



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2016 – 12:28 PM EDT

PDB ID : 5FCI
Title : Structure of the vacant uL3 W255C mutant 80S yeast ribosome
Authors : Mailliot, J.; Garreau de Loubresse, N.; Yusupova, G.; Dinman, J.D.; Yusupov, M.
Deposited on : 2015-12-15
Resolution : 3.40 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-20027674
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-20027674

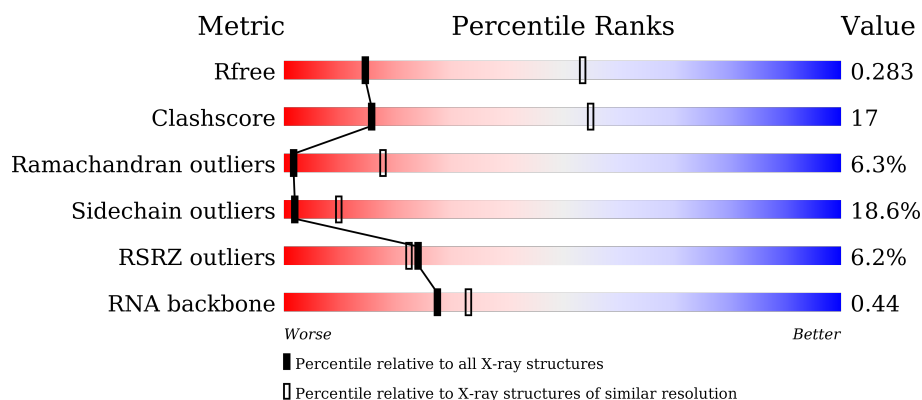
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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>31%</div> <div>48%</div> <div>18%</div> <div>..</div> </div>
1	6	1800	<div> <div>7%</div> <div>33%</div> <div>48%</div> <div>17%</div> <div>.</div> </div>
2	S0	251	<div> <div>11%</div> <div>23%</div> <div>46%</div> <div>11%</div> <div>.</div> <div>18%</div> </div>
2	s0	251	<div> <div>3%</div> <div>62%</div> <div>19%</div> <div>.</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
3	S1	254	
3	s1	254	
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	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	

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Mol	Chain	Length	Quality of chain
16	C4	136	
16	c4	136	
17	C5	141	
17	c5	141	
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	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	

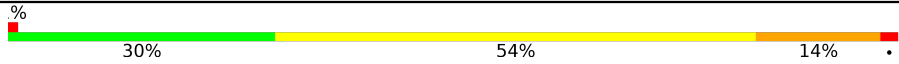

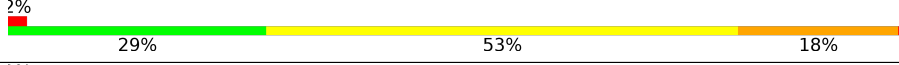

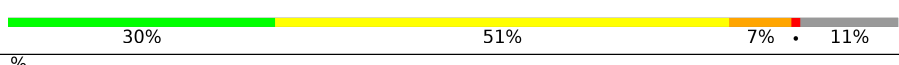
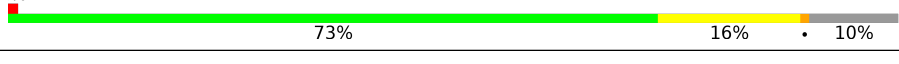
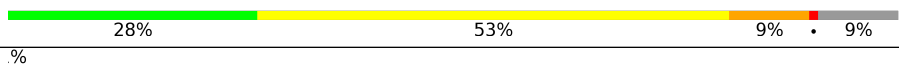

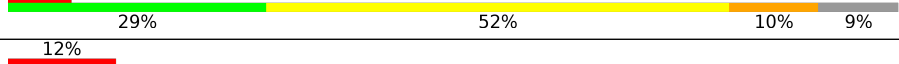

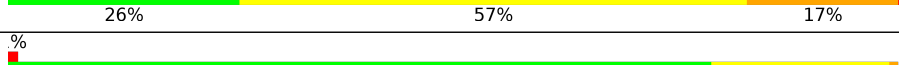
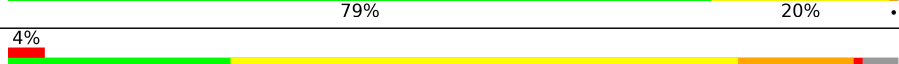

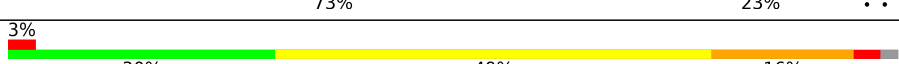
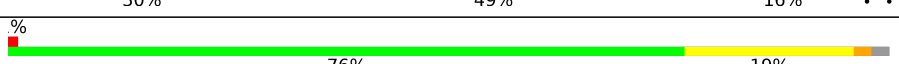
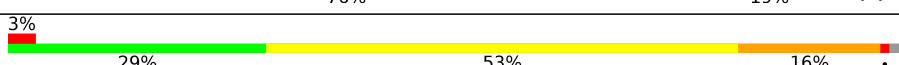
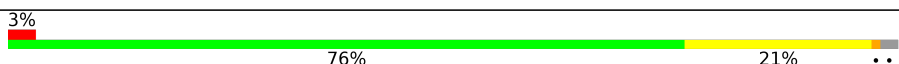
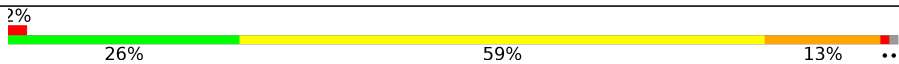
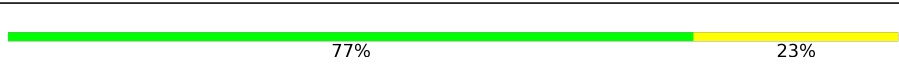


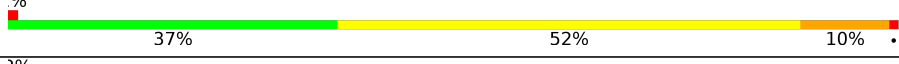
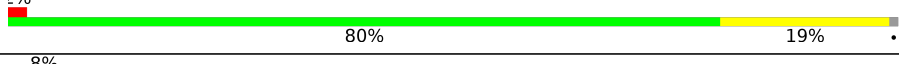
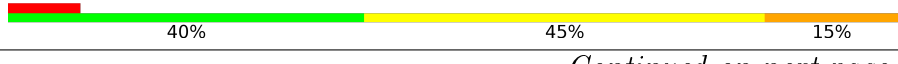

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Mol	Chain	Length	Quality of chain
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	182	
35	sM	182	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	


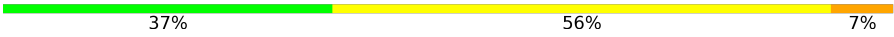

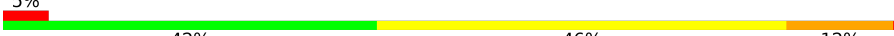

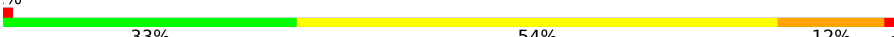
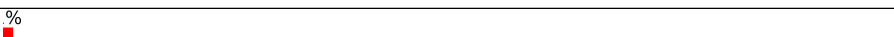

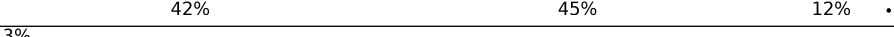

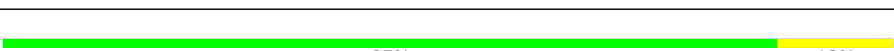


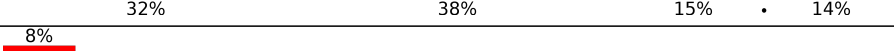




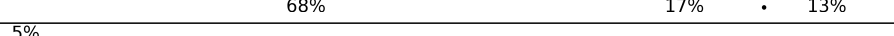
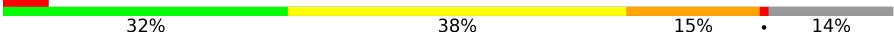

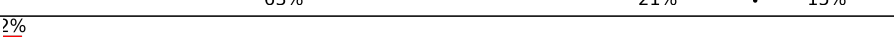



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Mol	Chain	Length	Quality of chain
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	

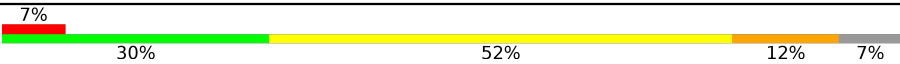


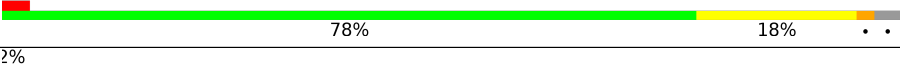
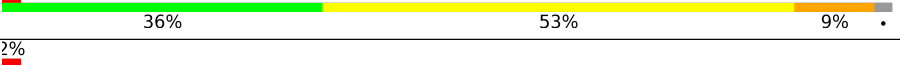
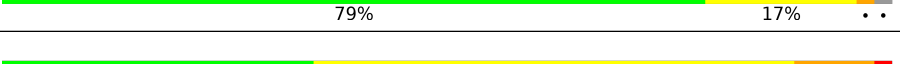
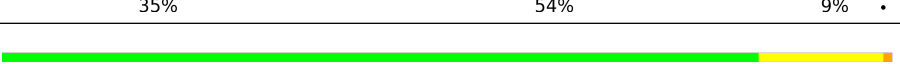
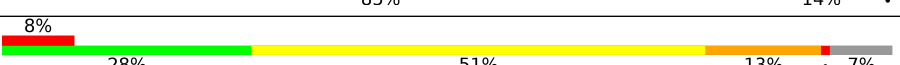
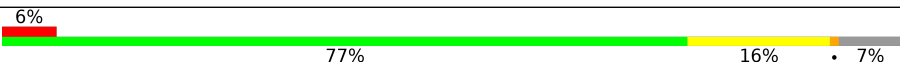

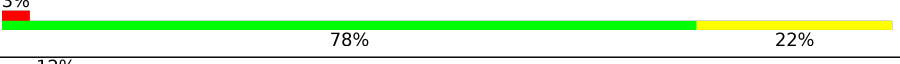
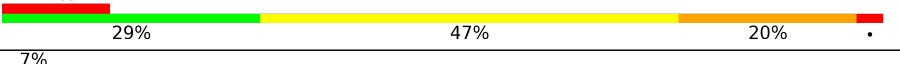



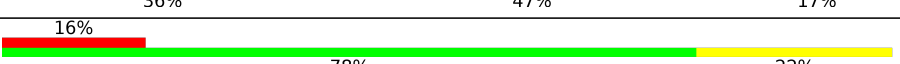
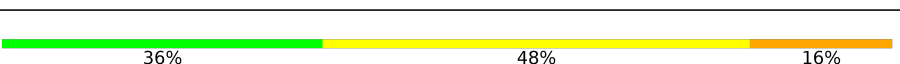
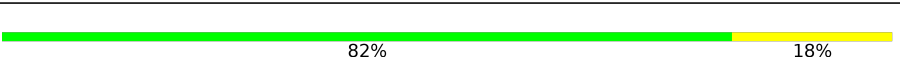
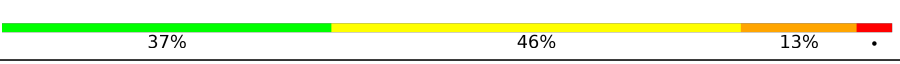






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Mol	Chain	Length	Quality of chain
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	

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Mol	Chain	Length	Quality of chain
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	120	
70	o4	120	
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	

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Mol	Chain	Length	Quality of chain
78	q2	105	
79	Q3	91	
79	q3	91	
80	c0	96	
81	m2	150	
82	p0	311	
83	p1	47	
84	p2	46	

