3604	OHX	1	0
86	5	3606	OHX	3	0
86	5	3608	OHX	1	0
86	5	3610	OHX	1	0
86	5	3611	OHX	1	0
86	5	3616	OHX	1	0
86	5	3618	OHX	2	0
86	5	3619	OHX	1	0
86	5	3622	OHX	1	0
86	5	3626	OHX	1	0
86	5	3631	OHX	1	0
86	5	3632	OHX	1	0
86	5	3633	OHX	1	0
86	5	3637	OHX	2	0
86	5	3638	OHX	1	0
86	5	3639	OHX	1	0
86	5	3640	OHX	1	0
86	5	3641	OHX	1	0
86	5	3643	OHX	1	0
86	5	3644	OHX	1	0
86	5	3645	OHX	1	0
86	5	3650	OHX	1	0
86	5	3653	OHX	1	0
86	5	3654	OHX	1	0
86	5	3656	OHX	3	0
86	5	3658	OHX	1	0
86	5	3659	OHX	1	0
86	5	3662	OHX	1	0
86	5	3664	OHX	1	0
86	5	3669	OHX	1	0
86	5	3670	OHX	1	0
86	5	3675	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	3676	OHX	1	0
86	5	3678	OHX	1	0
86	5	3680	OHX	1	0
86	5	3681	OHX	1	0
86	5	3682	OHX	2	0
86	5	3684	OHX	2	0
86	5	3685	OHX	2	0
86	5	3686	OHX	1	0
86	5	3687	OHX	1	0
86	5	3690	OHX	1	0
86	5	3691	OHX	8	0
86	5	3692	OHX	3	0
86	5	3693	OHX	5	0
86	5	3695	OHX	1	0
86	5	3696	OHX	1	0
86	5	3697	OHX	1	0
86	5	3706	OHX	1	0
86	5	3708	OHX	1	0
86	5	3710	OHX	1	0
86	5	3711	OHX	1	0
86	5	3713	OHX	3	0
86	5	3714	OHX	1	0
86	5	3715	OHX	1	0
86	5	3719	OHX	1	0
86	5	3720	OHX	1	0
86	6	1905	OHX	1	0
86	6	1908	OHX	2	0
86	6	1909	OHX	1	0
86	6	1910	OHX	1	0
86	6	1911	OHX	1	0
86	6	1913	OHX	1	0
86	6	1914	OHX	1	0
86	6	1917	OHX	1	0
86	6	1918	OHX	2	0
86	6	1919	OHX	2	0
86	6	1921	OHX	2	0
86	6	1922	OHX	5	0
86	6	1926	OHX	1	0
86	6	1927	OHX	1	0
86	6	1929	OHX	3	0
86	6	1930	OHX	2	0
86	6	1931	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	1934	OHX	2	0
86	6	1937	OHX	1	0
86	6	1938	OHX	1	0
86	6	1939	OHX	1	0
86	6	1940	OHX	1	0
86	6	1945	OHX	1	0
86	6	1947	OHX	1	0
86	6	1948	OHX	1	0
86	6	1951	OHX	1	0
86	6	1952	OHX	2	0
86	6	1953	OHX	1	0
86	6	1955	OHX	1	0
86	6	1956	OHX	4	0
86	6	1957	OHX	1	0
86	6	1958	OHX	3	0
86	6	1959	OHX	2	0
86	6	1961	OHX	1	0
86	6	1964	OHX	1	0
86	6	1965	OHX	2	0
86	6	1966	OHX	1	0
86	6	1973	OHX	2	0
86	6	1974	OHX	1	0
86	6	1975	OHX	1	0
86	6	1977	OHX	2	0
86	6	1980	OHX	1	0
86	6	1982	OHX	1	0
86	6	1983	OHX	2	0
86	6	1984	OHX	1	0
86	6	1988	OHX	1	0
86	6	1989	OHX	1	0
86	6	1990	OHX	2	0
86	6	1991	OHX	2	0
86	6	1995	OHX	2	0
86	6	1996	OHX	2	0
86	6	1997	OHX	1	0
86	6	1999	OHX	1	0
86	6	2000	OHX	1	0
86	6	2004	OHX	1	0
86	6	2006	OHX	1	0
86	6	2008	OHX	1	0
86	6	2009	OHX	2	0
86	6	2010	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2011	OHX	1	0
86	6	2012	OHX	1	0
86	6	2018	OHX	1	0
86	6	2021	OHX	1	0
86	6	2024	OHX	1	0
86	6	2025	OHX	1	0
86	6	2027	OHX	2	0
86	6	2030	OHX	1	0
86	6	2032	OHX	2	0
86	6	2033	OHX	3	0
86	6	2036	OHX	1	0
86	7	203	OHX	1	0
86	7	204	OHX	1	0
86	7	205	OHX	1	0
86	8	202	OHX	1	0
86	8	204	OHX	2	0
86	8	206	OHX	1	0
86	8	210	OHX	1	0
86	8	211	OHX	2	0
86	8	213	OHX	2	0
86	8	215	OHX	1	0
86	C1	201	OHX	1	0
86	C3	201	OHX	1	0
86	C5	201	OHX	5	0
86	C8	201	OHX	0	1
86	L3	401	OHX	2	0
86	L3	402	OHX	1	0
86	L4	401	OHX	3	0
86	M0	301	OHX	3	0
86	M9	201	OHX	1	0
86	N9	101	OHX	1	0
86	O1	201	OHX	5	0
86	O3	201	OHX	3	0
86	Q2	502	OHX	4	0
86	S8	301	OHX	2	0
86	S9	201	OHX	4	0
86	SR	401	OHX	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
82	m2	2
80	sM	1
68	O2	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	37.77
1	2	1716:C	O3'	1717:G	P	4.09
1	m2	23:UNK	C	28:UNK	N	3.84
1	m2	52:UNK	C	54:UNK	N	3.47
1	2	1685:G	O3'	1686:C	P	3.06

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1781/1800 (98%)	0.24	80 (4%) 34 16	54, 93, 190, 248	0
1	6	1795/1800 (99%)	0.13	73 (4%) 38 18	41, 80, 181, 246	0
2	S0	206/206 (100%)	0.69	26 (12%) 4 2	92, 107, 120, 134	0
2	s0	206/206 (100%)	0.60	10 (4%) 30 14	77, 95, 110, 124	0
3	S1	214/216 (99%)	1.28	54 (25%) 1 0	101, 136, 157, 161	0
3	s1	216/216 (100%)	0.89	25 (11%) 5 2	79, 98, 118, 131	0
4	S2	217/217 (100%)	0.30	4 (1%) 69 47	75, 88, 102, 114	0
4	s2	217/217 (100%)	0.30	8 (3%) 42 21	62, 78, 91, 106	0
5	S3	223/223 (100%)	0.67	16 (7%) 16 6	82, 97, 126, 136	0
5	s3	223/223 (100%)	1.08	43 (19%) 1 0	82, 119, 148, 156	0
6	S4	260/260 (100%)	0.92	35 (13%) 3 1	65, 93, 104, 136	0
6	s4	260/260 (100%)	0.46	3 (1%) 79 61	52, 76, 92, 126	0
7	S5	206/206 (100%)	1.07	38 (18%) 1 1	102, 125, 135, 149	0
7	s5	206/206 (100%)	0.92	30 (14%) 3 1	76, 104, 123, 130	0
8	S6	226/226 (100%)	0.72	18 (7%) 13 5	68, 109, 126, 143	0
8	s6	218/226 (96%)	0.36	10 (4%) 33 15	52, 86, 103, 121	0
9	S7	184/186 (98%)	0.94	29 (15%) 2 1	84, 117, 140, 147	0
9	s7	186/186 (100%)	0.79	26 (13%) 3 1	71, 111, 139, 148	0
10	S8	188/200 (94%)	0.48	10 (5%) 27 12	59, 77, 113, 129	0
10	s8	188/200 (94%)	0.63	17 (9%) 10 4	49, 71, 110, 133	0
11	S9	185/185 (100%)	1.30	41 (22%) 1 0	84, 101, 137, 158	0
11	s9	185/185 (100%)	0.81	18 (9%) 8 3	65, 82, 117, 141	0
12	C0	96/98 (97%)	1.00	13 (13%) 3 1	89, 114, 145, 157	0
12	c0	96/98 (97%)	2.72	53 (55%) 0 0	116, 151, 162, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	C1	155/156 (99%)	0.73	17 (10%)	6 2	61, 76, 122, 126	0
13	c1	146/156 (93%)	0.56	10 (6%)	18 7	50, 68, 96, 120	0
14	C2	124/124 (100%)	1.62	41 (33%)	0 0	147, 156, 166, 169	0
14	c2	124/124 (100%)	3.32	102 (82%)	0 0	196, 205, 217, 219	0
15	C3	150/150 (100%)	0.29	3 (2%)	65 44	70, 89, 102, 109	0
15	c3	150/150 (100%)	0.13	1 (0%)	87 75	63, 80, 98, 102	0
16	C4	127/128 (99%)	1.06	28 (22%)	1 0	71, 126, 142, 143	0
16	c4	128/128 (100%)	0.82	10 (7%)	14 5	57, 95, 104, 113	0
17	C5	124/142 (87%)	0.98	17 (13%)	3 1	88, 106, 128, 144	0
17	c5	135/142 (95%)	1.30	31 (22%)	1 0	77, 113, 129, 134	0
18	C6	141/142 (99%)	1.44	43 (30%)	0 0	84, 113, 119, 123	0
18	c6	142/142 (100%)	0.69	13 (9%)	10 3	72, 96, 114, 138	0
19	C7	120/136 (88%)	0.73	13 (10%)	6 2	93, 109, 132, 135	0
19	c7	117/136 (86%)	0.39	2 (1%)	70 49	83, 101, 117, 122	0
20	C8	145/145 (100%)	0.99	26 (17%)	2 1	84, 114, 141, 149	0
20	c8	145/145 (100%)	0.44	8 (5%)	26 11	78, 97, 115, 124	0
21	C9	143/143 (100%)	1.07	23 (16%)	2 1	96, 110, 124, 132	0
21	c9	143/143 (100%)	0.38	7 (4%)	30 14	70, 86, 106, 118	0
22	D0	107/110 (97%)	1.20	24 (22%)	1 0	78, 112, 139, 142	0
22	d0	110/110 (100%)	1.92	45 (40%)	0 0	78, 118, 151, 154	0
23	D1	87/87 (100%)	0.61	6 (6%)	18 7	88, 96, 111, 119	0
23	d1	87/87 (100%)	0.37	3 (3%)	46 23	71, 83, 106, 117	0
24	D2	129/129 (100%)	0.36	0	100 100	69, 83, 90, 99	0
24	d2	129/129 (100%)	0.15	0	100 100	56, 68, 78, 85	0
25	D3	144/144 (100%)	0.37	1 (0%)	87 75	61, 69, 83, 101	0
25	d3	144/144 (100%)	0.19	2 (1%)	75 57	51, 56, 70, 87	0
26	D4	134/134 (100%)	0.90	15 (11%)	6 2	83, 104, 120, 126	0
26	d4	134/134 (100%)	0.59	11 (8%)	12 5	61, 87, 101, 110	0
27	D5	70/70 (100%)	1.55	22 (31%)	0 0	123, 140, 145, 146	0
27	d5	69/70 (98%)	1.39	15 (21%)	1 0	92, 113, 123, 126	0
28	D6	97/97 (100%)	1.27	24 (24%)	1 0	78, 96, 144, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	0.48	4 (4%) 38 18	62, 78, 106, 112	0
29	D7	81/81 (100%)	0.83	10 (12%) 5 2	86, 104, 137, 138	0
29	d7	81/81 (100%)	0.66	8 (9%) 8 3	74, 92, 133, 136	0
30	D8	63/63 (100%)	1.42	17 (26%) 1 0	111, 131, 140, 142	0
30	d8	63/63 (100%)	1.66	20 (31%) 0 0	96, 115, 125, 132	0
31	D9	53/53 (100%)	0.64	4 (7%) 15 5	81, 86, 112, 118	0
31	d9	53/53 (100%)	1.37	14 (26%) 1 0	77, 94, 143, 158	0
32	E0	60/62 (96%)	1.43	14 (23%) 1 0	70, 103, 131, 136	0
32	e0	62/62 (100%)	0.82	8 (12%) 4 2	56, 84, 115, 127	0
33	E1	71/76 (93%)	1.52	19 (26%) 1 0	110, 142, 152, 154	0
33	e1	76/76 (100%)	3.08	48 (63%) 0 0	120, 187, 198, 200	0
34	SR	318/318 (100%)	1.12	67 (21%) 1 0	107, 124, 138, 158	0
34	sR	318/318 (100%)	1.32	79 (24%) 1 0	108, 128, 144, 156	0
35	SM	133/176 (75%)	0.99	21 (15%) 2 1	62, 94, 148, 159	0
36	1	3149/3396 (92%)	0.01	55 (1%) 70 49	31, 56, 138, 237	0
36	5	3150/3396 (92%)	-0.02	50 (1%) 72 51	29, 54, 127, 213	0
37	3	121/121 (100%)	-0.17	0 100 100	45, 83, 107, 113	0
37	7	121/121 (100%)	-0.26	0 100 100	36, 59, 72, 85	0
38	4	158/158 (100%)	-0.10	1 (0%) 89 77	36, 56, 97, 138	0
38	8	158/158 (100%)	-0.02	2 (1%) 77 59	42, 65, 107, 142	0
39	L2	252/252 (100%)	0.08	3 (1%) 79 61	37, 54, 70, 85	0
39	l2	252/252 (100%)	0.15	5 (1%) 65 44	40, 61, 80, 87	0
40	L3	386/386 (100%)	0.05	5 (1%) 77 59	39, 64, 80, 97	0
40	l3	386/386 (100%)	-0.16	2 (0%) 90 80	30, 46, 64, 92	0
41	L4	361/361 (100%)	-0.18	0 100 100	33, 49, 70, 78	0
41	l4	361/361 (100%)	-0.04	0 100 100	38, 57, 76, 87	0
42	L5	296/296 (100%)	0.73	34 (11%) 5 2	58, 91, 113, 136	0
42	l5	294/296 (99%)	0.16	7 (2%) 59 37	42, 64, 88, 109	0
43	L6	156/176 (88%)	0.02	2 (1%) 77 59	44, 55, 73, 84	0
43	l6	157/176 (89%)	0.05	2 (1%) 77 59	48, 56, 79, 92	0
44	L7	222/223 (99%)	-0.07	1 (0%) 90 80	39, 49, 80, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/223 (100%)	-0.14	0 100 100	35, 45, 86, 119	0
45	L8	233/233 (100%)	0.53	9 (3%) 40 19	62, 79, 117, 130	0
46	L9	191/191 (100%)	0.19	5 (2%) 56 33	64, 76, 90, 106	0
46	l9	191/191 (100%)	-0.10	2 (1%) 82 67	43, 52, 72, 86	0
47	M0	211/221 (95%)	0.49	6 (2%) 53 29	44, 67, 103, 110	0
47	m0	213/221 (96%)	0.24	4 (1%) 67 46	37, 55, 83, 102	0
48	M1	169/169 (100%)	0.53	11 (6%) 20 7	75, 94, 108, 118	0
48	m1	169/169 (100%)	0.08	1 (0%) 89 77	47, 69, 81, 85	0
49	M3	193/194 (99%)	0.11	3 (1%) 72 51	37, 60, 100, 131	0
49	m3	194/194 (100%)	0.62	14 (7%) 16 6	42, 72, 112, 125	0
50	M4	136/137 (99%)	-0.08	2 (1%) 74 54	51, 61, 78, 91	0
50	m4	137/137 (100%)	-0.25	1 (0%) 87 75	44, 51, 68, 84	0
51	M5	203/203 (100%)	-0.02	0 100 100	36, 50, 61, 64	0
51	m5	203/203 (100%)	0.21	1 (0%) 90 80	45, 63, 76, 80	0
52	M6	197/197 (100%)	-0.06	0 100 100	39, 50, 72, 78	0
52	m6	197/197 (100%)	-0.14	1 (0%) 90 80	31, 37, 68, 76	0
53	M7	183/183 (100%)	0.54	14 (7%) 14 5	40, 49, 107, 132	0
53	m7	155/183 (84%)	-0.02	0 100 100	36, 45, 61, 89	0
54	M8	185/185 (100%)	-0.10	0 100 100	39, 49, 65, 85	0
54	m8	185/185 (100%)	-0.01	0 100 100	38, 56, 68, 74	0
55	M9	188/188 (100%)	0.41	10 (5%) 27 12	57, 73, 146, 153	0
55	m9	188/188 (100%)	0.21	6 (3%) 48 25	52, 66, 133, 143	0
56	N0	172/172 (100%)	0.14	2 (1%) 79 61	50, 60, 75, 81	0
56	n0	172/172 (100%)	-0.10	0 100 100	37, 45, 59, 73	0
57	N1	159/159 (100%)	0.20	3 (1%) 67 46	43, 57, 103, 110	0
57	n1	159/159 (100%)	0.03	3 (1%) 67 46	40, 47, 91, 97	0
58	N2	100/100 (100%)	0.65	10 (10%) 8 3	90, 104, 113, 114	0
58	n2	98/100 (98%)	1.22	22 (22%) 1 0	80, 92, 102, 105	0
59	N3	136/136 (100%)	0.36	4 (2%) 52 28	47, 60, 74, 83	0
59	n3	136/136 (100%)	0.24	4 (2%) 52 28	32, 43, 59, 67	0
60	N4	98/98 (100%)	2.04	32 (32%) 0 0	59, 72, 144, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	N5	121/121 (100%)	0.29	3 (2%) 58 35	50, 66, 79, 104	0
61	n5	120/121 (99%)	0.37	2 (1%) 70 49	56, 72, 90, 106	0
62	N6	126/126 (100%)	0.29	5 (3%) 39 19	42, 58, 72, 85	0
62	n6	126/126 (100%)	0.43	2 (1%) 72 51	50, 67, 84, 91	0
63	N7	135/135 (100%)	0.98	16 (11%) 5 2	75, 91, 103, 109	0
63	n7	135/135 (100%)	1.15	28 (20%) 1 0	87, 102, 115, 123	0
64	N8	148/148 (100%)	0.01	1 (0%) 87 75	30, 52, 77, 86	0
64	n8	148/148 (100%)	0.15	1 (0%) 87 75	34, 58, 80, 84	0
65	N9	58/58 (100%)	0.33	3 (5%) 28 12	37, 60, 105, 119	0
65	n9	58/58 (100%)	0.11	1 (1%) 70 49	37, 58, 83, 93	0
66	O0	97/100 (97%)	0.45	5 (5%) 28 12	75, 85, 106, 114	0
66	o0	100/100 (100%)	0.68	8 (8%) 13 5	79, 90, 114, 122	0
67	O1	109/109 (100%)	0.56	5 (4%) 33 15	55, 68, 96, 104	0
67	o1	109/109 (100%)	0.35	3 (2%) 53 29	44, 58, 91, 114	0
68	O2	127/127 (100%)	0.11	3 (2%) 59 37	34, 45, 59, 78	0
68	o2	127/127 (100%)	0.21	2 (1%) 72 51	33, 52, 68, 89	0
69	O3	106/106 (100%)	-0.10	0 100 100	40, 46, 68, 83	0
69	o3	106/106 (100%)	-0.01	1 (0%) 84 69	35, 43, 68, 84	0
70	O4	112/112 (100%)	0.49	5 (4%) 34 16	49, 70, 107, 115	0
70	o4	112/112 (100%)	0.34	3 (2%) 55 30	53, 74, 114, 119	0
71	O5	119/119 (100%)	0.25	3 (2%) 58 35	47, 68, 77, 80	0
71	o5	119/119 (100%)	0.36	4 (3%) 46 23	60, 78, 89, 98	0
72	O6	99/99 (100%)	0.54	6 (6%) 22 9	57, 68, 99, 114	0
72	o6	99/99 (100%)	0.77	12 (12%) 5 2	66, 79, 100, 115	0
73	O7	87/87 (100%)	0.00	3 (3%) 46 23	39, 44, 65, 77	0
73	o7	87/87 (100%)	0.20	2 (2%) 61 39	40, 51, 81, 100	0
74	O8	77/77 (100%)	0.84	7 (9%) 10 4	80, 92, 104, 107	0
74	o8	77/77 (100%)	1.29	14 (18%) 1 1	85, 96, 106, 108	0
75	O9	50/50 (100%)	0.07	0 100 100	46, 52, 58, 59	0
75	o9	50/50 (100%)	0.15	1 (2%) 65 44	48, 56, 67, 70	0
76	Q0	52/52 (100%)	0.48	5 (9%) 9 3	55, 65, 84, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	q0	52/52 (100%)	-0.11	0 100 100	38, 43, 58, 62	0
77	Q1	25/25 (100%)	0.49	0 100 100	57, 59, 62, 62	0
77	q1	25/25 (100%)	0.29	0 100 100	46, 52, 57, 60	0
78	Q2	105/105 (100%)	0.85	10 (9%) 9 3	42, 63, 90, 117	0
78	q2	105/105 (100%)	0.32	5 (4%) 31 14	46, 61, 83, 105	0
79	Q3	91/91 (100%)	0.03	0 100 100	45, 58, 76, 83	0
79	q3	91/91 (100%)	0.14	1 (1%) 80 65	43, 62, 77, 89	0
80	sM	63/159 (39%)	1.31	10 (15%) 2 1	53, 109, 119, 121	0
81	l8	231/231 (100%)	0.80	20 (8%) 11 4	77, 92, 121, 130	0
82	m2	0/155	-	-	-	-
83	n4	135/135 (100%)	0.86	20 (14%) 3 1	43, 90, 125, 142	0
84	p0	143/312 (45%)	1.46	40 (27%) 1 0	91, 112, 173, 175	0
85	p1	0/47	-	-	-	-
85	p2	0/47	-	-	-	-
All	All	33027/34321 (96%)	0.38	2175 (6%) 19 7	29, 74, 138, 248	0

The worst 5 of 2175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	c0	98	THR	15.9
60	N4	86	SER	15.2
60	N4	85	ALA	13.6
1	2	1702	A	13.5
1	2	1693	A	12.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
87	MG	6	2062	1/1	0.92	0.48	107.08	51,51,51,51	0
87	MG	5	3913	1/1	0.97	0.53	97.93	41,41,41,41	0
87	MG	5	3849	1/1	0.98	0.84	54.77	36,36,36,36	0
86	OHX	5	3703	7/7	0.91	0.42	45.38	50,52,53,85	7
87	MG	1	3828	1/1	0.95	0.66	43.95	40,40,40,40	0
87	MG	1	3872	1/1	0.99	0.67	41.81	31,31,31,31	0
87	MG	1	3809	1/1	0.96	0.64	40.92	29,29,29,29	0
87	MG	5	3862	1/1	0.96	0.93	40.64	59,59,59,59	0
87	MG	1	3839	1/1	0.97	0.66	36.41	29,29,29,29	0
87	MG	1	3849	1/1	0.98	0.54	35.69	33,33,33,33	0
87	MG	5	3783	1/1	0.92	0.65	35.45	45,45,45,45	0
87	MG	1	3893	1/1	0.98	0.61	34.87	31,31,31,31	0
87	MG	1	3995	1/1	0.97	0.37	34.46	35,35,35,35	0
87	MG	1	3813	1/1	0.97	0.54	34.45	30,30,30,30	0
87	MG	5	3884	1/1	0.99	0.60	34.42	33,33,33,33	0
87	MG	5	3904	1/1	0.93	0.54	34.22	40,40,40,40	0
