



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 18, 2016 – 06:56 AM EDT

PDB ID : 5DAT
Title : Complex of yeast 80S ribosome with hypusine-containing eIF5A
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.;
Dever, T.E.; Yusupov, M.
Deposited on : 2015-08-20
Resolution : 3.15 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20027939

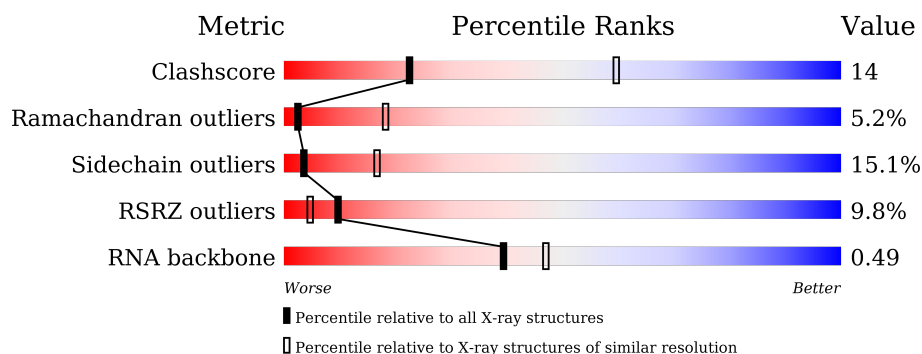
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)
RNA backbone	2183	1046 (3.62-2.70)

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>9%</div> <div>36%</div> <div>47%</div> <div>15%</div> <div>..</div> </div>
1	6	1800	<div> <div>5%</div> <div>42%</div> <div>43%</div> <div>14%</div> <div>.</div> </div>
2	S0	251	<div> <div>17%</div> <div>24%</div> <div>47%</div> <div>11%</div> <div>18%</div> </div>
2	s0	251	<div> <div>7%</div> <div>69%</div> <div>13%</div> <div>18%</div> </div>
3	S1	254	<div> <div>13%</div> <div>22%</div> <div>50%</div> <div>12%</div> <div>16%</div> </div>
3	s1	254	<div> <div>5%</div> <div>66%</div> <div>19%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	124	
14	c2	124	
15	C3	150	
15	c3	150	
16	C4	136	

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Mol	Chain	Length	Quality of chain
16	c4	136	
17	C5	137	
17	c5	137	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	

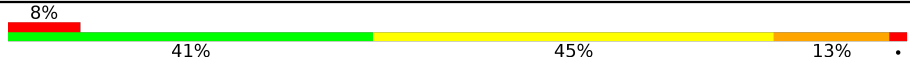



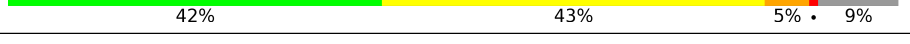
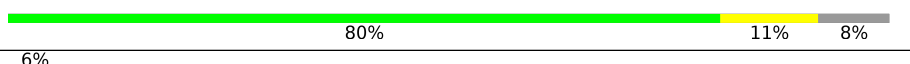
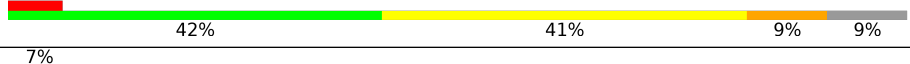

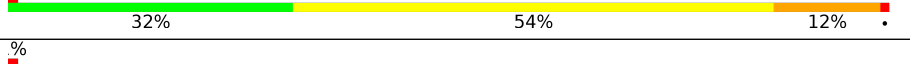


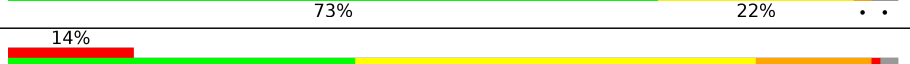
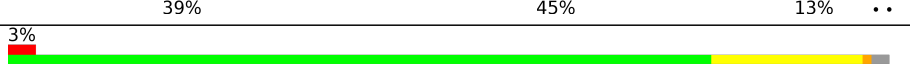
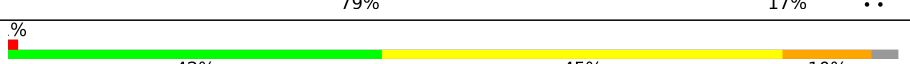

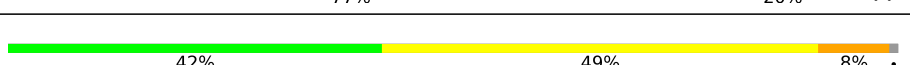
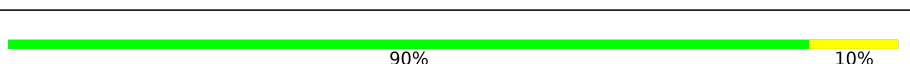
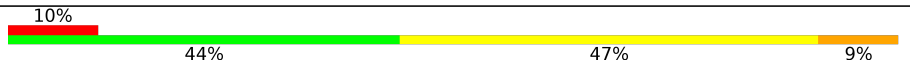
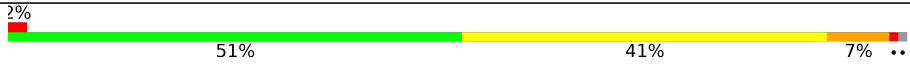


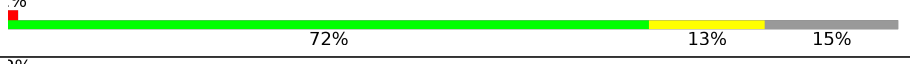



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Mol	Chain	Length	Quality of chain
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	

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Mol	Chain	Length	Quality of chain
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	204	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	

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Mol	Chain	Length	Quality of chain
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
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	104	
66	o0	104	
67	O1	112	

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Mol	Chain	Length	Quality of chain
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	

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Mol	Chain	Length	Quality of chain
80	d2	130	
81	m2	150	
82	m5	203	
83	p0	220	
84	p1	47	
84	p2	47	
85	f	157	
86	l1	213	

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
85	5CT	f	51	X	-	-	-
87	MG	1	3401	-	-	-	X
87	MG	1	3408	-	-	-	X
87	MG	1	3410	-	-	-	X
87	MG	1	3415	-	-	-	X
87	MG	1	3416	-	-	-	X
87	MG	1	3418	-	-	-	X
87	MG	1	3422	-	-	-	X
87	MG	1	3433	-	-	-	X
87	MG	1	3441	-	-	-	X
87	MG	1	3449	-	-	-	X
87	MG	1	3455	-	-	-	X
87	MG	1	3465	-	-	-	X
87	MG	1	3474	-	-	-	X
87	MG	1	3479	-	-	-	X
87	MG	1	3485	-	-	-	X
87	MG	1	3492	-	-	-	X
87	MG	1	3493	-	-	-	X
87	MG	1	3495	-	-	-	X
87	MG	1	3497	-	-	-	X
87	MG	1	3503	-	-	-	X
87	MG	1	3507	-	-	-	X
87	MG	1	3511	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	3512	-	-	-	X
87	MG	1	3513	-	-	-	X
87	MG	1	3523	-	-	-	X
87	MG	1	3525	-	-	-	X
87	MG	1	3527	-	-	-	X
87	MG	1	3534	-	-	-	X
87	MG	1	3535	-	-	-	X
87	MG	1	3536	-	-	-	X
87	MG	1	3541	-	-	-	X
87	MG	1	3547	-	-	-	X
87	MG	1	3550	-	-	-	X
87	MG	1	3552	-	-	-	X
87	MG	1	3554	-	-	-	X
87	MG	1	3556	-	-	-	X
87	MG	1	3557	-	-	-	X
87	MG	1	3559	-	-	-	X
87	MG	1	3567	-	-	-	X
87	MG	1	3568	-	-	-	X
87	MG	1	3570	-	-	-	X
87	MG	1	3571	-	-	-	X
87	MG	1	3573	-	-	-	X
87	MG	1	3575	-	-	-	X
87	MG	1	3577	-	-	-	X
87	MG	1	3578	-	-	-	X
87	MG	1	3580	-	-	-	X
87	MG	1	3584	-	-	-	X
87	MG	1	3590	-	-	-	X
87	MG	1	3623	-	-	-	X
87	MG	1	3642	-	-	-	X
87	MG	1	3667	-	-	-	X
87	MG	1	3670	-	-	-	X
87	MG	1	3673	-	-	-	X
87	MG	1	3674	-	-	-	X
87	MG	1	3683	-	-	-	X
87	MG	1	3686	-	-	-	X
87	MG	1	3687	-	-	-	X
87	MG	1	3692	-	-	-	X
87	MG	1	3701	-	-	-	X
87	MG	1	3706	-	-	-	X
87	MG	1	3707	-	-	-	X
87	MG	1	3731	-	-	-	X
87	MG	1	3732	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	1	3733	-	-	-	X
87	MG	1	3735	-	-	-	X
87	MG	1	3748	-	-	-	X
87	MG	1	4111	-	-	-	X
87	MG	1	4112	-	-	-	X
87	MG	1	4113	-	-	-	X
87	MG	2	1956	-	-	-	X
87	MG	2	1973	-	-	-	X
87	MG	3	220	-	-	-	X
87	MG	4	206	-	-	-	X
87	MG	4	215	-	-	-	X
87	MG	4	236	-	-	-	X
87	MG	5	3402	-	-	-	X
87	MG	5	3405	-	-	-	X
87	MG	5	3407	-	-	-	X
87	MG	5	3410	-	-	-	X
87	MG	5	3412	-	-	-	X
87	MG	5	3413	-	-	-	X
87	MG	5	3414	-	-	-	X
87	MG	5	3419	-	-	-	X
87	MG	5	3426	-	-	-	X
87	MG	5	3429	-	-	-	X
87	MG	5	3431	-	-	-	X
87	MG	5	3445	-	-	-	X
87	MG	5	3448	-	-	-	X
87	MG	5	3457	-	-	-	X
87	MG	5	3464	-	-	-	X
87	MG	5	3469	-	-	-	X
87	MG	5	3475	-	-	-	X
87	MG	5	3497	-	-	-	X
87	MG	5	3498	-	-	-	X
87	MG	5	3501	-	-	-	X
87	MG	5	3504	-	-	-	X
87	MG	5	3508	-	-	-	X
87	MG	5	3510	-	-	-	X
87	MG	5	3511	-	-	-	X
87	MG	5	3514	-	-	-	X
87	MG	5	3516	-	-	-	X
87	MG	5	3520	-	-	-	X
87	MG	5	3524	-	-	-	X
87	MG	5	3529	-	-	-	X
87	MG	5	3533	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	5	3540	-	-	-	X
87	MG	5	3544	-	-	-	X
87	MG	5	3546	-	-	-	X
87	MG	5	3547	-	-	-	X
87	MG	5	3549	-	-	-	X
87	MG	5	3556	-	-	-	X
87	MG	5	3561	-	-	-	X
87	MG	5	3562	-	-	-	X
87	MG	5	3564	-	-	-	X
87	MG	5	3565	-	-	-	X
87	MG	5	3570	-	-	-	X
87	MG	5	3571	-	-	-	X
87	MG	5	3578	-	-	-	X
87	MG	5	3582	-	-	-	X
87	MG	5	3583	-	-	-	X
87	MG	5	3585	-	-	-	X
87	MG	5	3587	-	-	-	X
87	MG	5	3589	-	-	-	X
87	MG	5	3590	-	-	-	X
87	MG	5	3591	-	-	-	X
87	MG	5	3592	-	-	-	X
87	MG	5	3593	-	-	-	X
87	MG	5	3594	-	-	-	X
87	MG	5	3595	-	-	-	X
87	MG	5	3600	-	-	-	X
87	MG	5	3630	-	-	-	X
87	MG	5	3633	-	-	-	X
87	MG	5	3635	-	-	-	X
87	MG	5	3665	-	-	-	X
87	MG	5	3670	-	-	-	X
87	MG	5	3714	-	-	-	X
87	MG	5	3715	-	-	-	X
87	MG	5	3720	-	-	-	X
87	MG	5	3731	-	-	-	X
87	MG	5	3751	-	-	-	X
87	MG	5	3761	-	-	-	X
87	MG	5	3767	-	-	-	X
87	MG	5	3769	-	-	-	X
87	MG	5	4162	-	-	-	X
87	MG	5	4165	-	-	-	X
87	MG	6	1908	-	-	-	X
87	MG	6	1915	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	6	1918	-	-	-	X
87	MG	6	1922	-	-	-	X
87	MG	6	1925	-	-	-	X
87	MG	6	1934	-	-	-	X
87	MG	6	1945	-	-	-	X
87	MG	6	1953	-	-	-	X
87	MG	6	1962	-	-	-	X
87	MG	6	1982	-	-	-	X
87	MG	6	1988	-	-	-	X
87	MG	6	1994	-	-	-	X
87	MG	6	2006	-	-	-	X
87	MG	6	2009	-	-	-	X
87	MG	7	208	-	-	-	X
87	MG	7	215	-	-	-	X
87	MG	7	228	-	-	-	X
87	MG	8	202	-	-	-	X
87	MG	8	204	-	-	-	X
87	MG	M7	202	-	-	-	X
87	MG	N3	201	-	-	-	X
87	MG	O2	201	-	-	-	X
87	MG	O3	201	-	-	-	X
87	MG	O7	104	-	-	-	X
87	MG	l2	303	-	-	-	X
87	MG	l3	401	-	-	-	X
87	MG	m7	201	-	-	-	X
87	MG	n0	202	-	-	-	X
87	MG	n3	201	-	-	-	X
87	MG	o9	101	-	-	-	X
88	OHX	1	3763	-	-	-	X
88	OHX	1	3771	-	-	-	X
88	OHX	1	3781	-	-	-	X
88	OHX	1	3784	-	-	-	X
88	OHX	1	3788	-	-	-	X
88	OHX	1	3793	-	-	-	X
88	OHX	1	3803	-	-	-	X
88	OHX	1	3807	-	-	-	X
88	OHX	1	3810	-	-	-	X
88	OHX	1	3812	-	-	-	X
88	OHX	1	3815	-	-	-	X
88	OHX	1	3820	-	-	-	X
88	OHX	1	3821	-	-	-	X
88	OHX	1	3825	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	OHX	1	3830	-	-	-	X
88	OHX	1	3837	-	-	-	X
88	OHX	1	3839	-	-	-	X
88	OHX	1	3842	-	-	-	X
88	OHX	1	3843	-	-	-	X
88	OHX	1	3846	-	-	-	X
88	OHX	1	3851	-	-	X	-
88	OHX	1	3853	-	-	-	X
88	OHX	1	3856	-	-	-	X
88	OHX	1	3859	-	-	-	X
88	OHX	1	3865	-	-	-	X
88	OHX	1	3866	-	-	-	X
88	OHX	1	3873	-	-	-	X
88	OHX	1	3877	-	-	-	X
88	OHX	1	3882	-	-	-	X
88	OHX	1	3886	-	-	-	X
88	OHX	1	3898	-	-	-	X
88	OHX	1	3899	-	-	-	X
88	OHX	1	3903	-	-	-	X
88	OHX	1	3914	-	-	-	X
88	OHX	1	3918	-	-	-	X
88	OHX	1	3923	-	-	-	X
88	OHX	1	3927	-	-	X	-
88	OHX	1	3939	-	-	X	-
88	OHX	1	3940	-	-	X	-
88	OHX	1	3947	-	-	-	X
88	OHX	1	3950	-	-	-	X
88	OHX	1	3953	-	-	-	X
88	OHX	1	3956	-	-	-	X
88	OHX	1	3968	-	-	-	X
88	OHX	1	3969	-	-	-	X
88	OHX	1	3975	-	-	-	X
88	OHX	1	3984	-	-	-	X
88	OHX	1	3992	-	-	-	X
88	OHX	1	4000	-	-	-	X
88	OHX	1	4001	-	-	X	-
88	OHX	1	4005	-	-	-	X
88	OHX	1	4006	-	-	-	X
88	OHX	1	4007	-	-	-	X
88	OHX	1	4008	-	-	-	X
88	OHX	1	4009	-	-	-	X
88	OHX	1	4010	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	OHX	1	4020	-	-	-	X
88	OHX	1	4022	-	-	-	X
88	OHX	1	4028	-	-	-	X
88	OHX	1	4031	-	-	-	X
88	OHX	1	4033	-	-	-	X
88	OHX	1	4042	-	-	-	X
88	OHX	1	4050	-	-	-	X
88	OHX	1	4051	-	-	-	X
88	OHX	1	4053	-	-	-	X
88	OHX	1	4060	-	-	-	X
88	OHX	1	4061	-	-	-	X
88	OHX	1	4064	-	-	-	X
88	OHX	1	4068	-	-	X	-
88	OHX	1	4069	-	-	-	X
88	OHX	1	4076	-	-	-	X
88	OHX	1	4077	-	-	X	-
88	OHX	1	4081	-	-	-	X
88	OHX	1	4090	-	-	-	X
88	OHX	1	4094	-	-	-	X
88	OHX	1	4097	-	-	-	X
88	OHX	1	4098	-	-	-	X
88	OHX	1	4101	-	-	-	X
88	OHX	1	4103	-	-	-	X
88	OHX	1	4106	-	-	-	X
88	OHX	1	4107	-	-	-	X
88	OHX	2	2010	-	-	-	X
88	OHX	2	2014	-	-	-	X
88	OHX	2	2023	-	-	-	X
88	OHX	2	2061	-	-	X	-
88	OHX	2	2092	-	-	X	-
88	OHX	2	2102	-	-	X	-
88	OHX	2	2118	-	-	-	X
88	OHX	2	2121	-	-	-	X
88	OHX	2	2124	-	-	-	X
88	OHX	2	2133	-	-	X	-
88	OHX	2	2142	-	-	-	X
88	OHX	2	2148	-	-	-	X
88	OHX	2	2150	-	-	X	-
88	OHX	3	211	-	-	-	X
88	OHX	3	215	-	-	-	X
88	OHX	3	219	-	-	-	X
88	OHX	4	222	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	OHX	4	226	-	-	-	X
88	OHX	4	229	-	-	-	X
88	OHX	4	234	-	-	-	X
88	OHX	4	235	-	-	-	X
88	OHX	5	3795	-	-	-	X
88	OHX	5	3800	-	-	-	X
88	OHX	5	3808	-	-	-	X
88	OHX	5	3810	-	-	-	X
88	OHX	5	3811	-	-	-	X
88	OHX	5	3812	-	-	-	X
88	OHX	5	3818	-	-	-	X
88	OHX	5	3826	-	-	-	X
88	OHX	5	3830	-	-	-	X
88	OHX	5	3837	-	-	-	X
88	OHX	5	3838	-	-	-	X
88	OHX	5	3840	-	-	-	X
88	OHX	5	3845	-	-	-	X
88	OHX	5	3846	-	-	-	X
88	OHX	5	3847	-	-	-	X
88	OHX	5	3849	-	-	-	X
88	OHX	5	3852	-	-	X	-
88	OHX	5	3856	-	-	-	X
88	OHX	5	3858	-	-	-	X
88	OHX	5	3861	-	-	-	X
88	OHX	5	3864	-	-	-	X
88	OHX	5	3867	-	-	-	X
88	OHX	5	3875	-	-	-	X
88	OHX	5	3884	-	-	-	X
88	OHX	5	3886	-	-	-	X
88	OHX	5	3887	-	-	-	X
88	OHX	5	3888	-	-	-	X
88	OHX	5	3896	-	-	-	X
88	OHX	5	3898	-	-	-	X
88	OHX	5	3900	-	-	X	-
88	OHX	5	3905	-	-	-	X
88	OHX	5	3911	-	-	-	X
88	OHX	5	3915	-	-	-	X
88	OHX	5	3918	-	-	-	X
88	OHX	5	3920	-	-	-	X
88	OHX	5	3923	-	-	-	X
88	OHX	5	3924	-	-	-	X
88	OHX	5	3931	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	OHX	5	3932	-	-	-	X
88	OHX	5	3939	-	-	-	X
88	OHX	5	3946	-	-	-	X
88	OHX	5	3947	-	-	-	X
88	OHX	5	3951	-	-	X	-
88	OHX	5	3953	-	-	-	X
88	OHX	5	3958	-	-	-	X
88	OHX	5	3959	-	-	-	X
88	OHX	5	3961	-	-	X	-
88	OHX	5	3962	-	-	-	X
88	OHX	5	3969	-	-	-	X
88	OHX	5	3973	-	-	-	X
88	OHX	5	3993	-	-	-	X
88	OHX	5	3995	-	-	-	X
88	OHX	5	3996	-	-	-	X
88	OHX	5	3998	-	-	-	X
88	OHX	5	4005	-	-	-	X
88	OHX	5	4011	-	-	-	X
88	OHX	5	4019	-	-	-	X
88	OHX	5	4024	-	-	-	X
88	OHX	5	4031	-	-	-	X
88	OHX	5	4035	-	-	-	X
88	OHX	5	4038	-	-	-	X
88	OHX	5	4055	-	-	-	X
88	OHX	5	4068	-	-	-	X
88	OHX	5	4069	-	-	-	X
88	OHX	5	4071	-	-	-	X
88	OHX	5	4081	-	-	-	X
88	OHX	5	4088	-	-	-	X
88	OHX	5	4093	-	-	-	X
88	OHX	5	4100	-	-	-	X
88	OHX	5	4103	-	-	-	X
88	OHX	5	4104	-	-	-	X
88	OHX	5	4106	-	-	X	-
88	OHX	5	4109	-	-	-	X
88	OHX	5	4117	-	-	-	X
88	OHX	5	4122	-	-	-	X
88	OHX	5	4126	-	-	X	-
88	OHX	5	4130	-	-	-	X
88	OHX	5	4147	-	-	-	X
88	OHX	5	4152	-	-	-	X
88	OHX	5	4157	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	OHX	6	2021	-	-	-	X
88	OHX	6	2028	-	-	-	X
88	OHX	6	2029	-	-	-	X
88	OHX	6	2040	-	-	X	-
88	OHX	6	2044	-	-	-	X
88	OHX	6	2049	-	-	-	X
88	OHX	6	2051	-	-	-	X
88	OHX	6	2064	-	-	-	X
88	OHX	6	2065	-	-	-	X
88	OHX	6	2067	-	-	X	X
88	OHX	6	2071	-	-	-	X
88	OHX	6	2086	-	-	X	-
88	OHX	6	2088	-	-	-	X
88	OHX	6	2096	-	-	X	-
88	OHX	6	2109	-	-	X	-
88	OHX	6	2114	-	-	-	X
88	OHX	6	2126	-	-	X	-
88	OHX	6	2127	-	-	X	-
88	OHX	6	2138	-	-	-	X
88	OHX	6	2142	-	-	X	-
88	OHX	6	2150	-	-	-	X
88	OHX	6	2154	-	-	-	X
88	OHX	6	2164	-	-	-	X
88	OHX	6	2185	-	-	-	X
88	OHX	7	216	-	-	-	X
88	OHX	7	218	-	-	-	X
88	OHX	7	219	-	-	-	X
88	OHX	7	221	-	-	-	X
88	OHX	7	222	-	-	-	X
88	OHX	7	223	-	-	-	X
88	OHX	8	217	-	-	-	X
88	OHX	8	219	-	-	-	X
88	OHX	8	220	-	-	-	X
88	OHX	8	225	-	-	-	X
88	OHX	8	226	-	-	-	X
88	OHX	8	227	-	-	-	X
88	OHX	C3	201	-	-	X	-
88	OHX	L4	401	-	-	X	-
88	OHX	M7	204	-	-	-	X
88	OHX	O9	101	-	-	-	X
88	OHX	S9	202	-	-	-	X
88	OHX	m0	304	-	-	-	X

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 414393 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	S	0	0	0
			1481	951	265	265				
9	s7	186	Total	C	N	O	S	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-A.

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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
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
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			
35	sM	104	Total	C	N	O	0	0	0
			679	402	140	137			

- 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	3169	Total	C	N	O	P	0	0	0
			67780	30276	12216	22120	3168			

- 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	17	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O	S	0	0	0
			1543	962	315	266				
49	m3	194	Total	C	N	O	S	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	204	Total	C	N	O	S	0	0	1
			1720	1077	361	281	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M5	170	LYS	-	insertion	UNP P05748

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 70 is a protein called 60S ribosomal protein L34-A (eL34).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	d2	130	Total	C	N	O	S	0	0	1
			1021	650	188	180	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d2	47	TYR	-	insertion	UNP P0C0W1

- Molecule 81 is a protein called 60S ribosomal protein L12-A (uL11).

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

- Molecule 82 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 84 is a protein called 60S ribosomal protein P1 alpha/P2 beta.

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

- Molecule 85 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	f	148	Total	C	N	O	S	0	0	0
			1122	696	189	228	9			

- Molecule 86 is a protein called 60S ribosomal protein L1-A (uL1).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
86	l1	213	Total	C	N	O	0	0	0
			1063	637	213	213			

- 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	N9	1	Total	Mg	0	0
			1	1		
87	n8	3	Total	Mg	0	0
			3	3		
87	6	115	Total	Mg	0	0
			115	115		
87	Q0	1	Total	Mg	0	0
			1	1		
87	sM	1	Total	Mg	0	0
			1	1		
87	O4	1	Total	Mg	0	0
			1	1		
87	o9	1	Total	Mg	0	0
			1	1		
87	l3	1	Total	Mg	0	0
			1	1		
87	d6	1	Total	Mg	0	0
			1	1		
87	2	96	Total	Mg	0	0
			96	96		
87	d2	1	Total	Mg	0	0
			1	1		
87	m6	2	Total	Mg	0	0
			2	2		
87	f	3	Total	Mg	0	0
			3	3		
87	l7	1	Total	Mg	0	0
			1	1		
87	n0	2	Total	Mg	0	0
			2	2		
87	m3	1	Total	Mg	0	0
			1	1		
87	N6	1	Total	Mg	0	0
			1	1		

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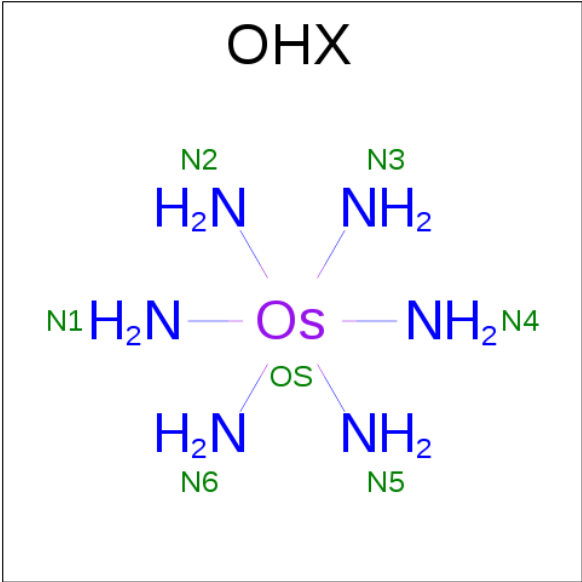
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	S9	1	Total 1	Mg 1	0	0
87	O3	2	Total 2	Mg 2	0	0
87	q0	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	o4	1	Total 1	Mg 1	0	0
87	M0	1	Total 1	Mg 1	0	0
87	n6	1	Total 1	Mg 1	0	0
87	5	400	Total 400	Mg 400	0	0
87	O7	3	Total 3	Mg 3	0	0
87	n9	2	Total 2	Mg 2	0	0
87	1	362	Total 362	Mg 362	0	0
87	O2	1	Total 1	Mg 1	0	0
87	Q2	1	Total 1	Mg 1	0	0
87	M8	1	Total 1	Mg 1	0	0
87	D9	1	Total 1	Mg 1	0	0
87	d3	1	Total 1	Mg 1	0	0
87	M3	2	Total 2	Mg 2	0	0
87	N3	3	Total 3	Mg 3	0	0
87	N8	4	Total 4	Mg 4	0	0
87	4	20	Total 20	Mg 20	0	0
87	D4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	S4	1	Total 1	Mg 1	0	0
87	L2	2	Total 2	Mg 2	0	0
87	l5	1	Total 1	Mg 1	0	0
87	m7	3	Total 3	Mg 3	0	0
87	M7	3	Total 3	Mg 3	0	0
87	L6	1	Total 1	Mg 1	0	0
87	s8	1	Total 1	Mg 1	0	0
87	o2	2	Total 2	Mg 2	0	0
87	c7	1	Total 1	Mg 1	0	0
87	7	16	Total 16	Mg 16	0	0
87	n3	1	Total 1	Mg 1	0	0
87	q1	1	Total 1	Mg 1	0	0
87	L3	3	Total 3	Mg 3	0	0
87	l2	3	Total 3	Mg 3	0	0
87	8	12	Total 12	Mg 12	0	0
87	m0	1	Total 1	Mg 1	0	0
87	M6	1	Total 1	Mg 1	0	0
87	N0	1	Total 1	Mg 1	0	0
87	3	9	Total 9	Mg 9	0	0

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	1	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
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88	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	2	1	Total	N	Os	1	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	2	1	Total	N	Os	0	0
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88	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
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88	S1	1	Total	N	Os	0	0
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88	S6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	S9	1	Total 7	N 6	Os 1	1	0
88	C1	1	Total 7	N 6	Os 1	0	0
88	C3	1	Total 7	N 6	Os 1	0	0
88	C5	1	Total 7	N 6	Os 1	0	0
88	C8	1	Total 7	N 6	Os 1	1	0
88	D9	1	Total 7	N 6	Os 1	0	0
88	SR	1	Total 7	N 6	Os 1	0	0
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88	1	1	Total 7	N 6	Os 1	2	0
88	1	1	Total 7	N 6	Os 1	1	0
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88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0
88	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
			7	6	1		
88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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88	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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88	4	1	Total	N	Os	0	0
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88	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	1	0
88	4	1	Total 7	N 6	Os 1	1	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	L3	1	Total 7	N 6	Os 1	0	0
88	L4	1	Total 7	N 6	Os 1	0	0
88	L5	1	Total 7	N 6	Os 1	0	0
88	M0	1	Total 7	N 6	Os 1	0	0
88	M0	1	Total 7	N 6	Os 1	0	0
88	M5	1	Total 7	N 6	Os 1	0	0
88	M7	1	Total 7	N 6	Os 1	0	0
88	M7	1	Total 7	N 6	Os 1	0	0
88	M8	1	Total 7	N 6	Os 1	0	0
88	M9	1	Total 7	N 6	Os 1	0	0
88	N1	1	Total 7	N 6	Os 1	0	0
88	N8	1	Total 7	N 6	Os 1	0	0
88	N9	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	O7	1	Total	N	Os	1	0
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88	O9	1	Total	N	Os	0	0
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88	Q2	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total	N	Os	1	0
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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	5	1	Total	N	Os	0	0
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88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	2	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total 7	N 6	Os 1	1	0
88	5	1	Total 7	N 6	Os 1	1	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	1	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	2	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	1	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	2	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	1	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	5	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	7	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	1	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	1	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	8	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	13	1	Total	N	Os	0	0
			7	6	1		
88	14	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	l4	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l5	1	Total	N	Os	0	0
			7	6	1		
88	l9	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m0	1	Total	N	Os	0	0
			7	6	1		
88	m5	1	Total	N	Os	0	0
			7	6	1		
88	m7	1	Total	N	Os	0	0
			7	6	1		
88	m9	1	Total	N	Os	0	0
			7	6	1		
88	n3	1	Total	N	Os	0	0
			7	6	1		
88	n6	1	Total	N	Os	0	0
			7	6	1		
88	n9	1	Total	N	Os	0	0
			7	6	1		
88	o3	1	Total	N	Os	0	0
			7	6	1		
88	o7	1	Total	N	Os	0	0
			7	6	1		
88	o9	1	Total	N	Os	0	0
			7	6	1		
88	q1	1	Total	N	Os	1	0
			7	6	1		
88	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

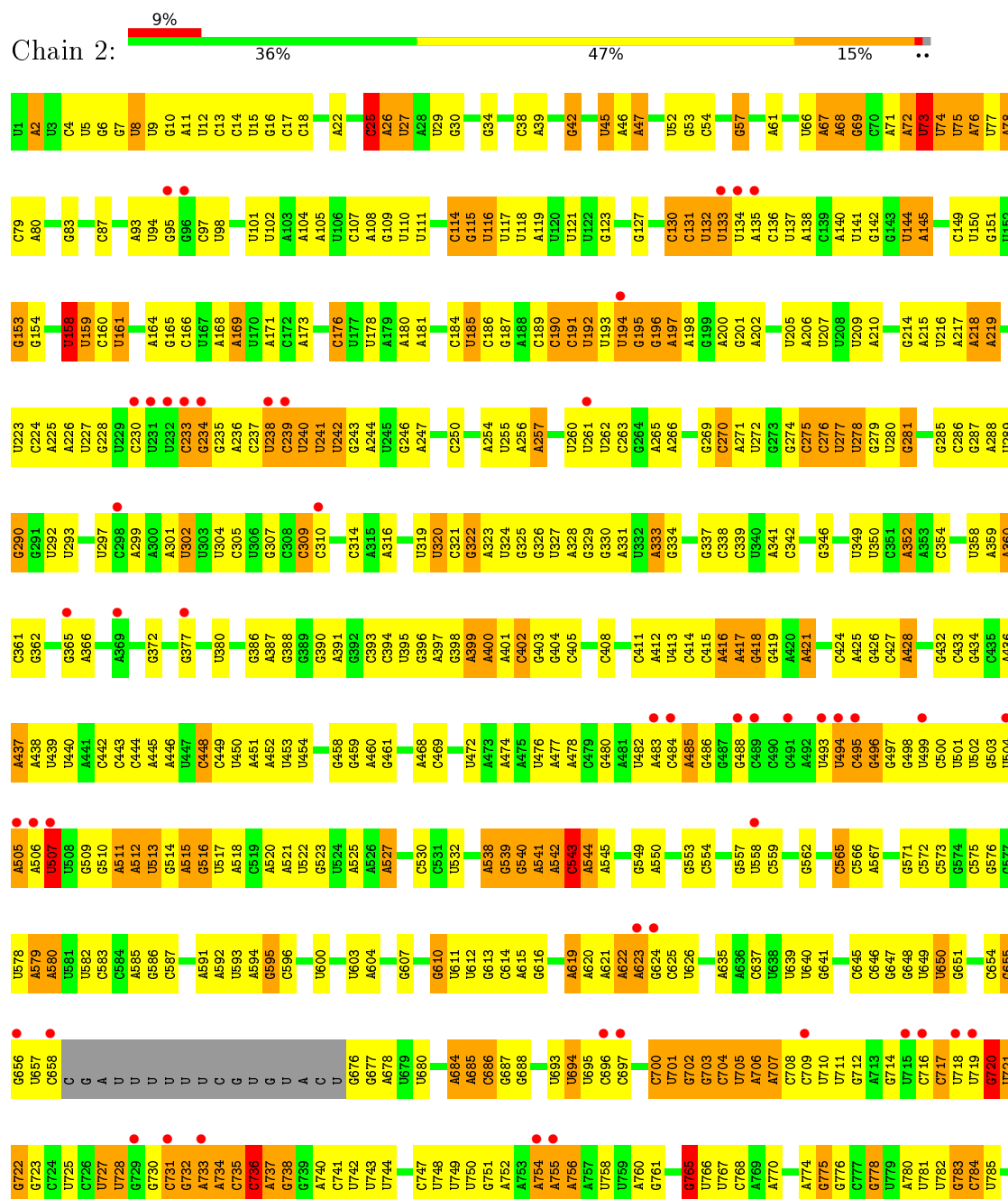
- Molecule 90 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
90	5	3	Total 3	O 3	0	0
90	f	9	Total 9	O 9	0	0

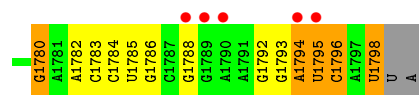
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

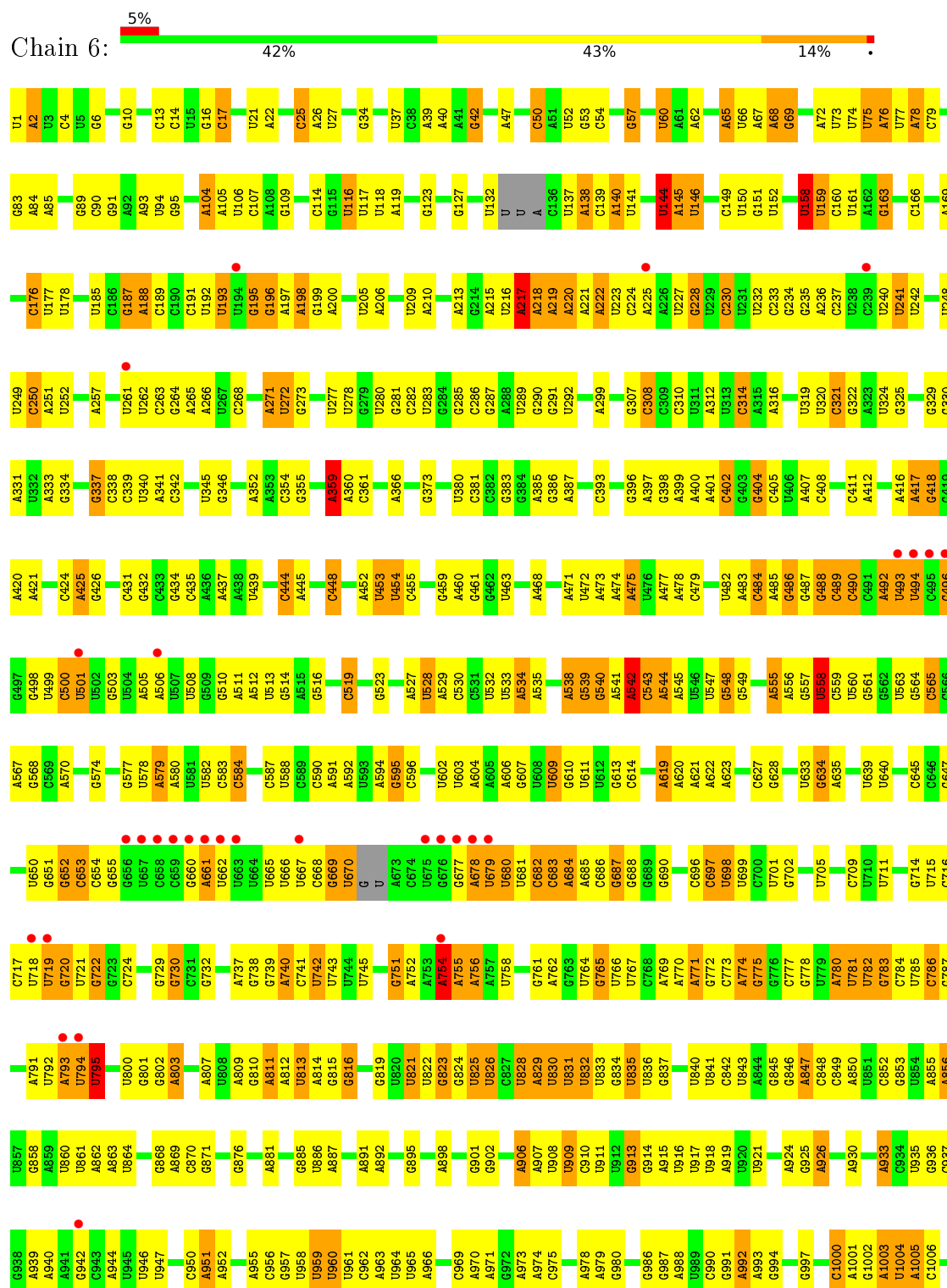
- Molecule 1: 18S ribosomal RNA

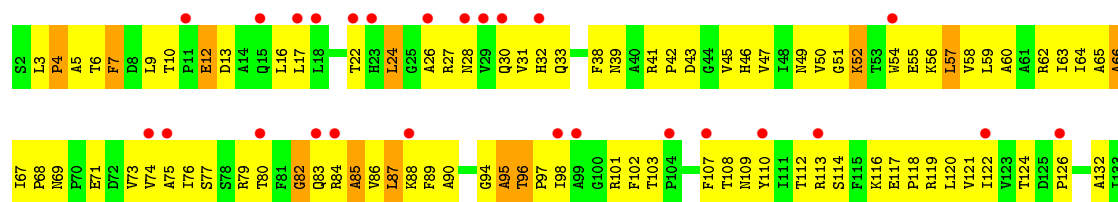


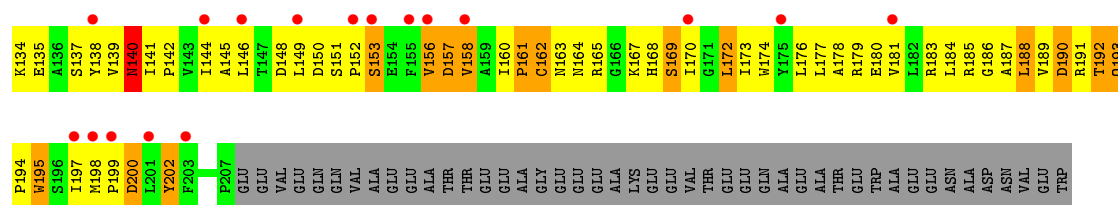
G1705	G1637	C1568	G1504	G1433	U1363	G1297	G1218	G1140	G1073	G1001	A930	A859	A788
C1706	G1638	A1569	A1505	U1434	G1364	U1298	C1222	G1141	G1074	G1002	C931	U860	A789
A1707	C1639	C1570	G1506	G1435	U1365	G1299	C1222	A1142	C1075	A1003	U932	U861	U792
C1708	C1640	C1571	G1507	U1443	U1366	U1300	A1226	A1143	A1076	U1004	A933	A862	U793
C1709	G1641	C1572	U1508	U1444	G1367	U1301	A1227	U1144	C1077	A1005	C934	A863	U794
U1710	G1642	A1573	U1511	U1445	G1368	U1302	G1228	U1145	C1078	A1006	U935	U864	U795
G1711	U1643	G1574	G1512	A1446	U1369	U1303	G1229	G1146	U1079	C1010	G936	A865	U796
G1712	G1644	G1575	G1513	U1447	U1370	U1304	G1229	A1147	U1080	G1011	A939	U866	A797
G1713	G1645	A1576	U1514	U1449	A1371	U1305	G1230	A1148	A1081	U1017	A940	U867	G797
G1714	U1646	U1577	U1515	U1450	C1372	U1306	U1232	G1149	C1082	A1012	U941	U868	U800
G1715	U1647	A1516	U1516	U1451	C1373	U1307	U1233	G1150	G1083	A1013	A942	U869	G801
G1716	A1648	U1517	U1517	U1452	C1374	U1310	U1234	A1151	A1086	U1014	G943	G872	G802
G1717	U1649	C1585	C1518	G1453	C1375	U1311	U1235	A1152	A1087	U1015	A944	U873	U805
G1718	U1650	A1586	U1519	G1454	C1376	U1312	U1236	G1153	A1088	U1016	U947	U874	U806
A1719	C1651	A1587	U1520	U1455	U1377	A1313	U1237	G1154	A1089	U1017	U948	U875	U807
G1720	C1652	C1588	G1521	C1456	C1378	A1314	U1238	G1155	A1090	U1018	U949	U876	G808
U1723	G1653	C1589	U1522	C1457	C1379	U1315	U1239	G1156	A1091	U1019	G949	U877	A809
U1728	G1654	C1591	U1523	G1458	A1382	U1316	U1240	A1157	A1092	C1021	C949	U878	G810
A1731	U1655	A1592	A1524	C1459	U1385	G1317	U1241	C1158	A1093	C1022	C950	G879	A811
A1732	U1656	A1593	A1525	C1460	G1385	U1318	U1242	C1159	A1094	A1023	A951	G880	A812
U1735	U1657	U1595	A1526	C1461	U1388	A1319	U1243	C1161	C1096	A1026	G952	U881	G815
U1738	U1658	G1594	C1527	C1462	A1388	U1320	U1244	G1165	U1097	C1027	G953	U882	G816
C1739	C1659	U1596	U1528	G1463	C1389	A1321	U1245	G1166	U1098	U1028	U960	U883	A817
U1746	U1660	A1597	U1529	C1464	U1390	A1322	U1246	G1167	U1099	U1029	U961	U884	G818
G1747	U1661	U1598	C1530	G1465	U1391	G1323	U1247	G1168	U1100	A1030	U962	U885	A819
G1748	G1662	U1599	U1531	G1466	U1392	G1324	U1248	G1169	G1101	U1031	G963	U886	U820
A1749	C1673	C1601	C1532	G1467	U1397	U1325	U1249	G1170	C1105	C1032	A966	U887	U821
A1750	U1674	G1602	U1533	U1468	U1398	G1326	U1250	G1171	U1106	C1033	U967	U888	U822
C1751	C1675	U1603	U1534	G1469	U1399	U1327	U1251	G1172	G1107	C1034	A968	U889	G823
U1752	U1681	U1604	U1535	C1470	A1400	G1328	U1252	U1175	G1108	A1039	A969	U890	G824
A1755	U1682	G1610	G1542	G1471	A1401	U1338	U1253	G1176	U1109	G1040	U969	U891	U825
A1756	C1683	A1611	A1545	C1472	G1402	U1339	U1254	G1177	G1110	G1041	U970	U892	U826
G1757	U1684	U1612	G1546	C1473	C1403	U1340	U1255	G1178	G1111	U1052	A971	U893	U827
U1758	C1685	U1613	A1547	G1474	C1404	A1341	U1256	G1179	G1112	G1042	A972	U894	U828
C1759	U1686	A1614	G1548	U1475	G1405	U1342	U1257	G1180	G1113	U1053	A973	U895	U829
G1760	U1687	C1615	C1549	C1476	G1406	A1343	U1258	U1181	U1114	G1046	C975	U896	U830
U1761	U1688	G1616	U1550	G1477	U1407	U1344	U1259	U1182	G1115	G1047	G976	U897	U831
A1762	A1689	U1621	U1551	C1481	A1410	U1345	U1260	U1183	U1116	G1048	A977	U898	U832
A1763	G1690	G1622	U1552	C1482	A1411	U1346	U1261	U1184	U1117	U1054	A978	U899	U833
C1764	A1691	U1623	U1553	A1483	G1412	A1347	U1262	U1185	G1118	U1055	A979	U900	U834
A1765	G1692	C1624	U1554	G1484	U1413	U1348	U1263	U1186	U1119	U1056	A980	U901	G838
A1766	A1693	C1625	U1555	U1485	U1414	A1349	U1264	U1187	G1120	U1057	A981	U902	U839
G1767	U1694	C1626	U1556	C1486	U1415	U1350	U1265	U1188	U1121	U1058	U982	U903	U840
G1768	G1695	U1628	U1557	G1487	G1416	G1351	U1266	U1189	G1122	U1059	A983	U904	U841
U1769	U1696	U1629	U1558	A1488	U1417	U1352	U1267	G1190	U1123	U1060	U984	U905	G846
U1770	G1697	U1630	U1559	U1489	A1418	U1353	U1268	U1191	C1124	U1061	A985	U906	A847
U1771	U1698	A1631	U1560	U1490	A1419	U1354	U1269	U1192	U1125	A1062	U986	U907	C848
C1772	G1699	C1632	U1561	U1491	U1420	U1355	U1270	U1193	U1126	U1063	A987	U908	U851
G1773	U1700	A1633	G1562	U1492	A1421	U1356	U1271	U1194	G1127	U1064	A988	U909	U852
G1774	A1701	C1634	C1563	A1493	U1422	U1357	U1272	U1195	U1128	A1065	A989	U910	G853
U1775	U1702	A1635	U1564	C1500	G1423	U1358	U1273	U1196	U1129	C1066	A990	U911	U854
U1776	C1703	A1635	U1565	U1501	G1424	U1359	U1274	U1197	U1130	C1067	A991	U912	A855
U1777	U1704	C1636	U1566	G1502	G1425	U1360	U1275	U1198	U1131	A1068	A992	U913	U856
				A1503	U1426	U1361	U1276	U1199	U1132	A1069	A993	U914	A924
					U1432	U1362	U1277	U1200	U1133	C1068	A994	U915	G925
							U1278	U1201	U1134	A1069	A995	U916	A926
							U1279	U1202	U1135	C1072	U996	U917	U857
							U1280	U1203	U1136			U918	G858
							U1281	U1204	U1137			U919	
							U1282	U1205	U1138			U920	
							U1283	U1206	U1139			U921	
							U1284	U1207	U1140			U922	
							U1285	U1208	U1141			U923	
							U1286	U1209	U1142			U924	
							U1287	U1210	U1143			U925	
							U1288	U1211	U1144			U926	
							U1289	U1212	U1145			U927	
							U1290	U1213	U1146				
							U1291	U1214	U1147				
							U1292	U1215	U1148				
							U1293	U1216	U1149				
							U1294	U1217	U1150				
							U1295	U1218	U1151				
							U1296	U1219	U1152				
							U1297	U1220	U1153				
							U1298	U1221	U1154				
							U1299	U1222	U1155				
							U1300	U1223	U1156				
							U1301	U1224	U1157				
							U1302	U1225	U1158				
							U1303	U1226	U1159				
							U1304	U1227	U1160				
							U1305	U1228	U1161				
							U1306	U1229	U1162				
							U1307	U1230	U1163				
							U1308	U1231	U1164				
							U1309	U1232	U1165				
							U1310	U1233	U1166				
							U1311	U1234	U1167				
							U1312	U1235	U1168				
							U1313	U1236	U1169				
							U1314	U1237	U1170				
							U1315	U1238	U1171				
							U1316	U1239	U1172				
							U1317	U1240	U1173				
							U1318	U1241	U1174				
							U1319	U1242	U1175				
							U1320	U1243	U1176				
							U1321	U1244	U1177				
							U1322	U1245	U1178				
							U1323	U1246	U1179				
							U1324	U1247	U1180				
							U1325	U1248	U1181				
							U1326	U1249	U1182				
							U1327	U1250	U1183				
							U1328	U1251	U1184				
							U1329	U1252	U1185				
							U1330	U1253	U1186				
							U1331	U1254	U1187				
							U1332	U1255	U1188				
							U1333	U1256	U1189				
							U1334	U1257	U1190				
							U1335	U1258	U1191				
							U1336	U1259	U1192				
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							U1339	U1262	U1195				
				</									



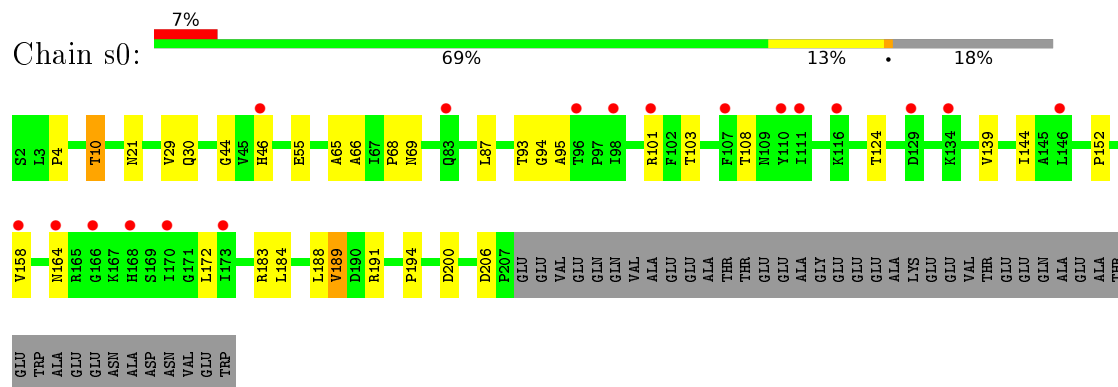
• Molecule 1: 18S ribosomal RNA



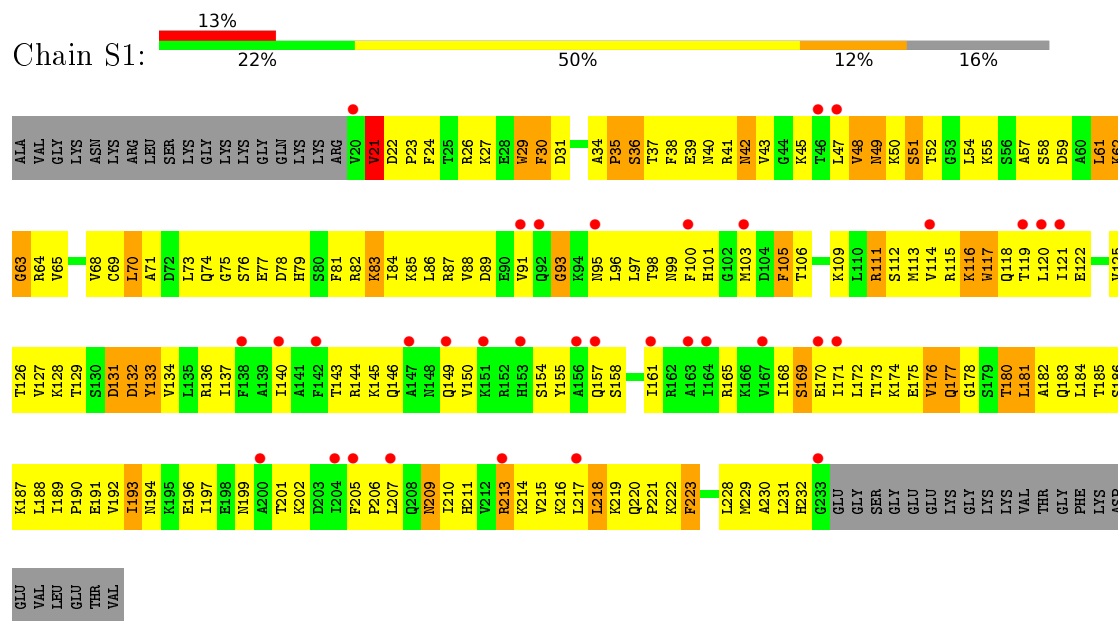




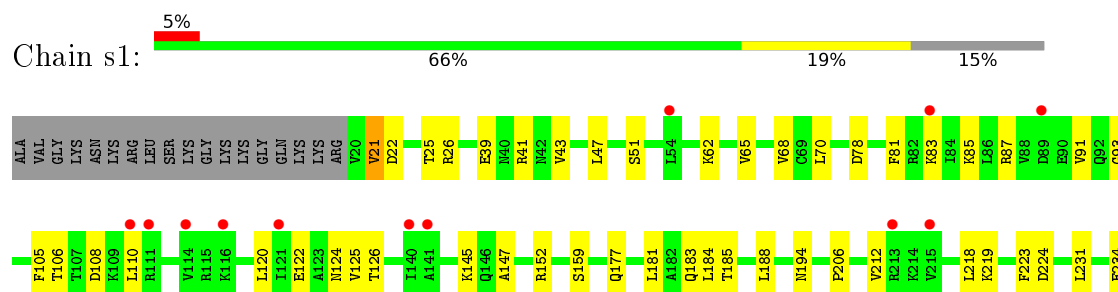
• Molecule 2: 40S ribosomal protein S0-A



• Molecule 3: 40S ribosomal protein S1-A



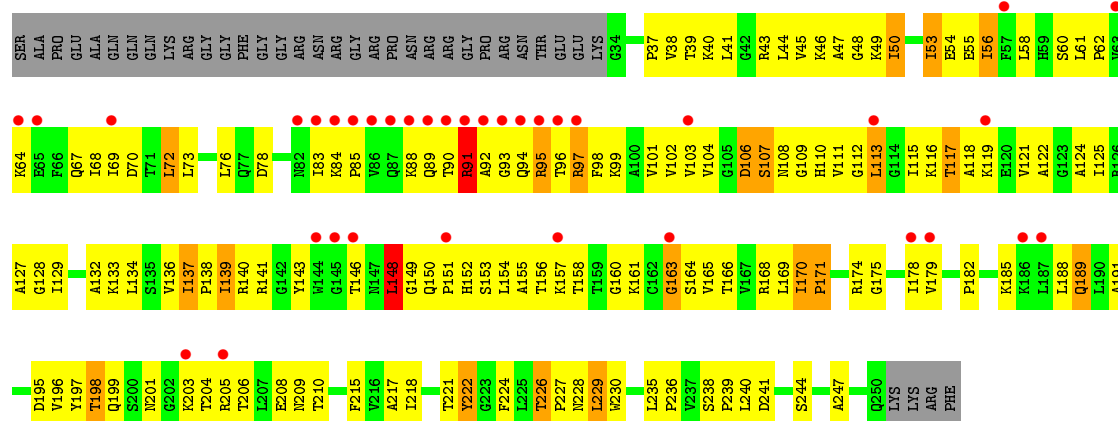
• Molecule 3: 40S ribosomal protein S1-A



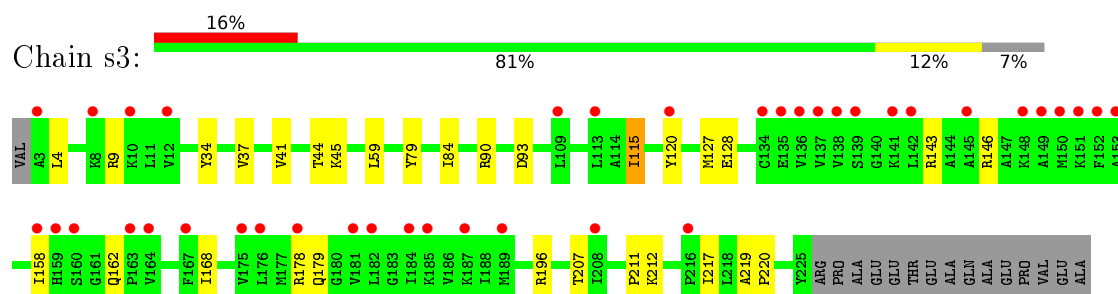
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GLU
GLU
LVS
GLY
LVS
LVS
VAL
THR
GLY
PHE
LVS
ASP
GLU
VAL
LEU
GLU
THR
VAL

• Molecule 4: 40S ribosomal protein S2

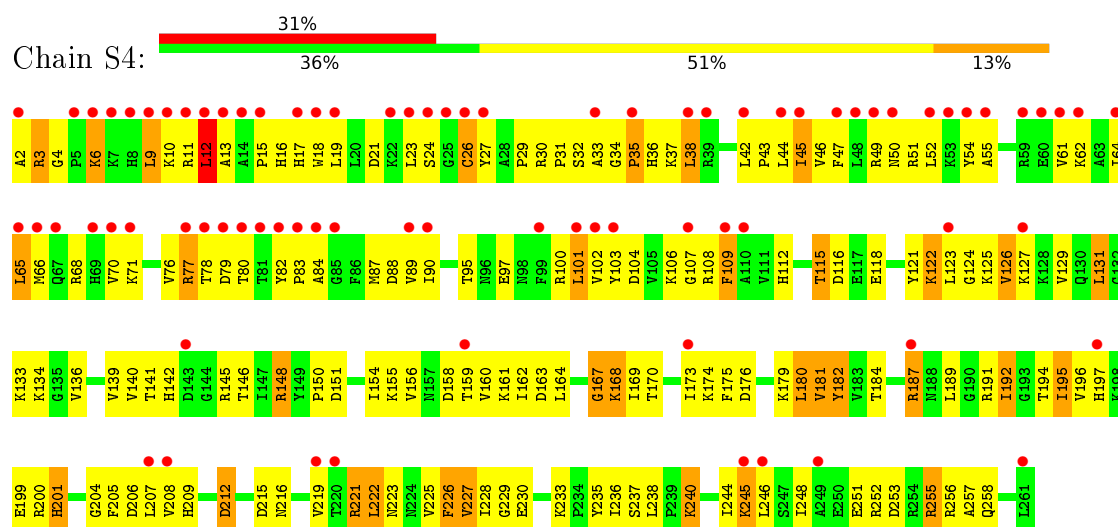
Chain S2: 14% 30% 47% 8% 14%



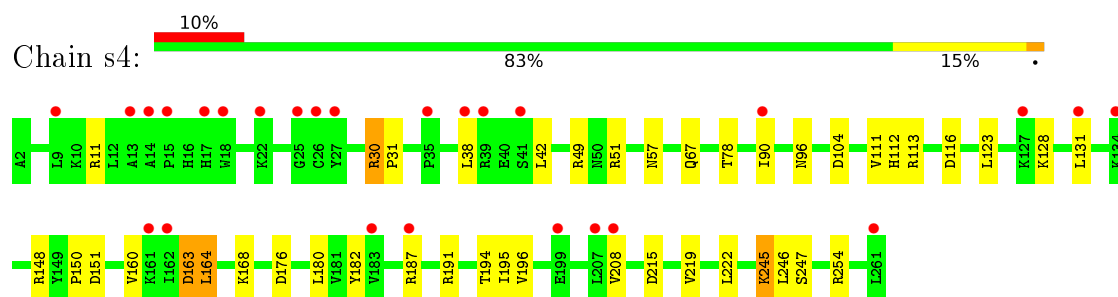
- Molecule 5: 40S ribosomal protein S3



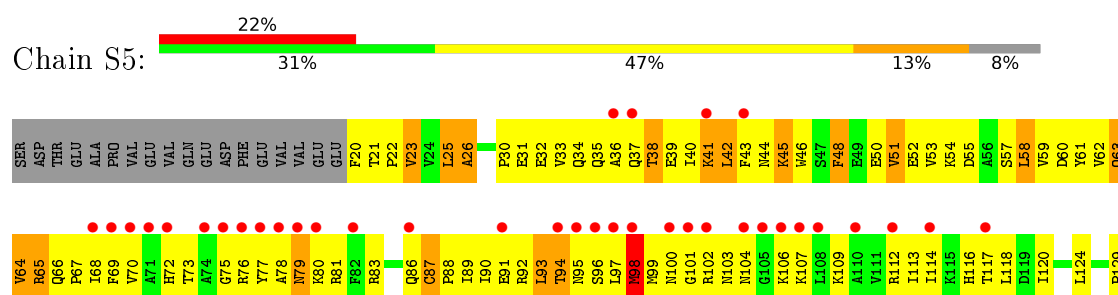
- Molecule 6: 40S ribosomal protein S4-A