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	OHX	1	3448	-	-	X	-
85	OHX	1	3475	-	-	X	-
85	OHX	1	3483	-	-	X	-
85	OHX	1	3490	-	-	-	X
85	OHX	1	3495	-	-	X	-
85	OHX	1	3497	-	-	X	-
85	OHX	1	3509	-	-	X	-
85	OHX	1	3510	-	-	-	X
85	OHX	1	3513	-	-	X	-
85	OHX	1	3515	-	-	-	X
85	OHX	1	3522	-	-	-	X
85	OHX	1	3527	-	-	-	X
85	OHX	1	3528	-	-	-	X
85	OHX	1	3537	-	-	-	X
85	OHX	1	3540	-	-	X	-
85	OHX	1	3542	-	-	-	X
85	OHX	1	3544	-	-	-	X
85	OHX	1	3556	-	-	X	-
85	OHX	1	3558	-	-	-	X
85	OHX	1	3564	-	-	-	X
85	OHX	1	3565	-	-	X	-
85	OHX	1	3569	-	-	X	-
85	OHX	1	3570	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	OHX	1	3582	-	-	X	-
85	OHX	1	3583	-	-	-	X
85	OHX	1	3584	-	-	-	X
85	OHX	1	3591	-	-	-	X
85	OHX	1	3592	-	-	X	-
85	OHX	1	3593	-	-	X	X
85	OHX	1	3594	-	-	X	X
85	OHX	1	3598	-	-	-	X
85	OHX	1	3603	-	-	-	X
85	OHX	1	3609	-	-	-	X
85	OHX	1	3611	-	-	-	X
85	OHX	1	3612	-	-	-	X
85	OHX	1	3616	-	-	X	X
85	OHX	1	3624	-	-	-	X
85	OHX	1	3625	-	-	-	X
85	OHX	1	3627	-	-	-	X
85	OHX	1	3630	-	-	-	X
85	OHX	1	3633	-	-	-	X
85	OHX	1	3634	-	-	-	X
85	OHX	1	3635	-	-	-	X
85	OHX	1	3645	-	-	-	X
85	OHX	1	3646	-	-	-	X
85	OHX	1	3647	-	-	-	X
85	OHX	1	3648	-	-	-	X
85	OHX	1	3649	-	-	-	X
85	OHX	1	3651	-	-	-	X
85	OHX	1	3652	-	-	-	X
85	OHX	1	3656	-	-	X	X
85	OHX	1	3657	-	-	-	X
85	OHX	1	3663	-	-	-	X
85	OHX	1	3666	-	-	-	X
85	OHX	1	3668	-	-	-	X
85	OHX	1	3670	-	-	-	X
85	OHX	1	3671	-	-	-	X
85	OHX	1	3672	-	-	-	X
85	OHX	1	3673	-	-	-	X
85	OHX	1	3676	-	-	-	X
85	OHX	1	3677	-	-	X	X
85	OHX	1	3680	-	-	-	X
85	OHX	1	3685	-	-	X	-
85	OHX	1	3687	-	-	-	X
85	OHX	1	3689	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	OHX	1	3691	-	-	-	X
85	OHX	1	3692	-	-	-	X
85	OHX	1	3694	-	-	X	-
85	OHX	1	3695	-	-	X	-
85	OHX	1	3697	-	-	-	X
85	OHX	1	3698	-	-	-	X
85	OHX	1	3702	-	-	X	-
85	OHX	1	3705	-	-	-	X
85	OHX	1	3707	-	-	-	X
85	OHX	1	3710	-	-	-	X
85	OHX	1	3711	-	-	X	-
85	OHX	1	3713	-	-	-	X
85	OHX	1	3714	-	-	-	X
85	OHX	1	3716	-	-	-	X
85	OHX	1	3719	-	-	-	X
85	OHX	1	3720	-	-	X	-
85	OHX	1	3721	-	-	-	X
85	OHX	1	3723	-	-	-	X
85	OHX	1	3724	-	-	-	X
85	OHX	1	3727	-	-	-	X
85	OHX	1	3731	-	-	-	X
85	OHX	1	3734	-	-	-	X
85	OHX	1	3736	-	-	-	X
85	OHX	1	3737	-	-	X	-
85	OHX	2	1909	-	-	X	-
85	OHX	2	1922	-	-	X	-
85	OHX	2	1942	-	-	-	X
85	OHX	2	1947	-	-	-	X
85	OHX	2	1953	-	-	X	X
85	OHX	2	1964	-	-	-	X
85	OHX	2	1968	-	-	X	-
85	OHX	2	1977	-	-	X	-
85	OHX	2	1981	-	-	-	X
85	OHX	2	1989	-	-	X	-
85	OHX	2	1991	-	-	-	X
85	OHX	2	1995	-	-	-	X
85	OHX	2	2004	-	-	-	X
85	OHX	2	2010	-	-	X	-
85	OHX	2	2013	-	-	-	X
85	OHX	2	2015	-	-	-	X
85	OHX	2	2022	-	-	-	X
85	OHX	2	2024	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	OHX	2	2025	-	-	X	-
85	OHX	2	2027	-	-	-	X
85	OHX	2	2034	-	-	-	X
85	OHX	2	2036	-	-	-	X
85	OHX	2	2039	-	-	-	X
85	OHX	2	2040	-	-	X	-
85	OHX	3	210	-	-	-	X
85	OHX	4	207	-	-	-	X
85	OHX	4	208	-	-	-	X
85	OHX	4	211	-	-	-	X
85	OHX	4	212	-	-	-	X
85	OHX	4	213	-	-	-	X
85	OHX	5	3444	-	-	X	-
85	OHX	5	3480	-	-	X	-
85	OHX	5	3496	-	-	-	X
85	OHX	5	3504	-	-	X	-
85	OHX	5	3505	-	-	X	X
85	OHX	5	3514	-	-	X	-
85	OHX	5	3524	-	-	X	-
85	OHX	5	3527	-	-	-	X
85	OHX	5	3530	-	-	-	X
85	OHX	5	3537	-	-	X	-
85	OHX	5	3539	-	-	X	-
85	OHX	5	3546	-	-	-	X
85	OHX	5	3553	-	-	-	X
85	OHX	5	3556	-	-	-	X
85	OHX	5	3558	-	-	-	X
85	OHX	5	3559	-	-	X	-
85	OHX	5	3570	-	-	X	-
85	OHX	5	3577	-	-	-	X
85	OHX	5	3583	-	-	-	X
85	OHX	5	3585	-	-	X	-
85	OHX	5	3590	-	-	-	X
85	OHX	5	3593	-	-	-	X
85	OHX	5	3594	-	-	X	-
85	OHX	5	3596	-	-	-	X
85	OHX	5	3604	-	-	-	X
85	OHX	5	3606	-	-	X	X
85	OHX	5	3609	-	-	-	X
85	OHX	5	3610	-	-	-	X
85	OHX	5	3611	-	-	-	X
85	OHX	5	3615	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	OHX	5	3616	-	-	-	X
85	OHX	5	3617	-	-	-	X
85	OHX	5	3622	-	-	-	X
85	OHX	5	3624	-	-	-	X
85	OHX	5	3625	-	-	-	X
85	OHX	5	3630	-	-	-	X
85	OHX	5	3631	-	-	-	X
85	OHX	5	3637	-	-	-	X
85	OHX	5	3639	-	-	-	X
85	OHX	5	3642	-	-	-	X
85	OHX	5	3644	-	-	-	X
85	OHX	5	3646	-	-	-	X
85	OHX	5	3647	-	-	X	-
85	OHX	5	3648	-	-	-	X
85	OHX	5	3650	-	-	-	X
85	OHX	5	3657	-	-	-	X
85	OHX	5	3658	-	-	-	X
85	OHX	5	3660	-	-	-	X
85	OHX	5	3663	-	-	-	X
85	OHX	5	3664	-	-	-	X
85	OHX	5	3665	-	-	-	X
85	OHX	5	3667	-	-	-	X
85	OHX	5	3668	-	-	-	X
85	OHX	5	3676	-	-	-	X
85	OHX	5	3678	-	-	-	X
85	OHX	5	3682	-	-	-	X
85	OHX	5	3688	-	-	-	X
85	OHX	5	3689	-	-	-	X
85	OHX	5	3690	-	-	-	X
85	OHX	5	3691	-	-	-	X
85	OHX	5	3693	-	-	X	X
85	OHX	5	3694	-	-	-	X
85	OHX	5	3695	-	-	-	X
85	OHX	5	3696	-	-	-	X
85	OHX	5	3697	-	-	-	X
85	OHX	5	3699	-	-	-	X
85	OHX	5	3700	-	-	-	X
85	OHX	5	3701	-	-	-	X
85	OHX	5	3702	-	-	-	X
85	OHX	5	3703	-	-	X	-
85	OHX	5	3704	-	-	X	-
85	OHX	5	3705	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	OHX	5	3706	-	-	X	-
85	OHX	5	3707	-	-	-	X
85	OHX	5	3709	-	-	-	X
85	OHX	5	3710	-	-	-	X
85	OHX	5	3715	-	-	-	X
85	OHX	5	3718	-	-	-	X
85	OHX	5	3720	-	-	-	X
85	OHX	5	3721	-	-	X	X
85	OHX	5	3728	-	-	-	X
85	OHX	5	3737	-	-	-	X
85	OHX	5	3738	-	-	-	X
85	OHX	5	3739	-	-	X	-
85	OHX	5	3740	-	-	-	X
85	OHX	5	3742	-	-	X	-
85	OHX	5	3743	-	-	X	-
85	OHX	6	1914	-	-	X	-
85	OHX	6	1964	-	-	-	X
85	OHX	6	1966	-	-	-	X
85	OHX	6	1967	-	-	-	X
85	OHX	6	1971	-	-	-	X
85	OHX	6	1975	-	-	X	-
85	OHX	6	1979	-	-	-	X
85	OHX	6	1980	-	-	-	X
85	OHX	6	1981	-	-	-	X
85	OHX	6	1987	-	-	-	X
85	OHX	6	1988	-	-	-	X
85	OHX	6	1990	-	-	-	X
85	OHX	6	1995	-	-	-	X
85	OHX	6	2001	-	-	X	X
85	OHX	6	2002	-	-	-	X
85	OHX	6	2005	-	-	-	X
85	OHX	6	2011	-	-	-	X
85	OHX	6	2015	-	-	-	X
85	OHX	6	2019	-	-	-	X
85	OHX	6	2022	-	-	-	X
85	OHX	6	2025	-	-	X	-
85	OHX	6	2028	-	-	-	X
85	OHX	6	2029	-	-	-	X
85	OHX	6	2030	-	-	-	X
85	OHX	6	2031	-	-	-	X
85	OHX	6	2032	-	-	-	X
85	OHX	6	2034	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	OHX	6	2038	-	-	-	X
85	OHX	6	2039	-	-	-	X
85	OHX	6	2043	-	-	-	X
85	OHX	6	2045	-	-	-	X
85	OHX	6	2049	-	-	-	X
85	OHX	7	203	-	-	X	-
85	OHX	7	209	-	-	X	X
85	OHX	7	211	-	-	X	X
85	OHX	7	212	-	-	-	X
85	OHX	8	203	-	-	X	-
85	OHX	8	208	-	-	-	X
85	OHX	8	211	-	-	X	-
85	OHX	8	212	-	-	-	X
85	OHX	8	213	-	-	-	X
85	OHX	8	215	-	-	-	X
85	OHX	D9	102	-	-	-	X
85	OHX	L4	401	-	-	X	-
85	OHX	M7	201	-	-	-	X
85	OHX	O4	201	-	-	-	X
85	OHX	Q2	502	-	-	X	-
85	OHX	S9	201	-	-	X	X
85	OHX	l3	402	-	-	-	X
85	OHX	m0	303	-	-	-	X
85	OHX	o4	201	-	-	-	X
85	OHX	o7	502	-	-	-	X
85	OHX	s9	201	-	-	-	X
86	MG	1	3738	-	-	-	X
86	MG	1	3740	-	-	-	X
86	MG	1	3743	-	-	-	X
86	MG	1	3744	-	-	-	X
86	MG	1	3746	-	-	-	X
86	MG	1	3750	-	-	-	X
86	MG	1	3752	-	-	-	X
86	MG	1	3753	-	-	-	X
86	MG	1	3758	-	-	-	X
86	MG	1	3768	-	-	-	X
86	MG	1	3782	-	-	-	X
86	MG	1	3786	-	-	-	X
86	MG	1	3787	-	-	-	X
86	MG	1	3795	-	-	-	X
86	MG	1	3796	-	-	-	X
86	MG	1	3801	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	1	3808	-	-	-	X
86	MG	1	3812	-	-	-	X
86	MG	1	3813	-	-	-	X
86	MG	1	3814	-	-	-	X
86	MG	1	3815	-	-	-	X
86	MG	1	3818	-	-	-	X
86	MG	1	3819	-	-	-	X
86	MG	1	3825	-	-	-	X
86	MG	1	3826	-	-	-	X
86	MG	1	3827	-	-	-	X
86	MG	1	3830	-	-	-	X
86	MG	1	3834	-	-	-	X
86	MG	1	3835	-	-	-	X
86	MG	1	3836	-	-	-	X
86	MG	1	3839	-	-	-	X
86	MG	1	3843	-	-	-	X
86	MG	1	3844	-	-	-	X
86	MG	1	3845	-	-	-	X
86	MG	1	3851	-	-	-	X
86	MG	1	3855	-	-	-	X
86	MG	1	3857	-	-	-	X
86	MG	1	3858	-	-	-	X
86	MG	1	3864	-	-	-	X
86	MG	1	3865	-	-	-	X
86	MG	1	3866	-	-	-	X
86	MG	1	3870	-	-	-	X
86	MG	1	3871	-	-	-	X
86	MG	1	3872	-	-	-	X
86	MG	1	3878	-	-	-	X
86	MG	1	3881	-	-	-	X
86	MG	1	3882	-	-	-	X
86	MG	1	3885	-	-	-	X
86	MG	1	3886	-	-	-	X
86	MG	1	3887	-	-	-	X
86	MG	1	3888	-	-	-	X
86	MG	1	3890	-	-	-	X
86	MG	1	3896	-	-	-	X
86	MG	1	3897	-	-	-	X
86	MG	1	3898	-	-	-	X
86	MG	1	3901	-	-	-	X
86	MG	1	3902	-	-	-	X
86	MG	1	3905	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	1	3907	-	-	-	X
86	MG	1	3908	-	-	-	X
86	MG	1	3910	-	-	-	X
86	MG	1	3912	-	-	-	X
86	MG	1	3913	-	-	-	X
86	MG	1	3914	-	-	-	X
86	MG	1	3920	-	-	-	X
86	MG	1	3921	-	-	-	X
86	MG	1	3929	-	-	-	X
86	MG	1	3942	-	-	-	X
86	MG	1	3946	-	-	-	X
86	MG	1	3954	-	-	-	X
86	MG	1	3961	-	-	-	X
86	MG	1	3973	-	-	-	X
86	MG	1	3977	-	-	-	X
86	MG	1	3981	-	-	-	X
86	MG	1	3983	-	-	-	X
86	MG	1	3990	-	-	-	X
86	MG	1	3993	-	-	-	X
86	MG	1	3995	-	-	-	X
86	MG	1	4003	-	-	-	X
86	MG	1	4013	-	-	-	X
86	MG	1	4014	-	-	-	X
86	MG	1	4030	-	-	-	X
86	MG	1	4031	-	-	-	X
86	MG	1	4033	-	-	-	X
86	MG	1	4037	-	-	-	X
86	MG	1	4040	-	-	-	X
86	MG	1	4041	-	-	-	X
86	MG	1	4049	-	-	-	X
86	MG	1	4053	-	-	-	X
86	MG	1	4057	-	-	-	X
86	MG	1	4060	-	-	-	X
86	MG	1	4061	-	-	-	X
86	MG	1	4062	-	-	-	X
86	MG	1	4063	-	-	-	X
86	MG	1	4066	-	-	-	X
86	MG	1	4068	-	-	-	X
86	MG	1	4084	-	-	-	X
86	MG	1	4094	-	-	-	X
86	MG	1	4104	-	-	-	X
86	MG	1	4105	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	1	4109	-	-	-	X
86	MG	1	4114	-	-	-	X
86	MG	1	4118	-	-	-	X
86	MG	1	4130	-	-	-	X
86	MG	1	4131	-	-	-	X
86	MG	1	4132	-	-	-	X
86	MG	2	2047	-	-	-	X
86	MG	2	2051	-	-	-	X
86	MG	2	2053	-	-	-	X
86	MG	2	2054	-	-	-	X
86	MG	2	2055	-	-	-	X
86	MG	2	2060	-	-	-	X
86	MG	2	2064	-	-	-	X
86	MG	2	2071	-	-	-	X
86	MG	2	2074	-	-	-	X
86	MG	2	2075	-	-	-	X
86	MG	2	2076	-	-	-	X
86	MG	2	2078	-	-	-	X
86	MG	2	2081	-	-	-	X
86	MG	2	2083	-	-	-	X
86	MG	2	2085	-	-	-	X
86	MG	2	2089	-	-	-	X
86	MG	2	2091	-	-	-	X
86	MG	2	2093	-	-	-	X
86	MG	2	2095	-	-	-	X
86	MG	2	2097	-	-	-	X
86	MG	2	2100	-	-	-	X
86	MG	2	2104	-	-	-	X
86	MG	2	2109	-	-	-	X
86	MG	2	2110	-	-	-	X
86	MG	2	2112	-	-	-	X
86	MG	4	219	-	-	-	X
86	MG	4	223	-	-	-	X
86	MG	5	3749	-	-	-	X
86	MG	5	3751	-	-	-	X
86	MG	5	3756	-	-	-	X
86	MG	5	3757	-	-	-	X
86	MG	5	3760	-	-	-	X
86	MG	5	3763	-	-	-	X
86	MG	5	3764	-	-	-	X
86	MG	5	3768	-	-	-	X
86	MG	5	3769	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	5	3772	-	-	-	X
86	MG	5	3774	-	-	-	X
86	MG	5	3782	-	-	-	X
86	MG	5	3788	-	-	-	X
86	MG	5	3792	-	-	-	X
86	MG	5	3800	-	-	-	X
86	MG	5	3803	-	-	-	X
86	MG	5	3804	-	-	-	X
86	MG	5	3810	-	-	-	X
86	MG	5	3814	-	-	-	X
86	MG	5	3815	-	-	-	X
86	MG	5	3830	-	-	-	X
86	MG	5	3832	-	-	-	X
86	MG	5	3833	-	-	-	X
86	MG	5	3835	-	-	-	X
86	MG	5	3837	-	-	-	X
86	MG	5	3839	-	-	-	X
86	MG	5	3844	-	-	-	X
86	MG	5	3845	-	-	-	X
86	MG	5	3846	-	-	-	X
86	MG	5	3847	-	-	-	X
86	MG	5	3850	-	-	-	X
86	MG	5	3851	-	-	-	X
86	MG	5	3852	-	-	-	X
86	MG	5	3858	-	-	-	X
86	MG	5	3861	-	-	-	X
86	MG	5	3862	-	-	-	X
86	MG	5	3866	-	-	-	X
86	MG	5	3869	-	-	-	X
86	MG	5	3876	-	-	-	X
86	MG	5	3878	-	-	-	X
86	MG	5	3880	-	-	-	X
86	MG	5	3883	-	-	-	X
86	MG	5	3884	-	-	-	X
86	MG	5	3885	-	-	-	X
86	MG	5	3887	-	-	-	X
86	MG	5	3889	-	-	-	X
86	MG	5	3892	-	-	-	X
86	MG	5	3894	-	-	-	X
86	MG	5	3895	-	-	-	X
86	MG	5	3899	-	-	-	X
86	MG	5	3900	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	5	3902	-	-	-	X
86	MG	5	3903	-	-	-	X
86	MG	5	3904	-	-	-	X
86	MG	5	3906	-	-	-	X
86	MG	5	3907	-	-	-	X
86	MG	5	3908	-	-	-	X
86	MG	5	3915	-	-	-	X
86	MG	5	3918	-	-	-	X
86	MG	5	3919	-	-	-	X
86	MG	5	3920	-	-	-	X
86	MG	5	3922	-	-	-	X
86	MG	5	3925	-	-	-	X
86	MG	5	3926	-	-	-	X
86	MG	5	3927	-	-	-	X
86	MG	5	3928	-	-	-	X
86	MG	5	3929	-	-	-	X
86	MG	5	3930	-	-	-	X
86	MG	5	3941	-	-	-	X
86	MG	5	3947	-	-	-	X
86	MG	5	3948	-	-	-	X
86	MG	5	3950	-	-	-	X
86	MG	5	3958	-	-	-	X
86	MG	5	3966	-	-	-	X
86	MG	5	3968	-	-	-	X
86	MG	5	3969	-	-	-	X
86	MG	5	3972	-	-	-	X
86	MG	5	3979	-	-	-	X
86	MG	5	3983	-	-	-	X
86	MG	5	3986	-	-	-	X
86	MG	5	3993	-	-	-	X
86	MG	5	3999	-	-	-	X
86	MG	5	4010	-	-	-	X
86	MG	5	4038	-	-	-	X
86	MG	5	4050	-	-	-	X
86	MG	5	4051	-	-	-	X
86	MG	5	4055	-	-	-	X
86	MG	5	4062	-	-	-	X
86	MG	5	4063	-	-	-	X
86	MG	5	4066	-	-	-	X
86	MG	5	4067	-	-	-	X
86	MG	5	4069	-	-	-	X
86	MG	5	4075	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	5	4076	-	-	-	X
86	MG	5	4087	-	-	-	X
86	MG	5	4089	-	-	-	X
86	MG	5	4090	-	-	-	X
86	MG	5	4091	-	-	-	X
86	MG	5	4104	-	-	-	X
86	MG	5	4107	-	-	-	X
86	MG	5	4108	-	-	-	X
86	MG	5	4110	-	-	-	X
86	MG	5	4113	-	-	-	X
86	MG	5	4115	-	-	-	X
86	MG	5	4119	-	-	-	X
86	MG	5	4124	-	-	-	X
86	MG	5	4125	-	-	-	X
86	MG	5	4135	-	-	-	X
86	MG	5	4137	-	-	-	X
86	MG	5	4140	-	-	-	X
86	MG	5	4146	-	-	-	X
86	MG	5	4154	-	-	-	X
86	MG	5	4163	-	-	-	X
86	MG	5	4165	-	-	-	X
86	MG	5	4166	-	-	-	X
86	MG	5	4170	-	-	-	X
86	MG	6	2051	-	-	-	X
86	MG	6	2053	-	-	-	X
86	MG	6	2054	-	-	-	X
86	MG	6	2056	-	-	-	X
86	MG	6	2058	-	-	-	X
86	MG	6	2059	-	-	-	X
86	MG	6	2060	-	-	-	X
86	MG	6	2061	-	-	-	X
86	MG	6	2064	-	-	-	X
86	MG	6	2067	-	-	-	X
86	MG	6	2070	-	-	-	X
86	MG	6	2072	-	-	-	X
86	MG	6	2073	-	-	-	X
86	MG	6	2076	-	-	-	X
86	MG	6	2081	-	-	-	X
86	MG	6	2085	-	-	-	X
86	MG	6	2086	-	-	-	X
86	MG	6	2091	-	-	-	X
86	MG	6	2092	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	6	2094	-	-	-	X
86	MG	6	2099	-	-	-	X
86	MG	6	2101	-	-	-	X
86	MG	6	2109	-	-	-	X
86	MG	6	2114	-	-	-	X
86	MG	6	2119	-	-	-	X
86	MG	6	2128	-	-	-	X
86	MG	6	2130	-	-	-	X
86	MG	6	2132	-	-	-	X
86	MG	6	2145	-	-	-	X
86	MG	6	2147	-	-	-	X
86	MG	6	2164	-	-	-	X
86	MG	6	2170	-	-	-	X
86	MG	6	2181	-	-	-	X
86	MG	8	219	-	-	-	X
86	MG	8	222	-	-	-	X
86	MG	C2	201	-	-	-	X
86	MG	C9	201	-	-	-	X
86	MG	L3	404	-	-	-	X
86	MG	L4	403	-	-	-	X
86	MG	M1	201	-	-	-	X
86	MG	M8	201	-	-	-	X
86	MG	MG	2224	-	-	-	X
86	MG	N0	201	-	-	-	X
86	MG	N3	201	-	-	-	X
86	MG	O1	201	-	-	-	X
86	MG	O2	201	-	-	-	X
86	MG	S4	301	-	-	-	X
86	MG	c1	202	-	-	-	X
86	MG	l3	403	-	-	-	X
86	MG	l3	404	-	-	-	X
86	MG	l3	406	-	-	-	X
86	MG	l7	301	-	-	-	X
86	MG	m0	305	-	-	-	X
86	MG	m6	203	-	-	-	X
86	MG	m7	201	-	-	-	X
86	MG	n0	202	-	-	-	X
86	MG	n0	203	-	-	-	X
86	MG	n0	204	-	-	-	X
86	MG	n3	202	-	-	-	X
86	MG	n6	201	-	-	-	X
86	MG	n6	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	MG	n8	201	-	-	-	X
86	MG	n9	103	-	-	-	X
86	MG	o1	201	-	-	-	X
86	MG	s1	301	-	-	-	X
86	MG	s4	302	-	-	-	X
86	MG	sM	402	-	-	-	X
87	ZN	d7	101	-	-	-	X