87	MG	1	3719	1/1	0.94	0.61	33.71	40,40,40,40	0
87	MG	1	3718	1/1	0.79	0.67	32.68	46,46,46,46	0
87	MG	2	2038	1/1	0.95	0.55	32.16	56,56,56,56	0
87	MG	1	3818	1/1	0.99	0.45	32.16	32,32,32,32	0
87	MG	6	2052	1/1	0.94	0.40	31.88	61,61,61,61	0
87	MG	1	4029	1/1	0.96	0.59	31.60	43,43,43,43	0
87	MG	6	2069	1/1	0.89	0.66	30.26	72,72,72,72	0
87	MG	1	3883	1/1	0.97	0.58	29.75	48,48,48,48	0
87	MG	5	3829	1/1	0.96	0.58	29.53	32,32,32,32	0
87	MG	5	3902	1/1	0.99	0.71	28.98	29,29,29,29	0
87	MG	6	2080	1/1	0.85	0.46	28.70	51,51,51,51	0
87	MG	1	3892	1/1	0.99	0.72	28.27	31,31,31,31	0
87	MG	1	3868	1/1	0.89	0.71	28.17	52,52,52,52	0
87	MG	1	3991	1/1	0.83	0.40	27.55	61,61,61,61	0
87	MG	6	2089	1/1	0.93	0.57	27.48	48,48,48,48	0
87	MG	5	3874	1/1	0.94	0.50	27.42	34,34,34,34	0
87	MG	1	3999	1/1	0.97	0.39	26.55	32,32,32,32	0
87	MG	1	3890	1/1	0.95	0.60	26.47	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3744	1/1	0.98	0.60	25.82	43,43,43,43	0
87	MG	1	3793	1/1	0.96	0.48	25.74	38,38,38,38	0
87	MG	2	2063	1/1	0.94	0.73	25.55	57,57,57,57	0
87	MG	1	3819	1/1	0.99	0.61	25.31	35,35,35,35	0
87	MG	1	3779	1/1	0.94	0.52	24.69	26,26,26,26	0
87	MG	5	3912	1/1	0.99	0.49	23.97	27,27,27,27	0
87	MG	5	3826	1/1	0.95	0.58	23.85	27,27,27,27	0
87	MG	5	3807	1/1	0.91	0.63	23.75	39,39,39,39	0
87	MG	5	3909	1/1	0.97	0.58	23.61	37,37,37,37	0
87	MG	5	3786	1/1	0.82	0.58	23.36	34,34,34,34	0
87	MG	1	3750	1/1	0.67	0.43	23.19	46,46,46,46	0
87	MG	5	4012	1/1	0.87	0.32	23.19	40,40,40,40	0
87	MG	2	2062	1/1	0.93	0.49	22.91	56,56,56,56	0
87	MG	5	3742	1/1	0.98	0.58	22.91	26,26,26,26	0
87	MG	1	3842	1/1	0.96	0.55	22.65	43,43,43,43	0
86	OHX	8	212	7/7	0.89	0.43	22.31	72,73,74,109	7
87	MG	4	221	1/1	0.89	0.53	22.00	48,48,48,48	0
87	MG	1	3975	1/1	0.93	0.37	21.92	43,43,43,43	0
87	MG	1	3841	1/1	0.94	0.50	21.26	40,40,40,40	0
87	MG	1	3895	1/1	0.99	0.62	21.20	16,16,16,16	0
87	MG	1	3870	1/1	0.95	0.49	20.74	29,29,29,29	0
87	MG	1	3857	1/1	0.96	0.55	20.37	47,47,47,47	0
87	MG	5	3822	1/1	0.94	0.54	20.31	35,35,35,35	0
87	MG	2	2095	1/1	0.77	0.41	19.98	69,69,69,69	0
87	MG	2	2060	1/1	0.55	0.51	19.77	76,76,76,76	0
87	MG	5	3832	1/1	0.99	0.56	19.72	33,33,33,33	0
87	MG	5	3908	1/1	0.95	0.61	19.64	36,36,36,36	0
87	MG	5	3784	1/1	0.96	0.60	19.40	39,39,39,39	0
87	MG	5	3871	1/1	0.93	0.56	19.39	40,40,40,40	0
87	MG	5	3911	1/1	0.98	0.47	18.90	39,39,39,39	0
87	MG	5	3938	1/1	0.82	0.31	18.84	37,37,37,37	0
87	MG	5	3828	1/1	0.97	0.49	18.76	31,31,31,31	0
87	MG	5	3763	1/1	0.98	0.49	18.63	35,35,35,35	0
87	MG	1	3742	1/1	0.90	0.36	18.34	44,44,44,44	0
87	MG	1	3908	1/1	0.89	0.38	18.21	42,42,42,42	0
87	MG	2	2033	1/1	0.93	0.55	18.06	63,63,63,63	0
87	MG	1	3808	1/1	0.92	0.55	17.96	35,35,35,35	0
87	MG	5	3840	1/1	0.91	0.45	17.95	34,34,34,34	0
87	MG	6	2038	1/1	0.85	0.52	17.80	51,51,51,51	0
87	MG	1	3934	1/1	0.98	0.42	17.79	39,39,39,39	0
87	MG	1	3827	1/1	0.89	0.42	17.62	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	MG	6	2055	1/1	0.98	0.48	17.56	44,44,44,44	0
87	MG	1	3866	1/1	0.96	0.55	17.51	34,34,34,34	0
87	MG	1	3875	1/1	0.92	0.46	17.50	31,31,31,31	0
87	MG	2	2080	1/1	0.84	0.54	17.23	88,88,88,88	0
86	OHX	5	3715	7/7	0.80	0.43	16.98	62,64,66,97	7
87	MG	1	3856	1/1	0.98	0.43	16.56	31,31,31,31	0
86	OHX	5	3658	7/7	0.89	0.25	16.53	56,57,60,98	7
87	MG	1	3769	1/1	0.96	0.53	16.50	34,34,34,34	0
87	MG	1	3863	1/1	0.96	0.49	16.47	38,38,38,38	0
87	MG	1	3840	1/1	0.94	0.41	16.46	30,30,30,30	0
87	MG	N8	202	1/1	0.79	0.50	16.42	41,41,41,41	0
87	MG	5	3842	1/1	0.93	0.45	16.12	40,40,40,40	0
87	MG	m7	201	1/1	0.97	0.65	16.06	35,35,35,35	0
87	MG	1	3867	1/1	0.90	0.48	15.98	25,25,25,25	0
87	MG	5	3731	1/1	0.73	0.34	15.97	49,49,49,49	0
87	MG	1	3871	1/1	0.90	0.45	15.84	45,45,45,45	0
86	OHX	1	3517	7/7	0.94	0.31	15.81	55,58,61,96	7
87	MG	2	2034	1/1	0.93	0.44	15.56	63,63,63,63	0
87	MG	1	3850	1/1	0.96	0.59	15.47	40,40,40,40	0
87	MG	1	3811	1/1	0.96	0.50	15.35	38,38,38,38	0
87	MG	5	3881	1/1	0.98	0.57	15.35	34,34,34,34	0
86	OHX	6	2034	7/7	0.74	0.48	15.34	84,85,86,112	7
87	MG	5	3901	1/1	0.98	0.57	15.34	36,36,36,36	0
87	MG	5	3819	1/1	0.97	0.30	15.33	33,33,33,33	0
87	MG	O2	201	1/1	0.93	0.35	15.07	33,33,33,33	0
87	MG	1	3805	1/1	0.98	0.38	14.95	43,43,43,43	0
86	OHX	1	3652	7/7	0.95	0.36	14.79	80,81,82,112	7
87	MG	4	224	1/1	0.98	0.39	14.72	37,37,37,37	0
87	MG	6	2079	1/1	0.96	0.51	14.62	67,67,67,67	0
87	MG	5	4106	1/1	0.93	0.62	14.58	50,50,50,50	0
87	MG	5	3890	1/1	0.98	0.42	14.52	30,30,30,30	0
87	MG	5	3865	1/1	0.92	0.29	14.49	58,58,58,58	0
87	MG	1	3898	1/1	0.96	0.36	14.37	35,35,35,35	0
87	MG	1	3821	1/1	0.94	0.40	14.37	38,38,38,38	0
87	MG	5	3920	1/1	0.90	0.37	14.33	39,39,39,39	0
87	MG	1	3888	1/1	0.93	0.40	14.10	61,61,61,61	0
87	MG	5	3886	1/1	0.96	0.48	13.93	36,36,36,36	0
87	MG	8	222	1/1	0.91	0.46	13.92	61,61,61,61	0
87	MG	2	2051	1/1	0.92	0.62	13.82	80,80,80,80	0
87	MG	1	3802	1/1	0.98	0.46	13.67	28,28,28,28	0
87	MG	5	3952	1/1	0.96	0.33	13.63	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	2082	1/1	0.91	0.57	13.56	58,58,58,58	0
87	MG	5	3778	1/1	0.90	0.35	13.52	34,34,34,34	0
86	OHX	1	3669	7/7	0.96	0.31	13.42	45,47,50,76	7
87	MG	5	3875	1/1	0.77	0.47	13.40	48,48,48,48	0
87	MG	1	3817	1/1	0.94	0.42	13.25	45,45,45,45	0
87	MG	5	4101	1/1	0.96	0.45	13.24	34,34,34,34	0
87	MG	6	2049	1/1	0.84	0.53	13.10	50,50,50,50	0
87	MG	5	3994	1/1	0.90	0.35	13.09	49,49,49,49	0
86	OHX	1	3677	7/7	0.91	0.30	12.95	68,69,69,96	7
87	MG	5	3834	1/1	0.94	0.50	12.91	33,33,33,33	0
87	MG	5	3858	1/1	0.97	0.73	12.79	30,30,30,30	0
87	MG	5	3905	1/1	0.97	0.53	12.76	34,34,34,34	0
87	MG	5	3910	1/1	0.96	0.43	12.73	41,41,41,41	0
87	MG	5	3962	1/1	0.96	0.37	12.67	40,40,40,40	0
87	MG	5	3914	1/1	0.93	0.48	12.53	33,33,33,33	0
87	MG	5	3906	1/1	0.94	0.36	12.51	35,35,35,35	0
87	MG	5	3887	1/1	0.81	0.55	12.44	37,37,37,37	0
87	MG	1	3823	1/1	0.96	0.55	12.38	40,40,40,40	0
87	MG	5	3797	1/1	0.92	0.36	12.30	37,37,37,37	0
86	OHX	5	3603	7/7	0.92	0.33	12.24	49,50,53,92	7
87	MG	5	3765	1/1	0.98	0.42	12.22	37,37,37,37	0
87	MG	1	3885	1/1	0.98	0.49	12.19	35,35,35,35	0
87	MG	6	2042	1/1	0.91	0.54	12.11	67,67,67,67	0
87	MG	5	4078	1/1	0.89	0.38	12.09	37,37,37,37	0
86	OHX	5	3709	7/7	0.83	0.43	12.05	45,45,47,82	7
87	MG	5	4018	1/1	0.93	0.27	12.04	38,38,38,38	0
87	MG	1	3873	1/1	0.94	0.52	12.03	29,29,29,29	0
87	MG	8	218	1/1	0.95	0.39	11.99	47,47,47,47	0
87	MG	6	2061	1/1	0.94	0.46	11.97	39,39,39,39	0
87	MG	n3	203	1/1	0.99	0.47	11.93	31,31,31,31	0
87	MG	5	3735	1/1	0.97	0.46	11.86	37,37,37,37	0
87	MG	5	3729	1/1	0.75	0.40	11.86	41,41,41,41	0
87	MG	1	3778	1/1	0.88	0.34	11.84	34,34,34,34	0
87	MG	1	3762	1/1	0.94	0.45	11.82	43,43,43,43	0
87	MG	2	2091	1/1	0.87	0.59	11.57	64,64,64,64	0
87	MG	5	3864	1/1	0.77	0.50	11.57	60,60,60,60	0
86	OHX	1	3705	7/7	0.86	0.23	11.54	61,62,64,96	7
86	OHX	5	3679	7/7	0.96	0.23	11.40	55,56,59,90	7
87	MG	6	2096	1/1	0.97	0.31	11.31	61,61,61,61	0
87	MG	1	4060	1/1	0.92	0.39	11.23	28,28,28,28	0
87	MG	M7	201	1/1	0.96	0.59	11.15	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	3706	7/7	0.89	0.29	11.15	57,58,59,88	7
86	OHX	5	3666	7/7	0.92	0.35	11.02	54,55,56,85	7
87	MG	5	3885	1/1	0.93	0.36	10.89	29,29,29,29	0
87	MG	2	2049	1/1	0.93	0.38	10.72	66,66,66,66	0
86	OHX	1	3658	7/7	0.91	0.32	10.62	93,93,94,127	7
87	MG	5	3891	1/1	0.97	0.36	10.49	37,37,37,37	0
87	MG	1	3852	1/1	0.87	0.51	10.38	38,38,38,38	0
87	MG	1	3800	1/1	0.93	0.38	10.35	35,35,35,35	0
87	MG	1	4001	1/1	0.92	0.24	10.34	54,54,54,54	0
87	MG	5	3811	1/1	0.85	0.34	10.30	50,50,50,50	0
87	MG	1	3886	1/1	0.97	0.35	10.30	43,43,43,43	0
87	MG	1	4026	1/1	0.81	0.31	10.23	29,29,29,29	0
86	OHX	1	3616	7/7	0.92	0.34	10.10	58,58,61,88	7
87	MG	1	3721	1/1	0.94	0.42	9.97	49,49,49,49	0
87	MG	2	2082	1/1	0.87	0.57	9.95	60,60,60,60	0
87	MG	1	3936	1/1	0.88	0.71	9.92	56,56,56,56	0
87	MG	2	2046	1/1	0.90	0.45	9.88	71,71,71,71	0
86	OHX	5	3698	7/7	0.91	0.40	9.83	66,66,68,99	7
87	MG	5	3882	1/1	0.92	0.32	9.71	30,30,30,30	0
87	MG	5	3897	1/1	0.99	0.46	9.70	35,35,35,35	0
87	MG	5	3876	1/1	0.95	0.35	9.69	37,37,37,37	0
87	MG	2	2087	1/1	0.89	0.45	9.66	84,84,84,84	0
87	MG	1	4057	1/1	0.97	0.40	9.55	44,44,44,44	0
87	MG	5	3922	1/1	0.94	0.40	9.40	32,32,32,32	0
87	MG	5	4076	1/1	0.94	0.42	9.39	43,43,43,43	0
86	OHX	5	3719	7/7	0.95	0.32	9.38	57,57,58,94	7
87	MG	6	2044	1/1	0.90	0.46	9.31	75,75,75,75	0
86	OHX	6	2020	7/7	0.81	0.37	9.27	58,58,60,94	7
86	OHX	5	3716	7/7	0.82	0.33	9.21	61,64,65,102	7
87	MG	5	3945	1/1	0.95	0.36	9.08	56,56,56,56	0
87	MG	L2	301	1/1	0.91	0.42	9.01	37,37,37,37	0
86	OHX	5	3563	7/7	0.95	0.28	8.96	66,68,69,96	7
86	OHX	1	3476	7/7	0.98	0.29	8.91	55,57,59,91	7
87	MG	5	3747	1/1	0.86	0.30	8.83	40,40,40,40	0
86	OHX	1	3564	7/7	0.95	0.29	8.81	49,51,52,90	7
86	OHX	5	3634	7/7	0.94	0.28	8.81	62,63,64,90	7
86	OHX	5	3601	7/7	0.89	0.26	8.77	83,85,88,109	7
87	MG	5	3730	1/1	0.93	0.33	8.76	42,42,42,42	0
87	MG	1	4017	1/1	0.95	0.32	8.73	37,37,37,37	0
87	MG	2	2074	1/1	0.79	0.34	8.66	107,107,107,107	0
87	MG	1	3835	1/1	0.87	0.47	8.58	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	4	217	7/7	0.88	0.40	8.53	61,63,64,98	7
87	MG	5	3833	1/1	0.91	0.29	8.51	38,38,38,38	0
87	MG	2	2090	1/1	0.88	0.36	8.33	60,60,60,60	0
86	OHX	1	3691	7/7	0.93	0.32	8.27	60,61,62,98	7
87	MG	5	4099	1/1	0.75	0.34	8.26	41,41,41,41	0
87	MG	1	3955	1/1	0.92	0.34	8.16	38,38,38,38	0
86	OHX	5	3690	7/7	0.94	0.27	8.16	66,68,70,102	7
87	MG	12	303	1/1	0.71	0.38	7.94	44,44,44,44	0
87	MG	1	3725	1/1	0.97	0.51	7.92	38,38,38,38	0
87	MG	6	2048	1/1	0.93	0.35	7.83	91,91,91,91	0
87	MG	5	4055	1/1	0.87	0.64	7.73	47,47,47,47	1
87	MG	6	2101	1/1	0.87	0.30	7.67	72,72,72,72	0
87	MG	5	3955	1/1	0.90	0.26	7.67	36,36,36,36	0
86	OHX	2	1997	7/7	0.94	0.29	7.55	69,70,72,98	7
87	MG	1	3727	1/1	0.77	0.26	7.51	50,50,50,50	0
86	OHX	5	3660	7/7	0.97	0.28	7.50	42,46,48,80	7
87	MG	5	3749	1/1	0.99	0.52	7.49	44,44,44,44	0
87	MG	1	3897	1/1	0.94	0.31	7.42	33,33,33,33	0
87	MG	L2	302	1/1	0.97	0.42	7.40	39,39,39,39	0
86	OHX	5	3613	7/7	0.96	0.23	7.31	41,43,45,72	7
87	MG	1	3790	1/1	0.95	0.49	7.27	44,44,44,44	0
87	MG	1	3967	1/1	0.93	0.24	7.14	50,50,50,50	0
87	MG	5	3852	1/1	0.95	0.26	7.12	56,56,56,56	0
87	MG	2	2042	1/1	0.92	0.41	6.98	71,71,71,71	0
87	MG	1	3746	1/1	0.98	0.33	6.95	39,39,39,39	0
87	MG	c1	201	1/1	0.85	0.48	6.81	52,52,52,52	0
86	OHX	8	210	7/7	0.95	0.25	6.80	86,87,88,113	7
86	OHX	5	3720	7/7	0.86	0.42	6.78	75,76,77,111	7
87	MG	2	2092	1/1	0.78	0.25	6.71	61,61,61,61	0
87	MG	L7	302	1/1	0.90	0.56	6.70	49,49,49,49	0
86	OHX	5	3713	7/7	0.93	0.27	6.69	44,44,45,87	7
86	OHX	5	3531	7/7	0.96	0.30	6.68	62,64,65,100	7
87	MG	1	3713	1/1	0.93	0.44	6.65	49,49,49,49	0
86	OHX	1	3693	7/7	0.82	0.38	6.62	55,57,58,91	7
87	MG	m5	301	1/1	0.97	0.40	6.57	44,44,44,44	0
86	OHX	1	3594	7/7	0.95	0.36	6.54	70,70,72,100	7
87	MG	1	3985	1/1	0.86	0.56	6.52	44,44,44,44	0
87	MG	5	3844	1/1	0.87	0.25	6.46	48,48,48,48	0
87	MG	5	3846	1/1	0.93	0.53	6.44	59,59,59,59	0
86	OHX	1	3641	7/7	0.88	0.26	6.29	77,77,78,103	7
86	OHX	7	208	7/7	0.93	0.30	6.25	51,53,55,82	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3696	7/7	0.90	0.28	6.21	45,47,49,83	7
87	MG	5	3791	1/1	0.86	0.33	6.20	39,39,39,39	0
87	MG	1	3971	1/1	0.91	0.29	6.13	39,39,39,39	0
87	MG	2	2069	1/1	0.95	0.40	5.99	63,63,63,63	0
87	MG	1	4063	1/1	0.92	0.38	5.93	34,34,34,34	0
86	OHX	5	3566	7/7	0.94	0.27	5.82	66,67,67,94	7
87	MG	1	3848	1/1	0.98	0.35	5.81	49,49,49,49	0
86	OHX	5	3650	7/7	0.92	0.26	5.71	44,46,47,79	7
87	MG	5	3767	1/1	0.96	0.29	5.70	31,31,31,31	0
87	MG	1	3860	1/1	0.95	0.30	5.65	51,51,51,51	0
86	OHX	5	3564	7/7	0.91	0.21	5.64	88,89,91,122	7
87	MG	6	2074	1/1	0.96	0.29	5.63	53,53,53,53	0
87	MG	5	3928	1/1	0.95	0.24	5.62	37,37,37,37	0
87	MG	5	3827	1/1	0.95	0.34	5.61	44,44,44,44	0
87	MG	2	2117	1/1	0.87	0.37	5.50	95,95,95,95	0
87	MG	5	4104	1/1	0.72	0.44	5.37	52,52,52,52	0
87	MG	5	3925	1/1	0.95	0.32	5.26	44,44,44,44	0
87	MG	2	2065	1/1	0.93	0.40	5.25	77,77,77,77	0
86	OHX	6	2024	7/7	0.86	0.28	5.20	90,90,92,119	7
87	MG	5	4054	1/1	0.98	0.29	5.17	30,30,30,30	0
86	OHX	1	3606	7/7	0.90	0.32	5.17	39,40,42,80	7
87	MG	1	3972	1/1	0.81	0.27	5.16	46,46,46,46	0
87	MG	5	3967	1/1	0.97	0.33	5.15	37,37,37,37	0
86	OHX	1	3686	7/7	0.92	0.27	5.13	74,75,76,104	7
87	MG	5	3746	1/1	0.94	0.31	5.09	64,64,64,64	0
86	OHX	5	3494	7/7	0.97	0.23	5.06	46,47,50,70	7
86	OHX	5	3643	7/7	0.92	0.25	5.04	50,52,54,79	7
86	OHX	5	3580	7/7	0.96	0.30	5.01	60,61,61,91	7
87	MG	5	3813	1/1	0.95	0.43	4.95	32,32,32,32	0
87	MG	5	3782	1/1	0.97	0.32	4.91	39,39,39,39	0
87	MG	5	3984	1/1	0.95	0.27	4.91	50,50,50,50	0
86	OHX	1	3454	7/7	0.96	0.28	4.88	53,58,59,80	7
86	OHX	1	3689	7/7	0.93	0.26	4.88	43,45,46,85	7
86	OHX	1	3651	7/7	0.88	0.38	4.85	62,63,67,100	7
87	MG	1	3753	1/1	0.96	0.51	4.85	45,45,45,45	0
86	OHX	1	3501	7/7	0.94	0.24	4.84	54,58,61,93	7
86	OHX	8	213	7/7	0.87	0.21	4.84	80,82,83,117	7
87	MG	1	3904	1/1	0.96	0.40	4.79	67,67,67,67	0
86	OHX	5	3618	7/7	0.93	0.26	4.75	68,68,71,92	7
86	OHX	6	1976	7/7	0.91	0.23	4.75	104,106,108,131	7
86	OHX	1	3545	7/7	0.91	0.25	4.71	68,69,71,105	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3882	1/1	0.97	0.47	4.69	51,51,51,51	0
87	MG	1	3946	1/1	0.79	0.29	4.66	32,32,32,32	0
86	OHX	5	3641	7/7	0.95	0.22	4.64	68,69,70,102	7
87	MG	5	4107	1/1	0.90	0.34	4.64	46,46,46,46	0
86	OHX	6	1958	7/7	0.85	0.25	4.63	67,68,70,109	7
87	MG	1	3796	1/1	0.97	0.21	4.62	49,49,49,49	0
87	MG	1	3731	1/1	0.85	0.24	4.54	39,39,39,39	0
87	MG	5	3969	1/1	0.95	0.29	4.53	39,39,39,39	0
86	OHX	5	3700	7/7	0.94	0.29	4.51	42,43,45,80	7
87	MG	6	2072	1/1	0.94	0.41	4.51	69,69,69,69	0
86	OHX	1	3491	7/7	0.93	0.23	4.46	48,53,56,87	7
86	OHX	6	1986	7/7	0.91	0.27	4.45	88,89,91,108	7
87	MG	1	3916	1/1	0.92	0.31	4.44	42,42,42,42	0
87	MG	5	3944	1/1	0.98	0.25	4.42	43,43,43,43	0
86	OHX	5	3600	7/7	0.96	0.24	4.35	51,53,54,89	7
87	MG	6	2041	1/1	0.91	0.34	4.34	76,76,76,76	0
86	OHX	1	3431	7/7	0.99	0.25	4.28	55,56,62,63	7