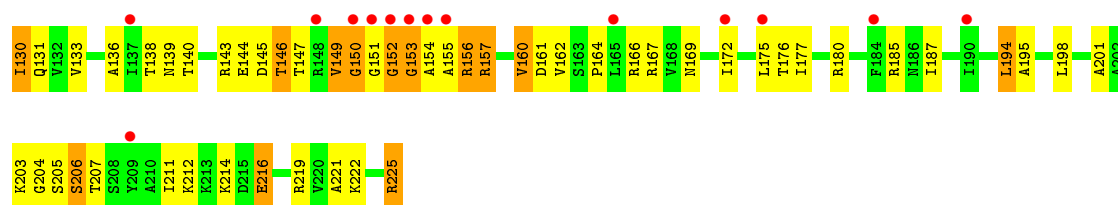


- Molecule 6: 40S ribosomal protein S4-A

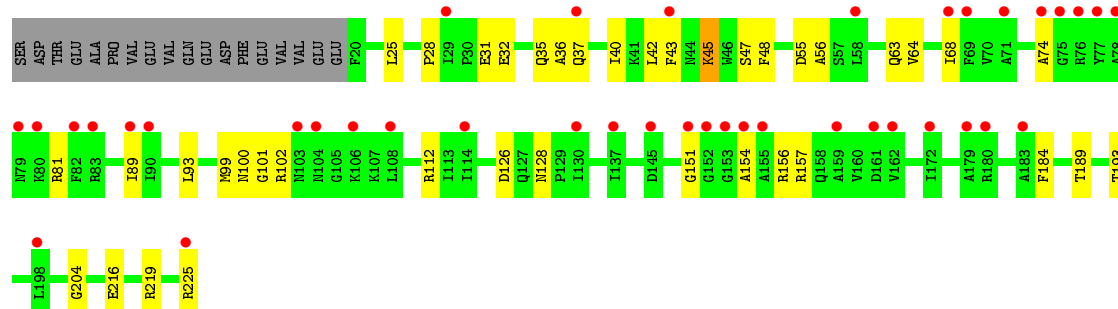
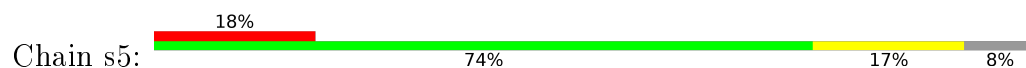


- Molecule 7: 40S ribosomal protein S5

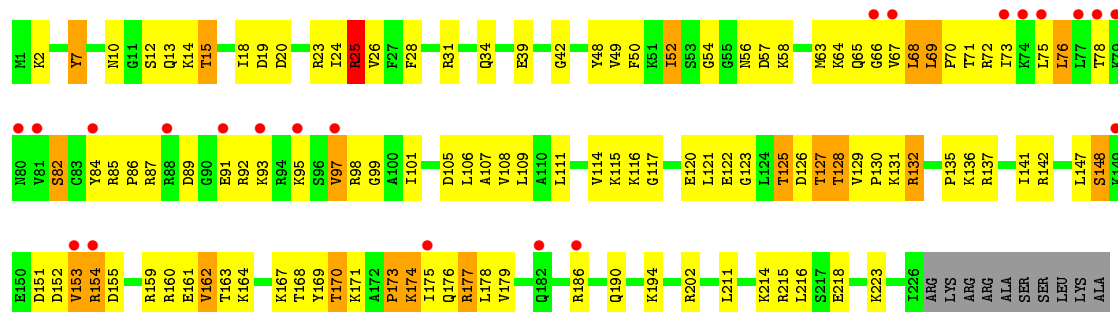




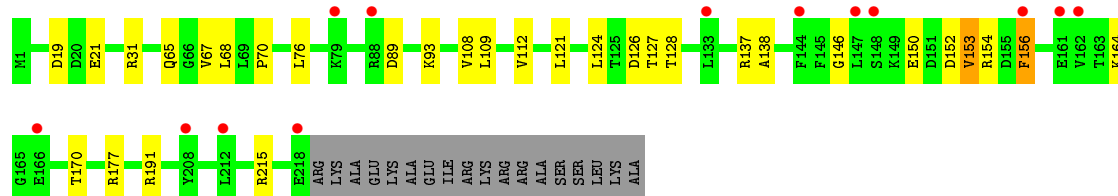
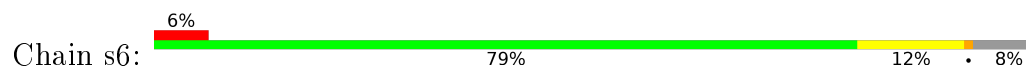
• Molecule 7: 40S ribosomal protein S5



• Molecule 8: 40S ribosomal protein S6-A

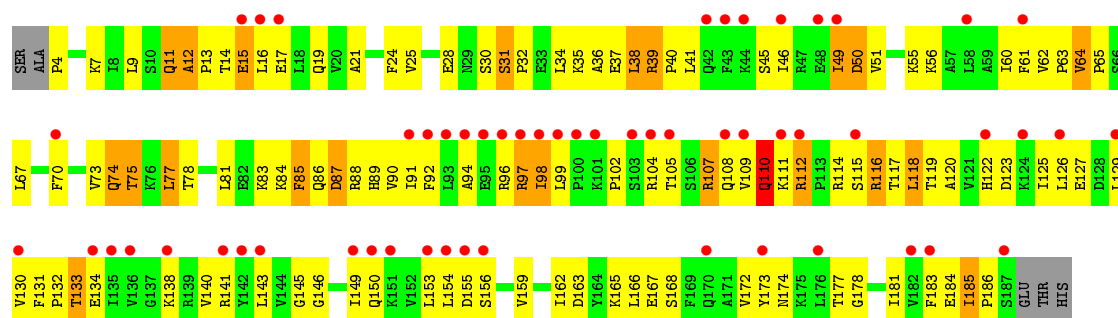


• Molecule 8: 40S ribosomal protein S6-A

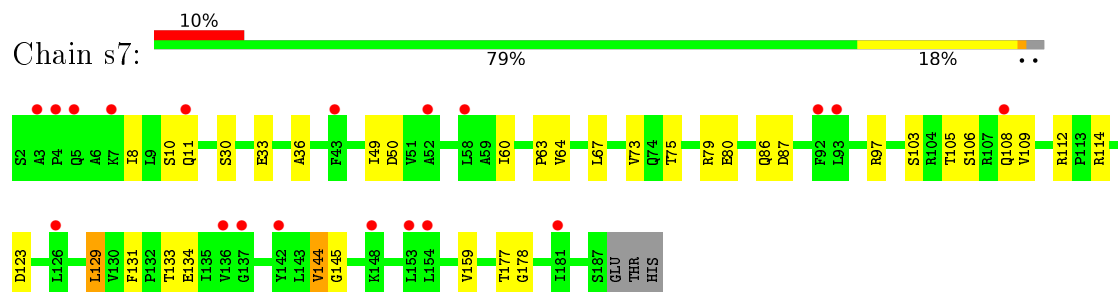


• Molecule 9: 40S ribosomal protein S7-A

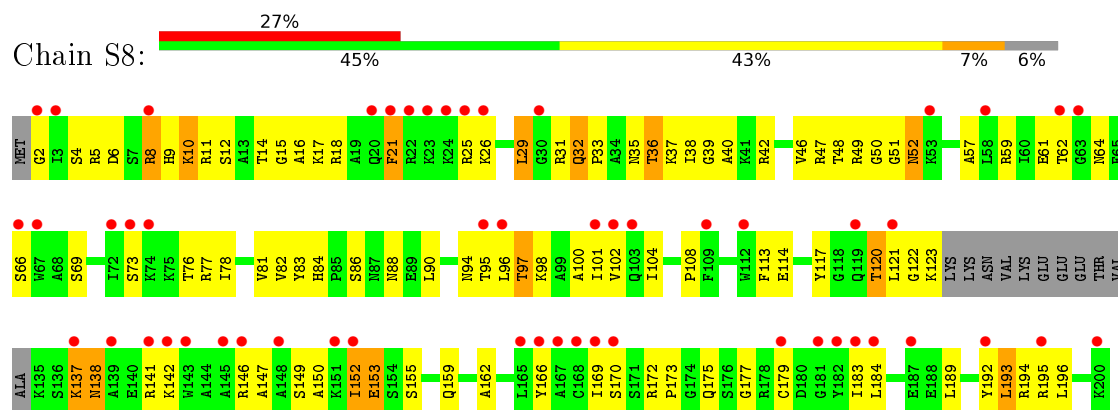




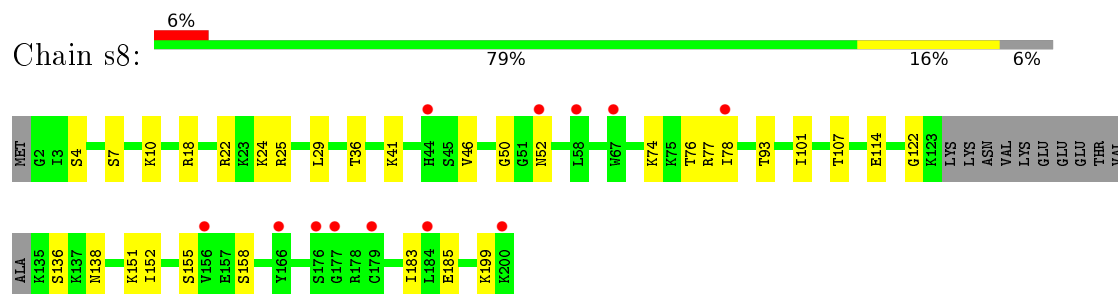
• Molecule 9: 40S ribosomal protein S7-A



• Molecule 10: 40S ribosomal protein S8-A

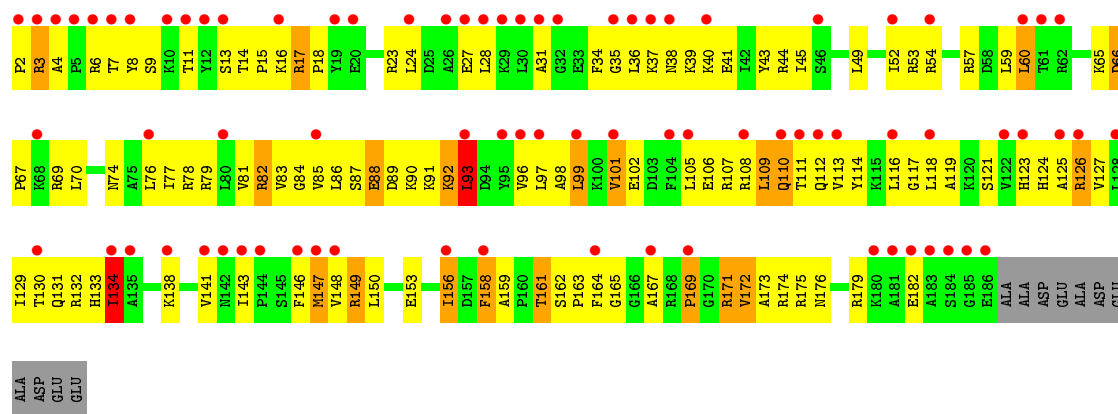


• Molecule 10: 40S ribosomal protein S8-A

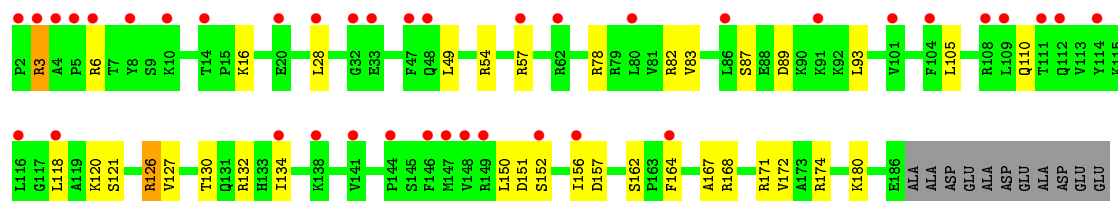
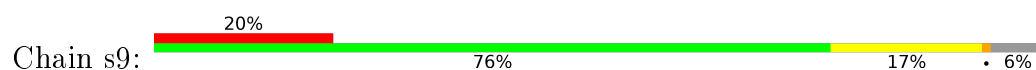


• Molecule 11: 40S ribosomal protein S9-A

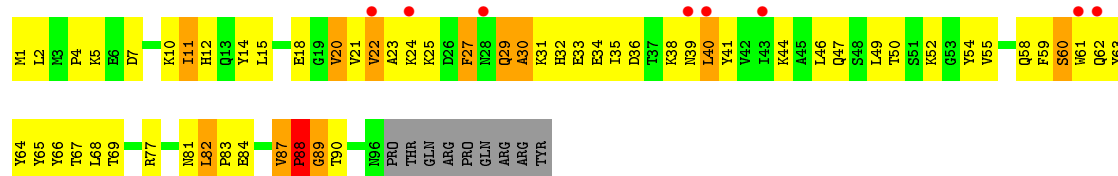




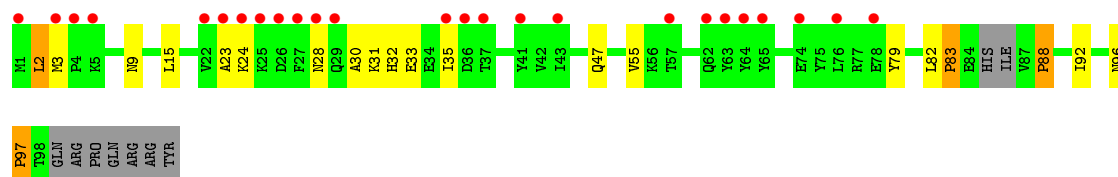
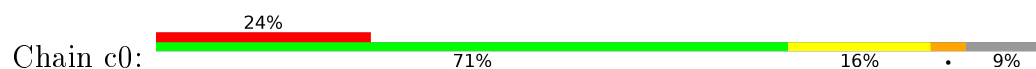
• Molecule 11: 40S ribosomal protein S9-A



• Molecule 12: 40S ribosomal protein S10-A

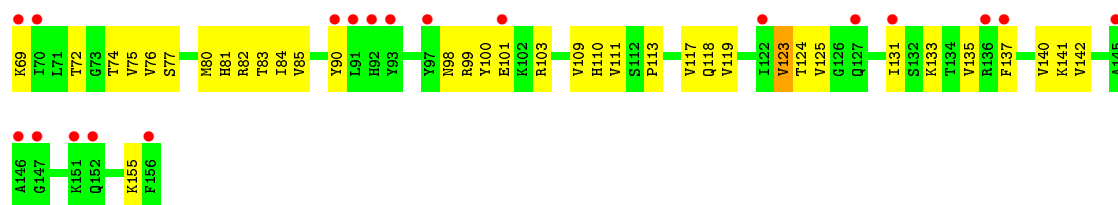


• Molecule 12: 40S ribosomal protein S10-A



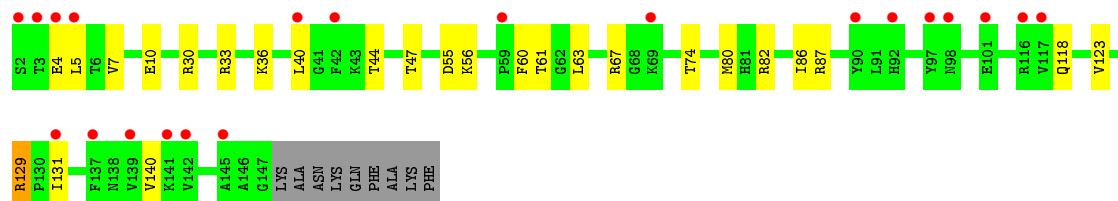
• Molecule 13: 40S ribosomal protein S11-A





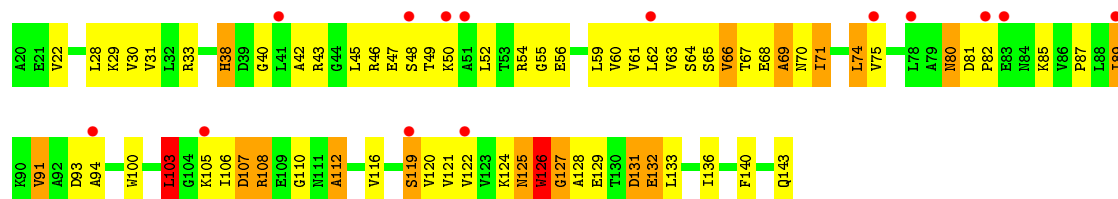
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



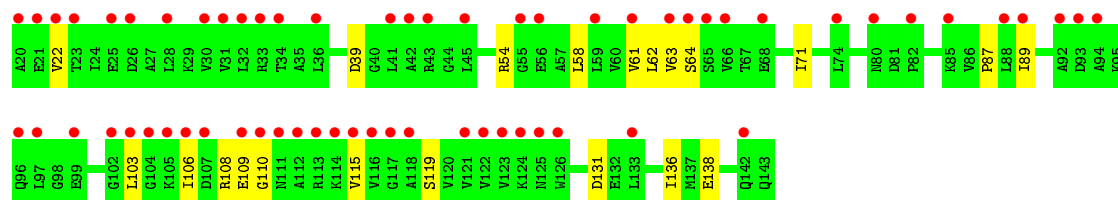
• Molecule 14: 40S ribosomal protein S12

Chain C2:



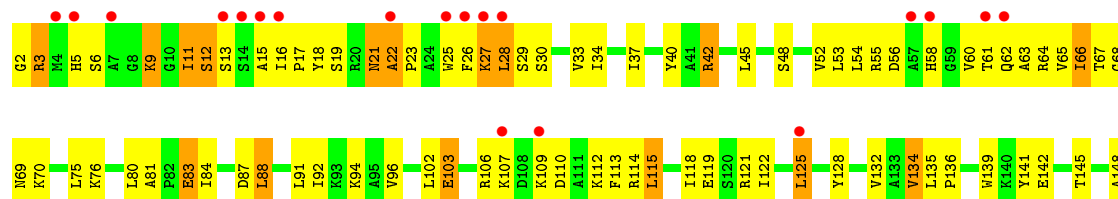
• Molecule 14: 40S ribosomal protein S12

Chain c2:



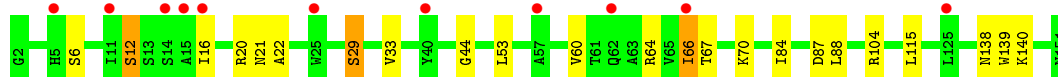
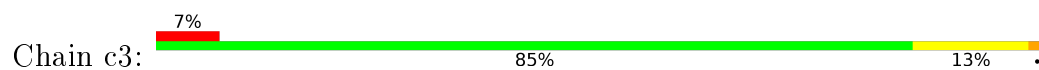
• Molecule 15: 40S ribosomal protein S13

Chain C3:

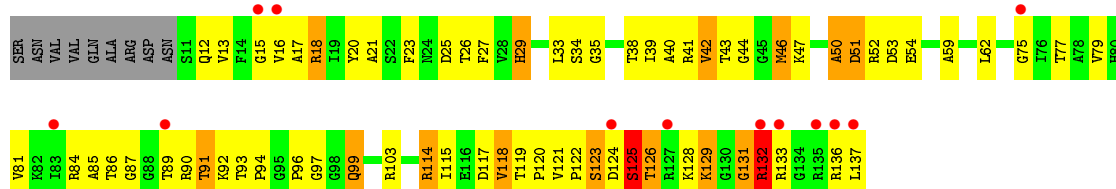
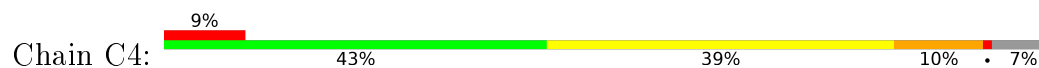




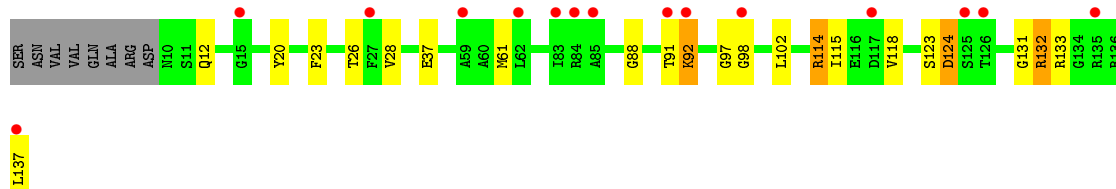
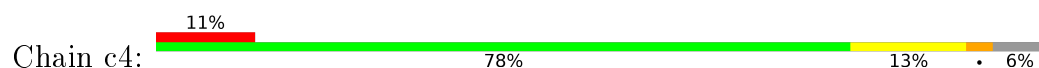
- Molecule 15: 40S ribosomal protein S13



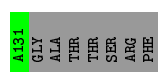
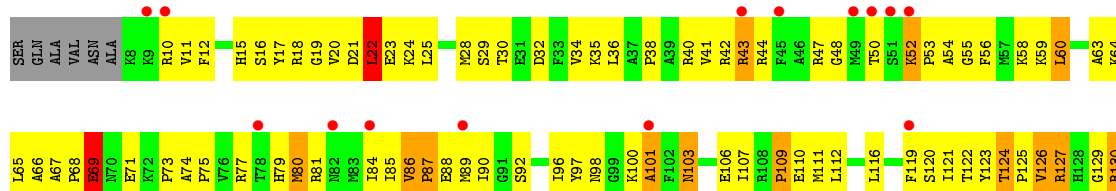
- Molecule 16: 40S ribosomal protein S14-A



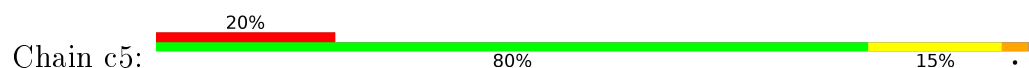
- Molecule 16: 40S ribosomal protein S14-A

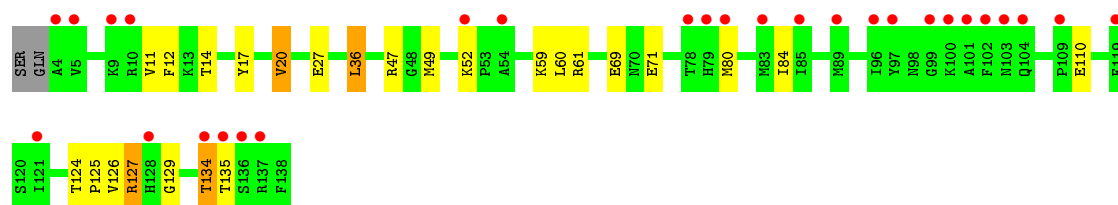


- Molecule 17: 40S ribosomal protein S15

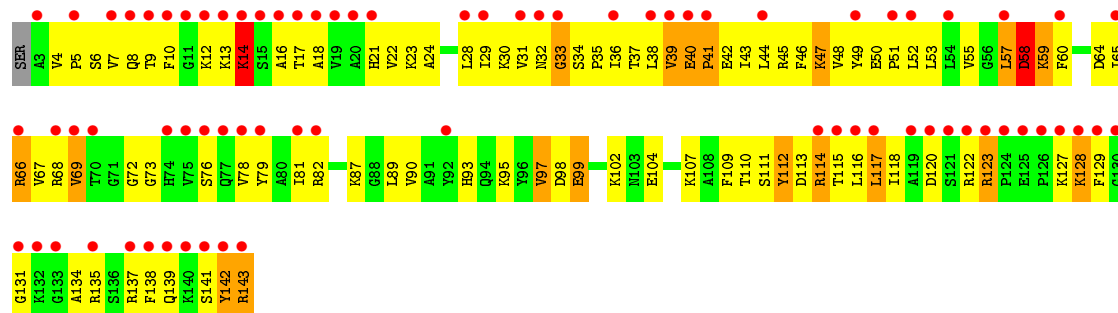


- Molecule 17: 40S ribosomal protein S15

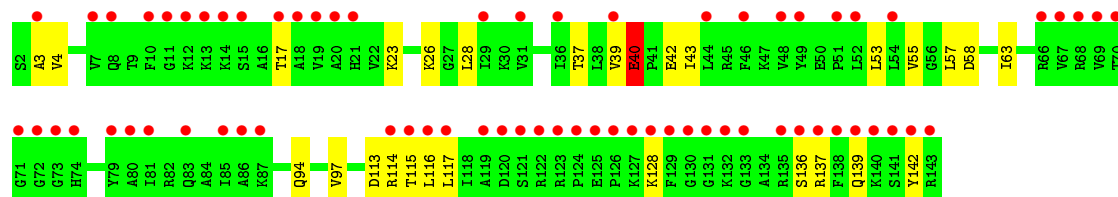
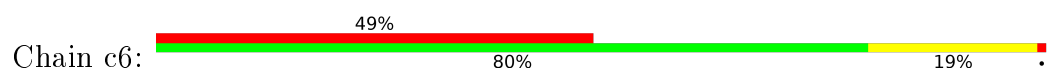




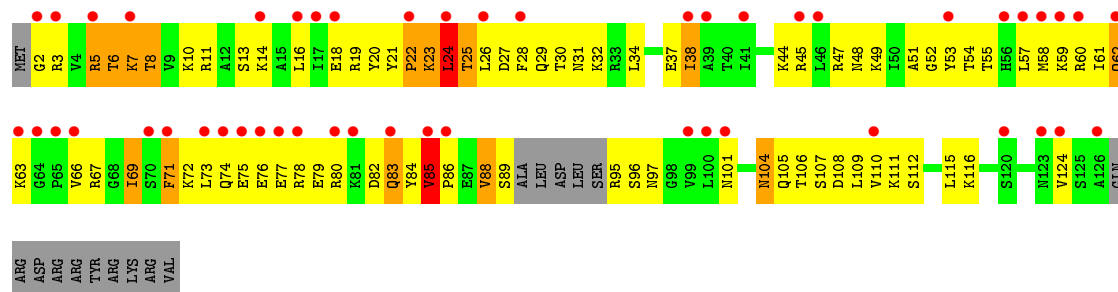
• Molecule 18: 40S ribosomal protein S16-A



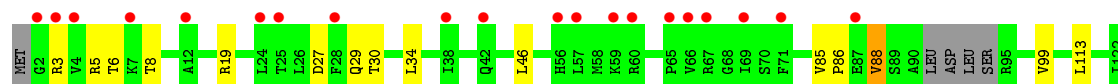
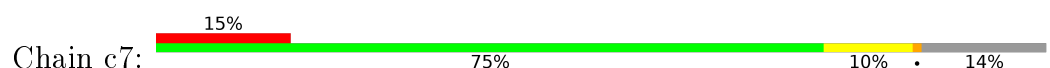
• Molecule 18: 40S ribosomal protein S16-A



• Molecule 19: 40S ribosomal protein S17-A

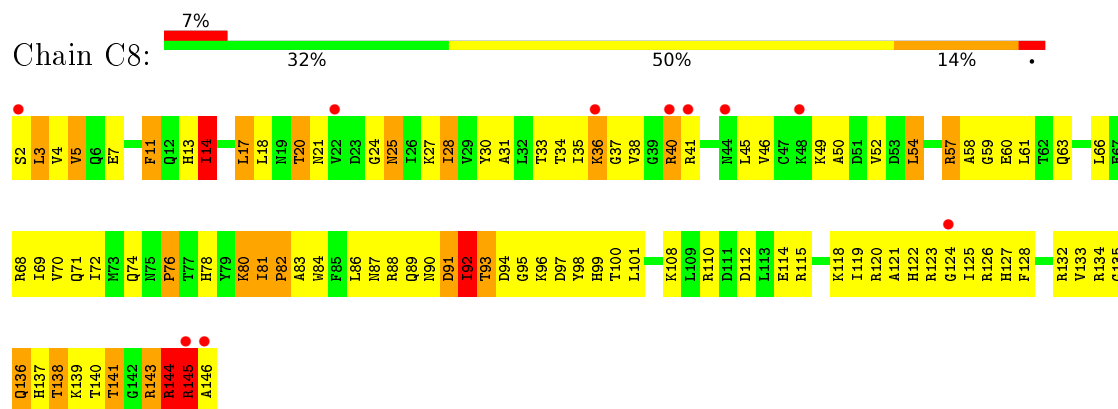


• Molecule 19: 40S ribosomal protein S17-A

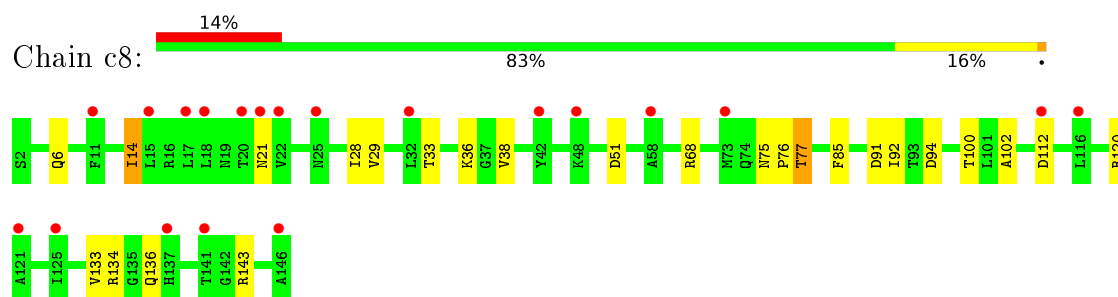


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VAL

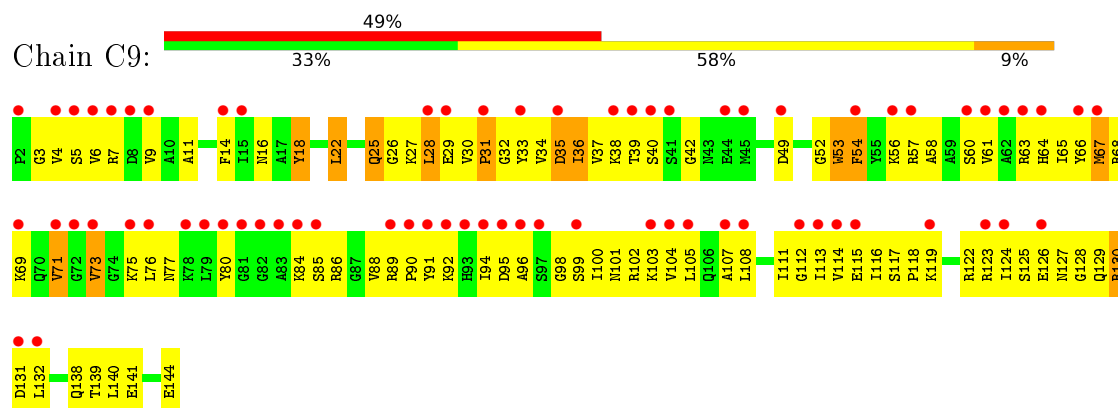
• Molecule 20: 40S ribosomal protein S18-A



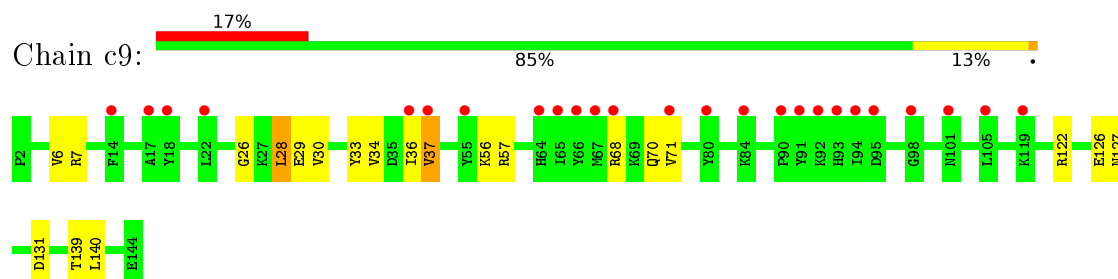
• Molecule 20: 40S ribosomal protein S18-A

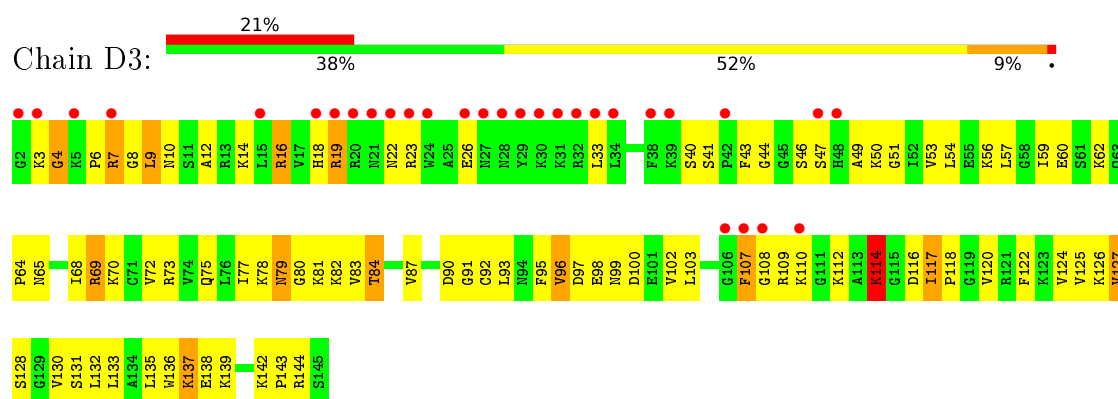


• Molecule 21: 40S ribosomal protein S19-A

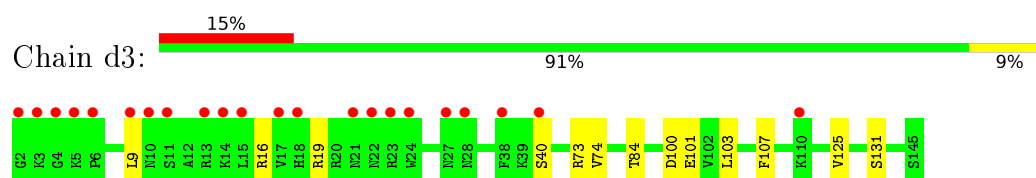


• Molecule 21: 40S ribosomal protein S19-A

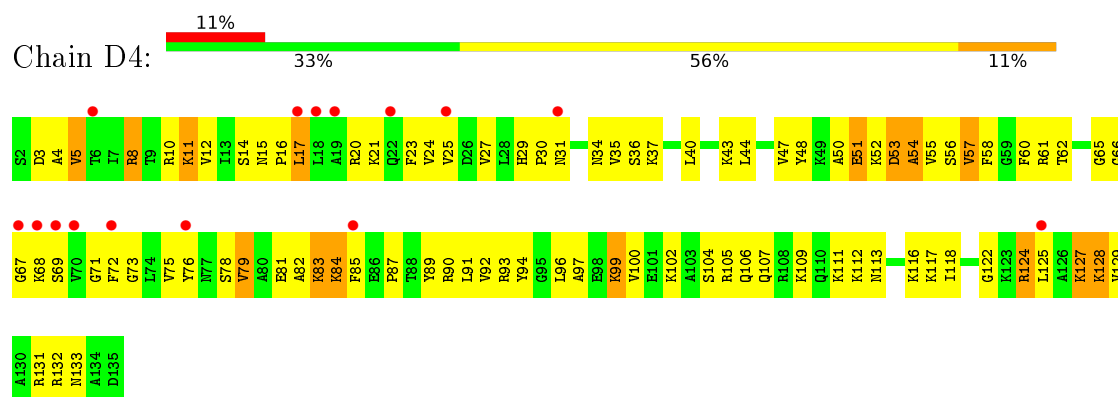




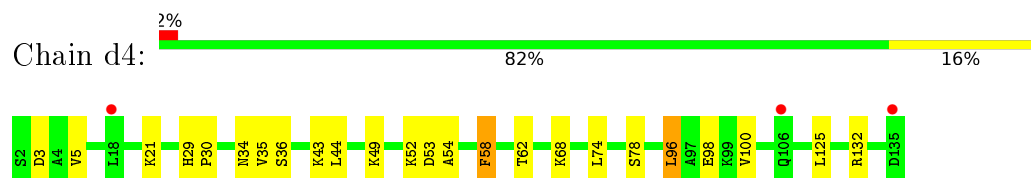
• Molecule 25: 40S ribosomal protein S23-A



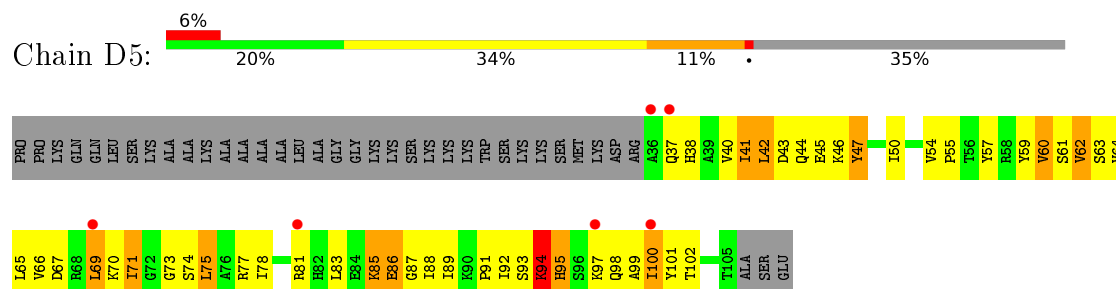
• Molecule 26: 40S ribosomal protein S24-A



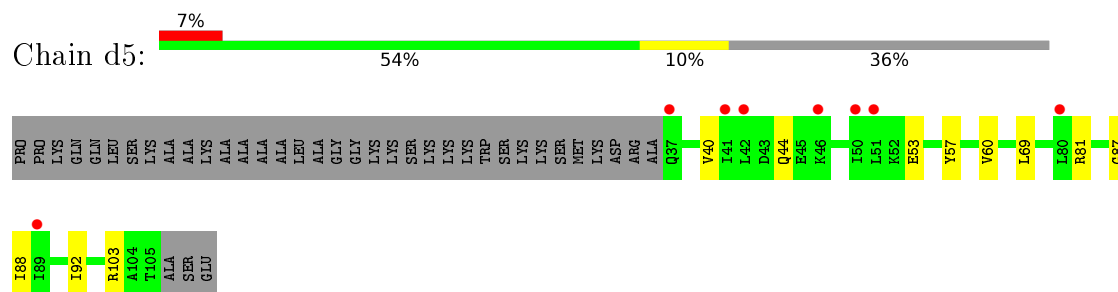
• Molecule 26: 40S ribosomal protein S24-A



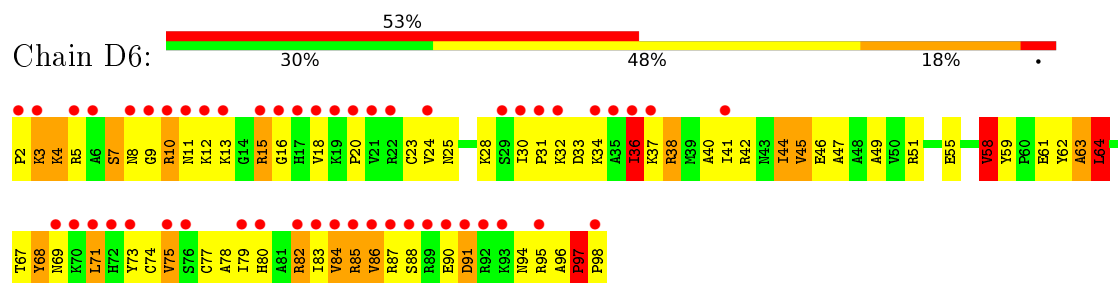
• Molecule 27: 40S ribosomal protein S25-A



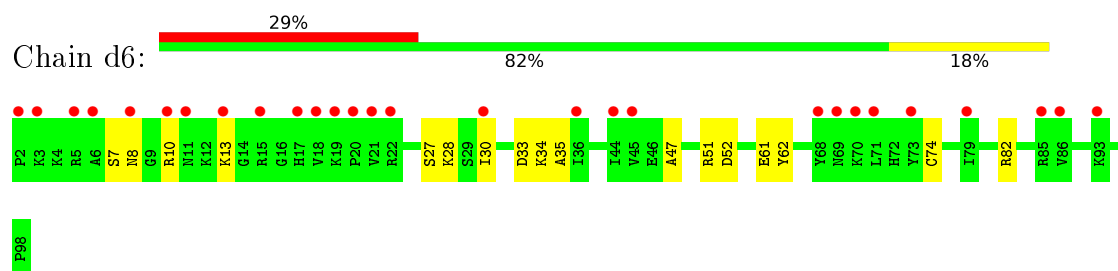
- Molecule 27: 40S ribosomal protein S25-A



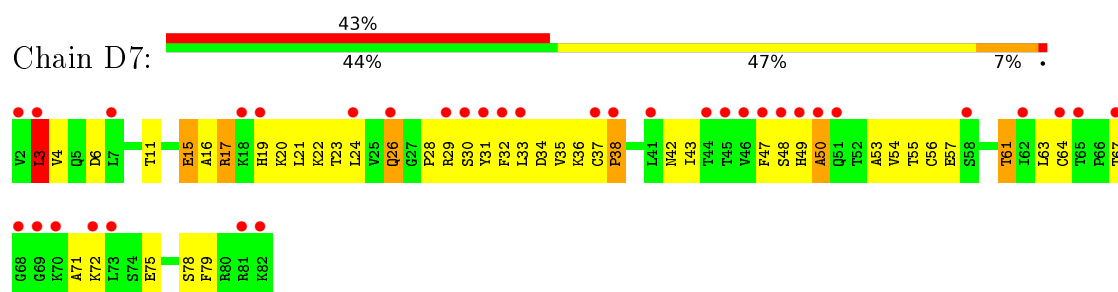
- Molecule 28: 40S ribosomal protein S26-B



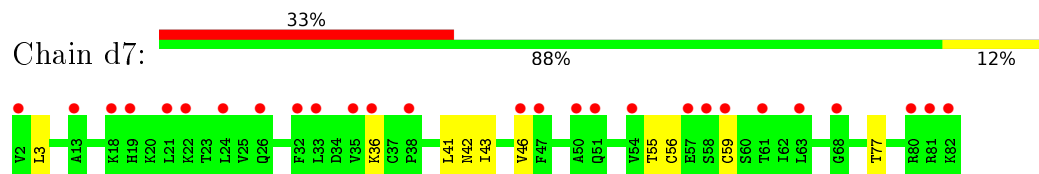
- Molecule 28: 40S ribosomal protein S26-B



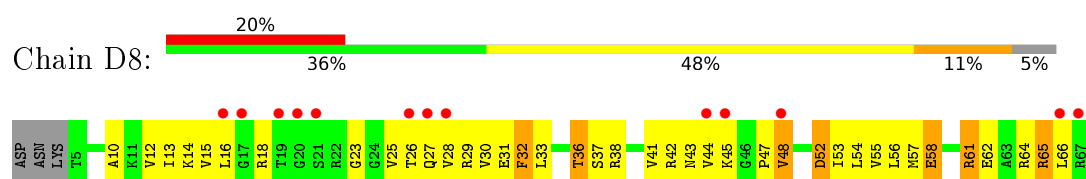
- Molecule 29: 40S ribosomal protein S27-A



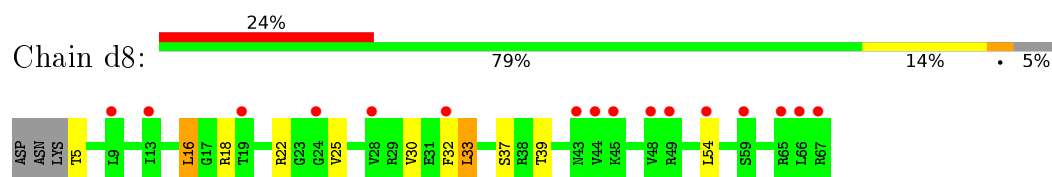
- Molecule 29: 40S ribosomal protein S27-A



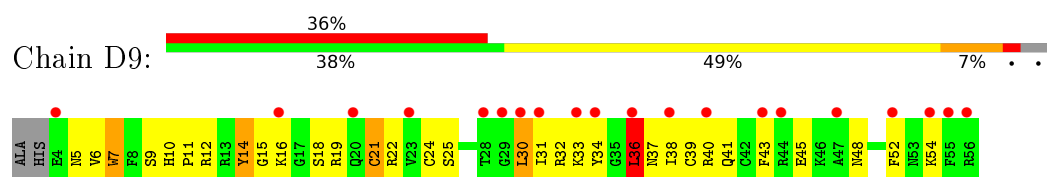
- Molecule 30: 40S ribosomal protein S28-A



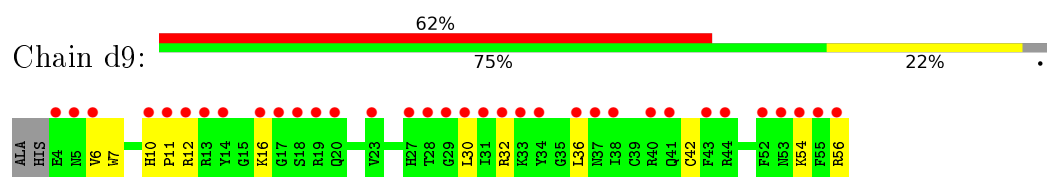
- Molecule 30: 40S ribosomal protein S28-A



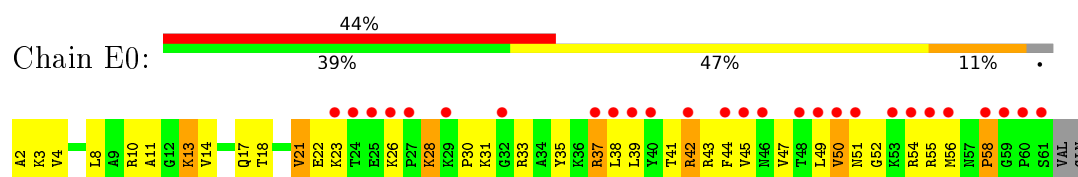
- Molecule 31: 40S ribosomal protein S29-A



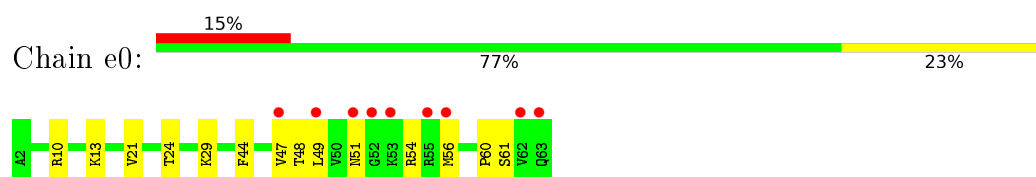
- Molecule 31: 40S ribosomal protein S29-A



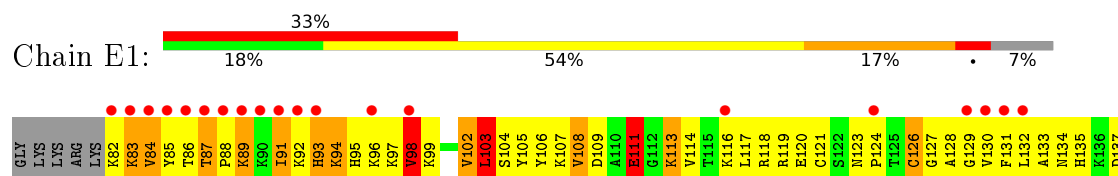
- Molecule 32: 40S ribosomal protein S30-A

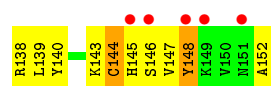


- Molecule 32: 40S ribosomal protein S30-A

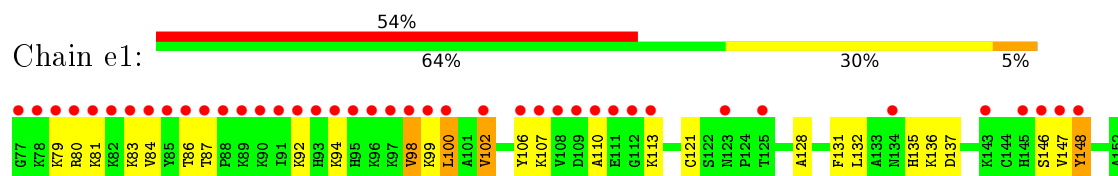


- Molecule 33: Ubiquitin-40S ribosomal protein S31

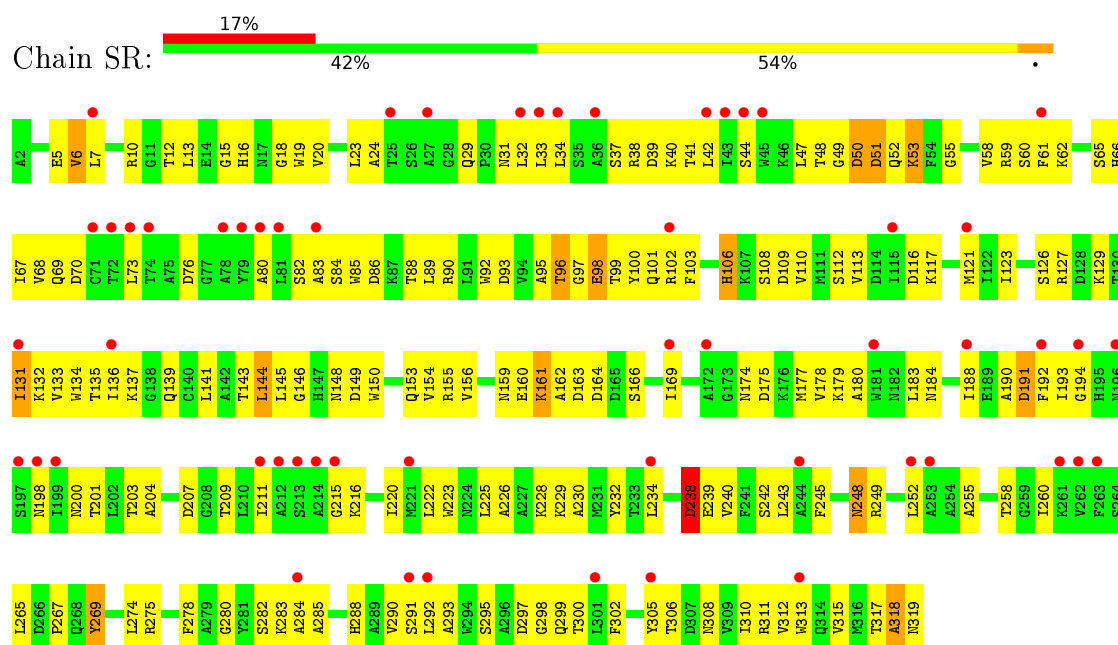




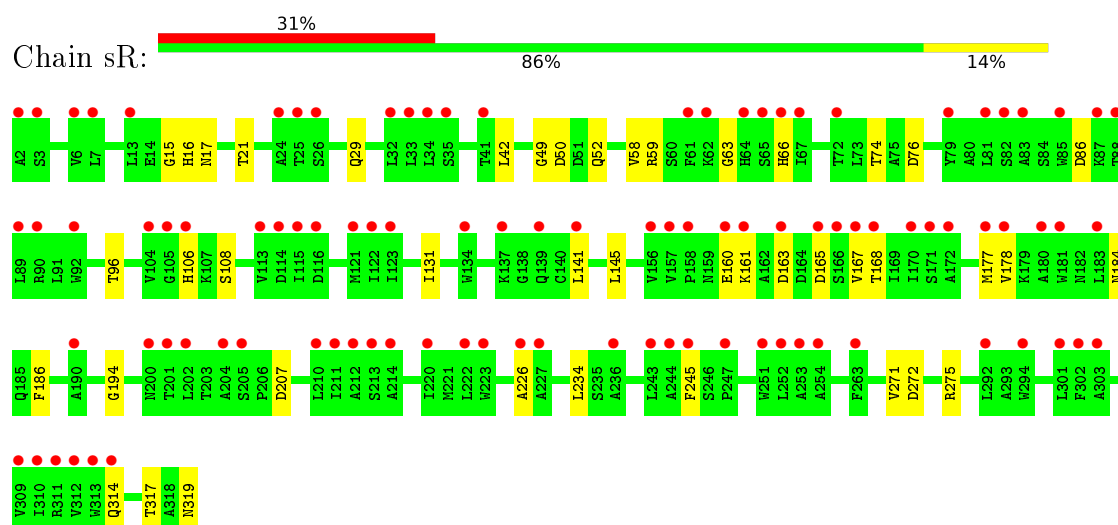
- Molecule 33: Ubiquitin-40S ribosomal protein S31



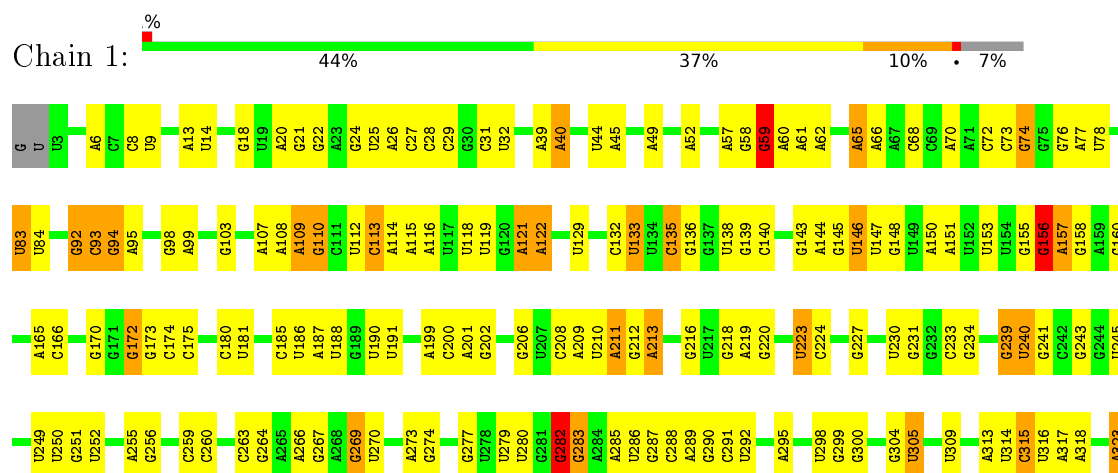
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



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



- Molecule 35: Suppressor protein STM1



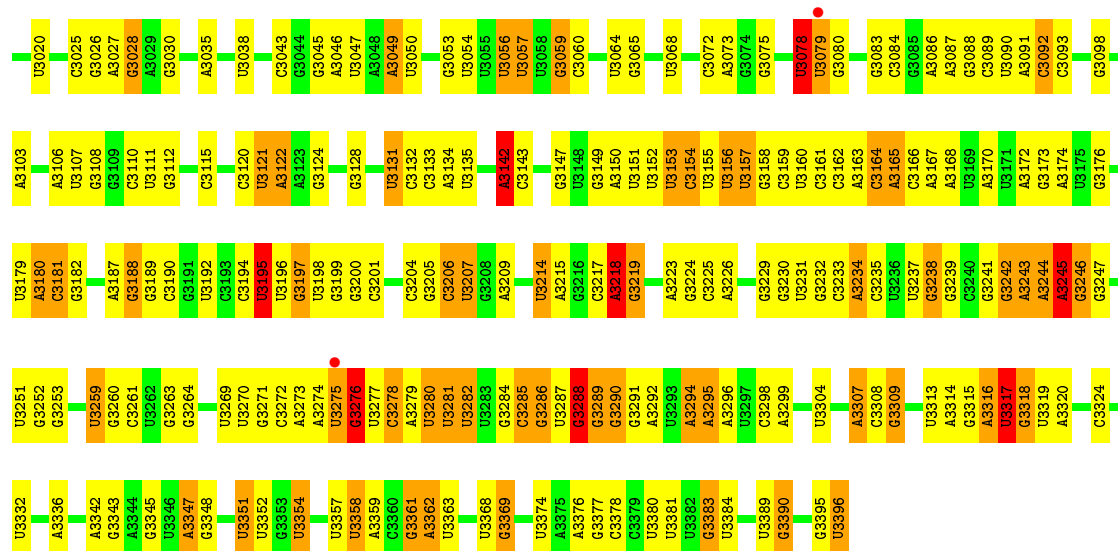
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U1572	G1486	G1392	G1311	G1236	G1149	G1066	U995	U897	U815		U642	C562	A416	
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G1576	A1489		C1316	A1240	A1153		G999	G901	C913	A738	C648	C566	G421	
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G1579	G1492	A1401	G1319	A1243	A1159	A1075	A1002	G909	U821	G742	G651	C569		C339
A1580	G1493		C1320	A1244	A1160		U1003	G910	C911	C743	A653	C573	U434	
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			C1327	G1248			A1006	A913	A828	U748		G579	C496	G345
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C1508	A1419	A1418	C1335	A1259	A1179	A1098	U1013	U922	G838	G760	C663	C592	U509	U359
				A1260	U1180	A1099	U1014	C923	U601	G761		U594	G510	G360
A1594	U1425		C1339	G1261	U1181	G1015	C840	G924	C839	G762	U670	U594	U511	A361
C1595	G1517		G1340	G1262	A1182	G1016	G1017	G924	C840	G763		G595	U512	
C1596				A1263	C1183	A1103	G1018	G934	A841	U764	A677	A598	A516	G364
C1597			U1347	G1264	G1104	A1104	G1019	U935	G944	C765	U678	C599	G517	A365
A1603	G1525	U1430	U1348	U1265	U1191	U108	G1020	U936	G944	U767	U679	G600	U	
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A1534	A1535	A1433	A1350	U1267	A1193	U109	G1024	G938	A848	C769	U682	A602	U	A373
A1535		G1434	U1351	G1268	A1196	U1110	A1025	U943	G853	G770		A603	U	
		A1435	A1352	U1269	C1197	U1111	U1028	U944		A771	G685	G604	C	G376
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G1542	G1543	U1438	G1354	C1271	A1200	G1115	A1030	C945		G773	G686	G610	U	U380
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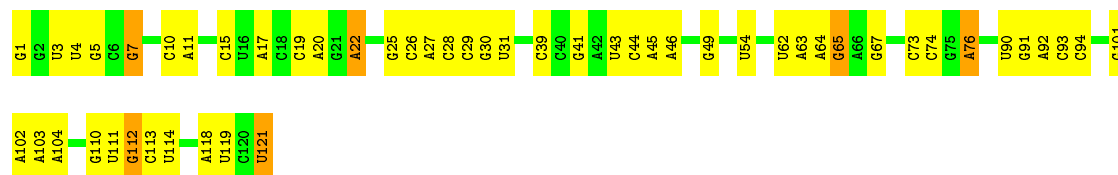
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G1769	G1677	G1590	C1508	A1419	U1330	A1245	C1155	G1072	G993	A904	G728	G728	C648	U563
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U1820	A1741	A1643	A1566	G1480	A1381	A1302	U1208		U1040	C958	G878	A785	C696	U623
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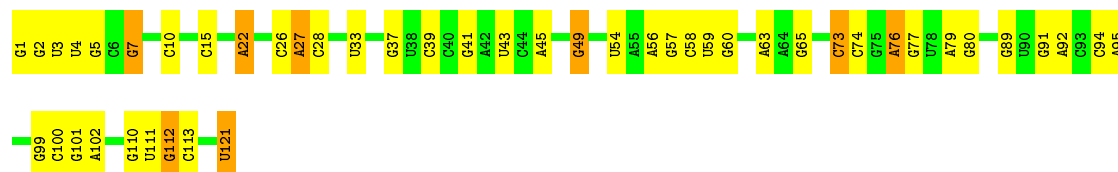
• Molecule 37: 5S ribosomal RNA