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 411776 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
			1612	1034	285	291	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1612	1034	285	291	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
			1820	1142	350	325	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			1492	957	267	268			

- 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			

- Molecule 13 is a protein called 40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17).

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
			892	562	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			892	562	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
			965	603	183	177	2			
19	c7	117	Total	C	N	O	S	0	0	0
			944	591	179	172	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			443	275	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			443	275	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 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
			2441	1543	418	472	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2445	1546	419	472	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			680	403	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	3150	Total	C	N	O	P	0	0	0
			67377	30095	12145	21987	3150			

- 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			
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
			1918	1193	389	335	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1918	1193	389	335	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
			3073	1948	583	533	9			
40	l3	386	Total	C	N	O	S	0	0	0
			3073	1948	583	533	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L3	255	CYS	TRP	engineered mutation	UNP P14126
l3	255	CYS	TRP	engineered mutation	UNP P14126

- 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
			2749	1730	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2749	1730	522	494	3			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1817	1159	326	329	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
			1717	1089	325	297	6			
47	m0	213	Total	C	N	O	S	0	0	0
			1733	1101	327	299	6			

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	S	0	0	0
			1442	896	287	259				
53	m7	155	Total	C	N	O	S	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	S	0	0	0
			1521	935	326	260				
55	m9	188	Total	C	N	O	S	0	0	0
			1521	935	326	260				

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	0	0	0
			796	516	131	149			
58	n2	98	Total	C	N	O	0	0	0
			778	505	127	146			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			800	508	159	132	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1089	682	219	187	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
			968	623	170	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
			890	565	168	156	1			
67	o1	109	Total	C	N	O	S	0	0	0
			890	565	168	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			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			881	546	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			881	546	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
			969	615	186	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
			771	481	156	132	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O	0	0	0
			612	391	115	106			
74	o8	77	Total	C	N	O	0	0	0
			612	391	115	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 S10-A.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c0	87	UNK	-	expression tag	UNP Q08745
c0	88	UNK	-	expression tag	UNP Q08745
c0	89	UNK	-	expression tag	UNP Q08745
c0	90	UNK	-	expression tag	UNP Q08745
c0	91	UNK	-	expression tag	UNP Q08745
c0	92	UNK	-	expression tag	UNP Q08745
c0	93	UNK	-	expression tag	UNP Q08745
c0	94	UNK	-	expression tag	UNP Q08745
c0	95	UNK	-	expression tag	UNP Q08745
c0	96	UNK	-	expression tag	UNP Q08745
c0	97	UNK	-	expression tag	UNP Q08745
c0	98	UNK	-	expression tag	UNP Q08745

- 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 acidic ribosomal protein P0.

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

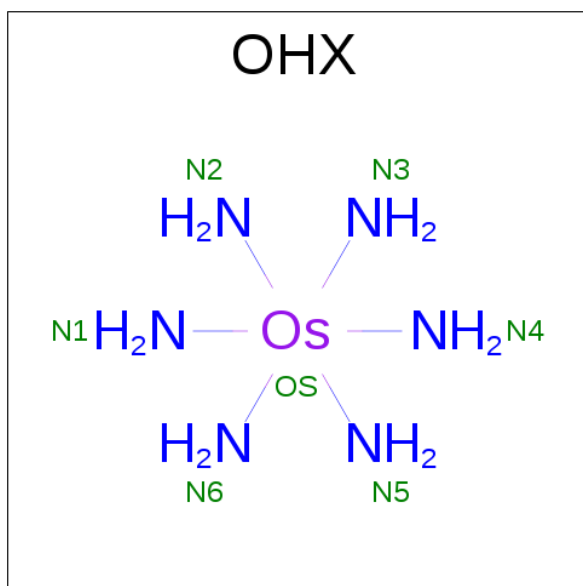
- Molecule 83 is a protein called 60S ribosomal protein P1 alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
83	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			