86	OHX	2	1960	7/7	0.95	0.20	4.27	80,82,83,112	7
86	OHX	1	3645	7/7	0.94	0.26	4.25	56,58,59,81	7
86	OHX	6	1932	7/7	0.91	0.26	4.22	75,82,85,110	7
86	OHX	1	3598	7/7	0.94	0.28	4.18	62,63,64,92	7
86	OHX	5	3651	7/7	0.86	0.29	4.18	47,47,49,84	7
86	OHX	7	203	7/7	0.94	0.23	4.16	53,59,62,95	7
86	OHX	3	203	7/7	0.96	0.25	4.16	70,71,73,104	7
86	OHX	1	3603	7/7	0.95	0.23	4.16	69,69,70,99	7
86	OHX	1	3620	7/7	0.91	0.30	4.12	60,62,63,97	7
86	OHX	8	209	7/7	0.96	0.21	4.10	71,72,74,99	7
87	MG	2	2057	1/1	0.91	0.25	4.06	66,66,66,66	0
87	MG	6	2105	1/1	0.96	0.28	4.06	45,45,45,45	0
86	OHX	5	3550	7/7	0.94	0.24	4.06	67,70,71,107	7
86	OHX	1	3541	7/7	0.95	0.27	4.06	68,69,70,102	7
86	OHX	N9	101	7/7	0.99	0.23	4.05	50,50,57,72	7
86	OHX	1	3475	7/7	0.96	0.26	4.00	57,60,62,90	7
86	OHX	1	3432	7/7	0.99	0.25	3.95	49,50,52,69	7
86	OHX	2	1999	7/7	0.93	0.33	3.94	75,75,76,103	7
86	OHX	5	3525	7/7	0.95	0.20	3.93	57,59,61,91	7
87	MG	5	4011	1/1	0.97	0.36	3.88	43,43,43,43	0
87	MG	1	3964	1/1	0.83	0.28	3.84	44,44,44,44	0
86	OHX	1	3646	7/7	0.91	0.20	3.84	69,71,71,109	7
87	MG	N3	201	1/1	0.89	0.28	3.81	43,43,43,43	0
86	OHX	5	3640	7/7	0.89	0.35	3.80	63,63,66,91	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3540	7/7	0.94	0.19	3.78	88,89,93,116	7
86	OHX	1	3589	7/7	0.94	0.24	3.78	84,86,88,115	7
86	OHX	5	3519	7/7	0.83	0.23	3.75	133,136,138,156	7
86	OHX	5	3612	7/7	0.96	0.21	3.71	64,64,65,96	7
87	MG	5	4038	1/1	0.96	0.28	3.70	54,54,54,54	0
87	MG	5	3981	1/1	0.80	0.26	3.70	84,84,84,84	0
86	OHX	4	214	7/7	0.91	0.26	3.68	58,59,63,92	7
86	OHX	2	1922	7/7	0.96	0.21	3.66	72,74,76,104	7
86	OHX	1	3624	7/7	0.97	0.22	3.65	54,54,55,85	7
86	OHX	5	3511	7/7	0.98	0.27	3.64	43,43,48,78	7
86	OHX	5	3689	7/7	0.86	0.28	3.63	80,80,81,104	7
86	OHX	5	3491	7/7	0.98	0.25	3.61	64,66,69,94	7
86	OHX	s4	301	7/7	0.89	0.27	3.60	85,86,87,117	7
87	MG	5	3924	1/1	0.94	0.23	3.60	35,35,35,35	0
87	MG	1	4058	1/1	0.88	0.24	3.57	38,38,38,38	0
86	OHX	6	1966	7/7	0.95	0.24	3.56	67,69,71,91	7
86	OHX	1	3556	7/7	0.96	0.28	3.50	72,73,76,107	7
87	MG	1	4013	1/1	0.97	0.32	3.49	42,42,42,42	0
87	MG	5	3817	1/1	0.99	0.26	3.49	40,40,40,40	0
86	OHX	5	3437	7/7	0.99	0.26	3.48	60,62,65,79	7
86	OHX	2	1928	7/7	0.97	0.24	3.44	74,74,76,99	7
86	OHX	6	1999	7/7	0.95	0.29	3.42	78,79,80,103	7
88	ZN	D7	101	1/1	0.44	0.55	3.39	159,159,159,159	0
86	OHX	5	3536	7/7	0.90	0.23	3.38	73,74,75,104	7
87	MG	1	4020	1/1	0.96	0.24	3.38	43,43,43,43	0
86	OHX	5	3538	7/7	0.96	0.26	3.37	72,76,77,99	7
86	OHX	4	211	7/7	0.97	0.22	3.36	45,47,49,83	7
87	MG	6	2122	1/1	0.92	0.40	3.36	70,70,70,70	0
87	MG	1	3881	1/1	0.96	0.42	3.34	59,59,59,59	0
89	UAM	6	2134	30/30	0.84	0.43	3.29	75,75,75,75	0
86	OHX	5	3431	7/7	0.99	0.25	3.27	48,50,53,62	7
86	OHX	2	1998	7/7	0.89	0.23	3.27	97,97,100,119	7
86	OHX	2	2026	7/7	0.85	0.27	3.23	104,105,106,127	7
87	MG	1	3789	1/1	0.86	0.24	3.22	43,43,43,43	0
86	OHX	1	3547	7/7	0.96	0.25	3.21	72,73,74,106	7
86	OHX	5	3416	7/7	0.99	0.22	3.19	46,47,50,76	7
87	MG	2	2077	1/1	0.88	0.53	3.19	95,95,95,95	0
86	OHX	5	3593	7/7	0.96	0.27	3.18	50,51,53,81	7
86	OHX	5	3721	7/7	0.90	0.20	3.18	111,113,114,141	7
86	OHX	1	3608	7/7	0.94	0.20	3.15	81,81,83,109	7
87	MG	2	2039	1/1	0.89	0.48	3.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3416	7/7	0.98	0.19	3.14	61,67,69,82	7
86	OHX	1	3521	7/7	0.99	0.24	3.13	45,46,47,84	7
86	OHX	6	1972	7/7	0.93	0.27	3.12	103,104,106,123	7
86	OHX	6	2001	7/7	0.97	0.28	3.10	61,62,63,93	7
86	OHX	5	3661	7/7	0.90	0.23	3.10	92,93,94,128	7
86	OHX	2	2021	7/7	0.89	0.26	3.08	64,65,66,101	7
87	MG	1	3780	1/1	0.98	0.27	3.02	41,41,41,41	0
86	OHX	6	1946	7/7	0.94	0.24	3.01	62,64,66,99	7
86	OHX	2	2005	7/7	0.93	0.21	3.00	81,81,81,110	7
86	OHX	5	3653	7/7	0.93	0.26	2.99	70,72,73,97	7
86	OHX	8	214	7/7	0.91	0.19	2.99	104,105,107,129	7
86	OHX	5	3529	7/7	0.96	0.27	2.97	48,51,53,92	7
86	OHX	2	1977	7/7	0.92	0.25	2.97	85,88,88,112	7
86	OHX	1	3680	7/7	0.95	0.24	2.96	57,58,60,100	7
86	OHX	2	2011	7/7	0.91	0.20	2.96	82,84,85,120	7
86	OHX	1	3513	7/7	0.96	0.27	2.95	56,59,62,84	7
86	OHX	1	3596	7/7	0.82	0.21	2.92	84,84,87,118	7
86	OHX	5	3645	7/7	0.95	0.22	2.90	67,67,68,96	7
86	OHX	1	3518	7/7	0.98	0.27	2.87	40,44,47,82	7
86	OHX	5	3535	7/7	0.96	0.21	2.86	65,68,72,92	7
87	MG	2	2071	1/1	0.92	0.23	2.79	60,60,60,60	0
86	OHX	6	2025	7/7	0.92	0.20	2.78	94,94,95,122	7
86	OHX	7	211	7/7	0.85	0.21	2.77	79,80,80,112	7
86	OHX	7	205	7/7	0.99	0.20	2.76	70,72,74,91	7
87	MG	6	2085	1/1	0.97	0.39	2.76	66,66,66,66	0
86	OHX	1	3642	7/7	0.90	0.26	2.72	50,50,53,86	7
87	MG	5	3936	1/1	0.97	0.29	2.72	51,51,51,51	0
86	OHX	6	1930	7/7	0.99	0.23	2.71	56,57,60,77	7
87	MG	n8	201	1/1	0.87	0.36	2.68	53,53,53,53	0
87	MG	1	4019	1/1	0.78	0.36	2.62	40,40,40,40	0
86	OHX	1	3561	7/7	0.98	0.22	2.61	54,54,56,73	7
86	OHX	6	1988	7/7	0.93	0.30	2.56	96,97,97,128	7
87	MG	1	3717	1/1	0.79	0.24	2.55	45,45,45,45	0
87	MG	1	3726	1/1	0.77	0.34	2.55	52,52,52,52	0
86	OHX	5	3692	7/7	0.90	0.26	2.55	55,57,59,90	7
86	OHX	6	1950	7/7	0.91	0.27	2.54	92,93,95,123	7
87	MG	2	2099	1/1	0.84	0.58	2.54	74,74,74,74	0
86	OHX	2	1968	7/7	0.88	0.26	2.52	113,114,115,142	7
86	OHX	1	3657	7/7	0.93	0.21	2.50	85,85,86,119	7
86	OHX	5	3558	7/7	0.95	0.18	2.49	97,97,98,125	7
86	OHX	1	3636	7/7	0.95	0.27	2.49	58,58,61,85	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3448	7/7	0.97	0.23	2.48	58,60,64,98	7
86	OHX	5	3464	7/7	0.97	0.25	2.47	64,65,67,98	7
86	OHX	1	3533	7/7	0.95	0.24	2.44	59,60,62,92	7
86	OHX	5	3490	7/7	0.99	0.20	2.43	55,55,59,86	7
87	MG	1	3829	1/1	0.95	0.21	2.41	50,50,50,50	0
86	OHX	5	3528	7/7	0.93	0.21	2.38	52,54,57,86	7
86	OHX	1	3490	7/7	0.93	0.24	2.37	72,74,78,102	7
86	OHX	1	3528	7/7	0.96	0.22	2.35	53,54,57,85	7
86	OHX	3	202	7/7	0.98	0.22	2.32	62,64,67,94	7
87	MG	1	3786	1/1	0.95	0.25	2.30	38,38,38,38	0
86	OHX	1	3538	7/7	0.95	0.23	2.28	55,58,60,83	7
86	OHX	5	3480	7/7	0.97	0.27	2.26	63,64,66,87	7
86	OHX	5	3465	7/7	0.99	0.23	2.25	55,56,58,64	7
86	OHX	5	3608	7/7	0.94	0.26	2.24	70,71,72,99	7
86	OHX	1	3522	7/7	0.96	0.22	2.23	49,50,52,73	7
86	OHX	2	1943	7/7	0.96	0.24	2.23	68,71,73,95	7
87	MG	5	3739	1/1	0.84	0.24	2.23	71,71,71,71	0
86	OHX	1	3447	7/7	0.97	0.22	2.22	54,55,59,84	7
86	OHX	5	3594	7/7	0.96	0.25	2.21	79,79,81,107	7
86	OHX	1	3514	7/7	0.97	0.24	2.20	41,46,51,81	7
86	OHX	5	3665	7/7	0.93	0.29	2.19	69,69,71,102	7
86	OHX	6	1989	7/7	0.83	0.30	2.19	72,73,75,105	7
86	OHX	5	3681	7/7	0.73	0.33	2.18	96,97,98,130	7
86	OHX	5	3523	7/7	0.95	0.20	2.17	47,49,55,86	7
86	OHX	6	1961	7/7	0.94	0.25	2.14	77,79,81,110	7
86	OHX	5	3586	7/7	0.94	0.20	2.12	62,63,64,98	7
86	OHX	6	2023	7/7	0.94	0.21	2.11	64,65,68,103	7
86	OHX	5	3459	7/7	0.96	0.19	2.10	57,59,65,93	7
86	OHX	6	1959	7/7	0.97	0.19	2.08	84,86,87,109	7
86	OHX	1	3676	7/7	0.95	0.25	2.07	68,68,70,94	7
86	OHX	5	3496	7/7	0.96	0.21	2.07	66,68,71,98	7
87	MG	6	2068	1/1	0.93	0.21	2.06	83,83,83,83	0
86	OHX	1	3498	7/7	0.97	0.19	2.05	68,71,72,92	7
87	MG	5	4006	1/1	0.97	0.23	2.03	34,34,34,34	0
86	OHX	5	3440	7/7	0.98	0.19	2.01	75,76,77,89	7
86	OHX	5	3470	7/7	0.96	0.17	1.99	80,84,84,102	7
86	OHX	1	3452	7/7	0.98	0.21	1.98	65,67,69,96	7
86	OHX	1	3704	7/7	0.89	0.26	1.96	68,69,70,101	7
86	OHX	5	3498	7/7	0.99	0.17	1.94	100,101,103,125	7
86	OHX	5	3631	7/7	0.94	0.20	1.92	74,76,78,110	7
86	OHX	1	3593	7/7	0.93	0.26	1.91	59,60,62,89	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3980	1/1	0.88	0.35	1.89	53,53,53,53	0
86	OHX	1	3505	7/7	0.97	0.27	1.89	46,48,52,85	7
86	OHX	6	2000	7/7	0.97	0.21	1.88	60,60,64,94	7
86	OHX	5	3620	7/7	0.91	0.20	1.87	76,77,78,110	7
86	OHX	5	3524	7/7	0.97	0.21	1.85	68,71,73,95	7
86	OHX	6	1915	7/7	0.99	0.20	1.85	57,58,63,80	7
86	OHX	1	3621	7/7	0.98	0.23	1.81	49,51,52,68	7
86	OHX	2	2002	7/7	0.90	0.26	1.80	111,111,114,134	7
86	OHX	5	3541	7/7	0.95	0.21	1.79	65,68,69,97	7
86	OHX	1	3434	7/7	0.97	0.21	1.77	73,75,76,93	7
86	OHX	6	2015	7/7	0.91	0.20	1.76	126,127,128,140	7
86	OHX	1	3643	7/7	0.93	0.22	1.75	51,52,53,83	7
86	OHX	1	3694	7/7	0.95	0.19	1.75	54,57,59,93	7
86	OHX	6	1909	7/7	0.98	0.18	1.74	86,86,90,100	7
86	OHX	5	3638	7/7	0.95	0.24	1.74	45,45,46,80	7
86	OHX	2	2014	7/7	0.92	0.21	1.72	62,65,67,103	7
86	OHX	1	3573	7/7	0.95	0.22	1.72	61,61,62,88	7
87	MG	2	2114	1/1	0.68	0.23	1.72	105,105,105,105	0
86	OHX	2	1956	7/7	0.96	0.20	1.72	76,76,78,103	7
86	OHX	5	3657	7/7	0.95	0.19	1.71	56,57,58,91	7
86	OHX	6	1970	7/7	0.97	0.17	1.68	90,91,92,111	7
86	OHX	2	1938	7/7	0.98	0.23	1.68	65,67,70,93	7
86	OHX	2	2003	7/7	0.83	0.25	1.68	81,83,83,114	7
86	OHX	5	3492	7/7	0.98	0.25	1.64	61,64,66,88	7
86	OHX	5	3425	7/7	0.99	0.20	1.63	57,61,62,83	0
87	MG	5	4052	1/1	0.87	0.21	1.63	34,34,34,34	0
87	MG	1	3763	1/1	0.91	0.34	1.62	60,60,60,60	0
86	OHX	1	3468	7/7	0.99	0.23	1.61	50,52,55,62	7
86	OHX	1	3492	7/7	0.96	0.23	1.60	52,54,57,78	7
86	OHX	5	3671	7/7	0.96	0.22	1.57	59,60,62,93	7
86	OHX	8	207	7/7	0.94	0.20	1.57	96,97,99,122	7
86	OHX	5	3555	7/7	0.95	0.22	1.57	45,46,48,77	7
86	OHX	4	204	7/7	0.97	0.22	1.56	59,60,63,80	7
86	OHX	1	3502	7/7	0.99	0.23	1.56	38,40,44,66	7
86	OHX	6	2032	7/7	0.87	0.28	1.56	76,77,78,101	7
86	OHX	6	1965	7/7	0.93	0.22	1.56	96,97,98,122	7
87	MG	2	2073	1/1	0.86	0.35	1.55	101,101,101,101	0
86	OHX	1	3558	7/7	0.98	0.21	1.55	59,60,62,84	7
86	OHX	7	204	7/7	0.98	0.20	1.53	49,50,53,71	7
87	MG	1	4025	1/1	0.93	0.24	1.52	42,42,42,42	0
86	OHX	5	3456	7/7	0.98	0.22	1.47	73,75,77,107	7
86	OHX	5	3614	7/7	0.96	0.23	1.46	48,49,52,78	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	2	2008	7/7	0.91	0.23	1.46	111,113,114,139	7
86	OHX	6	1998	7/7	0.97	0.28	1.46	76,77,78,103	7
86	OHX	2	1959	7/7	0.94	0.24	1.46	96,99,100,120	7
86	OHX	2	1921	7/7	0.94	0.25	1.45	93,94,101,115	7
86	OHX	5	3415	7/7	0.99	0.19	1.45	52,52,55,73	7
86	OHX	6	1977	7/7	0.95	0.19	1.45	61,62,64,90	7
87	MG	6	2075	1/1	0.90	0.20	1.44	34,34,34,34	0
86	OHX	5	3696	7/7	0.90	0.24	1.42	68,69,69,96	7
87	MG	1	3865	1/1	0.94	0.34	1.42	39,39,39,39	0
86	OHX	5	3501	7/7	0.95	0.23	1.42	48,49,52,80	7
86	OHX	1	3542	7/7	0.97	0.20	1.41	72,73,74,96	7
87	MG	5	3790	1/1	0.82	0.17	1.40	110,110,110,110	0
86	OHX	1	3685	7/7	0.80	0.26	1.39	106,107,109,129	7
86	OHX	5	3481	7/7	0.95	0.23	1.37	74,75,78,94	7
87	MG	5	3949	1/1	0.92	0.19	1.36	57,57,57,57	0
86	OHX	5	3644	7/7	0.85	0.24	1.34	53,57,59,103	7
86	OHX	1	3473	7/7	0.94	0.20	1.33	77,80,82,116	7
87	MG	n6	201	1/1	0.80	0.28	1.31	69,69,69,69	0
86	OHX	5	3441	7/7	0.98	0.19	1.31	63,65,71,95	7
87	MG	5	3726	1/1	0.97	0.24	1.31	34,34,34,34	0
88	ZN	q2	501	1/1	0.79	0.38	1.28	107,107,107,107	0
86	OHX	2	1918	7/7	0.95	0.19	1.27	82,83,87,106	7
86	OHX	5	3619	7/7	0.93	0.23	1.27	53,54,56,87	7
86	OHX	5	3414	7/7	0.99	0.18	1.25	61,63,64,73	0
86	OHX	5	3607	7/7	0.97	0.21	1.25	47,48,50,84	7
86	OHX	1	3516	7/7	0.98	0.22	1.25	61,61,64,85	7
86	OHX	1	3567	7/7	0.97	0.25	1.23	55,56,58,78	7
86	OHX	1	3710	7/7	0.91	0.16	1.23	93,94,94,124	7
86	OHX	6	1902	7/7	0.99	0.20	1.21	76,79,84,89	0
86	OHX	1	3580	7/7	0.99	0.20	1.21	51,52,55,82	7
86	OHX	1	3466	7/7	0.94	0.20	1.21	81,83,86,117	7
86	OHX	5	3461	7/7	0.99	0.18	1.20	40,43,48,69	7
86	OHX	2	2020	7/7	0.94	0.29	1.20	88,89,90,116	7
87	MG	5	3758	1/1	0.92	0.24	1.19	77,77,77,77	0
87	MG	1	3878	1/1	0.94	0.30	1.19	39,39,39,39	0
86	OHX	1	3462	7/7	0.98	0.22	1.18	67,68,71,90	7
86	OHX	1	3592	7/7	0.95	0.19	1.17	40,43,45,79	7
86	OHX	7	207	7/7	0.94	0.17	1.17	88,89,91,118	7
86	OHX	5	3547	7/7	0.95	0.20	1.16	48,52,54,83	7
86	OHX	5	3559	7/7	0.93	0.19	1.15	105,106,107,129	7
87	MG	5	3991	1/1	0.92	0.28	1.15	41,41,41,41	0
86	OHX	1	3470	7/7	0.98	0.24	1.15	66,69,72,89	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	1908	7/7	0.98	0.19	1.14	96,98,99,106	0
86	OHX	4	206	7/7	0.96	0.23	1.14	57,57,58,83	7
86	OHX	1	3679	7/7	0.90	0.25	1.14	74,75,76,101	7
86	OHX	2	1961	7/7	0.95	0.20	1.14	65,66,71,98	7
86	OHX	2	2025	7/7	0.94	0.22	1.13	98,98,100,121	7
86	OHX	6	1906	7/7	0.99	0.21	1.13	57,58,60,80	7
86	OHX	1	3537	7/7	0.99	0.23	1.11	48,50,52,69	7
86	OHX	1	3531	7/7	0.96	0.24	1.11	56,59,60,98	7
86	OHX	5	3569	7/7	0.93	0.26	1.11	58,61,64,89	7
86	OHX	3	207	7/7	0.90	0.17	1.10	108,108,110,132	7
87	MG	1	4028	1/1	0.93	0.24	1.08	39,39,39,39	0
86	OHX	2	1933	7/7	0.95	0.21	1.07	75,79,81,108	7
86	OHX	2	1909	7/7	0.93	0.19	1.06	99,102,106,112	0
86	OHX	5	3434	7/7	0.97	0.18	1.06	102,104,108,113	0
87	MG	1	3743	1/1	0.89	0.17	1.06	53,53,53,53	0
87	MG	3	216	1/1	0.91	0.27	1.05	75,75,75,75	0
86	OHX	5	3688	7/7	0.93	0.19	1.05	62,63,64,97	7
86	OHX	5	3685	7/7	0.88	0.17	1.03	66,67,68,108	7
86	OHX	2	1973	7/7	0.86	0.28	1.01	102,102,104,125	7
86	OHX	5	3622	7/7	0.93	0.21	1.00	73,73,74,97	7
86	OHX	6	2037	7/7	0.79	0.23	0.99	115,116,117,137	7
86	OHX	1	3458	7/7	0.96	0.15	0.98	109,110,114,130	7
86	OHX	1	3544	7/7	0.97	0.16	0.95	60,61,64,88	7
86	OHX	1	3463	7/7	0.99	0.22	0.95	49,53,53,61	7
86	OHX	1	3577	7/7	0.95	0.21	0.93	54,56,58,90	7
86	OHX	6	1992	7/7	0.95	0.19	0.93	87,88,89,113	7
86	OHX	6	1981	7/7	0.94	0.19	0.93	52,53,57,89	7
87	MG	5	4035	1/1	0.97	0.35	0.93	42,42,42,42	0
86	OHX	5	3599	7/7	0.94	0.18	0.92	83,84,87,112	7
86	OHX	6	1922	7/7	0.98	0.25	0.90	56,58,60,81	7
86	OHX	1	3415	7/7	0.99	0.17	0.90	64,64,69,79	0
86	OHX	m6	201	7/7	0.98	0.23	0.89	47,49,55,78	7
86	OHX	5	3451	7/7	0.97	0.21	0.88	57,59,60,78	7
86	OHX	5	3486	7/7	0.99	0.17	0.88	55,55,61,72	7
86	OHX	5	3530	7/7	0.96	0.22	0.87	41,43,48,79	7
86	OHX	1	3660	7/7	0.92	0.23	0.87	61,62,63,93	7
86	OHX	5	3554	7/7	0.97	0.21	0.87	54,57,58,90	7
86	OHX	5	3582	7/7	0.98	0.20	0.86	58,60,63,83	7
86	OHX	2	1927	7/7	0.96	0.19	0.83	98,99,102,123	7
86	OHX	5	3510	7/7	0.99	0.24	0.83	40,44,48,69	7
86	OHX	6	1974	7/7	0.87	0.26	0.82	67,70,73,106	7
86	OHX	1	3661	7/7	0.92	0.21	0.80	55,58,60,89	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2022	7/7	0.93	0.22	0.80	54,55,58,96	7
86	OHX	1	3445	7/7	0.98	0.17	0.80	59,62,63,91	7
87	MG	5	3843	1/1	0.97	0.26	0.78	32,32,32,32	0
86	OHX	1	3590	7/7	0.96	0.21	0.78	44,45,46,80	7
86	OHX	5	3516	7/7	0.97	0.23	0.78	42,45,50,70	7