Chain 3: 57% 38% 5%



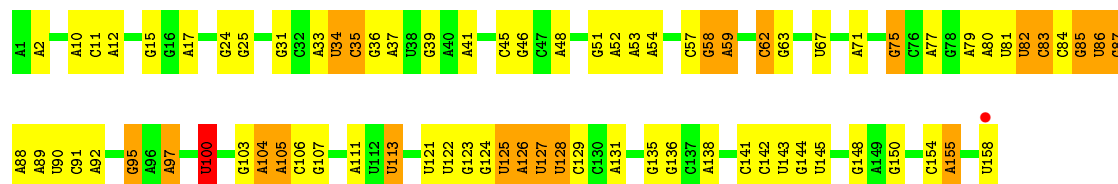
• Molecule 37: 5S ribosomal RNA

Chain 7: 61% 32% 7%



• Molecule 38: 5.8S ribosomal RNA

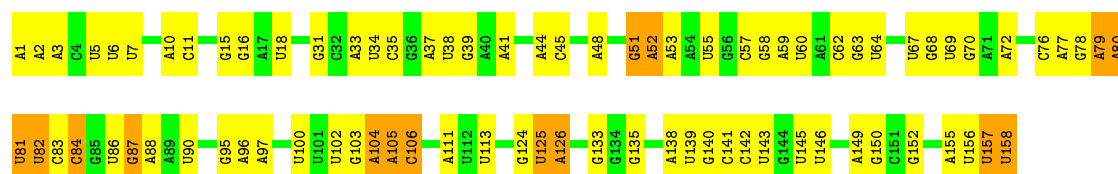
Chain 4: 50% 36% 13%



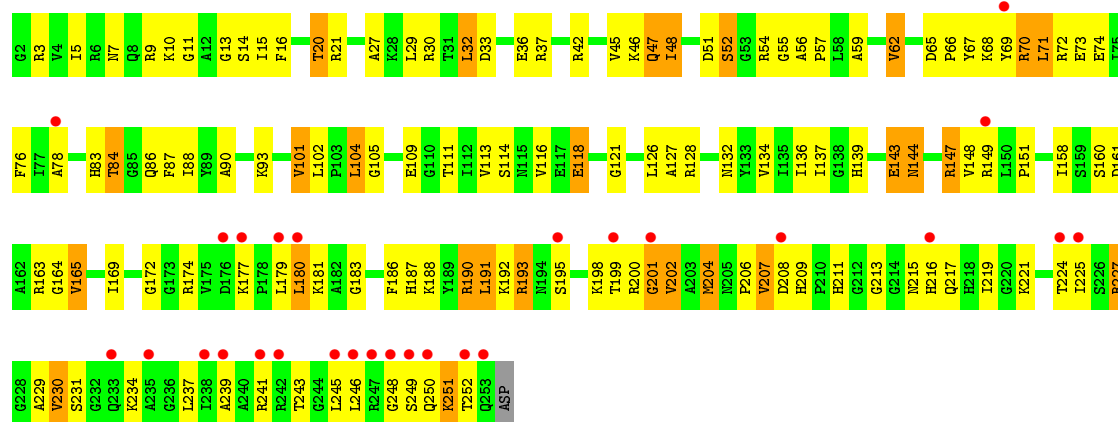
• Molecule 38: 5.8S ribosomal RNA

Chain 8: 48% 42% 9%

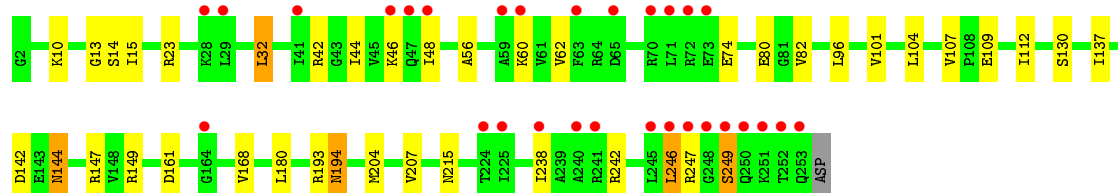
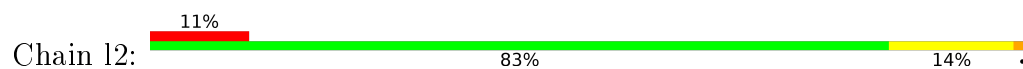




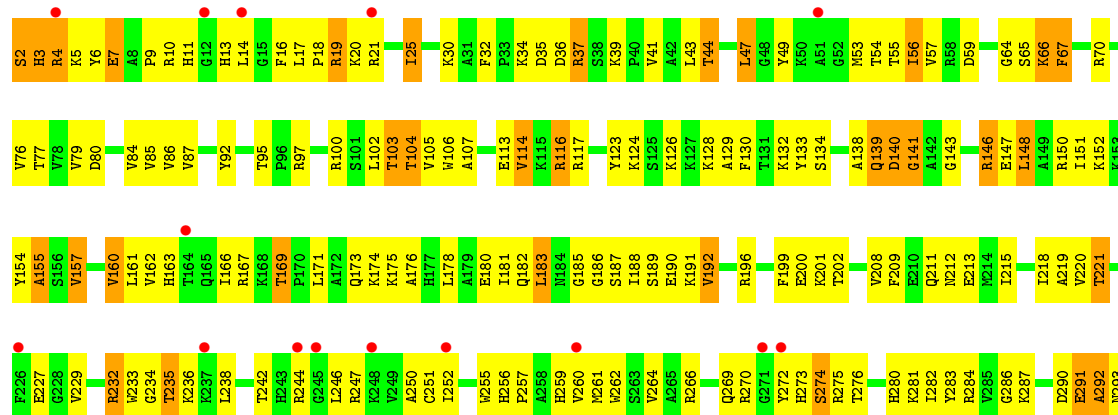
• Molecule 39: 60S ribosomal protein L2-A

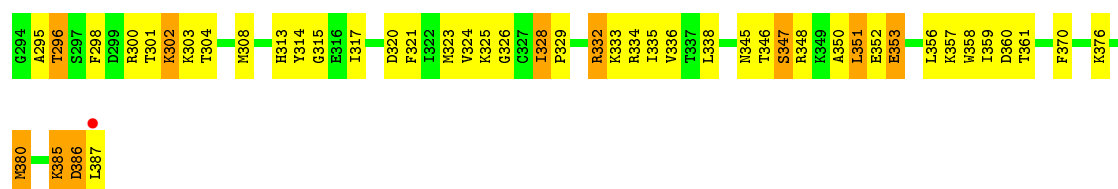


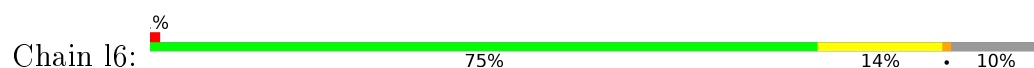
• Molecule 39: 60S ribosomal protein L2-A

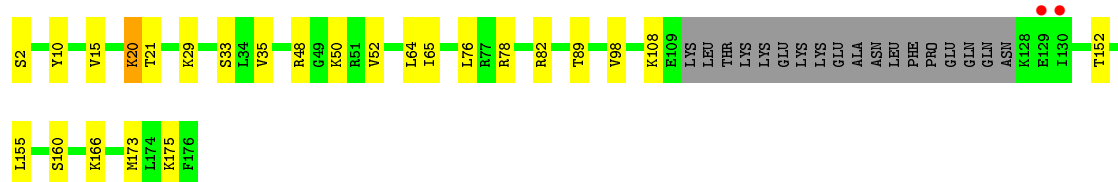


• Molecule 40: 60S ribosomal protein L3

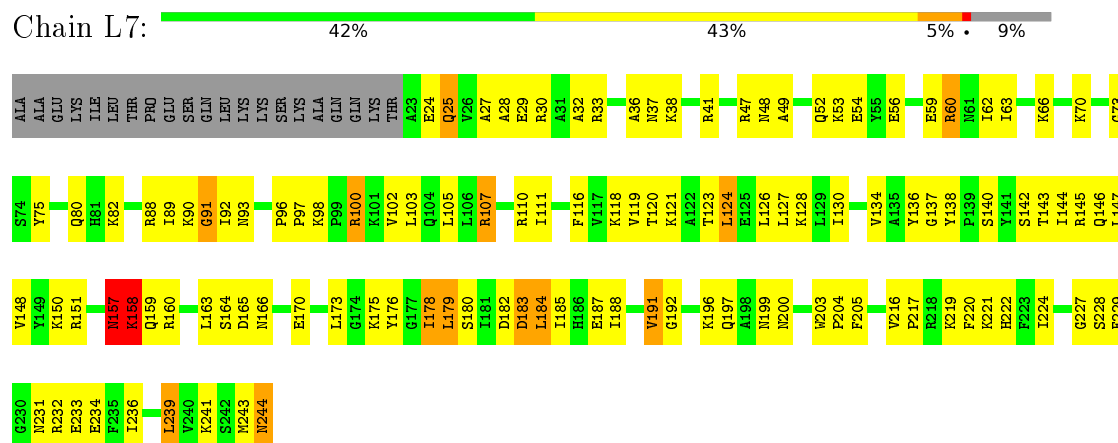




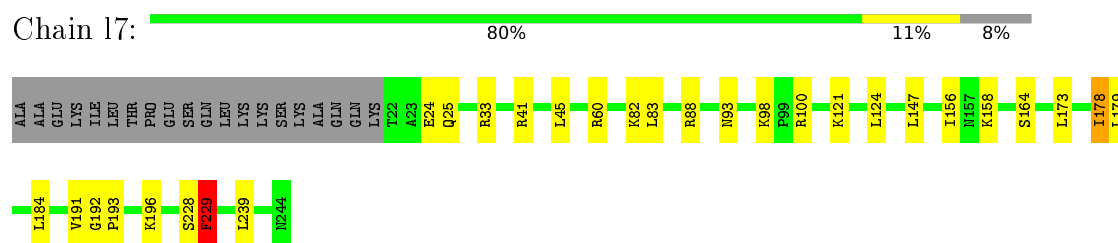




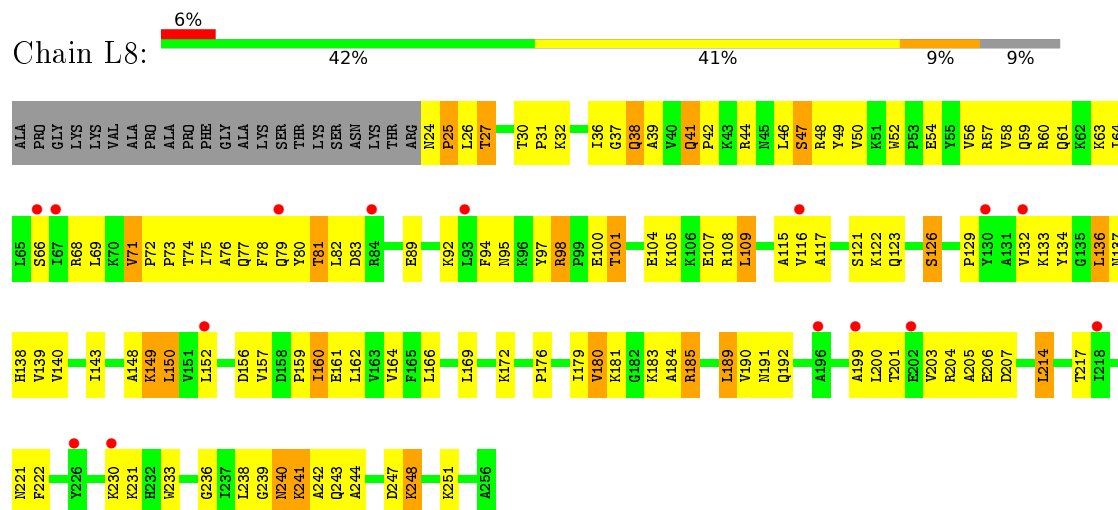
- Molecule 44: 60S ribosomal protein L7-A



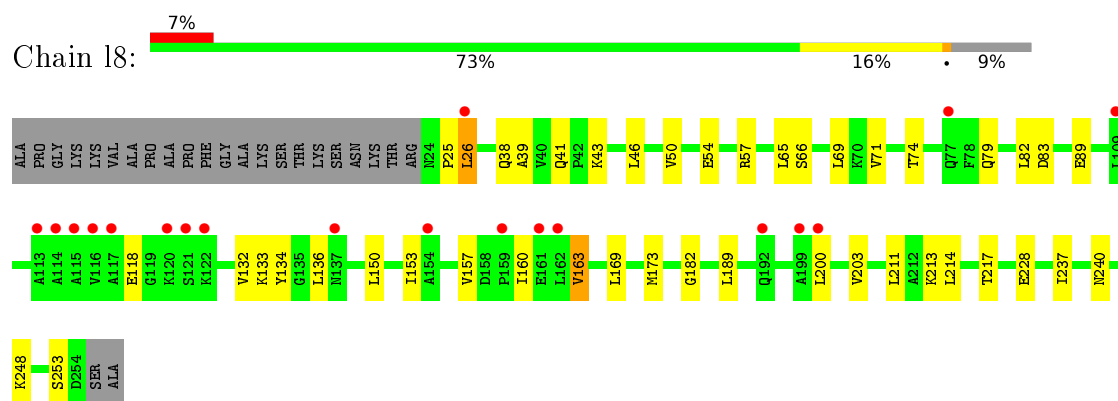
- Molecule 44: 60S ribosomal protein L7-A



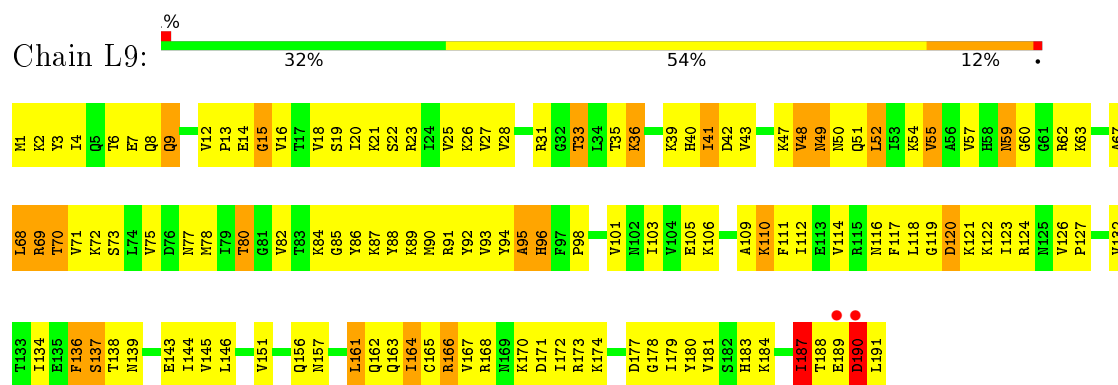
- Molecule 45: 60S ribosomal protein L8-A



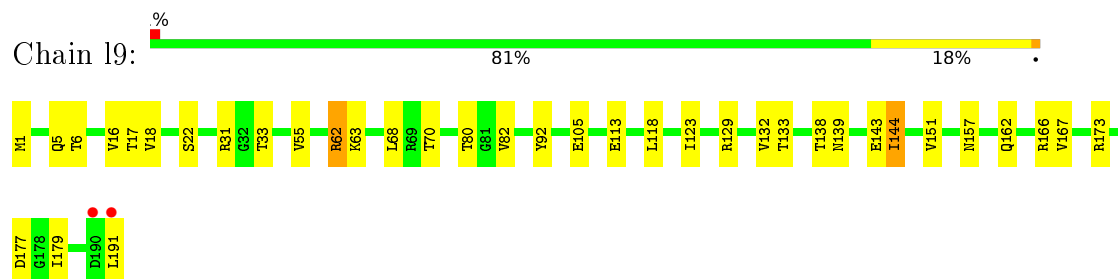
- Molecule 45: 60S ribosomal protein L8-A



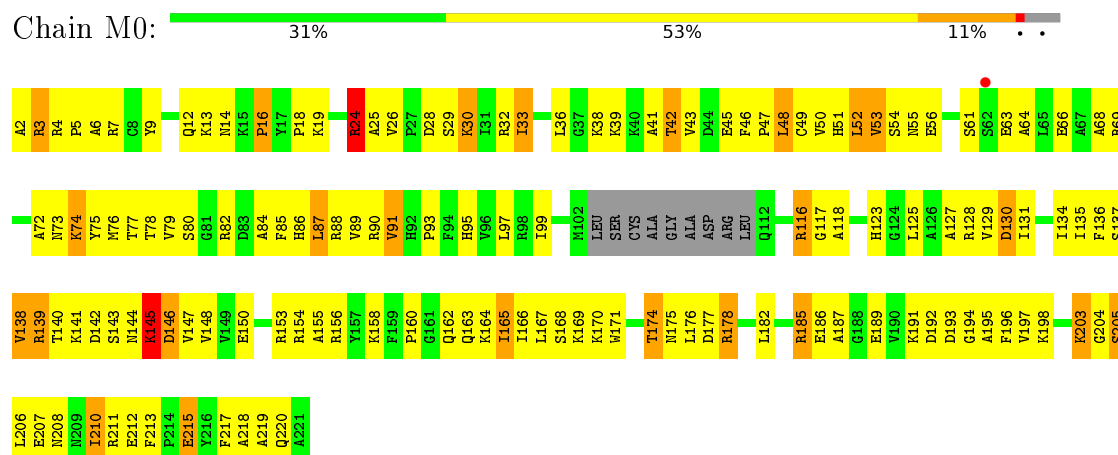
- Molecule 46: 60S ribosomal protein L9-A



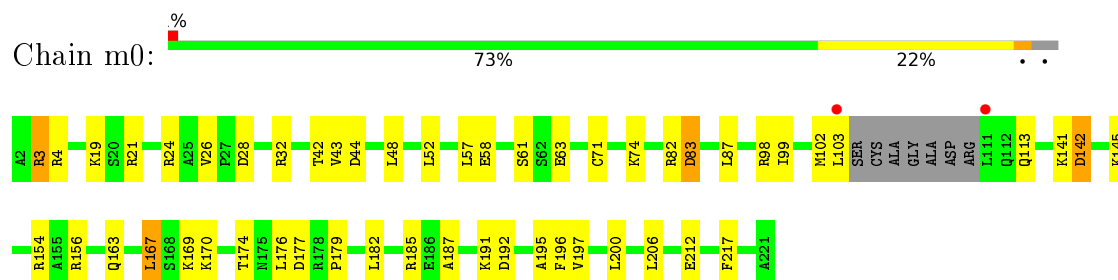
- Molecule 46: 60S ribosomal protein L9-A



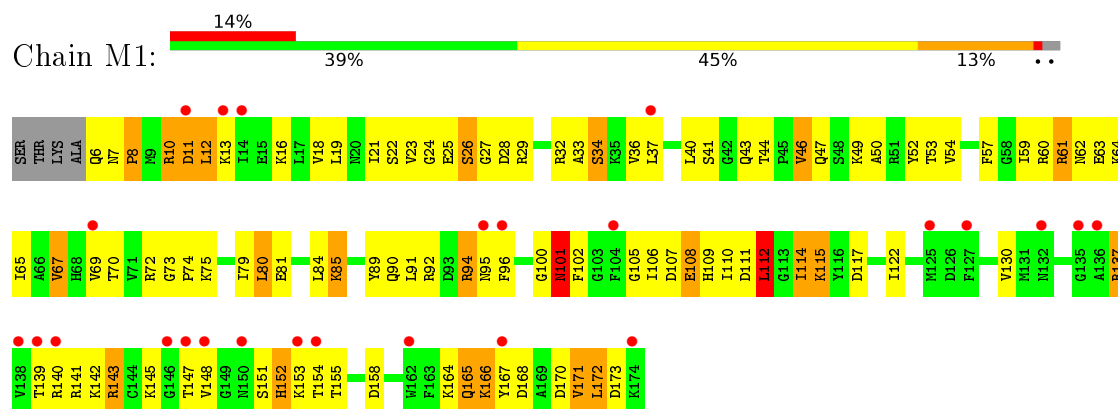
- Molecule 47: 60S ribosomal protein L10



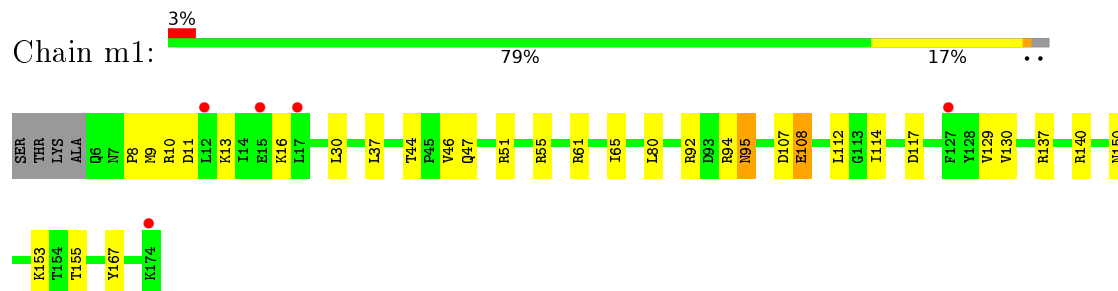
- Molecule 47: 60S ribosomal protein L10



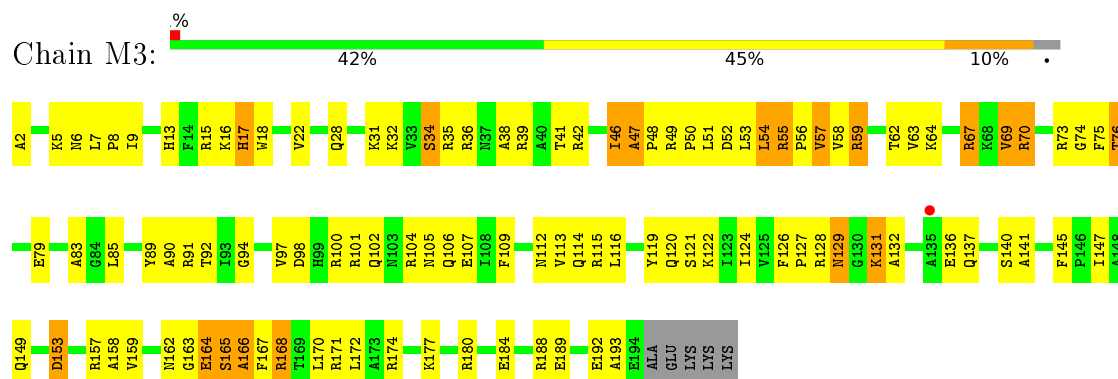
- Molecule 48: 60S ribosomal protein L11-B



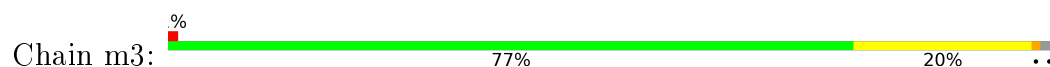
- Molecule 48: 60S ribosomal protein L11-B

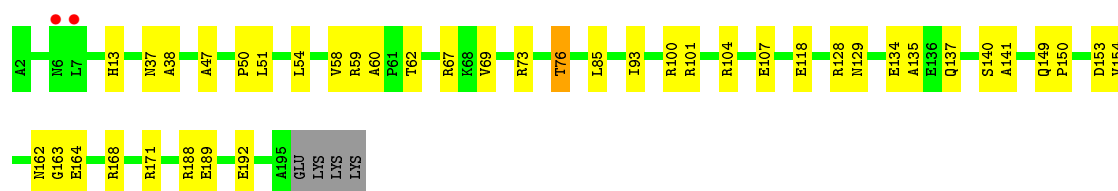


- Molecule 49: 60S ribosomal protein L13-A



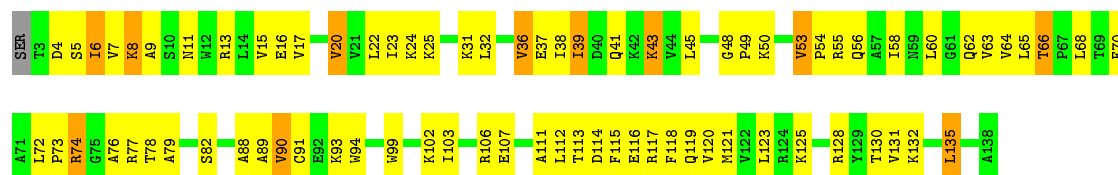
- Molecule 49: 60S ribosomal protein L13-A





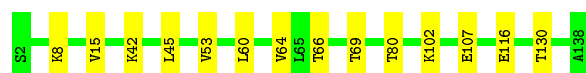
- Molecule 50: 60S ribosomal protein L14-A

Chain M4: 42% 49% 8% .



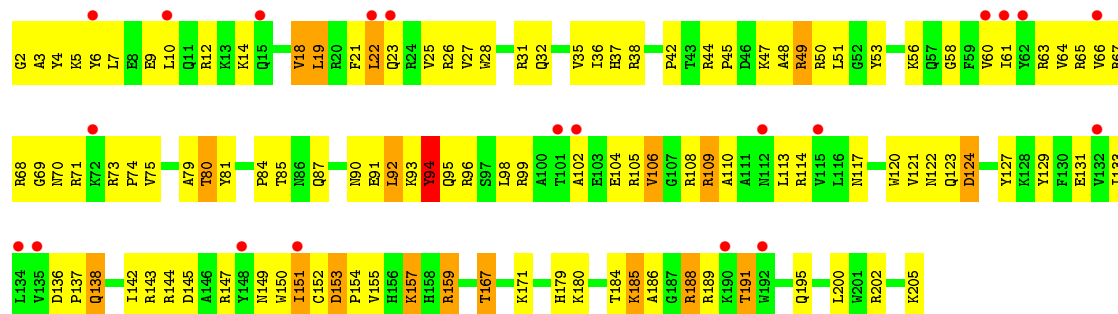
- Molecule 50: 60S ribosomal protein L14-A

Chain m4: 90% 10%



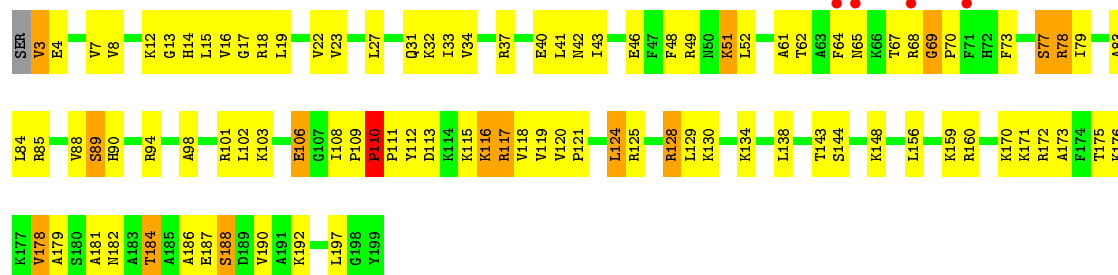
- Molecule 51: 60S ribosomal protein L15-A

Chain M5: 10% 44% 47% 9%

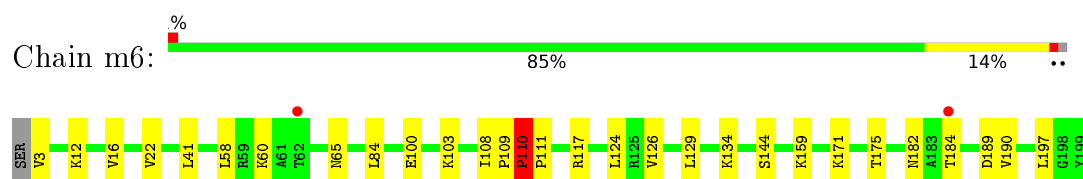


- Molecule 52: 60S ribosomal protein L16-A

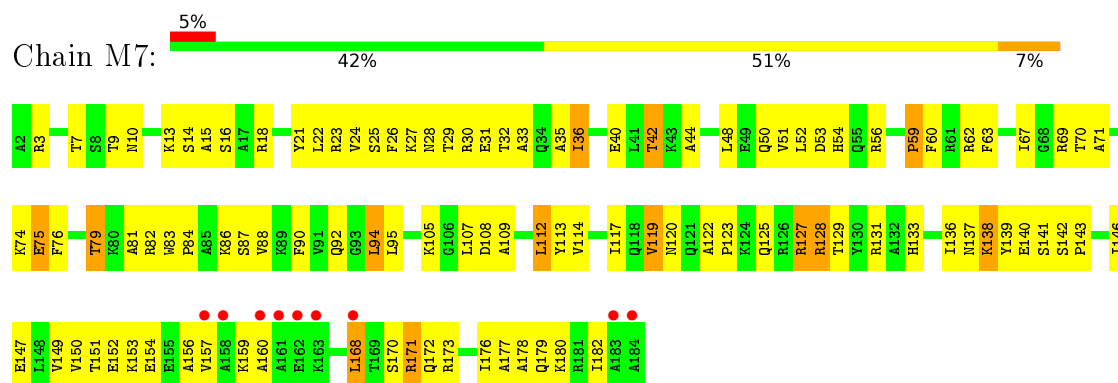
Chain M6: 2% 51% 41% 7% ..



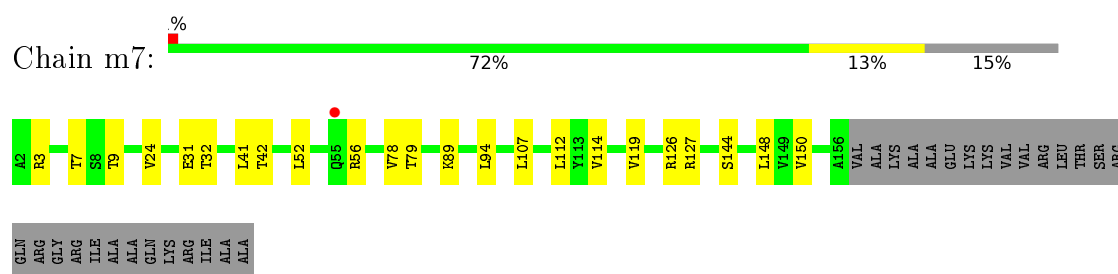
- Molecule 52: 60S ribosomal protein L16-A



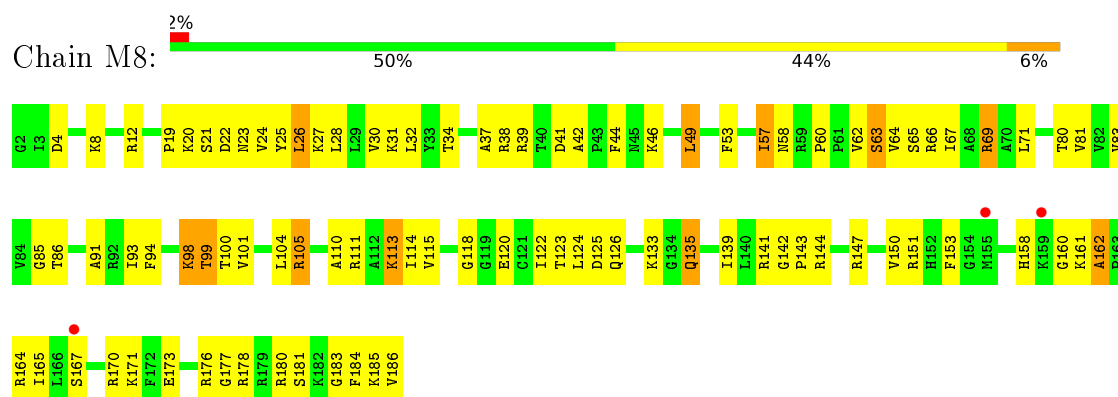
- Molecule 53: 60S ribosomal protein L17-A



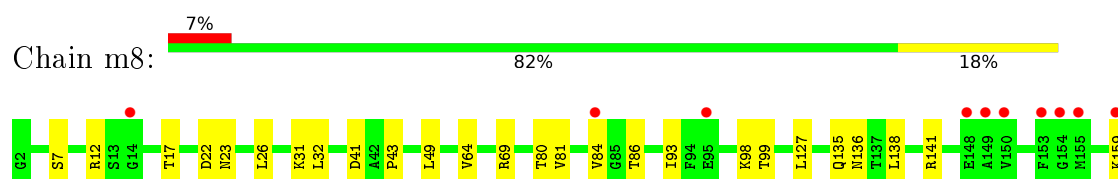
- Molecule 53: 60S ribosomal protein L17-A

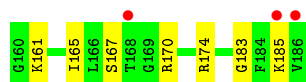


- Molecule 54: 60S ribosomal protein L18-A

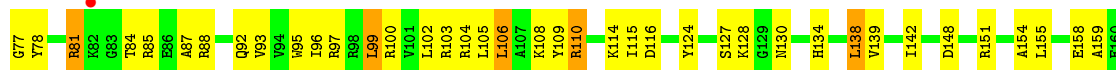


- Molecule 54: 60S ribosomal protein L18-A

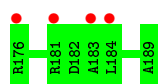
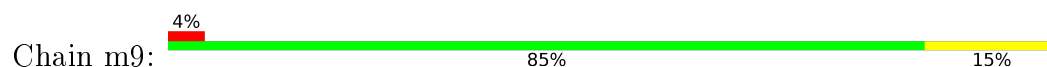




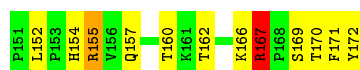
- Molecule 55: 60S ribosomal protein L19-A



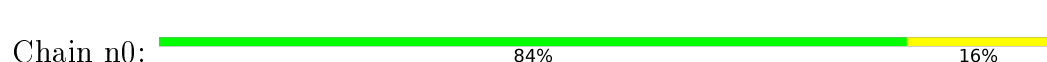
- Molecule 55: 60S ribosomal protein L19-A



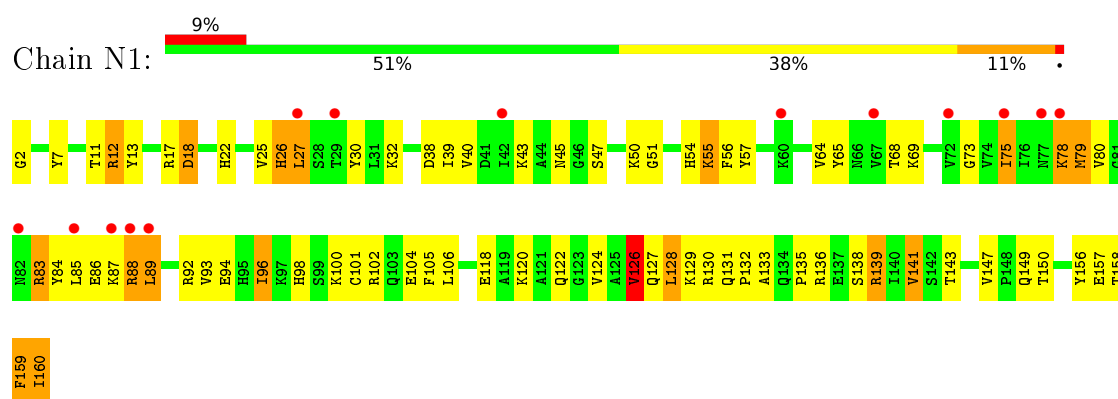
- Molecule 56: 60S ribosomal protein L20-A



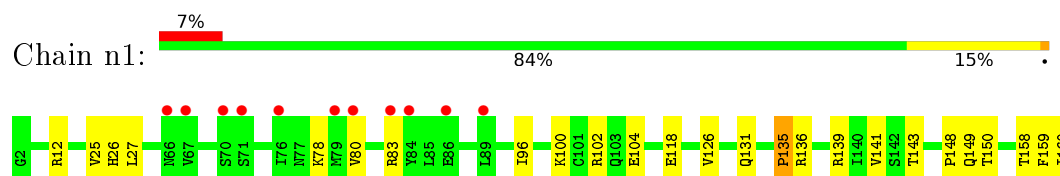
- Molecule 56: 60S ribosomal protein L20-A



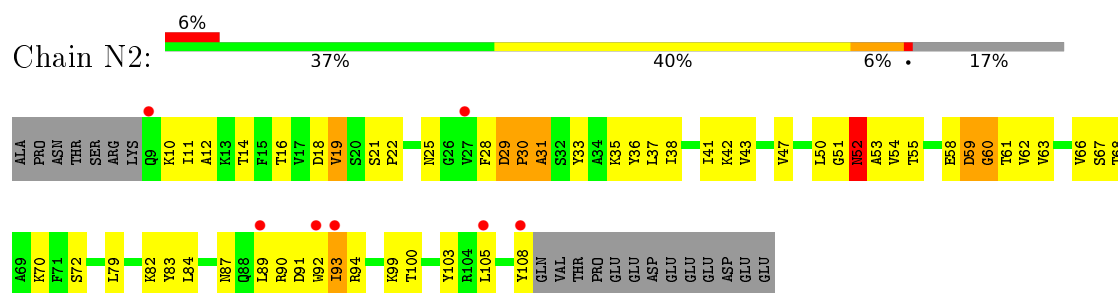
- Molecule 57: 60S ribosomal protein L21-A



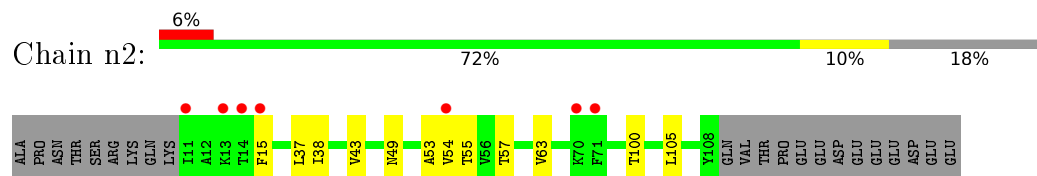
- Molecule 57: 60S ribosomal protein L21-A



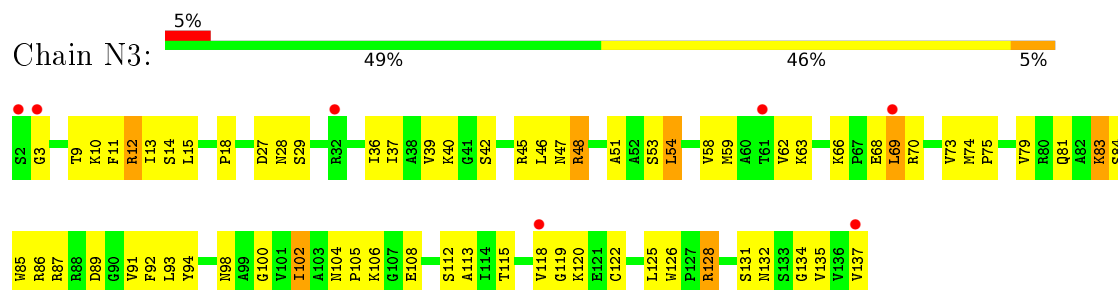
- Molecule 58: 60S ribosomal protein L22-A



- Molecule 58: 60S ribosomal protein L22-A

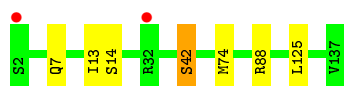


- Molecule 59: 60S ribosomal protein L23-A

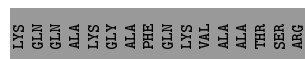
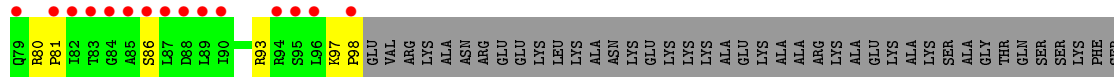
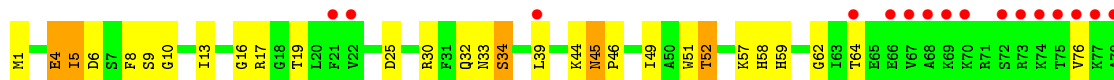
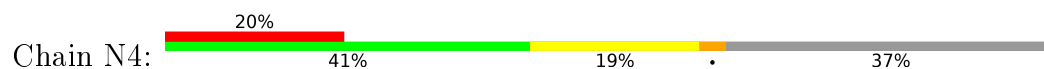


- Molecule 59: 60S ribosomal protein L23-A

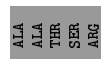
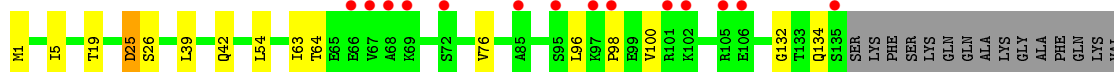
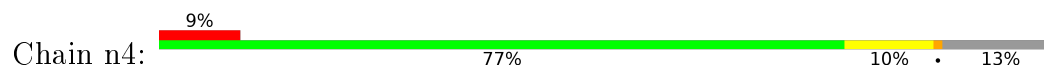




- Molecule 60: 60S ribosomal protein L24-A



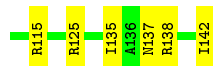
- Molecule 60: 60S ribosomal protein L24-A



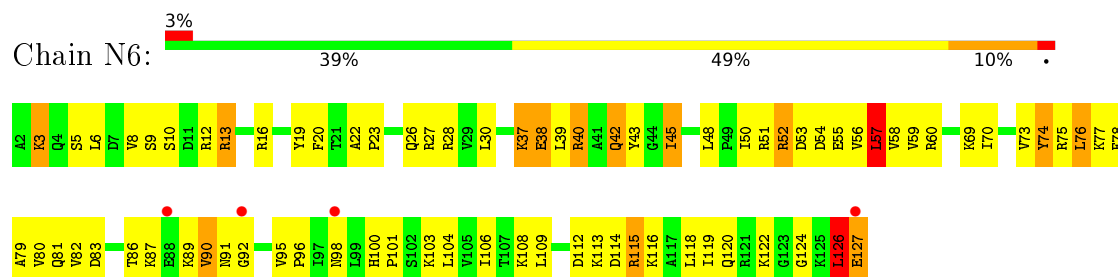
- Molecule 61: 60S ribosomal protein L25



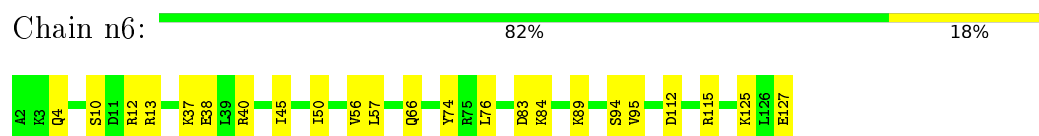
- Molecule 61: 60S ribosomal protein L25



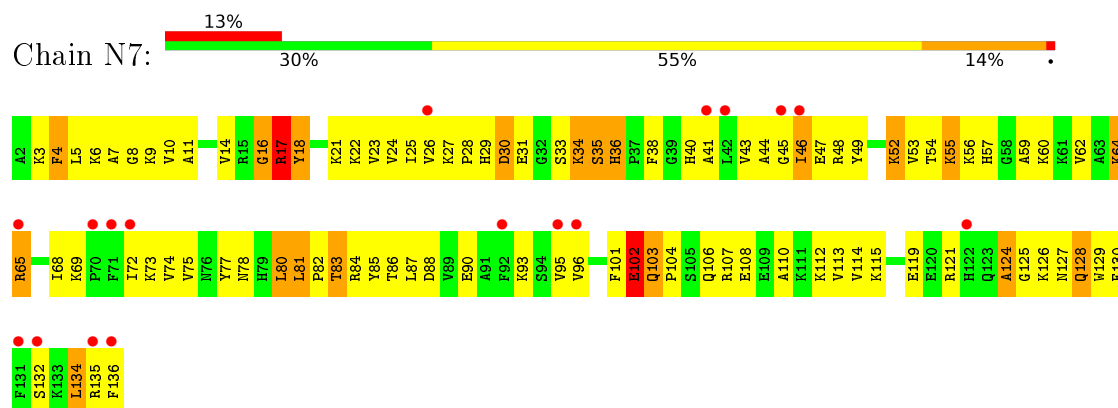
- Molecule 62: 60S ribosomal protein L26-A



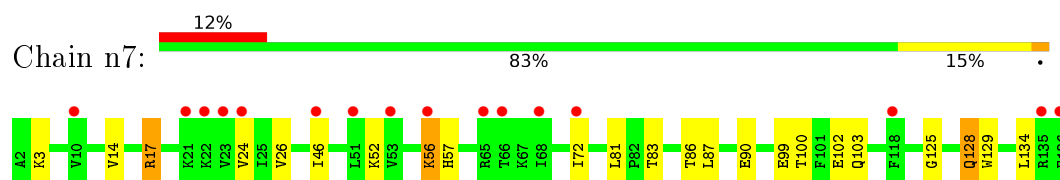
- Molecule 62: 60S ribosomal protein L26-A



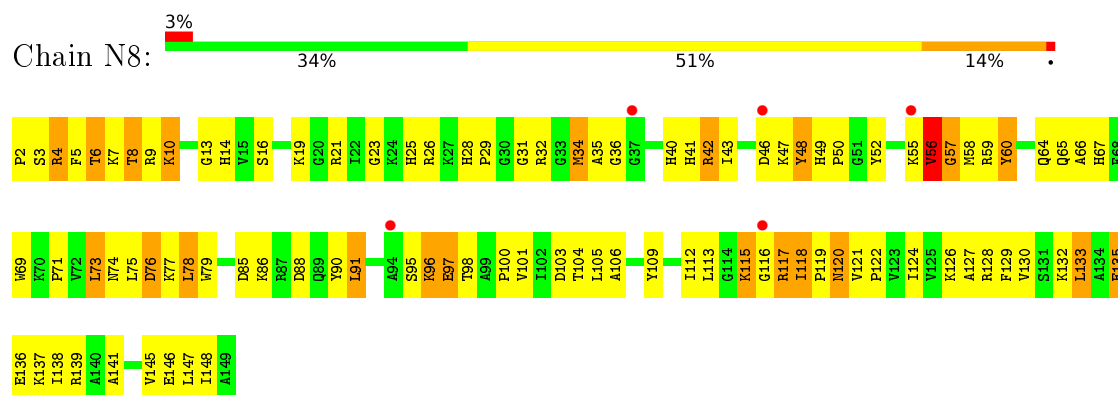
- Molecule 63: 60S ribosomal protein L27-A



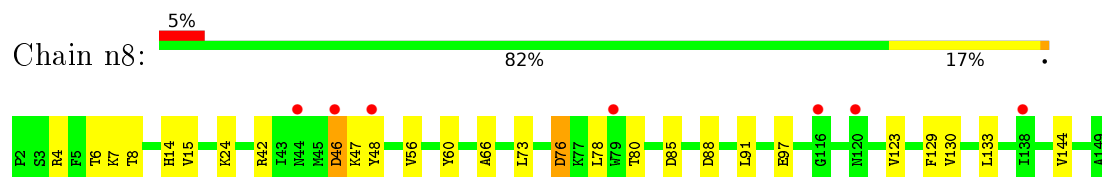
- Molecule 63: 60S ribosomal protein L27-A



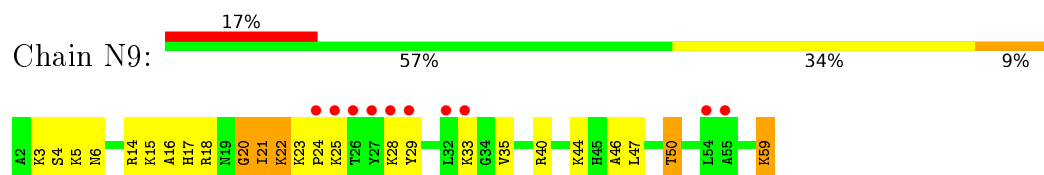
- Molecule 64: 60S ribosomal protein L28



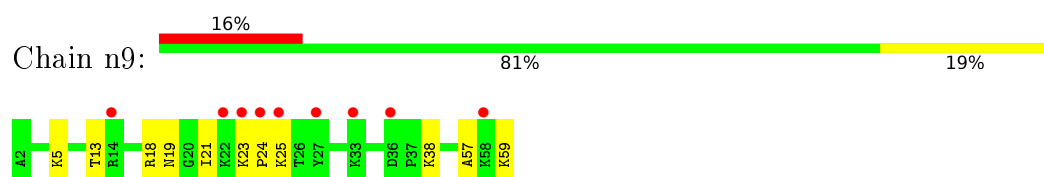
- Molecule 64: 60S ribosomal protein L28



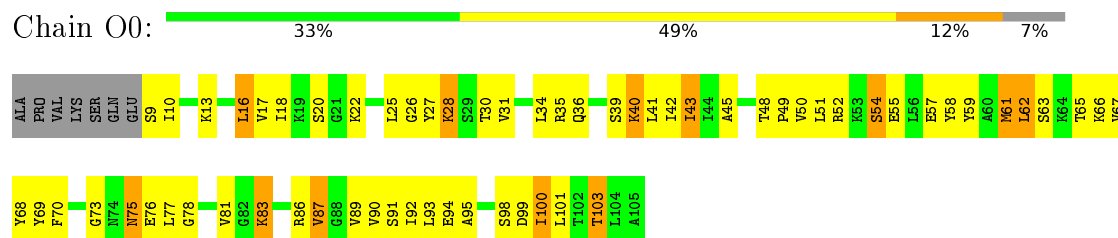
- Molecule 65: 60S ribosomal protein L29



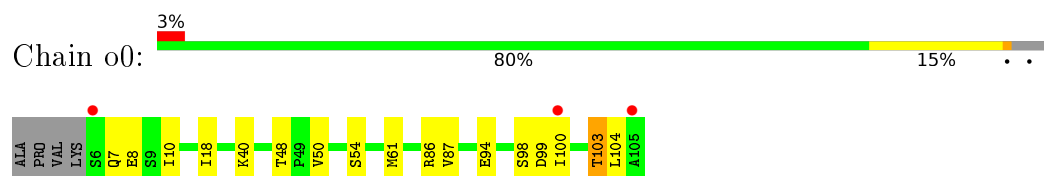
- Molecule 65: 60S ribosomal protein L29



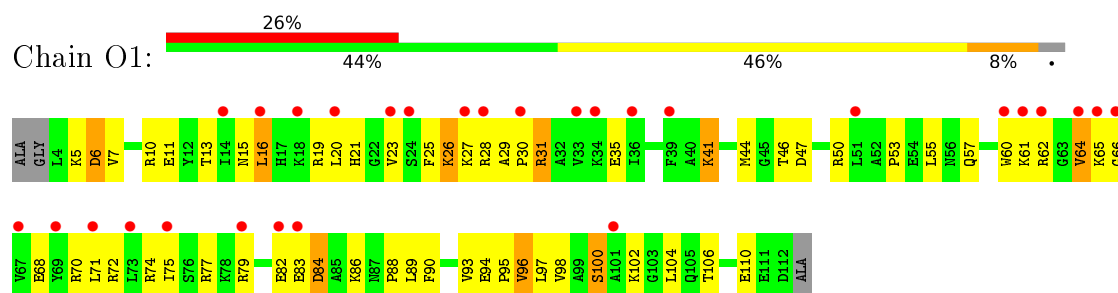
- Molecule 66: 60S ribosomal protein L30



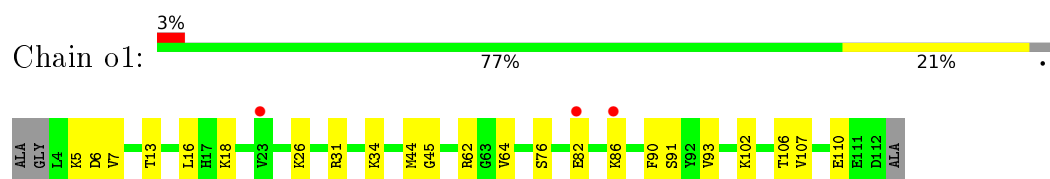
- Molecule 66: 60S ribosomal protein L30



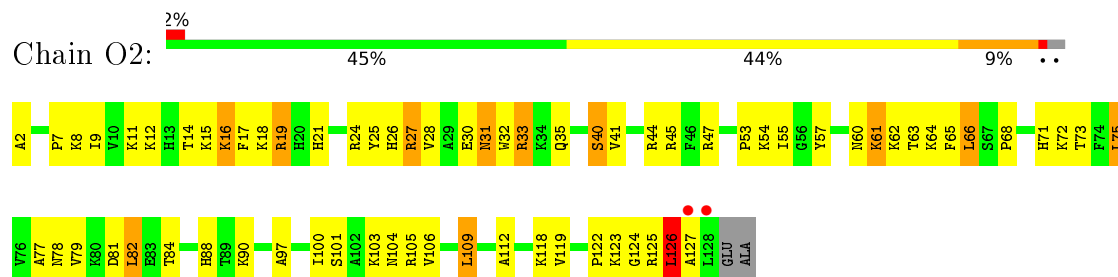
- Molecule 67: 60S ribosomal protein L31-A



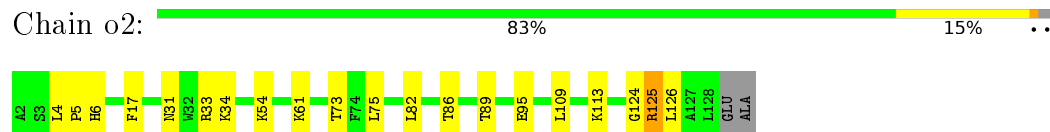
- Molecule 67: 60S ribosomal protein L31-A



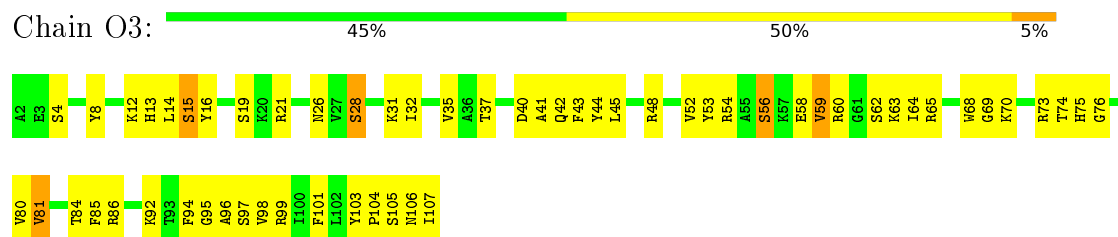
- Molecule 68: 60S ribosomal protein L32



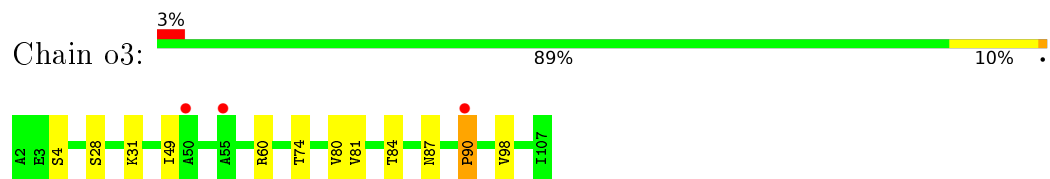
- Molecule 68: 60S ribosomal protein L32



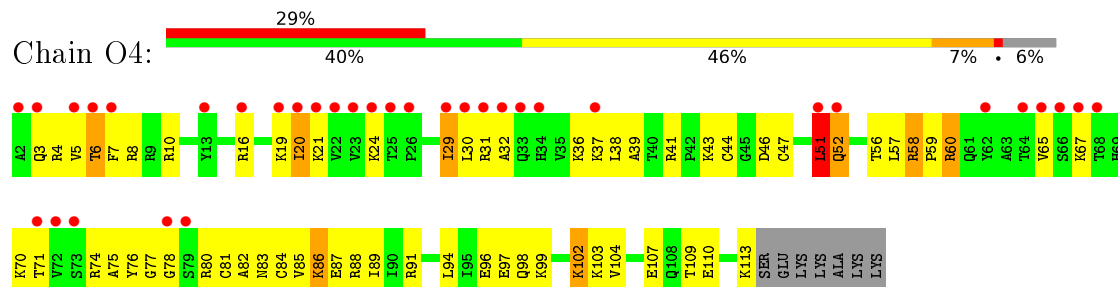
- Molecule 69: 60S ribosomal protein L33-A



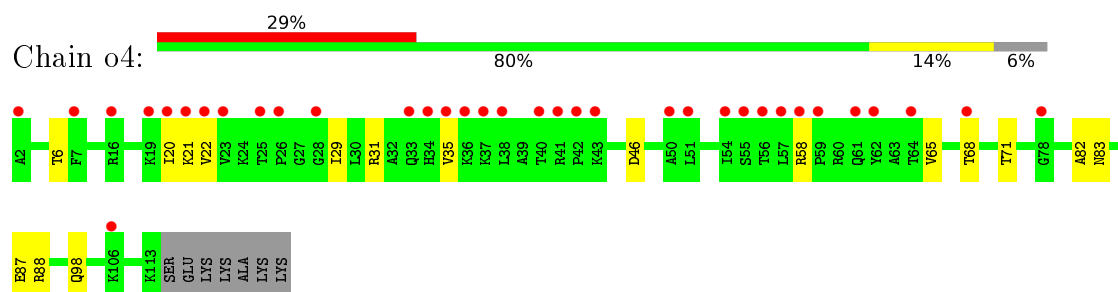
- Molecule 69: 60S ribosomal protein L33-A



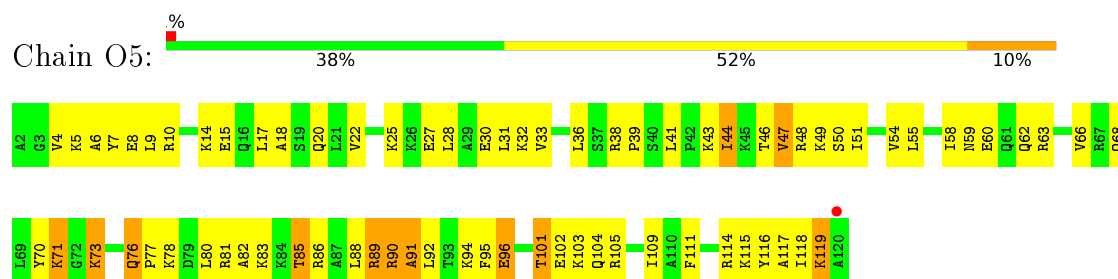
- Molecule 70: 60S ribosomal protein L34-A (eL34)



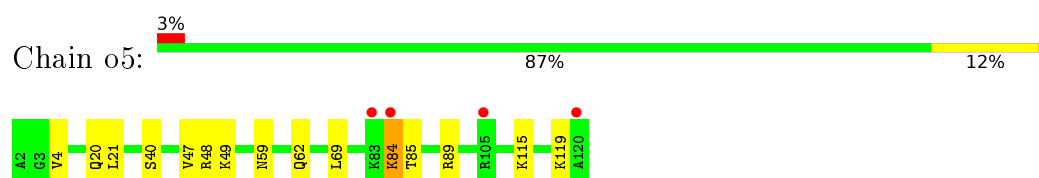
- Molecule 70: 60S ribosomal protein L34-A (eL34)



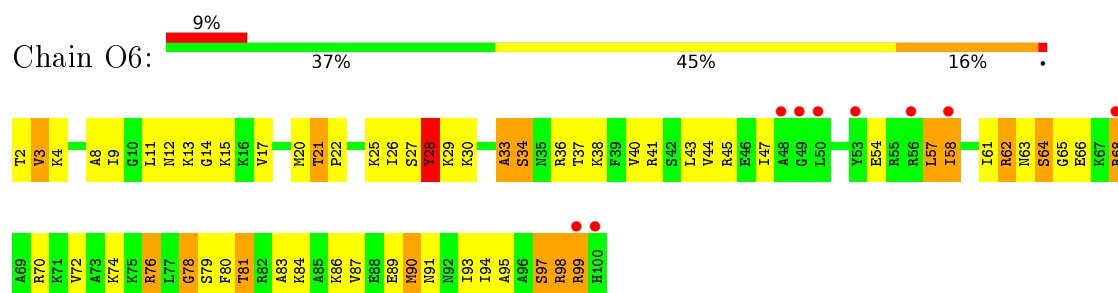
- Molecule 71: 60S ribosomal protein L35-A



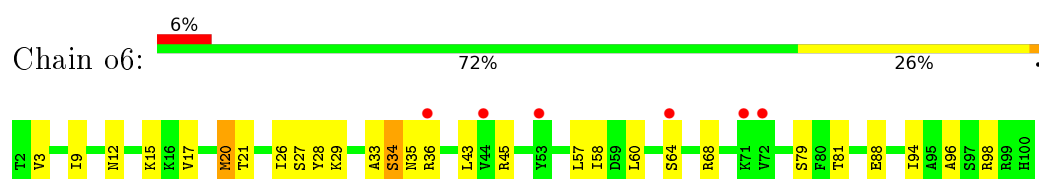
- Molecule 71: 60S ribosomal protein L35-A



- Molecule 72: 60S ribosomal protein L36-A

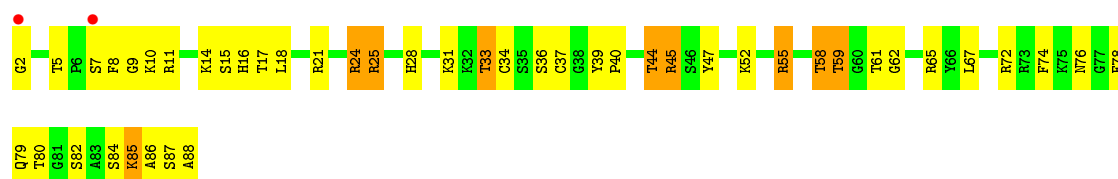


- Molecule 72: 60S ribosomal protein L36-A



- Molecule 73: 60S ribosomal protein L37-A

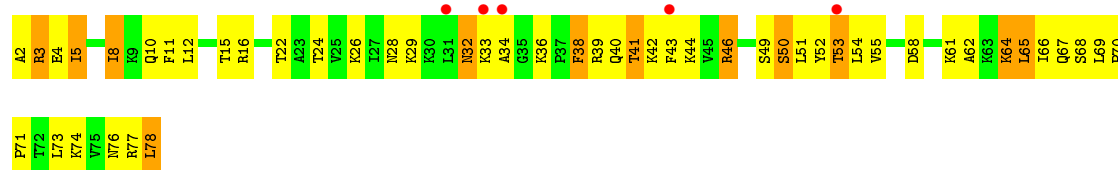




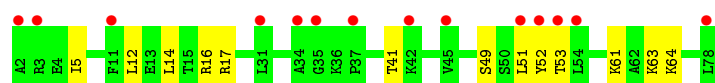
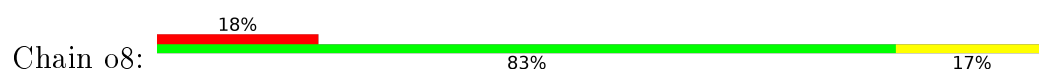
- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



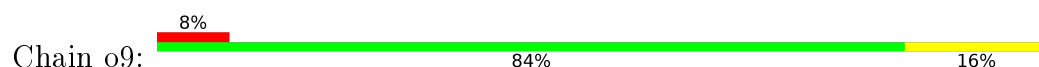
- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39

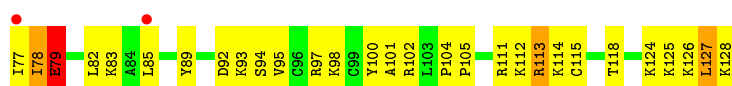


- Molecule 75: 60S ribosomal protein L39

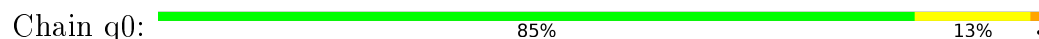


- Molecule 76: Ubiquitin-60S ribosomal protein L40

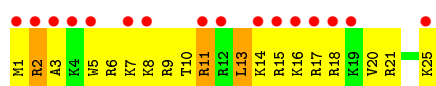




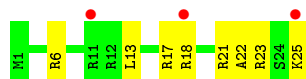
- Molecule 76: Ubiquitin-60S ribosomal protein L40



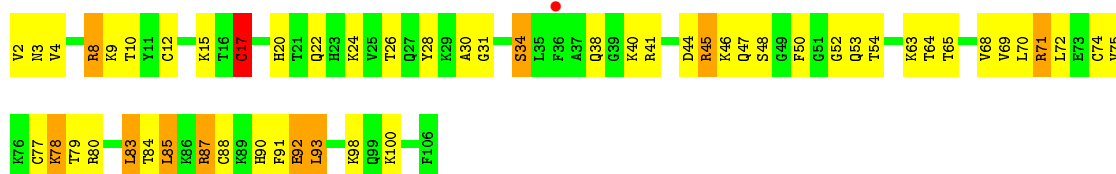
- Molecule 77: 60S ribosomal protein L41-A



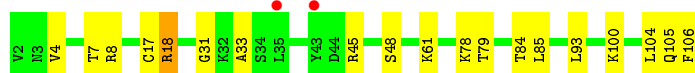
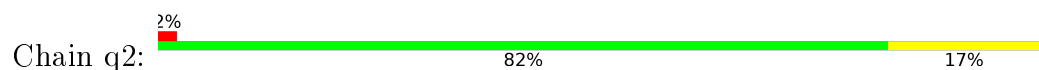
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A

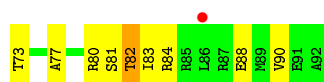


- Molecule 78: 60S ribosomal protein L42-A

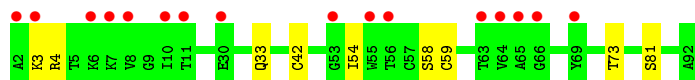
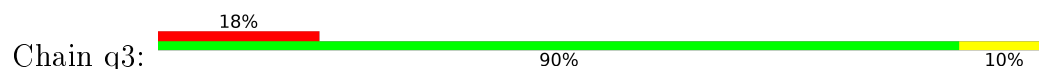


- Molecule 79: 60S ribosomal protein L43-A

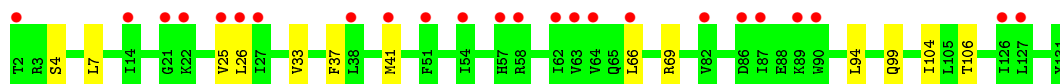




- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S22-A

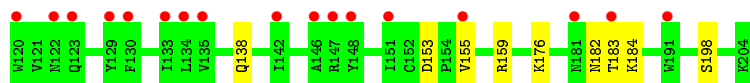
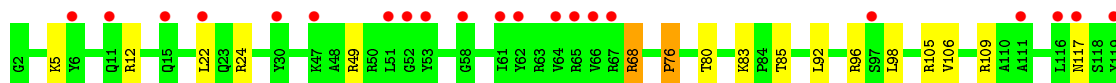


- Molecule 81: 60S ribosomal protein L12-A (uL11)

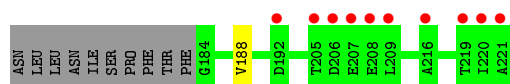
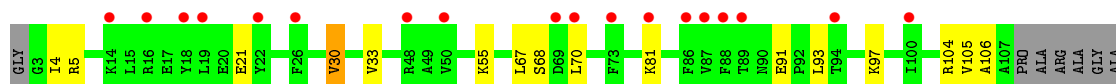


There are no outlier residues recorded for this chain.