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

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

- Molecule 85 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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			7	6	1		
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
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85	2	1	Total	N	Os	0	0
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85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	2	1	Total	N	Os	0	0
			7	6	1		
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85	S9	1	Total	N	Os	0	0
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85	C3	1	Total	N	Os	0	0
			7	6	1		
85	C5	1	Total	N	Os	0	0
			7	6	1		
85	C8	1	Total	N	Os	0	0
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85	D9	1	Total	N	Os	0	0
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85	SR	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	1	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
85	1	1	Total	N	Os	0	0
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			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
85	1	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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85	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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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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85	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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85	1	1	Total	N	Os	0	0
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	1	1	Total	N	Os	0	0
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85	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	3	1	Total	N	Os	0	0
			7	6	1		
85	3	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	4	1	Total	N	Os	0	0
			7	6	1		
85	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	L3	1	Total	N	Os	0	0
			7	6	1		
85	L4	1	Total	N	Os	0	0
			7	6	1		
85	M0	1	Total	N	Os	0	0
			7	6	1		
85	M5	1	Total	N	Os	0	0
			7	6	1		
85	M5	1	Total	N	Os	0	0
			7	6	1		
85	M7	1	Total	N	Os	0	0
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85	M7	1	Total	N	Os	0	0
			7	6	1		
85	M9	1	Total	N	Os	0	0
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85	N9	1	Total	N	Os	0	0
			7	6	1		
85	O3	1	Total	N	Os	0	0
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85	O4	1	Total	N	Os	0	0
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85	O7	1	Total	N	Os	0	0
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85	O7	1	Total	N	Os	0	0
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85	Q2	1	Total	N	Os	0	0
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85	6	1	Total	N	Os	0	0
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85	6	1	Total	N	Os	0	0
			7	6	1		
85	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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85	6	1	Total	N	Os	0	0
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85	6	1	Total	N	Os	0	0
			7	6	1		
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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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85	5	1	Total	N	Os	0	0
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85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	5	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	7	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	8	1	Total	N	Os	0	0
			7	6	1		
85	13	1	Total	N	Os	0	0
			7	6	1		
85	13	1	Total	N	Os	0	0
			7	6	1		
85	14	1	Total	N	Os	0	0
			7	6	1		
85	14	1	Total	N	Os	0	0
			7	6	1		
85	15	1	Total	N	Os	0	0
			7	6	1		
85	15	1	Total	N	Os	0	0
			7	6	1		
85	15	1	Total	N	Os	0	0
			7	6	1		
85	15	1	Total	N	Os	0	0
			7	6	1		
85	19	1	Total	N	Os	0	0
			7	6	1		
85	m0	1	Total	N	Os	0	0
			7	6	1		
85	m0	1	Total	N	Os	0	0
			7	6	1		
85	m0	1	Total	N	Os	0	0
			7	6	1		
85	m1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
85	m4	1	Total	N	Os	0	0
			7	6	1		
85	m5	1	Total	N	Os	0	0
			7	6	1		
85	n3	1	Total	N	Os	0	0
			7	6	1		
85	n5	1	Total	N	Os	0	0
			7	6	1		
85	n9	1	Total	N	Os	0	0
			7	6	1		
85	o2	1	Total	N	Os	0	0
			7	6	1		
85	o3	1	Total	N	Os	0	0
			7	6	1		
85	o4	1	Total	N	Os	0	0
			7	6	1		
85	o7	1	Total	N	Os	0	0
			7	6	1		
85	q2	1	Total	N	Os	0	0
			7	6	1		

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	1	Total	Mg	0	0
			1	1		
86	N9	1	Total	Mg	0	0
			1	1		
86	n8	1	Total	Mg	0	0
			1	1		
86	MG	6	Total	Mg	0	0
			6	6		
86	o1	1	Total	Mg	0	0
			1	1		
86	p0	1	Total	Mg	0	0
			1	1		
86	6	136	Total	Mg	0	0
			136	136		
86	sM	2	Total	Mg	0	0
			2	2		
86	q1	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	l3	5	Total 5	Mg 5	0	0
86	M1	1	Total 1	Mg 1	0	0
86	n0	4	Total 4	Mg 4	0	0
86	l4	1	Total 1	Mg 1	0	0
86	2	92	Total 92	Mg 92	0	0
86	N4	1	Total 1	Mg 1	0	0
86	L4	2	Total 2	Mg 2	0	0
86	l7	1	Total 1	Mg 1	0	0
86	M5	1	Total 1	Mg 1	0	0
86	m3	1	Total 1	Mg 1	0	0
86	N6	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	8	10	Total 10	Mg 10	0	0
86	M9	1	Total 1	Mg 1	0	0
86	q0	1	Total 1	Mg 1	0	0
86	SM	1	Total 1	Mg 1	0	0
86	c8	1	Total 1	Mg 1	0	0
86	M0	1	Total 1	Mg 1	0	0
86	c1	1	Total 1	Mg 1	0	0
86	5	428	Total 428	Mg 428	0	0
86	L5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	O7	2	Total 2	Mg 2	0	0
86	s6	1	Total 1	Mg 1	0	0
86	Q2	2	Total 2	Mg 2	0	0
86	M4	1	Total 1	Mg 1	0	0
86	n9	2	Total 2	Mg 2	0	0
86	1	395	Total 395	Mg 395	0	0
86	L9	1	Total 1	Mg 1	0	0
86	O2	1	Total 1	Mg 1	0	0
86	S8	1	Total 1	Mg 1	0	0
86	m1	1	Total 1	Mg 1	0	0
86	M8	1	Total 1	Mg 1	0	0
86	D9	2	Total 2	Mg 2	0	0
86	o3	1	Total 1	Mg 1	0	0
86	M3	1	Total 1	Mg 1	0	0
86	N3	2	Total 2	Mg 2	0	0
86	4	16	Total 16	Mg 16	0	0
86	n6	2	Total 2	Mg 2	0	0
86	S4	1	Total 1	Mg 1	0	0
86	L2	2	Total 2	Mg 2	0	0
86	m6	4	Total 4	Mg 4	0	0
86	m7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	M7	6	Total 6	Mg 6	0	0
86	m4	1	Total 1	Mg 1	0	0
86	o4	1	Total 1	Mg 1	0	0
86	N8	1	Total 1	Mg 1	0	0
86	s1	1	Total 1	Mg 1	0	0
86	D1	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	o2	1	Total 1	Mg 1	0	0
86	C9	1	Total 1	Mg 1	0	0
86	7	11	Total 11	Mg 11	0	0
86	n3	1	Total 1	Mg 1	0	0
86	Q1	1	Total 1	Mg 1	0	0
86	L3	2	Total 2	Mg 2	0	0
86	O5	1	Total 1	Mg 1	0	0
86	s4	1	Total 1	Mg 1	0	0
86	C2	7	Total 7	Mg 7	0	0
86	l9	1	Total 1	Mg 1	0	0
86	M6	2	Total 2	Mg 2	0	0
86	N0	1	Total 1	Mg 1	0	0
86	m0	2	Total 2	Mg 2	0	0
86	3	8	Total 8	Mg 8	0	0

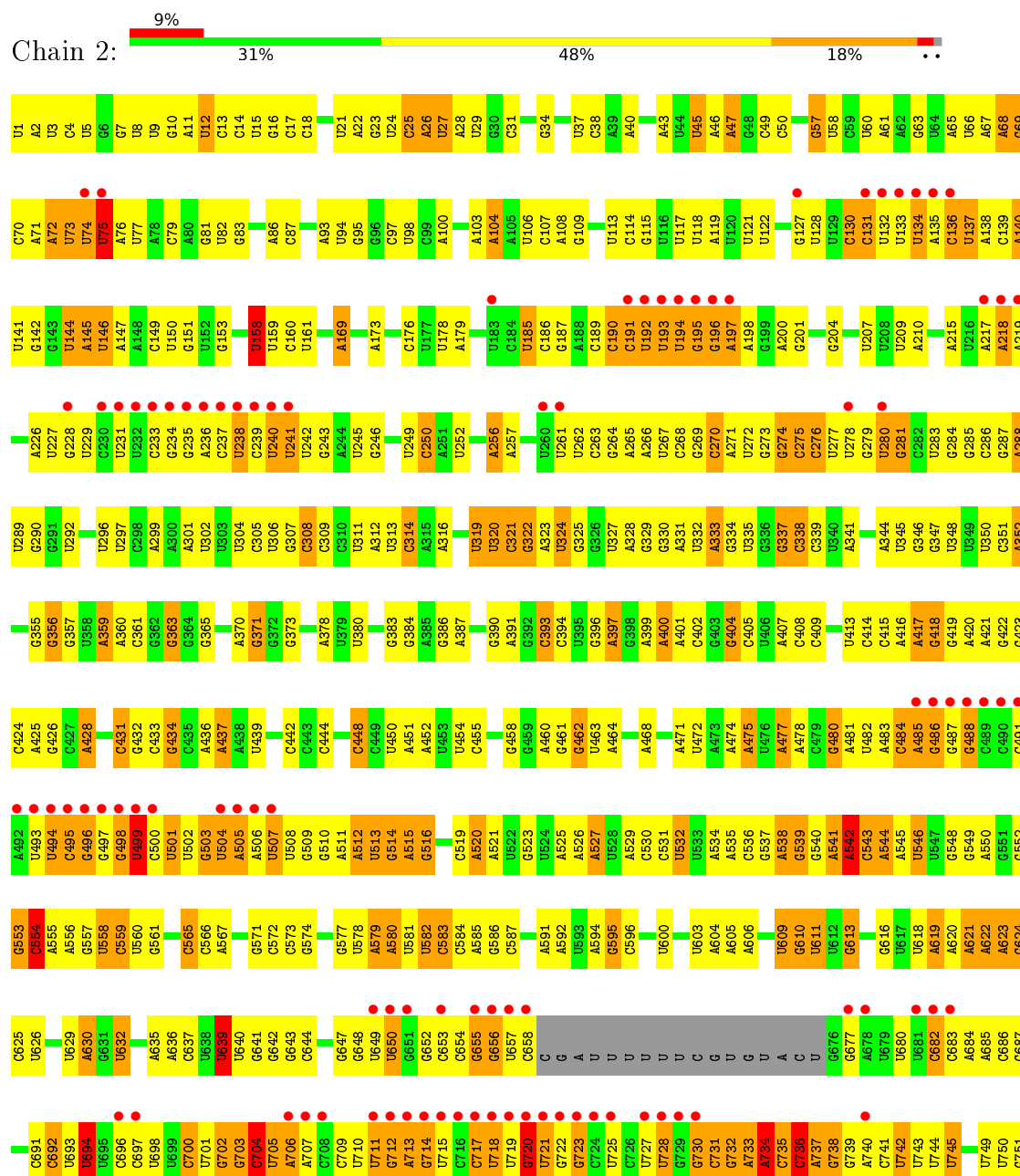
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total 1	Zn 1	0	0
87	D6	1	Total 1	Zn 1	0	0
87	Q2	1	Total 1	Zn 1	0	0
87	e1	1	Total 1	Zn 1	0	0
87	Q3	1	Total 1	Zn 1	0	0
87	D9	1	Total 1	Zn 1	0	0
87	E1	1	Total 1	Zn 1	0	0
87	Q0	1	Total 1	Zn 1	0	0
87	d7	1	Total 1	Zn 1	0	0
87	q3	1	Total 1	Zn 1	0	0
87	d9	1	Total 1	Zn 1	0	0
87	D7	1	Total 1	Zn 1	0	0
87	d6	1	Total 1	Zn 1	0	0
87	o7	1	Total 1	Zn 1	0	0
87	O7	1	Total 1	Zn 1	0	0
87	q2	1	Total 1	Zn 1	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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