86	OHX	5	3562	7/7	0.98	0.21	0.77	46,48,49,75	7
86	OHX	1	3425	7/7	0.99	0.20	0.76	54,59,64,84	0
86	OHX	1	3509	7/7	0.93	0.23	0.76	51,52,55,75	7
86	OHX	5	3683	7/7	0.94	0.15	0.75	92,92,94,121	7
86	OHX	5	3502	7/7	0.95	0.18	0.75	74,76,78,106	7
86	OHX	6	1940	7/7	0.93	0.15	0.75	118,121,123,134	7
86	OHX	8	205	7/7	0.97	0.24	0.74	71,71,74,91	7
86	OHX	1	3555	7/7	0.86	0.23	0.74	90,92,93,115	7
86	OHX	6	2003	7/7	0.95	0.17	0.73	91,91,92,122	7
86	OHX	8	206	7/7	0.96	0.20	0.73	72,72,73,103	7
86	OHX	2	1944	7/7	0.93	0.17	0.72	104,104,108,128	7
86	OHX	1	3673	7/7	0.87	0.22	0.72	97,98,101,124	7
86	OHX	1	3456	7/7	0.97	0.17	0.70	84,89,90,108	7
86	OHX	5	3539	7/7	0.95	0.15	0.68	108,109,111,129	7
86	OHX	6	1933	7/7	0.96	0.18	0.68	51,53,58,84	7
86	OHX	1	3439	7/7	0.99	0.15	0.68	63,65,67,81	7
86	OHX	6	1919	7/7	0.94	0.19	0.67	62,64,67,98	7
87	MG	1	3851	1/1	0.96	0.28	0.67	57,57,57,57	0
86	OHX	6	1945	7/7	0.97	0.17	0.66	71,72,74,100	7
86	OHX	5	3410	7/7	0.99	0.16	0.65	54,56,59,70	7
86	OHX	1	3700	7/7	0.89	0.23	0.65	67,68,69,95	7
86	OHX	1	3653	7/7	0.90	0.23	0.65	48,50,53,92	7
86	OHX	5	3635	7/7	0.96	0.21	0.65	54,55,56,88	7
86	OHX	6	2008	7/7	0.92	0.19	0.65	87,88,89,118	7
87	MG	1	4010	1/1	0.85	0.28	0.64	68,68,68,68	0
86	OHX	6	1994	7/7	0.89	0.17	0.63	127,128,128,142	7
86	OHX	5	3460	7/7	0.98	0.20	0.62	54,55,57,76	7
86	OHX	1	3453	7/7	0.98	0.15	0.62	79,80,82,101	7
86	OHX	6	1962	7/7	0.95	0.24	0.61	77,78,80,102	7
86	OHX	1	3424	7/7	0.99	0.15	0.61	78,79,81,89	0
86	OHX	n9	102	7/7	0.99	0.20	0.60	55,56,60,80	7
86	OHX	1	3613	7/7	0.92	0.21	0.60	62,65,66,97	7
86	OHX	6	1971	7/7	0.92	0.23	0.59	91,92,93,114	7
86	OHX	S9	201	7/7	0.89	0.25	0.58	85,86,87,114	7
86	OHX	1	3488	7/7	0.97	0.16	0.58	110,110,114,130	7
87	MG	n6	202	1/1	0.88	0.24	0.57	51,51,51,51	0
86	OHX	5	3436	7/7	0.99	0.17	0.57	57,57,60,76	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3732	1/1	0.94	0.22	0.56	33,33,33,33	0
86	OHX	6	1927	7/7	0.97	0.20	0.56	55,58,62,72	7
86	OHX	1	3585	7/7	0.96	0.19	0.55	56,57,59,92	7
86	OHX	8	216	7/7	0.89	0.24	0.53	84,85,86,112	7
86	OHX	5	3412	7/7	0.99	0.16	0.53	74,75,80,87	0
87	MG	6	2108	1/1	0.94	0.24	0.50	51,51,51,51	0
86	OHX	1	3609	7/7	0.95	0.18	0.48	72,74,75,102	7
86	OHX	2	1923	7/7	0.99	0.18	0.48	76,77,78,105	7
86	OHX	1	3575	7/7	0.95	0.19	0.48	63,64,65,85	7
86	OHX	1	3586	7/7	0.95	0.21	0.46	69,71,72,101	7
86	OHX	2	1905	7/7	0.99	0.21	0.46	65,66,67,82	7
86	OHX	1	3433	7/7	0.97	0.20	0.46	54,63,70,96	0
86	OHX	1	3435	7/7	0.99	0.19	0.45	69,70,70,74	7
86	OHX	5	3488	7/7	0.97	0.15	0.45	71,71,75,93	7
86	OHX	6	2011	7/7	0.95	0.21	0.44	64,65,66,95	7
86	OHX	1	3543	7/7	0.96	0.19	0.44	59,62,64,100	7
86	OHX	1	3479	7/7	0.99	0.20	0.43	52,53,55,79	7
86	OHX	5	3476	7/7	0.97	0.22	0.43	76,79,82,100	7
87	MG	5	4050	1/1	0.86	0.26	0.41	48,48,48,48	0
87	MG	1	4051	1/1	0.90	0.22	0.41	76,76,76,76	0
86	OHX	5	3589	7/7	0.97	0.18	0.39	48,50,52,84	7
86	OHX	5	3522	7/7	0.98	0.20	0.38	58,59,63,80	7
86	OHX	5	3499	7/7	0.97	0.18	0.37	77,79,80,102	7
86	OHX	5	3506	7/7	0.98	0.19	0.35	51,54,59,67	7
86	OHX	5	3693	7/7	0.92	0.19	0.35	64,66,67,88	7
86	OHX	2	1949	7/7	0.97	0.23	0.35	95,97,98,122	7
86	OHX	6	1934	7/7	0.98	0.17	0.34	86,87,89,102	7
86	OHX	1	3618	7/7	0.93	0.19	0.34	74,76,78,102	7
86	OHX	1	3417	7/7	0.99	0.18	0.33	41,42,48,68	7
86	OHX	1	3640	7/7	0.97	0.15	0.32	70,70,71,98	7
86	OHX	6	1910	7/7	0.99	0.19	0.32	62,62,66,82	7
86	OHX	5	3609	7/7	0.92	0.18	0.32	66,67,70,97	7
86	OHX	6	1907	7/7	0.98	0.16	0.31	79,82,84,95	0
86	OHX	5	3677	7/7	0.88	0.20	0.29	99,100,102,127	7
86	OHX	1	3500	7/7	0.96	0.16	0.29	101,104,108,126	7
86	OHX	5	3642	7/7	0.92	0.22	0.28	65,67,68,98	7
86	OHX	5	3500	7/7	0.94	0.17	0.28	74,78,81,100	7
86	OHX	1	3622	7/7	0.93	0.15	0.28	90,91,92,125	7
87	MG	2	2070	1/1	0.97	0.30	0.28	94,94,94,94	0
87	MG	m5	304	1/1	0.92	0.23	0.27	50,50,50,50	0
86	OHX	2	1935	7/7	0.95	0.24	0.27	98,100,101,122	7
86	OHX	5	3710	7/7	0.80	0.24	0.27	106,106,107,137	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3669	7/7	0.94	0.19	0.25	41,42,43,79	7
86	OHX	5	3438	7/7	0.99	0.18	0.25	50,54,58,71	7
86	OHX	7	201	7/7	0.99	0.19	0.24	64,69,70,92	7
86	OHX	5	3472	7/7	0.99	0.21	0.24	53,54,57,75	7
86	OHX	5	3680	7/7	0.94	0.20	0.24	74,75,77,106	7
86	OHX	1	3420	7/7	0.99	0.18	0.24	39,41,44,64	7
86	OHX	1	3530	7/7	0.98	0.18	0.23	76,76,78,96	7
86	OHX	5	3427	7/7	1.00	0.18	0.23	41,42,45,56	7
86	OHX	2	1902	7/7	0.99	0.16	0.23	77,77,81,93	0
86	OHX	1	3410	7/7	0.99	0.17	0.23	56,58,60,73	7
87	MG	1	3754	1/1	0.94	0.22	0.23	51,51,51,51	0
86	OHX	5	3439	7/7	0.99	0.16	0.22	82,83,86,93	0
86	OHX	5	3487	7/7	0.98	0.19	0.17	45,47,49,69	7
86	OHX	5	3543	7/7	0.94	0.16	0.16	62,62,64,85	7
86	OHX	2	1914	7/7	0.99	0.23	0.16	65,66,66,82	7
86	OHX	1	3536	7/7	0.97	0.17	0.16	50,55,57,76	7
86	OHX	o7	502	7/7	0.98	0.21	0.15	67,68,69,92	7
86	OHX	1	3427	7/7	0.99	0.15	0.15	85,86,90,94	0
86	OHX	2	1974	7/7	0.89	0.25	0.14	101,101,104,126	7
86	OHX	1	3681	7/7	0.93	0.19	0.13	56,60,61,86	7
86	OHX	1	3510	7/7	0.99	0.19	0.13	52,53,54,83	7
86	OHX	3	206	7/7	0.95	0.18	0.13	96,97,98,122	7
87	MG	1	3791	1/1	0.92	0.20	0.12	46,46,46,46	0
86	OHX	2	1947	7/7	0.97	0.20	0.12	68,69,70,98	7
86	OHX	5	3521	7/7	0.98	0.19	0.11	45,45,47,69	7
86	OHX	6	1979	7/7	0.90	0.20	0.11	87,88,90,120	7
86	OHX	1	3423	7/7	0.99	0.20	0.09	63,65,70,86	7
86	OHX	1	3656	7/7	0.94	0.16	0.08	83,84,85,110	7
86	OHX	1	3405	7/7	0.99	0.17	0.08	62,63,71,80	0
86	OHX	1	3449	7/7	0.98	0.16	0.07	71,73,75,99	7
86	OHX	5	3473	7/7	0.98	0.18	0.07	45,47,51,71	7
86	OHX	6	1913	7/7	0.98	0.19	0.06	76,77,80,94	7
86	OHX	2	1990	7/7	0.91	0.19	0.06	101,102,106,126	7
86	OHX	1	3422	7/7	0.99	0.17	0.04	64,65,67,75	7
86	OHX	1	3472	7/7	0.98	0.18	0.02	52,55,56,86	7
86	OHX	6	1978	7/7	0.94	0.18	0.02	79,80,83,103	7
86	OHX	2	1967	7/7	0.96	0.20	0.02	75,76,77,114	7
86	OHX	1	3579	7/7	0.96	0.18	0.01	60,61,63,89	7
86	OHX	5	3633	7/7	0.96	0.17	-0.01	75,76,79,99	7
86	OHX	5	3610	7/7	0.98	0.23	-0.01	52,54,55,76	7
86	OHX	n3	202	7/7	0.95	0.18	-0.01	60,62,65,94	7
86	OHX	5	3579	7/7	0.99	0.20	-0.01	56,58,59,80	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	2	1919	7/7	0.99	0.16	-0.02	77,80,82,97	7
86	OHX	6	1980	7/7	0.96	0.20	-0.02	61,62,63,100	7
86	OHX	1	3548	7/7	0.96	0.18	-0.02	80,80,82,99	7
86	OHX	5	3428	7/7	0.98	0.17	-0.02	49,51,57,88	0
86	OHX	1	3421	7/7	0.99	0.18	-0.02	63,65,66,82	7
86	OHX	1	3520	7/7	0.94	0.22	-0.02	60,60,63,89	7
87	MG	6	2103	1/1	0.95	0.18	-0.04	59,59,59,59	0
87	MG	2	2101	1/1	0.97	0.34	-0.05	78,78,78,78	0
86	OHX	2	1979	7/7	0.95	0.18	-0.05	63,64,65,94	7
86	OHX	2	1920	7/7	0.99	0.19	-0.05	82,84,86,96	7
86	OHX	1	3487	7/7	0.95	0.14	-0.06	120,121,123,137	7
86	OHX	6	1929	7/7	0.95	0.18	-0.07	137,138,140,147	7
86	OHX	2	1970	7/7	0.82	0.17	-0.07	132,137,138,157	7
86	OHX	2	1911	7/7	0.92	0.19	-0.07	109,111,116,131	7
86	OHX	1	3489	7/7	0.99	0.18	-0.07	64,66,67,88	7
86	OHX	1	3419	7/7	0.99	0.18	-0.09	51,55,56,76	7
86	OHX	1	3699	7/7	0.92	0.22	-0.11	75,76,77,106	7
86	OHX	1	3461	7/7	0.98	0.23	-0.11	50,52,60,78	7
86	OHX	6	1924	7/7	0.98	0.19	-0.12	76,81,82,103	7
87	MG	6	2109	1/1	0.97	0.17	-0.12	89,89,89,89	0
86	OHX	1	3601	7/7	0.94	0.19	-0.13	45,45,49,77	7
86	OHX	6	2027	7/7	0.89	0.21	-0.14	82,82,85,113	7
86	OHX	1	3675	7/7	0.95	0.16	-0.14	63,64,65,94	7
87	MG	1	3792	1/1	0.81	0.24	-0.14	53,53,53,53	0
86	OHX	2	1954	7/7	0.96	0.21	-0.15	87,91,94,113	7
86	OHX	1	3674	7/7	0.84	0.18	-0.15	114,116,116,146	7
86	OHX	6	1925	7/7	0.98	0.19	-0.17	59,59,62,76	7
86	OHX	2	1942	7/7	0.97	0.17	-0.17	76,79,80,96	7
86	OHX	2	1971	7/7	0.93	0.18	-0.17	153,154,154,170	7
86	OHX	1	3662	7/7	0.94	0.19	-0.18	63,64,66,94	7
86	OHX	6	1944	7/7	0.98	0.15	-0.18	111,111,113,127	7
86	OHX	1	3486	7/7	0.98	0.22	-0.20	63,65,68,95	7
86	OHX	6	1917	7/7	0.99	0.16	-0.20	65,66,68,84	7
86	OHX	6	1911	7/7	0.96	0.19	-0.21	87,89,94,103	7
86	OHX	1	3504	7/7	0.94	0.15	-0.22	85,86,89,113	7
86	OHX	6	2009	7/7	0.94	0.17	-0.23	66,67,70,99	7
86	OHX	8	203	7/7	0.98	0.18	-0.25	53,53,58,80	7
86	OHX	1	3559	7/7	0.96	0.16	-0.25	101,102,102,122	7
86	OHX	1	3614	7/7	0.91	0.20	-0.25	66,66,69,99	7
86	OHX	5	3574	7/7	0.96	0.15	-0.25	62,63,64,95	7
86	OHX	5	3649	7/7	0.95	0.22	-0.26	63,64,66,91	7
86	OHX	5	3611	7/7	0.95	0.14	-0.26	83,84,86,106	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	2	1907	7/7	0.95	0.15	-0.27	101,105,108,120	7
86	OHX	5	3577	7/7	0.93	0.18	-0.27	67,68,71,100	7
87	MG	5	3929	1/1	0.92	0.18	-0.27	52,52,52,52	0
86	OHX	5	3553	7/7	0.95	0.18	-0.28	54,55,56,87	7
86	OHX	1	3569	7/7	0.98	0.17	-0.29	49,53,56,82	7
87	MG	1	4006	1/1	0.98	0.21	-0.29	46,46,46,46	0
86	OHX	6	1953	7/7	0.98	0.16	-0.29	88,89,91,115	7
86	OHX	4	208	7/7	0.98	0.18	-0.29	82,83,85,104	7
86	OHX	1	3647	7/7	0.94	0.17	-0.29	73,75,76,102	7
87	MG	5	4002	1/1	0.96	0.19	-0.29	42,42,42,42	0
86	OHX	q2	502	7/7	0.98	0.20	-0.30	53,55,61,84	7
86	OHX	Q2	502	7/7	0.98	0.20	-0.30	41,45,48,82	7
86	OHX	1	3411	7/7	0.99	0.18	-0.31	41,47,50,78	0
87	MG	M0	302	1/1	0.91	0.23	-0.31	51,51,51,51	0
86	OHX	O3	201	7/7	0.98	0.20	-0.31	54,55,57,74	7
86	OHX	5	3443	7/7	0.96	0.17	-0.32	64,66,69,96	7
86	OHX	2	1904	7/7	0.99	0.16	-0.32	80,86,89,94	7
86	OHX	1	3474	7/7	0.98	0.18	-0.32	68,70,71,83	7
86	OHX	5	3517	7/7	0.98	0.17	-0.33	65,67,68,97	7
86	OHX	1	3508	7/7	0.97	0.18	-0.34	65,65,69,95	7
86	OHX	1	3712	7/7	0.87	0.21	-0.34	84,88,89,117	7
86	OHX	3	204	7/7	0.97	0.16	-0.36	96,98,98,118	7
86	OHX	5	3686	7/7	0.96	0.18	-0.37	63,63,64,95	7
86	OHX	5	3605	7/7	0.96	0.20	-0.37	73,75,77,112	7
86	OHX	2	1962	7/7	0.97	0.19	-0.38	89,89,91,118	7
86	OHX	4	203	7/7	0.99	0.18	-0.38	40,44,48,69	7
86	OHX	5	3474	7/7	0.97	0.22	-0.38	46,48,51,76	7
87	MG	1	3734	1/1	0.91	0.22	-0.39	42,42,42,42	0
86	OHX	5	3507	7/7	0.98	0.18	-0.39	62,64,65,95	7
86	OHX	5	3556	7/7	0.97	0.18	-0.41	58,59,60,83	7
86	OHX	5	3584	7/7	0.98	0.17	-0.41	53,53,56,68	7
86	OHX	6	1921	7/7	0.98	0.14	-0.41	125,126,127,128	0
86	OHX	2	2028	7/7	0.93	0.14	-0.42	130,130,131,153	7
86	OHX	5	3432	7/7	0.99	0.18	-0.43	48,48,52,66	7
86	OHX	5	3602	7/7	0.92	0.17	-0.43	119,121,122,143	7
86	OHX	s9	201	7/7	0.92	0.21	-0.43	68,68,71,98	7
86	OHX	2	1932	7/7	0.97	0.18	-0.43	92,93,94,116	7
86	OHX	6	1993	7/7	0.95	0.17	-0.44	85,86,89,116	7
86	OHX	5	3484	7/7	0.99	0.15	-0.44	54,58,62,71	7
86	OHX	2	2024	7/7	0.84	0.21	-0.44	116,116,118,142	7
86	OHX	2	2007	7/7	0.92	0.17	-0.44	101,101,104,120	7
86	OHX	5	3442	7/7	0.99	0.18	-0.45	59,61,63,72	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	3493	7/7	0.98	0.16	-0.45	67,68,71,91	7
86	OHX	5	3448	7/7	0.98	0.14	-0.47	70,73,77,93	7
86	OHX	5	3691	7/7	0.97	0.17	-0.47	51,53,55,88	7
86	OHX	1	3632	7/7	0.92	0.18	-0.47	105,105,106,124	7
86	OHX	1	3549	7/7	0.94	0.18	-0.47	88,88,90,108	7
87	MG	1	3992	1/1	0.94	0.17	-0.48	56,56,56,56	0
86	OHX	5	3468	7/7	0.99	0.20	-0.48	61,61,66,78	7
86	OHX	1	3471	7/7	0.99	0.14	-0.49	89,90,92,113	7
86	OHX	1	3631	7/7	0.96	0.18	-0.49	61,64,65,94	7
86	OHX	5	3695	7/7	0.90	0.22	-0.50	73,74,75,102	7
86	OHX	5	3403	7/7	1.00	0.16	-0.50	32,33,41,65	0
86	OHX	5	3401	7/7	0.99	0.16	-0.52	48,50,57,65	0
86	OHX	5	3526	7/7	0.99	0.16	-0.52	93,95,96,119	7
86	OHX	5	3630	7/7	0.94	0.16	-0.52	113,115,116,133	7
86	OHX	2	1996	7/7	0.96	0.24	-0.54	88,89,91,112	7
86	OHX	1	3429	7/7	0.99	0.18	-0.55	54,57,59,73	7
86	OHX	O1	201	7/7	0.89	0.18	-0.55	89,91,92,109	7
86	OHX	5	3408	7/7	0.99	0.18	-0.56	43,49,52,69	7
86	OHX	4	210	7/7	0.97	0.15	-0.57	82,83,85,107	7
86	OHX	1	3591	7/7	0.97	0.12	-0.58	106,107,108,136	7
87	MG	2	2119	1/1	0.98	0.15	-0.60	93,93,93,93	0
86	OHX	2	1972	7/7	0.96	0.15	-0.61	122,123,124,147	7
86	OHX	6	1942	7/7	0.98	0.18	-0.61	84,84,85,102	7
86	OHX	1	3588	7/7	0.94	0.16	-0.62	104,104,106,123	7
86	OHX	5	3503	7/7	0.97	0.17	-0.62	49,53,55,75	7
86	OHX	l3	401	7/7	0.98	0.18	-0.62	54,57,59,83	7
86	OHX	5	3532	7/7	0.96	0.15	-0.62	113,114,116,129	7
86	OHX	1	3659	7/7	0.84	0.16	-0.63	131,131,133,156	7
86	OHX	1	3402	7/7	1.00	0.16	-0.63	47,49,55,67	0
86	OHX	5	3444	7/7	0.98	0.16	-0.63	48,54,57,83	7
86	OHX	2	1903	7/7	0.98	0.20	-0.63	83,89,95,96	0
86	OHX	2	1940	7/7	0.93	0.17	-0.63	94,96,98,118	7
86	OHX	1	3418	7/7	0.99	0.17	-0.64	53,56,62,84	7
86	OHX	1	3539	7/7	0.97	0.18	-0.64	45,48,50,72	7
86	OHX	2	1915	7/7	0.96	0.15	-0.65	118,121,121,123	7
87	MG	2	2098	1/1	0.78	0.19	-0.66	107,107,107,107	0
87	MG	L7	301	1/1	0.86	0.18	-0.66	47,47,47,47	0
86	OHX	1	3527	7/7	0.99	0.17	-0.67	57,59,59,72	7
86	OHX	2	1964	7/7	0.95	0.16	-0.68	72,73,75,116	7
86	OHX	1	3485	7/7	0.97	0.15	-0.68	88,89,90,107	7
86	OHX	6	1904	7/7	0.99	0.15	-0.69	67,69,74,78	7
86	OHX	5	3423	7/7	0.99	0.17	-0.70	59,62,62,79	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	ZN	Q2	501	1/1	0.89	0.27	-0.71	107,107,107,107	0
86	OHX	7	206	7/7	0.98	0.15	-0.71	69,69,72,96	7
86	OHX	5	3405	7/7	0.99	0.16	-0.71	57,58,60,69	0
86	OHX	2	2000	7/7	0.95	0.15	-0.72	100,101,102,129	7
86	OHX	5	3513	7/7	0.97	0.16	-0.72	61,62,64,80	7
86	OHX	5	3471	7/7	0.97	0.15	-0.73	83,83,85,102	7
87	MG	1	3909	1/1	0.78	0.15	-0.74	71,71,71,71	0
86	OHX	5	3515	7/7	0.97	0.12	-0.74	138,139,140,151	7
86	OHX	1	3519	7/7	0.97	0.16	-0.74	85,85,87,108	7
86	OHX	2	1950	7/7	0.99	0.15	-0.75	83,84,86,106	7
86	OHX	6	1928	7/7	0.89	0.15	-0.75	138,141,142,159	7
86	OHX	2	1910	7/7	0.97	0.18	-0.75	88,89,92,110	7
86	OHX	5	3455	7/7	0.98	0.19	-0.75	81,84,85,99	7
86	OHX	8	202	7/7	0.99	0.17	-0.75	45,50,55,70	7
86	OHX	5	3406	7/7	0.99	0.16	-0.75	54,56,62,75	0
86	OHX	6	1901	7/7	0.99	0.15	-0.77	60,64,68,72	0
86	OHX	1	3496	7/7	0.98	0.19	-0.77	43,45,49,65	7
86	OHX	5	3509	7/7	0.97	0.13	-0.77	103,104,106,124	7
87	MG	5	3728	1/1	0.85	0.15	-0.77	46,46,46,46	0
88	ZN	Q0	500	1/1	0.98	0.14	-0.78	56,56,56,56	0
86	OHX	5	3682	7/7	0.86	0.19	-0.78	77,78,79,115	7
86	OHX	m0	302	7/7	0.91	0.22	-0.78	58,59,60,95	7
86	OHX	C1	201	7/7	0.96	0.18	-0.79	92,92,93,110	7
86	OHX	2	2015	7/7	0.93	0.16	-0.79	118,119,119,136	7
86	OHX	8	204	7/7	0.98	0.14	-0.80	88,89,92,114	7
86	OHX	1	3701	7/7	0.94	0.17	-0.80	63,64,66,101	7