- Molecule 82: 60S ribosomal protein L15-A



- Molecule 83: 60S acidic ribosomal protein P0



- Molecule 84: 60S ribosomal protein P1 alpha/P2 beta



There are no outlier residues recorded for this chain.

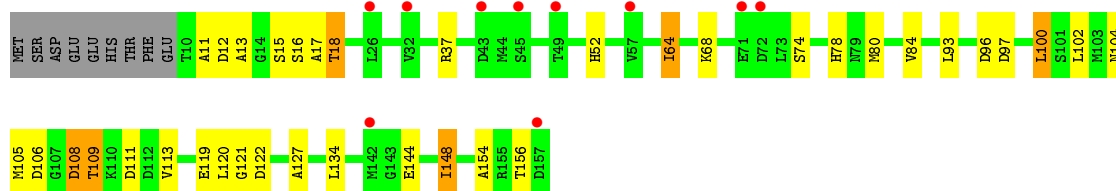
- Molecule 84: 60S ribosomal protein P1 alpha/P2 beta

Chain p2:  98%



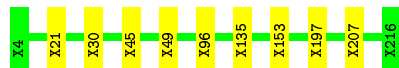
- Molecule 85: Eukaryotic translation initiation factor 5A-1

Chain f:  6% 71% 20% 6%



- Molecule 86: 60S ribosomal protein L1-A (uL1)

Chain l1:  96%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.63Å 286.45Å 303.41Å 90.00° 98.85° 90.00°	Depositor
Resolution (Å)	189.16 – 3.15 194.90 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (189.16-3.15) 99.8 (194.90-3.15)	Depositor EDS
R_{merge}	0.98	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.252 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	414393	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5CT, OHX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.43	0/42467	0.94	50/66169 (0.1%)
1	6	0.50	0/42790	0.98	58/66673 (0.1%)
2	S0	0.30	0/1617	0.51	0/2215
2	s0	0.33	0/1623	0.56	0/2222
3	S1	0.28	0/1735	0.52	0/2335
3	s1	0.35	0/1748	0.55	0/2352
4	S2	0.33	0/1665	0.53	0/2263
4	s2	0.38	0/1665	0.61	0/2263
5	S3	0.32	0/1759	0.52	0/2368
5	s3	0.31	0/1759	0.49	0/2368
6	S4	0.32	0/2109	0.56	0/2839
6	s4	0.36	0/2109	0.58	0/2839
7	S5	0.29	0/1629	0.51	0/2202
7	s5	0.30	0/1629	0.51	0/2202
8	S6	0.34	0/1823	0.50	0/2439
8	s6	0.37	0/1779	0.55	0/2379
9	S7	0.31	0/1506	0.54	0/2028
9	s7	0.32	0/1516	0.56	0/2043
10	S8	0.35	0/1514	0.53	0/2021
10	s8	0.38	0/1514	0.54	0/2021
11	S9	0.31	0/1519	0.52	0/2035
11	s9	0.36	0/1519	0.52	0/2035
12	C0	0.31	0/789	0.53	1/1067 (0.1%)
12	c0	0.29	0/776	0.58	3/1047 (0.3%)
13	C1	0.36	0/1239	0.53	0/1673
13	c1	0.40	0/1194	0.55	0/1610
14	C2	0.29	0/898	0.52	1/1220 (0.1%)
14	c2	0.26	0/898	0.50	0/1220
15	C3	0.34	0/1215	0.55	0/1638
15	c3	0.37	0/1215	0.52	0/1638
16	C4	0.28	0/901	0.55	0/1217
16	c4	0.34	0/960	0.58	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.32	0/998	0.56	0/1341
17	c5	0.36	0/1060	0.56	1/1426 (0.1%)
18	C6	0.32	0/1125	0.58	1/1510 (0.1%)
18	c6	0.34	0/1131	0.55	0/1518
19	C7	0.35	0/935	0.55	0/1254
19	c7	0.32	0/914	0.52	0/1224
20	C8	0.32	0/1211	0.54	0/1628
20	c8	0.34	0/1211	0.53	0/1628
21	C9	0.32	0/1130	0.52	0/1517
21	c9	0.31	0/1130	0.52	0/1517
22	D0	0.33	0/865	0.53	0/1169
22	d0	0.33	0/892	0.53	0/1205
23	D1	0.32	0/693	0.51	0/935
23	d1	0.36	0/693	0.55	0/935
24	D2	0.33	0/1038	0.60	1/1395 (0.1%)
25	D3	0.39	0/1139	0.58	0/1518
25	d3	0.42	0/1139	0.60	0/1518
26	D4	0.34	0/1087	0.50	0/1449
26	d4	0.36	0/1087	0.57	0/1449
27	D5	0.28	0/571	0.52	0/768
27	d5	0.29	0/566	0.52	0/761
28	D6	0.34	0/782	0.58	0/1047
28	d6	0.42	0/782	0.57	0/1047
29	D7	0.31	0/620	0.52	0/838
29	d7	0.32	0/620	0.54	0/838
30	D8	0.28	0/499	0.49	0/670
30	d8	0.32	0/499	0.53	0/670
31	D9	0.33	0/452	0.57	1/600 (0.2%)
31	d9	0.36	0/452	0.53	0/600
32	E0	0.29	0/483	0.49	0/643
32	e0	0.37	0/499	0.61	0/665
33	E1	0.32	0/577	0.60	0/770
33	e1	0.32	0/619	0.61	0/822
34	SR	0.29	0/2490	0.50	0/3389
34	sR	0.28	0/2495	0.48	0/3395
35	SM	0.35	0/1113	0.58	2/1502 (0.1%)
35	sM	0.37	0/682	0.52	0/921
36	1	0.66	11/75394 (0.0%)	1.10	227/117545 (0.2%)
36	5	0.69	7/75865 (0.0%)	1.12	209/118275 (0.2%)
37	3	0.55	0/2883	0.97	2/4491 (0.0%)
37	7	0.67	1/2883 (0.0%)	1.08	6/4491 (0.1%)
38	4	0.61	0/3746	1.06	2/5832 (0.0%)
38	8	0.61	0/3746	1.04	3/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.43	0/1948	0.62	0/2617
39	l2	0.46	0/1946	0.65	1/2614 (0.0%)
40	L3	0.46	0/3146	0.61	0/4228
40	l3	0.51	0/3146	0.63	0/4228
41	L4	0.47	0/2800	0.67	2/3790 (0.1%)
41	l4	0.47	1/2800 (0.0%)	0.66	2/3790 (0.1%)
42	L5	0.39	0/2425	0.57	0/3271
42	l5	0.46	0/2408	0.59	0/3248
43	L6	0.45	0/1260	0.58	0/1694
43	l6	0.49	0/1269	0.61	0/1705
44	L7	0.48	0/1821	0.63	0/2451
44	l7	0.51	0/1828	0.66	2/2461 (0.1%)
45	L8	0.37	0/1836	0.56	0/2481
45	l8	0.36	0/1795	0.55	0/2429
46	L9	0.45	0/1539	0.60	0/2073
46	l9	0.49	0/1539	0.62	0/2073
47	M0	0.48	0/1741	0.62	1/2335 (0.0%)
47	m0	0.50	0/1758	0.69	2/2358 (0.1%)
48	M1	0.36	0/1374	0.57	1/1842 (0.1%)
48	m1	0.43	0/1374	0.60	0/1842
49	M3	0.44	0/1568	0.59	0/2106
49	m3	0.44	0/1573	0.63	0/2113
50	M4	0.46	0/1068	0.58	0/1438
50	m4	0.48	0/1074	0.59	0/1446
51	M5	0.47	0/1755	0.64	0/2350
52	M6	0.53	0/1585	0.65	1/2128 (0.0%)
52	m6	0.60	0/1585	0.69	1/2128 (0.0%)
53	M7	0.48	0/1443	0.61	0/1944
53	m7	0.57	0/1250	0.65	0/1683
54	M8	0.45	0/1465	0.64	0/1965
54	m8	0.47	0/1465	0.66	0/1965
55	M9	0.33	0/1538	0.50	0/2050
55	m9	0.41	0/1538	0.53	0/2050
56	N0	0.47	0/1481	0.65	2/1990 (0.1%)
56	n0	0.52	0/1481	0.64	0/1990
57	N1	0.46	0/1300	0.58	0/1743
57	n1	0.51	0/1300	0.59	0/1743
58	N2	0.31	0/812	0.52	0/1099
58	n2	0.37	0/794	0.57	0/1076
59	N3	0.47	0/1018	0.61	0/1369
59	n3	0.53	0/1018	0.64	0/1369
60	N4	0.37	0/712	0.52	0/958
60	n4	0.42	0/1052	0.55	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	N5	0.43	0/979	0.60	0/1321
61	n5	0.43	0/974	0.60	0/1314
62	N6	0.47	0/1004	0.67	2/1341 (0.1%)
62	n6	0.43	0/1004	0.63	0/1341
63	N7	0.35	0/1118	0.56	0/1497
63	n7	0.35	0/1118	0.53	0/1497
64	N8	0.46	0/1204	0.66	0/1612
64	n8	0.49	0/1204	0.67	0/1612
65	N9	0.44	0/473	0.58	0/629
65	n9	0.50	0/473	0.69	0/629
66	O0	0.32	0/751	0.51	0/1008
66	o0	0.34	0/775	0.52	0/1040
67	O1	0.43	0/890	0.54	0/1196
67	o1	0.47	0/897	0.65	0/1205
68	O2	0.50	0/1041	0.63	0/1394
68	o2	0.54	0/1041	0.65	0/1394
69	O3	0.52	0/868	0.61	0/1168
69	o3	0.55	0/868	0.65	0/1168
70	O4	0.38	0/890	0.57	1/1189 (0.1%)
70	o4	0.41	0/890	0.60	0/1189
71	O5	0.44	0/978	0.61	0/1301
71	o5	0.39	0/974	0.56	0/1297
72	O6	0.41	0/778	0.61	0/1034
72	o6	0.42	0/777	0.59	0/1033
73	O7	0.48	0/696	0.68	0/923
73	o7	0.47	0/696	0.70	1/923 (0.1%)
74	O8	0.36	0/618	0.53	0/826
74	o8	0.36	0/614	0.56	0/822
75	O9	0.48	0/443	0.69	0/588
75	o9	0.52	0/443	0.62	0/588
76	Q0	0.45	0/423	0.66	0/562
76	q0	0.52	0/423	0.64	0/562
77	Q1	0.40	0/234	0.67	0/300
77	q1	0.51	0/234	0.66	0/300
78	Q2	0.58	1/860 (0.1%)	0.64	0/1136
78	q2	0.63	1/860 (0.1%)	0.70	1/1136 (0.1%)
79	Q3	0.42	0/701	0.59	0/934
79	q3	0.49	0/701	0.60	0/934
80	d2	0.37	0/1035	0.62	1/1388 (0.1%)
82	m5	0.43	0/1757	0.60	0/2354
83	p0	0.30	0/1092	0.48	0/1474
85	f	0.40	0/1121	0.64	0/1508
All	All	0.53	22/432423 (0.0%)	0.91	589/634777 (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
12	c0	0	1
16	c4	0	1
18	c6	0	1
19	C7	0	1
20	C8	0	1
27	D5	0	1
28	D6	0	2
44	L7	0	1
44	l7	0	1
52	M6	0	2
52	m6	0	1
64	n8	0	2
65	N9	0	1
85	f	1	0
86	l1	18	13
All	All	19	29

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	11.44	2.01	1.82
78	Q2	17	CYS	CB-SG	10.39	2.00	1.82
36	1	2954	U	C2-N3	9.03	1.44	1.37
36	5	1152	G	N9-C4	-8.08	1.31	1.38
36	1	2808	A	N3-C4	7.52	1.39	1.34

The worst 5 of 589 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-16.35	116.19	126.00
36	5	1152	G	N3-C4-C5	16.30	136.75	128.60
36	5	1152	G	C2-N3-C4	-13.10	105.35	111.90
36	5	2199	G	N1-C6-O6	12.73	127.54	119.90
36	5	2403	G	N1-C6-O6	10.83	126.40	119.90

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
85	f	51	5CT	C2
86	l1	4	UNK	CA
86	l1	21	UNK	CA
86	l1	23	UNK	CA
86	l1	27	UNK	CA

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
20	C8	81	ILE	Peptide
27	D5	94	LYS	Peptide
28	D6	10	ARG	Peptide
28	D6	97	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37970	0	19106	945	0
1	6	38260	0	19251	800	0
2	S0	1577	0	1567	152	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	125	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	140	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1816	107	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	160	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	140	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	108	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	112	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	134	0
11	s9	1494	0	1573	0	0
12	C0	772	0	727	53	0
12	c0	761	0	697	0	0
13	C1	1213	0	1257	61	0
13	c1	1168	0	1233	0	0
14	C2	890	0	887	67	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	82	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	89	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	93	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	90	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	111	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	94	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	79	0
22	d0	882	0	939	0	0
23	D1	684	0	672	69	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	62	0
25	D3	1121	0	1196	76	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	95	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	38	0
27	d5	558	0	598	0	0
28	D6	769	0	814	86	0
28	d6	769	0	814	0	0
29	D7	610	0	630	42	0
29	d7	610	0	631	0	0
30	D8	497	0	535	42	0
30	d8	497	0	535	0	0
31	D9	442	0	427	35	0
31	d9	442	0	428	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	E0	475	0	525	39	0
32	e0	491	0	542	0	0
33	E1	566	0	602	58	0
33	e1	608	0	657	0	0
34	SR	2437	0	2386	146	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	1002	65	0
35	sM	679	0	615	0	0
36	1	67355	0	33847	1247	0
36	5	67780	0	34064	1260	0
37	3	2579	0	1304	46	0
37	7	2579	0	1304	37	0
38	4	3353	0	1695	65	0
38	8	3353	0	1695	64	0
39	L2	1914	0	1981	125	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	193	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	206	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	165	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	77	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	112	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	112	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	133	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	136	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	86	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	122	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	69	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1778	113	0
52	M6	1555	0	1659	97	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	87	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	89	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1486	93	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	90	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	38	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	53	0
59	n3	1003	0	1047	0	0
60	N4	699	0	640	27	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	75	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	65	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	97	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	111	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	30	0
65	n9	462	0	491	0	0
66	O0	743	0	797	54	0
66	o0	767	0	816	0	0
67	O1	876	0	912	44	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	65	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	69	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	68	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	73	0
72	o6	770	0	846	0	0
73	O7	681	0	683	44	0
73	o7	681	0	683	0	0
74	O8	612	0	682	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	o8	608	0	671	0	0
75	O9	436	0	475	53	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	23	0
77	q1	233	0	284	0	0
78	Q2	847	0	914	54	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	41	0
79	q3	694	0	734	0	0
80	d2	1021	0	1057	0	0
81	m2	750	0	178	0	0
82	m5	1720	0	1779	0	0
83	p0	1077	0	1041	0	0
84	p1	235	0	53	0	0
84	p2	230	0	53	0	0
85	f	1122	0	1115	0	0
86	l1	1063	0	203	0	0
87	1	362	0	0	0	0
87	2	96	0	0	0	0
87	3	9	0	0	0	0
87	4	20	0	0	0	0
87	5	400	0	0	0	0
87	6	115	0	0	0	0
87	7	16	0	0	0	0
87	8	12	0	0	0	0
87	D4	1	0	0	0	0
87	D9	1	0	0	0	0
87	L2	2	0	0	0	0
87	L3	3	0	0	0	0
87	L6	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	M6	1	0	0	0	0
87	M7	3	0	0	0	0
87	M8	1	0	0	0	0
87	N0	1	0	0	0	0
87	N3	3	0	0	0	0
87	N6	1	0	0	0	0
87	N8	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	N9	1	0	0	0	0
87	O2	1	0	0	0	0
87	O3	2	0	0	0	0
87	O4	1	0	0	0	0
87	O7	3	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	0	0
87	S4	1	0	0	0	0
87	S9	1	0	0	0	0
87	SM	1	0	0	0	0
87	c7	1	0	0	0	0
87	d2	1	0	0	0	0
87	d3	1	0	0	0	0
87	d6	1	0	0	0	0
87	f	3	0	0	0	0
87	l2	3	0	0	0	0
87	l3	1	0	0	0	0
87	l5	1	0	0	0	0
87	l7	1	0	0	0	0
87	m0	1	0	0	0	0
87	m3	1	0	0	0	0
87	m6	2	0	0	0	0
87	m7	3	0	0	0	0
87	n0	2	0	0	0	0
87	n3	1	0	0	0	0
87	n6	1	0	0	0	0
87	n8	3	0	0	0	0
87	n9	2	0	0	0	0
87	o2	2	0	0	0	0
87	o4	1	0	0	0	0
87	o9	1	0	0	0	0
87	q0	1	0	0	0	0
87	q1	1	0	0	0	0
87	s8	1	0	0	0	0
87	sM	1	0	0	0	0
88	1	2457	0	0	243	0
88	2	1113	0	0	141	0
88	3	77	0	0	3	0
88	4	112	0	0	9	0
88	5	2562	0	0	262	0
88	6	1211	0	0	121	0
88	7	84	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	8	140	0	0	14	0
88	C1	7	0	0	0	0
88	C3	7	0	0	5	0
88	C5	7	0	0	2	0
88	C8	7	0	0	0	0
88	D9	7	0	0	1	0
88	L3	7	0	0	3	0
88	L4	7	0	0	4	0
88	L5	7	0	0	1	0
88	M0	14	0	0	4	0
88	M5	7	0	0	1	0
88	M7	14	0	0	3	0
88	M8	7	0	0	0	0
88	M9	7	0	0	2	0
88	N1	7	0	0	1	0
88	N8	7	0	0	0	0
88	N9	7	0	0	1	0
88	O3	7	0	0	1	0
88	O7	14	0	0	4	0
88	O9	7	0	0	1	0
88	Q2	7	0	0	1	0
88	S1	7	0	0	3	0
88	S6	7	0	0	3	0
88	S8	7	0	0	2	0
88	S9	7	0	0	1	0
88	SR	7	0	0	3	0
88	c3	7	0	0	0	0
88	c5	7	0	0	0	0
88	c8	7	0	0	0	0
88	l3	21	0	0	0	0
88	l4	14	0	0	0	0
88	l5	14	0	0	0	0
88	l9	7	0	0	0	0
88	m0	21	0	0	0	0
88	m5	7	0	0	0	0
88	m7	7	0	0	0	0
88	m9	7	0	0	0	0
88	n3	7	0	0	0	0
88	n6	7	0	0	0	0
88	n9	7	0	0	0	0
88	o3	7	0	0	0	0
88	o7	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	o9	7	0	0	0	0
88	q1	7	0	0	0	0
88	q2	7	0	0	0	0
88	s1	7	0	0	0	0
88	s4	7	0	0	0	0
88	s8	7	0	0	0	0
88	s9	7	0	0	0	0
88	sR	7	0	0	0	0
89	D6	1	0	0	0	0
89	D7	1	0	0	0	0
89	D9	1	0	0	0	0
89	E1	1	0	0	0	0
89	O7	1	0	0	0	0
89	Q0	1	0	0	0	0
89	Q2	1	0	0	0	0
89	Q3	1	0	0	0	0
89	d6	1	0	0	0	0
89	d7	1	0	0	0	0
89	d9	1	0	0	0	0
89	e1	1	0	0	0	0
89	o7	1	0	0	0	0
89	q0	1	0	0	0	0
89	q2	1	0	0	0	0
89	q3	1	0	0	0	0
90	5	3	0	0	0	0
90	f	9	0	0	0	0
All	All	414393	0	299160	9292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 9292 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	1.99	1.49
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.64	1.04
36:1:2820:A:H5''	36:1:2821:C:OP2	1.62	0.99
36:1:1481:A:O2'	36:1:1858:A:N3	1.96	0.97
24:D2:2:THR:N	1:6:1034:C:HO2'	337.95	0.97

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	204/251 (81%)	156 (76%)	29 (14%)	19 (9%)	1	4
2	s0	204/251 (81%)	159 (78%)	28 (14%)	17 (8%)	1	6
3	S1	212/254 (84%)	153 (72%)	34 (16%)	25 (12%)	0	2
3	s1	214/254 (84%)	172 (80%)	29 (14%)	13 (6%)	2	14
4	S2	215/253 (85%)	173 (80%)	33 (15%)	9 (4%)	3	24
4	s2	215/253 (85%)	176 (82%)	31 (14%)	8 (4%)	4	27
5	S3	221/239 (92%)	189 (86%)	24 (11%)	8 (4%)	4	28
5	s3	221/239 (92%)	180 (81%)	30 (14%)	11 (5%)	3	19
6	S4	258/260 (99%)	207 (80%)	35 (14%)	16 (6%)	2	13
6	s4	258/260 (99%)	211 (82%)	30 (12%)	17 (7%)	1	11
7	S5	204/224 (91%)	158 (78%)	32 (16%)	14 (7%)	1	10
7	s5	204/224 (91%)	157 (77%)	29 (14%)	18 (9%)	1	5
8	S6	224/236 (95%)	193 (86%)	22 (10%)	9 (4%)	4	25
8	s6	216/236 (92%)	188 (87%)	19 (9%)	9 (4%)	3	24
9	S7	182/189 (96%)	139 (76%)	28 (15%)	15 (8%)	1	6
9	s7	184/189 (97%)	147 (80%)	20 (11%)	17 (9%)	1	4
10	S8	184/200 (92%)	160 (87%)	16 (9%)	8 (4%)	3	23
10	s8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	3	20
11	S9	183/196 (93%)	145 (79%)	28 (15%)	10 (6%)	2	17
11	s9	183/196 (93%)	150 (82%)	23 (13%)	10 (6%)	2	17
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	8
12	c0	92/105 (88%)	60 (65%)	17 (18%)	15 (16%)	0	1
13	C1	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	3	21
13	c1	144/155 (93%)	120 (83%)	19 (13%)	5 (4%)	4	29
14	C2	122/124 (98%)	74 (61%)	33 (27%)	15 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/124 (98%)	76 (62%)	33 (27%)	13 (11%)	0	3
15	C3	148/150 (99%)	127 (86%)	17 (12%)	4 (3%)	6	37
15	c3	148/150 (99%)	118 (80%)	23 (16%)	7 (5%)	3	21
16	C4	125/136 (92%)	86 (69%)	25 (20%)	14 (11%)	0	3
16	c4	126/136 (93%)	98 (78%)	17 (14%)	11 (9%)	1	5
17	C5	122/137 (89%)	89 (73%)	20 (16%)	13 (11%)	0	3
17	c5	133/137 (97%)	99 (74%)	20 (15%)	14 (10%)	1	3
18	C6	139/142 (98%)	114 (82%)	13 (9%)	12 (9%)	1	5
18	c6	140/142 (99%)	117 (84%)	14 (10%)	9 (6%)	2	12
19	C7	116/136 (85%)	89 (77%)	16 (14%)	11 (10%)	1	4
19	c7	113/136 (83%)	87 (77%)	21 (19%)	5 (4%)	3	22
20	C8	143/145 (99%)	110 (77%)	24 (17%)	9 (6%)	2	12
20	c8	143/145 (99%)	110 (77%)	26 (18%)	7 (5%)	3	20
21	C9	141/143 (99%)	113 (80%)	22 (16%)	6 (4%)	3	23
21	c9	141/143 (99%)	121 (86%)	14 (10%)	6 (4%)	3	23
22	D0	105/120 (88%)	88 (84%)	15 (14%)	2 (2%)	10	48
22	d0	108/120 (90%)	89 (82%)	13 (12%)	6 (6%)	2	17
23	D1	85/87 (98%)	65 (76%)	14 (16%)	6 (7%)	1	9
23	d1	85/87 (98%)	66 (78%)	13 (15%)	6 (7%)	1	9
24	D2	127/129 (98%)	106 (84%)	18 (14%)	3 (2%)	7	41
25	D3	142/144 (99%)	116 (82%)	15 (11%)	11 (8%)	1	7
25	d3	142/144 (99%)	128 (90%)	12 (8%)	2 (1%)	14	55
26	D4	132/134 (98%)	112 (85%)	11 (8%)	9 (7%)	1	10
26	d4	132/134 (98%)	109 (83%)	14 (11%)	9 (7%)	1	10
27	D5	68/107 (64%)	49 (72%)	12 (18%)	7 (10%)	1	3
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	3	22
28	D6	95/97 (98%)	57 (60%)	21 (22%)	17 (18%)	0	0
28	d6	95/97 (98%)	68 (72%)	19 (20%)	8 (8%)	1	6
29	D7	79/81 (98%)	66 (84%)	5 (6%)	8 (10%)	1	4
29	d7	79/81 (98%)	60 (76%)	18 (23%)	1 (1%)	15	57
30	D8	61/66 (92%)	53 (87%)	6 (10%)	2 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	d8	61/66 (92%)	45 (74%)	12 (20%)	4 (7%)	1	11
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	4	26
31	d9	51/55 (93%)	40 (78%)	8 (16%)	3 (6%)	2	15
32	E0	58/62 (94%)	43 (74%)	11 (19%)	4 (7%)	1	10
32	e0	60/62 (97%)	45 (75%)	10 (17%)	5 (8%)	1	6
33	E1	69/76 (91%)	35 (51%)	20 (29%)	14 (20%)	0	0
33	e1	74/76 (97%)	40 (54%)	14 (19%)	20 (27%)	0	0
34	SR	316/318 (99%)	263 (83%)	40 (13%)	13 (4%)	3	25
34	sR	316/318 (99%)	257 (81%)	43 (14%)	16 (5%)	2	19
35	SM	155/273 (57%)	107 (69%)	27 (17%)	21 (14%)	0	1
35	sM	98/273 (36%)	60 (61%)	22 (22%)	16 (16%)	0	1
39	L2	250/253 (99%)	221 (88%)	20 (8%)	9 (4%)	4	28
39	l2	250/253 (99%)	216 (86%)	24 (10%)	10 (4%)	4	25
40	L3	384/386 (100%)	329 (86%)	41 (11%)	14 (4%)	4	28
40	l3	384/386 (100%)	344 (90%)	30 (8%)	10 (3%)	7	38
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	2	18
41	l4	359/361 (99%)	301 (84%)	40 (11%)	18 (5%)	3	19
42	L5	294/296 (99%)	239 (81%)	32 (11%)	23 (8%)	1	7
42	l5	292/296 (99%)	263 (90%)	19 (6%)	10 (3%)	5	29
43	L6	152/175 (87%)	132 (87%)	17 (11%)	3 (2%)	9	46
43	l6	153/175 (87%)	134 (88%)	16 (10%)	3 (2%)	9	46
44	L7	220/243 (90%)	199 (90%)	13 (6%)	8 (4%)	4	28
44	l7	221/243 (91%)	208 (94%)	8 (4%)	5 (2%)	8	42
45	L8	231/255 (91%)	188 (81%)	35 (15%)	8 (4%)	4	29
45	l8	229/255 (90%)	186 (81%)	30 (13%)	13 (6%)	2	16
46	L9	189/191 (99%)	161 (85%)	19 (10%)	9 (5%)	3	20
46	l9	189/191 (99%)	168 (89%)	18 (10%)	3 (2%)	12	52
47	M0	207/220 (94%)	172 (83%)	28 (14%)	7 (3%)	5	29
47	m0	209/220 (95%)	173 (83%)	19 (9%)	17 (8%)	1	6
48	M1	167/173 (96%)	125 (75%)	27 (16%)	15 (9%)	1	5
48	m1	167/173 (96%)	142 (85%)	18 (11%)	7 (4%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	161 (84%)	20 (10%)	10 (5%)	2	18
49	m3	192/198 (97%)	155 (81%)	19 (10%)	18 (9%)	1	4
50	M4	134/137 (98%)	119 (89%)	12 (9%)	3 (2%)	8	43
50	m4	135/137 (98%)	125 (93%)	8 (6%)	2 (2%)	13	53
51	M5	199/204 (98%)	174 (87%)	20 (10%)	5 (2%)	7	39
52	M6	195/198 (98%)	173 (89%)	18 (9%)	4 (2%)	9	44
52	m6	195/198 (98%)	177 (91%)	13 (7%)	5 (3%)	7	38
53	M7	181/183 (99%)	156 (86%)	20 (11%)	5 (3%)	6	36
53	m7	153/183 (84%)	139 (91%)	13 (8%)	1 (1%)	26	71
54	M8	183/185 (99%)	165 (90%)	13 (7%)	5 (3%)	6	37
54	m8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	5	30
55	M9	186/188 (99%)	160 (86%)	23 (12%)	3 (2%)	12	52
55	m9	186/188 (99%)	167 (90%)	15 (8%)	4 (2%)	8	43
56	N0	170/172 (99%)	154 (91%)	11 (6%)	5 (3%)	6	35
56	n0	170/172 (99%)	158 (93%)	10 (6%)	2 (1%)	16	58
57	N1	157/159 (99%)	141 (90%)	13 (8%)	3 (2%)	10	48
57	n1	157/159 (99%)	130 (83%)	24 (15%)	3 (2%)	10	48
58	N2	98/120 (82%)	74 (76%)	16 (16%)	8 (8%)	1	6
58	n2	96/120 (80%)	79 (82%)	14 (15%)	3 (3%)	5	32
59	N3	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	8	43
59	n3	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	26	71
60	N4	96/155 (62%)	72 (75%)	19 (20%)	5 (5%)	2	18
60	n4	133/155 (86%)	108 (81%)	18 (14%)	7 (5%)	2	18
61	N5	119/141 (84%)	107 (90%)	9 (8%)	3 (2%)	7	39
61	n5	118/141 (84%)	99 (84%)	9 (8%)	10 (8%)	1	5
62	N6	124/126 (98%)	108 (87%)	14 (11%)	2 (2%)	12	52
62	n6	124/126 (98%)	110 (89%)	9 (7%)	5 (4%)	4	25
63	N7	133/135 (98%)	103 (77%)	16 (12%)	14 (10%)	1	3
63	n7	133/135 (98%)	103 (77%)	22 (16%)	8 (6%)	2	14
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	3	20
64	n8	146/148 (99%)	121 (83%)	19 (13%)	6 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	N9	56/58 (97%)	45 (80%)	9 (16%)	2 (4%)	4	28
65	n9	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	5
66	O0	95/104 (91%)	84 (88%)	11 (12%)	0	100	100
66	o0	98/104 (94%)	84 (86%)	8 (8%)	6 (6%)	2	14
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	2	17
67	o1	107/112 (96%)	82 (77%)	20 (19%)	5 (5%)	3	21
68	O2	125/129 (97%)	113 (90%)	9 (7%)	3 (2%)	7	41
68	o2	125/129 (97%)	109 (87%)	11 (9%)	5 (4%)	4	25
69	O3	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
69	o3	104/106 (98%)	92 (88%)	11 (11%)	1 (1%)	19	63
70	O4	110/119 (92%)	99 (90%)	11 (10%)	0	100	100
70	o4	110/119 (92%)	94 (86%)	15 (14%)	1 (1%)	21	65
71	O5	117/119 (98%)	97 (83%)	18 (15%)	2 (2%)	11	50
71	o5	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	7	38
72	O6	97/99 (98%)	77 (79%)	11 (11%)	9 (9%)	1	4
72	o6	97/99 (98%)	79 (81%)	10 (10%)	8 (8%)	1	6
73	O7	85/87 (98%)	71 (84%)	12 (14%)	2 (2%)	7	41
73	o7	85/87 (98%)	71 (84%)	13 (15%)	1 (1%)	16	58
74	O8	75/77 (97%)	65 (87%)	8 (11%)	2 (3%)	6	37
74	o8	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	4	25
75	O9	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	9	44
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
76	Q0	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	9	46
76	q0	50/52 (96%)	44 (88%)	5 (10%)	1 (2%)	9	46
77	Q1	23/25 (92%)	23 (100%)	0	0	100	100
77	q1	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	3	23
78	Q2	103/105 (98%)	84 (82%)	16 (16%)	3 (3%)	6	35
78	q2	103/105 (98%)	90 (87%)	8 (8%)	5 (5%)	3	20
79	Q3	89/91 (98%)	77 (86%)	9 (10%)	3 (3%)	5	29
79	q3	89/91 (98%)	79 (89%)	9 (10%)	1 (1%)	17	61
80	d2	125/130 (96%)	114 (91%)	10 (8%)	1 (1%)	24	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	m5	201/203 (99%)	178 (89%)	19 (10%)	4 (2%)	9	46
83	p0	139/220 (63%)	112 (81%)	20 (14%)	7 (5%)	3	19
85	f	145/157 (92%)	96 (66%)	29 (20%)	20 (14%)	0	1
All	All	22474/24167 (93%)	18605 (83%)	2710 (12%)	1159 (5%)	2	18

5 of 1159 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	191	ARG
2	S0	192	THR
2	S0	202	TYR

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	164/209 (78%)	139 (85%)	25 (15%)	3	16
2	s0	165/209 (79%)	146 (88%)	19 (12%)	7	29
3	S1	191/223 (86%)	167 (87%)	24 (13%)	5	25
3	s1	192/223 (86%)	156 (81%)	36 (19%)	2	10
4	S2	176/204 (86%)	151 (86%)	25 (14%)	4	19
4	s2	176/204 (86%)	140 (80%)	36 (20%)	1	7
5	S3	182/194 (94%)	155 (85%)	27 (15%)	4	17
5	s3	182/194 (94%)	162 (89%)	20 (11%)	8	31
6	S4	221/221 (100%)	190 (86%)	31 (14%)	4	19
6	s4	221/221 (100%)	191 (86%)	30 (14%)	5	21
7	S5	173/190 (91%)	146 (84%)	27 (16%)	3	14
7	s5	173/190 (91%)	150 (87%)	23 (13%)	5	22
8	S6	188/201 (94%)	164 (87%)	24 (13%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	s6	187/201 (93%)	163 (87%)	24 (13%)	5	24
9	S7	165/169 (98%)	141 (86%)	24 (14%)	4	18
9	s7	165/169 (98%)	144 (87%)	21 (13%)	5	24
10	S8	150/161 (93%)	136 (91%)	14 (9%)	11	40
10	s8	150/161 (93%)	128 (85%)	22 (15%)	4	18
11	S9	158/165 (96%)	136 (86%)	22 (14%)	4	20
11	s9	158/165 (96%)	130 (82%)	28 (18%)	2	11
12	C0	77/98 (79%)	69 (90%)	8 (10%)	9	33
12	c0	73/98 (74%)	67 (92%)	6 (8%)	14	48
13	C1	129/136 (95%)	122 (95%)	7 (5%)	27	67
13	c1	129/136 (95%)	107 (83%)	22 (17%)	2	12
14	C2	88/100 (88%)	79 (90%)	9 (10%)	9	35
14	c2	88/100 (88%)	80 (91%)	8 (9%)	12	41
15	C3	127/127 (100%)	107 (84%)	20 (16%)	3	14
15	c3	127/127 (100%)	108 (85%)	19 (15%)	3	17
16	C4	81/104 (78%)	68 (84%)	13 (16%)	3	14
16	c4	97/104 (93%)	83 (86%)	14 (14%)	4	19
17	C5	101/113 (89%)	87 (86%)	14 (14%)	4	20
17	c5	103/113 (91%)	89 (86%)	14 (14%)	5	21
18	C6	117/118 (99%)	101 (86%)	16 (14%)	4	21
18	c6	118/118 (100%)	98 (83%)	20 (17%)	2	12
19	C7	94/124 (76%)	77 (82%)	17 (18%)	2	10
19	c7	92/124 (74%)	81 (88%)	11 (12%)	6	27
20	C8	128/128 (100%)	105 (82%)	23 (18%)	2	11
20	c8	128/128 (100%)	108 (84%)	20 (16%)	3	14
21	C9	115/115 (100%)	101 (88%)	14 (12%)	6	26
21	c9	115/115 (100%)	98 (85%)	17 (15%)	4	17
22	D0	100/113 (88%)	87 (87%)	13 (13%)	5	23
22	d0	103/113 (91%)	86 (84%)	17 (16%)	3	13
23	D1	74/74 (100%)	64 (86%)	10 (14%)	5	22
23	d1	74/74 (100%)	63 (85%)	11 (15%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	D2	110/110 (100%)	92 (84%)	18 (16%)	3	13
25	D3	119/119 (100%)	103 (87%)	16 (13%)	5	22
25	d3	119/119 (100%)	108 (91%)	11 (9%)	11	40
26	D4	112/112 (100%)	101 (90%)	11 (10%)	10	37
26	d4	112/112 (100%)	95 (85%)	17 (15%)	3	16
27	D5	61/88 (69%)	48 (79%)	13 (21%)	1	6
27	d5	61/88 (69%)	53 (87%)	8 (13%)	5	23
28	D6	83/83 (100%)	70 (84%)	13 (16%)	3	14
28	d6	83/83 (100%)	74 (89%)	9 (11%)	8	32
29	D7	70/70 (100%)	64 (91%)	6 (9%)	13	45
29	d7	70/70 (100%)	61 (87%)	9 (13%)	5	24
30	D8	56/59 (95%)	49 (88%)	7 (12%)	6	25
30	d8	56/59 (95%)	47 (84%)	9 (16%)	3	13
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	12
31	d9	47/48 (98%)	38 (81%)	9 (19%)	2	10
32	E0	51/53 (96%)	45 (88%)	6 (12%)	6	28
32	e0	53/53 (100%)	44 (83%)	9 (17%)	2	12
33	E1	62/66 (94%)	51 (82%)	11 (18%)	2	11
33	e1	66/66 (100%)	55 (83%)	11 (17%)	3	12
34	SR	259/261 (99%)	239 (92%)	20 (8%)	16	52
34	sR	260/261 (100%)	233 (90%)	27 (10%)	9	33
35	SM	97/228 (42%)	73 (75%)	24 (25%)	1	3
35	sM	54/228 (24%)	48 (89%)	6 (11%)	8	31
39	L2	193/195 (99%)	163 (84%)	30 (16%)	3	15
39	l2	192/195 (98%)	157 (82%)	35 (18%)	2	10
40	L3	319/322 (99%)	263 (82%)	56 (18%)	2	11
40	l3	320/322 (99%)	259 (81%)	61 (19%)	2	10
41	L4	288/288 (100%)	241 (84%)	47 (16%)	3	13
41	l4	288/288 (100%)	238 (83%)	50 (17%)	2	12
42	L5	244/244 (100%)	196 (80%)	48 (20%)	1	8
42	l5	243/244 (100%)	199 (82%)	44 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	L6	134/152 (88%)	113 (84%)	21 (16%)	3	14
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	12
44	L7	186/204 (91%)	166 (89%)	20 (11%)	8	32
44	l7	187/204 (92%)	162 (87%)	25 (13%)	5	22
45	L8	187/207 (90%)	155 (83%)	32 (17%)	2	12
45	l8	177/207 (86%)	144 (81%)	33 (19%)	2	10
46	L9	171/171 (100%)	143 (84%)	28 (16%)	3	13
46	l9	171/171 (100%)	135 (79%)	36 (21%)	1	7
47	M0	177/186 (95%)	148 (84%)	29 (16%)	3	13
47	m0	179/186 (96%)	142 (79%)	37 (21%)	1	7
48	M1	147/150 (98%)	121 (82%)	26 (18%)	2	11
48	m1	147/150 (98%)	120 (82%)	27 (18%)	2	10
49	M3	154/158 (98%)	136 (88%)	18 (12%)	7	29
49	m3	154/158 (98%)	130 (84%)	24 (16%)	3	14
50	M4	107/108 (99%)	87 (81%)	20 (19%)	2	10
50	m4	108/108 (100%)	96 (89%)	12 (11%)	8	31
51	M5	175/176 (99%)	149 (85%)	26 (15%)	4	17
52	M6	160/161 (99%)	143 (89%)	17 (11%)	8	33
52	m6	160/161 (99%)	136 (85%)	24 (15%)	3	17
53	M7	140/145 (97%)	121 (86%)	19 (14%)	5	21
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	11
54	M8	150/150 (100%)	133 (89%)	17 (11%)	7	30
54	m8	150/150 (100%)	123 (82%)	27 (18%)	2	11
55	M9	153/153 (100%)	137 (90%)	16 (10%)	8	33
55	m9	153/153 (100%)	128 (84%)	25 (16%)	3	13
56	N0	156/156 (100%)	126 (81%)	30 (19%)	2	9
56	n0	156/156 (100%)	131 (84%)	25 (16%)	3	14
57	N1	136/136 (100%)	113 (83%)	23 (17%)	2	12
57	n1	136/136 (100%)	113 (83%)	23 (17%)	2	12
58	N2	87/106 (82%)	78 (90%)	9 (10%)	9	34
58	n2	85/106 (80%)	76 (89%)	9 (11%)	8	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	N3	104/104 (100%)	91 (88%)	13 (12%)	6	25
59	n3	104/104 (100%)	97 (93%)	7 (7%)	20	58
60	N4	57/129 (44%)	50 (88%)	7 (12%)	6	26
60	n4	100/129 (78%)	90 (90%)	10 (10%)	9	36
61	N5	104/117 (89%)	82 (79%)	22 (21%)	1	7
61	n5	104/117 (89%)	83 (80%)	21 (20%)	1	7
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	12
62	n6	109/109 (100%)	91 (84%)	18 (16%)	3	13
63	N7	115/115 (100%)	97 (84%)	18 (16%)	3	14
63	n7	115/115 (100%)	97 (84%)	18 (16%)	3	14
64	N8	118/118 (100%)	102 (86%)	16 (14%)	5	21
64	n8	118/118 (100%)	97 (82%)	21 (18%)	2	11
65	N9	46/46 (100%)	41 (89%)	5 (11%)	8	31
65	n9	46/46 (100%)	40 (87%)	6 (13%)	5	23
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1	8
66	o0	84/87 (97%)	72 (86%)	12 (14%)	4	19
67	O1	92/96 (96%)	76 (83%)	16 (17%)	2	12
67	o1	94/96 (98%)	76 (81%)	18 (19%)	2	10
68	O2	109/110 (99%)	90 (83%)	19 (17%)	2	12
68	o2	109/110 (99%)	93 (85%)	16 (15%)	4	18
69	O3	90/90 (100%)	78 (87%)	12 (13%)	5	22
69	o3	90/90 (100%)	78 (87%)	12 (13%)	5	22
70	O4	95/101 (94%)	80 (84%)	15 (16%)	3	14
70	o4	95/101 (94%)	79 (83%)	16 (17%)	2	12
71	O5	104/104 (100%)	88 (85%)	16 (15%)	3	15
71	o5	103/104 (99%)	90 (87%)	13 (13%)	5	25
72	O6	81/81 (100%)	70 (86%)	11 (14%)	5	21
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0	2
73	O7	70/70 (100%)	58 (83%)	12 (17%)	2	12
73	o7	70/70 (100%)	62 (89%)	8 (11%)	7	30
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	o8	67/68 (98%)	57 (85%)	10 (15%)	4	17
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	8
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	11
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	12
76	q0	47/47 (100%)	39 (83%)	8 (17%)	2	12
77	Q1	23/23 (100%)	20 (87%)	3 (13%)	5	23
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	1
78	Q2	90/90 (100%)	75 (83%)	15 (17%)	3	12
78	q2	90/90 (100%)	76 (84%)	14 (16%)	3	14
79	Q3	71/71 (100%)	58 (82%)	13 (18%)	2	10
79	q3	71/71 (100%)	63 (89%)	8 (11%)	7	30
80	d2	110/111 (99%)	99 (90%)	11 (10%)	9	36
82	m5	175/175 (100%)	151 (86%)	24 (14%)	4	21
83	p0	105/186 (56%)	94 (90%)	11 (10%)	8	33
85	f	123/132 (93%)	100 (81%)	23 (19%)	2	10
All	All	18849/20264 (93%)	16010 (85%)	2839 (15%)	3	17

5 of 2839 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	O5	102	GLU
10	s8	36	THR
64	n8	123	VAL
74	O8	67	GLN
4	s2	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
74	O8	32	ASN
6	s4	142	HIS
63	n7	127	ASN
3	s1	209	ASN
9	s7	71	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	448 (25%)	41 (2%)
1	6	1791/1800 (99%)	444 (24%)	32 (1%)
36	1	3145/3396 (92%)	646 (20%)	55 (1%)
36	5	3163/3396 (93%)	632 (19%)	59 (1%)
37	3	120/121 (99%)	10 (8%)	0
37	7	120/121 (99%)	17 (14%)	1 (0%)
38	4	157/158 (99%)	35 (22%)	4 (2%)
38	8	157/158 (99%)	32 (20%)	0
All	All	10429/10950 (95%)	2264 (21%)	192 (1%)

5 of 2264 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	8	U
1	2	25	C
1	2	26	A

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3056	U
1	6	542	A
36	5	2586	G
36	1	3228	C
38	4	85	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	5CT	f	51	85	12,14,15	2.33	4 (33%)	12,15,17	1.66	3 (25%)

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
85	5CT	f	51	85	1/1/2/4	0/12/14/16	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	f	51	5CT	O1-C2	-6.54	1.24	1.43
85	f	51	5CT	C1-NZ	-3.32	1.41	1.47
85	f	51	5CT	CB-CA	2.05	1.56	1.53
85	f	51	5CT	C1-C2	2.48	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	f	51	5CT	O-C-CA	-2.09	120.11	125.72
85	f	51	5CT	O1-C2-C3	3.16	118.39	109.36
85	f	51	5CT	O1-C2-C1	3.34	120.64	109.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
85	f	51	5CT	C2