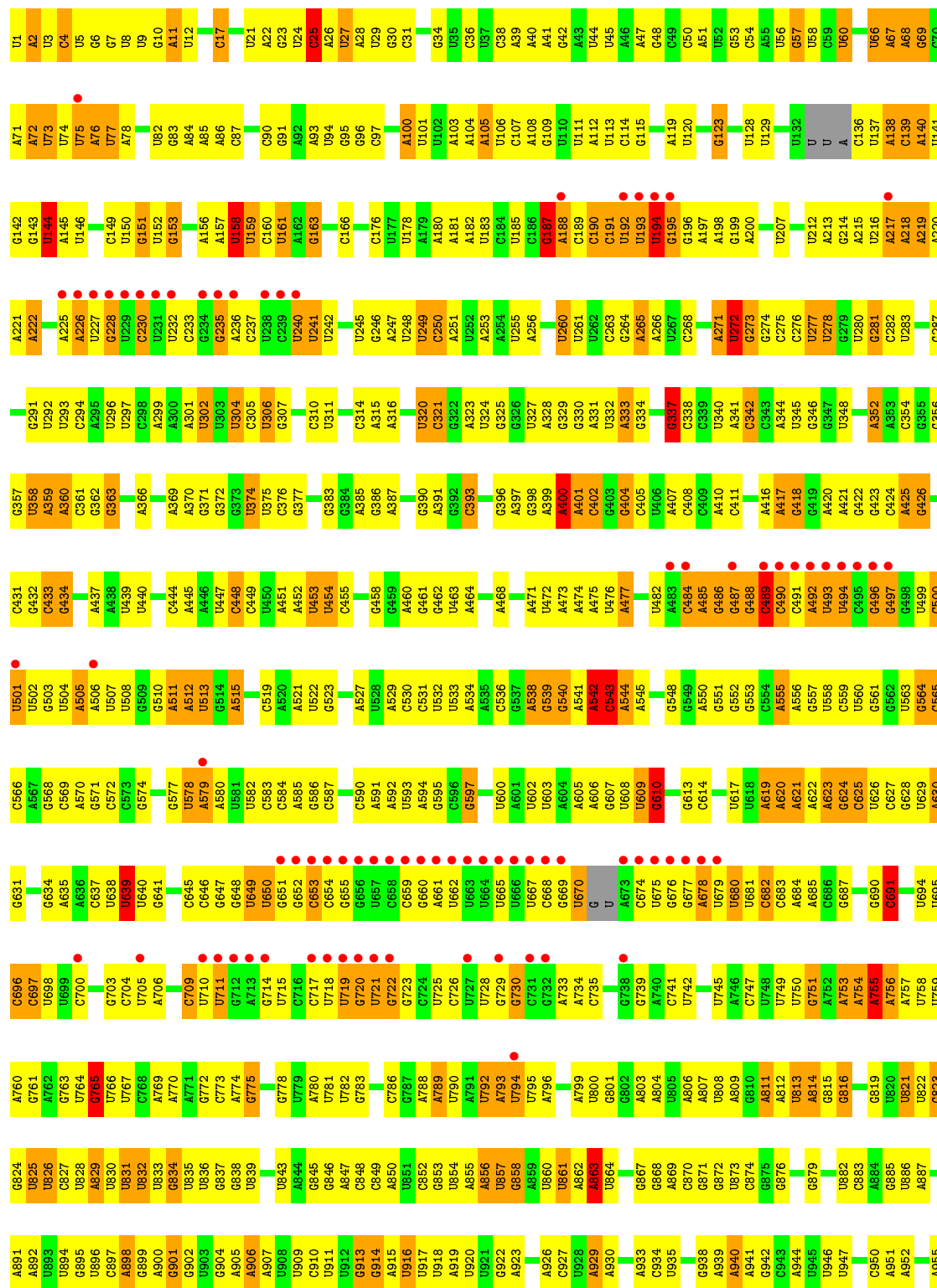
- Molecule 1: 18S ribosomal RNA

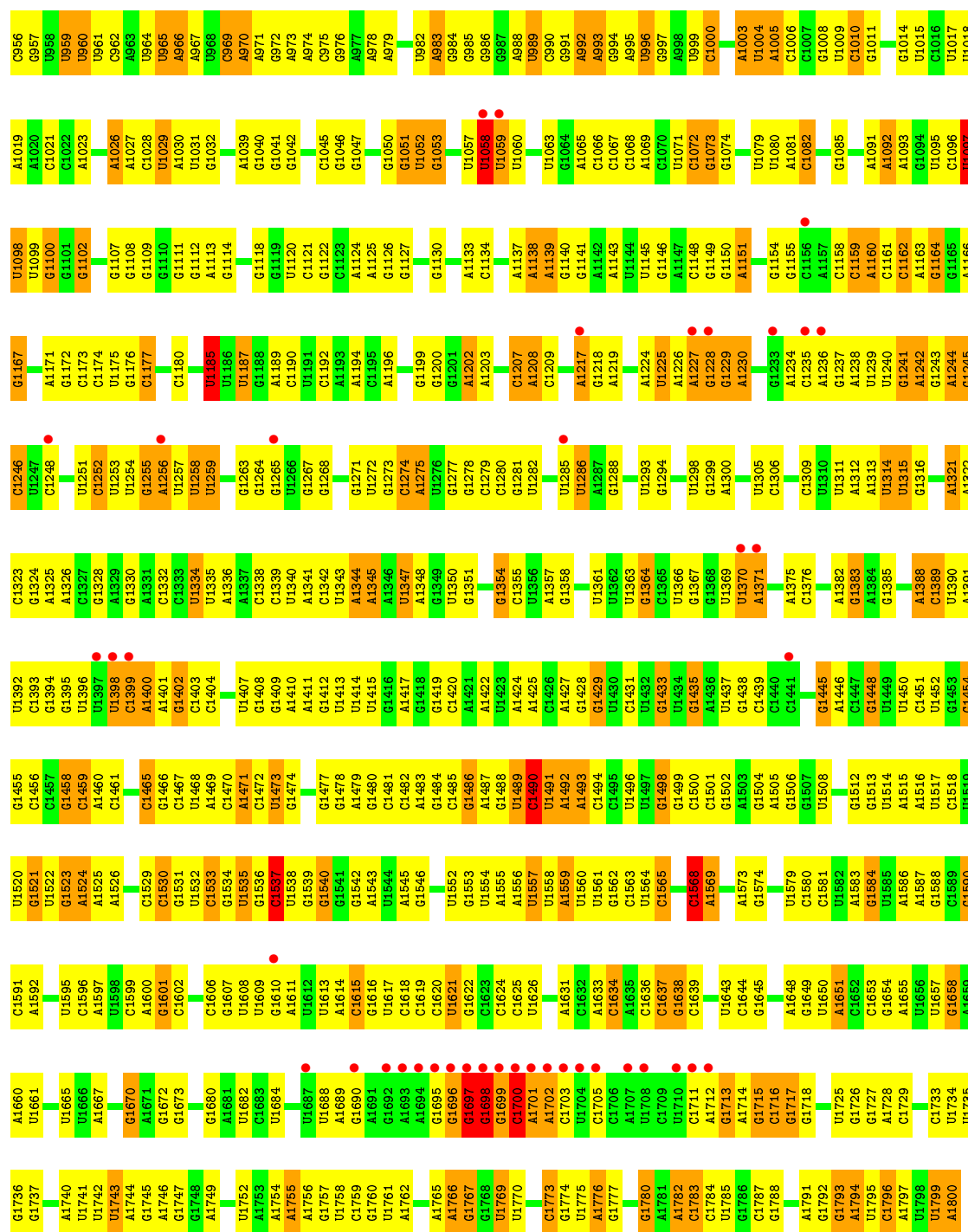




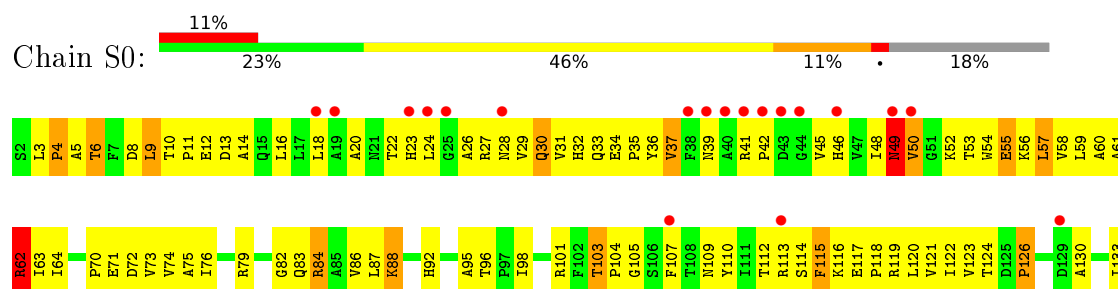


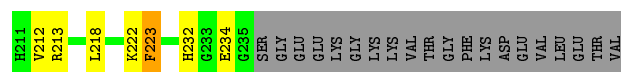
• Molecule 1: 18S ribosomal RNA



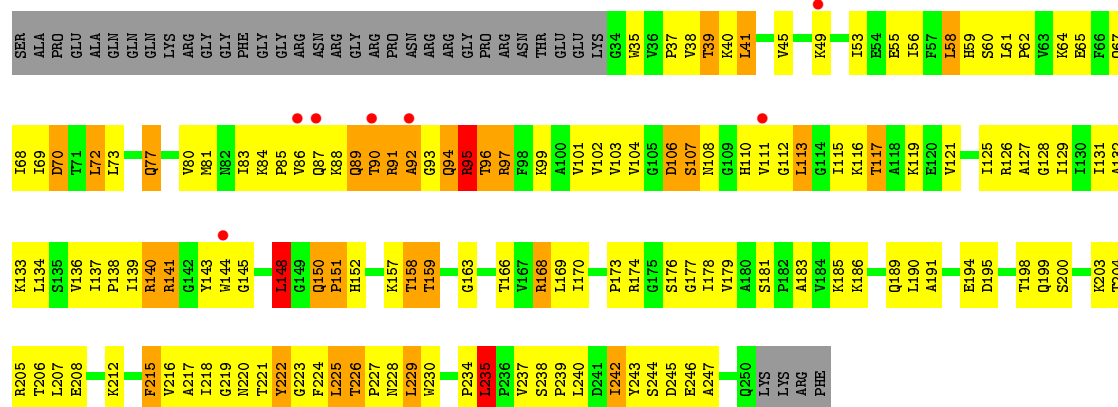


• Molecule 2: 40S ribosomal protein S0-A

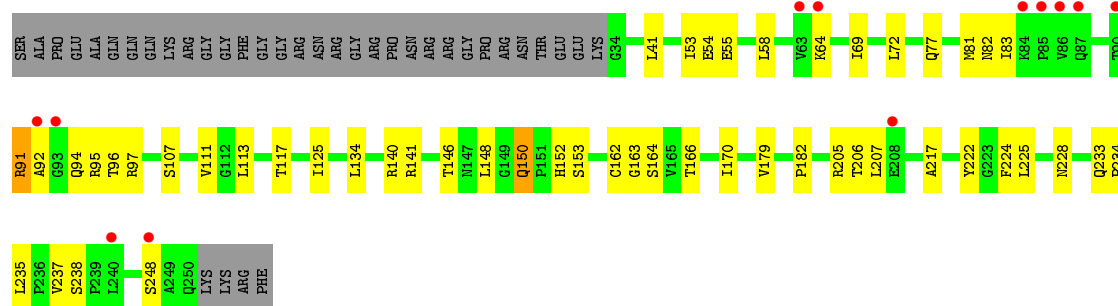




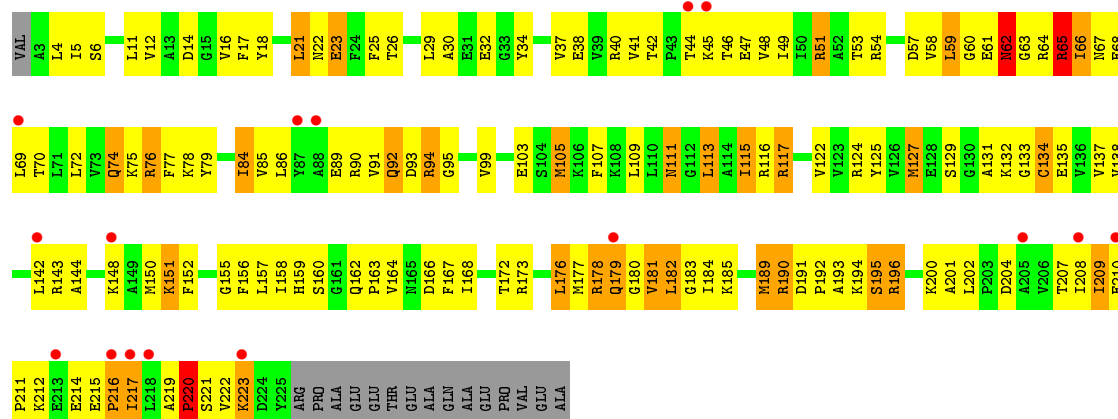
• Molecule 4: 40S ribosomal protein S2



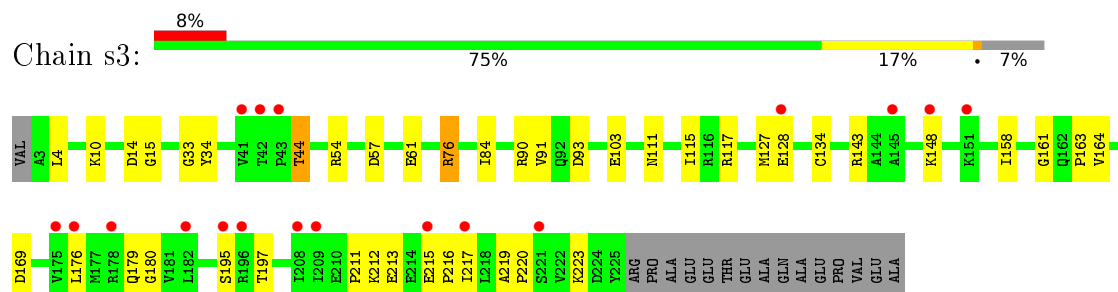
• Molecule 4: 40S ribosomal protein S2



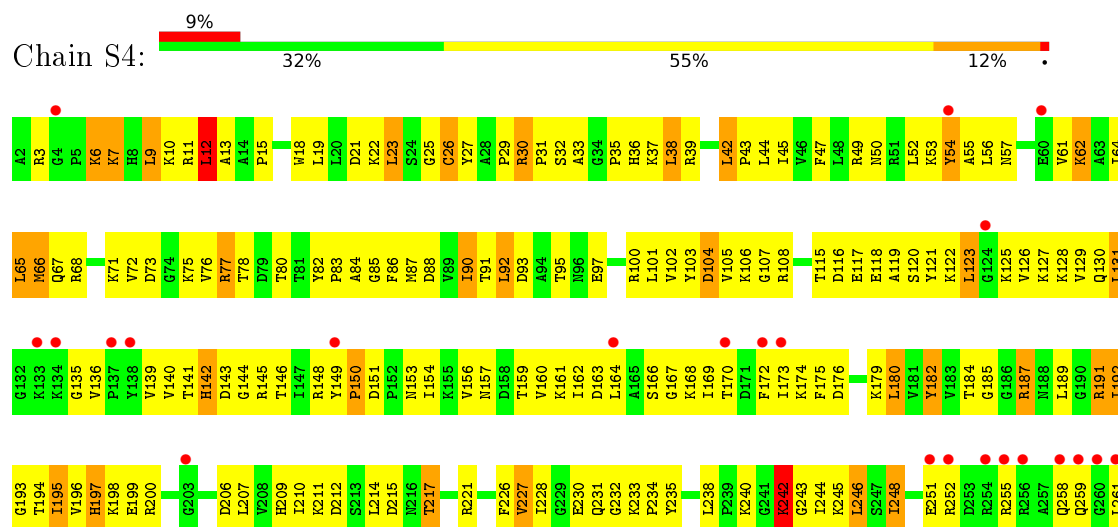
• Molecule 5: 40S ribosomal protein S3



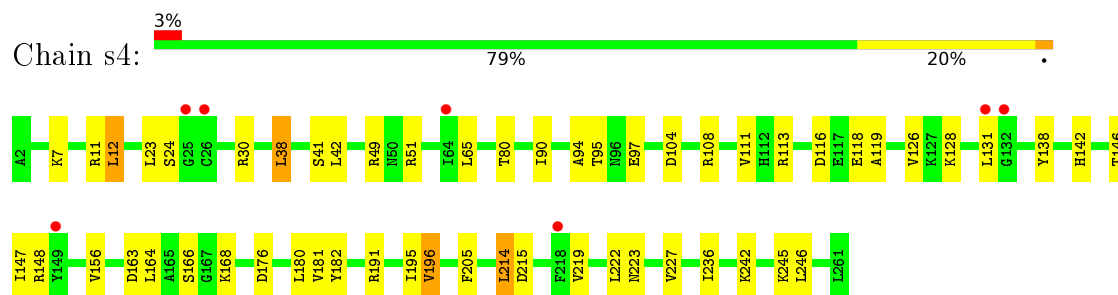
- Molecule 5: 40S ribosomal protein S3



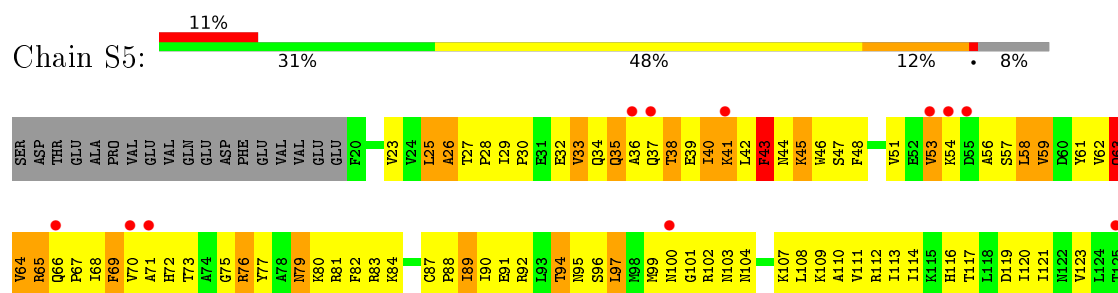
- Molecule 6: 40S ribosomal protein S4-A