86	OHX	L3	402	7/7	0.96	0.17	-0.80	74,75,79,102	7
86	OHX	2	2001	7/7	0.96	0.17	-0.80	74,75,77,107	7
88	ZN	d7	101	1/1	0.86	0.23	-0.81	142,142,142,142	0
86	OHX	M5	301	7/7	0.97	0.18	-0.82	70,70,72,103	7
87	MG	1	4061	1/1	0.93	0.19	-0.82	33,33,33,33	0
86	OHX	2	1945	7/7	0.90	0.13	-0.82	110,111,113,137	7
86	OHX	1	3412	7/7	1.00	0.22	-0.83	57,62,65,72	7
86	OHX	5	3576	7/7	0.98	0.14	-0.83	51,52,53,76	7
86	OHX	1	3413	7/7	0.99	0.18	-0.83	52,54,56,71	7
86	OHX	5	3417	7/7	0.99	0.16	-0.83	55,58,60,79	7
86	OHX	5	3591	7/7	0.98	0.15	-0.84	47,47,50,76	7
87	MG	5	3771	1/1	0.92	0.16	-0.84	46,46,46,46	0
87	MG	5	4046	1/1	0.95	0.17	-0.84	49,49,49,49	0
86	OHX	1	3495	7/7	0.97	0.16	-0.85	56,56,60,79	7
86	OHX	2	1981	7/7	0.96	0.17	-0.86	74,75,77,106	7
86	OHX	19	201	7/7	0.92	0.19	-0.86	70,70,71,107	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3483	7/7	0.96	0.15	-0.86	79,81,83,107	7
86	OHX	5	3592	7/7	0.98	0.17	-0.87	54,57,58,85	7
86	OHX	1	3576	7/7	0.96	0.15	-0.87	71,72,74,106	7
86	OHX	5	3404	7/7	0.99	0.16	-0.88	30,36,40,66	0
86	OHX	6	1996	7/7	0.96	0.14	-0.88	102,103,104,128	7
86	OHX	1	3403	7/7	1.00	0.15	-0.88	44,45,48,62	0
86	OHX	6	1918	7/7	0.99	0.15	-0.89	61,62,65,83	7
86	OHX	1	3441	7/7	0.99	0.18	-0.91	49,52,56,62	7
86	OHX	5	3561	7/7	0.94	0.15	-0.93	112,112,114,136	7
86	OHX	1	3529	7/7	0.98	0.13	-0.94	123,125,126,138	7
86	OHX	5	3463	7/7	0.97	0.15	-0.95	73,74,77,102	7
86	OHX	2	1936	7/7	0.98	0.16	-0.95	70,71,74,96	7
86	OHX	6	1982	7/7	0.94	0.13	-0.96	105,106,108,132	7
86	OHX	1	3581	7/7	0.94	0.13	-0.97	83,86,88,119	7
86	OHX	1	3428	7/7	0.97	0.18	-0.98	74,74,77,92	0
86	OHX	5	3617	7/7	0.97	0.18	-0.98	52,53,54,77	7
86	OHX	2	1917	7/7	0.97	0.16	-0.98	81,82,84,103	7
86	OHX	1	3503	7/7	0.97	0.17	-0.99	65,66,70,87	7
86	OHX	2	1925	7/7	0.97	0.10	-0.99	125,126,127,140	7
86	OHX	1	3630	7/7	0.96	0.18	-1.00	57,60,63,93	7
86	OHX	1	3572	7/7	0.98	0.16	-1.00	45,46,49,72	7
86	OHX	1	3443	7/7	0.99	0.16	-1.00	57,58,59,81	7
86	OHX	5	3418	7/7	0.99	0.18	-1.01	44,50,54,67	7
86	OHX	5	3421	7/7	0.99	0.17	-1.01	67,68,73,82	0
86	OHX	5	3684	7/7	0.87	0.16	-1.01	73,74,76,109	7
86	OHX	6	2021	7/7	0.94	0.14	-1.01	102,103,103,127	7
86	OHX	5	3673	7/7	0.96	0.16	-1.02	67,67,68,98	7
86	OHX	1	3484	7/7	0.99	0.15	-1.02	52,56,59,80	7
86	OHX	2	1901	7/7	0.99	0.16	-1.03	71,74,79,94	0
86	OHX	1	3638	7/7	0.96	0.12	-1.03	67,69,70,105	7
87	MG	5	3741	1/1	0.87	0.14	-1.03	29,29,29,29	0
86	OHX	6	2005	7/7	0.96	0.18	-1.04	67,68,71,103	7
86	OHX	6	1985	7/7	0.96	0.17	-1.04	84,84,85,111	7
86	OHX	C8	201	7/7	0.98	0.14	-1.05	114,115,117,130	7
86	OHX	5	3429	7/7	0.99	0.17	-1.05	61,62,66,78	7
86	OHX	6	1990	7/7	0.95	0.16	-1.05	89,91,93,122	7
86	OHX	6	1939	7/7	0.97	0.17	-1.06	79,80,82,113	7
86	OHX	2	1983	7/7	0.97	0.15	-1.06	100,102,103,115	7
87	MG	6	2135	1/1	0.76	0.18	-1.07	61,61,61,61	0
86	OHX	5	3514	7/7	0.96	0.17	-1.07	69,71,73,95	7
86	OHX	1	3438	7/7	0.99	0.16	-1.08	51,54,60,75	7
86	OHX	m0	301	7/7	0.93	0.18	-1.08	97,98,101,130	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	MG	6	2046	1/1	0.97	0.18	-1.09	121,121,121,121	0
87	MG	5	3802	1/1	0.86	0.13	-1.09	74,74,74,74	0
86	OHX	6	1908	7/7	0.99	0.16	-1.10	66,67,72,92	0
86	OHX	1	3450	7/7	0.99	0.19	-1.10	69,69,69,89	7
86	OHX	2	1937	7/7	0.97	0.17	-1.10	102,103,106,123	7
86	OHX	5	3413	7/7	0.99	0.17	-1.11	43,45,51,64	7
86	OHX	L3	401	7/7	0.98	0.17	-1.11	65,67,68,91	7
86	OHX	6	1947	7/7	0.98	0.16	-1.11	80,81,83,106	7
86	OHX	6	1903	7/7	0.99	0.16	-1.12	64,67,68,80	0
86	OHX	5	3426	7/7	0.99	0.16	-1.12	45,48,49,69	7
86	OHX	6	1920	7/7	0.98	0.16	-1.13	79,80,82,104	7
86	OHX	5	3452	7/7	0.98	0.13	-1.13	109,110,112,119	0
86	OHX	1	3404	7/7	0.99	0.14	-1.13	56,60,63,69	0
87	MG	1	4065	1/1	0.96	0.13	-1.14	69,69,69,69	0
87	MG	5	4004	1/1	0.92	0.13	-1.14	65,65,65,65	0
86	OHX	1	3444	7/7	0.99	0.16	-1.14	74,75,75,104	7
86	OHX	6	1914	7/7	0.98	0.13	-1.14	94,95,96,108	7
86	OHX	6	1997	7/7	0.94	0.18	-1.15	103,104,105,124	7
88	ZN	d6	101	1/1	0.99	0.13	-1.15	67,67,67,67	0
86	OHX	n1	201	7/7	0.99	0.17	-1.15	39,45,52,70	7
86	OHX	5	3467	7/7	0.97	0.15	-1.15	90,93,94,113	7
86	OHX	2	1924	7/7	0.98	0.14	-1.16	87,88,90,111	7
86	OHX	5	3458	7/7	0.99	0.17	-1.16	59,60,62,82	7
86	OHX	2	1913	7/7	0.98	0.16	-1.16	84,85,88,111	7
86	OHX	1	3532	7/7	0.96	0.14	-1.16	107,109,111,126	7
86	OHX	6	1954	7/7	0.90	0.14	-1.16	152,153,154,166	7
86	OHX	2	1988	7/7	0.98	0.16	-1.17	89,89,91,111	7
86	OHX	2	1993	7/7	0.96	0.12	-1.17	114,114,115,138	7
86	OHX	l5	301	7/7	0.91	0.11	-1.18	104,105,106,134	7
88	ZN	d9	101	1/1	0.99	0.10	-1.18	98,98,98,98	0
86	OHX	2	2017	7/7	0.90	0.13	-1.20	145,145,146,164	7
86	OHX	4	213	7/7	0.97	0.11	-1.20	102,103,104,129	7
86	OHX	l3	402	7/7	0.92	0.17	-1.21	86,87,88,111	7
86	OHX	1	3430	7/7	0.99	0.14	-1.21	69,72,74,80	7
86	OHX	2	1941	7/7	0.98	0.14	-1.21	98,98,100,115	7
86	OHX	5	3504	7/7	0.97	0.19	-1.23	32,39,43,64	7
86	OHX	1	3584	7/7	0.96	0.09	-1.25	106,106,108,131	7
87	MG	1	4064	1/1	0.78	0.13	-1.25	66,66,66,66	0
86	OHX	2	1952	7/7	0.98	0.17	-1.26	68,69,71,98	7
86	OHX	5	3419	7/7	0.99	0.16	-1.27	40,45,51,71	7
86	OHX	1	3401	7/7	1.00	0.17	-1.28	37,41,45,62	0
86	OHX	5	3495	7/7	0.97	0.14	-1.29	86,87,88,111	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	d3	201	1/1	0.93	0.17	-1.29	51,51,51,51	0
88	ZN	O7	101	1/1	1.00	0.17	-1.29	42,42,42,42	0
86	OHX	1	3480	7/7	0.99	0.18	-1.30	53,54,59,81	7
86	OHX	2	1946	7/7	0.97	0.14	-1.30	125,126,127,136	7
86	OHX	1	3464	7/7	0.99	0.14	-1.35	102,103,104,112	7
86	OHX	5	3581	7/7	0.95	0.14	-1.35	84,84,86,111	7
86	OHX	1	3665	7/7	0.91	0.16	-1.36	59,60,61,105	7
86	OHX	l5	302	7/7	0.92	0.15	-1.36	101,102,102,130	7
86	OHX	2	1916	7/7	0.98	0.15	-1.36	82,86,87,105	7
86	OHX	5	3687	7/7	0.87	0.14	-1.37	143,144,145,163	7
86	OHX	2	2009	7/7	0.97	0.10	-1.37	133,134,134,148	7
88	ZN	D9	101	1/1	0.98	0.09	-1.39	85,85,85,85	0
86	OHX	1	3637	7/7	0.96	0.12	-1.39	116,116,117,131	7
86	OHX	2	2016	7/7	0.93	0.10	-1.39	126,126,127,150	7
86	OHX	5	3667	7/7	0.93	0.12	-1.40	134,134,135,149	7
86	OHX	5	3449	7/7	0.99	0.12	-1.40	80,81,83,107	7
86	OHX	1	3515	7/7	0.98	0.19	-1.41	47,50,52,75	7
86	OHX	5	3717	7/7	0.93	0.15	-1.41	121,122,123,139	7
86	OHX	6	2036	7/7	0.92	0.13	-1.41	101,103,104,124	7
86	OHX	5	3542	7/7	0.97	0.09	-1.43	155,156,156,166	7
86	OHX	s8	301	7/7	0.90	0.14	-1.44	105,105,106,130	7
87	MG	5	3988	1/1	0.87	0.13	-1.46	64,64,64,64	0
88	ZN	E1	501	1/1	0.95	0.07	-1.46	138,138,138,138	0
86	OHX	1	3426	7/7	0.99	0.17	-1.46	53,55,62,79	7
86	OHX	5	3537	7/7	0.94	0.13	-1.47	95,96,100,118	7
86	OHX	5	3411	7/7	1.00	0.17	-1.48	40,41,45,59	7
86	OHX	5	3424	7/7	0.99	0.20	-1.49	67,70,71,78	7
86	OHX	n3	201	7/7	0.99	0.14	-1.50	57,59,60,76	7
86	OHX	5	3409	7/7	0.99	0.21	-1.50	55,56,60,79	7
86	OHX	5	3652	7/7	0.96	0.16	-1.52	63,64,66,100	7
86	OHX	2	1931	7/7	0.94	0.12	-1.56	112,112,116,133	7
86	OHX	5	3483	7/7	0.99	0.14	-1.57	48,49,51,67	7
86	OHX	1	3583	7/7	0.95	0.12	-1.59	83,84,86,110	7
86	OHX	1	3552	7/7	0.96	0.16	-1.60	64,67,67,92	7
86	OHX	5	3590	7/7	0.97	0.16	-1.61	44,45,46,87	7
86	OHX	M0	301	7/7	0.93	0.19	-1.62	68,70,73,97	7
86	OHX	1	3650	7/7	0.97	0.16	-1.63	53,53,55,79	7
87	MG	6	2136	1/1	0.94	0.12	-1.64	76,76,76,76	0
86	OHX	SR	401	7/7	0.96	0.09	-1.67	142,143,143,158	7
88	ZN	q0	201	1/1	1.00	0.13	-1.77	41,41,41,41	0
86	OHX	6	1952	7/7	0.91	0.12	-1.77	159,160,161,172	7
86	OHX	6	2013	7/7	0.85	0.15	-1.78	163,163,164,174	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	1923	7/7	0.99	0.15	-1.79	65,67,69,79	7
88	ZN	e1	501	1/1	0.96	0.12	-1.79	191,191,191,191	0
86	OHX	5	3402	7/7	0.99	0.16	-1.79	34,39,46,63	0
87	MG	sM	301	1/1	0.90	0.09	-1.81	52,52,52,52	0
86	OHX	o3	201	7/7	0.99	0.16	-1.82	56,56,59,85	7
86	OHX	5	3454	7/7	0.99	0.16	-1.84	44,46,48,64	7
86	OHX	1	3708	7/7	0.91	0.11	-1.85	170,171,172,180	7
86	OHX	L4	401	7/7	0.92	0.18	-1.87	74,74,76,102	7
88	ZN	o7	501	1/1	1.00	0.18	-1.88	57,57,57,57	0
87	MG	5	4058	1/1	0.86	0.17	-1.91	33,33,33,33	0
86	OHX	6	1995	7/7	0.96	0.14	-1.91	91,93,94,119	7
87	MG	2	2118	1/1	0.77	0.16	-1.94	75,75,75,75	0
86	OHX	1	3599	7/7	0.98	0.15	-1.95	49,50,51,76	7
86	OHX	6	1991	7/7	0.92	0.15	-1.96	79,80,81,108	7
86	OHX	5	3604	7/7	0.89	0.12	-1.99	110,112,113,139	7
86	OHX	1	3482	7/7	0.98	0.12	-2.03	61,66,70,88	7
87	MG	5	4053	1/1	0.97	0.16	-2.05	48,48,48,48	0
86	OHX	5	3479	7/7	0.99	0.15	-2.07	49,53,56,81	7
88	ZN	Q3	501	1/1	0.99	0.10	-2.13	71,71,71,71	0
86	OHX	5	3724	7/7	0.75	0.20	-2.14	181,181,182,194	7
86	OHX	1	3566	7/7	0.96	0.09	-2.14	104,105,105,128	7
86	OHX	1	3535	7/7	0.94	0.12	-2.14	125,125,126,142	7
88	ZN	D6	500	1/1	0.98	0.08	-2.16	85,85,85,85	0
88	ZN	q3	501	1/1	1.00	0.10	-2.22	76,76,76,76	0
86	OHX	1	3467	7/7	0.97	0.12	-2.32	91,92,95,114	7
86	OHX	m5	302	7/7	0.96	0.16	-2.33	85,86,86,110	7
86	OHX	5	3540	7/7	0.99	0.17	-2.35	49,50,52,75	7
86	OHX	1	3406	7/7	1.00	0.18	-2.35	41,44,49,68	0
86	OHX	5	3670	7/7	0.98	0.17	-2.37	44,48,50,73	7
86	OHX	5	3430	7/7	0.99	0.15	-2.41	54,55,59,67	7
86	OHX	1	3578	7/7	0.95	0.11	-2.48	108,110,110,135	7
86	OHX	6	1956	7/7	0.98	0.09	-2.52	157,158,158,169	7
86	OHX	5	3497	7/7	0.98	0.14	-2.54	49,52,55,74	7
86	OHX	S8	301	7/7	0.90	0.15	-2.61	113,114,115,138	7
87	MG	5	3780	1/1	0.80	0.12	-2.63	47,47,47,47	0
86	OHX	1	3683	7/7	0.96	0.13	-2.77	79,81,81,109	7
86	OHX	sR	401	7/7	0.90	0.14	-2.82	136,137,137,158	7
87	MG	5	3745	1/1	0.90	0.11	-2.85	40,40,40,40	0
86	OHX	5	3664	7/7	0.96	0.10	-2.87	99,100,101,126	7
86	OHX	C5	201	7/7	0.93	0.10	-2.90	129,129,130,150	7
86	OHX	5	3606	7/7	0.96	0.15	-2.91	50,53,55,90	7
86	OHX	6	1957	7/7	0.97	0.10	-2.93	90,92,94,115	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3414	7/7	0.99	0.18	-2.97	46,50,52,58	7
87	MG	1	3880	1/1	0.87	0.10	-3.03	51,51,51,51	0
87	MG	5	3927	1/1	0.93	0.11	-3.05	40,40,40,40	0
86	OHX	2	1976	7/7	0.98	0.09	-3.07	108,108,109,127	7
87	MG	1	3939	1/1	0.99	0.08	-3.22	38,38,38,38	0
86	OHX	5	3485	7/7	0.99	0.12	-3.32	54,55,58,74	7
87	MG	5	4017	1/1	0.89	0.10	-3.34	68,68,68,68	0
86	OHX	1	3526	7/7	0.97	0.13	-3.37	76,77,79,96	7
86	OHX	5	3551	7/7	0.97	0.08	-3.39	113,114,115,135	7
86	OHX	1	3440	7/7	0.98	0.16	-3.40	77,79,81,87	7
86	OHX	5	3407	7/7	0.99	0.16	-3.52	51,57,59,69	0
87	MG	1	3899	1/1	0.95	0.14	-3.54	41,41,41,41	0
86	OHX	2	1978	7/7	0.92	0.10	-3.87	179,179,180,188	7
86	OHX	2	1948	7/7	0.98	0.09	-4.46	107,108,109,129	7
86	OHX	c5	201	7/7	0.90	0.12	-5.28	134,134,135,148	7
86	OHX	5	3578	7/7	0.96	0.11	-5.35	153,154,155,165	7
86	OHX	6	1969	7/7	0.98	0.13	-5.36	79,80,80,104	7
86	OHX	1	3570	7/7	0.99	0.16	-6.77	52,55,56,78	7
87	MG	1	3902	1/1	0.94	0.08	-8.14	58,58,58,58	0
87	MG	5	3917	1/1	0.94	0.08	-8.61	48,48,48,48	0
86	OHX	6	1938	7/7	0.97	0.12	-10.15	89,90,93,109	7
87	MG	5	3795	1/1	0.93	0.45	-	57,57,57,57	0
87	MG	1	3960	1/1	0.86	0.40	-	53,53,53,53	0
87	MG	5	3941	1/1	0.83	0.21	-	53,53,53,53	0
87	MG	1	3806	1/1	0.99	0.30	-	39,39,39,39	0
86	OHX	6	1964	7/7	0.98	0.12	-	57,60,61,83	7
87	MG	1	3764	1/1	0.80	0.47	-	60,60,60,60	0
86	OHX	1	3437	7/7	0.98	0.19	-	61,64,67,86	7
86	OHX	2	1963	7/7	0.96	0.24	-	72,74,75,98	7
87	MG	5	3825	1/1	0.92	0.73	-	39,39,39,39	0
87	MG	5	3810	1/1	0.93	0.23	-	51,51,51,51	0
87	MG	1	4054	1/1	0.93	0.59	-	48,48,48,48	0
87	MG	5	3806	1/1	0.96	0.34	-	60,60,60,60	0
87	MG	5	4043	1/1	0.92	0.24	-	77,77,77,77	0
87	MG	8	224	1/1	0.72	0.85	-	59,59,59,59	0
87	MG	6	2104	1/1	0.95	0.41	-	74,74,74,74	0
87	MG	5	3752	1/1	0.92	0.21	-	39,39,39,39	0
87	MG	5	3971	1/1	0.91	0.39	-	65,65,65,65	0
87	MG	2	2078	1/1	0.71	0.37	-	68,68,68,68	0
87	MG	5	4005	1/1	0.82	0.40	-	43,43,43,43	0
86	OHX	1	3678	7/7	0.95	0.38	-	57,57,58,89	7
86	OHX	5	3662	7/7	0.94	0.18	-	69,70,71,107	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	2	2111	1/1	0.86	0.42	-	91,91,91,91	0
87	MG	5	4049	1/1	0.96	0.39	-	59,59,59,59	0
87	MG	5	3983	1/1	0.92	0.56	-	52,52,52,52	0
87	MG	6	2110	1/1	0.78	0.16	-	49,49,49,49	0
86	OHX	5	3420	7/7	0.99	0.16	-	64,65,66,78	7
87	MG	5	3872	1/1	0.90	0.64	-	49,49,49,49	0
87	MG	5	4105	1/1	0.94	0.19	-	40,40,40,40	0
87	MG	1	3714	1/1	0.96	0.80	-	46,46,46,46	0
87	MG	1	3732	1/1	0.83	0.41	-	50,50,50,50	0
87	MG	5	3959	1/1	0.92	0.32	-	56,56,56,56	0
87	MG	1	4033	1/1	0.99	0.39	-	40,40,40,40	0
87	MG	1	4011	1/1	0.95	0.41	-	41,41,41,41	0
86	OHX	1	3664	7/7	0.98	0.26	-	62,63,65,93	7
87	MG	1	4040	1/1	0.92	0.20	-	62,62,62,62	0
87	MG	4	218	1/1	0.92	0.63	-	53,53,53,53	0
87	MG	o7	503	1/1	0.95	0.39	-	78,78,78,78	0
87	MG	1	3931	1/1	0.94	0.52	-	51,51,51,51	0
87	MG	5	3761	1/1	0.84	0.56	-	48,48,48,48	0
87	MG	5	4072	1/1	0.87	0.36	-	67,67,67,67	0
86	OHX	2	1982	7/7	0.92	0.19	-	85,85,87,112	7
87	MG	5	4007	1/1	0.82	0.20	-	56,56,56,56	0
87	MG	5	3796	1/1	0.88	0.23	-	36,36,36,36	0
87	MG	1	3744	1/1	0.96	0.36	-	49,49,49,49	0
86	OHX	6	1936	7/7	0.98	0.14	-	68,69,73,88	7
86	OHX	6	2006	7/7	0.83	0.34	-	87,87,88,112	7
87	MG	5	3805	1/1	0.58	0.57	-	63,63,63,63	0
87	MG	5	4074	1/1	0.75	0.81	-	55,55,55,55	0
87	MG	1	3761	1/1	0.98	0.47	-	52,52,52,52	0
87	MG	5	4073	1/1	0.85	0.31	-	40,40,40,40	0
86	OHX	1	3627	7/7	0.88	0.20	-	94,94,96,126	7
86	OHX	2	1989	7/7	0.86	0.26	-	94,95,97,121	7
87	MG	5	4045	1/1	0.92	0.61	-	29,29,29,29	0
87	MG	5	4036	1/1	0.92	0.33	-	39,39,39,39	0
87	MG	1	3906	1/1	0.92	0.41	-	46,46,46,46	0
87	MG	5	3982	1/1	0.77	0.25	-	52,52,52,52	0
87	MG	6	2130	1/1	0.45	0.77	-	95,95,95,95	0
87	MG	3	212	1/1	0.91	0.52	-	40,40,40,40	0
87	MG	5	4090	1/1	0.91	0.68	-	41,41,41,41	0
87	MG	2	2036	1/1	0.90	0.32	-	82,82,82,82	0
86	OHX	1	3655	7/7	0.94	0.29	-	87,87,87,115	7
87	MG	5	4083	1/1	0.84	0.23	-	53,53,53,53	0
87	MG	1	3953	1/1	0.94	0.20	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3663	7/7	0.91	0.30	-	73,74,75,117	7
87	MG	4	230	1/1	0.90	0.72	-	72,72,72,72	0
86	OHX	5	3704	7/7	0.94	0.09	-	151,151,151,167	7
86	OHX	1	3523	7/7	0.95	0.15	-	83,84,87,111	7
87	MG	1	4034	1/1	0.97	0.65	-	57,57,57,57	0
86	OHX	5	3655	7/7	0.96	0.20	-	61,64,64,89	7
87	MG	1	3970	1/1	0.95	0.26	-	58,58,58,58	0