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2290 ligands modelled in this entry, 1124 are monoatomic - leaving 1166 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
88	OHX	1	3757	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3758	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3759	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3760	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3761	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3762	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3763	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3764	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3765	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3766	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3767	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3768	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3769	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3770	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3771	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3772	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3773	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3774	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3775	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3776	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3777	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3778	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3779	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3780	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3781	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3782	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3783	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3784	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3785	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3786	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3787	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3788	-	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
88	OHX	1	3789	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3790	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3791	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3792	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3793	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3794	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3795	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3796	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3797	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3798	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3799	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3800	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3801	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3802	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3804	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3805	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3806	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3807	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3808	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3809	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3810	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3811	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3812	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3813	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3814	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3815	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3816	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3817	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3818	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3819	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3820	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3821	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3822	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3823	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3824	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3825	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3826	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3827	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3828	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3829	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3830	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3831	-	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
88	OHX	1	3832	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3833	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3834	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3835	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3836	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3837	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3838	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3839	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3840	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3841	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3842	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3843	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3844	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3845	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3846	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3847	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3848	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3849	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3850	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3851	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3852	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3853	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3854	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3855	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3856	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3857	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3858	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3859	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3860	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3861	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3862	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3874	-	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
88	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3917	-	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
88	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3960	-	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
88	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4003	-	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
88	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4046	-	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
88	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4089	-	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
88	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2018	-	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
88	OHX	2	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2061	-	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
88	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2102	1	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2104	-	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
88	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2147	-	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
88	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	210	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	212	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	213	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	214	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3794	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3795	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3796	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3797	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3798	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3799	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3800	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3801	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3802	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3804	-	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
88	OHX	5	3805	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3806	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3807	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3808	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3809	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3810	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3811	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3812	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3813	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3814	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3815	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3816	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3817	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3818	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3819	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3820	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3821	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3822	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3823	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3824	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3825	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3826	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3827	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3828	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3829	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3830	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3831	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3832	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3833	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3834	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3835	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3836	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3837	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3838	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3839	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3840	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3841	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3842	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3843	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3844	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3845	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3846	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3847	-	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
88	OHX	5	3848	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3849	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3850	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3851	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3852	36	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3853	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3854	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3855	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3856	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3857	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3858	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3859	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3860	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3861	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3862	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3863	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3890	-	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
88	OHX	5	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3933	-	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
88	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3976	-	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
88	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4019	-	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
88	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4062	-	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
88	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4068	36	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4105	-	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
88	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4126	36	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4148	-	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
88	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2044	-	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
88	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2067	1	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2087	-	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
88	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2130	-	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
88	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2173	-	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
88	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	231	-	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
88	OHX	8	232	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	D9	103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	N8	205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	N9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O7	105	73	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O7	106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	S1	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	S6	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	S8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	S9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c5	800	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	304	-	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
88	OHX	m5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n9	103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	q1	702	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s1	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	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
88	OHX	1	3757	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3758	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3759	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3760	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3761	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3762	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3763	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3764	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3765	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3766	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3767	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3768	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3769	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3770	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3771	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3772	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3773	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3774	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3775	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3776	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3777	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3778	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3779	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3780	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3781	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3782	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3783	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3784	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3785	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3786	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3787	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3788	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3789	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3790	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3791	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3792	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3793	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3794	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3795	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3796	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3797	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3798	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3799	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3800	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3801	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3802	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3803	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3804	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3805	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3806	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3807	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3808	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3809	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3810	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3811	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3812	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3813	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3814	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3815	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3816	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3817	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3818	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3819	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3820	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3821	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3822	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3823	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3824	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3825	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3826	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3827	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3828	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3829	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3830	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3831	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3832	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3833	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3834	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3835	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3836	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3837	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3838	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3839	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3840	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3841	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3842	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3843	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3844	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3845	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3846	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3847	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3848	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3849	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3850	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3851	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3852	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3853	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3854	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3855	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3856	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3857	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3858	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3859	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3860	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3861	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3862	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3863	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3864	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3865	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3866	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3867	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3902	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3944	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3986	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4028	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4070	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
88	OHX	2	1994	-	-	0/0/0/0	0/0/0/0
88	OHX	2	1995	-	-	0/0/0/0	0/0/0/0
88	OHX	2	1996	-	-	0/0/0/0	0/0/0/0
88	OHX	2	1997	-	-	0/0/0/0	0/0/0/0
88	OHX	2	1998	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	1999	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2000	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2001	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2002	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2003	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2004	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2005	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2006	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2007	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2008	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2009	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2010	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2011	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2012	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2013	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2014	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2015	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2016	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2017	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2018	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2019	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2020	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2021	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2040	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2082	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2102	1	-	0/0/0/0	0/0/0/0
88	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2124	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
88	OHX	3	209	-	-	0/0/0/0	0/0/0/0
88	OHX	3	210	-	-	0/0/0/0	0/0/0/0
88	OHX	3	211	-	-	0/0/0/0	0/0/0/0
88	OHX	3	212	-	-	0/0/0/0	0/0/0/0
88	OHX	3	213	-	-	0/0/0/0	0/0/0/0
88	OHX	3	214	-	-	0/0/0/0	0/0/0/0
88	OHX	3	215	-	-	0/0/0/0	0/0/0/0
88	OHX	3	216	-	-	0/0/0/0	0/0/0/0
88	OHX	3	217	-	-	0/0/0/0	0/0/0/0
88	OHX	3	218	-	-	0/0/0/0	0/0/0/0
88	OHX	3	219	-	-	0/0/0/0	0/0/0/0
88	OHX	4	220	-	-	0/0/0/0	0/0/0/0
88	OHX	4	221	-	-	0/0/0/0	0/0/0/0
88	OHX	4	222	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	4	223	-	-	0/0/0/0	0/0/0/0
88	OHX	4	224	-	-	0/0/0/0	0/0/0/0
88	OHX	4	225	-	-	0/0/0/0	0/0/0/0
88	OHX	4	226	-	-	0/0/0/0	0/0/0/0
88	OHX	4	227	-	-	0/0/0/0	0/0/0/0
88	OHX	4	228	-	-	0/0/0/0	0/0/0/0
88	OHX	4	229	-	-	0/0/0/0	0/0/0/0
88	OHX	4	230	-	-	0/0/0/0	0/0/0/0
88	OHX	4	231	-	-	0/0/0/0	0/0/0/0
88	OHX	4	232	-	-	0/0/0/0	0/0/0/0
88	OHX	4	233	-	-	0/0/0/0	0/0/0/0
88	OHX	4	234	-	-	0/0/0/0	0/0/0/0
88	OHX	4	235	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3794	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3795	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3796	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3797	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3798	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3799	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3800	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3801	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3802	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3803	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3804	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3805	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3806	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3807	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3808	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3809	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3810	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3811	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3812	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3813	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3814	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3815	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3816	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3817	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3818	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3819	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3820	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3821	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3822	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3823	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3824	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3825	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3826	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3827	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3828	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3829	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3830	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3831	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3832	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3833	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3834	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3835	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3836	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3837	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3838	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3839	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3840	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3841	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3842	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3843	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3844	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3845	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3846	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3847	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3848	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3849	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3850	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3851	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3852	36	-	0/0/0/0	0/0/0/0
88	OHX	5	3853	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3854	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3855	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3856	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3857	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3858	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3859	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3860	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3861	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3862	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3863	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3864	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3865	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3866	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3867	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3868	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3869	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3870	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3871	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3872	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3873	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3874	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3875	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3876	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3877	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3878	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3879	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3880	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3881	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3882	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3883	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3884	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3885	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3886	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3887	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3888	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3889	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3890	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3891	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3892	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3893	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3894	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3895	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3896	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3897	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3906	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3948	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3990	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4032	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4068	36	-	0/0/0/0	0/0/0/0
88	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4074	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4116	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4126	36	-	0/0/0/0	0/0/0/0
88	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4158	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2013	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2014	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2015	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2016	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2017	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2018	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2019	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2020	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2021	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2022	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2023	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2024	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2025	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2026	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2027	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2028	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2029	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2030	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2031	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2032	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2033	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2034	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2035	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2036	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2037	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2038	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2039	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2040	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2041	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2042	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2043	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2053	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2067	1	-	0/0/0/0	0/0/0/0
88	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2095	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2137	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2179	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
88	OHX	7	216	-	-	0/0/0/0	0/0/0/0
88	OHX	7	217	-	-	0/0/0/0	0/0/0/0
88	OHX	7	218	-	-	0/0/0/0	0/0/0/0
88	OHX	7	219	-	-	0/0/0/0	0/0/0/0
88	OHX	7	220	-	-	0/0/0/0	0/0/0/0
88	OHX	7	221	-	-	0/0/0/0	0/0/0/0
88	OHX	7	222	-	-	0/0/0/0	0/0/0/0
88	OHX	7	223	-	-	0/0/0/0	0/0/0/0
88	OHX	7	224	-	-	0/0/0/0	0/0/0/0
88	OHX	7	225	-	-	0/0/0/0	0/0/0/0
88	OHX	7	226	-	-	0/0/0/0	0/0/0/0
88	OHX	7	227	-	-	0/0/0/0	0/0/0/0
88	OHX	8	213	-	-	0/0/0/0	0/0/0/0
88	OHX	8	214	-	-	0/0/0/0	0/0/0/0
88	OHX	8	215	-	-	0/0/0/0	0/0/0/0
88	OHX	8	216	-	-	0/0/0/0	0/0/0/0
88	OHX	8	217	-	-	0/0/0/0	0/0/0/0
88	OHX	8	218	-	-	0/0/0/0	0/0/0/0
88	OHX	8	219	-	-	0/0/0/0	0/0/0/0
88	OHX	8	220	-	-	0/0/0/0	0/0/0/0
88	OHX	8	221	-	-	0/0/0/0	0/0/0/0
88	OHX	8	222	-	-	0/0/0/0	0/0/0/0
88	OHX	8	223	-	-	0/0/0/0	0/0/0/0
88	OHX	8	224	-	-	0/0/0/0	0/0/0/0
88	OHX	8	225	-	-	0/0/0/0	0/0/0/0
88	OHX	8	226	-	-	0/0/0/0	0/0/0/0
88	OHX	8	227	-	-	0/0/0/0	0/0/0/0
88	OHX	8	228	-	-	0/0/0/0	0/0/0/0
88	OHX	8	229	-	-	0/0/0/0	0/0/0/0
88	OHX	8	230	-	-	0/0/0/0	0/0/0/0
88	OHX	8	231	-	-	0/0/0/0	0/0/0/0
88	OHX	8	232	-	-	0/0/0/0	0/0/0/0
88	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C8	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	D9	103	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
88	OHX	L4	401	-	-	0/0/0/0	0/0/0/0
88	OHX	L5	301	-	-	0/0/0/0	0/0/0/0
88	OHX	M0	302	-	-	0/0/0/0	0/0/0/0
88	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
88	OHX	M5	301	-	-	0/0/0/0	0/0/0/0
88	OHX	M7	204	-	-	0/0/0/0	0/0/0/0
88	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
88	OHX	M8	202	-	-	0/0/0/0	0/0/0/0
88	OHX	M9	201	-	-	0/0/0/0	0/0/0/0
88	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
88	OHX	N8	205	-	-	0/0/0/0	0/0/0/0
88	OHX	N9	102	-	-	0/0/0/0	0/0/0/0
88	OHX	O3	203	-	-	0/0/0/0	0/0/0/0
88	OHX	O7	105	73	-	0/0/0/0	0/0/0/0
88	OHX	O7	106	-	-	0/0/0/0	0/0/0/0
88	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
88	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
88	OHX	S1	301	-	-	0/0/0/0	0/0/0/0
88	OHX	S6	301	-	-	0/0/0/0	0/0/0/0
88	OHX	S8	301	-	-	0/0/0/0	0/0/0/0
88	OHX	S9	202	-	-	0/0/0/0	0/0/0/0
88	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
88	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	c5	800	-	-	0/0/0/0	0/0/0/0
88	OHX	c8	201	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
88	OHX	l4	401	-	-	0/0/0/0	0/0/0/0
88	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	302	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
88	OHX	l9	201	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	304	-	-	0/0/0/0	0/0/0/0
88	OHX	m5	301	-	-	0/0/0/0	0/0/0/0
88	OHX	m7	204	-	-	0/0/0/0	0/0/0/0
88	OHX	m9	201	-	-	0/0/0/0	0/0/0/0
88	OHX	n3	202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	n6	202	-	-	0/0/0/0	0/0/0/0
88	OHX	n9	103	-	-	0/0/0/0	0/0/0/0
88	OHX	o3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
88	OHX	o9	102	-	-	0/0/0/0	0/0/0/0
88	OHX	q1	702	-	-	0/0/0/0	0/0/0/0
88	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
88	OHX	s1	301	-	-	0/0/0/0	0/0/0/0
88	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
88	OHX	s8	302	-	-	0/0/0/0	0/0/0/0
88	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
88	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

582 monomers are involved in 844 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3758	OHX	1	0
88	1	3762	OHX	2	0
88	1	3764	OHX	1	0
88	1	3766	OHX	1	0
88	1	3767	OHX	1	0
88	1	3768	OHX	1	0
88	1	3770	OHX	1	0
88	1	3773	OHX	2	0
88	1	3775	OHX	2	0
88	1	3776	OHX	2	0
88	1	3778	OHX	1	0
88	1	3779	OHX	1	0
88	1	3781	OHX	1	0
88	1	3782	OHX	2	0
88	1	3783	OHX	1	0
88	1	3788	OHX	1	0
88	1	3792	OHX	1	0
88	1	3795	OHX	1	0
88	1	3801	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3802	OHX	1	0
88	1	3804	OHX	2	0
88	1	3805	OHX	1	0
88	1	3806	OHX	1	0
88	1	3808	OHX	1	0
88	1	3810	OHX	1	0
88	1	3813	OHX	1	0
88	1	3814	OHX	1	0
88	1	3818	OHX	1	0
88	1	3819	OHX	2	0
88	1	3821	OHX	2	0
88	1	3823	OHX	1	0
88	1	3825	OHX	3	0
88	1	3826	OHX	1	0
88	1	3829	OHX	1	0
88	1	3833	OHX	1	0
88	1	3836	OHX	2	0
88	1	3841	OHX	1	0
88	1	3844	OHX	1	0
88	1	3845	OHX	1	0
88	1	3847	OHX	1	0
88	1	3849	OHX	1	0
88	1	3850	OHX	1	0
88	1	3851	OHX	6	0
88	1	3852	OHX	2	0
88	1	3855	OHX	1	0
88	1	3860	OHX	1	0
88	1	3862	OHX	2	0
88	1	3864	OHX	1	0
88	1	3868	OHX	1	0
88	1	3870	OHX	2	0
88	1	3871	OHX	2	0
88	1	3873	OHX	1	0
88	1	3874	OHX	1	0
88	1	3875	OHX	2	0
88	1	3876	OHX	3	0
88	1	3879	OHX	1	0
88	1	3880	OHX	1	0
88	1	3882	OHX	2	0
88	1	3884	OHX	1	0
88	1	3886	OHX	1	0
88	1	3888	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3892	OHX	2	0
88	1	3893	OHX	1	0
88	1	3894	OHX	1	0
88	1	3897	OHX	2	0
88	1	3898	OHX	1	0
88	1	3899	OHX	1	0
88	1	3902	OHX	1	0
88	1	3903	OHX	2	0
88	1	3904	OHX	2	0
88	1	3909	OHX	1	0
88	1	3913	OHX	1	0
88	1	3915	OHX	1	0
88	1	3920	OHX	2	0
88	1	3923	OHX	2	0
88	1	3927	OHX	5	0
88	1	3928	OHX	1	0
88	1	3930	OHX	1	0
88	1	3935	OHX	2	0
88	1	3936	OHX	1	0
88	1	3937	OHX	2	0
88	1	3938	OHX	1	0
88	1	3939	OHX	4	0
88	1	3940	OHX	4	0
88	1	3942	OHX	2	0
88	1	3943	OHX	1	0
88	1	3946	OHX	1	0
88	1	3949	OHX	1	0
88	1	3950	OHX	2	0
88	1	3951	OHX	3	0
88	1	3952	OHX	1	0
88	1	3953	OHX	2	0
88	1	3955	OHX	1	0
88	1	3957	OHX	1	0
88	1	3961	OHX	1	0
88	1	3962	OHX	1	0
88	1	3964	OHX	1	0
88	1	3965	OHX	1	0
88	1	3969	OHX	1	0
88	1	3970	OHX	1	0
88	1	3971	OHX	1	0
88	1	3975	OHX	1	0
88	1	3979	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	3980	OHX	2	0
88	1	3982	OHX	1	0
88	1	3983	OHX	2	0
88	1	3984	OHX	1	0
88	1	3985	OHX	2	0
88	1	3990	OHX	1	0
88	1	3991	OHX	1	0
88	1	3993	OHX	1	0
88	1	3995	OHX	1	0
88	1	3998	OHX	1	0
88	1	3999	OHX	1	0
88	1	4001	OHX	6	0
88	1	4002	OHX	1	0
88	1	4003	OHX	1	0
88	1	4006	OHX	2	0
88	1	4009	OHX	1	0
88	1	4010	OHX	1	0
88	1	4011	OHX	1	0
88	1	4012	OHX	1	0
88	1	4016	OHX	2	0
88	1	4017	OHX	1	0
88	1	4020	OHX	3	0
88	1	4023	OHX	1	0
88	1	4025	OHX	1	0
88	1	4028	OHX	1	0
88	1	4032	OHX	2	0
88	1	4033	OHX	1	0
88	1	4035	OHX	1	0
88	1	4036	OHX	1	0
88	1	4037	OHX	1	0
88	1	4038	OHX	1	0
88	1	4039	OHX	1	0
88	1	4040	OHX	2	0
88	1	4042	OHX	1	0
88	1	4045	OHX	2	0
88	1	4046	OHX	2	0
88	1	4050	OHX	2	0
88	1	4051	OHX	1	0
88	1	4053	OHX	1	0
88	1	4055	OHX	2	0
88	1	4056	OHX	1	0
88	1	4060	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	1	4062	OHX	1	0
88	1	4063	OHX	3	0
88	1	4064	OHX	2	0
88	1	4065	OHX	1	0
88	1	4068	OHX	6	0
88	1	4069	OHX	2	0
88	1	4070	OHX	1	0
88	1	4071	OHX	1	0
88	1	4072	OHX	1	0
88	1	4075	OHX	1	0
88	1	4077	OHX	4	0
88	1	4080	OHX	2	0
88	1	4084	OHX	1	0
88	1	4086	OHX	1	0
88	1	4089	OHX	1	0
88	1	4090	OHX	2	0
88	1	4096	OHX	1	0
88	1	4097	OHX	1	0
88	1	4099	OHX	1	0
88	1	4100	OHX	2	0
88	1	4101	OHX	1	0
88	1	4102	OHX	1	0
88	1	4103	OHX	1	0
88	1	4104	OHX	1	0
88	1	4107	OHX	2	0
88	2	1994	OHX	2	0
88	2	1996	OHX	1	0
88	2	1997	OHX	2	0
88	2	1999	OHX	1	0
88	2	2002	OHX	1	0
88	2	2003	OHX	1	0
88	2	2005	OHX	2	0
88	2	2006	OHX	1	0
88	2	2007	OHX	1	0
88	2	2008	OHX	2	0
88	2	2009	OHX	2	0
88	2	2010	OHX	2	0
88	2	2011	OHX	1	0
88	2	2013	OHX	1	0
88	2	2015	OHX	1	0
88	2	2016	OHX	1	0
88	2	2017	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	2	2020	OHX	1	0
88	2	2021	OHX	1	0
88	2	2022	OHX	1	0
88	2	2023	OHX	1	0
88	2	2024	OHX	2	0
88	2	2028	OHX	1	0
88	2	2029	OHX	1	0
88	2	2030	OHX	1	0
88	2	2031	OHX	1	0
88	2	2033	OHX	1	0
88	2	2034	OHX	1	0
88	2	2036	OHX	1	0
88	2	2037	OHX	1	0
88	2	2040	OHX	1	0
88	2	2041	OHX	1	0
88	2	2042	OHX	1	0
88	2	2044	OHX	2	0
88	2	2045	OHX	1	0
88	2	2049	OHX	1	0
88	2	2052	OHX	1	0
88	2	2053	OHX	1	0
88	2	2055	OHX	2	0
88	2	2056	OHX	1	0
88	2	2058	OHX	1	0
88	2	2061	OHX	8	0
88	2	2062	OHX	1	0
88	2	2064	OHX	2	0
88	2	2067	OHX	1	0
88	2	2068	OHX	2	0
88	2	2071	OHX	2	0
88	2	2074	OHX	3	0
88	2	2075	OHX	2	0
88	2	2076	OHX	1	0
88	2	2079	OHX	3	0
88	2	2082	OHX	3	0
88	2	2086	OHX	2	0
88	2	2087	OHX	1	0
88	2	2090	OHX	1	0
88	2	2091	OHX	1	0
88	2	2092	OHX	4	0
88	2	2097	OHX	1	0
88	2	2098	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	2	2100	OHX	1	0
88	2	2101	OHX	1	0
88	2	2102	OHX	4	0
88	2	2104	OHX	3	0
88	2	2105	OHX	1	0
88	2	2107	OHX	1	0
88	2	2108	OHX	1	0
88	2	2111	OHX	2	0
88	2	2113	OHX	1	0
88	2	2116	OHX	1	0
88	2	2117	OHX	2	0
88	2	2119	OHX	2	0
88	2	2122	OHX	1	0
88	2	2125	OHX	1	0
88	2	2126	OHX	2	0
88	2	2127	OHX	1	0
88	2	2129	OHX	3	0
88	2	2130	OHX	1	0
88	2	2131	OHX	1	0
88	2	2132	OHX	1	0
88	2	2133	OHX	4	0
88	2	2134	OHX	1	0
88	2	2135	OHX	1	0
88	2	2137	OHX	1	0
88	2	2138	OHX	3	0
88	2	2142	OHX	1	0
88	2	2143	OHX	1	0
88	2	2147	OHX	2	0
88	2	2148	OHX	1	0
88	2	2150	OHX	5	0
88	3	209	OHX	1	0
88	3	211	OHX	1	0
88	3	214	OHX	1	0
88	3	218	OHX	1	0
88	4	221	OHX	2	0
88	4	222	OHX	1	0
88	4	223	OHX	1	0
88	4	224	OHX	1	0
88	4	225	OHX	1	0
88	4	228	OHX	1	0
88	4	231	OHX	1	0
88	4	235	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	3795	OHX	1	0
88	5	3796	OHX	2	0
88	5	3797	OHX	2	0
88	5	3799	OHX	2	0
88	5	3803	OHX	1	0
88	5	3804	OHX	1	0
88	5	3805	OHX	1	0
88	5	3806	OHX	1	0
88	5	3807	OHX	2	0
88	5	3809	OHX	2	0
88	5	3810	OHX	1	0
88	5	3813	OHX	1	0
88	5	3814	OHX	1	0
88	5	3818	OHX	1	0
88	5	3822	OHX	1	0
88	5	3823	OHX	2	0
88	5	3828	OHX	1	0
88	5	3829	OHX	1	0
88	5	3831	OHX	1	0
88	5	3832	OHX	1	0
88	5	3833	OHX	1	0
88	5	3834	OHX	1	0
88	5	3836	OHX	1	0
88	5	3838	OHX	1	0
88	5	3839	OHX	1	0
88	5	3840	OHX	1	0
88	5	3843	OHX	1	0
88	5	3845	OHX	1	0
88	5	3847	OHX	1	0
88	5	3848	OHX	1	0
88	5	3851	OHX	3	0
88	5	3852	OHX	4	0
88	5	3853	OHX	1	0
88	5	3854	OHX	1	0
88	5	3855	OHX	2	0
88	5	3858	OHX	1	0
88	5	3859	OHX	1	0
88	5	3860	OHX	2	0
88	5	3861	OHX	2	0
88	5	3863	OHX	1	0
88	5	3864	OHX	1	0
88	5	3868	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	3870	OHX	1	0
88	5	3873	OHX	1	0
88	5	3876	OHX	2	0
88	5	3881	OHX	2	0
88	5	3884	OHX	1	0
88	5	3885	OHX	2	0
88	5	3886	OHX	1	0
88	5	3890	OHX	1	0
88	5	3891	OHX	1	0
88	5	3896	OHX	1	0
88	5	3898	OHX	1	0
88	5	3899	OHX	1	0
88	5	3900	OHX	6	0
88	5	3904	OHX	1	0
88	5	3905	OHX	2	0
88	5	3911	OHX	2	0
88	5	3912	OHX	1	0
88	5	3913	OHX	1	0
88	5	3916	OHX	2	0
88	5	3918	OHX	1	0
88	5	3920	OHX	1	0
88	5	3921	OHX	2	0
88	5	3923	OHX	1	0
88	5	3925	OHX	1	0
88	5	3926	OHX	1	0
88	5	3928	OHX	2	0
88	5	3930	OHX	3	0
88	5	3931	OHX	1	0
88	5	3933	OHX	2	0
88	5	3934	OHX	1	0
88	5	3935	OHX	2	0
88	5	3937	OHX	2	0
88	5	3939	OHX	1	0
88	5	3940	OHX	1	0
88	5	3941	OHX	1	0
88	5	3943	OHX	1	0
88	5	3945	OHX	2	0
88	5	3946	OHX	1	0
88	5	3947	OHX	1	0
88	5	3948	OHX	1	0
88	5	3949	OHX	1	0
88	5	3950	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	3951	OHX	4	0
88	5	3952	OHX	1	0
88	5	3955	OHX	1	0
88	5	3959	OHX	1	0
88	5	3961	OHX	4	0
88	5	3962	OHX	2	0
88	5	3966	OHX	1	0
88	5	3967	OHX	1	0
88	5	3968	OHX	1	0
88	5	3970	OHX	3	0
88	5	3971	OHX	1	0
88	5	3972	OHX	1	0
88	5	3975	OHX	3	0
88	5	3976	OHX	3	0
88	5	3978	OHX	1	0
88	5	3979	OHX	1	0
88	5	3982	OHX	1	0
88	5	3987	OHX	3	0
88	5	3988	OHX	1	0
88	5	3990	OHX	1	0
88	5	3994	OHX	1	0
88	5	3995	OHX	2	0
88	5	3996	OHX	2	0
88	5	3997	OHX	2	0
88	5	3998	OHX	1	0
88	5	4000	OHX	3	0
88	5	4001	OHX	1	0
88	5	4003	OHX	2	0
88	5	4004	OHX	1	0
88	5	4005	OHX	1	0
88	5	4013	OHX	2	0
88	5	4016	OHX	1	0
88	5	4018	OHX	1	0
88	5	4021	OHX	2	0
88	5	4022	OHX	1	0
88	5	4024	OHX	2	0
88	5	4025	OHX	1	0
88	5	4032	OHX	2	0
88	5	4034	OHX	1	0
88	5	4036	OHX	1	0
88	5	4038	OHX	1	0
88	5	4040	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	4041	OHX	1	0
88	5	4042	OHX	1	0
88	5	4047	OHX	1	0
88	5	4048	OHX	1	0
88	5	4051	OHX	1	0
88	5	4052	OHX	1	0
88	5	4053	OHX	2	0
88	5	4055	OHX	2	0
88	5	4058	OHX	1	0
88	5	4059	OHX	2	0
88	5	4064	OHX	1	0
88	5	4065	OHX	1	0
88	5	4067	OHX	1	0
88	5	4068	OHX	3	0
88	5	4071	OHX	2	0
88	5	4072	OHX	1	0
88	5	4074	OHX	1	0
88	5	4075	OHX	1	0
88	5	4078	OHX	1	0
88	5	4079	OHX	1	0
88	5	4080	OHX	2	0
88	5	4081	OHX	2	0
88	5	4082	OHX	2	0
88	5	4083	OHX	1	0
88	5	4084	OHX	1	0
88	5	4085	OHX	1	0
88	5	4088	OHX	2	0
88	5	4089	OHX	1	0
88	5	4091	OHX	1	0
88	5	4092	OHX	1	0
88	5	4094	OHX	1	0
88	5	4095	OHX	1	0
88	5	4096	OHX	1	0
88	5	4099	OHX	2	0
88	5	4102	OHX	1	0
88	5	4106	OHX	5	0
88	5	4107	OHX	3	0
88	5	4108	OHX	1	0
88	5	4110	OHX	1	0
88	5	4111	OHX	1	0
88	5	4112	OHX	2	0
88	5	4118	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	5	4121	OHX	2	0
88	5	4124	OHX	2	0
88	5	4126	OHX	6	0
88	5	4130	OHX	1	0
88	5	4132	OHX	1	0
88	5	4134	OHX	1	0
88	5	4137	OHX	3	0
88	5	4138	OHX	1	0
88	5	4139	OHX	1	0
88	5	4140	OHX	1	0
88	5	4142	OHX	1	0
88	5	4143	OHX	1	0
88	5	4149	OHX	1	0
88	5	4150	OHX	1	0
88	5	4152	OHX	1	0
88	5	4153	OHX	1	0
88	5	4154	OHX	1	0
88	5	4156	OHX	1	0
88	5	4157	OHX	4	0
88	5	4159	OHX	1	0
88	6	2014	OHX	1	0
88	6	2016	OHX	1	0
88	6	2020	OHX	1	0
88	6	2022	OHX	1	0
88	6	2025	OHX	1	0
88	6	2027	OHX	1	0
88	6	2028	OHX	1	0
88	6	2029	OHX	1	0
88	6	2032	OHX	1	0
88	6	2033	OHX	1	0
88	6	2036	OHX	1	0
88	6	2037	OHX	1	0
88	6	2038	OHX	1	0
88	6	2040	OHX	4	0
88	6	2044	OHX	1	0
88	6	2045	OHX	2	0
88	6	2050	OHX	1	0
88	6	2051	OHX	1	0
88	6	2053	OHX	1	0
88	6	2055	OHX	1	0
88	6	2060	OHX	2	0
88	6	2063	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	6	2064	OHX	1	0
88	6	2066	OHX	1	0
88	6	2067	OHX	4	0
88	6	2069	OHX	2	0
88	6	2070	OHX	1	0
88	6	2074	OHX	2	0
88	6	2075	OHX	1	0
88	6	2076	OHX	1	0
88	6	2079	OHX	1	0
88	6	2081	OHX	2	0
88	6	2084	OHX	1	0
88	6	2085	OHX	2	0
88	6	2086	OHX	4	0
88	6	2087	OHX	1	0
88	6	2089	OHX	1	0
88	6	2091	OHX	1	0
88	6	2092	OHX	1	0
88	6	2095	OHX	1	0
88	6	2096	OHX	4	0
88	6	2097	OHX	1	0
88	6	2101	OHX	1	0
88	6	2102	OHX	1	0
88	6	2104	OHX	2	0
88	6	2106	OHX	1	0
88	6	2109	OHX	4	0
88	6	2110	OHX	1	0
88	6	2116	OHX	1	0
88	6	2121	OHX	2	0
88	6	2126	OHX	4	0
88	6	2127	OHX	4	0
88	6	2134	OHX	2	0
88	6	2135	OHX	1	0
88	6	2136	OHX	2	0
88	6	2137	OHX	1	0
88	6	2139	OHX	1	0
88	6	2140	OHX	1	0
88	6	2141	OHX	1	0
88	6	2142	OHX	4	0
88	6	2144	OHX	1	0
88	6	2145	OHX	1	0
88	6	2146	OHX	1	0
88	6	2148	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	6	2151	OHX	1	0
88	6	2152	OHX	2	0
88	6	2153	OHX	1	0
88	6	2156	OHX	2	0
88	6	2159	OHX	2	0
88	6	2160	OHX	2	0
88	6	2164	OHX	1	0
88	6	2166	OHX	1	0
88	6	2169	OHX	1	0
88	6	2170	OHX	1	0
88	6	2173	OHX	1	0
88	6	2174	OHX	3	0
88	6	2175	OHX	2	0
88	6	2177	OHX	1	0
88	6	2179	OHX	1	0
88	6	2182	OHX	1	0
88	6	2184	OHX	1	0
88	7	218	OHX	1	0
88	7	219	OHX	1	0
88	7	221	OHX	1	0
88	7	224	OHX	1	0
88	7	225	OHX	1	0
88	8	214	OHX	1	0
88	8	215	OHX	1	0
88	8	216	OHX	1	0
88	8	219	OHX	1	0
88	8	220	OHX	1	0
88	8	221	OHX	1	0
88	8	222	OHX	2	0
88	8	223	OHX	1	0
88	8	225	OHX	1	0
88	8	227	OHX	1	0
88	8	229	OHX	1	0
88	8	230	OHX	1	0
88	8	231	OHX	1	0
88	C3	201	OHX	5	0
88	C5	201	OHX	2	0
88	D9	103	OHX	1	0
88	L3	404	OHX	3	0
88	L4	401	OHX	4	0
88	L5	301	OHX	1	0
88	M0	302	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	M0	303	OHX	3	0
88	M5	301	OHX	1	0
88	M7	204	OHX	1	0
88	M7	205	OHX	2	0
88	M9	201	OHX	2	0
88	N1	201	OHX	1	0
88	N9	102	OHX	1	0
88	O3	203	OHX	1	0
88	O7	105	OHX	3	0
88	O7	106	OHX	1	0
88	O9	101	OHX	1	0
88	Q2	503	OHX	1	0
88	S1	301	OHX	3	0
88	S6	301	OHX	3	0
88	S8	301	OHX	2	0
88	S9	202	OHX	1	0
88	SR	401	OHX	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
86	l1	46
1	2	2
81	m2	2
36	5	1

The worst 5 of 51 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	5.68
1	l1	132:UNK	C	133:UNK	N	4.51
1	m2	23:UNK	C	28:UNK	N	4.14
1	l1	81:UNK	C	82:UNK	N	3.84
1	5	2437:G	O3'	2438:A	P	3.63

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%)	0.76	159 (8%) 12 6	57, 96, 178, 219	0
1	6	1795/1800 (99%)	0.51	86 (4%) 34 20	44, 84, 166, 211	0
2	S0	206/251 (82%)	1.12	43 (20%) 1 1	100, 115, 126, 138	0
2	s0	206/251 (82%)	0.62	18 (8%) 13 6	81, 98, 114, 118	0
3	S1	214/254 (84%)	0.80	34 (15%) 3 1	104, 134, 156, 161	0
3	s1	216/254 (85%)	0.49	12 (5%) 28 14	77, 91, 111, 123	0
4	S2	217/253 (85%)	0.91	36 (16%) 2 1	81, 93, 109, 115	0
4	s2	217/253 (85%)	1.13	48 (22%) 1 1	65, 81, 96, 112	0
5	S3	223/239 (93%)	1.34	68 (30%) 1 0	84, 97, 119, 130	0
5	s3	223/239 (93%)	0.80	39 (17%) 2 1	80, 109, 133, 136	0
6	S4	260/260 (100%)	1.33	80 (30%) 1 0	71, 96, 106, 121	0
6	s4	260/260 (100%)	0.71	26 (10%) 9 4	59, 86, 100, 121	0
7	S5	206/224 (91%)	1.11	50 (24%) 1 1	103, 122, 131, 135	0
7	s5	206/224 (91%)	0.93	40 (19%) 1 1	83, 106, 121, 129	0
8	S6	226/236 (95%)	0.49	22 (9%) 10 5	72, 102, 122, 133	0
8	s6	218/236 (92%)	0.48	13 (5%) 25 13	60, 90, 110, 121	0
9	S7	184/189 (97%)	1.31	56 (30%) 1 0	98, 122, 142, 148	0
9	s7	186/189 (98%)	0.67	19 (10%) 9 4	79, 107, 134, 139	0
10	S8	188/200 (94%)	1.47	54 (28%) 1 0	67, 83, 116, 129	0
10	s8	188/200 (94%)	0.71	12 (6%) 23 11	56, 74, 119, 135	0
11	S9	185/196 (94%)	1.94	80 (43%) 0 0	86, 103, 129, 145	0
11	s9	185/196 (94%)	1.21	39 (21%) 1 1	72, 90, 120, 138	0
12	C0	96/105 (91%)	0.33	8 (8%) 14 6	89, 110, 128, 138	0
12	c0	96/105 (91%)	1.13	25 (26%) 1 0	101, 132, 145, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	C1	155/155 (100%)	1.50	42 (27%)	1	0	71, 82, 114, 129	0
13	c1	146/155 (94%)	1.21	21 (14%)	3	2	59, 71, 99, 122	0
14	C2	124/124 (100%)	0.72	14 (11%)	7	3	135, 143, 151, 154	0
14	c2	124/124 (100%)	2.28	62 (50%)	0	0	172, 187, 200, 208	0
15	C3	150/150 (100%)	0.64	19 (12%)	5	2	77, 91, 111, 115	0
15	c3	150/150 (100%)	0.65	11 (7%)	18	9	64, 80, 95, 100	0
16	C4	127/136 (93%)	0.38	12 (9%)	11	5	78, 131, 145, 150	0
16	c4	128/136 (94%)	0.78	15 (11%)	6	3	58, 92, 102, 108	0
17	C5	124/137 (90%)	0.70	14 (11%)	7	3	84, 100, 116, 128	0
17	c5	135/137 (98%)	1.18	28 (20%)	1	1	76, 101, 113, 119	0
18	C6	141/142 (99%)	2.41	75 (53%)	0	0	89, 110, 115, 118	0
18	c6	142/142 (100%)	2.18	69 (48%)	0	0	75, 99, 113, 127	0
19	C7	120/136 (88%)	1.75	49 (40%)	0	0	96, 110, 133, 135	0
19	c7	117/136 (86%)	0.88	20 (17%)	2	1	83, 98, 116, 118	0
20	C8	145/145 (100%)	0.47	10 (6%)	20	10	83, 109, 130, 138	0
20	c8	145/145 (100%)	0.70	20 (13%)	4	2	82, 97, 120, 130	0
21	C9	143/143 (100%)	1.98	70 (48%)	0	0	94, 108, 119, 126	0
21	c9	143/143 (100%)	1.08	25 (17%)	2	1	78, 93, 110, 119	0
22	D0	107/120 (89%)	2.12	47 (43%)	0	0	82, 112, 129, 132	0
22	d0	110/120 (91%)	2.21	57 (51%)	0	0	79, 110, 138, 141	0
23	D1	87/87 (100%)	0.83	14 (16%)	3	1	96, 104, 120, 127	0
23	d1	87/87 (100%)	0.33	3 (3%)	49	32	78, 87, 109, 119	0
24	D2	129/129 (100%)	2.43	75 (58%)	0	0	80, 93, 99, 108	0
25	D3	144/144 (100%)	1.04	30 (20%)	1	1	67, 73, 81, 95	0
25	d3	144/144 (100%)	0.70	22 (15%)	3	1	54, 61, 72, 82	0
26	D4	134/134 (100%)	0.62	15 (11%)	7	3	80, 104, 115, 122	0
26	d4	134/134 (100%)	0.17	3 (2%)	65	49	68, 91, 103, 109	0
27	D5	70/107 (65%)	0.51	6 (8%)	13	6	119, 133, 139, 141	0
27	d5	69/107 (64%)	0.91	8 (11%)	6	3	97, 117, 127, 130	0
28	D6	97/97 (100%)	2.03	51 (52%)	0	0	82, 95, 140, 144	0
28	d6	97/97 (100%)	1.43	28 (28%)	1	0	62, 74, 105, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
29	D7	81/81 (100%)	1.91	35 (43%)	0	0	95, 109, 134, 140	0
29	d7	81/81 (100%)	1.69	27 (33%)	0	0	79, 93, 127, 132	0
30	D8	63/66 (95%)	0.84	13 (20%)	1	1	111, 126, 137, 141	0
30	d8	63/66 (95%)	1.18	16 (25%)	1	0	98, 113, 124, 135	0
31	D9	53/55 (96%)	1.69	20 (37%)	0	0	83, 87, 103, 110	0
31	d9	53/55 (96%)	2.92	34 (64%)	0	0	77, 88, 125, 139	0
32	E0	60/62 (96%)	2.27	27 (45%)	0	0	74, 101, 125, 127	0
32	e0	62/62 (100%)	0.67	9 (14%)	3	2	62, 89, 112, 115	0
33	E1	71/76 (93%)	1.56	25 (35%)	0	0	103, 132, 143, 147	0
33	e1	76/76 (100%)	2.80	41 (53%)	0	0	108, 162, 178, 183	0
34	SR	318/318 (100%)	1.01	55 (17%)	2	1	106, 117, 131, 147	0
34	sR	318/318 (100%)	1.44	99 (31%)	1	0	106, 124, 137, 148	0
35	SM	159/273 (58%)	0.90	33 (20%)	1	1	58, 94, 141, 144	0
35	sM	104/273 (38%)	0.36	7 (6%)	21	11	50, 106, 179, 186	0
36	1	3149/3396 (92%)	0.33	37 (1%)	81	69	35, 57, 128, 216	0
36	5	3169/3396 (93%)	0.38	40 (1%)	79	67	33, 53, 126, 187	0
37	3	121/121 (100%)	0.18	0	100	100	41, 72, 85, 91	0
37	7	121/121 (100%)	0.21	0	100	100	39, 58, 68, 77	0
38	4	158/158 (100%)	0.19	1 (0%)	90	84	43, 58, 94, 137	0
38	8	158/158 (100%)	0.21	0	100	100	43, 59, 94, 128	0
39	L2	252/253 (99%)	0.90	28 (11%)	7	3	44, 61, 76, 85	0
39	l2	252/253 (99%)	1.03	29 (11%)	6	3	40, 56, 73, 80	0
40	L3	386/386 (100%)	0.38	16 (4%)	41	25	40, 59, 72, 87	0
40	l3	386/386 (100%)	0.21	5 (1%)	79	67	34, 48, 62, 78	0
41	L4	361/361 (100%)	0.03	1 (0%)	94	92	38, 53, 69, 74	0
41	l4	361/361 (100%)	0.04	0	100	100	39, 55, 72, 84	0
42	L5	296/296 (100%)	0.66	25 (8%)	14	6	55, 79, 95, 114	0
42	l5	294/296 (99%)	0.38	7 (2%)	62	45	46, 62, 87, 102	0
43	L6	156/175 (89%)	0.09	0	100	100	47, 54, 70, 83	0
43	l6	157/175 (89%)	0.11	2 (1%)	79	67	48, 56, 76, 87	0
44	L7	222/243 (91%)	0.08	0	100	100	38, 48, 76, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	0.04	0 100 100	38, 47, 77, 109	0
45	L8	233/255 (91%)	0.61	15 (6%) 23 11	67, 81, 110, 120	0
45	l8	231/255 (90%)	0.58	19 (8%) 14 7	69, 82, 109, 118	0
46	L9	191/191 (100%)	0.15	2 (1%) 84 74	54, 65, 77, 87	0
46	l9	191/191 (100%)	0.11	2 (1%) 84 74	43, 55, 71, 81	0
47	M0	211/220 (95%)	0.24	1 (0%) 91 87	41, 55, 88, 106	0
47	m0	213/220 (96%)	0.28	2 (0%) 85 77	39, 56, 80, 97	0
48	M1	169/173 (97%)	0.87	25 (14%) 3 2	63, 81, 93, 100	0
48	m1	169/173 (97%)	0.42	5 (2%) 54 37	51, 65, 76, 83	0
49	M3	193/198 (97%)	0.29	1 (0%) 91 87	38, 63, 100, 123	0
49	m3	194/198 (97%)	0.17	2 (1%) 84 74	39, 66, 96, 120	0
50	M4	136/137 (99%)	-0.03	0 100 100	49, 56, 68, 78	0
50	m4	137/137 (100%)	-0.07	0 100 100	45, 52, 66, 80	0
51	M5	204/204 (100%)	1.00	21 (10%) 9 4	40, 54, 66, 70	0
52	M6	197/198 (99%)	0.34	4 (2%) 68 52	39, 44, 64, 67	20 (10%)
52	m6	197/198 (99%)	0.28	2 (1%) 84 74	34, 40, 63, 65	18 (9%)
53	M7	183/183 (100%)	0.58	9 (4%) 33 19	43, 50, 97, 121	0
53	m7	155/183 (84%)	0.32	1 (0%) 90 84	37, 45, 59, 88	0
54	M8	185/185 (100%)	0.37	3 (1%) 74 61	41, 54, 69, 90	0
54	m8	185/185 (100%)	0.60	13 (7%) 19 10	40, 55, 64, 69	0
55	M9	188/188 (100%)	0.42	16 (8%) 13 6	60, 74, 144, 150	0
55	m9	188/188 (100%)	0.32	8 (4%) 39 23	49, 62, 125, 137	0
56	N0	172/172 (100%)	0.41	8 (4%) 35 20	46, 54, 65, 73	0
56	n0	172/172 (100%)	0.06	0 100 100	41, 48, 61, 70	0
57	N1	159/159 (100%)	0.70	14 (8%) 12 6	41, 54, 96, 103	0
57	n1	159/159 (100%)	0.65	11 (6%) 20 10	38, 48, 82, 89	0
58	N2	100/120 (83%)	0.41	7 (7%) 19 10	89, 104, 117, 121	0
58	n2	98/120 (81%)	0.67	7 (7%) 19 10	73, 85, 93, 97	0
59	N3	136/136 (100%)	0.55	7 (5%) 32 17	46, 56, 68, 76	0
59	n3	136/136 (100%)	0.54	2 (1%) 76 62	35, 45, 56, 60	0
60	N4	98/155 (63%)	2.10	31 (31%) 1 0	57, 69, 134, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	n4	135/155 (87%)	0.77	14 (10%) 8 4	45, 93, 120, 132	0
61	N5	121/141 (85%)	0.47	4 (3%) 50 33	55, 66, 82, 107	0
61	n5	120/141 (85%)	0.27	3 (2%) 61 45	53, 66, 81, 93	0
62	N6	126/126 (100%)	0.49	4 (3%) 51 34	46, 60, 71, 77	0
62	n6	126/126 (100%)	0.45	0 100 100	49, 63, 75, 82	0
63	N7	135/135 (100%)	0.97	17 (12%) 5 3	81, 93, 105, 113	0
63	n7	135/135 (100%)	0.70	16 (11%) 6 3	74, 88, 99, 104	0
64	N8	148/148 (100%)	0.46	5 (3%) 49 32	35, 56, 78, 89	0
64	n8	148/148 (100%)	0.64	7 (4%) 35 20	35, 55, 76, 80	0
65	N9	58/58 (100%)	1.10	10 (17%) 2 1	37, 60, 96, 109	0
65	n9	58/58 (100%)	0.83	9 (15%) 3 1	37, 56, 77, 87	0
66	O0	97/104 (93%)	-0.25	0 100 100	81, 89, 107, 111	0
66	o0	100/104 (96%)	-0.04	3 (3%) 54 37	72, 80, 100, 109	0
67	O1	109/112 (97%)	1.23	29 (26%) 1 0	57, 69, 91, 98	0
67	o1	109/112 (97%)	0.66	3 (2%) 56 40	45, 57, 88, 104	0
68	O2	127/129 (98%)	0.27	2 (1%) 74 61	36, 48, 61, 74	0
68	o2	127/129 (98%)	0.22	0 100 100	34, 51, 64, 70	0
69	O3	106/106 (100%)	0.31	0 100 100	39, 45, 64, 74	0
69	o3	106/106 (100%)	0.52	3 (2%) 56 40	38, 45, 69, 77	0
70	O4	112/119 (94%)	1.29	35 (31%) 1 0	55, 71, 106, 113	0
70	o4	112/119 (94%)	1.43	35 (31%) 1 0	48, 66, 102, 107	0
71	O5	119/119 (100%)	0.03	1 (0%) 87 79	51, 68, 76, 81	0
71	o5	119/119 (100%)	0.19	4 (3%) 49 32	55, 68, 83, 92	0
72	O6	99/99 (100%)	0.49	9 (9%) 11 5	59, 69, 97, 110	0
72	o6	99/99 (100%)	0.76	6 (6%) 25 12	63, 71, 88, 106	0
73	O7	87/87 (100%)	0.58	2 (2%) 64 47	42, 48, 66, 85	0
73	o7	87/87 (100%)	0.72	3 (3%) 49 32	39, 47, 73, 92	0
74	O8	77/77 (100%)	0.42	5 (6%) 22 11	77, 90, 107, 112	0
74	o8	77/77 (100%)	0.88	14 (18%) 2 1	73, 86, 99, 101	0
75	O9	50/50 (100%)	0.73	3 (6%) 25 13	49, 55, 58, 58	0
75	o9	50/50 (100%)	0.97	4 (8%) 15 7	47, 52, 60, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	Q0	52/52 (100%)	0.57	2 (3%) 44 27	46, 52, 67, 73	0
76	q0	52/52 (100%)	0.31	0 100 100	39, 45, 55, 58	0
77	Q1	25/25 (100%)	2.41	16 (64%) 0 0	58, 64, 68, 69	0
77	q1	25/25 (100%)	1.28	3 (12%) 6 3	50, 53, 56, 57	0
78	Q2	105/105 (100%)	0.25	1 (0%) 84 74	42, 56, 75, 99	0
78	q2	105/105 (100%)	0.17	2 (1%) 70 54	41, 54, 69, 107	0
79	Q3	91/91 (100%)	0.66	6 (6%) 22 11	51, 64, 78, 86	0
79	q3	91/91 (100%)	1.11	16 (17%) 2 1	44, 56, 72, 82	0
80	d2	130/130 (100%)	1.20	24 (18%) 2 1	63, 75, 82, 91	0
81	m2	0/150	-	-	-	-
82	m5	203/203 (100%)	1.30	38 (18%) 2 1	41, 56, 68, 73	0
83	p0	143/220 (65%)	0.99	28 (19%) 1 1	103, 124, 217, 227	0
84	p1	0/47	-	-	-	-
84	p2	0/47	-	-	-	-
85	f	147/157 (93%)	0.42	10 (6%) 20 10	48, 81, 147, 150	4 (2%)
86	l1	0/213	-	-	-	-
All	All	33262/35574 (93%)	0.66	3268 (9%) 10 5	33, 73, 133, 227	42 (0%)

The worst 5 of 3268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	1694	A	15.4
1	2	1693	A	14.9
60	N4	86	SER	14.5
60	N4	75	THR	14.4
1	2	1708	U	14.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	5CT	f	51	15/16	0.89	0.49	-	46,46,46,46	15