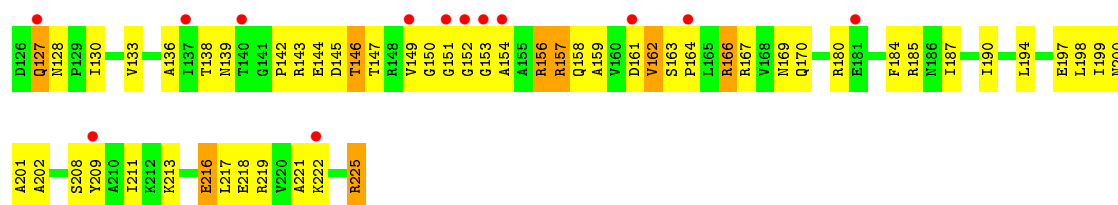


- Molecule 6: 40S ribosomal protein S4-A

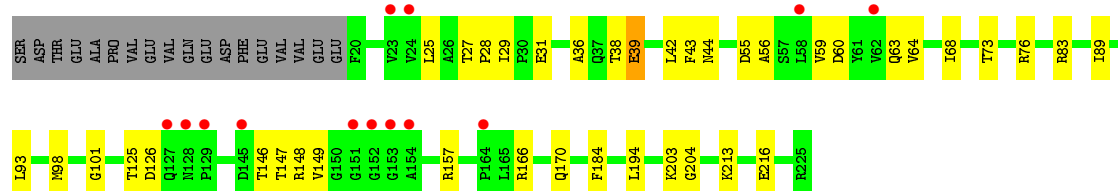
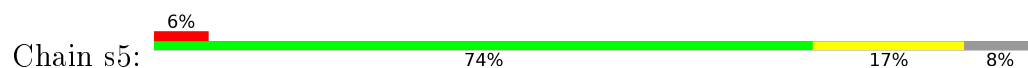


- Molecule 7: 40S ribosomal protein S5

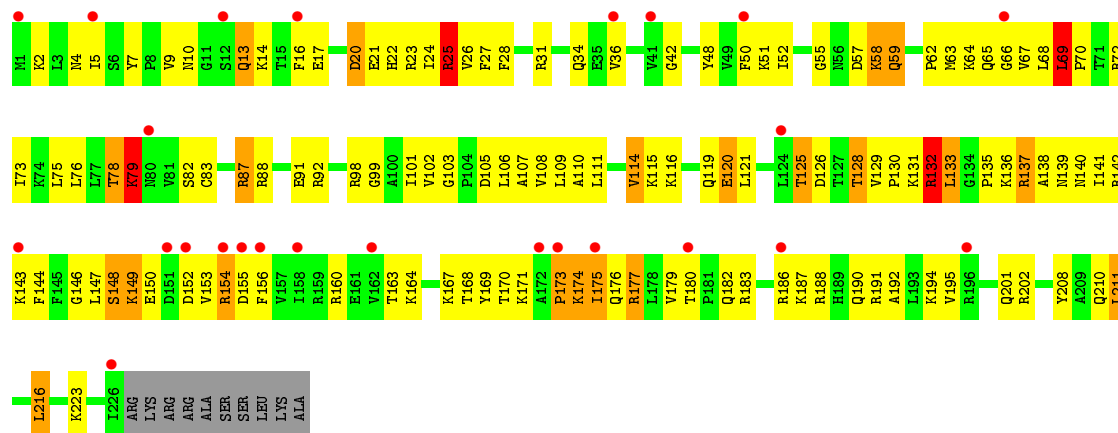




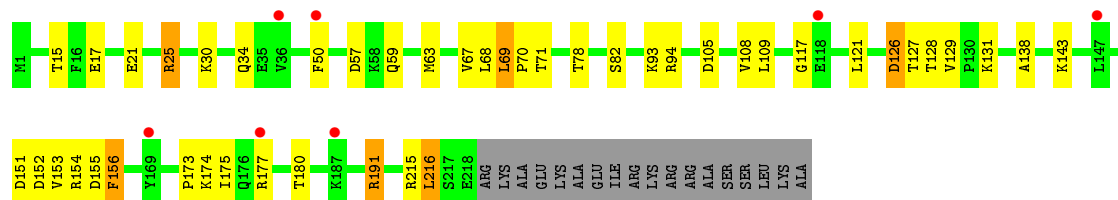
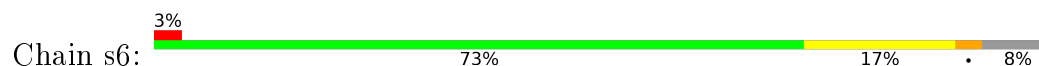
• Molecule 7: 40S ribosomal protein S5



• Molecule 8: 40S ribosomal protein S6-A

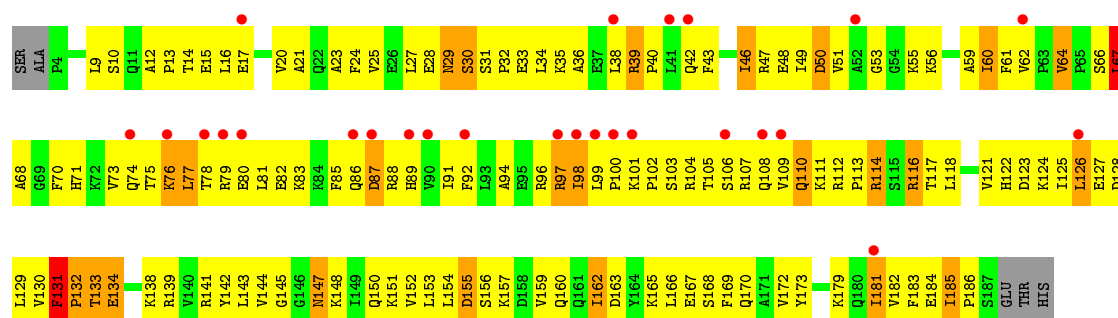


• Molecule 8: 40S ribosomal protein S6-A

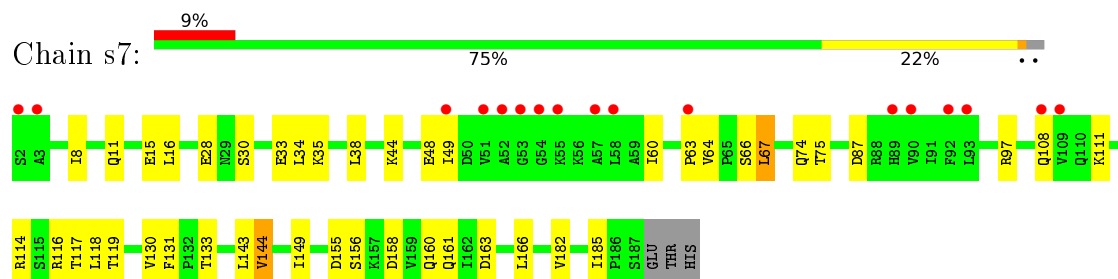


• Molecule 9: 40S ribosomal protein S7-A

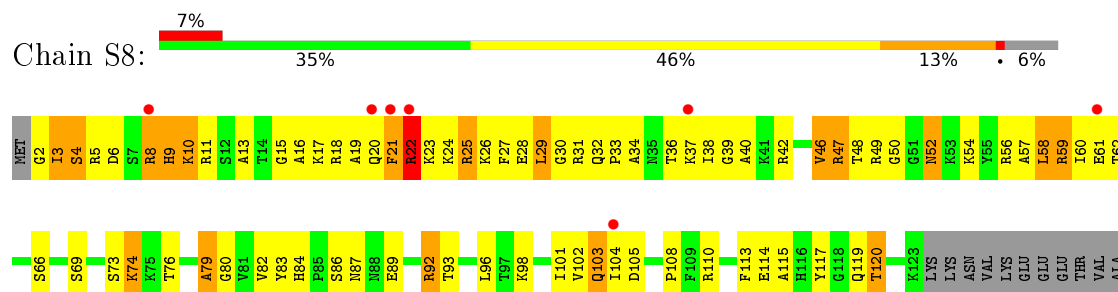




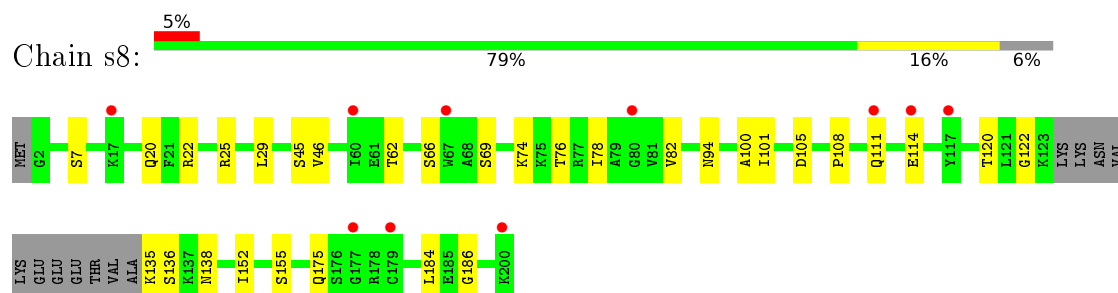
- Molecule 9: 40S ribosomal protein S7-A



- Molecule 10: 40S ribosomal protein S8-A

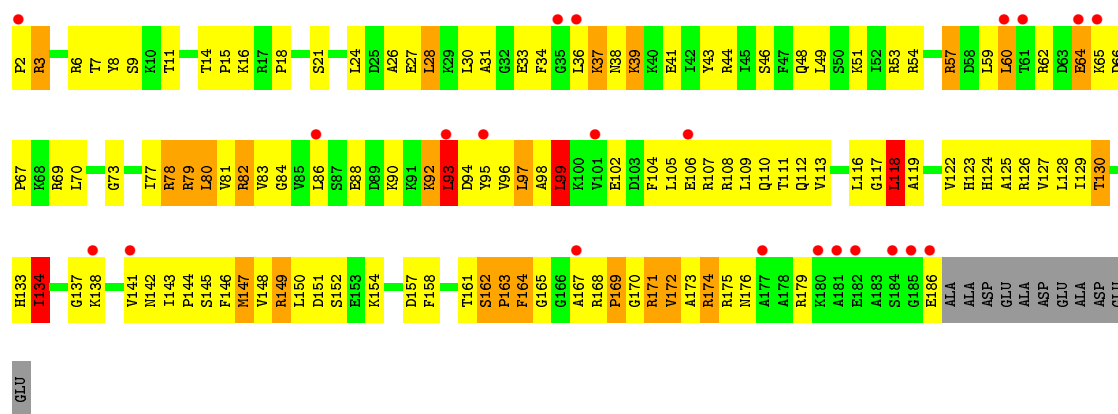


- Molecule 10: 40S ribosomal protein S8-A

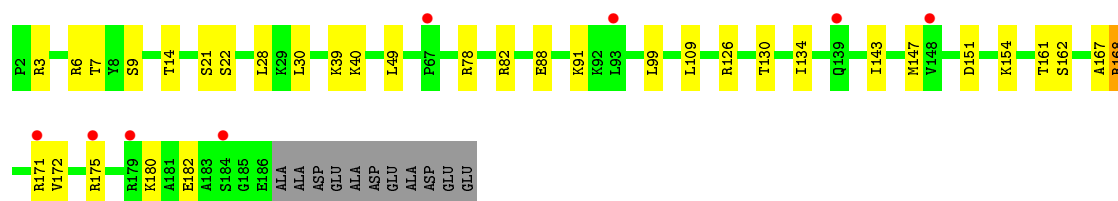
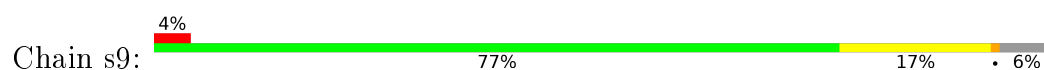


- Molecule 11: 40S ribosomal protein S9-A

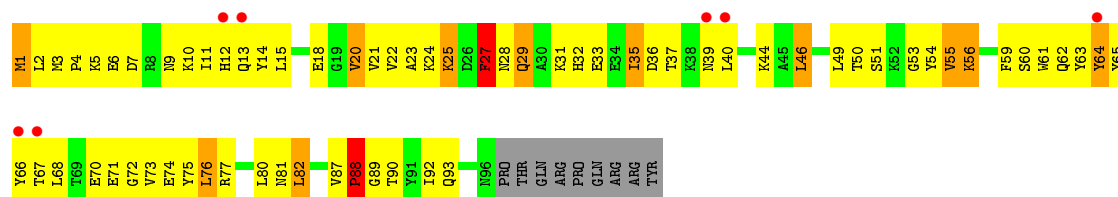




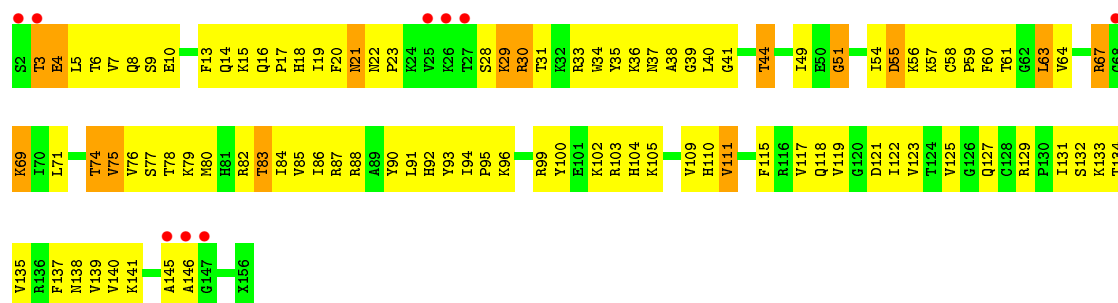
• Molecule 11: 40S ribosomal protein S9-A