86	OHX	5	3663	7/7	0.96	0.23	-	51,52,54,83	7
86	OHX	6	1935	7/7	0.98	0.23	-	66,67,69,92	7
87	MG	5	3961	1/1	0.91	0.57	-	40,40,40,40	0
86	OHX	5	3615	7/7	0.94	0.23	-	60,60,62,84	7
86	OHX	5	3450	7/7	0.97	0.16	-	81,84,87,105	7
87	MG	5	3951	1/1	0.77	0.38	-	57,57,57,57	0
87	MG	5	4027	1/1	0.88	0.22	-	56,56,56,56	0
87	MG	5	4089	1/1	0.94	0.27	-	69,69,69,69	0
87	MG	2	2041	1/1	0.66	0.32	-	74,74,74,74	0
87	MG	5	3816	1/1	0.85	0.52	-	51,51,51,51	0
86	OHX	1	3709	7/7	0.89	0.19	-	79,80,81,112	7
87	MG	1	4009	1/1	0.84	0.59	-	65,65,65,65	0
87	MG	5	4037	1/1	0.88	0.39	-	52,52,52,52	0
87	MG	5	3895	1/1	0.98	0.47	-	28,28,28,28	0
87	MG	6	2106	1/1	0.86	0.32	-	48,48,48,48	0
87	MG	5	3769	1/1	0.95	0.38	-	49,49,49,49	0
86	OHX	5	3648	7/7	0.92	0.37	-	84,85,87,110	7
87	MG	5	3998	1/1	0.82	0.85	-	71,71,71,71	0
86	OHX	6	2026	7/7	0.90	0.32	-	64,64,66,98	7
87	MG	6	2128	1/1	0.88	0.55	-	54,54,54,54	0
87	MG	1	3940	1/1	0.93	0.24	-	55,55,55,55	0
87	MG	5	3787	1/1	0.82	0.36	-	59,59,59,59	0
87	MG	1	3927	1/1	0.84	0.25	-	50,50,50,50	0
87	MG	6	2065	1/1	0.90	0.69	-	61,61,61,61	0
87	MG	5	4069	1/1	0.87	0.42	-	70,70,70,70	0
87	MG	6	2127	1/1	0.90	0.45	-	49,49,49,49	0
86	OHX	1	3481	7/7	0.98	0.16	-	85,88,90,104	7
87	MG	5	3948	1/1	0.89	0.19	-	40,40,40,40	0
87	MG	1	3912	1/1	0.80	0.54	-	63,63,63,63	0
87	MG	1	4043	1/1	0.77	0.40	-	54,54,54,54	0
86	OHX	1	3711	7/7	0.93	0.21	-	80,80,82,109	7
87	MG	5	3996	1/1	0.85	0.28	-	50,50,50,50	0
87	MG	5	4065	1/1	0.98	0.53	-	59,59,59,59	0
87	MG	5	3734	1/1	0.89	0.29	-	53,53,53,53	0
87	MG	5	4085	1/1	0.96	0.55	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3524	7/7	0.98	0.20	-	63,65,67,94	7
87	MG	1	3755	1/1	0.94	0.18	-	53,53,53,53	0
86	OHX	5	3699	7/7	0.95	0.17	-	68,69,70,100	7
87	MG	1	3869	1/1	0.98	0.50	-	36,36,36,36	0
87	MG	1	4003	1/1	0.95	0.14	-	51,51,51,51	0
86	OHX	4	212	7/7	0.94	0.14	-	113,115,117,141	7
87	MG	5	3736	1/1	0.90	0.34	-	39,39,39,39	0
87	MG	2	2054	1/1	0.85	0.42	-	53,53,53,53	0
87	MG	6	2121	1/1	0.75	0.30	-	49,49,49,49	0
87	MG	5	3986	1/1	0.78	0.17	-	49,49,49,49	0
87	MG	1	3910	1/1	0.94	0.32	-	51,51,51,51	0
87	MG	1	3729	1/1	0.96	0.34	-	78,78,78,78	0
87	MG	m7	202	1/1	0.93	0.24	-	45,45,45,45	0
87	MG	5	3733	1/1	0.90	0.25	-	46,46,46,46	0
87	MG	5	3915	1/1	0.91	0.08	-	47,47,47,47	0
87	MG	2	2031	1/1	0.86	0.65	-	50,50,50,50	0
87	MG	5	4098	1/1	0.96	0.19	-	56,56,56,56	0
87	MG	2	2104	1/1	0.88	0.31	-	65,65,65,65	0
87	MG	1	3838	1/1	0.96	0.37	-	42,42,42,42	0
87	MG	5	3937	1/1	0.91	0.33	-	49,49,49,49	0
86	OHX	1	3605	7/7	0.86	0.24	-	72,74,76,101	7
87	MG	2	2053	1/1	0.94	0.57	-	84,84,84,84	0
86	OHX	5	3659	7/7	0.93	0.21	-	48,50,52,90	7
87	MG	1	3862	1/1	0.88	0.37	-	38,38,38,38	0
87	MG	2	2096	1/1	0.84	0.12	-	107,107,107,107	0
87	MG	5	3926	1/1	0.97	0.36	-	51,51,51,51	0
87	MG	1	3887	1/1	0.87	0.46	-	39,39,39,39	0
87	MG	M7	203	1/1	0.80	0.45	-	69,69,69,69	0
87	MG	5	3836	1/1	0.89	0.60	-	27,27,27,27	0
87	MG	6	2039	1/1	0.92	0.31	-	60,60,60,60	0
87	MG	1	3822	1/1	0.86	0.39	-	50,50,50,50	0
87	MG	1	3810	1/1	0.88	0.42	-	48,48,48,48	0
87	MG	2	2086	1/1	0.92	0.45	-	70,70,70,70	0
86	OHX	2	1985	7/7	0.94	0.12	-	107,108,109,128	7
86	OHX	5	3722	7/7	0.83	0.33	-	69,69,70,99	7
87	MG	5	3976	1/1	0.92	0.15	-	57,57,57,57	0
87	MG	2	2056	1/1	0.93	0.34	-	68,68,68,68	0
86	OHX	3	205	7/7	0.90	0.18	-	88,89,90,118	7
87	MG	5	3985	1/1	0.70	0.58	-	50,50,50,50	0
87	MG	1	3759	1/1	0.76	0.48	-	48,48,48,48	0
87	MG	1	3807	1/1	0.91	0.74	-	42,42,42,42	0
87	MG	5	3788	1/1	0.82	0.38	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3629	7/7	0.89	0.20	-	99,99,101,126	7
87	MG	3	210	1/1	0.90	0.59	-	47,47,47,47	0
87	MG	4	225	1/1	0.90	0.64	-	50,50,50,50	0
86	OHX	1	3617	7/7	0.93	0.19	-	83,83,84,103	7
87	MG	2	2075	1/1	0.96	0.31	-	63,63,63,63	0
87	MG	6	2120	1/1	0.89	0.81	-	58,58,58,58	0
87	MG	1	4037	1/1	0.80	0.49	-	62,62,62,62	0
87	MG	5	3774	1/1	0.78	0.35	-	46,46,46,46	0
87	MG	1	3748	1/1	0.95	0.76	-	45,45,45,45	0
87	MG	1	3749	1/1	0.97	0.73	-	40,40,40,40	0
87	MG	6	2113	1/1	0.89	0.31	-	75,75,75,75	0
87	MG	5	4013	1/1	0.91	0.28	-	49,49,49,49	0
86	OHX	4	207	7/7	0.96	0.13	-	77,78,81,100	7
86	OHX	5	3708	7/7	0.82	0.20	-	86,87,88,116	7
87	MG	5	3770	1/1	0.96	0.21	-	43,43,43,43	0
86	OHX	6	1951	7/7	0.97	0.10	-	115,116,117,131	7
87	MG	5	4009	1/1	0.94	0.48	-	72,72,72,72	0
87	MG	2	2081	1/1	0.86	0.78	-	60,60,60,60	0
86	OHX	5	3639	7/7	0.87	0.17	-	84,84,85,116	7
87	MG	5	3801	1/1	0.88	0.59	-	37,37,37,37	0
86	OHX	1	3602	7/7	0.95	0.25	-	62,62,65,86	7
87	MG	1	3784	1/1	0.76	0.73	-	54,54,54,54	0
87	MG	1	3756	1/1	0.95	0.43	-	34,34,34,34	0
87	MG	5	3815	1/1	0.98	0.49	-	33,33,33,33	0
87	MG	1	3963	1/1	0.28	0.32	-	74,74,74,74	0
87	MG	1	3903	1/1	0.88	0.31	-	68,68,68,68	0
87	MG	5	4020	1/1	0.90	0.18	-	47,47,47,47	0
86	OHX	C3	201	7/7	0.92	0.18	-	105,107,107,135	7
87	MG	7	222	1/1	0.90	0.17	-	59,59,59,59	0
86	OHX	5	3654	7/7	0.92	0.18	-	83,84,84,117	7
87	MG	5	3879	1/1	0.99	0.51	-	32,32,32,32	0
87	MG	1	3830	1/1	0.95	0.52	-	40,40,40,40	0
87	MG	1	3943	1/1	0.81	0.37	-	78,78,78,78	0
86	OHX	2	2006	7/7	0.89	0.16	-	114,116,116,135	7
86	OHX	5	3621	7/7	0.96	0.13	-	92,93,95,111	7
87	MG	1	3782	1/1	0.96	0.61	-	47,47,47,47	0
87	MG	1	3739	1/1	0.98	0.53	-	60,60,60,60	0
86	OHX	1	3550	7/7	0.98	0.22	-	73,74,75,100	7
87	MG	1	3826	1/1	0.98	0.39	-	36,36,36,36	0
87	MG	1	3938	1/1	0.85	0.56	-	48,48,48,48	0
86	OHX	5	3595	7/7	0.92	0.17	-	69,70,73,104	7
87	MG	6	2070	1/1	0.95	0.44	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3929	1/1	0.97	0.26	-	40,40,40,40	0
87	MG	5	4066	1/1	0.89	0.69	-	60,60,60,60	0
87	MG	1	3989	1/1	0.49	0.31	-	82,82,82,82	0
86	OHX	6	1948	7/7	0.99	0.16	-	69,69,71,98	7
87	MG	d6	102	1/1	0.68	0.44	-	66,66,66,66	0
86	OHX	5	3694	7/7	0.90	0.28	-	59,60,60,88	7
86	OHX	6	2002	7/7	0.93	0.28	-	90,90,91,117	7
87	MG	5	3818	1/1	0.94	0.48	-	39,39,39,39	0
87	MG	6	2066	1/1	0.96	0.36	-	51,51,51,51	0
87	MG	5	4026	1/1	0.95	0.33	-	53,53,53,53	0
87	MG	6	2071	1/1	0.81	0.58	-	52,52,52,52	0
87	MG	1	3935	1/1	0.90	0.53	-	40,40,40,40	0
87	MG	1	3990	1/1	0.92	0.25	-	58,58,58,58	0
87	MG	2	2108	1/1	0.65	0.88	-	131,131,131,131	0
87	MG	1	3915	1/1	0.77	0.36	-	63,63,63,63	0
87	MG	7	212	1/1	0.94	0.36	-	57,57,57,57	0
86	OHX	2	1957	7/7	0.96	0.12	-	136,137,137,147	7
87	MG	5	4071	1/1	0.83	0.37	-	55,55,55,55	0
87	MG	1	4024	1/1	0.90	0.46	-	63,63,63,63	0
87	MG	1	3948	1/1	0.90	0.32	-	49,49,49,49	0
87	MG	5	3773	1/1	0.91	0.37	-	35,35,35,35	0
87	MG	6	2118	1/1	0.53	0.31	-	109,109,109,109	0
87	MG	1	3922	1/1	0.72	0.66	-	63,63,63,63	0
86	OHX	5	3570	7/7	0.95	0.18	-	86,86,87,110	7
87	MG	2	2043	1/1	0.95	0.57	-	57,57,57,57	0
86	OHX	5	3545	7/7	0.97	0.23	-	50,52,54,85	7
87	MG	5	3737	1/1	0.78	0.29	-	49,49,49,49	0
87	MG	6	2124	1/1	0.75	0.57	-	84,84,84,84	0
86	OHX	2	2018	7/7	0.89	0.18	-	116,117,118,136	7
86	OHX	6	2029	7/7	0.77	0.29	-	125,126,128,147	7
86	OHX	6	2033	7/7	0.96	0.16	-	86,87,88,106	7
87	MG	2	2115	1/1	0.80	0.66	-	66,66,66,66	0
87	MG	S2	301	1/1	0.87	0.81	-	68,68,68,68	0
87	MG	1	3777	1/1	0.94	0.47	-	39,39,39,39	0
86	OHX	1	3460	7/7	0.98	0.20	-	73,74,77,86	7
86	OHX	6	1968	7/7	0.91	0.23	-	89,91,94,128	7
86	OHX	2	2010	7/7	0.92	0.30	-	104,107,108,129	7
87	MG	1	3781	1/1	0.86	0.37	-	42,42,42,42	0
87	MG	1	3724	1/1	0.93	0.93	-	62,62,62,62	0
87	MG	2	2079	1/1	0.86	0.47	-	58,58,58,58	0
87	MG	m5	303	1/1	0.95	0.61	-	45,45,45,45	0
87	MG	6	2112	1/1	0.90	0.36	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3907	1/1	0.91	0.53	-	39,39,39,39	0
86	OHX	5	3453	7/7	0.98	0.15	-	77,79,80,99	7
87	MG	6	2111	1/1	0.87	0.28	-	54,54,54,54	0
87	MG	5	4001	1/1	0.82	0.21	-	49,49,49,49	0
87	MG	1	3758	1/1	0.86	0.27	-	47,47,47,47	0
87	MG	q2	503	1/1	0.91	0.40	-	51,51,51,51	0
87	MG	5	3878	1/1	0.94	0.72	-	36,36,36,36	0
87	MG	8	221	1/1	0.95	0.31	-	53,53,53,53	0
87	MG	5	3841	1/1	0.92	0.40	-	46,46,46,46	0
86	OHX	1	3668	7/7	0.91	0.13	-	84,84,85,110	7
87	MG	1	3965	1/1	0.90	0.34	-	46,46,46,46	0
86	OHX	5	3422	7/7	0.99	0.18	-	56,58,60,65	7
86	OHX	14	401	7/7	0.85	0.28	-	62,62,63,86	7
86	OHX	2	1975	7/7	0.93	0.15	-	110,111,112,131	7
86	OHX	6	1937	7/7	0.99	0.15	-	72,72,75,85	7
86	OHX	5	3557	7/7	0.98	0.18	-	58,58,60,83	7
87	MG	5	4031	1/1	0.98	0.83	-	60,60,60,60	0
87	MG	5	3979	1/1	0.84	0.21	-	53,53,53,53	0
86	OHX	5	3626	7/7	0.96	0.12	-	78,78,79,103	7
87	MG	1	3832	1/1	0.94	0.47	-	35,35,35,35	0
86	OHX	c8	201	7/7	0.95	0.18	-	107,107,108,127	7
87	MG	6	2077	1/1	0.80	0.65	-	75,75,75,75	0
87	MG	1	3968	1/1	0.89	0.57	-	49,49,49,49	0
87	MG	2	2076	1/1	0.88	0.51	-	51,51,51,51	0
86	OHX	1	3629	7/7	0.97	0.12	-	104,104,106,123	7
87	MG	2	2084	1/1	0.96	0.53	-	69,69,69,69	0
87	MG	5	3804	1/1	0.96	0.75	-	46,46,46,46	0
86	OHX	5	3482	7/7	0.98	0.24	-	49,52,55,72	7
87	MG	1	3913	1/1	0.81	0.34	-	54,54,54,54	0
87	MG	1	3914	1/1	0.92	0.30	-	47,47,47,47	0
86	OHX	2	1951	7/7	0.94	0.13	-	134,135,136,149	7
87	MG	o7	504	1/1	0.94	0.49	-	65,65,65,65	0
87	MG	5	3775	1/1	0.91	0.58	-	36,36,36,36	0
86	OHX	1	3436	7/7	0.97	0.17	-	81,83,86,103	7
87	MG	4	227	1/1	0.78	0.49	-	56,56,56,56	0
87	MG	6	2076	1/1	0.96	0.44	-	42,42,42,42	0
86	OHX	1	3442	7/7	0.97	0.15	-	72,75,81,91	7
87	MG	1	3932	1/1	0.94	0.65	-	110,110,110,110	0
87	MG	1	3877	1/1	0.96	0.35	-	43,43,43,43	0
87	MG	5	4022	1/1	0.90	0.36	-	59,59,59,59	0
87	MG	5	4097	1/1	0.96	0.47	-	22,22,22,22	0
86	OHX	5	3718	7/7	0.87	0.25	-	76,78,79,104	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3408	7/7	0.99	0.17	-	42,47,53,66	7
87	MG	5	4047	1/1	0.84	0.28	-	44,44,44,44	0
87	MG	1	4052	1/1	0.83	0.21	-	75,75,75,75	0
87	MG	1	3930	1/1	0.81	0.29	-	50,50,50,50	0
86	OHX	2	2019	7/7	0.87	0.18	-	112,113,113,139	7
87	MG	5	3939	1/1	0.93	0.23	-	52,52,52,52	0
87	MG	2	2035	1/1	0.97	0.52	-	64,64,64,64	0
86	OHX	1	3682	7/7	0.90	0.24	-	86,87,88,115	7
87	MG	4	228	1/1	0.92	0.24	-	41,41,41,41	0
86	OHX	5	3636	7/7	0.93	0.30	-	70,71,72,104	7
87	MG	5	3918	1/1	0.91	0.40	-	45,45,45,45	0
87	MG	6	2097	1/1	0.94	0.71	-	59,59,59,59	0
87	MG	5	3900	1/1	0.96	0.43	-	31,31,31,31	0
86	OHX	1	3465	7/7	0.99	0.17	-	62,65,68,81	7
87	MG	1	3812	1/1	0.89	0.64	-	34,34,34,34	0
87	MG	6	2040	1/1	0.55	0.52	-	54,54,54,54	0
87	MG	5	3808	1/1	0.84	0.30	-	41,41,41,41	0
87	MG	5	3972	1/1	0.91	0.54	-	45,45,45,45	0
87	MG	1	4045	1/1	0.94	0.57	-	42,42,42,42	0
87	MG	5	3762	1/1	0.98	0.35	-	57,57,57,57	0
86	OHX	5	3678	7/7	0.92	0.23	-	71,71,74,106	7
86	OHX	M9	201	7/7	0.86	0.16	-	98,98,99,123	7
86	OHX	2	1912	7/7	0.98	0.13	-	105,106,108,115	7
87	MG	1	3816	1/1	0.98	0.48	-	39,39,39,39	0
87	MG	1	4015	1/1	0.95	0.08	-	66,66,66,66	0
87	MG	5	4086	1/1	0.96	0.69	-	45,45,45,45	0
86	OHX	1	3697	7/7	0.94	0.20	-	75,76,77,104	7
86	OHX	m4	201	7/7	0.86	0.24	-	124,124,124,140	7
87	MG	5	3893	1/1	0.94	0.38	-	38,38,38,38	0
86	OHX	1	3409	7/7	0.99	0.18	-	57,59,61,75	7
86	OHX	2	1958	7/7	0.90	0.22	-	97,98,99,129	7
86	OHX	1	3494	7/7	0.99	0.13	-	71,71,74,88	7
87	MG	L3	403	1/1	0.94	0.19	-	48,48,48,48	0
87	MG	1	3747	1/1	0.96	0.35	-	50,50,50,50	0
87	MG	5	3889	1/1	0.90	0.47	-	45,45,45,45	0
86	OHX	5	3475	7/7	0.96	0.17	-	81,83,88,104	7
87	MG	1	3905	1/1	0.88	0.35	-	51,51,51,51	0
87	MG	1	3799	1/1	0.86	0.44	-	48,48,48,48	0
86	OHX	5	3714	7/7	0.93	0.12	-	127,127,127,145	7
86	OHX	5	3656	7/7	0.95	0.26	-	46,48,50,85	7
87	MG	5	3999	1/1	0.85	0.52	-	67,67,67,67	0
87	MG	5	3794	1/1	0.91	0.33	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	2084	1/1	0.95	0.39	-	79,79,79,79	0
87	MG	c6	201	1/1	0.61	0.40	-	91,91,91,91	0
86	OHX	2	1986	7/7	0.97	0.14	-	90,91,92,113	7
87	MG	1	3876	1/1	0.93	0.45	-	36,36,36,36	0
86	OHX	5	3647	7/7	0.96	0.18	-	50,52,54,92	7
87	MG	5	3896	1/1	0.94	0.39	-	38,38,38,38	0
87	MG	5	3859	1/1	0.96	0.42	-	35,35,35,35	0
87	MG	5	3980	1/1	0.82	0.43	-	77,77,77,77	0
87	MG	5	4025	1/1	0.97	0.17	-	56,56,56,56	0
87	MG	6	2063	1/1	0.81	0.40	-	52,52,52,52	0
87	MG	5	4028	1/1	0.84	0.38	-	80,80,80,80	0
86	OHX	1	3587	7/7	0.97	0.24	-	83,84,85,107	7
87	MG	1	3843	1/1	0.92	0.25	-	34,34,34,34	0
87	MG	6	2092	1/1	0.79	0.48	-	61,61,61,61	0
86	OHX	5	3575	7/7	0.94	0.27	-	65,68,69,94	7
87	MG	1	3803	1/1	0.94	0.63	-	47,47,47,47	0
87	MG	6	2102	1/1	0.83	0.36	-	61,61,61,61	0
87	MG	5	4102	1/1	0.95	0.28	-	41,41,41,41	0
87	MG	1	4055	1/1	0.92	0.62	-	51,51,51,51	0
86	OHX	5	3646	7/7	0.85	0.25	-	77,78,79,104	7
86	OHX	5	3518	7/7	0.98	0.19	-	65,65,68,94	7
86	OHX	6	1973	7/7	0.98	0.15	-	76,78,80,103	7
86	OHX	5	3597	7/7	0.92	0.23	-	97,97,99,124	7
87	MG	5	4067	1/1	0.77	0.17	-	68,68,68,68	0
87	MG	2	2052	1/1	0.90	0.70	-	66,66,66,66	0
87	MG	6	2060	1/1	0.85	0.41	-	86,86,86,86	0
86	OHX	1	3560	7/7	0.95	0.14	-	111,113,114,136	7
87	MG	1	4035	1/1	0.48	0.49	-	111,111,111,111	0
87	MG	5	3934	1/1	0.89	0.52	-	52,52,52,52	0
87	MG	1	3937	1/1	0.94	0.74	-	52,52,52,52	0
87	MG	5	4010	1/1	0.93	0.44	-	40,40,40,40	0
87	MG	5	3738	1/1	0.92	0.58	-	34,34,34,34	0
87	MG	1	4005	1/1	0.94	0.71	-	54,54,54,54	0
86	OHX	5	3616	7/7	0.92	0.17	-	77,79,80,101	7
86	OHX	2	1984	7/7	0.89	0.20	-	85,85,89,120	7
87	MG	6	2099	1/1	0.92	0.40	-	91,91,91,91	0
87	MG	2	2116	1/1	0.82	0.30	-	64,64,64,64	0
87	MG	5	4094	1/1	0.89	0.24	-	70,70,70,70	0
86	OHX	2	1966	7/7	0.94	0.33	-	86,87,88,114	7
86	OHX	5	3478	7/7	0.98	0.27	-	62,63,66,102	7
87	MG	5	3750	1/1	0.97	0.28	-	39,39,39,39	0
87	MG	5	3935	1/1	0.78	0.42	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	4059	1/1	0.79	0.39	-	69,69,69,69	0
87	MG	5	4084	1/1	0.95	0.48	-	33,33,33,33	0
87	MG	5	3757	1/1	0.98	0.52	-	39,39,39,39	0
86	OHX	7	210	7/7	0.94	0.24	-	52,53,54,90	7
87	MG	6	2114	1/1	0.91	0.15	-	76,76,76,76	0
86	OHX	5	3457	7/7	0.97	0.16	-	69,75,78,101	7
87	MG	5	3798	1/1	0.90	0.45	-	71,71,71,71	0
87	MG	5	3743	1/1	0.89	0.52	-	74,74,74,74	0
87	MG	1	3824	1/1	0.96	0.62	-	34,34,34,34	0
87	MG	6	2090	1/1	0.95	0.49	-	61,61,61,61	0
86	OHX	5	3477	7/7	0.98	0.18	-	68,69,71,94	7
87	MG	5	4088	1/1	0.94	0.74	-	65,65,65,65	0
87	MG	1	3722	1/1	0.93	0.50	-	42,42,42,42	0
87	MG	8	219	1/1	0.87	0.69	-	62,62,62,62	0
87	MG	5	3764	1/1	0.95	0.70	-	44,44,44,44	0