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
87	MG	1	3735	1/1	0.95	1.82	50.63	38,38,38,38	0
87	MG	1	3674	1/1	0.86	0.63	41.51	75,75,75,75	0
87	MG	6	1988	1/1	0.56	0.77	40.28	61,61,61,61	0
87	MG	5	3769	1/1	0.96	0.94	39.04	43,43,43,43	1
87	MG	1	3707	1/1	0.93	1.14	35.84	45,45,45,45	1
87	MG	5	3670	1/1	0.82	1.34	35.32	36,36,36,36	1
87	MG	6	1934	1/1	0.93	0.52	30.74	79,79,79,79	0
87	MG	O7	104	1/1	0.93	2.39	28.93	43,43,43,43	1
88	OHX	5	4081	7/7	0.90	0.53	25.50	72,72,72,72	4
87	MG	5	3665	1/1	0.88	0.48	24.04	39,39,39,39	1
88	OHX	6	2071	7/7	0.89	0.37	23.89	57,57,57,57	3
87	MG	1	3667	1/1	0.98	0.64	23.50	38,38,38,38	1
87	MG	5	3593	1/1	0.99	0.53	23.46	28,28,28,28	0
87	MG	1	3547	1/1	0.95	0.47	23.29	38,38,38,38	0
87	MG	5	3761	1/1	0.90	1.13	23.11	41,41,41,41	1
87	MG	5	4162	1/1	0.95	1.68	22.17	36,36,36,36	1
88	OHX	5	3918	7/7	0.92	0.41	22.08	46,46,46,46	3
87	MG	7	215	1/1	0.98	1.08	22.06	54,54,54,54	1
87	MG	5	3497	1/1	0.80	0.68	20.83	48,48,48,48	1
88	OHX	5	4068	7/7	0.96	0.32	20.22	38,38,38,38	4
87	MG	5	4165	1/1	0.96	1.10	19.96	39,39,39,39	1
88	OHX	5	4093	7/7	0.87	0.32	19.72	80,80,80,80	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	4	215	1/1	0.95	0.94	19.62	51,51,51,51	1
88	OHX	1	3950	7/7	0.90	0.31	18.88	99,99,99,99	5
87	MG	5	3529	1/1	0.96	0.50	18.80	28,28,28,28	0
87	MG	1	4112	1/1	0.97	0.81	18.68	35,35,35,35	1
88	OHX	5	3920	7/7	0.95	0.33	17.91	48,48,48,48	2
87	MG	6	1994	1/1	0.88	0.76	17.72	57,57,57,57	1
87	MG	1	3497	1/1	0.97	0.42	17.59	34,34,34,34	0
88	OHX	1	3853	7/7	0.94	0.37	17.36	70,70,70,70	1
88	OHX	1	3843	7/7	0.95	0.25	16.85	111,111,111,111	1
87	MG	O3	201	1/1	0.86	0.95	16.73	44,44,44,44	1
88	OHX	1	4098	7/7	0.91	0.44	16.16	45,45,45,45	5
88	OHX	5	4019	7/7	0.82	0.36	15.84	60,60,60,60	5
87	MG	1	3687	1/1	0.96	0.47	15.69	41,41,41,41	1
87	MG	2	1956	1/1	0.94	0.55	15.63	90,90,90,90	0
87	MG	5	3516	1/1	0.97	0.41	15.20	36,36,36,36	0
87	MG	5	3731	1/1	0.82	0.47	15.03	44,44,44,44	0
87	MG	1	3733	1/1	0.93	1.15	14.84	37,37,37,37	1
87	MG	1	3416	1/1	0.88	0.39	14.82	42,42,42,42	0
87	MG	5	3504	1/1	0.93	0.41	14.20	36,36,36,36	0
88	OHX	1	4000	7/7	0.97	0.28	14.06	104,104,104,104	5
87	MG	5	3547	1/1	0.86	0.40	13.97	51,51,51,51	0
87	MG	1	3511	1/1	0.93	0.32	13.49	36,36,36,36	0
87	MG	1	3556	1/1	0.96	0.37	13.32	29,29,29,29	0
87	MG	5	3429	1/1	0.99	0.44	13.27	30,30,30,30	0
87	MG	5	3520	1/1	0.98	0.57	13.05	39,39,39,39	0
87	MG	1	3554	1/1	0.99	0.52	13.05	30,30,30,30	0
87	MG	5	3587	1/1	0.96	0.40	13.04	39,39,39,39	0
87	MG	6	2009	1/1	0.91	0.43	12.94	73,73,73,73	0
87	MG	1	3512	1/1	0.95	0.45	12.71	37,37,37,37	0
88	OHX	6	2029	7/7	0.96	0.31	12.67	67,67,67,67	5
87	MG	1	3580	1/1	0.98	0.52	12.54	27,27,27,27	0
87	MG	5	3595	1/1	0.89	0.41	12.37	35,35,35,35	0
87	MG	1	3573	1/1	0.94	0.38	12.12	53,53,53,53	0
88	OHX	1	3846	7/7	0.88	0.37	12.11	43,43,43,43	3
87	MG	1	3577	1/1	0.98	0.48	12.02	27,27,27,27	0
88	OHX	5	3932	7/7	0.95	0.36	11.46	88,88,88,88	3
87	MG	1	3541	1/1	0.98	0.42	11.31	39,39,39,39	0
87	MG	O2	201	1/1	0.95	0.65	11.09	36,36,36,36	1
87	MG	5	3582	1/1	0.98	0.46	10.86	34,34,34,34	0
87	MG	1	3686	1/1	0.96	0.64	10.78	47,47,47,47	1
87	MG	1	3535	1/1	0.86	0.49	10.73	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	5	3405	1/1	0.97	0.40	10.69	34,34,34,34	0
87	MG	1	3570	1/1	0.95	0.40	10.49	37,37,37,37	0
87	MG	1	3568	1/1	0.89	0.45	10.48	40,40,40,40	0
87	MG	5	3714	1/1	0.97	0.80	10.36	39,39,39,39	1
87	MG	5	3419	1/1	0.83	0.30	10.31	51,51,51,51	0
88	OHX	3	219	7/7	0.69	0.33	10.24	78,78,78,78	5
87	MG	5	3594	1/1	0.89	0.42	10.23	36,36,36,36	0
87	MG	5	3767	1/1	0.84	0.49	10.12	40,40,40,40	0
87	MG	5	3633	1/1	0.97	0.30	10.03	43,43,43,43	0
88	OHX	3	211	7/7	0.97	0.34	9.98	55,55,55,55	2
88	OHX	1	4009	7/7	0.93	0.29	9.93	42,42,42,42	3
87	MG	5	3448	1/1	0.96	0.33	9.81	34,34,34,34	0
87	MG	1	3410	1/1	0.97	0.38	9.74	55,55,55,55	0
88	OHX	5	4152	7/7	0.88	0.35	9.73	50,50,50,50	3
87	MG	6	1945	1/1	0.78	0.36	9.65	66,66,66,66	0
88	OHX	5	4147	7/7	0.74	0.44	9.59	52,52,52,52	5
87	MG	5	3508	1/1	0.97	0.40	9.58	34,34,34,34	0
87	MG	1	4113	1/1	0.86	1.27	9.55	55,55,55,55	1
88	OHX	5	3998	7/7	0.94	0.33	9.41	101,101,101,101	4
87	MG	1	3670	1/1	0.74	0.38	9.37	44,44,44,44	0
88	OHX	7	223	7/7	0.96	0.29	9.24	65,65,65,65	1
87	MG	6	1908	1/1	0.82	0.31	9.24	58,58,58,58	0
88	OHX	5	3959	7/7	0.94	0.29	9.15	78,78,78,78	2
88	OHX	1	3923	7/7	0.93	0.34	9.04	36,36,36,36	2
88	OHX	5	3838	7/7	0.97	0.36	8.98	62,62,62,62	3
87	MG	5	3720	1/1	0.93	0.33	8.85	42,42,42,42	0
88	OHX	5	4069	7/7	0.93	0.32	8.84	143,143,143,143	7
88	OHX	5	3826	7/7	0.98	0.28	8.83	47,47,47,47	3
88	OHX	5	3923	7/7	0.88	0.38	8.80	37,37,37,37	4
87	MG	5	3561	1/1	0.97	0.40	8.64	35,35,35,35	0
88	OHX	1	4053	7/7	0.94	0.29	8.62	51,51,51,51	4
87	MG	1	3465	1/1	0.94	0.40	8.45	30,30,30,30	0
88	OHX	1	4076	7/7	0.90	0.83	8.37	48,48,48,48	3
87	MG	4	206	1/1	0.98	0.38	8.11	40,40,40,40	0
87	MG	1	3455	1/1	0.96	0.40	8.07	32,32,32,32	0
88	OHX	4	234	7/7	0.91	0.30	8.03	64,64,64,64	5
87	MG	1	3559	1/1	0.93	0.36	7.87	33,33,33,33	0
88	OHX	5	3886	7/7	0.97	0.29	7.71	66,66,66,66	3
87	MG	5	3578	1/1	0.99	0.41	7.68	38,38,38,38	0
87	MG	1	3731	1/1	0.94	0.51	7.64	47,47,47,47	1
88	OHX	8	220	7/7	0.96	0.26	7.57	75,75,75,75	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	4055	7/7	0.93	0.26	7.48	44,44,44,44	3
87	MG	5	3751	1/1	0.87	0.47	7.35	51,51,51,51	0
87	MG	6	1922	1/1	0.98	0.36	7.28	60,60,60,60	0
88	OHX	7	218	7/7	0.97	0.30	7.25	56,56,56,56	2
87	MG	1	3503	1/1	0.97	0.48	7.23	34,34,34,34	0
87	MG	1	3692	1/1	0.90	0.36	7.21	58,58,58,58	1
88	OHX	1	4103	7/7	0.88	0.34	7.17	46,46,46,46	4
88	OHX	5	3858	7/7	0.96	0.31	7.17	45,45,45,45	4
88	OHX	1	3856	7/7	0.94	0.28	7.17	45,45,45,45	4
87	MG	5	3431	1/1	0.96	0.43	7.12	44,44,44,44	0
87	MG	1	3578	1/1	0.99	0.43	7.11	34,34,34,34	0
88	OHX	1	3956	7/7	0.88	0.28	7.10	65,65,65,65	3
88	OHX	1	3812	7/7	0.97	0.30	7.01	100,100,100,100	3
88	OHX	1	4031	7/7	0.89	0.21	7.00	116,116,116,116	3
87	MG	5	3475	1/1	0.92	0.30	6.96	34,34,34,34	0
88	OHX	1	4028	7/7	0.97	0.30	6.91	70,70,70,70	4
87	MG	1	3527	1/1	0.93	0.33	6.74	40,40,40,40	0
88	OHX	5	3847	7/7	0.98	0.33	6.70	87,87,87,87	3
88	OHX	1	3859	7/7	0.93	0.32	6.67	82,82,82,82	5
87	MG	1	3552	1/1	0.89	0.41	6.65	52,52,52,52	0
88	OHX	5	3840	7/7	0.95	0.33	6.53	65,65,65,65	2
87	MG	5	3585	1/1	0.95	0.48	6.51	38,38,38,38	0
87	MG	1	3493	1/1	0.95	0.40	6.51	30,30,30,30	0
88	OHX	1	4060	7/7	0.85	0.30	6.50	61,61,61,61	4
87	MG	1	3623	1/1	0.96	0.38	6.49	48,48,48,48	0
87	MG	n3	201	1/1	0.98	0.40	6.48	31,31,31,31	0
88	OHX	1	3903	7/7	0.95	0.27	6.46	52,52,52,52	3
87	MG	5	3600	1/1	0.93	0.31	6.35	45,45,45,45	0
88	OHX	1	4050	7/7	0.77	0.27	6.34	106,106,106,106	5
88	OHX	5	3911	7/7	0.98	0.28	6.30	137,137,137,137	3
88	OHX	5	4088	7/7	0.83	0.55	6.26	41,41,41,41	6
87	MG	5	3583	1/1	0.98	0.45	6.23	28,28,28,28	0
87	MG	5	3544	1/1	0.96	0.40	6.22	54,54,54,54	0
87	MG	5	3464	1/1	0.80	0.35	6.19	118,118,118,118	0
88	OHX	8	225	7/7	0.91	0.29	6.17	70,70,70,70	5
87	MG	5	3414	1/1	0.95	0.36	6.17	34,34,34,34	0
88	OHX	7	221	7/7	0.99	0.27	6.15	67,67,67,67	2
88	OHX	5	3887	7/7	0.98	0.31	6.15	87,87,87,87	3
87	MG	5	3533	1/1	0.96	0.30	6.14	54,54,54,54	0
88	OHX	5	4100	7/7	0.83	0.71	6.13	50,50,50,50	4
88	OHX	1	3820	7/7	0.96	0.28	6.06	86,86,86,86	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	7	222	7/7	0.98	0.31	6.04	66,66,66,66	2
88	OHX	5	3846	7/7	0.99	0.27	5.93	88,88,88,88	1
87	MG	6	1962	1/1	0.83	0.27	5.81	95,95,95,95	0
87	MG	5	3564	1/1	0.88	0.38	5.79	33,33,33,33	0
88	OHX	1	3842	7/7	0.98	0.28	5.77	109,109,109,109	3
88	OHX	M7	204	7/7	0.81	0.56	5.76	43,43,43,43	4
88	OHX	1	3992	7/7	0.97	0.31	5.73	82,82,82,82	5
88	OHX	6	2065	7/7	0.94	0.22	5.67	141,141,141,141	6
87	MG	1	3732	1/1	0.96	0.40	5.64	37,37,37,37	0
87	MG	3	220	1/1	0.97	0.34	5.59	49,49,49,49	1
88	OHX	6	2064	7/7	0.94	0.28	5.53	97,97,97,97	3
88	OHX	1	4101	7/7	0.75	0.26	5.51	85,85,85,85	6
88	OHX	1	3886	7/7	0.97	0.22	5.50	124,124,124,124	4
88	OHX	1	4090	7/7	0.90	0.24	5.38	46,46,46,46	4
87	MG	1	3534	1/1	0.94	0.34	5.35	40,40,40,40	0
88	OHX	1	3810	7/7	0.97	0.28	5.35	89,89,89,89	4
88	OHX	1	3815	7/7	0.99	0.30	5.31	51,51,51,51	3
88	OHX	5	4117	7/7	0.90	0.34	5.29	36,36,36,36	2
87	MG	1	3422	1/1	0.98	0.35	5.26	58,58,58,58	0
88	OHX	5	3915	7/7	0.89	0.26	5.25	127,127,127,127	5
88	OHX	5	3884	7/7	0.99	0.28	5.21	53,53,53,53	3
88	OHX	1	3825	7/7	0.98	0.27	5.20	90,90,90,90	3
88	OHX	1	3899	7/7	0.89	0.44	5.17	50,50,50,50	5
88	OHX	5	3905	7/7	0.95	0.27	5.10	118,118,118,118	3
88	OHX	1	3821	7/7	0.98	0.23	5.06	83,83,83,83	3
87	MG	5	3549	1/1	0.97	0.37	5.05	56,56,56,56	0
88	OHX	1	4069	7/7	0.82	0.36	5.04	51,51,51,51	3
87	MG	5	3501	1/1	0.97	0.33	4.98	33,33,33,33	0
88	OHX	2	2148	7/7	0.93	0.54	4.91	67,67,67,67	4
88	OHX	5	3810	7/7	1.00	0.22	4.89	69,69,69,69	0
87	MG	1	3513	1/1	0.96	0.26	4.89	50,50,50,50	0
88	OHX	1	3968	7/7	0.97	0.30	4.88	72,72,72,72	3
87	MG	1	3683	1/1	0.86	0.33	4.84	46,46,46,46	0
87	MG	5	3510	1/1	0.96	0.36	4.80	35,35,35,35	0
88	OHX	5	4109	7/7	0.96	0.33	4.78	68,68,68,68	6
88	OHX	1	4107	7/7	0.96	0.23	4.76	151,151,151,151	6
87	MG	6	1982	1/1	0.94	0.31	4.75	61,61,61,61	0
88	OHX	5	3993	7/7	0.89	0.30	4.74	58,58,58,58	3
87	MG	1	3525	1/1	0.96	0.33	4.74	35,35,35,35	0
87	MG	6	1925	1/1	0.87	0.33	4.74	52,52,52,52	0
87	MG	5	3498	1/1	0.98	0.28	4.73	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	3845	7/7	0.98	0.28	4.72	79,79,79,79	4
88	OHX	5	3875	7/7	0.98	0.28	4.71	53,53,53,53	3
87	MG	1	3701	1/1	0.91	0.29	4.70	35,35,35,35	0
88	OHX	8	217	7/7	0.97	0.26	4.67	85,85,85,85	3
88	OHX	1	3918	7/7	0.98	0.30	4.66	70,70,70,70	3
88	OHX	6	2051	7/7	0.96	0.26	4.60	123,123,123,123	5
88	OHX	2	2124	7/7	0.84	0.51	4.52	88,88,88,88	7
87	MG	1	3408	1/1	0.96	0.31	4.51	38,38,38,38	0
87	MG	5	3571	1/1	0.97	0.41	4.50	39,39,39,39	0
87	MG	5	3514	1/1	0.98	0.43	4.48	36,36,36,36	0
87	MG	5	3511	1/1	0.98	0.42	4.47	31,31,31,31	0
87	MG	5	3592	1/1	0.94	0.39	4.46	45,45,45,45	0
87	MG	1	3449	1/1	0.86	0.29	4.46	42,42,42,42	0
88	OHX	1	3781	7/7	0.99	0.25	4.45	92,92,92,92	4
88	OHX	1	3898	7/7	0.97	0.30	4.41	80,80,80,80	5
88	OHX	1	4061	7/7	0.84	0.31	4.40	53,53,53,53	3
87	MG	1	3673	1/1	0.94	0.61	4.39	61,61,61,61	0
87	MG	2	1973	1/1	0.40	0.34	4.37	107,107,107,107	0
88	OHX	5	3962	7/7	0.91	0.28	4.36	61,61,61,61	4
87	MG	6	1918	1/1	0.95	0.35	4.34	48,48,48,48	0
88	OHX	1	4097	7/7	0.79	0.31	4.33	74,74,74,74	5
88	OHX	5	3931	7/7	0.95	0.27	4.33	55,55,55,55	3
88	OHX	1	4005	7/7	0.95	0.29	4.31	60,60,60,60	5
88	OHX	1	3865	7/7	0.85	0.42	4.30	46,46,46,46	4
88	OHX	1	4006	7/7	0.91	0.23	4.29	68,68,68,68	4
88	OHX	5	3795	7/7	0.87	0.35	4.26	38,38,38,38	1
88	OHX	1	4007	7/7	0.93	0.28	4.25	40,40,40,40	4
87	MG	5	3590	1/1	0.96	0.39	4.22	37,37,37,37	0
87	MG	1	3474	1/1	0.96	0.32	4.21	43,43,43,43	0
88	OHX	1	3771	7/7	0.99	0.26	4.16	68,68,68,68	2
88	OHX	4	229	7/7	0.97	0.21	4.11	92,92,92,92	3
87	MG	1	3536	1/1	0.84	0.32	4.09	43,43,43,43	0
87	MG	5	3524	1/1	0.92	0.35	4.07	35,35,35,35	0
88	OHX	5	3867	7/7	0.99	0.22	4.07	75,75,75,75	1
88	OHX	1	3975	7/7	0.87	0.33	4.06	59,59,59,59	5
88	OHX	6	2164	7/7	0.84	0.38	4.05	81,81,81,81	5
87	MG	1	3571	1/1	0.95	0.40	3.98	48,48,48,48	0
88	OHX	1	3984	7/7	0.90	0.30	3.98	72,72,72,72	4
87	MG	5	3402	1/1	0.70	0.33	3.96	47,47,47,47	0
88	OHX	5	3973	7/7	0.97	0.22	3.92	153,153,153,153	7
88	OHX	2	2118	7/7	0.93	0.34	3.89	82,82,82,82	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	m7	201	1/1	0.96	0.40	3.86	40,40,40,40	0
88	OHX	5	3830	7/7	0.99	0.25	3.85	95,95,95,95	2
88	OHX	6	2114	7/7	0.98	0.28	3.79	65,65,65,65	2
88	OHX	5	4038	7/7	0.97	0.25	3.76	65,65,65,65	4
87	MG	7	228	1/1	0.92	0.27	3.73	38,38,38,38	0
87	MG	5	3412	1/1	0.80	0.28	3.71	37,37,37,37	0
87	MG	5	3562	1/1	0.99	0.28	3.71	31,31,31,31	0
87	MG	1	3523	1/1	0.96	0.42	3.70	33,33,33,33	0
87	MG	8	204	1/1	0.87	0.27	3.69	52,52,52,52	0
88	OHX	5	3864	7/7	0.97	0.25	3.69	87,87,87,87	3
88	OHX	5	3898	7/7	0.92	0.29	3.69	70,70,70,70	5
88	OHX	1	3969	7/7	0.95	0.26	3.66	64,64,64,64	4
87	MG	5	3457	1/1	0.91	0.29	3.63	34,34,34,34	0
87	MG	5	3445	1/1	0.99	0.32	3.63	38,38,38,38	0
88	OHX	8	219	7/7	0.95	0.25	3.62	59,59,59,59	2
88	OHX	1	3914	7/7	0.95	0.26	3.62	70,70,70,70	4
87	MG	1	3418	1/1	0.81	0.49	3.60	78,78,78,78	0
87	MG	l3	401	1/1	0.96	0.44	3.57	31,31,31,31	0
88	OHX	5	4071	7/7	0.89	0.31	3.55	42,42,42,42	4
88	OHX	5	4024	7/7	0.97	0.32	3.54	74,74,74,74	5
88	OHX	1	3837	7/7	0.98	0.28	3.52	64,64,64,64	3
88	OHX	1	3763	7/7	0.99	0.27	3.52	72,72,72,72	2
88	OHX	6	2154	7/7	0.93	0.30	3.51	69,69,69,69	5
88	OHX	5	4122	7/7	0.90	0.40	3.50	55,55,55,55	4
87	MG	n0	202	1/1	0.84	0.33	3.49	48,48,48,48	0
87	MG	1	3485	1/1	0.98	0.41	3.48	32,32,32,32	0
87	MG	1	3401	1/1	0.94	0.44	3.45	46,46,46,46	0
88	OHX	5	3849	7/7	0.99	0.21	3.45	127,127,127,127	2
88	OHX	8	227	7/7	0.91	0.27	3.44	56,56,56,56	4
88	OHX	5	3808	7/7	1.00	0.25	3.44	71,71,71,71	2
87	MG	5	3556	1/1	0.97	0.35	3.43	33,33,33,33	0
87	MG	5	3407	1/1	0.96	0.32	3.42	36,36,36,36	0
87	MG	5	3540	1/1	0.96	0.39	3.42	36,36,36,36	0
88	OHX	5	3939	7/7	0.95	0.33	3.38	46,46,46,46	3
88	OHX	1	4081	7/7	0.90	0.34	3.38	61,61,61,61	5
88	OHX	5	3996	7/7	0.87	0.29	3.37	116,116,116,116	3
87	MG	1	4111	1/1	0.98	0.31	3.36	44,44,44,44	1
87	MG	1	3584	1/1	0.97	0.36	3.30	43,43,43,43	0
88	OHX	5	3946	7/7	0.97	0.23	3.30	100,100,100,100	3
88	OHX	1	4033	7/7	0.91	0.34	3.29	52,52,52,52	5
88	OHX	5	3924	7/7	0.95	0.27	3.28	45,45,45,45	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	6	2185	7/7	0.70	0.28	3.28	75,75,75,75	4
88	OHX	5	3856	7/7	0.97	0.28	3.26	60,60,60,60	2
87	MG	1	3748	1/1	0.90	0.30	3.26	45,45,45,45	0
88	OHX	1	3793	7/7	0.99	0.25	3.25	62,62,62,62	1
87	MG	5	3546	1/1	0.89	0.31	3.20	56,56,56,56	0
88	OHX	5	3818	7/7	1.00	0.23	3.14	63,63,63,63	3
87	MG	N3	201	1/1	0.95	0.32	3.13	39,39,39,39	0
88	OHX	6	2049	7/7	0.97	0.25	3.13	95,95,95,95	2
88	OHX	2	2010	7/7	0.95	0.27	3.12	86,86,86,86	5
88	OHX	5	3896	7/7	0.99	0.30	3.12	106,106,106,106	1
88	OHX	6	2138	7/7	0.92	0.61	3.12	62,62,62,62	5
88	OHX	3	215	7/7	0.93	0.20	3.12	80,80,80,80	2
87	MG	5	3570	1/1	0.96	0.30	3.11	38,38,38,38	0
88	OHX	7	216	7/7	0.98	0.33	3.11	71,71,71,71	2
88	OHX	1	3877	7/7	0.97	0.25	3.10	44,44,44,44	1
88	OHX	6	2088	7/7	0.90	0.26	3.10	107,107,107,107	3
88	OHX	5	4011	7/7	0.93	0.28	3.10	56,56,56,56	1
87	MG	1	3495	1/1	0.96	0.31	3.10	40,40,40,40	0
88	OHX	6	2021	7/7	0.99	0.22	3.06	95,95,95,95	3
87	MG	1	3590	1/1	0.96	0.39	3.02	70,70,70,70	0
88	OHX	1	3830	7/7	0.98	0.26	3.02	57,57,57,57	1
88	OHX	1	4010	7/7	0.95	0.36	3.02	50,50,50,50	6
88	OHX	5	3812	7/7	0.99	0.25	2.99	58,58,58,58	1
88	OHX	1	3803	7/7	0.98	0.26	2.99	60,60,60,60	3
88	OHX	1	3947	7/7	0.92	0.24	2.96	92,92,92,92	5
88	OHX	1	3807	7/7	0.97	0.26	2.92	86,86,86,86	3
88	OHX	5	3837	7/7	0.99	0.31	2.89	74,74,74,74	2
88	OHX	4	226	7/7	0.98	0.20	2.88	75,75,75,75	1
88	OHX	2	2014	7/7	0.94	0.28	2.86	75,75,75,75	4
87	MG	4	236	1/1	0.98	0.55	2.85	56,56,56,56	0
87	MG	1	3575	1/1	0.97	0.37	2.84	35,35,35,35	0
88	OHX	5	3969	7/7	0.98	0.25	2.84	54,54,54,54	4
87	MG	1	3507	1/1	0.98	0.41	2.82	36,36,36,36	0
88	OHX	O9	101	7/7	0.89	0.41	2.81	47,47,47,47	4
88	OHX	1	3873	7/7	0.96	0.27	2.79	50,50,50,50	2
88	OHX	1	3784	7/7	1.00	0.23	2.78	74,74,74,74	2
87	MG	5	3630	1/1	0.96	0.27	2.77	55,55,55,55	0
88	OHX	4	222	7/7	0.97	0.24	2.76	57,57,57,57	3
88	OHX	5	4130	7/7	0.87	0.26	2.76	54,54,54,54	5
87	MG	5	3410	1/1	0.95	0.29	2.72	37,37,37,37	0
88	OHX	1	4008	7/7	0.96	0.25	2.69	53,53,53,53	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	4022	7/7	0.90	0.32	2.69	50,50,50,50	4
88	OHX	5	3811	7/7	0.99	0.26	2.67	59,59,59,59	1
88	OHX	1	3866	7/7	0.98	0.23	2.66	53,53,53,53	3
87	MG	1	3492	1/1	0.94	0.32	2.66	39,39,39,39	0
88	OHX	5	3947	7/7	0.97	0.24	2.60	53,53,53,53	5
88	OHX	1	4020	7/7	0.88	0.32	2.59	46,46,46,46	4
87	MG	5	3715	1/1	0.97	0.33	2.58	39,39,39,39	0
87	MG	5	3589	1/1	0.87	0.37	2.58	33,33,33,33	0
87	MG	1	3550	1/1	0.98	0.32	2.53	32,32,32,32	0
88	OHX	5	4104	7/7	0.85	0.32	2.50	54,54,54,54	3
87	MG	6	1915	1/1	0.75	0.27	2.49	82,82,82,82	0
88	OHX	5	3800	7/7	1.00	0.24	2.49	57,57,57,57	4
88	OHX	m0	304	7/7	0.85	0.34	2.48	44,44,44,44	5
88	OHX	6	2150	7/7	0.92	0.26	2.48	66,66,66,66	1
88	OHX	5	3953	7/7	0.96	0.25	2.46	101,101,101,101	2
88	OHX	2	2023	7/7	0.96	0.29	2.46	111,111,111,111	2
88	OHX	1	4042	7/7	0.91	0.36	2.43	52,52,52,52	5
87	MG	1	3441	1/1	0.96	0.29	2.39	56,56,56,56	0
88	OHX	6	2044	7/7	0.96	0.25	2.38	51,51,51,51	3
88	OHX	1	3882	7/7	0.99	0.21	2.37	65,65,65,65	5
88	OHX	5	4103	7/7	0.84	0.24	2.35	63,63,63,63	7
88	OHX	8	226	7/7	0.95	0.23	2.32	92,92,92,92	5
88	OHX	7	219	7/7	0.99	0.26	2.31	44,44,44,44	2
87	MG	7	208	1/1	0.87	0.34	2.31	55,55,55,55	0
87	MG	12	303	1/1	0.97	0.48	2.30	45,45,45,45	0
88	OHX	5	3861	7/7	0.97	0.27	2.29	55,55,55,55	2
88	OHX	5	4005	7/7	0.95	0.20	2.27	78,78,78,78	6
87	MG	M7	202	1/1	0.91	0.36	2.25	41,41,41,41	0
88	OHX	1	3839	7/7	0.96	0.27	2.24	55,55,55,55	3
88	OHX	1	4064	7/7	0.89	0.23	2.23	62,62,62,62	5
88	OHX	4	235	7/7	0.88	0.28	2.21	59,59,59,59	3
87	MG	1	3706	1/1	0.95	0.27	2.20	36,36,36,36	0
87	MG	5	3469	1/1	0.96	0.28	2.19	38,38,38,38	0
88	OHX	5	4035	7/7	0.92	0.30	2.18	42,42,42,42	4
87	MG	5	3635	1/1	0.95	0.26	2.16	42,42,42,42	0
88	OHX	1	4051	7/7	0.87	0.26	2.16	59,59,59,59	4
87	MG	8	202	1/1	0.86	0.28	2.15	44,44,44,44	0
88	OHX	6	2028	7/7	0.99	0.23	2.13	67,67,67,67	2
88	OHX	5	3995	7/7	0.96	0.28	2.13	68,68,68,68	5
87	MG	5	3565	1/1	0.98	0.30	2.13	34,34,34,34	0
88	OHX	1	3953	7/7	0.94	0.26	2.11	131,131,131,131	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3642	1/1	0.87	0.25	2.11	37,37,37,37	0
88	OHX	1	4106	7/7	0.93	0.52	2.11	60,60,60,60	4
87	MG	1	3479	1/1	0.98	0.24	2.08	54,54,54,54	0
88	OHX	1	4094	7/7	0.88	0.32	2.07	60,60,60,60	3
87	MG	1	3433	1/1	0.96	0.28	2.07	37,37,37,37	0
88	OHX	6	2067	7/7	0.99	0.19	2.07	157,157,157,157	5
87	MG	5	3426	1/1	0.89	0.26	2.05	65,65,65,65	0
87	MG	1	3557	1/1	0.91	0.36	2.03	33,33,33,33	0
88	OHX	1	3788	7/7	0.99	0.27	2.02	67,67,67,67	3
88	OHX	5	3958	7/7	0.95	0.26	2.02	52,52,52,52	2
87	MG	5	3413	1/1	0.99	0.24	2.02	41,41,41,41	0
88	OHX	5	3888	7/7	0.99	0.24	2.02	51,51,51,51	1
87	MG	5	3591	1/1	0.98	0.30	2.00	45,45,45,45	0
87	MG	6	1953	1/1	0.94	0.43	1.99	51,51,51,51	0
88	OHX	6	2068	7/7	0.95	0.22	1.98	99,99,99,99	3
88	OHX	5	4037	7/7	0.90	0.25	1.97	62,62,62,62	6
88	OHX	1	3802	7/7	0.96	0.35	1.97	66,66,66,66	3
88	OHX	1	4099	7/7	0.89	0.26	1.93	72,72,72,72	6
87	MG	6	1965	1/1	0.95	0.31	1.92	63,63,63,63	0
88	OHX	2	2100	7/7	0.91	0.23	1.87	70,70,70,70	5
88	OHX	1	4001	7/7	0.90	0.17	1.85	200,200,200,200	7
88	OHX	5	4065	7/7	0.96	0.25	1.85	82,82,82,82	3
88	OHX	6	2167	7/7	0.81	0.36	1.85	48,48,48,48	2
88	OHX	5	4031	7/7	0.93	0.47	1.84	60,60,60,60	5
88	OHX	5	3909	7/7	0.88	0.32	1.84	54,54,54,54	3
88	OHX	5	4044	7/7	0.90	0.26	1.82	54,54,54,54	3
88	OHX	2	2126	7/7	0.82	0.26	1.81	111,111,111,111	5
87	MG	1	3668	1/1	0.96	0.21	1.79	51,51,51,51	0
88	OHX	2	2051	7/7	0.91	0.17	1.78	136,136,136,136	4
88	OHX	5	4049	7/7	0.93	0.30	1.77	40,40,40,40	2
88	OHX	14	401	7/7	0.96	0.34	1.76	69,69,69,69	5
88	OHX	1	4012	7/7	0.95	0.28	1.74	41,41,41,41	4
88	OHX	5	4120	7/7	0.95	0.28	1.73	38,38,38,38	3
88	OHX	1	3927	7/7	0.97	0.26	1.73	48,48,48,48	4
88	OHX	1	4025	7/7	0.92	0.30	1.72	42,42,42,42	3
88	OHX	5	4154	7/7	0.89	0.27	1.72	42,42,42,42	3
88	OHX	5	4028	7/7	0.90	0.35	1.72	39,39,39,39	3
87	MG	1	3483	1/1	0.91	0.28	1.70	39,39,39,39	0
87	MG	5	3553	1/1	0.95	0.32	1.69	36,36,36,36	0
87	MG	5	3656	1/1	0.97	0.35	1.69	42,42,42,42	0
88	OHX	1	4017	7/7	0.95	0.32	1.65	50,50,50,50	5
88	OHX	7	225	7/7	0.95	0.25	1.65	43,43,43,43	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3759	7/7	1.00	0.24	1.65	55,55,55,55	2
88	OHX	5	3893	7/7	0.98	0.20	1.64	76,76,76,76	4
87	MG	5	3669	1/1	0.89	0.25	1.64	76,76,76,76	0
88	OHX	8	224	7/7	0.90	0.28	1.62	46,46,46,46	4
87	MG	1	3415	1/1	0.95	0.47	1.61	57,57,57,57	0
88	OHX	8	222	7/7	0.96	0.23	1.58	59,59,59,59	3
88	OHX	6	2032	7/7	0.97	0.22	1.56	131,131,131,131	3
88	OHX	5	3925	7/7	0.98	0.23	1.56	46,46,46,46	4
88	OHX	1	3936	7/7	0.98	0.21	1.55	103,103,103,103	3
88	OHX	2	2144	7/7	0.83	0.38	1.55	97,97,97,97	6
88	OHX	7	227	7/7	0.93	0.22	1.54	59,59,59,59	3
88	OHX	1	4018	7/7	0.90	0.30	1.54	42,42,42,42	1
88	OHX	5	4013	7/7	0.95	0.23	1.51	67,67,67,67	4
87	MG	1	3526	1/1	0.95	0.29	1.50	38,38,38,38	0
88	OHX	5	4150	7/7	0.91	0.38	1.50	41,41,41,41	6
87	MG	1	3567	1/1	0.93	0.44	1.50	48,48,48,48	0
87	MG	1	3501	1/1	0.94	0.31	1.50	47,47,47,47	0
88	OHX	3	210	7/7	0.98	0.23	1.49	48,48,48,48	3
88	OHX	2	2147	7/7	0.79	0.30	1.48	102,102,102,102	6
88	OHX	1	3816	7/7	0.97	0.28	1.48	66,66,66,66	5
88	OHX	5	4095	7/7	0.88	0.28	1.48	60,60,60,60	4
88	OHX	5	3899	7/7	0.97	0.26	1.47	72,72,72,72	2
88	OHX	5	3907	7/7	0.98	0.26	1.47	41,41,41,41	2
88	OHX	5	3997	7/7	0.95	0.24	1.42	42,42,42,42	3
87	MG	5	3567	1/1	0.92	0.30	1.42	38,38,38,38	0
87	MG	5	3467	1/1	0.73	0.23	1.42	125,125,125,125	0
88	OHX	1	3951	7/7	0.95	0.24	1.42	41,41,41,41	3
88	OHX	1	3869	7/7	0.80	0.37	1.42	56,56,56,56	4
87	MG	1	3602	1/1	0.95	0.25	1.42	43,43,43,43	0
88	OHX	1	3779	7/7	0.99	0.21	1.41	82,82,82,82	2
88	OHX	2	2037	7/7	0.96	0.24	1.40	102,102,102,102	3
87	MG	1	3628	1/1	0.95	0.32	1.40	51,51,51,51	0
88	OHX	5	4078	7/7	0.93	0.29	1.39	38,38,38,38	5
88	OHX	3	212	7/7	0.99	0.28	1.39	76,76,76,76	2
87	MG	L3	402	1/1	0.87	0.31	1.37	58,58,58,58	0
88	OHX	1	4013	7/7	0.94	0.22	1.37	60,60,60,60	3
88	OHX	5	3871	7/7	0.95	0.39	1.36	42,42,42,42	3
88	OHX	5	4082	7/7	0.86	0.22	1.35	99,99,99,99	5
88	OHX	1	3782	7/7	0.99	0.25	1.35	67,67,67,67	3
88	OHX	1	4062	7/7	0.91	0.30	1.34	39,39,39,39	3
88	OHX	1	3829	7/7	0.97	0.24	1.34	60,60,60,60	2
88	OHX	1	3966	7/7	0.73	0.29	1.34	55,55,55,55	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3679	1/1	0.74	0.30	1.32	45,45,45,45	0
87	MG	1	3444	1/1	0.96	0.22	1.31	44,44,44,44	0
88	OHX	5	4041	7/7	0.88	0.29	1.31	47,47,47,47	3
88	OHX	5	4106	7/7	0.95	0.25	1.31	52,52,52,52	3
88	OHX	1	3761	7/7	0.99	0.26	1.30	66,66,66,66	2
88	OHX	1	3938	7/7	0.95	0.26	1.30	53,53,53,53	3
88	OHX	1	3772	7/7	0.99	0.26	1.30	51,51,51,51	2
88	OHX	5	3894	7/7	0.96	0.26	1.29	56,56,56,56	4
88	OHX	5	3814	7/7	0.99	0.23	1.29	54,54,54,54	4
88	OHX	1	3770	7/7	0.99	0.21	1.28	71,71,71,71	2
88	OHX	1	4084	7/7	0.86	0.36	1.27	47,47,47,47	4
87	MG	2	1921	1/1	0.97	0.27	1.25	69,69,69,69	0
88	OHX	5	3951	7/7	0.98	0.26	1.23	49,49,49,49	3
88	OHX	2	2110	7/7	0.94	0.35	1.22	61,61,61,61	5
88	OHX	o9	102	7/7	0.89	0.34	1.20	47,47,47,47	5
87	MG	5	3651	1/1	0.90	0.37	1.20	45,45,45,45	0
87	MG	1	3464	1/1	0.91	0.24	1.19	39,39,39,39	0
88	OHX	5	3937	7/7	0.98	0.20	1.17	136,136,136,136	1
87	MG	1	3555	1/1	0.94	0.28	1.17	45,45,45,45	0
87	MG	6	1933	1/1	0.86	0.20	1.16	90,90,90,90	0
88	OHX	5	4061	7/7	0.87	0.23	1.15	61,61,61,61	1
88	OHX	1	3989	7/7	0.89	0.27	1.15	78,78,78,78	3
87	MG	5	3525	1/1	0.94	0.24	1.14	46,46,46,46	0
88	OHX	5	4040	7/7	0.97	0.24	1.13	40,40,40,40	4
88	OHX	O7	105	7/7	0.90	0.33	1.11	76,76,76,76	4
87	MG	2	1910	1/1	0.93	0.30	1.11	65,65,65,65	0
87	MG	1	3502	1/1	0.95	0.28	1.11	38,38,38,38	0
87	MG	5	3602	1/1	0.94	0.28	1.09	35,35,35,35	0
87	MG	1	3663	1/1	0.92	0.24	1.09	52,52,52,52	0
88	OHX	3	217	7/7	0.94	0.23	1.08	78,78,78,78	5
88	OHX	1	3838	7/7	0.94	0.28	1.07	78,78,78,78	3
88	OHX	5	3883	7/7	0.98	0.23	1.07	54,54,54,54	4
87	MG	o9	101	1/1	0.92	0.40	1.06	53,53,53,53	0
88	OHX	6	2027	7/7	0.99	0.24	1.06	77,77,77,77	1
88	OHX	2	2019	7/7	0.97	0.24	1.05	93,93,93,93	3
88	OHX	5	3950	7/7	0.94	0.28	1.05	40,40,40,40	4
88	OHX	S9	202	7/7	0.88	0.50	1.05	87,87,87,87	5
88	OHX	1	3827	7/7	0.96	0.24	1.05	73,73,73,73	1
88	OHX	1	4068	7/7	0.96	0.27	1.04	50,50,50,50	6
88	OHX	6	2176	7/7	0.89	0.32	1.04	63,63,63,63	4
88	OHX	5	3940	7/7	0.97	0.23	1.04	42,42,42,42	2
88	OHX	5	3797	7/7	1.00	0.25	1.03	55,55,55,55	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	3799	7/7	0.99	0.24	1.01	54,54,54,54	2
88	OHX	1	3884	7/7	0.96	0.25	1.01	54,54,54,54	3
88	OHX	L4	401	7/7	0.96	0.31	1.00	61,61,61,61	6
88	OHX	5	3897	7/7	0.97	0.22	0.98	76,76,76,76	2
87	MG	5	3411	1/1	0.95	0.24	0.98	37,37,37,37	0
88	OHX	5	3926	7/7	0.97	0.28	0.96	41,41,41,41	5
88	OHX	1	3758	7/7	0.99	0.24	0.96	61,61,61,61	1
88	OHX	5	3821	7/7	0.99	0.23	0.96	69,69,69,69	1
88	OHX	4	221	7/7	0.99	0.23	0.95	64,64,64,64	3
88	OHX	6	2161	7/7	0.90	0.17	0.94	133,133,133,133	7
88	OHX	5	3841	7/7	0.99	0.26	0.93	51,51,51,51	1
88	OHX	6	2031	7/7	0.98	0.23	0.91	81,81,81,81	3
88	OHX	1	3967	7/7	0.93	0.32	0.91	37,37,37,37	4
88	OHX	1	3939	7/7	0.94	0.23	0.86	76,76,76,76	4
88	OHX	4	230	7/7	0.88	0.30	0.86	47,47,47,47	3
87	MG	5	3548	1/1	0.81	0.36	0.84	45,45,45,45	0
88	OHX	5	4137	7/7	0.75	0.28	0.82	96,96,96,96	6
87	MG	6	1954	1/1	0.98	0.34	0.82	51,51,51,51	0
88	OHX	1	3948	7/7	0.94	0.24	0.80	73,73,73,73	3
88	OHX	2	2111	7/7	0.94	0.26	0.79	73,73,73,73	5
88	OHX	M0	302	7/7	0.95	0.30	0.78	50,50,50,50	4
88	OHX	6	2060	7/7	0.97	0.21	0.78	96,96,96,96	3
87	MG	4	209	1/1	0.99	0.23	0.77	58,58,58,58	0
88	OHX	1	3911	7/7	0.96	0.22	0.77	64,64,64,64	4
88	OHX	6	2040	7/7	0.99	0.19	0.76	130,130,130,130	5
88	OHX	15	303	7/7	0.85	0.27	0.75	94,94,94,94	6
88	OHX	5	3824	7/7	0.98	0.25	0.74	62,62,62,62	2
87	MG	6	2006	1/1	0.98	0.51	0.74	83,83,83,83	0
87	MG	5	3466	1/1	0.89	0.24	0.74	44,44,44,44	0
88	OHX	5	3801	7/7	1.00	0.27	0.74	63,63,63,63	2
88	OHX	1	4002	7/7	0.90	0.25	0.73	55,55,55,55	2
87	MG	5	3675	1/1	0.93	0.25	0.73	42,42,42,42	0
88	OHX	8	214	7/7	0.95	0.30	0.72	80,80,80,80	4
88	OHX	5	3966	7/7	0.95	0.25	0.71	55,55,55,55	4
88	OHX	5	4015	7/7	0.95	0.23	0.70	66,66,66,66	4
88	OHX	2	2065	7/7	0.89	0.24	0.70	117,117,117,117	3
88	OHX	6	2130	7/7	0.92	0.23	0.70	61,61,61,61	3
88	OHX	1	3870	7/7	0.95	0.25	0.70	43,43,43,43	3
88	OHX	n3	202	7/7	0.98	0.21	0.69	63,63,63,63	3
88	OHX	6	2146	7/7	0.85	0.35	0.69	53,53,53,53	3
88	OHX	6	2058	7/7	0.98	0.21	0.68	77,77,77,77	3
88	OHX	5	4066	7/7	0.92	0.27	0.68	53,53,53,53	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3435	1/1	0.98	0.26	0.66	39,39,39,39	0
88	OHX	1	3776	7/7	0.99	0.20	0.65	72,72,72,72	1
87	MG	5	3566	1/1	0.93	0.29	0.65	40,40,40,40	0
87	MG	6	1949	1/1	0.91	0.28	0.65	80,80,80,80	0
88	OHX	6	2149	7/7	0.94	0.26	0.64	49,49,49,49	4
88	OHX	5	4102	7/7	0.91	0.21	0.64	53,53,53,53	5
88	OHX	15	302	7/7	0.89	0.23	0.63	105,105,105,105	5
87	MG	2	1944	1/1	0.79	0.24	0.62	80,80,80,80	0
88	OHX	5	4033	7/7	0.93	0.31	0.62	37,37,37,37	5
88	OHX	5	4133	7/7	0.92	0.27	0.62	38,38,38,38	4
88	OHX	1	3766	7/7	0.99	0.24	0.61	55,55,55,55	1
87	MG	5	3611	1/1	0.94	0.29	0.60	46,46,46,46	0
88	OHX	5	3964	7/7	0.97	0.24	0.60	53,53,53,53	5
88	OHX	2	2028	7/7	0.97	0.21	0.59	74,74,74,74	4
88	OHX	1	3760	7/7	0.99	0.26	0.59	64,64,64,64	3
88	OHX	1	3874	7/7	0.98	0.25	0.58	43,43,43,43	3
88	OHX	5	3976	7/7	0.97	0.24	0.58	50,50,50,50	4
87	MG	6	1968	1/1	0.99	0.23	0.57	55,55,55,55	0
88	OHX	1	3888	7/7	0.97	0.26	0.57	45,45,45,45	3
88	OHX	2	2131	7/7	0.93	0.35	0.57	86,86,86,86	6
87	MG	N8	201	1/1	0.85	0.32	0.56	57,57,57,57	0
88	OHX	5	4114	7/7	0.94	0.27	0.56	47,47,47,47	4
87	MG	1	3533	1/1	0.97	0.30	0.56	50,50,50,50	0
87	MG	L7	301	1/1	0.97	0.24	0.55	41,41,41,41	0
88	OHX	1	4023	7/7	0.95	0.22	0.53	69,69,69,69	6
87	MG	1	3609	1/1	0.80	0.24	0.53	44,44,44,44	0
88	OHX	2	2067	7/7	0.96	0.19	0.52	124,124,124,124	5
88	OHX	C8	201	7/7	0.98	0.25	0.52	106,106,106,106	3
88	OHX	5	4108	7/7	0.94	0.26	0.52	64,64,64,64	4
88	OHX	8	231	7/7	0.94	0.20	0.51	62,62,62,62	3
88	OHX	6	2137	7/7	0.83	0.33	0.50	85,85,85,85	5
88	OHX	1	3994	7/7	0.95	0.22	0.50	47,47,47,47	2
87	MG	6	1909	1/1	0.97	0.21	0.48	109,109,109,109	0
88	OHX	L5	301	7/7	0.89	0.38	0.48	81,81,81,81	7
87	MG	5	3699	1/1	0.90	0.25	0.47	35,35,35,35	0
88	OHX	1	3780	7/7	0.99	0.25	0.47	72,72,72,72	2
88	OHX	2	2138	7/7	0.95	0.36	0.47	72,72,72,72	6
88	OHX	5	4060	7/7	0.97	0.25	0.47	38,38,38,38	4
88	OHX	6	2066	7/7	0.95	0.19	0.46	161,161,161,161	6
88	OHX	5	3806	7/7	0.99	0.22	0.46	58,58,58,58	1
88	OHX	5	3948	7/7	0.97	0.22	0.45	50,50,50,50	3
88	OHX	6	2179	7/7	0.92	0.18	0.45	99,99,99,99	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	4086	7/7	0.92	0.23	0.44	45,45,45,45	4
88	OHX	5	3829	7/7	0.98	0.24	0.43	56,56,56,56	2
87	MG	5	4160	1/1	0.88	0.29	0.43	39,39,39,39	0
88	OHX	19	201	7/7	0.93	0.28	0.42	65,65,65,65	2
88	OHX	1	3826	7/7	0.99	0.24	0.41	52,52,52,52	2
88	OHX	5	3835	7/7	0.98	0.24	0.40	55,55,55,55	3
88	OHX	1	4032	7/7	0.91	0.23	0.40	56,56,56,56	5
88	OHX	5	4029	7/7	0.97	0.24	0.39	49,49,49,49	4
88	OHX	4	220	7/7	0.99	0.24	0.39	60,60,60,60	3
88	OHX	3	214	7/7	0.97	0.21	0.39	77,77,77,77	4
88	OHX	5	4138	7/7	0.73	0.26	0.39	138,138,138,138	6
88	OHX	1	4019	7/7	0.94	0.21	0.38	65,65,65,65	2
88	OHX	1	4075	7/7	0.91	0.34	0.38	74,74,74,74	5
88	OHX	6	2158	7/7	0.90	0.25	0.38	70,70,70,70	1
88	OHX	5	3983	7/7	0.93	0.26	0.38	42,42,42,42	3
87	MG	2	1950	1/1	0.86	0.30	0.37	99,99,99,99	0
87	MG	5	3625	1/1	0.80	0.30	0.37	52,52,52,52	0
87	MG	5	3641	1/1	0.72	0.23	0.36	39,39,39,39	0
87	MG	1	3466	1/1	0.98	0.24	0.36	42,42,42,42	0
88	OHX	8	213	7/7	0.99	0.24	0.36	58,58,58,58	2
88	OHX	1	3995	7/7	0.94	0.18	0.35	98,98,98,98	7
88	OHX	5	3873	7/7	0.97	0.27	0.35	65,65,65,65	3
87	MG	5	4166	1/1	0.85	0.32	0.35	68,68,68,68	0
88	OHX	5	4057	7/7	0.94	0.26	0.34	73,73,73,73	6
88	OHX	2	2121	7/7	0.87	0.41	0.34	60,60,60,60	5
88	OHX	5	4017	7/7	0.96	0.21	0.34	69,69,69,69	4
88	OHX	1	4100	7/7	0.83	0.29	0.33	71,71,71,71	3
87	MG	1	3606	1/1	0.98	0.25	0.32	44,44,44,44	0
87	MG	1	3669	1/1	0.96	0.25	0.32	38,38,38,38	0
88	OHX	2	1994	7/7	1.00	0.21	0.32	85,85,85,85	0
87	MG	n0	201	1/1	0.83	0.24	0.32	45,45,45,45	0
88	OHX	5	4023	7/7	0.97	0.19	0.31	97,97,97,97	5
87	MG	M0	301	1/1	0.96	0.28	0.31	42,42,42,42	0
88	OHX	1	3765	7/7	0.99	0.23	0.31	59,59,59,59	2
88	OHX	5	3798	7/7	1.00	0.25	0.30	58,58,58,58	2
88	OHX	1	3931	7/7	0.97	0.28	0.29	53,53,53,53	4
88	OHX	6	2111	7/7	0.90	0.29	0.29	94,94,94,94	7
87	MG	1	3540	1/1	0.99	0.25	0.28	35,35,35,35	0
88	OHX	5	4113	7/7	0.93	0.40	0.28	53,53,53,53	3
87	MG	5	3613	1/1	0.97	0.26	0.28	45,45,45,45	0
88	OHX	1	3933	7/7	0.96	0.26	0.27	53,53,53,53	4
88	OHX	2	2043	7/7	0.99	0.20	0.27	80,80,80,80	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	6	2082	7/7	0.97	0.17	0.26	93,93,93,93	4
88	OHX	5	4070	7/7	0.88	0.26	0.26	69,69,69,69	3
88	OHX	6	2153	7/7	0.93	0.21	0.25	75,75,75,75	3
88	OHX	5	3823	7/7	1.00	0.23	0.25	43,43,43,43	1
89	ZN	D7	101	1/1	0.74	0.33	0.24	152,152,152,152	0
88	OHX	5	3796	7/7	0.94	0.28	0.24	52,52,52,52	2
88	OHX	1	3806	7/7	0.98	0.24	0.23	73,73,73,73	2
88	OHX	2	2039	7/7	0.86	0.22	0.23	133,133,133,133	5
88	OHX	1	3824	7/7	0.97	0.27	0.22	57,57,57,57	2
88	OHX	2	2002	7/7	0.95	0.23	0.22	109,109,109,109	4
88	OHX	5	3975	7/7	0.97	0.22	0.22	70,70,70,70	2
88	OHX	5	3913	7/7	0.99	0.19	0.22	55,55,55,55	3
88	OHX	6	2102	7/7	0.89	0.29	0.21	69,69,69,69	3
88	OHX	6	2018	7/7	0.99	0.24	0.21	64,64,64,64	3
88	OHX	1	3775	7/7	0.99	0.23	0.21	49,49,49,49	3
88	OHX	1	3757	7/7	1.00	0.24	0.20	56,56,56,56	1
88	OHX	2	2012	7/7	0.99	0.21	0.20	80,80,80,80	5
88	OHX	5	3880	7/7	0.99	0.23	0.19	45,45,45,45	2
88	OHX	1	4080	7/7	0.90	0.22	0.17	60,60,60,60	5
88	OHX	6	2092	7/7	0.92	0.28	0.17	61,61,61,61	3
88	OHX	1	4049	7/7	0.94	0.19	0.17	99,99,99,99	3
88	OHX	6	2129	7/7	0.90	0.22	0.17	58,58,58,58	3
88	OHX	6	2142	7/7	0.93	0.29	0.17	68,68,68,68	5
88	OHX	1	3907	7/7	0.94	0.30	0.17	69,69,69,69	3
88	OHX	s9	201	7/7	0.93	0.36	0.17	73,73,73,73	5
88	OHX	2	2075	7/7	0.95	0.22	0.16	60,60,60,60	4
88	OHX	5	3882	7/7	0.99	0.21	0.16	56,56,56,56	4
88	OHX	2	2117	7/7	0.83	0.20	0.16	95,95,95,95	5
88	OHX	2	2142	7/7	0.89	0.43	0.15	101,101,101,101	6
88	OHX	6	2095	7/7	0.96	0.24	0.15	104,104,104,104	3
88	OHX	8	221	7/7	0.97	0.24	0.14	42,42,42,42	4
88	OHX	1	3999	7/7	0.93	0.25	0.14	55,55,55,55	5
88	OHX	1	4040	7/7	0.90	0.20	0.14	59,59,59,59	2
88	OHX	5	3836	7/7	0.99	0.19	0.13	78,78,78,78	3
88	OHX	1	4055	7/7	0.90	0.30	0.13	71,71,71,71	5
88	OHX	5	3853	7/7	0.96	0.29	0.13	69,69,69,69	2
87	MG	1	3450	1/1	0.81	0.32	0.13	62,62,62,62	0
88	OHX	5	4000	7/7	0.96	0.26	0.12	48,48,48,48	4
88	OHX	5	3974	7/7	0.98	0.23	0.12	49,49,49,49	3
88	OHX	2	2114	7/7	0.84	0.37	0.11	99,99,99,99	4
88	OHX	m0	302	7/7	0.95	0.27	0.11	97,97,97,97	4
87	MG	c7	201	1/1	0.77	0.31	0.11	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	3912	7/7	0.95	0.27	0.10	43,43,43,43	4
88	OHX	1	3787	7/7	0.97	0.28	0.10	70,70,70,70	3
88	OHX	1	4057	7/7	0.91	0.25	0.10	77,77,77,77	3
88	OHX	6	2034	7/7	0.99	0.20	0.09	70,70,70,70	3
88	OHX	5	3930	7/7	0.95	0.23	0.09	49,49,49,49	3
87	MG	8	206	1/1	0.98	0.21	0.09	58,58,58,58	0
88	OHX	5	3822	7/7	0.99	0.23	0.09	49,49,49,49	1
88	OHX	5	4058	7/7	0.94	0.23	0.09	50,50,50,50	4
88	OHX	1	3789	7/7	0.99	0.20	0.08	70,70,70,70	3
88	OHX	5	3928	7/7	0.97	0.22	0.08	101,101,101,101	3
88	OHX	5	3942	7/7	0.98	0.24	0.06	46,46,46,46	3
88	OHX	5	3834	7/7	1.00	0.21	0.05	52,52,52,52	5
87	MG	6	1978	1/1	0.93	0.17	0.05	88,88,88,88	0
87	MG	M7	203	1/1	0.83	0.23	0.05	44,44,44,44	0
87	MG	1	3471	1/1	0.98	0.20	0.04	36,36,36,36	0
87	MG	n8	202	1/1	0.95	0.27	0.03	51,51,51,51	0
88	OHX	1	4086	7/7	0.87	0.34	0.03	136,136,136,136	7
88	OHX	1	3902	7/7	0.98	0.23	0.01	51,51,51,51	1
88	OHX	1	4078	7/7	0.94	0.27	0.01	45,45,45,45	6
87	MG	1	3740	1/1	0.94	0.29	0.01	62,62,62,62	0
88	OHX	5	3892	7/7	0.98	0.24	0.01	45,45,45,45	3
87	MG	6	1911	1/1	0.96	0.23	-0.00	91,91,91,91	0
88	OHX	5	4135	7/7	0.92	0.23	-0.01	68,68,68,68	3
87	MG	5	4164	1/1	0.96	0.36	-0.02	55,55,55,55	0
87	MG	5	3766	1/1	0.93	0.24	-0.02	33,33,33,33	0
88	OHX	5	4126	7/7	0.97	0.24	-0.03	53,53,53,53	6
87	MG	O3	202	1/1	0.91	0.26	-0.03	40,40,40,40	0
88	OHX	1	3777	7/7	0.99	0.22	-0.04	74,74,74,74	3
88	OHX	C5	201	7/7	0.87	0.20	-0.04	116,116,116,116	5
88	OHX	1	3785	7/7	0.99	0.24	-0.04	49,49,49,49	3
88	OHX	5	4042	7/7	0.93	0.26	-0.04	47,47,47,47	3
88	OHX	sR	401	7/7	0.90	0.23	-0.05	125,125,125,125	5
87	MG	1	3549	1/1	0.96	0.27	-0.05	39,39,39,39	0
87	MG	6	1955	1/1	0.97	0.36	-0.06	64,64,64,64	0
88	OHX	2	2135	7/7	0.78	0.25	-0.06	194,194,194,194	7
87	MG	n6	201	1/1	0.93	0.29	-0.06	59,59,59,59	0
88	OHX	5	3862	7/7	0.99	0.21	-0.09	47,47,47,47	4
88	OHX	O7	106	7/7	0.97	0.25	-0.09	55,55,55,55	3
88	OHX	6	2115	7/7	0.87	0.24	-0.09	70,70,70,70	4
88	OHX	5	3877	7/7	0.98	0.26	-0.09	54,54,54,54	3
87	MG	6	1970	1/1	0.97	0.22	-0.10	52,52,52,52	0
88	OHX	6	2059	7/7	0.97	0.23	-0.10	67,67,67,67	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3819	7/7	0.99	0.20	-0.10	68,68,68,68	3
88	OHX	6	2089	7/7	0.98	0.20	-0.11	58,58,58,58	3
87	MG	5	3694	1/1	0.92	0.23	-0.11	45,45,45,45	0
88	OHX	5	3876	7/7	0.99	0.22	-0.11	54,54,54,54	1
88	OHX	6	2013	7/7	1.00	0.21	-0.12	69,69,69,69	1
88	OHX	1	4087	7/7	0.93	0.22	-0.13	45,45,45,45	4
88	OHX	1	4093	7/7	0.94	0.37	-0.14	42,42,42,42	5
88	OHX	5	3863	7/7	0.99	0.23	-0.15	89,89,89,89	2
88	OHX	4	224	7/7	0.98	0.23	-0.15	81,81,81,81	4
87	MG	6	1944	1/1	0.96	0.26	-0.15	70,70,70,70	0
88	OHX	5	3833	7/7	0.99	0.23	-0.16	52,52,52,52	2
88	OHX	6	2126	7/7	0.93	0.19	-0.16	74,74,74,74	5
88	OHX	2	2072	7/7	0.95	0.20	-0.16	104,104,104,104	5
88	OHX	8	215	7/7	0.98	0.23	-0.17	59,59,59,59	2
88	OHX	1	3993	7/7	0.95	0.26	-0.17	53,53,53,53	2
87	MG	1	3677	1/1	0.85	0.20	-0.17	49,49,49,49	0
88	OHX	5	3972	7/7	0.97	0.22	-0.17	60,60,60,60	4
87	MG	2	1943	1/1	0.94	0.29	-0.17	78,78,78,78	0
87	MG	1	3551	1/1	0.97	0.23	-0.17	32,32,32,32	0
88	OHX	5	4131	7/7	0.87	0.32	-0.18	59,59,59,59	2
88	OHX	m0	303	7/7	0.97	0.26	-0.18	49,49,49,49	1
87	MG	5	3422	1/1	0.97	0.25	-0.18	40,40,40,40	0
88	OHX	5	3868	7/7	0.98	0.21	-0.18	77,77,77,77	4
88	OHX	1	3862	7/7	0.98	0.23	-0.19	54,54,54,54	4
88	OHX	2	2017	7/7	0.98	0.17	-0.19	118,118,118,118	5
88	OHX	5	4085	7/7	0.96	0.24	-0.20	66,66,66,66	3
87	MG	5	3509	1/1	0.97	0.25	-0.21	43,43,43,43	0
88	OHX	5	4012	7/7	0.94	0.23	-0.21	49,49,49,49	3
88	OHX	5	3957	7/7	0.97	0.25	-0.21	38,38,38,38	2
87	MG	5	3432	1/1	0.79	0.20	-0.22	46,46,46,46	0
88	OHX	5	4072	7/7	0.98	0.22	-0.23	42,42,42,42	4
88	OHX	6	2107	7/7	0.94	0.18	-0.23	114,114,114,114	7
87	MG	1	3738	1/1	0.86	0.29	-0.24	62,62,62,62	0
88	OHX	6	2041	7/7	0.99	0.22	-0.24	61,61,61,61	2
88	OHX	S6	301	7/7	0.85	0.20	-0.24	105,105,105,105	5
88	OHX	1	3970	7/7	0.98	0.19	-0.25	53,53,53,53	4
87	MG	2	1915	1/1	0.89	0.25	-0.25	78,78,78,78	0
88	OHX	1	3860	7/7	0.98	0.24	-0.25	40,40,40,40	2
88	OHX	2	2041	7/7	0.97	0.15	-0.25	110,110,110,110	5
88	OHX	2	2078	7/7	0.92	0.21	-0.25	77,77,77,77	5
88	OHX	N9	102	7/7	0.99	0.23	-0.25	63,63,63,63	1
88	OHX	2	2000	7/7	0.98	0.18	-0.26	102,102,102,102	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	c5	800	7/7	0.90	0.26	-0.26	117,117,117,117	5
87	MG	1	3491	1/1	0.96	0.27	-0.26	44,44,44,44	0
88	OHX	5	3827	7/7	0.99	0.22	-0.27	40,40,40,40	3
88	OHX	1	3773	7/7	0.99	0.23	-0.27	63,63,63,63	3
88	OHX	2	2061	7/7	0.92	0.27	-0.27	63,63,63,63	4
88	OHX	6	2145	7/7	0.93	0.31	-0.28	88,88,88,88	6
88	OHX	5	3949	7/7	0.98	0.23	-0.28	50,50,50,50	4
87	MG	N9	101	1/1	0.81	0.25	-0.28	33,33,33,33	0
88	OHX	2	2001	7/7	0.97	0.19	-0.29	104,104,104,104	2