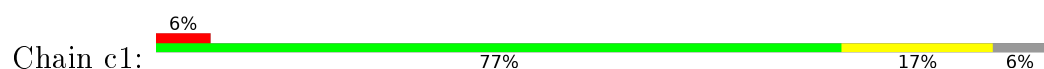
• Molecule 12: 40S ribosomal protein S10-A



• Molecule 13: 40S ribosomal protein S11-A, 40S ribosomal protein S11-A (uS17)

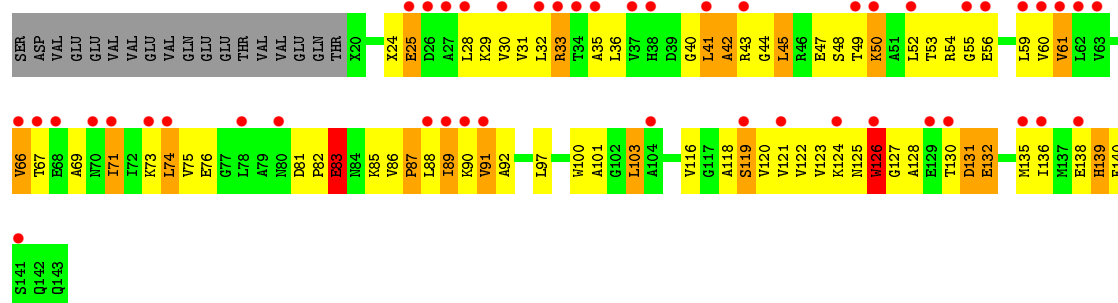


• Molecule 13: 40S ribosomal protein S11-A, 40S ribosomal protein S11-A (uS17)

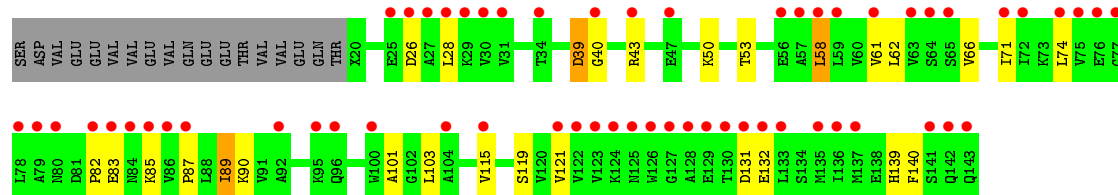
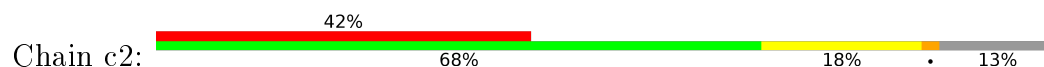




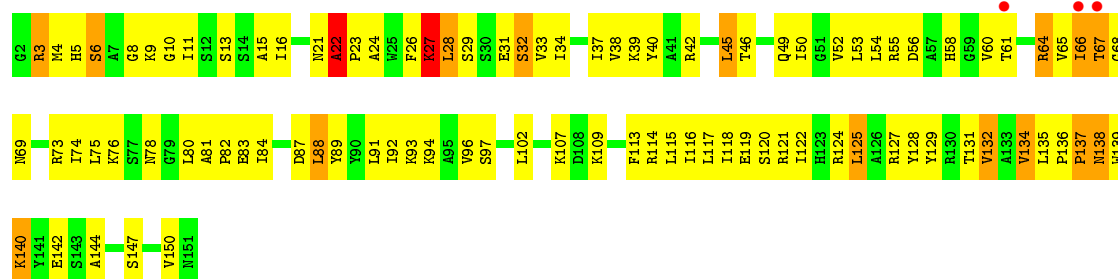
• Molecule 14: 40S ribosomal protein S12



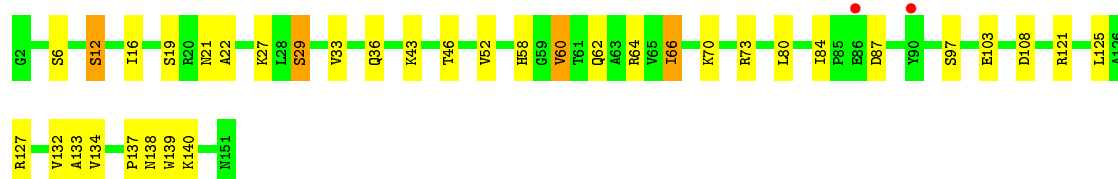
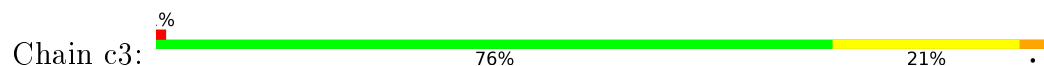
• Molecule 14: 40S ribosomal protein S12



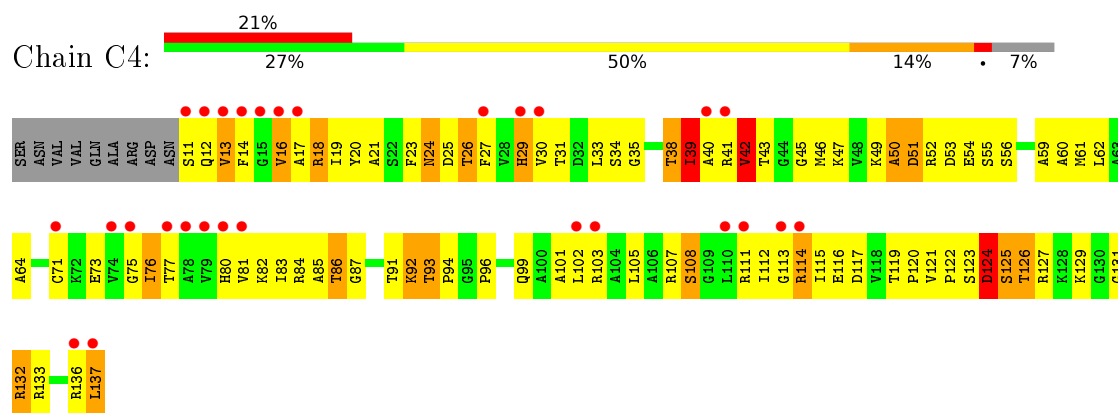
• Molecule 15: 40S ribosomal protein S13



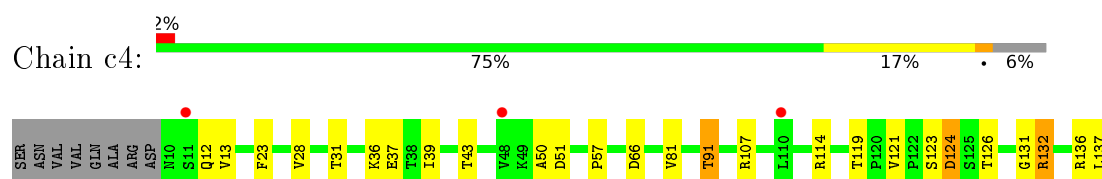
• Molecule 15: 40S ribosomal protein S13



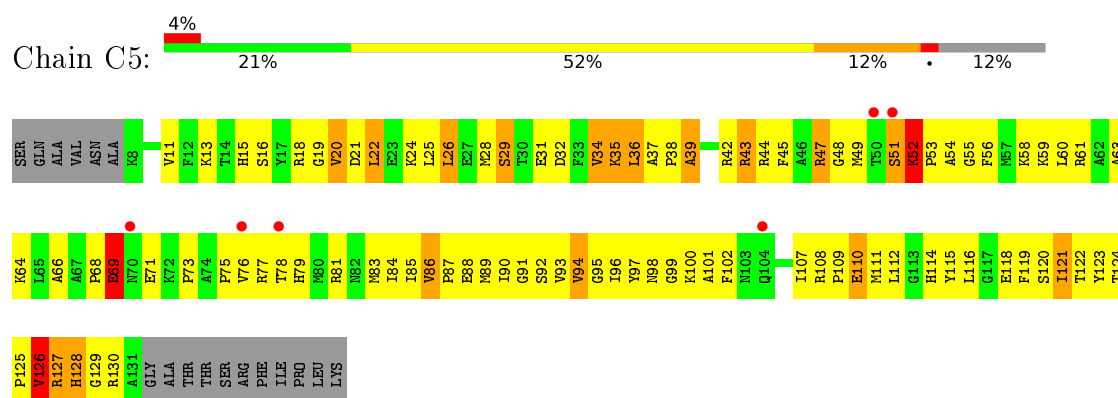
- Molecule 16: 40S ribosomal protein S14-A



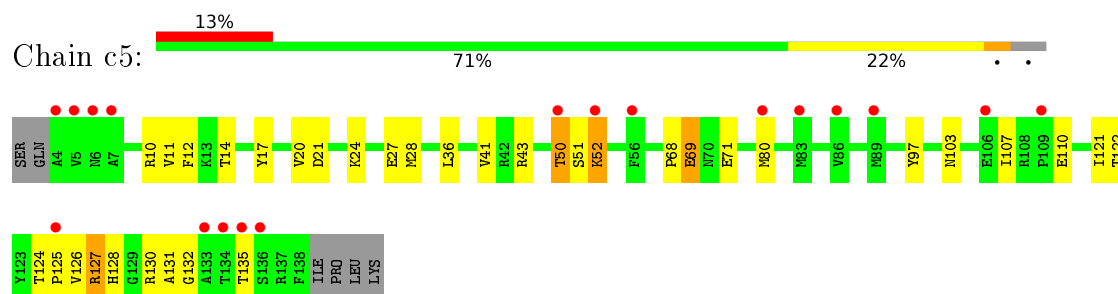
- Molecule 16: 40S ribosomal protein S14-A



- Molecule 17: 40S ribosomal protein S15

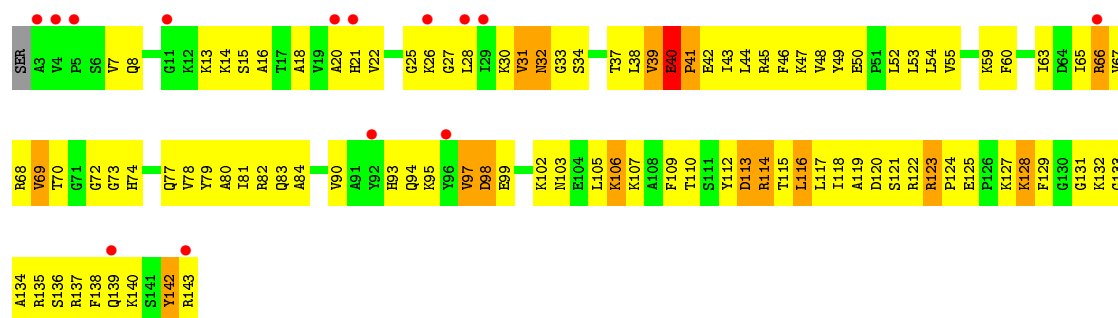


- Molecule 17: 40S ribosomal protein S15

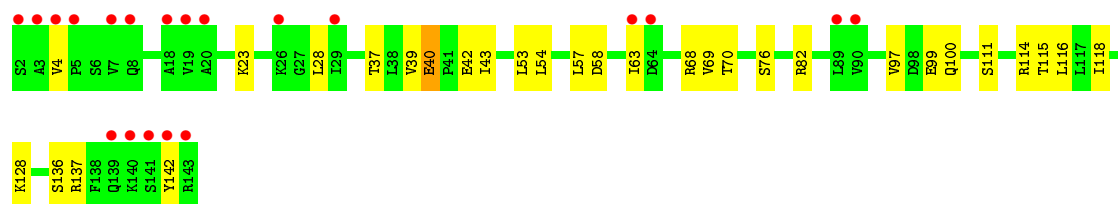
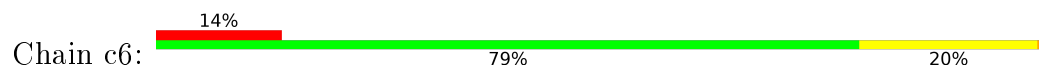


- Molecule 18: 40S ribosomal protein S16-A

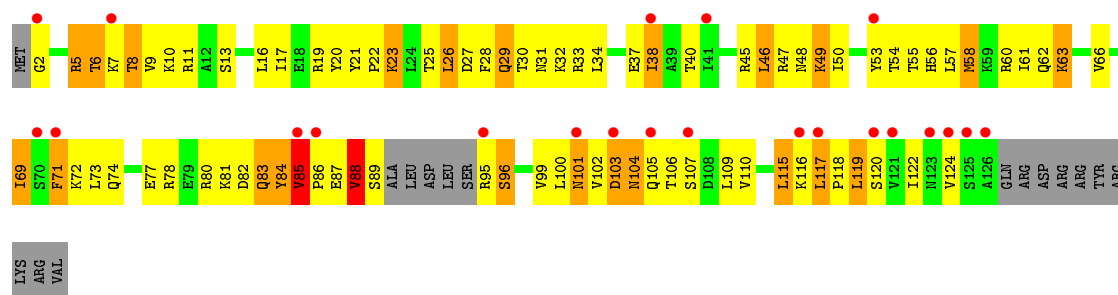




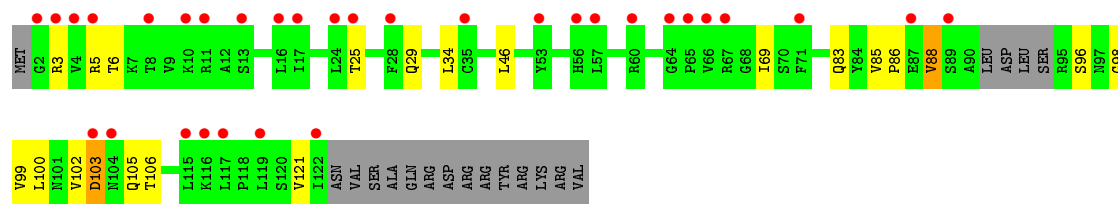
- Molecule 18: 40S ribosomal protein S16-A



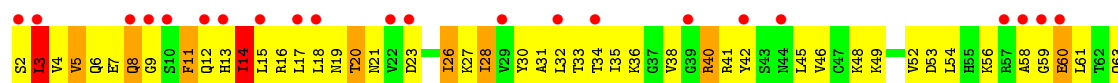
- Molecule 19: 40S ribosomal protein S17-A