87	MG	5	4019	1/1	0.93	0.21	-	53,53,53,53	0
87	MG	5	3987	1/1	0.90	0.36	-	43,43,43,43	0
87	MG	5	3883	1/1	0.93	0.44	-	44,44,44,44	0
87	MG	5	4057	1/1	0.94	0.20	-	38,38,38,38	0
87	MG	5	3957	1/1	0.89	0.35	-	65,65,65,65	0
87	MG	5	3966	1/1	0.92	0.25	-	51,51,51,51	0
87	MG	6	2133	1/1	0.97	0.23	-	58,58,58,58	0
87	MG	1	3993	1/1	0.94	0.23	-	40,40,40,40	0
86	OHX	1	3707	7/7	0.91	0.16	-	84,84,85,114	7
86	OHX	5	3548	7/7	0.96	0.17	-	83,84,86,107	7
86	OHX	5	3675	7/7	0.96	0.09	-	132,133,134,150	7
87	MG	5	3785	1/1	0.93	0.41	-	53,53,53,53	0
86	OHX	5	3544	7/7	0.94	0.29	-	58,60,63,99	7
86	OHX	2	2012	7/7	0.87	0.19	-	128,128,129,143	7
87	MG	1	4046	1/1	0.98	0.40	-	94,94,94,94	0
87	MG	1	4042	1/1	0.88	0.32	-	55,55,55,55	0
87	MG	7	214	1/1	0.98	0.40	-	59,59,59,59	0
87	MG	2	2089	1/1	0.78	0.90	-	84,84,84,84	0
87	MG	1	3957	1/1	0.87	0.34	-	50,50,50,50	0
87	MG	6	2107	1/1	0.87	0.62	-	61,61,61,61	0
87	MG	2	2110	1/1	0.91	0.57	-	59,59,59,59	0
87	MG	6	2132	1/1	0.71	0.45	-	85,85,85,85	0
87	MG	7	217	1/1	0.81	0.43	-	44,44,44,44	0
86	OHX	1	3635	7/7	0.96	0.17	-	72,73,74,101	7
87	MG	5	3960	1/1	0.88	0.52	-	54,54,54,54	0
87	MG	1	3981	1/1	0.72	0.18	-	66,66,66,66	0
87	MG	2	2068	1/1	0.76	0.57	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3738	1/1	0.95	0.57	-	51,51,51,51	0
87	MG	5	4061	1/1	0.92	0.23	-	55,55,55,55	0
87	MG	2	2085	1/1	0.86	0.49	-	74,74,74,74	0
87	MG	1	4032	1/1	0.97	0.23	-	68,68,68,68	0
86	OHX	5	3585	7/7	0.92	0.16	-	94,96,99,127	7
87	MG	5	3814	1/1	0.93	0.33	-	42,42,42,42	0
86	OHX	1	3667	7/7	0.82	0.41	-	57,58,60,89	7
87	MG	2	2030	1/1	0.94	0.78	-	47,47,47,47	0
87	MG	5	3824	1/1	0.97	0.46	-	34,34,34,34	0
87	MG	5	3850	1/1	0.99	0.50	-	43,43,43,43	0
87	MG	5	4029	1/1	0.95	0.21	-	43,43,43,43	0
87	MG	1	3716	1/1	0.72	0.43	-	123,123,123,123	0
86	OHX	1	3695	7/7	0.92	0.13	-	118,118,118,140	7
86	OHX	6	2019	7/7	0.94	0.27	-	82,83,84,106	7
86	OHX	5	3573	7/7	0.97	0.17	-	64,65,68,85	7
87	MG	5	3809	1/1	0.91	0.43	-	48,48,48,48	0
87	MG	5	3894	1/1	0.98	0.54	-	35,35,35,35	0
86	OHX	1	3623	7/7	0.95	0.08	-	124,124,124,144	7
87	MG	5	3755	1/1	0.91	0.24	-	44,44,44,44	0
87	MG	5	3899	1/1	0.94	0.59	-	43,43,43,43	0
87	MG	4	201	1/1	0.88	0.22	-	56,56,56,56	0
87	MG	5	3753	1/1	0.89	0.17	-	65,65,65,65	0
86	OHX	5	3668	7/7	0.89	0.39	-	101,102,103,131	7
87	MG	1	4007	1/1	0.90	0.38	-	52,52,52,52	0
87	MG	2	2112	1/1	0.79	0.50	-	88,88,88,88	0
87	MG	1	3797	1/1	0.84	0.44	-	52,52,52,52	0
87	MG	1	3772	1/1	0.84	0.29	-	44,44,44,44	0
87	MG	5	4000	1/1	0.79	0.15	-	61,61,61,61	0
87	MG	6	2087	1/1	0.95	0.42	-	55,55,55,55	0
87	MG	1	3847	1/1	0.94	0.48	-	38,38,38,38	0
87	MG	5	3860	1/1	0.80	0.43	-	40,40,40,40	0
87	MG	1	3854	1/1	0.97	0.59	-	41,41,41,41	0
87	MG	5	3942	1/1	0.56	0.37	-	94,94,94,94	0
87	MG	M3	201	1/1	0.62	0.43	-	98,98,98,98	0
87	MG	1	3825	1/1	0.87	0.43	-	38,38,38,38	0
87	MG	1	3926	1/1	0.91	0.40	-	45,45,45,45	0
87	MG	2	2055	1/1	0.76	0.38	-	86,86,86,86	0
87	MG	2	2058	1/1	0.96	0.51	-	64,64,64,64	0
87	MG	1	3925	1/1	0.89	0.37	-	44,44,44,44	0
87	MG	5	3990	1/1	0.98	0.52	-	52,52,52,52	0
86	OHX	5	3628	7/7	0.94	0.21	-	55,58,59,80	7
87	MG	5	4060	1/1	0.76	0.27	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2035	7/7	0.86	0.43	-	113,114,115,138	7
86	OHX	1	3625	7/7	0.91	0.15	-	102,103,105,121	7
87	MG	1	3728	1/1	0.92	0.53	-	56,56,56,56	0
86	OHX	6	1960	7/7	0.90	0.28	-	66,68,71,107	7
87	MG	5	3921	1/1	0.86	0.48	-	58,58,58,58	0
86	OHX	8	211	7/7	0.96	0.10	-	114,114,115,137	7
87	MG	5	3946	1/1	0.78	0.61	-	50,50,50,50	0
87	MG	6	2050	1/1	0.97	0.60	-	38,38,38,38	0
86	OHX	2	2004	7/7	0.96	0.21	-	70,71,71,94	7
87	MG	1	4000	1/1	0.62	0.47	-	39,39,39,39	0
86	OHX	1	3553	7/7	0.96	0.10	-	113,114,115,137	7
87	MG	6	2100	1/1	0.89	0.37	-	73,73,73,73	0
86	OHX	6	1949	7/7	0.93	0.17	-	99,100,102,117	7
86	OHX	1	3615	7/7	0.94	0.13	-	96,97,98,121	7
87	MG	5	3779	1/1	0.94	0.60	-	52,52,52,52	0
87	MG	D3	201	1/1	0.81	0.18	-	64,64,64,64	0
87	MG	7	218	1/1	0.62	0.32	-	67,67,67,67	0
87	MG	1	3834	1/1	0.93	0.65	-	38,38,38,38	0
87	MG	5	4091	1/1	0.89	0.42	-	52,52,52,52	0
86	OHX	5	3549	7/7	0.97	0.22	-	59,60,60,86	7
87	MG	5	3974	1/1	0.82	0.13	-	84,84,84,84	0
87	MG	6	2083	1/1	0.94	0.43	-	46,46,46,46	0
86	OHX	1	3568	7/7	0.92	0.29	-	71,72,73,98	7
87	MG	6	2091	1/1	0.80	0.49	-	60,60,60,60	0
87	MG	5	4080	1/1	0.90	0.35	-	52,52,52,52	0
87	MG	5	3848	1/1	0.97	0.44	-	33,33,33,33	0
86	OHX	1	3639	7/7	0.96	0.19	-	79,80,81,109	7
87	MG	1	3770	1/1	0.98	0.50	-	28,28,28,28	0
86	OHX	7	209	7/7	0.90	0.30	-	77,78,81,100	7
86	OHX	1	3554	7/7	0.97	0.13	-	69,69,70,97	7
87	MG	1	4049	1/1	0.93	0.08	-	79,79,79,79	0
87	MG	1	3760	1/1	0.93	0.31	-	39,39,39,39	0
87	MG	1	3998	1/1	0.88	0.26	-	44,44,44,44	0
87	MG	4	220	1/1	0.81	0.57	-	53,53,53,53	0
87	MG	1	3962	1/1	0.64	0.59	-	59,59,59,59	0
87	MG	2	2064	1/1	0.93	0.55	-	61,61,61,61	0
87	MG	5	3777	1/1	0.82	0.34	-	32,32,32,32	0
87	MG	5	4056	1/1	0.92	0.38	-	48,48,48,48	0
86	OHX	1	3633	7/7	0.97	0.18	-	69,70,72,98	7
86	OHX	5	3598	7/7	0.95	0.26	-	52,52,54,77	7
86	OHX	2	1955	7/7	0.97	0.23	-	82,83,86,99	7
87	MG	5	3823	1/1	0.93	0.34	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3533	7/7	0.97	0.21	-	51,51,52,79	7
87	MG	1	3861	1/1	0.93	0.56	-	47,47,47,47	0
86	OHX	6	2017	7/7	0.88	0.21	-	96,96,98,122	7
86	OHX	1	3684	7/7	0.93	0.21	-	107,107,108,130	7
86	OHX	7	202	7/7	0.97	0.19	-	58,63,64,77	7
87	MG	L4	402	1/1	0.91	0.29	-	50,50,50,50	0
87	MG	6	2088	1/1	0.90	0.45	-	45,45,45,45	0
87	MG	5	3958	1/1	0.78	0.19	-	48,48,48,48	0
87	MG	1	3879	1/1	0.83	0.43	-	39,39,39,39	0
87	MG	6	2064	1/1	0.93	0.34	-	68,68,68,68	0
86	OHX	1	3611	7/7	0.94	0.19	-	59,60,62,92	7
87	MG	2	2037	1/1	0.81	0.38	-	77,77,77,77	0
87	MG	1	3987	1/1	0.92	0.23	-	49,49,49,49	0
87	MG	1	3945	1/1	0.83	0.53	-	57,57,57,57	0
86	OHX	5	3552	7/7	0.98	0.14	-	57,57,59,84	7
86	OHX	1	3619	7/7	0.93	0.24	-	70,70,72,99	7
87	MG	5	3759	1/1	0.94	0.24	-	31,31,31,31	0
87	MG	5	3793	1/1	0.78	0.38	-	43,43,43,43	0
87	MG	1	3884	1/1	0.98	0.85	-	36,36,36,36	0
87	MG	5	4093	1/1	0.70	0.45	-	78,78,78,78	0
86	OHX	5	3674	7/7	0.97	0.31	-	70,71,72,102	7
87	MG	5	3754	1/1	0.82	0.35	-	39,39,39,39	0
86	OHX	1	3634	7/7	0.89	0.43	-	72,73,74,107	7
86	OHX	5	3588	7/7	0.97	0.19	-	77,78,78,101	7
87	MG	1	3733	1/1	0.83	0.27	-	51,51,51,51	0
87	MG	6	2058	1/1	0.94	0.38	-	61,61,61,61	0
87	MG	1	3959	1/1	0.90	0.49	-	45,45,45,45	0
87	MG	1	4004	1/1	0.93	0.26	-	52,52,52,52	0
87	MG	2	2066	1/1	0.95	0.43	-	64,64,64,64	0
86	OHX	6	2007	7/7	0.89	0.24	-	85,86,87,119	7
87	MG	5	4087	1/1	0.95	0.29	-	42,42,42,42	0
87	MG	2	2040	1/1	0.81	0.50	-	80,80,80,80	0
86	OHX	5	3520	7/7	0.97	0.14	-	103,104,106,122	7
87	MG	1	3795	1/1	0.66	0.38	-	77,77,77,77	0
87	MG	1	3944	1/1	0.68	1.26	-	59,59,59,59	0
87	MG	2	2107	1/1	0.98	0.68	-	71,71,71,71	0
87	MG	q1	101	1/1	0.91	0.20	-	47,47,47,47	0
87	MG	8	223	1/1	0.90	0.57	-	55,55,55,55	0
86	OHX	1	3703	7/7	0.83	0.34	-	55,57,58,89	7
87	MG	5	3963	1/1	0.89	0.40	-	55,55,55,55	0
87	MG	1	4041	1/1	0.94	0.35	-	58,58,58,58	0
87	MG	5	3863	1/1	0.95	0.32	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	2095	1/1	0.89	0.52	-	52,52,52,52	0
86	OHX	8	215	7/7	0.90	0.28	-	70,71,75,101	7
87	MG	5	3977	1/1	0.88	0.42	-	79,79,79,79	0
87	MG	5	4063	1/1	0.90	0.44	-	48,48,48,48	0
87	MG	1	3997	1/1	0.95	0.70	-	58,58,58,58	0
87	MG	5	4051	1/1	0.95	0.52	-	40,40,40,40	0
87	MG	5	3954	1/1	0.70	0.60	-	65,65,65,65	0
87	MG	6	2047	1/1	0.85	0.41	-	53,53,53,53	0
87	MG	2	2088	1/1	0.58	0.36	-	83,83,83,83	0
87	MG	3	213	1/1	0.96	0.58	-	38,38,38,38	0
87	MG	1	3958	1/1	0.80	0.36	-	45,45,45,45	0
87	MG	5	3950	1/1	0.77	0.69	-	61,61,61,61	0
87	MG	1	3907	1/1	0.82	0.41	-	42,42,42,42	0
87	MG	6	2115	1/1	0.78	0.17	-	56,56,56,56	0
86	OHX	1	3649	7/7	0.92	0.18	-	68,68,70,99	7
86	OHX	1	3644	7/7	0.81	0.20	-	140,141,142,164	7
86	OHX	1	3512	7/7	0.93	0.19	-	69,72,76,102	7
86	OHX	2	2022	7/7	0.66	0.16	-	250,250,250,254	7
86	OHX	1	3690	7/7	0.94	0.23	-	72,73,73,110	7
86	OHX	2	2013	7/7	0.89	0.14	-	120,120,121,141	7
87	MG	1	3774	1/1	0.95	0.51	-	53,53,53,53	0
87	MG	2	2102	1/1	0.94	0.75	-	61,61,61,61	0
87	MG	6	2119	1/1	0.95	0.66	-	49,49,49,49	0
87	MG	1	3751	1/1	0.95	0.46	-	31,31,31,31	0
87	MG	1	3941	1/1	0.91	0.27	-	44,44,44,44	0
87	MG	1	4030	1/1	0.95	0.34	-	45,45,45,45	0
86	OHX	1	3626	7/7	0.94	0.17	-	89,91,92,118	7
86	OHX	2	1992	7/7	0.92	0.18	-	88,90,90,111	7
87	MG	1	3952	1/1	0.93	0.45	-	52,52,52,52	0
87	MG	8	217	1/1	0.93	0.47	-	60,60,60,60	0
87	MG	1	3745	1/1	0.89	0.26	-	44,44,44,44	0
87	MG	5	4048	1/1	0.94	0.27	-	50,50,50,50	0
86	OHX	3	208	7/7	0.90	0.26	-	96,97,97,118	7
87	MG	4	202	1/1	0.90	0.24	-	53,53,53,53	0
87	MG	1	3949	1/1	0.85	0.34	-	47,47,47,47	0
86	OHX	1	3688	7/7	0.76	0.24	-	158,158,159,172	7
86	OHX	1	3551	7/7	0.97	0.15	-	77,78,80,101	7
87	MG	5	3756	1/1	0.86	0.33	-	61,61,61,61	0
86	OHX	6	1912	7/7	0.99	0.16	-	62,63,66,82	7
87	MG	5	4044	1/1	0.88	0.35	-	42,42,42,42	0
87	MG	4	223	1/1	0.89	0.77	-	31,31,31,31	0
87	MG	5	3861	1/1	0.94	0.43	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	MG	5	4014	1/1	0.91	0.40	-	47,47,47,47	0
87	MG	5	3800	1/1	0.94	0.33	-	53,53,53,53	0
87	MG	3	209	1/1	0.89	0.18	-	89,89,89,89	0
86	OHX	1	3557	7/7	0.93	0.24	-	62,64,65,97	7
86	OHX	6	2016	7/7	0.93	0.30	-	64,65,67,102	7
87	MG	7	215	1/1	0.89	0.53	-	30,30,30,30	0
86	OHX	5	3632	7/7	0.86	0.19	-	146,147,148,168	7
86	OHX	6	1943	7/7	0.97	0.13	-	87,88,89,109	7
87	MG	5	4092	1/1	0.97	0.34	-	42,42,42,42	0
87	MG	4	229	1/1	0.91	0.23	-	57,57,57,57	0
87	MG	1	4014	1/1	0.91	0.19	-	55,55,55,55	0
86	OHX	6	2018	7/7	0.95	0.16	-	75,75,76,108	7
86	OHX	1	3493	7/7	0.99	0.17	-	56,57,58,82	7
87	MG	5	4040	1/1	0.89	0.22	-	40,40,40,40	0
87	MG	6	2081	1/1	0.96	0.52	-	44,44,44,44	0
87	MG	1	4002	1/1	0.96	0.17	-	37,37,37,37	0
87	MG	1	3740	1/1	0.91	0.57	-	48,48,48,48	0
86	OHX	4	215	7/7	0.92	0.20	-	87,88,89,114	7
86	OHX	5	3534	7/7	0.95	0.23	-	56,58,61,96	7
86	OHX	1	3478	7/7	0.98	0.21	-	64,65,70,91	7
87	MG	7	219	1/1	0.96	0.27	-	42,42,42,42	0
87	MG	n9	101	1/1	0.65	0.35	-	46,46,46,46	0
87	MG	5	3847	1/1	0.87	0.40	-	34,34,34,34	0
86	OHX	M7	202	7/7	0.92	0.25	-	69,69,70,100	7
87	MG	1	3891	1/1	0.96	0.66	-	33,33,33,33	0
86	OHX	1	3671	7/7	0.93	0.21	-	69,69,70,100	7
87	MG	Q2	503	1/1	0.94	0.18	-	68,68,68,68	0
87	MG	6	2116	1/1	0.95	0.38	-	55,55,55,55	0
87	MG	1	3820	1/1	0.92	0.64	-	41,41,41,41	0
87	MG	5	4062	1/1	0.86	0.39	-	36,36,36,36	1
86	OHX	5	3508	7/7	0.91	0.34	-	79,80,82,117	7
86	OHX	1	3692	7/7	0.93	0.20	-	70,71,71,92	7
86	OHX	2	1930	7/7	0.98	0.12	-	74,75,76,94	7
87	MG	5	3837	1/1	0.94	0.45	-	28,28,28,28	0
87	MG	1	3837	1/1	0.96	0.71	-	35,35,35,35	0
86	OHX	5	3637	7/7	0.97	0.10	-	59,61,61,95	7
87	MG	2	2113	1/1	0.86	0.53	-	61,61,61,61	0
87	MG	5	3830	1/1	0.96	0.23	-	39,39,39,39	0
86	OHX	1	3648	7/7	0.93	0.25	-	63,65,66,99	7
87	MG	1	3947	1/1	0.91	0.69	-	51,51,51,51	0
87	MG	1	3757	1/1	0.78	0.23	-	50,50,50,50	0
86	OHX	5	3462	7/7	0.98	0.16	-	65,67,69,94	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	2053	1/1	0.96	0.50	-	61,61,61,61	0
87	MG	5	3727	1/1	0.95	0.54	-	58,58,58,58	0
87	MG	1	3896	1/1	0.93	0.18	-	47,47,47,47	0
87	MG	5	3855	1/1	0.96	0.84	-	41,41,41,41	0
87	MG	1	3919	1/1	0.97	0.40	-	51,51,51,51	0
86	OHX	2	1987	7/7	0.95	0.34	-	100,100,101,124	7
87	MG	5	4030	1/1	0.87	0.46	-	81,81,81,81	0
86	OHX	1	3534	7/7	0.95	0.12	-	157,158,158,170	7
86	OHX	5	3446	7/7	0.99	0.18	-	50,53,56,67	7
87	MG	1	3785	1/1	0.98	0.54	-	45,45,45,45	0
87	MG	1	3858	1/1	0.95	0.69	-	34,34,34,34	0
87	MG	N8	201	1/1	0.88	0.31	-	33,33,33,33	0
86	OHX	1	3654	7/7	0.92	0.29	-	75,75,77,106	7
86	OHX	3	201	7/7	0.97	0.20	-	82,89,90,102	7
87	MG	1	4016	1/1	0.94	0.44	-	32,32,32,32	0
87	MG	2	2106	1/1	0.95	0.32	-	87,87,87,87	0
87	MG	6	2078	1/1	0.97	0.50	-	42,42,42,42	0
86	OHX	4	216	7/7	0.93	0.25	-	69,70,70,98	7
87	MG	1	3775	1/1	0.94	0.22	-	44,44,44,44	0
87	MG	q0	202	1/1	0.88	0.20	-	53,53,53,53	0
87	MG	7	221	1/1	0.66	0.33	-	63,63,63,63	0
87	MG	5	4042	1/1	0.90	0.12	-	39,39,39,39	0
87	MG	6	2129	1/1	0.94	0.44	-	77,77,77,77	0
86	OHX	1	3563	7/7	0.95	0.21	-	93,95,98,115	7
87	MG	5	3851	1/1	0.95	0.41	-	34,34,34,34	0
86	OHX	2	1934	7/7	0.95	0.16	-	97,98,99,115	7
86	OHX	5	3572	7/7	0.89	0.32	-	61,63,65,101	7
87	MG	1	3966	1/1	0.85	0.52	-	50,50,50,50	0
87	MG	5	3923	1/1	0.94	0.40	-	36,36,36,36	0
87	MG	2	2100	1/1	0.81	0.56	-	68,68,68,68	0
87	MG	5	3772	1/1	0.89	0.39	-	41,41,41,41	1
87	MG	1	3794	1/1	0.83	0.43	-	61,61,61,61	0
87	MG	5	3839	1/1	0.95	0.70	-	42,42,42,42	0
87	MG	5	3740	1/1	0.84	0.35	-	40,40,40,40	0
86	OHX	1	3574	7/7	0.91	0.17	-	101,103,104,129	7
87	MG	1	4012	1/1	0.93	0.43	-	48,48,48,48	0
87	MG	5	4016	1/1	0.97	0.39	-	29,29,29,29	0
87	MG	5	3932	1/1	0.94	0.20	-	52,52,52,52	0
87	MG	1	3920	1/1	0.89	0.28	-	44,44,44,44	0
87	MG	5	3892	1/1	0.96	0.59	-	40,40,40,40	0
86	OHX	5	3672	7/7	0.92	0.18	-	66,66,67,96	7
87	MG	5	3854	1/1	0.92	0.35	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3815	1/1	0.96	0.54	-	36,36,36,36	0
87	MG	5	4075	1/1	0.96	0.81	-	42,42,42,42	0
86	OHX	1	3451	7/7	0.97	0.17	-	60,62,67,86	7
87	MG	1	4056	1/1	0.97	0.27	-	43,43,43,43	0
87	MG	1	3767	1/1	0.76	0.73	-	59,59,59,59	0
86	OHX	1	3469	7/7	0.98	0.17	-	62,65,69,89	7
87	MG	5	4033	1/1	0.97	0.22	-	45,45,45,45	0
86	OHX	5	3505	7/7	0.95	0.21	-	78,79,83,110	7
86	OHX	5	3676	7/7	0.93	0.20	-	83,84,85,114	7
87	MG	1	3900	1/1	0.98	0.30	-	39,39,39,39	0
87	MG	4	219	1/1	0.92	0.66	-	59,59,59,59	0
86	OHX	5	3560	7/7	0.98	0.14	-	57,59,60,79	7
87	MG	1	3950	1/1	0.85	0.14	-	61,61,61,61	0
87	MG	5	3869	1/1	0.78	0.45	-	47,47,47,47	0
87	MG	1	3804	1/1	0.98	0.59	-	32,32,32,32	0
86	OHX	6	2004	7/7	0.87	0.17	-	96,97,99,128	7
87	MG	1	3918	1/1	0.75	0.58	-	58,58,58,58	0
86	OHX	5	3435	7/7	0.99	0.22	-	48,49,53,79	7
87	MG	2	2044	1/1	0.95	0.47	-	47,47,47,47	0
86	OHX	1	3407	7/7	0.99	0.15	-	61,66,69,75	0
86	OHX	2	1929	7/7	0.97	0.15	-	69,71,74,86	7
87	MG	M5	303	1/1	0.87	0.25	-	49,49,49,49	0
87	MG	5	3760	1/1	0.79	0.29	-	42,42,42,42	0
87	MG	5	3989	1/1	0.86	0.37	-	40,40,40,40	0