88	OHX	5	4026	7/7	0.97	0.20	-0.29	68,68,68,68	6
88	OHX	2	2108	7/7	0.85	0.23	-0.29	83,83,83,83	3
88	OHX	5	3999	7/7	0.95	0.26	-0.29	53,53,53,53	1
89	ZN	q3	501	1/1	0.99	0.18	-0.29	63,63,63,63	0
88	OHX	5	3879	7/7	0.97	0.23	-0.29	61,61,61,61	3
87	MG	6	1976	1/1	0.97	0.27	-0.30	54,54,54,54	0
88	OHX	5	4004	7/7	0.98	0.23	-0.30	49,49,49,49	2
88	OHX	1	3808	7/7	0.98	0.24	-0.30	52,52,52,52	1
88	OHX	5	4039	7/7	0.94	0.22	-0.30	55,55,55,55	3
88	OHX	6	2077	7/7	0.93	0.25	-0.30	87,87,87,87	4
88	OHX	1	3795	7/7	0.99	0.22	-0.30	51,51,51,51	3
88	OHX	5	3954	7/7	0.96	0.23	-0.31	73,73,73,73	3
88	OHX	6	2025	7/7	0.99	0.21	-0.31	98,98,98,98	2
88	OHX	5	3813	7/7	0.99	0.21	-0.32	63,63,63,63	1
88	OHX	5	3985	7/7	0.97	0.23	-0.32	46,46,46,46	4
88	OHX	1	3952	7/7	0.96	0.22	-0.33	46,46,46,46	5
88	OHX	s1	301	7/7	0.98	0.21	-0.33	91,91,91,91	2
88	OHX	5	4123	7/7	0.93	0.22	-0.33	47,47,47,47	3
88	OHX	N8	205	7/7	0.91	0.20	-0.33	105,105,105,105	7
88	OHX	1	3797	7/7	0.99	0.22	-0.33	55,55,55,55	2
87	MG	2	1936	1/1	0.93	0.26	-0.33	63,63,63,63	0
87	MG	2	2154	1/1	0.88	0.21	-0.33	105,105,105,105	0
88	OHX	5	4096	7/7	0.97	0.24	-0.34	55,55,55,55	4
87	MG	5	3759	1/1	0.92	0.23	-0.34	44,44,44,44	0
88	OHX	1	3818	7/7	0.99	0.20	-0.34	106,106,106,106	3
88	OHX	6	2136	7/7	0.88	0.20	-0.35	165,165,165,165	7
88	OHX	6	2090	7/7	0.93	0.27	-0.35	84,84,84,84	6
87	MG	1	3475	1/1	0.90	0.25	-0.35	49,49,49,49	0
88	OHX	6	2170	7/7	0.88	0.25	-0.37	76,76,76,76	6
88	OHX	6	2160	7/7	0.88	0.18	-0.37	98,98,98,98	7
88	OHX	6	2093	7/7	0.96	0.21	-0.37	47,47,47,47	2
87	MG	1	3486	1/1	0.85	0.25	-0.38	49,49,49,49	0
88	OHX	4	231	7/7	0.95	0.19	-0.39	56,56,56,56	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	7	220	7/7	0.98	0.22	-0.40	43,43,43,43	3
88	OHX	s8	302	7/7	0.94	0.24	-0.42	108,108,108,108	5
87	MG	1	3478	1/1	0.95	0.24	-0.42	39,39,39,39	0
87	MG	1	3632	1/1	0.94	0.29	-0.43	41,41,41,41	0
88	OHX	5	4097	7/7	0.94	0.21	-0.43	132,132,132,132	5
88	OHX	1	4046	7/7	0.92	0.17	-0.43	105,105,105,105	5
88	OHX	5	4036	7/7	0.91	0.24	-0.44	47,47,47,47	3
88	OHX	M8	202	7/7	0.87	0.26	-0.44	49,49,49,49	2
88	OHX	6	2162	7/7	0.93	0.20	-0.44	87,87,87,87	4
87	MG	2	1964	1/1	0.97	0.22	-0.44	69,69,69,69	0
88	OHX	5	3815	7/7	0.99	0.22	-0.45	56,56,56,56	3
88	OHX	1	3858	7/7	0.98	0.20	-0.45	61,61,61,61	3
88	OHX	6	2083	7/7	0.96	0.32	-0.45	85,85,85,85	7
88	OHX	1	3872	7/7	0.98	0.23	-0.46	47,47,47,47	2
87	MG	1	3660	1/1	0.71	0.20	-0.46	52,52,52,52	0
88	OHX	n6	202	7/7	0.98	0.20	-0.46	89,89,89,89	5
88	OHX	1	3767	7/7	0.99	0.22	-0.46	68,68,68,68	3
88	OHX	2	2040	7/7	0.97	0.23	-0.46	68,68,68,68	4
88	OHX	5	3802	7/7	1.00	0.23	-0.47	62,62,62,62	3
88	OHX	1	4039	7/7	0.91	0.23	-0.47	76,76,76,76	5
88	OHX	5	3817	7/7	1.00	0.20	-0.47	66,66,66,66	1
88	OHX	6	2147	7/7	0.93	0.29	-0.48	82,82,82,82	5
87	MG	2	1914	1/1	0.98	0.21	-0.48	77,77,77,77	0
88	OHX	5	4007	7/7	0.98	0.23	-0.48	35,35,35,35	3
87	MG	2	1937	1/1	0.88	0.25	-0.48	66,66,66,66	0
88	OHX	2	2064	7/7	0.91	0.29	-0.49	79,79,79,79	3
88	OHX	5	3848	7/7	0.98	0.24	-0.49	58,58,58,58	3
88	OHX	6	2173	7/7	0.89	0.17	-0.49	88,88,88,88	6
88	OHX	1	3876	7/7	0.97	0.20	-0.51	56,56,56,56	4
88	OHX	6	2152	7/7	0.90	0.29	-0.51	87,87,87,87	5
88	OHX	1	3893	7/7	0.95	0.20	-0.52	131,131,131,131	5
88	OHX	1	3890	7/7	0.95	0.16	-0.52	106,106,106,106	5
88	OHX	1	3851	7/7	0.99	0.22	-0.52	42,42,42,42	4
88	OHX	6	2106	7/7	0.92	0.18	-0.52	80,80,80,80	3
87	MG	4	212	1/1	0.86	0.19	-0.52	54,54,54,54	0
88	OHX	6	2061	7/7	0.96	0.21	-0.53	84,84,84,84	2
88	OHX	5	3805	7/7	0.99	0.23	-0.53	63,63,63,63	2
88	OHX	6	2174	7/7	0.97	0.17	-0.53	86,86,86,86	6
88	OHX	l3	404	7/7	0.89	0.24	-0.53	71,71,71,71	3
88	OHX	6	2063	7/7	0.97	0.18	-0.54	138,138,138,138	4
88	OHX	2	2092	7/7	0.95	0.22	-0.54	113,113,113,113	5
88	OHX	1	3895	7/7	0.99	0.21	-0.54	50,50,50,50	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	6	2020	7/7	0.99	0.23	-0.55	77,77,77,77	3
87	MG	6	1961	1/1	0.77	0.19	-0.55	68,68,68,68	0
88	OHX	1	3833	7/7	0.99	0.20	-0.55	61,61,61,61	3
88	OHX	1	3875	7/7	0.96	0.21	-0.56	86,86,86,86	3
88	OHX	n9	103	7/7	0.99	0.24	-0.57	59,59,59,59	3
88	OHX	2	2011	7/7	0.99	0.20	-0.57	80,80,80,80	2
88	OHX	1	3949	7/7	0.95	0.22	-0.57	37,37,37,37	2
88	OHX	1	3930	7/7	0.98	0.23	-0.57	42,42,42,42	4
88	OHX	2	2129	7/7	0.83	0.14	-0.58	118,118,118,118	6
88	OHX	1	3980	7/7	0.95	0.15	-0.58	182,182,182,182	7
88	OHX	6	2062	7/7	0.98	0.18	-0.59	114,114,114,114	4
88	OHX	5	4092	7/7	0.91	0.25	-0.59	64,64,64,64	5
88	OHX	2	2013	7/7	0.93	0.22	-0.59	105,105,105,105	3
88	OHX	2	2068	7/7	0.95	0.17	-0.60	144,144,144,144	6
88	OHX	2	2038	7/7	0.96	0.18	-0.60	110,110,110,110	3
88	OHX	2	2103	7/7	0.96	0.27	-0.61	77,77,77,77	3
87	MG	5	3680	1/1	0.84	0.21	-0.61	41,41,41,41	0
88	OHX	q1	702	7/7	0.95	0.20	-0.62	48,48,48,48	3
88	OHX	5	4008	7/7	0.96	0.28	-0.62	40,40,40,40	3
88	OHX	6	2118	7/7	0.91	0.25	-0.62	62,62,62,62	3
88	OHX	1	3943	7/7	0.97	0.18	-0.62	89,89,89,89	3
88	OHX	6	2035	7/7	0.97	0.21	-0.63	82,82,82,82	3
87	MG	1	3653	1/1	0.99	0.25	-0.64	57,57,57,57	1
87	MG	6	1901	1/1	0.97	0.25	-0.64	55,55,55,55	0
88	OHX	2	2115	7/7	0.92	0.17	-0.65	103,103,103,103	5
87	MG	2	2155	1/1	0.83	0.27	-0.65	83,83,83,83	0
88	OHX	1	3979	7/7	0.96	0.20	-0.65	69,69,69,69	3
88	OHX	2	2077	7/7	0.98	0.19	-0.65	73,73,73,73	3
88	OHX	2	2070	7/7	0.94	0.27	-0.66	100,100,100,100	5
87	MG	1	4109	1/1	0.96	0.20	-0.66	56,56,56,56	0
88	OHX	2	2007	7/7	0.96	0.19	-0.66	136,136,136,136	6
88	OHX	2	2073	7/7	0.96	0.21	-0.66	64,64,64,64	4
88	OHX	o7	502	7/7	0.99	0.20	-0.67	57,57,57,57	1
88	OHX	1	4003	7/7	0.97	0.18	-0.67	57,57,57,57	4
88	OHX	2	2036	7/7	0.96	0.25	-0.67	75,75,75,75	5
88	OHX	2	2058	7/7	0.96	0.22	-0.67	61,61,61,61	3
88	OHX	1	3857	7/7	0.99	0.22	-0.68	38,38,38,38	3
88	OHX	1	3959	7/7	0.98	0.21	-0.68	51,51,51,51	2
88	OHX	6	2112	7/7	0.96	0.21	-0.68	69,69,69,69	3
88	OHX	N1	201	7/7	0.99	0.23	-0.69	56,56,56,56	2
87	MG	5	3653	1/1	0.86	0.20	-0.69	37,37,37,37	0
88	OHX	1	3762	7/7	0.99	0.23	-0.69	59,59,59,59	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
89	ZN	q0	201	1/1	0.99	0.21	-0.70	45,45,45,45	0
88	OHX	5	3839	7/7	0.99	0.23	-0.70	53,53,53,53	2
87	MG	N0	201	1/1	0.80	0.24	-0.70	51,51,51,51	0
88	OHX	5	3809	7/7	1.00	0.22	-0.70	54,54,54,54	2
88	OHX	1	3792	7/7	1.00	0.21	-0.70	54,54,54,54	2
88	OHX	5	4149	7/7	0.89	0.19	-0.70	101,101,101,101	7
88	OHX	5	3852	7/7	0.98	0.20	-0.70	75,75,75,75	2
88	OHX	1	3937	7/7	0.96	0.21	-0.71	54,54,54,54	4
88	OHX	1	3822	7/7	0.99	0.23	-0.71	46,46,46,46	2
88	OHX	5	4001	7/7	0.97	0.21	-0.72	40,40,40,40	3
88	OHX	6	2098	7/7	0.95	0.21	-0.72	75,75,75,75	4
88	OHX	6	2070	7/7	0.96	0.19	-0.72	86,86,86,86	3
88	OHX	6	2122	7/7	0.97	0.20	-0.72	64,64,64,64	3
88	OHX	5	3921	7/7	0.98	0.22	-0.73	83,83,83,83	3
88	OHX	2	2097	7/7	0.96	0.21	-0.73	88,88,88,88	4
88	OHX	l3	402	7/7	0.98	0.22	-0.73	50,50,50,50	2
88	OHX	6	2109	7/7	0.88	0.20	-0.73	100,100,100,100	5
88	OHX	2	2101	7/7	0.93	0.19	-0.74	100,100,100,100	5
87	MG	2	1985	1/1	0.96	0.18	-0.74	81,81,81,81	0
88	OHX	6	2024	7/7	0.99	0.20	-0.74	83,83,83,83	2
88	OHX	1	4030	7/7	0.83	0.23	-0.74	73,73,73,73	3
88	OHX	2	2093	7/7	0.98	0.17	-0.75	91,91,91,91	7
88	OHX	1	3778	7/7	0.99	0.22	-0.75	69,69,69,69	2
88	OHX	2	2066	7/7	0.98	0.13	-0.75	139,139,139,139	6
87	MG	1	3583	1/1	0.97	0.25	-0.75	42,42,42,42	0
88	OHX	q2	502	7/7	0.97	0.23	-0.76	46,46,46,46	3
88	OHX	1	3917	7/7	0.97	0.22	-0.76	52,52,52,52	5
88	OHX	2	2080	7/7	0.97	0.17	-0.76	107,107,107,107	7
88	OHX	6	2091	7/7	0.97	0.20	-0.77	90,90,90,90	5
88	OHX	4	227	7/7	0.97	0.22	-0.77	42,42,42,42	3
88	OHX	M0	303	7/7	0.88	0.19	-0.77	97,97,97,97	7
88	OHX	2	1998	7/7	0.99	0.19	-0.78	73,73,73,73	3
88	OHX	6	2036	7/7	0.98	0.20	-0.78	58,58,58,58	2
88	OHX	1	3963	7/7	0.96	0.19	-0.78	58,58,58,58	3
88	OHX	1	3841	7/7	0.99	0.21	-0.79	48,48,48,48	2
88	OHX	2	2096	7/7	0.91	0.21	-0.79	100,100,100,100	4
87	MG	1	3582	1/1	0.93	0.20	-0.79	38,38,38,38	0
88	OHX	1	3901	7/7	0.98	0.19	-0.80	63,63,63,63	5
89	ZN	d7	101	1/1	0.84	0.32	-0.80	142,142,142,142	0
87	MG	n9	101	1/1	0.93	0.21	-0.80	32,32,32,32	0
88	OHX	1	4021	7/7	0.95	0.19	-0.80	48,48,48,48	5
88	OHX	5	3970	7/7	0.97	0.20	-0.81	57,57,57,57	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3920	7/7	0.98	0.22	-0.82	44,44,44,44	4
88	OHX	1	3934	7/7	0.97	0.16	-0.83	65,65,65,65	3
88	OHX	6	2140	7/7	0.88	0.19	-0.83	119,119,119,119	7
87	MG	6	1966	1/1	0.91	0.18	-0.84	83,83,83,83	0
88	OHX	5	3982	7/7	0.98	0.22	-0.85	43,43,43,43	3
88	OHX	2	2081	7/7	0.96	0.23	-0.85	78,78,78,78	6
88	OHX	1	3817	7/7	0.99	0.20	-0.86	50,50,50,50	4
87	MG	12	302	1/1	0.86	0.24	-0.86	50,50,50,50	0
88	OHX	6	2030	7/7	0.99	0.20	-0.86	60,60,60,60	1
88	OHX	5	3878	7/7	0.99	0.23	-0.86	44,44,44,44	2
88	OHX	2	2094	7/7	0.91	0.23	-0.87	79,79,79,79	5
88	OHX	o3	201	7/7	0.98	0.22	-0.87	49,49,49,49	3
88	OHX	2	2048	7/7	0.95	0.18	-0.87	97,97,97,97	3
88	OHX	1	3850	7/7	0.99	0.19	-0.88	57,57,57,57	3
88	OHX	1	4059	7/7	0.92	0.24	-0.88	65,65,65,65	4
88	OHX	5	3984	7/7	0.99	0.21	-0.89	42,42,42,42	3
88	OHX	2	2056	7/7	0.94	0.14	-0.90	108,108,108,108	5
88	OHX	2	2003	7/7	0.99	0.17	-0.90	98,98,98,98	2
87	MG	5	3681	1/1	0.92	0.14	-0.90	130,130,130,130	0
87	MG	1	3476	1/1	0.97	0.21	-0.92	43,43,43,43	0
88	OHX	1	3834	7/7	0.99	0.20	-0.92	47,47,47,47	2
88	OHX	6	2094	7/7	0.92	0.17	-0.92	106,106,106,106	5
87	MG	5	3612	1/1	0.92	0.24	-0.93	38,38,38,38	0
88	OHX	Q2	503	7/7	0.98	0.22	-0.94	45,45,45,45	2
88	OHX	1	3798	7/7	0.99	0.21	-0.94	71,71,71,71	1
88	OHX	5	3855	7/7	0.99	0.20	-0.94	59,59,59,59	4
87	MG	1	3414	1/1	0.97	0.21	-0.94	45,45,45,45	0
88	OHX	C1	201	7/7	0.98	0.19	-0.94	97,97,97,97	5
87	MG	5	3640	1/1	0.97	0.23	-0.96	38,38,38,38	0
88	OHX	5	3910	7/7	0.97	0.19	-0.97	64,64,64,64	4
88	OHX	5	3961	7/7	0.94	0.21	-0.98	56,56,56,56	3
88	OHX	1	3774	7/7	0.99	0.22	-0.98	63,63,63,63	4
88	OHX	2	2116	7/7	0.92	0.17	-0.99	146,146,146,146	7
87	MG	2	1938	1/1	0.90	0.21	-1.00	67,67,67,67	0
87	MG	6	1907	1/1	0.92	0.16	-1.00	76,76,76,76	0
88	OHX	2	2069	7/7	0.96	0.13	-1.00	122,122,122,122	3
88	OHX	2	2032	7/7	0.98	0.17	-1.00	92,92,92,92	4
88	OHX	L3	404	7/7	0.97	0.19	-1.00	68,68,68,68	2
87	MG	1	4110	1/1	0.77	0.15	-1.01	73,73,73,73	0
87	MG	6	1905	1/1	0.90	0.18	-1.01	67,67,67,67	0
88	OHX	5	3832	7/7	1.00	0.20	-1.01	55,55,55,55	2
88	OHX	5	3906	7/7	0.99	0.23	-1.02	40,40,40,40	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3915	7/7	0.92	0.23	-1.03	72,72,72,72	3
88	OHX	2	2137	7/7	0.81	0.13	-1.04	148,148,148,148	6
88	OHX	5	4084	7/7	0.95	0.19	-1.04	48,48,48,48	5
88	OHX	1	3900	7/7	0.94	0.20	-1.04	51,51,51,51	3
88	OHX	5	4112	7/7	0.95	0.18	-1.05	57,57,57,57	3
88	OHX	5	3903	7/7	0.98	0.19	-1.05	55,55,55,55	1
88	OHX	M5	301	7/7	0.97	0.20	-1.05	66,66,66,66	4
88	OHX	6	2148	7/7	0.96	0.15	-1.06	93,93,93,93	5
88	OHX	1	3786	7/7	0.99	0.23	-1.06	46,46,46,46	2
89	ZN	Q0	201	1/1	0.99	0.18	-1.07	49,49,49,49	0
88	OHX	5	4014	7/7	0.99	0.13	-1.07	72,72,72,72	4
88	OHX	5	3870	7/7	0.99	0.21	-1.07	48,48,48,48	3
88	OHX	5	3825	7/7	0.99	0.22	-1.08	62,62,62,62	3
88	OHX	6	2033	7/7	0.99	0.19	-1.08	60,60,60,60	5
88	OHX	S8	301	7/7	0.93	0.16	-1.08	109,109,109,109	6
88	OHX	S1	301	7/7	0.97	0.18	-1.09	117,117,117,117	3
88	OHX	2	2027	7/7	0.97	0.15	-1.09	94,94,94,94	5
87	MG	m0	301	1/1	0.97	0.22	-1.09	45,45,45,45	0
88	OHX	3	213	7/7	0.97	0.17	-1.11	76,76,76,76	4
88	OHX	6	2039	7/7	0.97	0.17	-1.11	123,123,123,123	3
88	OHX	2	2062	7/7	0.90	0.22	-1.11	93,93,93,93	4
88	OHX	1	4035	7/7	0.95	0.20	-1.11	64,64,64,64	4
88	OHX	1	3840	7/7	0.98	0.15	-1.12	90,90,90,90	5
87	MG	5	3597	1/1	0.87	0.17	-1.12	48,48,48,48	0
88	OHX	2	2105	7/7	0.95	0.16	-1.13	106,106,106,106	4
88	OHX	2	2082	7/7	0.93	0.22	-1.13	86,86,86,86	5
89	ZN	d9	101	1/1	0.98	0.14	-1.13	89,89,89,89	0
88	OHX	6	2133	7/7	0.86	0.14	-1.13	148,148,148,148	7
88	OHX	5	3803	7/7	1.00	0.20	-1.14	60,60,60,60	2
88	OHX	5	4073	7/7	0.96	0.20	-1.14	47,47,47,47	2
88	OHX	1	3801	7/7	0.99	0.22	-1.14	55,55,55,55	2
88	OHX	5	3857	7/7	0.98	0.24	-1.14	52,52,52,52	3
89	ZN	Q3	501	1/1	0.99	0.14	-1.15	74,74,74,74	0
88	OHX	5	3851	7/7	0.98	0.22	-1.15	41,41,41,41	3
88	OHX	2	2006	7/7	0.99	0.17	-1.15	72,72,72,72	4
87	MG	5	3494	1/1	0.96	0.25	-1.16	35,35,35,35	0
88	OHX	1	3925	7/7	0.98	0.20	-1.17	56,56,56,56	7
88	OHX	1	3935	7/7	0.94	0.23	-1.17	55,55,55,55	2
88	OHX	2	2088	7/7	0.92	0.23	-1.17	99,99,99,99	3
88	OHX	6	2019	7/7	0.99	0.18	-1.18	87,87,87,87	2
88	OHX	6	2103	7/7	0.96	0.27	-1.19	90,90,90,90	7
88	OHX	1	3828	7/7	0.99	0.19	-1.20	65,65,65,65	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3883	7/7	0.99	0.19	-1.20	48,48,48,48	5
88	OHX	1	3983	7/7	0.99	0.21	-1.20	52,52,52,52	4
88	OHX	2	2125	7/7	0.96	0.09	-1.20	113,113,113,113	4
88	OHX	D9	103	7/7	0.91	0.24	-1.20	89,89,89,89	5
89	ZN	D9	101	1/1	0.96	0.11	-1.20	86,86,86,86	0
88	OHX	6	2056	7/7	0.99	0.18	-1.20	75,75,75,75	3
88	OHX	2	1996	7/7	0.98	0.21	-1.21	99,99,99,99	2
88	OHX	1	3878	7/7	0.98	0.20	-1.21	46,46,46,46	4
88	OHX	6	2055	7/7	0.99	0.14	-1.21	110,110,110,110	2
87	MG	5	3433	1/1	0.97	0.18	-1.22	60,60,60,60	0
88	OHX	5	3927	7/7	0.96	0.22	-1.22	48,48,48,48	2
88	OHX	2	2009	7/7	0.99	0.17	-1.22	86,86,86,86	5
88	OHX	2	2102	7/7	0.93	0.13	-1.23	161,161,161,161	7
87	MG	d2	201	1/1	0.91	0.19	-1.24	71,71,71,71	0
88	OHX	2	2008	7/7	0.98	0.20	-1.25	89,89,89,89	3
88	OHX	2	1997	7/7	0.99	0.18	-1.26	89,89,89,89	2
88	OHX	O3	203	7/7	0.98	0.23	-1.27	47,47,47,47	3
88	OHX	5	4094	7/7	0.95	0.19	-1.27	64,64,64,64	5
88	OHX	5	3936	7/7	0.97	0.20	-1.27	51,51,51,51	1
88	OHX	5	3819	7/7	1.00	0.21	-1.28	65,65,65,65	2
88	OHX	2	2047	7/7	0.94	0.20	-1.28	88,88,88,88	5
88	OHX	1	3897	7/7	0.96	0.21	-1.28	51,51,51,51	5
88	OHX	1	3889	7/7	0.96	0.20	-1.30	49,49,49,49	3
87	MG	6	2187	1/1	0.92	0.15	-1.30	93,93,93,93	0
88	OHX	1	3864	7/7	0.98	0.20	-1.30	65,65,65,65	2
88	OHX	2	2005	7/7	0.98	0.19	-1.32	90,90,90,90	3
88	OHX	5	3978	7/7	0.97	0.20	-1.32	45,45,45,45	3
89	ZN	E1	501	1/1	0.91	0.12	-1.32	132,132,132,132	0
88	OHX	1	3977	7/7	0.96	0.21	-1.32	51,51,51,51	3
88	OHX	6	2125	7/7	0.95	0.16	-1.33	76,76,76,76	2
87	MG	sM	301	1/1	0.94	0.19	-1.33	50,50,50,50	0
87	MG	5	3658	1/1	0.93	0.19	-1.34	39,39,39,39	0
87	MG	5	3523	1/1	0.92	0.25	-1.35	38,38,38,38	0
87	MG	5	3483	1/1	0.96	0.16	-1.36	68,68,68,68	0
88	OHX	2	2031	7/7	0.96	0.17	-1.36	102,102,102,102	1
88	OHX	6	2108	7/7	0.98	0.20	-1.37	91,91,91,91	5
88	OHX	6	2043	7/7	0.94	0.20	-1.38	91,91,91,91	4
88	OHX	1	3871	7/7	0.98	0.21	-1.39	50,50,50,50	4
88	OHX	6	2099	7/7	0.95	0.19	-1.40	64,64,64,64	5
88	OHX	SR	401	7/7	0.94	0.14	-1.40	133,133,133,133	5
87	MG	O4	201	1/1	0.87	0.19	-1.41	73,73,73,73	0
87	MG	5	3406	1/1	0.92	0.18	-1.41	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3982	7/7	0.95	0.20	-1.42	50,50,50,50	2
88	OHX	2	2104	7/7	0.95	0.23	-1.42	106,106,106,106	7
87	MG	5	3604	1/1	0.91	0.21	-1.42	39,39,39,39	0
87	MG	1	3562	1/1	0.83	0.23	-1.43	49,49,49,49	0
88	OHX	1	3769	7/7	1.00	0.22	-1.44	64,64,64,64	4
88	OHX	6	2053	7/7	0.98	0.20	-1.45	86,86,86,86	5
87	MG	2	1965	1/1	0.83	0.16	-1.45	81,81,81,81	0
87	MG	L2	302	1/1	0.86	0.19	-1.47	44,44,44,44	0
88	OHX	8	216	7/7	0.98	0.20	-1.48	60,60,60,60	4
88	OHX	2	2098	7/7	0.98	0.17	-1.48	70,70,70,70	3
88	OHX	2	2050	7/7	0.96	0.21	-1.48	77,77,77,77	3
87	MG	6	2186	1/1	0.91	0.20	-1.48	67,67,67,67	0
88	OHX	5	3935	7/7	0.98	0.21	-1.49	45,45,45,45	3
88	OHX	1	3804	7/7	0.99	0.23	-1.50	74,74,74,74	3
88	OHX	1	3932	7/7	0.96	0.19	-1.50	87,87,87,87	2
87	MG	l7	301	1/1	0.94	0.18	-1.51	46,46,46,46	0
88	OHX	5	3900	7/7	0.98	0.20	-1.51	39,39,39,39	3
89	ZN	o7	501	1/1	0.99	0.17	-1.52	48,48,48,48	0
87	MG	6	1937	1/1	0.90	0.24	-1.52	71,71,71,71	0
88	OHX	2	2150	7/7	0.86	0.11	-1.53	140,140,140,140	7
88	OHX	2	2079	7/7	0.97	0.15	-1.53	122,122,122,122	6
87	MG	8	210	1/1	0.80	0.10	-1.54	86,86,86,86	0
88	OHX	1	3845	7/7	0.97	0.22	-1.54	70,70,70,70	2
87	MG	L2	301	1/1	0.90	0.15	-1.56	43,43,43,43	0
88	OHX	1	3974	7/7	0.97	0.16	-1.56	61,61,61,61	5
87	MG	L7	302	1/1	0.89	0.22	-1.56	47,47,47,47	0
87	MG	4	207	1/1	0.86	0.17	-1.57	37,37,37,37	0
87	MG	6	1981	1/1	0.94	0.16	-1.57	85,85,85,85	0
88	OHX	1	4024	7/7	0.93	0.21	-1.59	61,61,61,61	1
88	OHX	1	4052	7/7	0.98	0.21	-1.59	58,58,58,58	2
87	MG	2	1947	1/1	0.96	0.20	-1.60	98,98,98,98	0
88	OHX	2	2046	7/7	0.93	0.25	-1.61	98,98,98,98	5
87	MG	1	3407	1/1	0.71	0.19	-1.63	52,52,52,52	0
87	MG	5	3626	1/1	0.87	0.24	-1.65	53,53,53,53	0
88	OHX	2	2042	7/7	0.97	0.16	-1.66	100,100,100,100	4
89	ZN	e1	501	1/1	0.81	0.06	-1.66	168,168,168,168	0
87	MG	6	2188	1/1	0.81	0.06	-1.68	81,81,81,81	0
88	OHX	1	3835	7/7	0.99	0.20	-1.69	60,60,60,60	3
88	OHX	6	2072	7/7	0.97	0.18	-1.70	70,70,70,70	3
87	MG	1	3420	1/1	0.84	0.19	-1.71	39,39,39,39	0
88	OHX	2	2113	7/7	0.94	0.16	-1.72	99,99,99,99	4
87	MG	2	2153	1/1	0.88	0.17	-1.73	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3844	7/7	0.99	0.20	-1.73	56,56,56,56	3
88	OHX	5	3890	7/7	0.99	0.19	-1.73	56,56,56,56	3
88	OHX	1	3986	7/7	0.98	0.19	-1.74	41,41,41,41	2
89	ZN	O7	101	1/1	0.99	0.15	-1.75	49,49,49,49	0
88	OHX	1	4045	7/7	0.97	0.19	-1.75	45,45,45,45	4
87	MG	2	1969	1/1	0.86	0.11	-1.75	93,93,93,93	0
88	OHX	2	2035	7/7	0.94	0.21	-1.77	100,100,100,100	6
87	MG	2	1929	1/1	0.97	0.20	-1.78	75,75,75,75	0
88	OHX	5	4148	7/7	0.95	0.17	-1.79	45,45,45,45	6
87	MG	o2	202	1/1	0.75	0.17	-1.80	52,52,52,52	0
88	OHX	5	3865	7/7	0.99	0.21	-1.80	49,49,49,49	2
88	OHX	6	2015	7/7	0.99	0.19	-1.80	73,73,73,73	2
89	ZN	D6	500	1/1	0.99	0.12	-1.80	89,89,89,89	0
87	MG	1	3720	1/1	0.95	0.17	-1.83	48,48,48,48	0
88	OHX	5	3804	7/7	0.99	0.24	-1.83	56,56,56,56	1
89	ZN	Q2	501	1/1	0.97	0.07	-1.83	79,79,79,79	0
87	MG	2	1961	1/1	0.96	0.17	-1.84	101,101,101,101	0
88	OHX	2	1995	7/7	0.99	0.21	-1.85	90,90,90,90	2
88	OHX	1	3928	7/7	0.99	0.20	-1.87	52,52,52,52	3
88	OHX	1	3885	7/7	0.98	0.18	-1.88	51,51,51,51	3
88	OHX	6	2084	7/7	0.94	0.22	-1.89	98,98,98,98	5
87	MG	6	1950	1/1	0.96	0.18	-1.89	76,76,76,76	0
87	MG	1	4108	1/1	0.92	0.17	-1.90	41,41,41,41	0
88	OHX	5	3945	7/7	0.98	0.19	-1.90	59,59,59,59	5
88	OHX	5	3987	7/7	0.98	0.17	-1.91	69,69,69,69	5
88	OHX	m5	301	7/7	0.99	0.17	-1.92	72,72,72,72	3
88	OHX	5	3794	7/7	1.00	0.22	-1.92	50,50,50,50	3
87	MG	5	3423	1/1	0.91	0.20	-1.94	38,38,38,38	0
88	OHX	5	4048	7/7	0.97	0.21	-1.95	41,41,41,41	5
88	OHX	5	3820	7/7	1.00	0.20	-1.95	65,65,65,65	4
87	MG	2	1939	1/1	0.94	0.18	-1.98	79,79,79,79	0
88	OHX	1	3942	7/7	0.96	0.17	-1.98	87,87,87,87	3
88	OHX	1	3896	7/7	0.97	0.17	-1.99	57,57,57,57	4
88	OHX	6	2014	7/7	0.99	0.19	-1.99	85,85,85,85	2
88	OHX	1	4077	7/7	0.93	0.20	-2.00	56,56,56,56	5
88	OHX	2	2084	7/7	0.97	0.17	-2.00	87,87,87,87	3
89	ZN	d6	101	1/1	0.97	0.11	-2.01	71,71,71,71	0
88	OHX	1	3945	7/7	0.97	0.18	-2.02	52,52,52,52	1
88	OHX	1	3768	7/7	0.99	0.20	-2.03	63,63,63,63	5
87	MG	6	2004	1/1	0.97	0.15	-2.07	90,90,90,90	0
87	MG	1	3655	1/1	0.88	0.20	-2.07	44,44,44,44	0
88	OHX	6	2057	7/7	0.97	0.21	-2.08	65,65,65,65	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	2	2099	7/7	0.92	0.20	-2.08	99,99,99,99	4
88	OHX	5	3981	7/7	0.95	0.18	-2.11	60,60,60,60	5
88	OHX	5	4067	7/7	0.96	0.17	-2.11	41,41,41,41	4
88	OHX	2	2086	7/7	0.97	0.21	-2.13	94,94,94,94	4
88	OHX	5	3860	7/7	0.99	0.20	-2.13	73,73,73,73	2
88	OHX	2	2059	7/7	0.97	0.14	-2.13	90,90,90,90	1
87	MG	1	3406	1/1	0.76	0.23	-2.14	48,48,48,48	0
88	OHX	6	2105	7/7	0.96	0.16	-2.14	83,83,83,83	2
88	OHX	5	3807	7/7	1.00	0.22	-2.16	49,49,49,49	2
88	OHX	5	3881	7/7	1.00	0.19	-2.17	51,51,51,51	1
87	MG	1	3690	1/1	0.87	0.15	-2.17	46,46,46,46	0
88	OHX	2	2049	7/7	0.98	0.20	-2.19	78,78,78,78	6
88	OHX	2	2033	7/7	0.97	0.15	-2.20	91,91,91,91	7
88	OHX	6	2101	7/7	0.97	0.15	-2.21	88,88,88,88	3
88	OHX	1	3894	7/7	0.97	0.19	-2.21	49,49,49,49	4
88	OHX	6	2074	7/7	0.97	0.19	-2.22	71,71,71,71	2
88	OHX	2	2134	7/7	0.93	0.18	-2.22	85,85,85,85	4
88	OHX	1	3887	7/7	0.98	0.21	-2.23	63,63,63,63	1
87	MG	1	3565	1/1	0.94	0.17	-2.27	50,50,50,50	0
88	OHX	6	2116	7/7	0.97	0.18	-2.29	62,62,62,62	3
87	MG	5	3606	1/1	0.95	0.15	-2.31	40,40,40,40	0
87	MG	5	3420	1/1	0.91	0.15	-2.38	35,35,35,35	0
87	MG	5	3631	1/1	0.91	0.15	-2.39	50,50,50,50	0
87	MG	5	4161	1/1	0.89	0.14	-2.44	39,39,39,39	0
88	OHX	5	3889	7/7	0.99	0.22	-2.44	47,47,47,47	3
87	MG	12	301	1/1	0.98	0.12	-2.49	40,40,40,40	0
88	OHX	5	4006	7/7	0.97	0.21	-2.49	49,49,49,49	2
87	MG	2	1923	1/1	0.90	0.15	-2.52	89,89,89,89	0
88	OHX	2	2016	7/7	0.99	0.17	-2.57	87,87,87,87	4
88	OHX	5	3895	7/7	0.99	0.20	-2.59	47,47,47,47	3
89	ZN	q2	501	1/1	0.91	0.08	-2.60	79,79,79,79	0
87	MG	5	3430	1/1	0.94	0.13	-2.61	41,41,41,41	0
88	OHX	6	2184	7/7	0.92	0.10	-2.62	115,115,115,115	6
87	MG	1	3743	1/1	0.99	0.15	-2.62	49,49,49,49	0
88	OHX	6	2078	7/7	0.98	0.18	-2.66	66,66,66,66	2
87	MG	2	1941	1/1	0.71	0.15	-2.70	81,81,81,81	0
88	OHX	5	3869	7/7	0.99	0.20	-2.71	45,45,45,45	3
88	OHX	2	2024	7/7	0.96	0.16	-2.71	98,98,98,98	6
87	MG	1	3477	1/1	0.96	0.16	-2.75	41,41,41,41	0
88	OHX	2	2122	7/7	0.94	0.20	-2.76	83,83,83,83	3
88	OHX	6	2100	7/7	0.96	0.18	-2.77	65,65,65,65	4
88	OHX	5	3828	7/7	1.00	0.20	-2.77	49,49,49,49	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	2	2055	7/7	0.99	0.15	-2.84	83,83,83,83	5
87	MG	2	1971	1/1	0.84	0.19	-2.86	64,64,64,64	0
87	MG	1	3734	1/1	0.97	0.16	-2.88	35,35,35,35	0
88	OHX	6	2104	7/7	0.97	0.16	-2.96	83,83,83,83	5
88	OHX	2	2034	7/7	0.98	0.17	-2.99	79,79,79,79	5
88	OHX	6	2045	7/7	0.99	0.15	-3.05	87,87,87,87	5
88	OHX	2	2091	7/7	0.95	0.15	-3.08	85,85,85,85	4
88	OHX	2	2030	7/7	0.98	0.18	-3.12	71,71,71,71	4
87	MG	5	3696	1/1	0.96	0.11	-3.13	56,56,56,56	0
87	MG	5	3744	1/1	0.96	0.11	-3.16	42,42,42,42	0
87	MG	5	3771	1/1	0.96	0.17	-3.19	38,38,38,38	0
88	OHX	5	4124	7/7	0.89	0.12	-3.33	163,163,163,163	7
88	OHX	5	3971	7/7	0.97	0.17	-3.38	43,43,43,43	2
87	MG	5	3416	1/1	0.76	0.12	-3.39	49,49,49,49	0
87	MG	2	1986	1/1	0.87	0.15	-3.44	99,99,99,99	0
88	OHX	5	3919	7/7	0.99	0.16	-3.44	53,53,53,53	1
88	OHX	2	2015	7/7	0.99	0.18	-3.58	81,81,81,81	1
88	OHX	6	2038	7/7	0.99	0.19	-3.60	63,63,63,63	5
87	MG	5	3515	1/1	0.97	0.10	-3.68	42,42,42,42	0
88	OHX	2	2029	7/7	0.98	0.15	-3.76	103,103,103,103	4
87	MG	5	3459	1/1	0.82	0.17	-3.85	43,43,43,43	0
87	MG	5	3707	1/1	0.94	0.13	-3.88	44,44,44,44	0
87	MG	5	3679	1/1	0.96	0.14	-3.91	50,50,50,50	0
87	MG	1	3626	1/1	0.96	0.19	-3.91	43,43,43,43	0
88	OHX	6	2081	7/7	0.98	0.16	-3.93	74,74,74,74	3
87	MG	5	3451	1/1	0.85	0.14	-4.03	44,44,44,44	0
87	MG	5	3716	1/1	0.92	0.18	-4.03	40,40,40,40	0
88	OHX	8	232	7/7	0.96	0.15	-4.08	48,48,48,48	3
88	OHX	1	3891	7/7	0.97	0.18	-4.17	63,63,63,63	3
87	MG	5	3484	1/1	0.87	0.14	-4.30	48,48,48,48	0
87	MG	5	3428	1/1	0.96	0.13	-4.30	34,34,34,34	0
88	OHX	5	4051	7/7	0.98	0.17	-4.71	51,51,51,51	2
87	MG	1	3468	1/1	0.76	0.17	-4.73	48,48,48,48	0
87	MG	1	3587	1/1	0.91	0.09	-4.86	63,63,63,63	0
87	MG	5	3418	1/1	0.84	0.13	-4.91	41,41,41,41	0
87	MG	5	3671	1/1	0.86	0.17	-5.53	44,44,44,44	0
88	OHX	6	2022	7/7	0.99	0.19	-5.62	66,66,66,66	3
87	MG	1	3430	1/1	0.94	0.12	-6.00	50,50,50,50	0
88	OHX	1	3783	7/7	1.00	0.21	-6.08	57,57,57,57	2
87	MG	5	3503	1/1	0.96	0.09	-6.14	47,47,47,47	0
87	MG	5	3598	1/1	0.97	0.11	-6.27	50,50,50,50	0
88	OHX	2	2106	7/7	0.91	0.17	-6.98	108,108,108,108	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3719	1/1	0.87	0.11	-7.21	60,60,60,60	0
87	MG	6	1939	1/1	0.96	0.14	-7.78	57,57,57,57	0
87	MG	6	1930	1/1	0.90	0.09	-8.57	63,63,63,63	0
87	MG	1	3645	1/1	0.92	0.32	-	57,57,57,57	0
88	OHX	1	3854	7/7	0.99	0.22	-	53,53,53,53	3
87	MG	1	3605	1/1	0.54	0.46	-	55,55,55,55	0
88	OHX	1	3922	7/7	0.97	0.26	-	74,74,74,74	4
87	MG	5	3659	1/1	0.95	0.27	-	49,49,49,49	0
87	MG	1	3548	1/1	0.96	0.40	-	35,35,35,35	0
87	MG	5	3698	1/1	0.97	0.27	-	65,65,65,65	0
87	MG	1	3713	1/1	0.88	0.44	-	72,72,72,72	0
87	MG	1	3434	1/1	0.95	0.24	-	59,59,59,59	0
88	OHX	1	3863	7/7	0.99	0.23	-	69,69,69,69	4
87	MG	6	1904	1/1	0.92	0.27	-	82,82,82,82	0
87	MG	6	1977	1/1	0.97	0.09	-	70,70,70,70	0
88	OHX	1	4066	7/7	0.92	0.23	-	37,37,37,37	3
88	OHX	6	2183	7/7	0.94	0.15	-	101,101,101,101	6
87	MG	1	3403	1/1	0.91	0.17	-	43,43,43,43	0
87	MG	1	3532	1/1	0.85	0.29	-	43,43,43,43	0
87	MG	2	1987	1/1	0.88	0.36	-	96,96,96,96	0
88	OHX	5	3844	7/7	0.98	0.25	-	47,47,47,47	1
87	MG	5	3735	1/1	0.81	0.23	-	49,49,49,49	1
87	MG	d6	102	1/1	0.89	0.72	-	65,65,65,65	0
88	OHX	1	4095	7/7	0.92	0.26	-	45,45,45,45	3
88	OHX	1	4092	7/7	0.94	0.20	-	49,49,49,49	4
87	MG	5	3780	1/1	0.87	0.39	-	43,43,43,43	0
87	MG	5	3481	1/1	0.85	0.60	-	48,48,48,48	0
88	OHX	1	3764	7/7	0.99	0.22	-	54,54,54,54	3
88	OHX	5	3831	7/7	0.99	0.24	-	54,54,54,54	2
87	MG	1	3599	1/1	0.89	0.26	-	61,61,61,61	0
87	MG	5	3617	1/1	0.89	0.29	-	35,35,35,35	0
87	MG	1	3470	1/1	0.91	0.30	-	47,47,47,47	0
87	MG	1	3739	1/1	0.94	0.41	-	45,45,45,45	0
87	MG	5	3409	1/1	0.95	0.31	-	41,41,41,41	0
88	OHX	1	3987	7/7	0.98	0.26	-	65,65,65,65	5
87	MG	N8	203	1/1	0.77	0.22	-	52,52,52,52	0
88	OHX	1	3879	7/7	0.98	0.19	-	82,82,82,82	3
87	MG	1	3700	1/1	0.75	0.22	-	63,63,63,63	0
87	MG	1	3603	1/1	0.92	0.24	-	45,45,45,45	0
87	MG	5	3573	1/1	0.97	0.48	-	41,41,41,41	0
87	MG	3	207	1/1	0.93	0.27	-	68,68,68,68	0
88	OHX	1	4037	7/7	0.94	0.20	-	60,60,60,60	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	6	2141	7/7	0.95	0.15	-	87,87,87,87	5
87	MG	1	3601	1/1	0.96	0.37	-	47,47,47,47	0
88	OHX	5	4046	7/7	0.95	0.23	-	46,46,46,46	2
87	MG	6	1942	1/1	0.88	0.37	-	78,78,78,78	0
87	MG	5	3703	1/1	0.94	0.38	-	48,48,48,48	0
87	MG	2	1984	1/1	0.96	0.31	-	57,57,57,57	0
87	MG	3	202	1/1	0.98	0.47	-	54,54,54,54	0
87	MG	8	201	1/1	0.96	0.15	-	51,51,51,51	0
88	OHX	6	2128	7/7	0.92	0.39	-	56,56,56,56	3
87	MG	1	3448	1/1	0.85	0.33	-	54,54,54,54	0
87	MG	1	3680	1/1	0.75	0.31	-	66,66,66,66	0
87	MG	5	3526	1/1	0.96	0.40	-	35,35,35,35	0
87	MG	1	3429	1/1	0.91	0.16	-	42,42,42,42	0
87	MG	M3	202	1/1	0.87	0.20	-	44,44,44,44	0
87	MG	7	210	1/1	0.96	0.32	-	49,49,49,49	0
88	OHX	5	3866	7/7	0.98	0.25	-	61,61,61,61	2
88	OHX	1	3998	7/7	0.96	0.20	-	67,67,67,67	3
87	MG	1	3737	1/1	0.93	0.16	-	53,53,53,53	0
87	MG	5	3447	1/1	0.92	0.26	-	46,46,46,46	0
87	MG	1	3498	1/1	0.97	0.42	-	32,32,32,32	0
87	MG	5	3535	1/1	0.98	0.31	-	41,41,41,41	0
87	MG	1	3618	1/1	0.83	0.28	-	53,53,53,53	0
88	OHX	2	2107	7/7	0.89	0.15	-	108,108,108,108	4
87	MG	1	3576	1/1	0.98	0.39	-	31,31,31,31	0
87	MG	5	3471	1/1	0.95	0.31	-	59,59,59,59	0
88	OHX	2	2076	7/7	0.97	0.14	-	78,78,78,78	2
87	MG	5	3762	1/1	0.94	0.98	-	45,45,45,45	1
87	MG	2	1981	1/1	0.83	0.32	-	60,60,60,60	0
87	MG	5	3688	1/1	0.91	0.14	-	66,66,66,66	0
87	MG	1	3656	1/1	0.95	0.35	-	44,44,44,44	0
87	MG	5	3785	1/1	0.61	0.28	-	52,52,52,52	0
87	MG	6	2008	1/1	0.96	0.26	-	83,83,83,83	0
87	MG	5	3700	1/1	0.84	0.21	-	53,53,53,53	0
87	MG	1	3519	1/1	0.88	0.33	-	55,55,55,55	0
87	MG	5	3557	1/1	0.92	0.20	-	49,49,49,49	0
87	MG	8	203	1/1	0.94	0.14	-	52,52,52,52	0
88	OHX	5	4053	7/7	0.94	0.24	-	67,67,67,67	4
87	MG	M3	201	1/1	0.59	0.44	-	97,97,97,97	0
88	OHX	6	2073	7/7	0.95	0.24	-	68,68,68,68	5
87	MG	4	210	1/1	0.90	0.35	-	61,61,61,61	0
88	OHX	2	2087	7/7	0.91	0.23	-	100,100,100,100	6
87	MG	6	2000	1/1	0.87	0.26	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3729	1/1	0.92	0.17	-	51,51,51,51	0
88	OHX	5	3967	7/7	0.93	0.28	-	45,45,45,45	2
87	MG	1	3704	1/1	0.81	0.21	-	53,53,53,53	0
87	MG	1	3747	1/1	0.77	0.35	-	55,55,55,55	0
88	OHX	1	3921	7/7	0.98	0.21	-	73,73,73,73	3
87	MG	1	3624	1/1	0.95	0.25	-	38,38,38,38	0
87	MG	5	3777	1/1	0.90	0.13	-	67,67,67,67	0
87	MG	2	1992	1/1	0.87	0.16	-	86,86,86,86	0
88	OHX	5	4054	7/7	0.91	0.25	-	46,46,46,46	2
87	MG	Q2	502	1/1	0.81	0.20	-	72,72,72,72	0
87	MG	2	1979	1/1	0.79	0.18	-	68,68,68,68	0
87	MG	6	1910	1/1	0.95	0.21	-	59,59,59,59	0
88	OHX	2	2074	7/7	0.85	0.15	-	179,179,179,179	7
88	OHX	5	3854	7/7	0.97	0.29	-	80,80,80,80	3
87	MG	5	3470	1/1	0.95	0.25	-	49,49,49,49	0
88	OHX	1	4047	7/7	0.94	0.25	-	48,48,48,48	3
88	OHX	5	4020	7/7	0.97	0.30	-	40,40,40,40	2
88	OHX	8	218	7/7	0.96	0.27	-	73,73,73,73	2
87	MG	1	3699	1/1	0.87	0.20	-	48,48,48,48	0
88	OHX	1	3929	7/7	0.98	0.28	-	116,116,116,116	5
87	MG	1	3615	1/1	0.88	0.12	-	67,67,67,67	0
87	MG	5	3468	1/1	0.91	0.35	-	49,49,49,49	0
88	OHX	6	2050	7/7	0.97	0.21	-	87,87,87,87	3
87	MG	6	1951	1/1	0.80	0.45	-	74,74,74,74	0
87	MG	1	3694	1/1	0.85	0.35	-	81,81,81,81	0
87	MG	6	1990	1/1	0.92	0.34	-	72,72,72,72	0
87	MG	1	3431	1/1	0.82	0.12	-	52,52,52,52	0
87	MG	1	3726	1/1	0.80	0.22	-	60,60,60,60	0
88	OHX	5	4079	7/7	0.90	0.25	-	45,45,45,45	3
88	OHX	1	4096	7/7	0.92	0.26	-	52,52,52,52	3
87	MG	4	219	1/1	0.87	0.35	-	58,58,58,58	0
87	MG	1	3754	1/1	0.88	0.22	-	39,39,39,39	0
87	MG	6	1920	1/1	0.85	0.23	-	53,53,53,53	0
88	OHX	5	3901	7/7	0.97	0.29	-	67,67,67,67	2
87	MG	1	3695	1/1	0.95	0.46	-	59,59,59,59	0
88	OHX	1	3880	7/7	0.97	0.24	-	62,62,62,62	4
87	MG	1	3509	1/1	0.96	0.16	-	39,39,39,39	0
87	MG	M6	201	1/1	0.89	0.21	-	47,47,47,47	0
88	OHX	1	3971	7/7	0.95	0.28	-	61,61,61,61	3
88	OHX	1	4058	7/7	0.95	0.13	-	106,106,106,106	6
87	MG	1	3574	1/1	0.97	0.18	-	41,41,41,41	0
88	OHX	2	2045	7/7	0.97	0.34	-	65,65,65,65	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3412	1/1	0.89	0.29	-	46,46,46,46	0
88	OHX	1	3944	7/7	0.97	0.20	-	44,44,44,44	1
87	MG	5	3518	1/1	0.96	0.41	-	31,31,31,31	0
87	MG	5	3775	1/1	0.74	0.21	-	63,63,63,63	0
87	MG	1	3528	1/1	0.87	0.30	-	40,40,40,40	0
87	MG	5	3472	1/1	0.98	0.20	-	44,44,44,44	0
88	OHX	5	3965	7/7	0.96	0.34	-	61,61,61,61	3
87	MG	1	3736	1/1	0.85	0.25	-	54,54,54,54	0
88	OHX	2	2054	7/7	0.97	0.15	-	104,104,104,104	5
88	OHX	5	4089	7/7	0.88	0.37	-	67,67,67,67	5
87	MG	2	1942	1/1	0.72	0.29	-	77,77,77,77	0
87	MG	1	3742	1/1	0.85	0.18	-	68,68,68,68	0
88	OHX	5	4030	7/7	0.94	0.31	-	48,48,48,48	1
87	MG	1	3614	1/1	0.84	0.26	-	55,55,55,55	0
87	MG	1	3522	1/1	0.97	0.21	-	48,48,48,48	0
87	MG	2	1908	1/1	0.93	0.18	-	84,84,84,84	0
87	MG	1	3496	1/1	0.93	0.26	-	40,40,40,40	0
88	OHX	1	4054	7/7	0.92	0.23	-	43,43,43,43	3
87	MG	2	1972	1/1	0.93	0.23	-	91,91,91,91	0
87	MG	4	205	1/1	0.96	0.28	-	40,40,40,40	0
88	OHX	1	4073	7/7	0.88	0.21	-	55,55,55,55	2
88	OHX	1	3848	7/7	0.99	0.18	-	45,45,45,45	2
88	OHX	1	3794	7/7	0.99	0.23	-	65,65,65,65	3
87	MG	6	1960	1/1	0.97	0.18	-	52,52,52,52	0
87	MG	1	3413	1/1	0.76	0.18	-	66,66,66,66	0
87	MG	7	209	1/1	0.88	0.15	-	59,59,59,59	0
88	OHX	1	4105	7/7	0.90	0.17	-	98,98,98,98	3
88	OHX	2	2143	7/7	0.91	0.63	-	61,61,61,61	5
87	MG	5	3683	1/1	0.81	0.23	-	41,41,41,41	0
87	MG	1	3524	1/1	0.84	0.56	-	62,62,62,62	0
87	MG	6	2011	1/1	0.83	0.26	-	79,79,79,79	0
88	OHX	5	4025	7/7	0.90	0.23	-	133,133,133,133	6
87	MG	2	1963	1/1	0.54	0.30	-	95,95,95,95	0
87	MG	1	3457	1/1	0.94	0.33	-	32,32,32,32	0
87	MG	6	1938	1/1	0.94	0.49	-	98,98,98,98	0
87	MG	5	3551	1/1	0.87	0.20	-	46,46,46,46	0
87	MG	5	3772	1/1	0.93	0.14	-	65,65,65,65	0
87	MG	1	3460	1/1	0.92	0.23	-	59,59,59,59	0
87	MG	5	3713	1/1	0.91	0.39	-	55,55,55,55	0
87	MG	1	3445	1/1	0.91	0.30	-	46,46,46,46	0
88	OHX	1	4044	7/7	0.95	0.23	-	62,62,62,62	4
87	MG	1	3688	1/1	0.93	0.25	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3978	7/7	0.96	0.19	-	74,74,74,74	5
87	MG	6	2003	1/1	0.91	0.68	-	51,51,51,51	0
87	MG	5	3427	1/1	0.85	0.22	-	40,40,40,40	0
87	MG	2	1959	1/1	0.78	0.37	-	84,84,84,84	0
87	MG	5	3473	1/1	0.97	0.48	-	59,59,59,59	0
87	MG	n9	102	1/1	0.90	0.61	-	41,41,41,41	0
87	MG	5	3506	1/1	0.92	0.35	-	34,34,34,34	0
87	MG	5	3677	1/1	0.90	0.15	-	69,69,69,69	0
87	MG	o2	201	1/1	0.87	0.26	-	37,37,37,37	0
87	MG	1	3715	1/1	0.94	0.18	-	49,49,49,49	0
88	OHX	5	3914	7/7	0.98	0.21	-	54,54,54,54	4
88	OHX	5	4032	7/7	0.97	0.30	-	51,51,51,51	3
87	MG	1	3613	1/1	0.79	0.35	-	60,60,60,60	0
88	OHX	5	4101	7/7	0.93	0.28	-	54,54,54,54	5
87	MG	1	3636	1/1	0.95	0.32	-	58,58,58,58	0
88	OHX	5	4076	7/7	0.92	0.21	-	38,38,38,38	2
87	MG	1	3427	1/1	0.56	0.32	-	53,53,53,53	0
87	MG	1	3729	1/1	0.88	0.15	-	55,55,55,55	0
88	OHX	5	4134	7/7	0.88	0.24	-	50,50,50,50	6
88	OHX	2	2133	7/7	0.87	0.18	-	108,108,108,108	6
87	MG	1	3718	1/1	0.63	0.38	-	108,108,108,108	0
88	OHX	5	3908	7/7	0.98	0.24	-	58,58,58,58	2
87	MG	5	3552	1/1	0.83	0.39	-	46,46,46,46	0
88	OHX	1	3892	7/7	0.95	0.23	-	149,149,149,149	5
88	OHX	1	3972	7/7	0.94	0.27	-	53,53,53,53	2
88	OHX	2	2139	7/7	0.84	0.29	-	164,164,164,164	7
87	MG	6	1985	1/1	0.81	0.16	-	90,90,90,90	0
87	MG	5	3531	1/1	0.60	0.24	-	48,48,48,48	0
87	MG	6	1972	1/1	0.95	0.10	-	60,60,60,60	0
87	MG	1	3592	1/1	0.93	0.33	-	47,47,47,47	0
88	OHX	5	3922	7/7	0.98	0.27	-	59,59,59,59	3
88	OHX	1	4063	7/7	0.94	0.26	-	55,55,55,55	4
87	MG	2	1954	1/1	0.33	0.26	-	82,82,82,82	0
87	MG	1	3621	1/1	0.78	0.21	-	56,56,56,56	0
87	MG	6	1992	1/1	0.90	0.26	-	84,84,84,84	0
88	OHX	5	3992	7/7	0.93	0.31	-	41,41,41,41	4
87	MG	5	3614	1/1	0.96	0.19	-	44,44,44,44	0
87	MG	1	3452	1/1	0.96	0.31	-	36,36,36,36	0
87	MG	2	1924	1/1	0.91	0.15	-	75,75,75,75	0
87	MG	5	3541	1/1	0.98	0.47	-	38,38,38,38	0
87	MG	5	3753	1/1	0.94	0.18	-	42,42,42,42	0
87	MG	2	1968	1/1	0.93	0.17	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3560	1/1	0.96	0.60	-	35,35,35,35	0
87	MG	N6	201	1/1	0.88	0.33	-	64,64,64,64	0
87	MG	5	3723	1/1	0.94	0.60	-	55,55,55,55	0
88	OHX	1	3941	7/7	0.97	0.25	-	46,46,46,46	3
88	OHX	2	2095	7/7	0.92	0.18	-	70,70,70,70	5
88	OHX	1	4048	7/7	0.96	0.17	-	52,52,52,52	3
88	OHX	1	3985	7/7	0.93	0.19	-	114,114,114,114	4
87	MG	1	3594	1/1	0.97	0.42	-	50,50,50,50	0
88	OHX	2	2123	7/7	0.92	0.18	-	94,94,94,94	4
87	MG	5	3763	1/1	0.89	0.18	-	41,41,41,41	0
87	MG	D4	201	1/1	0.91	0.33	-	69,69,69,69	0
88	OHX	1	3855	7/7	0.98	0.24	-	102,102,102,102	4
87	MG	1	3553	1/1	0.96	0.28	-	41,41,41,41	0
87	MG	5	3486	1/1	0.81	0.25	-	45,45,45,45	0
87	MG	5	3774	1/1	0.92	0.18	-	50,50,50,50	0
87	MG	5	3728	1/1	0.84	0.22	-	47,47,47,47	0
87	MG	5	3543	1/1	0.96	0.24	-	41,41,41,41	0
87	MG	5	3748	1/1	0.89	0.12	-	45,45,45,45	0
88	OHX	5	4110	7/7	0.92	0.28	-	54,54,54,54	5
87	MG	6	1927	1/1	0.96	0.27	-	54,54,54,54	0
87	MG	8	212	1/1	0.61	0.31	-	67,67,67,67	0
87	MG	5	3747	1/1	0.94	0.24	-	46,46,46,46	1
88	OHX	5	3929	7/7	0.97	0.26	-	42,42,42,42	4
88	OHX	2	2149	7/7	0.80	0.21	-	134,134,134,134	6
87	MG	1	3616	1/1	0.91	0.23	-	44,44,44,44	0
87	MG	5	3743	1/1	0.95	0.23	-	45,45,45,45	0
87	MG	6	1964	1/1	0.87	0.30	-	75,75,75,75	0
87	MG	5	3485	1/1	0.87	0.47	-	73,73,73,73	0
87	MG	7	205	1/1	0.91	0.52	-	34,34,34,34	0
88	OHX	5	4107	7/7	0.97	0.27	-	48,48,48,48	5
87	MG	2	1919	1/1	0.80	0.27	-	70,70,70,70	0
87	MG	6	1969	1/1	0.81	0.23	-	73,73,73,73	0
88	OHX	5	4128	7/7	0.91	0.18	-	99,99,99,99	4
88	OHX	5	4142	7/7	0.80	0.52	-	37,37,37,37	6
88	OHX	5	4047	7/7	0.93	0.22	-	52,52,52,52	3
87	MG	5	3690	1/1	0.91	0.51	-	68,68,68,68	0
87	MG	5	3438	1/1	0.93	0.41	-	48,48,48,48	0
87	MG	2	1917	1/1	0.94	0.17	-	65,65,65,65	0
87	MG	1	3661	1/1	0.86	0.33	-	46,46,46,46	0
88	OHX	2	2022	7/7	0.98	0.18	-	78,78,78,78	2
87	MG	6	2010	1/1	0.83	0.19	-	66,66,66,66	0
87	MG	n8	203	1/1	0.90	0.20	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3712	1/1	0.91	0.19	-	40,40,40,40	0
87	MG	1	3622	1/1	0.89	0.21	-	44,44,44,44	0
87	MG	2	1922	1/1	0.85	0.20	-	60,60,60,60	0
87	MG	6	1914	1/1	0.74	0.23	-	78,78,78,78	0
87	MG	1	3659	1/1	0.85	0.34	-	86,86,86,86	0
88	OHX	6	2182	7/7	0.86	0.22	-	152,152,152,152	7
88	OHX	5	4111	7/7	0.85	0.29	-	77,77,77,77	6
88	OHX	6	2157	7/7	0.96	0.28	-	51,51,51,51	3
87	MG	1	3664	1/1	0.89	0.18	-	60,60,60,60	0
88	OHX	1	3940	7/7	0.98	0.26	-	47,47,47,47	4
87	MG	5	3709	1/1	0.92	0.40	-	56,56,56,56	0
88	OHX	5	3968	7/7	0.98	0.19	-	58,58,58,58	3
88	OHX	2	2128	7/7	0.87	0.33	-	62,62,62,62	3
87	MG	1	3607	1/1	0.95	0.18	-	45,45,45,45	0
88	OHX	7	217	7/7	0.99	0.22	-	61,61,61,61	5
87	MG	6	1923	1/1	0.94	0.34	-	82,82,82,82	0
87	MG	Q0	202	1/1	0.94	0.76	-	56,56,56,56	0
87	MG	2	1988	1/1	0.91	0.20	-	66,66,66,66	0
87	MG	1	3487	1/1	0.97	0.35	-	35,35,35,35	0
88	OHX	1	4014	7/7	0.96	0.22	-	53,53,53,53	3
87	MG	5	3662	1/1	0.90	0.12	-	55,55,55,55	0
87	MG	5	3770	1/1	0.86	0.30	-	40,40,40,40	0
87	MG	1	3722	1/1	0.94	0.35	-	56,56,56,56	0
87	MG	5	3610	1/1	0.89	0.51	-	45,45,45,45	0
87	MG	1	3649	1/1	0.94	0.41	-	45,45,45,45	0
88	OHX	6	2151	7/7	0.89	0.22	-	58,58,58,58	4
87	MG	5	3782	1/1	0.95	0.28	-	52,52,52,52	0
87	MG	5	3619	1/1	0.83	0.30	-	53,53,53,53	0
87	MG	5	3637	1/1	0.89	0.32	-	57,57,57,57	0
88	OHX	5	3843	7/7	0.99	0.21	-	47,47,47,47	3
87	MG	5	3576	1/1	0.96	0.21	-	35,35,35,35	0
87	MG	5	3642	1/1	0.88	0.45	-	54,54,54,54	0
87	MG	5	3673	1/1	0.86	0.11	-	48,48,48,48	1
87	MG	8	211	1/1	0.88	0.23	-	56,56,56,56	0
87	MG	6	1913	1/1	0.94	0.26	-	44,44,44,44	0
87	MG	5	3783	1/1	0.86	0.30	-	70,70,70,70	0
87	MG	5	3580	1/1	0.97	0.47	-	44,44,44,44	0
87	MG	2	1951	1/1	0.94	0.21	-	106,106,106,106	0
88	OHX	5	4121	7/7	0.91	0.20	-	145,145,145,145	7
88	OHX	6	2123	7/7	0.94	0.21	-	70,70,70,70	4
87	MG	N3	203	1/1	0.89	0.18	-	55,55,55,55	0
87	MG	2	1940	1/1	0.93	0.18	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	6	2026	7/7	0.99	0.22	-	69,69,69,69	2
87	MG	1	3703	1/1	0.88	0.21	-	59,59,59,59	0
87	MG	1	3499	1/1	0.95	0.31	-	40,40,40,40	0
87	MG	1	3662	1/1	0.70	0.28	-	43,43,43,43	0
88	OHX	6	2172	7/7	0.92	0.31	-	73,73,73,73	6
87	MG	1	3440	1/1	0.97	0.24	-	52,52,52,52	0
87	MG	1	3438	1/1	0.92	0.31	-	36,36,36,36	0
87	MG	5	3710	1/1	0.83	0.31	-	46,46,46,46	0
87	MG	5	3627	1/1	0.87	0.22	-	48,48,48,48	0
87	MG	1	3627	1/1	0.90	0.28	-	44,44,44,44	0
87	MG	4	208	1/1	0.97	0.33	-	49,49,49,49	0
88	OHX	5	3986	7/7	0.96	0.21	-	46,46,46,46	3
87	MG	5	3768	1/1	0.76	0.28	-	62,62,62,62	0
88	OHX	6	2023	7/7	0.99	0.21	-	73,73,73,73	2
88	OHX	1	4041	7/7	0.84	0.23	-	200,200,200,200	7
88	OHX	5	3938	7/7	0.97	0.26	-	41,41,41,41	4
87	MG	5	3628	1/1	0.92	0.20	-	42,42,42,42	0
87	MG	3	203	1/1	0.87	0.30	-	38,38,38,38	0
87	MG	1	3721	1/1	0.78	0.18	-	60,60,60,60	0
87	MG	1	3617	1/1	0.83	0.55	-	44,44,44,44	0
88	OHX	6	2086	7/7	0.92	0.37	-	68,68,68,68	5
88	OHX	6	2076	7/7	0.97	0.19	-	54,54,54,54	5
87	MG	6	1980	1/1	0.87	0.28	-	83,83,83,83	0
88	OHX	5	4016	7/7	0.95	0.26	-	78,78,78,78	3
87	MG	1	3458	1/1	0.89	0.41	-	43,43,43,43	0
87	MG	5	3545	1/1	0.86	0.33	-	44,44,44,44	0
87	MG	m7	202	1/1	0.97	0.29	-	37,37,37,37	0
87	MG	2	1911	1/1	0.89	0.26	-	65,65,65,65	0
87	MG	6	1974	1/1	0.76	0.53	-	94,94,94,94	0
88	OHX	6	2052	7/7	0.96	0.26	-	73,73,73,73	2
87	MG	5	3603	1/1	0.97	0.24	-	38,38,38,38	0
87	MG	5	3505	1/1	0.96	0.23	-	52,52,52,52	0
87	MG	2	1906	1/1	0.79	0.17	-	67,67,67,67	0
87	MG	2	1945	1/1	0.88	0.38	-	90,90,90,90	0
87	MG	2	1912	1/1	0.68	0.47	-	88,88,88,88	0
87	MG	5	3644	1/1	0.83	0.29	-	43,43,43,43	0
87	MG	4	213	1/1	0.98	0.38	-	49,49,49,49	0
87	MG	5	3776	1/1	0.95	0.19	-	49,49,49,49	0
87	MG	5	3579	1/1	0.95	0.35	-	32,32,32,32	0
87	MG	1	3520	1/1	0.94	0.39	-	53,53,53,53	0
87	MG	2	1966	1/1	0.85	0.16	-	90,90,90,90	0
87	MG	1	3459	1/1	0.85	0.40	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	4074	7/7	0.94	0.32	-	53,53,53,53	4
87	MG	5	3652	1/1	0.97	0.29	-	44,44,44,44	0
88	OHX	5	3850	7/7	0.98	0.30	-	72,72,72,72	1
87	MG	5	3791	1/1	0.92	0.26	-	42,42,42,42	0
87	MG	6	2001	1/1	0.96	0.81	-	51,51,51,51	0
88	OHX	6	2079	7/7	0.97	0.22	-	52,52,52,52	4
87	MG	O7	103	1/1	0.91	0.84	-	55,55,55,55	1
87	MG	5	3746	1/1	0.92	0.17	-	59,59,59,59	0
88	OHX	2	2025	7/7	0.97	0.21	-	74,74,74,74	4
88	OHX	5	4156	7/7	0.89	0.25	-	78,78,78,78	7
88	OHX	5	3904	7/7	0.95	0.30	-	67,67,67,67	3
88	OHX	5	3891	7/7	0.99	0.20	-	60,60,60,60	3
87	MG	1	3484	1/1	0.77	0.37	-	81,81,81,81	0
88	OHX	2	2120	7/7	0.93	0.15	-	123,123,123,123	5
88	OHX	2	2145	7/7	0.89	0.19	-	88,88,88,88	3
88	OHX	5	4002	7/7	0.96	0.27	-	63,63,63,63	4
87	MG	5	3745	1/1	0.88	0.21	-	39,39,39,39	0
87	MG	6	1931	1/1	0.98	0.32	-	54,54,54,54	0
87	MG	2	1974	1/1	0.89	0.24	-	71,71,71,71	0
88	OHX	5	4125	7/7	0.90	0.25	-	51,51,51,51	3
88	OHX	5	4045	7/7	0.93	0.22	-	56,56,56,56	4
88	OHX	2	2060	7/7	0.93	0.19	-	73,73,73,73	1
87	MG	5	3621	1/1	0.57	0.55	-	99,99,99,99	0
87	MG	1	3442	1/1	0.96	0.33	-	45,45,45,45	0
87	MG	5	3538	1/1	0.86	0.27	-	45,45,45,45	0
88	OHX	5	4043	7/7	0.97	0.23	-	46,46,46,46	5
87	MG	5	3711	1/1	0.92	0.41	-	63,63,63,63	0
88	OHX	1	3881	7/7	0.97	0.30	-	60,60,60,60	1
87	MG	5	3663	1/1	0.91	0.43	-	84,84,84,84	0
88	OHX	2	2146	7/7	0.80	0.43	-	82,82,82,82	5
87	MG	5	3639	1/1	0.80	0.41	-	69,69,69,69	0
88	OHX	5	3944	7/7	0.97	0.24	-	50,50,50,50	4
87	MG	q1	701	1/1	0.92	0.15	-	52,52,52,52	0
87	MG	2	1905	1/1	0.82	0.19	-	65,65,65,65	0
87	MG	5	3668	1/1	0.73	0.29	-	64,64,64,64	0
88	OHX	5	4059	7/7	0.95	0.26	-	40,40,40,40	2
87	MG	5	3708	1/1	0.85	0.32	-	46,46,46,46	0
88	OHX	5	3902	7/7	0.98	0.19	-	39,39,39,39	3
87	MG	5	3646	1/1	0.93	0.24	-	38,38,38,38	0
88	OHX	5	3963	7/7	0.96	0.33	-	64,64,64,64	2
88	OHX	2	1999	7/7	0.97	0.22	-	104,104,104,104	2
88	OHX	5	3977	7/7	0.93	0.26	-	41,41,41,41	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3584	1/1	0.97	0.33	-	31,31,31,31	0
88	OHX	6	2085	7/7	0.98	0.16	-	69,69,69,69	2
87	MG	5	3616	1/1	0.84	0.26	-	63,63,63,63	0
87	MG	M7	201	1/1	0.73	0.45	-	73,73,73,73	0
87	MG	5	3550	1/1	0.90	0.31	-	37,37,37,37	0
88	OHX	1	4004	7/7	0.96	0.26	-	59,59,59,59	4
87	MG	1	3712	1/1	0.89	0.27	-	40,40,40,40	0
87	MG	1	3610	1/1	0.94	0.20	-	39,39,39,39	1
88	OHX	1	4071	7/7	0.92	0.26	-	40,40,40,40	4
87	MG	5	3623	1/1	0.70	0.65	-	95,95,95,95	0
88	OHX	6	2135	7/7	0.96	0.11	-	88,88,88,88	5
87	MG	2	1960	1/1	0.79	0.37	-	75,75,75,75	0
87	MG	2	1991	1/1	0.96	0.13	-	76,76,76,76	0
87	MG	5	3449	1/1	0.88	0.26	-	37,37,37,37	0
87	MG	5	3752	1/1	0.95	0.37	-	41,41,41,41	1
87	MG	1	3591	1/1	0.89	0.29	-	52,52,52,52	0
88	OHX	6	2132	7/7	0.98	0.15	-	61,61,61,61	5
88	OHX	5	3934	7/7	0.96	0.28	-	98,98,98,98	2
88	OHX	5	4127	7/7	0.91	0.30	-	45,45,45,45	5
87	MG	5	3727	1/1	0.95	0.36	-	46,46,46,46	1
87	MG	1	3691	1/1	0.88	0.30	-	65,65,65,65	0
87	MG	2	1946	1/1	0.87	0.34	-	66,66,66,66	0
87	MG	5	3779	1/1	0.92	0.26	-	51,51,51,51	0
87	MG	1	3510	1/1	0.98	0.27	-	36,36,36,36	0
87	MG	5	3605	1/1	0.87	0.32	-	56,56,56,56	0
88	OHX	4	225	7/7	0.98	0.19	-	57,57,57,57	3
88	OHX	1	3924	7/7	0.90	0.32	-	64,64,64,64	4
88	OHX	6	2131	7/7	0.96	0.26	-	53,53,53,53	4
88	OHX	1	4016	7/7	0.93	0.18	-	63,63,63,63	3
88	OHX	1	3852	7/7	0.98	0.21	-	79,79,79,79	2
87	MG	1	3675	1/1	0.69	0.36	-	65,65,65,65	0
87	MG	6	1959	1/1	0.81	0.22	-	80,80,80,80	0
88	OHX	6	2047	7/7	0.98	0.20	-	68,68,68,68	4
87	MG	6	1983	1/1	0.92	0.17	-	60,60,60,60	0
87	MG	5	3454	1/1	0.83	0.40	-	48,48,48,48	0
87	MG	5	3706	1/1	0.74	0.38	-	69,69,69,69	0
87	MG	5	3537	1/1	0.93	0.35	-	42,42,42,42	0
87	MG	5	3689	1/1	0.96	1.09	-	39,39,39,39	1
88	OHX	M7	205	7/7	0.92	0.29	-	57,57,57,57	5
87	MG	8	208	1/1	0.92	0.35	-	46,46,46,46	0
87	MG	5	3555	1/1	0.95	0.32	-	36,36,36,36	0
87	MG	1	3494	1/1	0.88	0.57	-	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	5	3755	1/1	0.73	0.17	-	64,64,64,64	0
88	OHX	5	3917	7/7	0.99	0.20	-	41,41,41,41	2
87	MG	2	1953	1/1	0.90	0.33	-	65,65,65,65	0
87	MG	5	3572	1/1	0.96	0.46	-	32,32,32,32	0
87	MG	S9	201	1/1	0.80	0.35	-	99,99,99,99	0
87	MG	1	3517	1/1	0.94	0.44	-	40,40,40,40	0
88	OHX	1	3791	7/7	0.98	0.27	-	58,58,58,58	3
87	MG	1	3417	1/1	0.88	0.26	-	50,50,50,50	0
87	MG	5	3527	1/1	0.96	0.27	-	39,39,39,39	0
87	MG	5	3705	1/1	0.86	0.24	-	50,50,50,50	0
88	OHX	5	4009	7/7	0.97	0.26	-	41,41,41,41	3
87	MG	3	201	1/1	0.95	0.37	-	71,71,71,71	0
87	MG	8	209	1/1	0.91	0.34	-	50,50,50,50	0
87	MG	SM	301	1/1	0.88	0.30	-	58,58,58,58	0
88	OHX	1	3799	7/7	0.98	0.25	-	61,61,61,61	1
87	MG	5	3488	1/1	0.87	0.40	-	34,34,34,34	0
88	OHX	5	3979	7/7	0.97	0.35	-	84,84,84,84	3
87	MG	1	3515	1/1	0.87	0.18	-	54,54,54,54	0
88	OHX	6	2165	7/7	0.85	0.22	-	119,119,119,119	7
87	MG	5	3685	1/1	0.87	0.25	-	44,44,44,44	0
87	MG	5	3507	1/1	0.96	0.45	-	37,37,37,37	0
87	MG	5	3624	1/1	0.92	0.34	-	41,41,41,41	0
88	OHX	6	2069	7/7	0.97	0.20	-	74,74,74,74	4
88	OHX	5	4119	7/7	0.92	0.30	-	51,51,51,51	4
87	MG	5	3733	1/1	0.92	0.44	-	39,39,39,39	0
87	MG	1	3585	1/1	0.98	0.28	-	45,45,45,45	0
88	OHX	s4	301	7/7	0.94	0.20	-	82,82,82,82	2
88	OHX	8	230	7/7	0.81	0.33	-	65,65,65,65	5
88	OHX	6	2168	7/7	0.91	0.25	-	72,72,72,72	3
88	OHX	5	4153	7/7	0.83	0.32	-	50,50,50,50	6
87	MG	3	205	1/1	0.93	0.50	-	60,60,60,60	0
88	OHX	5	3933	7/7	0.93	0.25	-	64,64,64,64	3
88	OHX	2	2151	7/7	0.87	0.28	-	109,109,109,109	6
87	MG	5	3618	1/1	0.91	0.20	-	56,56,56,56	0
88	OHX	5	4116	7/7	0.91	0.22	-	47,47,47,47	3
87	MG	2	1990	1/1	0.85	0.27	-	74,74,74,74	0
87	MG	1	3685	1/1	0.84	0.28	-	50,50,50,50	0
88	OHX	5	4145	7/7	0.92	0.29	-	47,47,47,47	4
87	MG	5	3638	1/1	0.93	0.28	-	41,41,41,41	0
88	OHX	5	4144	7/7	0.92	0.32	-	49,49,49,49	5
87	MG	5	3786	1/1	0.76	0.49	-	90,90,90,90	0
87	MG	1	3711	1/1	0.77	0.72	-	59,59,59,59	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3666	1/1	0.79	0.25	-	66,66,66,66	0
87	MG	5	3536	1/1	0.85	0.50	-	36,36,36,36	0
87	MG	1	3710	1/1	0.86	0.19	-	45,45,45,45	0
88	OHX	6	2178	7/7	0.94	0.16	-	97,97,97,97	5
87	MG	2	1993	1/1	0.84	0.11	-	76,76,76,76	0
87	MG	2	1902	1/1	0.81	0.24	-	59,59,59,59	0
88	OHX	5	3874	7/7	0.98	0.25	-	62,62,62,62	3
87	MG	5	3532	1/1	0.97	0.40	-	37,37,37,37	0
87	MG	1	3657	1/1	0.95	0.33	-	50,50,50,50	0
87	MG	O7	102	1/1	0.78	0.56	-	67,67,67,67	0
88	OHX	1	4026	7/7	0.96	0.21	-	51,51,51,51	2
87	MG	1	3631	1/1	0.92	0.39	-	79,79,79,79	0
88	OHX	5	4087	7/7	0.96	0.30	-	45,45,45,45	6
87	MG	1	3529	1/1	0.91	0.17	-	49,49,49,49	0
88	OHX	2	2018	7/7	0.98	0.19	-	83,83,83,83	3
87	MG	1	3435	1/1	0.96	0.46	-	35,35,35,35	0
88	OHX	1	3964	7/7	0.94	0.24	-	54,54,54,54	4
87	MG	5	3522	1/1	0.95	0.48	-	45,45,45,45	0
87	MG	1	3641	1/1	0.87	0.51	-	58,58,58,58	0
88	OHX	5	3990	7/7	0.92	0.28	-	80,80,80,80	3
87	MG	1	3564	1/1	0.93	0.47	-	47,47,47,47	0
87	MG	1	3755	1/1	0.94	0.28	-	53,53,53,53	0
87	MG	5	3455	1/1	0.98	0.17	-	45,45,45,45	0
87	MG	5	3512	1/1	0.96	0.13	-	40,40,40,40	0
87	MG	1	3447	1/1	0.97	0.24	-	41,41,41,41	0
88	OHX	2	2090	7/7	0.93	0.18	-	84,84,84,84	3
87	MG	2	1933	1/1	0.86	0.23	-	84,84,84,84	0
87	MG	6	1906	1/1	0.98	0.43	-	51,51,51,51	0
87	MG	5	3491	1/1	0.95	0.23	-	46,46,46,46	0
88	OHX	8	223	7/7	0.93	0.29	-	95,95,95,95	3
87	MG	1	3684	1/1	0.95	0.15	-	57,57,57,57	0
87	MG	1	3561	1/1	0.92	0.43	-	46,46,46,46	0
87	MG	5	3519	1/1	0.95	0.34	-	32,32,32,32	0
88	OHX	6	2046	7/7	0.98	0.21	-	60,60,60,60	3
87	MG	5	3629	1/1	0.98	0.27	-	43,43,43,43	0
87	MG	1	3746	1/1	0.86	0.29	-	56,56,56,56	0
87	MG	5	3661	1/1	0.93	0.34	-	43,43,43,43	0
87	MG	m7	203	1/1	0.95	0.30	-	35,35,35,35	0
87	MG	m6	201	1/1	0.90	0.36	-	42,42,42,42	0
87	MG	s8	301	1/1	0.74	0.31	-	63,63,63,63	0
87	MG	1	3756	1/1	0.94	0.16	-	54,54,54,54	0
87	MG	1	3426	1/1	0.94	0.42	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3671	1/1	0.87	0.14	-	47,47,47,47	0
88	OHX	5	3994	7/7	0.94	0.26	-	45,45,45,45	3
87	MG	1	3678	1/1	0.84	0.34	-	69,69,69,69	0
88	OHX	5	3941	7/7	0.98	0.17	-	60,60,60,60	1
88	OHX	6	2175	7/7	0.89	0.23	-	57,57,57,57	5
87	MG	5	3596	1/1	0.96	0.18	-	46,46,46,46	0
87	MG	5	3490	1/1	0.81	0.15	-	51,51,51,51	0
87	MG	6	1967	1/1	0.82	0.21	-	64,64,64,64	0
87	MG	1	3633	1/1	0.96	0.26	-	52,52,52,52	0
87	MG	7	202	1/1	0.95	0.42	-	26,26,26,26	0
87	MG	6	1948	1/1	0.93	0.20	-	55,55,55,55	0
87	MG	6	1971	1/1	0.98	0.22	-	56,56,56,56	0
88	OHX	2	2141	7/7	0.91	0.44	-	78,78,78,78	5
88	OHX	1	3849	7/7	0.99	0.18	-	65,65,65,65	2
88	OHX	6	2159	7/7	0.92	0.10	-	135,135,135,135	6
87	MG	5	3502	1/1	0.76	0.28	-	44,44,44,44	0
87	MG	4	203	1/1	0.83	0.40	-	52,52,52,52	0
87	MG	6	1956	1/1	0.95	0.34	-	61,61,61,61	0
87	MG	5	3496	1/1	0.98	0.28	-	38,38,38,38	0
88	OHX	5	4083	7/7	0.93	0.26	-	74,74,74,74	5
87	MG	5	3636	1/1	0.84	0.11	-	54,54,54,54	0
87	MG	1	3597	1/1	0.70	0.14	-	68,68,68,68	0
87	MG	2	1930	1/1	0.77	0.17	-	76,76,76,76	0
87	MG	6	1928	1/1	0.90	0.24	-	70,70,70,70	0
87	MG	5	3788	1/1	0.95	0.61	-	40,40,40,40	0
87	MG	1	3473	1/1	0.88	0.36	-	58,58,58,58	0
87	MG	1	3612	1/1	0.95	0.11	-	58,58,58,58	0
87	MG	5	3441	1/1	0.99	0.34	-	35,35,35,35	0
88	OHX	5	4027	7/7	0.95	0.20	-	45,45,45,45	4
87	MG	1	3504	1/1	0.93	0.23	-	42,42,42,42	0
88	OHX	6	2075	7/7	0.96	0.19	-	71,71,71,71	2
87	MG	5	3489	1/1	0.96	0.33	-	40,40,40,40	0
87	MG	5	3528	1/1	0.94	0.24	-	34,34,34,34	0
88	OHX	4	232	7/7	0.94	0.24	-	45,45,45,45	4
88	OHX	6	2139	7/7	0.93	0.21	-	91,91,91,91	4
87	MG	5	3446	1/1	0.83	0.33	-	43,43,43,43	0
88	OHX	3	218	7/7	0.91	0.28	-	49,49,49,49	4
88	OHX	6	2127	7/7	0.89	0.21	-	98,98,98,98	5
88	OHX	2	2020	7/7	0.95	0.23	-	73,73,73,73	4
87	MG	5	3474	1/1	0.95	0.17	-	39,39,39,39	0
87	MG	2	1907	1/1	0.94	0.36	-	65,65,65,65	0
87	MG	5	3647	1/1	0.94	0.23	-	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	L3	401	1/1	0.96	0.19	-	41,41,41,41	0
88	OHX	6	2110	7/7	0.89	0.26	-	65,65,65,65	3
87	MG	5	3437	1/1	0.94	0.30	-	33,33,33,33	0
88	OHX	2	2021	7/7	0.98	0.18	-	71,71,71,71	4
87	MG	7	203	1/1	0.97	0.39	-	57,57,57,57	0
87	MG	5	3738	1/1	0.87	0.19	-	51,51,51,51	0
88	OHX	5	4075	7/7	0.94	0.20	-	49,49,49,49	3
87	MG	1	3542	1/1	0.96	0.31	-	36,36,36,36	0
87	MG	1	3544	1/1	0.99	0.10	-	58,58,58,58	0
87	MG	1	3652	1/1	0.88	0.27	-	46,46,46,46	0
88	OHX	5	3916	7/7	0.98	0.23	-	90,90,90,90	5
87	MG	1	3530	1/1	0.79	0.38	-	63,63,63,63	0
87	MG	2	1967	1/1	0.26	0.47	-	130,130,130,130	0
87	MG	1	3581	1/1	0.91	0.21	-	42,42,42,42	0
87	MG	1	3538	1/1	0.93	0.42	-	46,46,46,46	0
87	MG	1	3741	1/1	0.87	0.29	-	46,46,46,46	0
88	OHX	2	2112	7/7	0.95	0.15	-	103,103,103,103	6
87	MG	5	3453	1/1	0.93	0.24	-	38,38,38,38	0
88	OHX	1	3836	7/7	0.99	0.30	-	78,78,78,78	3
87	MG	5	3792	1/1	0.82	0.33	-	44,44,44,44	1
87	MG	5	3608	1/1	0.87	0.12	-	47,47,47,47	0
88	OHX	1	4015	7/7	0.89	0.28	-	52,52,52,52	4
87	MG	5	3725	1/1	0.87	0.26	-	53,53,53,53	0
87	MG	5	3434	1/1	0.93	0.30	-	44,44,44,44	0
87	MG	6	1921	1/1	0.85	0.22	-	71,71,71,71	0
87	MG	6	1941	1/1	0.97	0.43	-	47,47,47,47	0
88	OHX	1	3906	7/7	0.95	0.19	-	59,59,59,59	2
88	OHX	1	4011	7/7	0.86	0.26	-	117,117,117,117	4
88	OHX	5	4136	7/7	0.82	0.35	-	85,85,85,85	6
88	OHX	1	3904	7/7	0.94	0.22	-	55,55,55,55	3
88	OHX	2	2071	7/7	0.95	0.25	-	104,104,104,104	5
87	MG	1	3629	1/1	0.87	0.24	-	52,52,52,52	0
88	OHX	1	3990	7/7	0.88	0.25	-	80,80,80,80	4
87	MG	5	3492	1/1	0.93	0.30	-	46,46,46,46	0
87	MG	5	3757	1/1	0.69	0.23	-	59,59,59,59	0
87	MG	5	3697	1/1	0.95	0.38	-	40,40,40,40	0
88	OHX	2	2057	7/7	0.91	0.20	-	96,96,96,96	3
87	MG	1	3625	1/1	0.90	0.20	-	56,56,56,56	0
88	OHX	2	2089	7/7	0.97	0.18	-	88,88,88,88	3
88	OHX	5	4155	7/7	0.88	0.24	-	58,58,58,58	4
87	MG	6	1989	1/1	0.76	0.26	-	81,81,81,81	0
88	OHX	1	3790	7/7	0.99	0.24	-	77,77,77,77	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3682	1/1	0.92	0.39	-	50,50,50,50	0
87	MG	N3	202	1/1	0.57	0.19	-	65,65,65,65	0
87	MG	5	3577	1/1	0.87	0.49	-	39,39,39,39	0
88	OHX	1	3981	7/7	0.96	0.24	-	49,49,49,49	3
88	OHX	1	4089	7/7	0.91	0.34	-	63,63,63,63	3
87	MG	7	207	1/1	0.83	0.36	-	40,40,40,40	0
88	OHX	1	3996	7/7	0.98	0.23	-	55,55,55,55	5
87	MG	1	3423	1/1	0.81	0.26	-	49,49,49,49	0
87	MG	7	214	1/1	0.84	0.28	-	66,66,66,66	0
88	OHX	6	2121	7/7	0.97	0.16	-	89,89,89,89	5
87	MG	1	3638	1/1	0.86	0.40	-	69,69,69,69	0
87	MG	5	3476	1/1	0.82	0.15	-	46,46,46,46	0
87	MG	6	2005	1/1	0.81	0.64	-	72,72,72,72	0
87	MG	2	1932	1/1	0.94	0.15	-	78,78,78,78	0
88	OHX	1	3958	7/7	0.96	0.25	-	47,47,47,47	4
87	MG	5	3588	1/1	0.98	0.29	-	37,37,37,37	0
88	OHX	5	3956	7/7	0.96	0.28	-	81,81,81,81	3
88	OHX	5	3859	7/7	0.99	0.20	-	58,58,58,58	1
87	MG	1	3402	1/1	0.85	0.39	-	53,53,53,53	0
88	OHX	5	4132	7/7	0.81	0.28	-	72,72,72,72	5
87	MG	1	3539	1/1	0.94	0.30	-	45,45,45,45	0
87	MG	1	3409	1/1	0.98	0.36	-	37,37,37,37	0
88	OHX	5	4050	7/7	0.93	0.21	-	39,39,39,39	4
87	MG	1	3723	1/1	0.80	0.21	-	70,70,70,70	0
87	MG	5	3739	1/1	0.70	0.35	-	63,63,63,63	0
87	MG	1	3702	1/1	0.88	0.45	-	42,42,42,42	0
87	MG	6	2012	1/1	0.77	0.14	-	72,72,72,72	0
88	OHX	2	2140	7/7	0.92	0.52	-	65,65,65,65	4
87	MG	5	3620	1/1	0.93	0.40	-	44,44,44,44	0
88	OHX	1	3809	7/7	0.97	0.28	-	77,77,77,77	3
87	MG	1	3411	1/1	0.88	0.24	-	46,46,46,46	0
88	OHX	5	4077	7/7	0.96	0.28	-	53,53,53,53	5
87	MG	5	3732	1/1	0.94	0.11	-	49,49,49,49	0
88	OHX	2	2119	7/7	0.87	0.23	-	84,84,84,84	3
87	MG	5	3479	1/1	0.91	0.24	-	54,54,54,54	0
88	OHX	5	3816	7/7	0.99	0.24	-	69,69,69,69	1
87	MG	6	1996	1/1	0.93	0.36	-	60,60,60,60	0
87	MG	6	1929	1/1	0.96	0.29	-	68,68,68,68	0
88	OHX	1	3814	7/7	0.98	0.24	-	76,76,76,76	5
87	MG	5	3787	1/1	0.95	0.15	-	42,42,42,42	0
87	MG	6	1935	1/1	0.96	0.35	-	50,50,50,50	0
87	MG	1	3650	1/1	0.98	0.14	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3521	1/1	0.93	0.51	-	43,43,43,43	0
88	OHX	5	3980	7/7	0.97	0.28	-	54,54,54,54	3
88	OHX	6	2124	7/7	0.91	0.42	-	81,81,81,81	4
88	OHX	c3	201	7/7	0.92	0.19	-	89,89,89,89	3
87	MG	6	1946	1/1	0.95	0.30	-	48,48,48,48	0
87	MG	5	3450	1/1	0.89	0.34	-	48,48,48,48	0
87	MG	4	218	1/1	0.77	0.28	-	41,41,41,41	0
87	MG	1	3439	1/1	0.89	0.42	-	55,55,55,55	0
88	OHX	8	229	7/7	0.83	0.28	-	49,49,49,49	4
88	OHX	6	2113	7/7	0.94	0.17	-	66,66,66,66	2
87	MG	5	3778	1/1	0.92	0.24	-	64,64,64,64	0
87	MG	5	3443	1/1	0.89	0.17	-	46,46,46,46	0
88	OHX	5	4115	7/7	0.96	0.21	-	92,92,92,92	2
87	MG	1	3489	1/1	0.98	0.24	-	44,44,44,44	0
87	MG	5	3650	1/1	0.93	0.47	-	43,43,43,43	0
87	MG	L6	201	1/1	0.81	0.26	-	53,53,53,53	0
87	MG	l5	301	1/1	0.84	0.36	-	56,56,56,56	0
87	MG	1	3698	1/1	0.90	0.41	-	57,57,57,57	0
88	OHX	6	2048	7/7	0.99	0.21	-	64,64,64,64	2
87	MG	6	1957	1/1	0.93	0.52	-	65,65,65,65	0
87	MG	n8	201	1/1	0.93	0.20	-	34,34,34,34	0
87	MG	1	3665	1/1	0.84	0.28	-	63,63,63,63	0
88	OHX	1	4070	7/7	0.86	0.22	-	71,71,71,71	4
88	OHX	1	3926	7/7	0.95	0.26	-	50,50,50,50	3
87	MG	4	217	1/1	0.61	0.26	-	60,60,60,60	0
87	MG	2	1970	1/1	0.70	0.20	-	91,91,91,91	0
88	OHX	5	3872	7/7	0.96	0.33	-	71,71,71,71	3
88	OHX	1	3796	7/7	0.99	0.31	-	77,77,77,77	3
88	OHX	5	4052	7/7	0.92	0.20	-	58,58,58,58	5
87	MG	1	3595	1/1	0.96	0.35	-	45,45,45,45	0
87	MG	8	207	1/1	0.82	0.19	-	50,50,50,50	0
87	MG	1	3421	1/1	0.80	0.30	-	44,44,44,44	0
87	MG	5	3704	1/1	0.93	0.42	-	44,44,44,44	0
87	MG	5	3773	1/1	0.90	0.53	-	40,40,40,40	0
88	OHX	5	3943	7/7	0.97	0.21	-	69,69,69,69	2
88	OHX	5	4099	7/7	0.83	0.24	-	75,75,75,75	5
87	MG	5	3686	1/1	0.92	0.15	-	40,40,40,40	0
88	OHX	7	226	7/7	0.90	0.36	-	61,61,61,61	4
87	MG	1	3708	1/1	0.82	0.25	-	50,50,50,50	0
87	MG	1	3566	1/1	0.95	0.45	-	53,53,53,53	0
87	MG	5	3781	1/1	0.89	0.65	-	56,56,56,56	0
87	MG	3	206	1/1	0.85	0.19	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3463	1/1	0.91	0.25	-	56,56,56,56	0
88	OHX	5	3952	7/7	0.99	0.21	-	45,45,45,45	3
88	OHX	5	4158	7/7	0.85	0.19	-	49,49,49,49	1
87	MG	L7	303	1/1	0.95	0.14	-	51,51,51,51	0
88	OHX	6	2096	7/7	0.98	0.14	-	86,86,86,86	5
88	OHX	1	4091	7/7	0.93	0.40	-	44,44,44,44	5
87	MG	d3	201	1/1	0.80	0.19	-	60,60,60,60	0
87	MG	1	3651	1/1	0.96	0.19	-	58,58,58,58	0
88	OHX	5	4098	7/7	0.91	0.18	-	74,74,74,74	6
87	MG	7	206	1/1	0.89	0.52	-	54,54,54,54	0
87	MG	2	1920	1/1	0.95	0.27	-	61,61,61,61	0
87	MG	1	3514	1/1	0.97	0.35	-	35,35,35,35	0
88	OHX	2	2052	7/7	0.90	0.18	-	94,94,94,94	3
87	MG	1	3644	1/1	0.85	0.21	-	51,51,51,51	0
88	OHX	1	4029	7/7	0.92	0.22	-	51,51,51,51	3
87	MG	6	1903	1/1	0.96	0.15	-	53,53,53,53	0
87	MG	2	1958	1/1	0.95	0.11	-	70,70,70,70	0
87	MG	6	1917	1/1	0.62	0.44	-	78,78,78,78	0
87	MG	5	3741	1/1	0.92	0.21	-	39,39,39,39	0
88	OHX	5	3988	7/7	0.93	0.28	-	54,54,54,54	2
87	MG	4	211	1/1	0.89	0.36	-	66,66,66,66	0
88	OHX	m9	201	7/7	0.85	0.21	-	61,61,61,61	4
87	MG	5	3460	1/1	0.99	0.38	-	34,34,34,34	0
87	MG	6	1912	1/1	0.76	0.26	-	59,59,59,59	0
87	MG	1	3462	1/1	0.86	0.38	-	50,50,50,50	0
87	MG	1	3588	1/1	0.96	0.28	-	55,55,55,55	0
88	OHX	4	233	7/7	0.92	0.33	-	63,63,63,63	2
88	OHX	1	3965	7/7	0.89	0.24	-	64,64,64,64	5
88	OHX	1	4043	7/7	0.90	0.18	-	125,125,125,125	6
88	OHX	5	4091	7/7	0.75	0.38	-	34,34,34,34	4
87	MG	1	3745	1/1	0.85	0.23	-	47,47,47,47	0
87	MG	1	3472	1/1	0.94	0.36	-	58,58,58,58	0
87	MG	1	3480	1/1	0.96	0.17	-	55,55,55,55	0
87	MG	2	1975	1/1	0.61	0.17	-	74,74,74,74	0
88	OHX	1	3991	7/7	0.95	0.40	-	88,88,88,88	5
88	OHX	1	4088	7/7	0.88	0.28	-	58,58,58,58	7
87	MG	2	1909	1/1	0.74	0.33	-	84,84,84,84	0
87	MG	5	3478	1/1	0.93	0.37	-	58,58,58,58	0
88	OHX	6	2017	7/7	0.98	0.23	-	79,79,79,79	5
87	MG	1	3506	1/1	0.90	0.30	-	51,51,51,51	0
87	MG	5	3634	1/1	0.95	0.24	-	47,47,47,47	0
87	MG	2	1982	1/1	0.98	0.07	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3513	1/1	0.96	0.30	-	48,48,48,48	0
87	MG	1	3705	1/1	0.92	0.23	-	48,48,48,48	0
87	MG	N8	202	1/1	0.93	0.33	-	44,44,44,44	0
87	MG	5	3465	1/1	0.89	0.29	-	36,36,36,36	0
87	MG	7	213	1/1	0.78	0.48	-	60,60,60,60	0
87	MG	1	3543	1/1	0.97	0.27	-	36,36,36,36	0
87	MG	1	3752	1/1	0.91	0.13	-	51,51,51,51	0
87	MG	5	3674	1/1	0.88	0.28	-	50,50,50,50	0
88	OHX	1	4027	7/7	0.84	0.33	-	50,50,50,50	4
87	MG	5	3790	1/1	0.78	0.27	-	70,70,70,70	0
87	MG	5	3687	1/1	0.93	0.25	-	47,47,47,47	0
87	MG	6	1952	1/1	0.92	0.33	-	58,58,58,58	0
87	MG	5	3737	1/1	0.79	0.16	-	51,51,51,51	0
87	MG	1	3589	1/1	0.94	0.17	-	53,53,53,53	0
88	OHX	2	2083	7/7	0.95	0.17	-	100,100,100,100	6
87	MG	f	1002	1/1	0.97	0.22	-	58,58,58,58	0
87	MG	4	216	1/1	0.82	0.17	-	65,65,65,65	0
87	MG	5	3666	1/1	0.83	0.23	-	39,39,39,39	0
87	MG	6	2007	1/1	0.69	0.56	-	100,100,100,100	0
87	MG	1	3419	1/1	0.88	0.32	-	47,47,47,47	0
87	MG	2	1903	1/1	0.87	0.14	-	59,59,59,59	0
88	OHX	6	2080	7/7	0.94	0.25	-	76,76,76,76	2
87	MG	1	3676	1/1	0.95	0.72	-	49,49,49,49	0
88	OHX	1	3916	7/7	0.96	0.23	-	45,45,45,45	2
87	MG	8	205	1/1	0.92	0.22	-	45,45,45,45	0
87	MG	5	3542	1/1	0.87	0.26	-	38,38,38,38	0
88	OHX	1	3957	7/7	0.97	0.19	-	48,48,48,48	3
87	MG	o4	201	1/1	0.79	0.26	-	50,50,50,50	0
87	MG	5	3672	1/1	0.86	0.19	-	48,48,48,48	0
87	MG	1	3697	1/1	0.85	0.45	-	56,56,56,56	0
87	MG	5	3569	1/1	0.68	0.37	-	40,40,40,40	0
87	MG	5	3758	1/1	0.94	0.43	-	58,58,58,58	0
87	MG	1	3593	1/1	0.88	0.22	-	48,48,48,48	0
87	MG	5	3480	1/1	0.98	0.32	-	44,44,44,44	0
87	MG	2	1934	1/1	0.88	0.37	-	93,93,93,93	0
87	MG	5	3436	1/1	0.95	0.24	-	46,46,46,46	0
87	MG	5	3664	1/1	0.84	0.21	-	44,44,44,44	0
87	MG	1	3646	1/1	0.87	0.40	-	41,41,41,41	0
88	OHX	2	2109	7/7	0.94	0.25	-	73,73,73,73	4
87	MG	1	3558	1/1	0.98	0.18	-	38,38,38,38	0
88	OHX	5	4018	7/7	0.95	0.28	-	87,87,87,87	4
87	MG	5	3560	1/1	0.96	0.43	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	2	1913	1/1	0.87	0.29	-	69,69,69,69	0
88	OHX	6	2134	7/7	0.88	0.18	-	88,88,88,88	6
87	MG	5	3645	1/1	0.87	0.27	-	48,48,48,48	0
88	OHX	6	2156	7/7	0.92	0.21	-	62,62,62,62	4
88	OHX	1	3861	7/7	0.97	0.32	-	99,99,99,99	3
88	OHX	1	3955	7/7	0.98	0.28	-	100,100,100,100	2
87	MG	7	211	1/1	0.88	0.26	-	52,52,52,52	0
87	MG	2	1955	1/1	0.93	0.37	-	78,78,78,78	0
87	MG	1	3681	1/1	0.77	0.30	-	54,54,54,54	0
88	OHX	2	2044	7/7	0.96	0.16	-	130,130,130,130	7
88	OHX	5	3885	7/7	0.98	0.24	-	42,42,42,42	3
87	MG	5	3563	1/1	0.87	0.42	-	45,45,45,45	0
87	MG	5	3736	1/1	0.74	0.42	-	80,80,80,80	0
87	MG	2	1904	1/1	0.86	0.53	-	75,75,75,75	0
87	MG	5	3693	1/1	0.85	0.26	-	47,47,47,47	0
87	MG	5	3660	1/1	0.92	0.15	-	50,50,50,50	0
88	OHX	1	3988	7/7	0.96	0.27	-	68,68,68,68	3
88	OHX	2	2127	7/7	0.88	0.15	-	146,146,146,146	6
87	MG	5	3415	1/1	0.93	0.55	-	55,55,55,55	0
88	OHX	2	2132	7/7	0.93	0.23	-	81,81,81,81	5
88	OHX	m7	204	7/7	0.81	0.42	-	50,50,50,50	4
88	OHX	1	4074	7/7	0.91	0.20	-	156,156,156,156	7
87	MG	2	1927	1/1	0.96	0.29	-	95,95,95,95	0
87	MG	1	3461	1/1	0.92	0.26	-	46,46,46,46	0
87	MG	2	1978	1/1	0.85	0.24	-	58,58,58,58	0
87	MG	5	3554	1/1	0.92	0.35	-	47,47,47,47	0
87	MG	1	3598	1/1	0.78	0.40	-	70,70,70,70	0
88	OHX	5	4159	7/7	0.81	0.17	-	162,162,162,162	7
87	MG	5	3676	1/1	0.84	0.29	-	62,62,62,62	0
88	OHX	l3	403	7/7	0.99	0.19	-	47,47,47,47	2
87	MG	2	1962	1/1	0.86	0.20	-	66,66,66,66	0
87	MG	5	3401	1/1	0.93	0.19	-	42,42,42,42	0
87	MG	5	3692	1/1	0.88	0.18	-	59,59,59,59	0
87	MG	1	3437	1/1	0.89	0.18	-	51,51,51,51	0
87	MG	5	3421	1/1	0.80	0.39	-	63,63,63,63	0
87	MG	1	3490	1/1	0.95	0.38	-	40,40,40,40	0
87	MG	5	3695	1/1	0.95	0.22	-	39,39,39,39	0
87	MG	5	3756	1/1	0.88	0.42	-	39,39,39,39	0
87	MG	5	3493	1/1	0.92	0.20	-	38,38,38,38	0
88	OHX	5	3991	7/7	0.92	0.32	-	96,96,96,96	4
87	MG	1	3454	1/1	0.92	0.27	-	43,43,43,43	0
87	MG	2	1957	1/1	0.88	0.14	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	6	2117	7/7	0.89	0.24	-	94,94,94,94	5
87	MG	5	3655	1/1	0.92	0.19	-	42,42,42,42	0
87	MG	5	3499	1/1	0.83	0.22	-	50,50,50,50	0
87	MG	5	3461	1/1	0.95	0.51	-	48,48,48,48	0
88	OHX	6	2016	7/7	0.99	0.22	-	83,83,83,83	4
87	MG	6	1999	1/1	0.88	0.29	-	57,57,57,57	0
87	MG	1	3404	1/1	0.93	0.21	-	60,60,60,60	0
88	OHX	5	4146	7/7	0.91	0.26	-	39,39,39,39	2
88	OHX	2	2130	7/7	0.93	0.18	-	103,103,103,103	7
87	MG	5	3575	1/1	0.91	0.48	-	42,42,42,42	0
87	MG	5	3760	1/1	0.90	0.31	-	48,48,48,48	0
88	OHX	6	2163	7/7	0.94	0.20	-	62,62,62,62	7
88	OHX	1	3946	7/7	0.97	0.19	-	56,56,56,56	3
87	MG	6	1943	1/1	0.93	0.51	-	51,51,51,51	0
88	OHX	5	4141	7/7	0.96	0.23	-	74,74,74,74	3
87	MG	1	3604	1/1	0.70	0.64	-	90,90,90,90	0
88	OHX	1	3973	7/7	0.97	0.26	-	52,52,52,52	3
87	MG	5	3730	1/1	0.85	0.28	-	44,44,44,44	0
88	OHX	6	2054	7/7	0.99	0.21	-	89,89,89,89	2
88	OHX	6	2169	7/7	0.91	0.16	-	61,61,61,61	5
88	OHX	6	2180	7/7	0.84	0.13	-	137,137,137,137	6
87	MG	f	1001	1/1	0.99	0.41	-	42,42,42,42	0
87	MG	6	1932	1/1	0.83	0.20	-	60,60,60,60	0
87	MG	6	1991	1/1	0.71	0.29	-	65,65,65,65	0
87	MG	1	3456	1/1	0.89	0.38	-	33,33,33,33	0
87	MG	5	3444	1/1	0.89	0.49	-	55,55,55,55	0
87	MG	1	3488	1/1	0.96	0.33	-	46,46,46,46	0
87	MG	5	3574	1/1	0.97	0.37	-	41,41,41,41	0
87	MG	5	3648	1/1	0.73	0.26	-	55,55,55,55	0
88	OHX	1	4056	7/7	0.87	0.27	-	74,74,74,74	4
87	MG	6	1995	1/1	0.82	0.44	-	67,67,67,67	0
88	OHX	1	3910	7/7	0.96	0.20	-	75,75,75,75	3
87	MG	2	1925	1/1	0.29	0.33	-	99,99,99,99	0
88	OHX	5	4063	7/7	0.95	0.21	-	54,54,54,54	2
88	OHX	1	3997	7/7	0.94	0.33	-	49,49,49,49	2
87	MG	1	3432	1/1	0.97	0.14	-	51,51,51,51	0
88	OHX	1	4102	7/7	0.85	0.30	-	58,58,58,58	2
87	MG	1	3630	1/1	0.96	0.13	-	40,40,40,40	0
87	MG	1	3728	1/1	0.95	0.26	-	75,75,75,75	0
87	MG	5	3452	1/1	0.94	0.26	-	35,35,35,35	0
87	MG	5	3701	1/1	0.67	0.26	-	48,48,48,48	0
87	MG	5	3530	1/1	0.94	0.32	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3632	1/1	0.90	0.29	-	51,51,51,51	0
87	MG	5	3789	1/1	0.78	0.23	-	59,59,59,59	0
88	OHX	4	228	7/7	0.96	0.26	-	96,96,96,96	3
87	MG	1	3545	1/1	0.91	0.29	-	42,42,42,42	0
88	OHX	6	2097	7/7	0.95	0.18	-	97,97,97,97	3
88	OHX	2	2063	7/7	0.98	0.15	-	80,80,80,80	4
88	OHX	5	3989	7/7	0.95	0.26	-	48,48,48,48	3
87	MG	6	1997	1/1	0.87	0.40	-	122,122,122,122	0
88	OHX	4	223	7/7	0.95	0.27	-	67,67,67,67	3
88	OHX	6	2120	7/7	0.91	0.23	-	84,84,84,84	5
87	MG	2	1935	1/1	0.93	0.43	-	67,67,67,67	0
87	MG	5	3404	1/1	0.93	0.38	-	35,35,35,35	0
87	MG	1	3639	1/1	0.97	0.17	-	58,58,58,58	0
87	MG	5	3691	1/1	0.78	0.30	-	52,52,52,52	0
87	MG	5	3539	1/1	0.95	0.34	-	29,29,29,29	0
87	MG	1	3443	1/1	0.80	0.36	-	36,36,36,36	0
87	MG	1	3654	1/1	0.89	0.22	-	56,56,56,56	0
88	OHX	1	3868	7/7	0.97	0.27	-	68,68,68,68	3
87	MG	1	3753	1/1	0.91	0.28	-	64,64,64,64	0
88	OHX	1	3832	7/7	0.98	0.31	-	88,88,88,88	3
87	MG	5	3643	1/1	0.89	0.12	-	60,60,60,60	0
87	MG	1	3600	1/1	0.96	0.28	-	48,48,48,48	0
87	MG	5	3678	1/1	0.91	0.22	-	52,52,52,52	0
88	OHX	1	3976	7/7	0.89	0.28	-	83,83,83,83	4
87	MG	5	3649	1/1	0.98	0.17	-	47,47,47,47	0
88	OHX	2	2085	7/7	0.95	0.19	-	83,83,83,83	3
87	MG	2	1948	1/1	0.93	0.19	-	66,66,66,66	0
88	OHX	3	216	7/7	0.91	0.31	-	62,62,62,62	3
87	MG	1	3424	1/1	0.94	0.12	-	61,61,61,61	0
87	MG	1	3717	1/1	0.43	0.26	-	61,61,61,61	0
87	MG	6	1916	1/1	0.96	0.16	-	71,71,71,71	0
87	MG	5	3722	1/1	0.75	0.71	-	46,46,46,46	1
88	OHX	1	3811	7/7	0.99	0.26	-	58,58,58,58	3
87	MG	1	3693	1/1	0.93	0.29	-	53,53,53,53	0
87	MG	1	3672	1/1	0.94	0.23	-	68,68,68,68	0
87	MG	5	3764	1/1	0.92	0.45	-	110,110,110,110	0
87	MG	1	3750	1/1	0.83	0.28	-	55,55,55,55	0
88	OHX	5	4129	7/7	0.89	0.26	-	58,58,58,58	3
88	OHX	5	4118	7/7	0.91	0.24	-	67,67,67,67	5
87	MG	5	3462	1/1	0.89	0.16	-	39,39,39,39	0
87	MG	1	3640	1/1	0.98	0.50	-	66,66,66,66	0
87	MG	4	201	1/1	0.84	0.51	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3634	1/1	0.92	0.31	-	60,60,60,60	0
87	MG	1	3569	1/1	0.92	0.50	-	35,35,35,35	0
87	MG	1	3719	1/1	0.66	0.29	-	58,58,58,58	0
87	MG	5	3609	1/1	0.91	0.24	-	38,38,38,38	0
87	MG	5	3726	1/1	0.89	0.24	-	47,47,47,47	0
87	MG	1	3725	1/1	0.96	0.26	-	43,43,43,43	0
87	MG	1	3563	1/1	0.86	0.46	-	40,40,40,40	0
87	MG	5	3439	1/1	0.92	0.31	-	46,46,46,46	0
87	MG	5	3742	1/1	0.80	0.35	-	61,61,61,61	0
87	MG	6	1979	1/1	0.74	0.19	-	54,54,54,54	0
87	MG	7	204	1/1	0.93	0.42	-	46,46,46,46	0
88	OHX	1	3867	7/7	0.98	0.23	-	84,84,84,84	3
88	OHX	C3	201	7/7	0.90	0.26	-	94,94,94,94	3
87	MG	M8	201	1/1	0.60	0.42	-	51,51,51,51	0
87	MG	5	3521	1/1	0.94	0.34	-	45,45,45,45	0
87	MG	1	3714	1/1	0.89	0.26	-	46,46,46,46	0
87	MG	1	3482	1/1	0.94	0.29	-	51,51,51,51	0
87	MG	1	3608	1/1	0.94	0.14	-	49,49,49,49	0
87	MG	5	3599	1/1	0.89	0.20	-	42,42,42,42	0
87	MG	2	1983	1/1	0.93	0.20	-	71,71,71,71	0
87	MG	1	3658	1/1	0.93	0.28	-	43,43,43,43	0
87	MG	5	3442	1/1	0.92	0.27	-	36,36,36,36	0
87	MG	1	3648	1/1	0.97	0.15	-	46,46,46,46	0
87	MG	5	3765	1/1	0.97	0.15	-	47,47,47,47	0
88	OHX	1	3908	7/7	0.93	0.26	-	80,80,80,80	2
87	MG	1	3635	1/1	0.78	0.31	-	61,61,61,61	0
87	MG	1	3405	1/1	0.76	0.70	-	118,118,118,118	0
87	MG	1	3467	1/1	0.91	0.27	-	54,54,54,54	0
87	MG	6	1993	1/1	0.84	0.27	-	56,56,56,56	0
88	OHX	5	4080	7/7	0.95	0.19	-	111,111,111,111	4
87	MG	2	1928	1/1	0.95	0.32	-	74,74,74,74	0
87	MG	6	1973	1/1	0.75	0.38	-	102,102,102,102	0
87	MG	N8	204	1/1	0.85	0.20	-	56,56,56,56	0
87	MG	1	3716	1/1	0.86	0.32	-	44,44,44,44	0
87	MG	5	3456	1/1	0.94	0.19	-	40,40,40,40	0
88	OHX	2	2053	7/7	0.92	0.19	-	120,120,120,120	5
88	OHX	5	4056	7/7	0.96	0.23	-	49,49,49,49	5
87	MG	5	3615	1/1	0.84	0.17	-	35,35,35,35	0
87	MG	5	3654	1/1	0.98	0.28	-	33,33,33,33	0
87	MG	5	3458	1/1	0.92	0.31	-	39,39,39,39	0
88	OHX	1	4072	7/7	0.82	0.24	-	68,68,68,68	5
87	MG	6	1902	1/1	0.94	0.12	-	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	3734	1/1	0.73	0.69	-	93,93,93,93	0
87	MG	5	3749	1/1	0.58	0.27	-	70,70,70,70	0
87	MG	1	3500	1/1	0.90	0.43	-	40,40,40,40	0
87	MG	6	1998	1/1	0.78	0.20	-	55,55,55,55	0
87	MG	2	1918	1/1	0.83	0.26	-	65,65,65,65	0
87	MG	4	204	1/1	0.91	0.43	-	48,48,48,48	0
87	MG	1	3469	1/1	0.94	0.35	-	63,63,63,63	0
88	OHX	M9	201	7/7	0.86	0.15	-	75,75,75,75	3
88	OHX	1	3813	7/7	0.99	0.22	-	54,54,54,54	1
88	OHX	6	2181	7/7	0.72	0.79	-	92,92,92,92	5
87	MG	4	202	1/1	0.93	0.41	-	53,53,53,53	0
87	MG	6	1963	1/1	0.95	0.19	-	89,89,89,89	0
87	MG	2	1952	1/1	0.92	0.16	-	71,71,71,71	0
87	MG	5	3495	1/1	0.91	0.20	-	34,34,34,34	0
88	OHX	6	2155	7/7	0.91	0.14	-	108,108,108,108	5
87	MG	1	3730	1/1	0.89	0.19	-	72,72,72,72	0
88	OHX	1	4082	7/7	0.84	0.39	-	44,44,44,44	4
87	MG	q0	202	1/1	0.88	0.41	-	50,50,50,50	0
87	MG	5	3724	1/1	0.87	0.24	-	44,44,44,44	0
87	MG	5	3721	1/1	0.86	0.21	-	54,54,54,54	0
87	MG	2	1976	1/1	0.75	0.18	-	75,75,75,75	0
87	MG	1	3436	1/1	0.90	0.24	-	40,40,40,40	0
87	MG	1	3696	1/1	0.80	0.23	-	62,62,62,62	0
88	OHX	c8	201	7/7	0.95	0.22	-	94,94,94,94	5
88	OHX	5	4151	7/7	0.83	0.36	-	60,60,60,60	6
87	MG	f	1003	1/1	0.78	0.20	-	50,50,50,50	0
87	MG	6	1924	1/1	0.53	0.61	-	84,84,84,84	0
88	OHX	1	3954	7/7	0.96	0.25	-	54,54,54,54	3
87	MG	5	3403	1/1	0.95	0.39	-	41,41,41,41	0
87	MG	5	3657	1/1	0.80	0.21	-	42,42,42,42	0
88	OHX	1	4085	7/7	0.88	0.31	-	42,42,42,42	3
87	MG	2	1980	1/1	0.79	0.26	-	89,89,89,89	0
88	OHX	1	4038	7/7	0.88	0.27	-	83,83,83,83	4
87	MG	6	1947	1/1	0.94	0.21	-	58,58,58,58	0
88	OHX	1	3805	7/7	0.99	0.24	-	60,60,60,60	3
87	MG	5	3586	1/1	0.96	0.38	-	31,31,31,31	0
88	OHX	5	3960	7/7	0.98	0.25	-	108,108,108,108	4
87	MG	6	1940	1/1	0.92	0.28	-	40,40,40,40	0
87	MG	5	3417	1/1	0.98	0.26	-	38,38,38,38	0
88	OHX	5	4010	7/7	0.97	0.26	-	62,62,62,62	4
88	OHX	6	2144	7/7	0.88	0.19	-	139,139,139,139	7
87	MG	5	3601	1/1	0.81	0.21	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3611	1/1	0.92	0.37	-	59,59,59,59	0
87	MG	1	3643	1/1	0.97	0.32	-	35,35,35,35	0
87	MG	5	3718	1/1	0.84	0.28	-	59,59,59,59	0
88	OHX	6	2119	7/7	0.94	0.19	-	62,62,62,62	2
88	OHX	5	4157	7/7	0.91	0.28	-	85,85,85,85	5
87	MG	1	3531	1/1	0.92	0.40	-	52,52,52,52	0
87	MG	5	3534	1/1	0.93	0.32	-	41,41,41,41	0
87	MG	1	3637	1/1	0.85	0.27	-	47,47,47,47	0
88	OHX	1	4034	7/7	0.92	0.38	-	50,50,50,50	5
87	MG	5	3482	1/1	0.91	0.43	-	30,30,30,30	0
87	MG	5	3559	1/1	0.98	0.46	-	31,31,31,31	0
87	MG	5	3408	1/1	0.88	0.31	-	48,48,48,48	0
87	MG	m6	202	1/1	0.81	0.30	-	52,52,52,52	0
87	MG	5	3784	1/1	0.94	0.28	-	41,41,41,41	0
88	OHX	1	3913	7/7	0.98	0.19	-	55,55,55,55	2
87	MG	5	3750	1/1	0.95	0.14	-	47,47,47,47	0
88	OHX	1	3962	7/7	0.95	0.24	-	42,42,42,42	3
87	MG	3	204	1/1	0.94	0.43	-	37,37,37,37	0
87	MG	5	3558	1/1	0.91	0.33	-	37,37,37,37	0
88	OHX	2	2152	7/7	0.82	0.18	-	104,104,104,104	5
87	MG	2	1949	1/1	0.61	0.31	-	90,90,90,90	0
88	OHX	1	4036	7/7	0.94	0.28	-	70,70,70,70	3
87	MG	1	3689	1/1	0.88	0.24	-	55,55,55,55	0
88	OHX	2	2136	7/7	0.93	0.27	-	72,72,72,72	5
87	MG	6	1958	1/1	0.95	0.47	-	51,51,51,51	0
87	MG	6	1984	1/1	0.83	0.40	-	72,72,72,72	0
87	MG	6	1987	1/1	0.95	0.30	-	58,58,58,58	0
88	OHX	5	4143	7/7	0.93	0.14	-	116,116,116,116	5
87	MG	2	1916	1/1	0.98	0.17	-	60,60,60,60	0
87	MG	6	1975	1/1	0.91	0.25	-	58,58,58,58	0
87	MG	6	1936	1/1	0.82	0.20	-	59,59,59,59	0
87	MG	1	3453	1/1	0.97	0.25	-	51,51,51,51	0
88	OHX	6	2037	7/7	0.98	0.18	-	95,95,95,95	3
87	MG	1	3709	1/1	0.85	0.63	-	44,44,44,44	0
87	MG	1	3572	1/1	0.97	0.31	-	44,44,44,44	0
88	OHX	6	2087	7/7	0.94	0.18	-	100,100,100,100	5
87	MG	5	3424	1/1	0.94	0.23	-	51,51,51,51	0
87	MG	2	1926	1/1	0.81	0.33	-	61,61,61,61	0
87	MG	1	3481	1/1	0.92	0.27	-	40,40,40,40	0
87	MG	1	3751	1/1	0.86	0.26	-	61,61,61,61	0
87	MG	1	3727	1/1	0.95	0.36	-	46,46,46,46	0
87	MG	D9	102	1/1	0.88	0.22	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3619	1/1	0.85	0.22	-	49,49,49,49	0
87	MG	6	2002	1/1	0.90	0.21	-	55,55,55,55	0
87	MG	1	3647	1/1	0.87	0.21	-	58,58,58,58	0
87	MG	1	3537	1/1	0.91	0.36	-	36,36,36,36	0
88	OHX	6	2171	7/7	0.93	0.14	-	131,131,131,131	7
88	OHX	2	2004	7/7	0.99	0.20	-	112,112,112,112	3
87	MG	1	3724	1/1	0.92	0.12	-	86,86,86,86	0
88	OHX	1	4083	7/7	0.95	0.22	-	90,90,90,90	4
87	MG	m3	201	1/1	0.95	0.19	-	40,40,40,40	0
88	OHX	5	4003	7/7	0.93	0.26	-	41,41,41,41	2
87	MG	4	214	1/1	0.83	0.27	-	71,71,71,71	0
87	MG	2	1901	1/1	0.52	0.40	-	87,87,87,87	0
88	OHX	2	2026	7/7	0.96	0.18	-	99,99,99,99	3
87	MG	2	1977	1/1	0.90	0.24	-	83,83,83,83	0
87	MG	1	3586	1/1	0.92	0.23	-	51,51,51,51	0
87	MG	2	1989	1/1	0.87	0.27	-	103,103,103,103	0
88	OHX	14	402	7/7	0.91	0.26	-	52,52,52,52	5
88	OHX	5	4140	7/7	0.92	0.26	-	52,52,52,52	5
87	MG	5	3622	1/1	0.93	0.30	-	38,38,38,38	0
88	OHX	3	209	7/7	0.99	0.28	-	68,68,68,68	3
88	OHX	5	4139	7/7	0.88	0.29	-	58,58,58,58	5
88	OHX	5	4090	7/7	0.86	0.23	-	83,83,83,83	4
87	MG	1	3620	1/1	0.93	0.32	-	39,39,39,39	0
87	MG	1	3508	1/1	0.97	0.35	-	37,37,37,37	0
88	OHX	5	3955	7/7	0.97	0.20	-	42,42,42,42	2
88	OHX	1	4067	7/7	0.83	0.30	-	104,104,104,104	4
88	OHX	6	2042	7/7	0.99	0.17	-	66,66,66,66	2
87	MG	1	3446	1/1	0.88	0.31	-	53,53,53,53	0
87	MG	5	3517	1/1	0.93	0.24	-	42,42,42,42	0
87	MG	1	3451	1/1	0.62	0.46	-	64,64,64,64	0
88	OHX	1	4065	7/7	0.92	0.28	-	98,98,98,98	7
87	MG	1	3546	1/1	0.90	0.18	-	48,48,48,48	0
88	OHX	8	228	7/7	0.93	0.27	-	67,67,67,67	3
87	MG	1	3579	1/1	0.98	0.42	-	38,38,38,38	0
88	OHX	1	3909	7/7	0.97	0.19	-	68,68,68,68	3
88	OHX	6	2177	7/7	0.91	0.26	-	68,68,68,68	5
87	MG	5	3754	1/1	0.83	0.33	-	49,49,49,49	0
87	MG	S4	301	1/1	0.65	2.11	-	88,88,88,88	0
87	MG	2	1931	1/1	0.90	0.33	-	70,70,70,70	0
88	OHX	1	4079	7/7	0.90	0.20	-	120,120,120,120	7
87	MG	6	1986	1/1	0.84	0.07	-	63,63,63,63	0
88	OHX	5	4105	7/7	0.95	0.26	-	44,44,44,44	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3463	1/1	0.81	0.27	-	51,51,51,51	0
88	OHX	5	4034	7/7	0.91	0.22	-	72,72,72,72	3
88	OHX	5	4021	7/7	0.96	0.21	-	41,41,41,41	5
87	MG	5	3440	1/1	0.75	0.50	-	81,81,81,81	0
88	OHX	5	4022	7/7	0.94	0.22	-	96,96,96,96	6
87	MG	7	201	1/1	0.93	0.36	-	51,51,51,51	0
87	MG	1	3744	1/1	0.96	0.36	-	34,34,34,34	0
88	OHX	5	3842	7/7	0.98	0.30	-	77,77,77,77	3
88	OHX	1	3919	7/7	0.96	0.17	-	96,96,96,96	3
87	MG	1	3425	1/1	0.97	0.33	-	48,48,48,48	0
87	MG	6	1926	1/1	0.85	0.21	-	57,57,57,57	0
87	MG	L3	403	1/1	0.89	0.11	-	52,52,52,52	0
87	MG	7	212	1/1	0.89	0.52	-	70,70,70,70	0
87	MG	1	3505	1/1	0.97	0.42	-	36,36,36,36	0
88	OHX	5	4062	7/7	0.92	0.24	-	50,50,50,50	5
87	MG	1	3516	1/1	0.96	0.36	-	36,36,36,36	0
88	OHX	1	3831	7/7	0.95	0.29	-	85,85,85,85	3
87	MG	5	3487	1/1	0.92	0.20	-	52,52,52,52	0
87	MG	5	3684	1/1	0.76	0.17	-	75,75,75,75	0
87	MG	5	3568	1/1	0.98	0.38	-	33,33,33,33	0
87	MG	5	3682	1/1	0.63	0.52	-	50,50,50,50	0
88	OHX	1	3800	7/7	0.98	0.28	-	91,91,91,91	3
87	MG	5	3425	1/1	0.94	0.38	-	37,37,37,37	0
87	MG	3	208	1/1	0.69	0.27	-	67,67,67,67	0
87	MG	5	3667	1/1	0.84	0.35	-	54,54,54,54	0
88	OHX	1	3823	7/7	0.99	0.21	-	57,57,57,57	2
87	MG	6	1919	1/1	0.82	0.13	-	66,66,66,66	0
88	OHX	1	3912	7/7	0.94	0.30	-	112,112,112,112	4
87	MG	1	3596	1/1	0.86	0.31	-	64,64,64,64	0
87	MG	1	3428	1/1	0.91	0.24	-	52,52,52,52	0
87	MG	5	3607	1/1	0.86	0.25	-	52,52,52,52	0
88	OHX	6	2143	7/7	0.95	0.16	-	74,74,74,74	5
87	MG	5	3793	1/1	0.89	0.30	-	49,49,49,49	0
88	OHX	1	3847	7/7	0.98	0.25	-	42,42,42,42	2
87	MG	5	3581	1/1	0.95	0.48	-	28,28,28,28	0
88	OHX	7	224	7/7	0.95	0.27	-	51,51,51,51	4
87	MG	5	3717	1/1	0.92	0.24	-	44,44,44,44	0
87	MG	5	3500	1/1	0.96	0.30	-	41,41,41,41	0
87	MG	5	3477	1/1	0.90	0.22	-	76,76,76,76	0
87	MG	5	4163	1/1	0.90	0.25	-	34,34,34,34	0
87	MG	5	3702	1/1	0.80	0.26	-	62,62,62,62	0
88	OHX	1	4104	7/7	0.88	0.27	-	56,56,56,56	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3961	7/7	0.96	0.23	-	41,41,41,41	4
88	OHX	1	3905	7/7	0.97	0.26	-	52,52,52,52	2
88	OHX	6	2166	7/7	0.91	0.39	-	65,65,65,65	5
88	OHX	5	4064	7/7	0.93	0.37	-	38,38,38,38	3
87	MG	1	3518	1/1	0.95	0.47	-	41,41,41,41	0
88	OHX	1	3960	7/7	0.97	0.26	-	110,110,110,110	2
87	MG	1	3749	1/1	0.86	0.20	-	48,48,48,48	0
87	MG	5	3740	1/1	0.96	0.33	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.