87	MG	6	2067	1/1	0.79	0.72	-	65,65,65,65	0
87	MG	1	3874	1/1	0.93	0.53	-	36,36,36,36	0
87	MG	1	3723	1/1	0.92	0.47	-	51,51,51,51	0
87	MG	2	2109	1/1	0.96	0.58	-	57,57,57,57	0
87	MG	1	3994	1/1	0.78	0.38	-	58,58,58,58	0
87	MG	5	3965	1/1	0.92	0.29	-	48,48,48,48	0
87	MG	1	3984	1/1	0.93	0.28	-	43,43,43,43	0
87	MG	1	3986	1/1	0.48	0.52	-	93,93,93,93	0
87	MG	M5	302	1/1	0.98	0.47	-	41,41,41,41	0
86	OHX	5	3565	7/7	0.97	0.09	-	124,125,127,141	7
87	MG	5	4008	1/1	0.81	0.29	-	52,52,52,52	0
86	OHX	6	1916	7/7	0.99	0.17	-	62,62,65,81	7
87	MG	1	3798	1/1	0.95	0.35	-	38,38,38,38	0
87	MG	1	3735	1/1	0.98	0.20	-	46,46,46,46	0
87	MG	5	4003	1/1	0.95	0.57	-	43,43,43,43	0
87	MG	1	3974	1/1	0.93	0.45	-	58,58,58,58	0
87	MG	5	3880	1/1	0.97	0.76	-	40,40,40,40	0
86	OHX	1	3702	7/7	0.88	0.21	-	94,95,96,121	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	MG	6	2045	1/1	0.72	0.36	-	52,52,52,52	0
87	MG	1	3730	1/1	0.94	0.70	-	42,42,42,42	0
86	OHX	2	2027	7/7	0.70	0.49	-	72,73,74,103	7
87	MG	1	3855	1/1	0.87	0.51	-	47,47,47,47	0
87	MG	1	3976	1/1	0.90	0.18	-	51,51,51,51	0
87	MG	1	4018	1/1	0.93	0.29	-	54,54,54,54	0
87	MG	M3	202	1/1	0.88	0.40	-	38,38,38,38	0
86	OHX	8	208	7/7	0.96	0.13	-	89,89,90,115	7
86	OHX	1	3525	7/7	0.97	0.16	-	80,81,84,112	7
87	MG	6	2056	1/1	0.76	0.92	-	64,64,64,64	0
86	OHX	1	3698	7/7	0.87	0.12	-	168,168,168,180	7
87	MG	4	231	1/1	0.76	0.32	-	50,50,50,50	0
87	MG	1	3814	1/1	0.95	0.56	-	29,29,29,29	0
86	OHX	1	3610	7/7	0.93	0.16	-	84,85,86,112	7
87	MG	6	2059	1/1	0.96	0.27	-	67,67,67,67	0
86	OHX	5	3583	7/7	0.97	0.26	-	48,49,50,65	7
87	MG	1	4022	1/1	0.88	0.19	-	53,53,53,53	0
87	MG	l3	403	1/1	0.94	0.43	-	28,28,28,28	0
87	MG	1	3973	1/1	0.78	0.14	-	57,57,57,57	0
87	MG	2	2048	1/1	0.93	0.53	-	57,57,57,57	0
87	MG	5	4095	1/1	0.91	0.21	-	77,77,77,77	0
87	MG	2	2093	1/1	0.88	0.72	-	61,61,61,61	0
87	MG	6	2057	1/1	0.90	0.47	-	48,48,48,48	0
86	OHX	1	3497	7/7	0.98	0.19	-	83,85,87,105	7
87	MG	5	3870	1/1	0.90	0.81	-	50,50,50,50	0
87	MG	5	3943	1/1	0.76	0.40	-	84,84,84,84	0
87	MG	1	4036	1/1	0.80	0.55	-	54,54,54,54	0
87	MG	5	3748	1/1	0.83	0.22	-	47,47,47,47	0
87	MG	1	4039	1/1	0.87	0.22	-	55,55,55,55	0
86	OHX	6	2030	7/7	0.84	0.38	-	68,69,70,102	7
87	MG	5	4021	1/1	0.88	0.27	-	44,44,44,44	0
87	MG	5	4077	1/1	0.95	0.12	-	39,39,39,39	0
87	MG	1	3773	1/1	0.98	0.39	-	46,46,46,46	0
87	MG	1	3911	1/1	0.96	0.22	-	41,41,41,41	1
86	OHX	5	3702	7/7	0.89	0.21	-	79,80,80,110	7
87	MG	1	3996	1/1	0.87	0.28	-	47,47,47,47	0
87	MG	1	3942	1/1	0.86	0.45	-	47,47,47,47	0
87	MG	7	220	1/1	0.88	0.27	-	56,56,56,56	0
87	MG	5	3821	1/1	0.98	0.23	-	48,48,48,48	0
87	MG	M9	202	1/1	0.81	0.21	-	79,79,79,79	0
86	OHX	6	2031	7/7	0.93	0.18	-	81,82,83,108	7
86	OHX	5	3489	7/7	0.96	0.18	-	95,96,99,122	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	2086	1/1	0.91	0.54	-	67,67,67,67	0
87	MG	6	2131	1/1	0.82	0.69	-	60,60,60,60	0
86	OHX	1	3612	7/7	0.98	0.15	-	62,63,64,83	7
86	OHX	6	1905	7/7	0.98	0.19	-	74,77,79,87	7
86	OHX	2	1953	7/7	0.89	0.20	-	85,86,88,118	7
87	MG	5	3975	1/1	0.89	0.24	-	42,42,42,42	0
87	MG	1	3845	1/1	0.77	0.23	-	73,73,73,73	0
86	OHX	1	3600	7/7	0.97	0.11	-	124,124,125,147	7
87	MG	1	3894	1/1	0.94	0.68	-	41,41,41,41	0
87	MG	12	301	1/1	0.87	0.91	-	53,53,53,53	0
87	MG	1	3783	1/1	0.94	0.35	-	66,66,66,66	0
87	MG	5	3835	1/1	0.97	0.37	-	41,41,41,41	0
86	OHX	5	3571	7/7	0.92	0.16	-	71,73,75,105	7
87	MG	5	3940	1/1	0.95	0.45	-	42,42,42,42	0
86	OHX	1	3499	7/7	0.98	0.17	-	58,59,63,83	7
87	MG	1	4044	1/1	0.82	0.65	-	57,57,57,57	0
87	MG	3	214	1/1	0.91	0.44	-	75,75,75,75	0
86	OHX	2	1991	7/7	0.93	0.17	-	111,112,112,136	7
87	MG	5	3768	1/1	0.96	0.21	-	39,39,39,39	0
87	MG	5	3799	1/1	0.95	0.48	-	46,46,46,46	0
87	MG	1	3776	1/1	0.91	0.57	-	54,54,54,54	0
86	OHX	2	1994	7/7	0.96	0.14	-	89,90,91,113	7
86	OHX	1	3595	7/7	0.96	0.12	-	125,127,128,150	7
86	OHX	1	3706	7/7	0.92	0.25	-	51,52,54,82	7
87	MG	1	3988	1/1	0.95	0.23	-	39,39,39,39	0
86	OHX	4	205	7/7	0.98	0.23	-	61,63,64,91	7
87	MG	5	3867	1/1	0.96	0.51	-	55,55,55,55	0
87	MG	1	4027	1/1	0.94	0.16	-	53,53,53,53	0
86	OHX	5	3624	7/7	0.96	0.13	-	90,91,92,112	7
87	MG	5	3812	1/1	0.85	0.15	-	51,51,51,51	0
86	OHX	6	2028	7/7	0.95	0.16	-	74,76,76,101	7
87	MG	1	4050	1/1	0.66	0.62	-	55,55,55,55	0
87	MG	4	226	1/1	0.95	0.15	-	57,57,57,57	0
87	MG	5	4034	1/1	0.92	0.19	-	38,38,38,38	0
86	OHX	1	3446	7/7	0.98	0.16	-	78,81,85,98	0
86	OHX	2	1906	7/7	0.98	0.22	-	92,93,98,110	0
86	OHX	5	3466	7/7	0.98	0.16	-	95,96,98,108	0
86	OHX	1	3507	7/7	0.98	0.15	-	79,79,82,95	7
86	OHX	6	1983	7/7	0.94	0.16	-	89,90,92,122	7
87	MG	5	3978	1/1	0.87	0.22	-	39,39,39,39	0
86	OHX	6	1926	7/7	0.97	0.15	-	96,100,101,114	7
87	MG	6	2051	1/1	0.87	0.42	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	1980	7/7	0.95	0.28	-	81,81,82,106	7
87	MG	1	4023	1/1	0.56	0.18	-	59,59,59,59	0
87	MG	5	3956	1/1	0.92	0.31	-	61,61,61,61	0
87	MG	1	3889	1/1	0.87	0.75	-	45,45,45,45	0
87	MG	7	216	1/1	0.97	0.37	-	37,37,37,37	0
87	MG	1	3788	1/1	0.93	0.37	-	54,54,54,54	0
87	MG	1	3969	1/1	0.87	0.43	-	57,57,57,57	0
87	MG	4	222	1/1	0.95	0.24	-	43,43,43,43	0
87	MG	2	2050	1/1	0.74	0.67	-	67,67,67,67	0
86	OHX	5	3567	7/7	0.98	0.17	-	68,69,71,99	7
87	MG	6	2117	1/1	0.90	0.57	-	69,69,69,69	0
87	MG	M7	204	1/1	0.87	0.41	-	42,42,42,42	0
87	MG	5	3838	1/1	0.82	0.38	-	42,42,42,42	0
87	MG	1	3833	1/1	0.97	0.42	-	38,38,38,38	0
87	MG	1	3982	1/1	0.78	0.40	-	56,56,56,56	0
87	MG	3	211	1/1	0.91	0.35	-	78,78,78,78	0
87	MG	5	4070	1/1	0.91	0.15	-	45,45,45,45	0
87	MG	6	2125	1/1	0.91	0.25	-	69,69,69,69	0
87	MG	1	3801	1/1	0.90	0.56	-	74,74,74,74	0
86	OHX	5	3723	7/7	0.93	0.30	-	95,95,95,117	7
87	MG	5	3776	1/1	0.95	0.77	-	50,50,50,50	0
87	MG	2	2029	1/1	0.94	0.50	-	81,81,81,81	0
86	OHX	5	3627	7/7	0.97	0.25	-	57,58,59,90	7
87	MG	5	4081	1/1	0.96	0.53	-	44,44,44,44	0
87	MG	5	4039	1/1	0.81	0.44	-	45,45,45,45	0
86	OHX	1	3628	7/7	0.92	0.14	-	93,95,97,122	7
87	MG	5	3792	1/1	0.93	0.35	-	53,53,53,53	0
87	MG	5	4079	1/1	0.94	0.38	-	45,45,45,45	0
87	MG	1	4048	1/1	0.92	0.56	-	59,59,59,59	0
87	MG	8	201	1/1	0.95	0.18	-	46,46,46,46	0
87	MG	8	220	1/1	0.98	0.66	-	44,44,44,44	0
87	MG	5	4068	1/1	0.85	0.63	-	61,61,61,61	0
86	OHX	5	3625	7/7	0.92	0.12	-	102,102,104,128	7
87	MG	5	3973	1/1	0.92	0.33	-	48,48,48,48	0
86	OHX	1	3597	7/7	0.93	0.24	-	59,60,63,92	7
86	OHX	5	3712	7/7	0.90	0.25	-	94,95,95,113	7
87	MG	5	3888	1/1	0.97	0.49	-	26,26,26,26	0
87	MG	1	4038	1/1	0.93	0.45	-	41,41,41,41	0
87	MG	3	215	1/1	0.73	0.56	-	62,62,62,62	0
87	MG	6	2043	1/1	0.97	0.41	-	47,47,47,47	0
87	MG	7	213	1/1	0.82	0.44	-	27,27,27,27	0
87	MG	12	302	1/1	0.81	0.38	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	2	2083	1/1	0.78	0.57	-	98,98,98,98	0
86	OHX	2	1965	7/7	0.93	0.17	-	92,93,94,124	7
86	OHX	1	3604	7/7	0.88	0.29	-	54,56,56,93	7
86	OHX	5	3697	7/7	0.91	0.18	-	111,111,112,137	7
87	MG	1	3954	1/1	0.85	0.36	-	54,54,54,54	0
87	MG	5	3930	1/1	0.94	0.33	-	49,49,49,49	0
87	MG	5	3751	1/1	0.96	0.27	-	32,32,32,32	0
86	OHX	5	3469	7/7	0.98	0.18	-	62,63,66,75	7
87	MG	6	2123	1/1	0.83	0.16	-	62,62,62,62	0
87	MG	2	2061	1/1	0.95	0.57	-	59,59,59,59	0
87	MG	5	3856	1/1	0.95	0.25	-	50,50,50,50	0
87	MG	5	3820	1/1	0.94	0.42	-	42,42,42,42	0
86	OHX	1	3477	7/7	0.95	0.13	-	96,98,104,122	7
87	MG	1	3983	1/1	0.94	0.23	-	41,41,41,41	0
86	OHX	1	3506	7/7	0.97	0.17	-	103,104,108,129	7
87	MG	1	3787	1/1	0.98	0.53	-	54,54,54,54	0
87	MG	5	3993	1/1	0.94	0.20	-	88,88,88,88	0
87	MG	1	3846	1/1	0.92	0.32	-	53,53,53,53	0
86	OHX	6	2012	7/7	0.96	0.22	-	66,66,67,88	7
87	MG	1	3771	1/1	0.90	0.38	-	33,33,33,33	0
87	MG	5	3853	1/1	0.98	0.61	-	40,40,40,40	0
86	OHX	5	3512	7/7	0.99	0.19	-	65,66,70,89	7
86	OHX	5	3527	7/7	0.95	0.16	-	69,74,75,104	7
87	MG	5	4059	1/1	0.75	0.34	-	47,47,47,47	1
87	MG	5	3868	1/1	0.98	0.63	-	41,41,41,41	0
86	OHX	1	3546	7/7	0.97	0.17	-	69,70,70,95	7
87	MG	5	3873	1/1	0.92	0.73	-	46,46,46,46	0
87	MG	1	3736	1/1	0.85	0.45	-	44,44,44,44	0
86	OHX	6	2010	7/7	0.95	0.24	-	58,58,59,88	7
86	OHX	5	3445	7/7	0.98	0.13	-	78,79,86,98	7
87	MG	5	3916	1/1	0.89	0.12	-	46,46,46,46	0
86	OHX	5	3711	7/7	0.94	0.27	-	67,70,71,97	7
87	MG	5	4100	1/1	0.91	0.30	-	41,41,41,41	0
87	MG	5	3831	1/1	0.97	0.25	-	47,47,47,47	0
86	OHX	5	3623	7/7	0.94	0.12	-	83,85,86,117	7
87	MG	2	2059	1/1	0.91	0.51	-	63,63,63,63	0
87	MG	1	3741	1/1	0.93	0.44	-	49,49,49,49	0
87	MG	1	3768	1/1	0.99	0.58	-	40,40,40,40	0
86	OHX	5	3587	7/7	0.96	0.24	-	59,60,61,91	7
87	MG	1	3978	1/1	0.93	0.41	-	41,41,41,41	0
86	OHX	5	3447	7/7	0.97	0.18	-	44,46,52,76	7
87	MG	6	2054	1/1	0.77	0.47	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	1941	7/7	0.96	0.19	-	72,72,76,96	7
87	MG	1	3933	1/1	0.90	0.22	-	49,49,49,49	0
87	MG	1	3901	1/1	0.82	0.17	-	46,46,46,46	0
86	OHX	2	2023	7/7	0.88	0.31	-	76,77,79,101	7
87	MG	1	4047	1/1	0.83	0.46	-	59,59,59,59	0
87	MG	5	4041	1/1	0.91	0.37	-	66,66,66,66	0
87	MG	1	3928	1/1	0.93	0.20	-	46,46,46,46	0
87	MG	5	3866	1/1	0.93	0.66	-	48,48,48,48	0
87	MG	5	3898	1/1	0.91	0.41	-	39,39,39,39	0
87	MG	1	3836	1/1	0.96	0.50	-	48,48,48,48	0
87	MG	1	3720	1/1	0.95	0.45	-	42,42,42,42	0
87	MG	1	3924	1/1	0.86	0.19	-	61,61,61,61	0
87	MG	2	2032	1/1	0.38	0.34	-	77,77,77,77	0
87	MG	1	3844	1/1	0.96	0.53	-	54,54,54,54	0
87	MG	6	2126	1/1	0.89	0.51	-	63,63,63,63	0
87	MG	5	4024	1/1	0.79	0.19	-	55,55,55,55	0
87	MG	1	4053	1/1	0.91	0.20	-	64,64,64,64	0
87	MG	5	4032	1/1	0.92	0.39	-	40,40,40,40	0
86	OHX	6	1975	7/7	0.95	0.22	-	105,106,106,128	7
86	OHX	1	3459	7/7	0.99	0.22	-	57,61,62,77	7
86	OHX	2	1926	7/7	0.99	0.12	-	85,87,88,100	7
87	MG	1	3831	1/1	0.95	0.30	-	51,51,51,51	0
87	MG	1	3752	1/1	0.76	0.26	-	68,68,68,68	0
86	OHX	6	1987	7/7	0.94	0.30	-	68,69,70,97	7
86	OHX	1	3562	7/7	0.94	0.15	-	96,98,99,118	7
87	MG	5	3789	1/1	0.94	0.25	-	33,33,33,33	0
86	OHX	1	3457	7/7	0.97	0.30	-	52,56,59,79	7
87	MG	1	3979	1/1	0.83	0.23	-	54,54,54,54	0
87	MG	1	3917	1/1	0.95	0.55	-	43,43,43,43	0
87	MG	1	4021	1/1	0.64	0.37	-	43,43,43,43	1
86	OHX	6	1931	7/7	0.98	0.17	-	70,72,75,96	7
87	MG	2	2094	1/1	0.91	0.38	-	74,74,74,74	0
87	MG	1	3951	1/1	0.66	0.33	-	51,51,51,51	0
87	MG	1	3853	1/1	0.70	0.52	-	35,35,35,35	0
87	MG	1	3977	1/1	0.69	0.39	-	79,79,79,79	0
87	MG	5	3992	1/1	0.95	0.20	-	50,50,50,50	0
86	OHX	2	1939	7/7	0.98	0.15	-	98,99,100,120	7
87	MG	5	3997	1/1	0.93	0.53	-	51,51,51,51	0
86	OHX	1	3607	7/7	0.93	0.13	-	97,97,100,127	7
87	MG	5	3953	1/1	0.94	0.26	-	57,57,57,57	0
86	OHX	c3	201	7/7	0.89	0.19	-	102,103,104,130	7
87	MG	2	2103	1/1	0.79	0.28	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3864	1/1	0.92	0.36	-	49,49,49,49	0
87	MG	5	4082	1/1	0.85	0.28	-	48,48,48,48	0
87	MG	2	2067	1/1	0.90	0.20	-	71,71,71,71	0
86	OHX	5	3707	7/7	0.92	0.36	-	63,64,66,96	7
87	MG	2	2105	1/1	0.89	0.79	-	57,57,57,57	0
86	OHX	1	3666	7/7	0.92	0.25	-	67,69,72,97	7
86	OHX	1	3670	7/7	0.94	0.19	-	117,118,119,142	7
87	MG	2	2045	1/1	0.89	0.56	-	50,50,50,50	0
86	OHX	1	3571	7/7	0.98	0.18	-	121,121,122,139	7
86	OHX	1	3672	7/7	0.94	0.16	-	74,74,75,99	7
87	MG	O7	102	1/1	0.92	0.41	-	61,61,61,61	0
86	OHX	5	3705	7/7	0.91	0.30	-	62,62,63,90	7
87	MG	1	4062	1/1	0.65	0.23	-	56,56,56,56	0
87	MG	5	3947	1/1	0.90	0.90	-	52,52,52,52	0
87	MG	1	3956	1/1	0.86	0.90	-	69,69,69,69	0
87	MG	1	3859	1/1	0.98	0.54	-	33,33,33,33	0
87	MG	5	3968	1/1	0.91	0.29	-	34,34,34,34	0
87	MG	5	4023	1/1	0.92	0.49	-	44,44,44,44	0
87	MG	4	232	1/1	0.89	0.67	-	59,59,59,59	0
87	MG	5	3931	1/1	0.93	0.44	-	44,44,44,44	0
86	OHX	5	3596	7/7	0.95	0.18	-	68,70,72,98	7
86	OHX	2	1995	7/7	0.91	0.28	-	75,76,78,101	7
86	OHX	6	1955	7/7	0.94	0.12	-	169,169,170,177	7
86	OHX	1	3511	7/7	0.97	0.17	-	88,90,93,110	7
87	MG	1	3737	1/1	0.92	0.28	-	60,60,60,60	0
87	MG	1	3961	1/1	0.84	0.26	-	63,63,63,63	0
87	MG	6	2093	1/1	0.91	0.46	-	46,46,46,46	0
87	MG	5	4015	1/1	0.93	0.20	-	60,60,60,60	0
86	OHX	5	3701	7/7	0.93	0.18	-	83,83,84,113	7
86	OHX	1	3582	7/7	0.95	0.19	-	51,52,56,80	7
86	OHX	1	3687	7/7	0.93	0.17	-	72,72,74,100	7
87	MG	5	3803	1/1	0.80	0.22	-	53,53,53,53	0
87	MG	1	3923	1/1	0.74	0.13	-	69,69,69,69	0
87	MG	2	2097	1/1	0.79	0.50	-	65,65,65,65	0
87	MG	5	3877	1/1	0.98	0.50	-	37,37,37,37	0
87	MG	5	3845	1/1	0.99	0.75	-	41,41,41,41	0
87	MG	1	4031	1/1	0.95	0.27	-	96,96,96,96	0
87	MG	5	4064	1/1	0.94	0.47	-	61,61,61,61	0
86	OHX	1	3565	7/7	0.95	0.14	-	75,76,77,108	7
87	MG	5	3933	1/1	0.89	0.92	-	60,60,60,60	0
86	OHX	6	1963	7/7	0.98	0.21	-	83,83,84,109	7
87	MG	6	2094	1/1	0.90	0.25	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	MG	5	3781	1/1	0.97	0.56	-	39,39,39,39	0
86	OHX	2	1969	7/7	0.97	0.09	-	133,134,134,153	7
86	OHX	4	209	7/7	0.96	0.16	-	59,62,64,92	7
86	OHX	6	1967	7/7	0.98	0.19	-	56,57,59,80	7
86	OHX	5	3546	7/7	0.98	0.12	-	70,71,73,96	7
87	MG	5	3964	1/1	0.89	0.68	-	49,49,49,49	0
87	MG	1	4008	1/1	0.93	0.54	-	50,50,50,50	0
87	MG	1	3765	1/1	0.95	0.38	-	35,35,35,35	0
87	MG	5	3919	1/1	0.77	0.55	-	46,46,46,46	0
87	MG	2	2072	1/1	0.70	0.50	-	99,99,99,99	0
87	MG	5	3766	1/1	0.98	0.42	-	43,43,43,43	0
87	MG	n8	202	1/1	0.80	0.29	-	51,51,51,51	0
87	MG	5	3857	1/1	0.95	0.44	-	31,31,31,31	0
87	MG	1	3921	1/1	0.95	0.44	-	69,69,69,69	0
87	MG	5	3903	1/1	0.92	0.34	-	30,30,30,30	0
87	MG	5	4103	1/1	0.90	0.31	-	49,49,49,49	0
87	MG	2	2047	1/1	0.70	0.51	-	61,61,61,61	0
86	OHX	5	3568	7/7	0.94	0.14	-	78,79,80,116	7
87	MG	6	2073	1/1	0.87	0.53	-	94,94,94,94	0
86	OHX	5	3433	7/7	0.98	0.17	-	48,50,55,73	7
87	MG	L7	303	1/1	0.85	0.19	-	48,48,48,48	0
87	MG	5	3725	1/1	0.96	0.54	-	40,40,40,40	0
86	OHX	6	1984	7/7	0.93	0.16	-	100,102,102,129	7
86	OHX	6	2014	7/7	0.90	0.27	-	94,95,97,120	7
87	MG	5	3995	1/1	0.83	0.39	-	53,53,53,53	0
87	MG	5	3970	1/1	0.99	0.55	-	51,51,51,51	0
86	OHX	1	3455	7/7	0.97	0.14	-	76,78,82,100	7
87	MG	6	2098	1/1	0.93	0.21	-	87,87,87,87	0
87	MG	1	3766	1/1	0.94	0.38	-	43,43,43,43	0
87	MG	1	3715	1/1	0.98	0.35	-	45,45,45,45	0
87	MG	5	4096	1/1	0.61	0.21	-	73,73,73,73	0

6.5 Other polymers

There are no such residues in this entry.