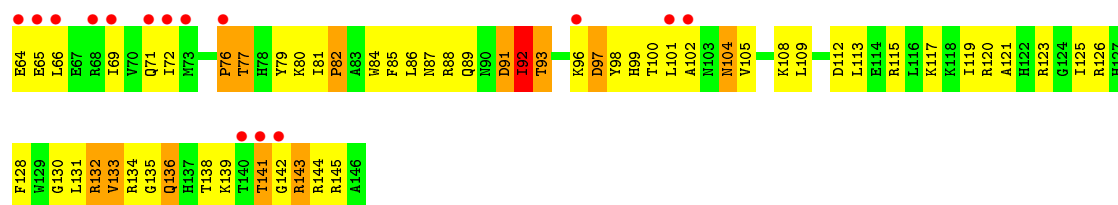


- Molecule 19: 40S ribosomal protein S17-A

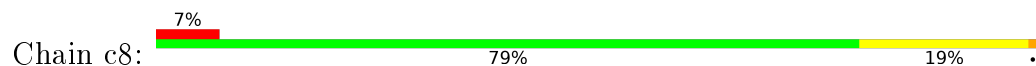


- Molecule 20: 40S ribosomal protein S18-A

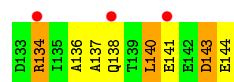
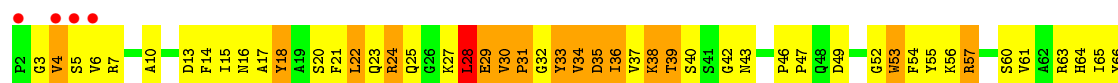




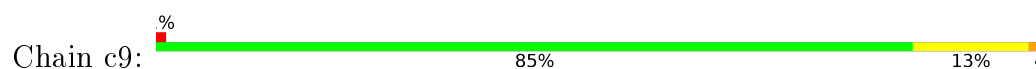
- Molecule 20: 40S ribosomal protein S18-A



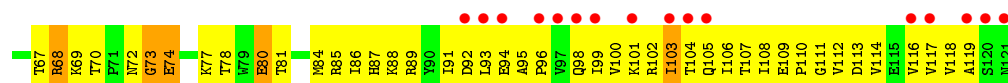
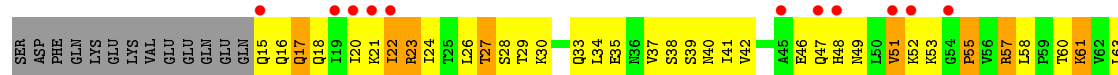
- Molecule 21: 40S ribosomal protein S19-A



- Molecule 21: 40S ribosomal protein S19-A

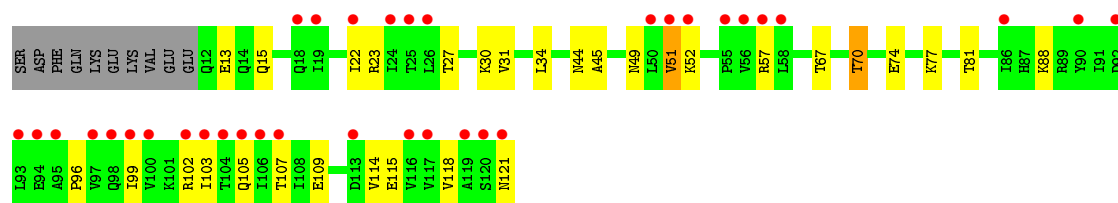


- Molecule 22: 40S ribosomal protein S20

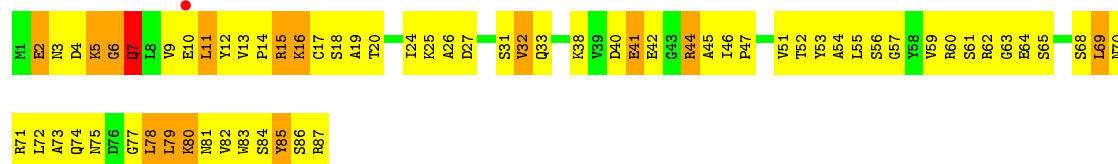


- Molecule 22: 40S ribosomal protein S20

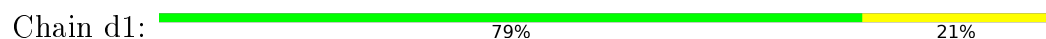




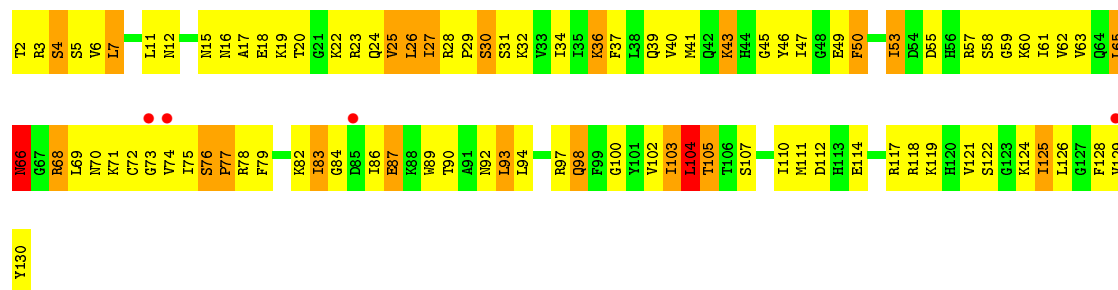
- Molecule 23: 40S ribosomal protein S21-A



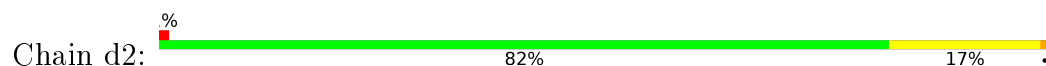
- Molecule 23: 40S ribosomal protein S21-A



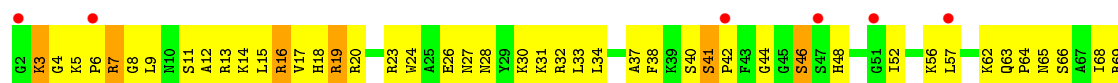
- Molecule 24: 40S ribosomal protein S22-A

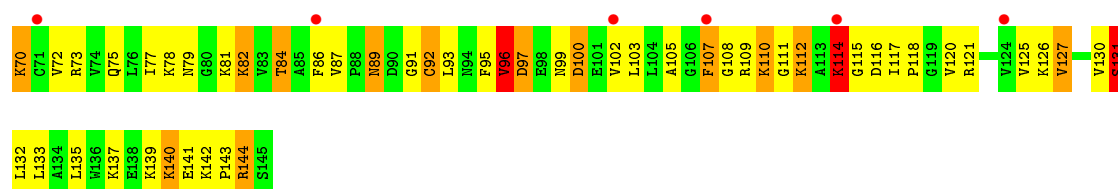


- Molecule 24: 40S ribosomal protein S22-A



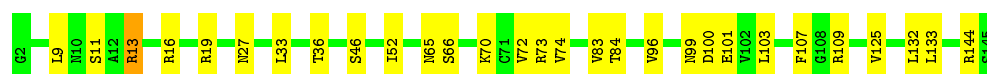
- Molecule 25: 40S ribosomal protein S23-A





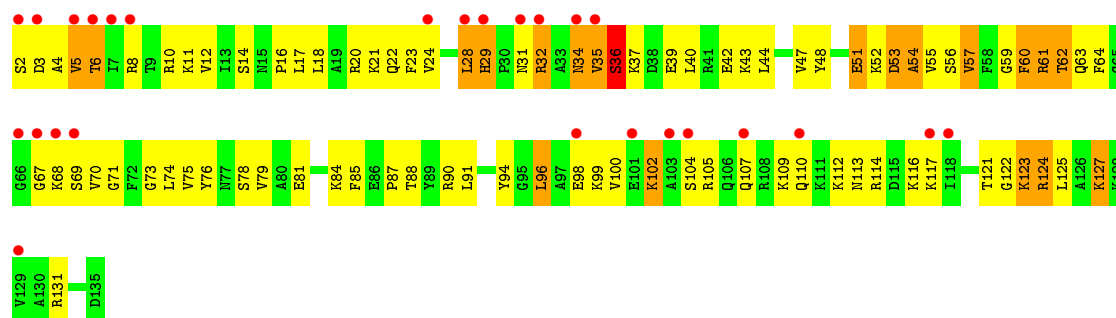
- Molecule 25: 40S ribosomal protein S23-A

Chain d3: 80% 19% .



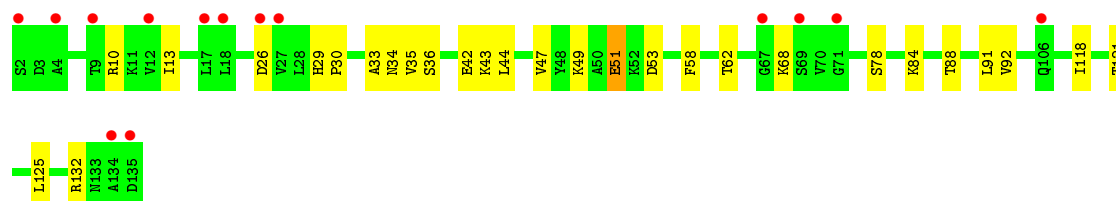
- Molecule 26: 40S ribosomal protein S24-A

Chain D4: 19% 35% 50% 14% .



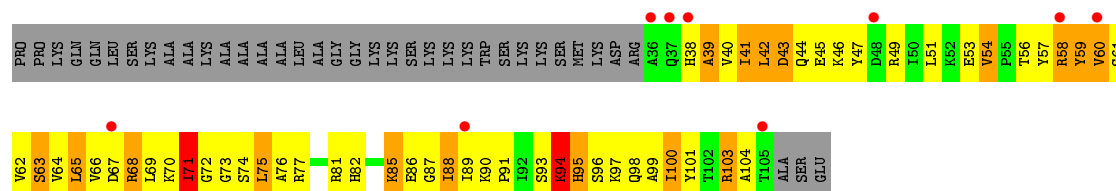
- Molecule 26: 40S ribosomal protein S24-A

Chain d4: 10% 79% 20% .

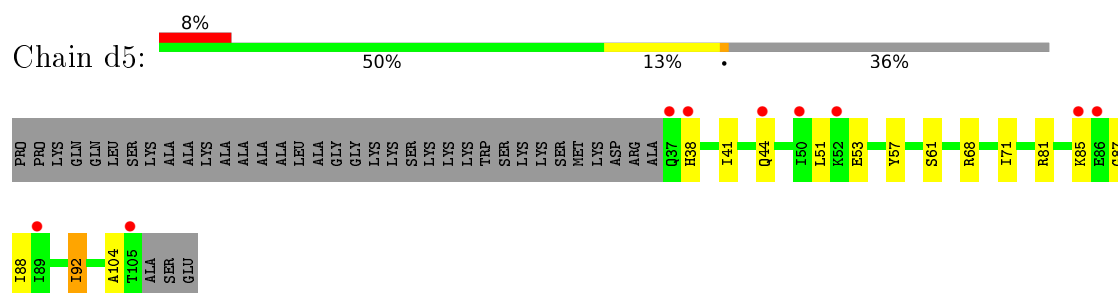


- Molecule 27: 40S ribosomal protein S25-A

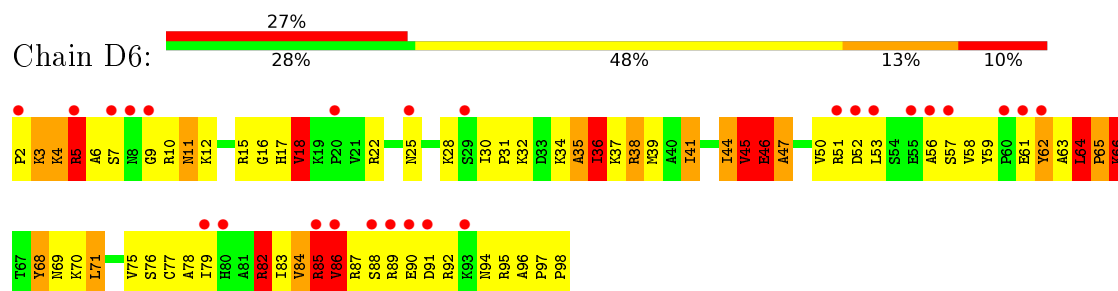
Chain D5: 8% 13% 35% 16% 35% .



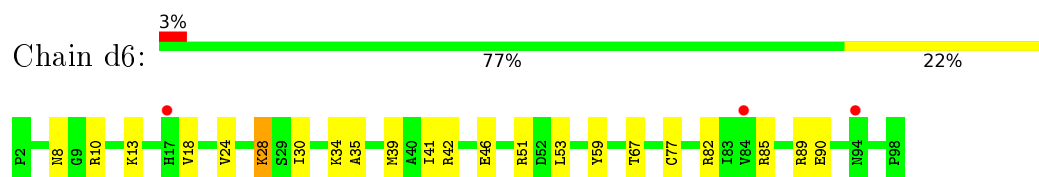
- Molecule 27: 40S ribosomal protein S25-A



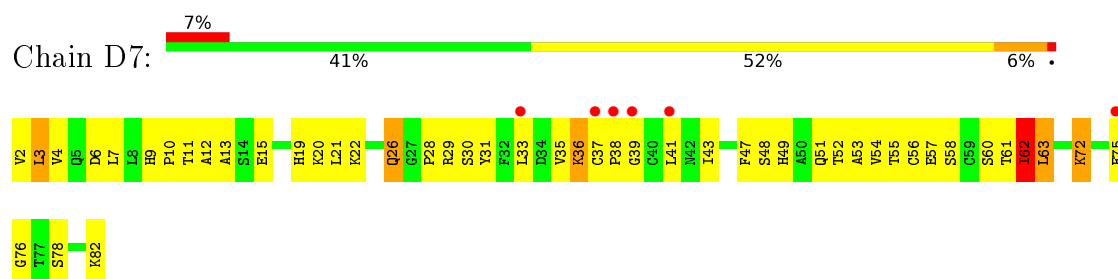
- Molecule 28: 40S ribosomal protein S26-A



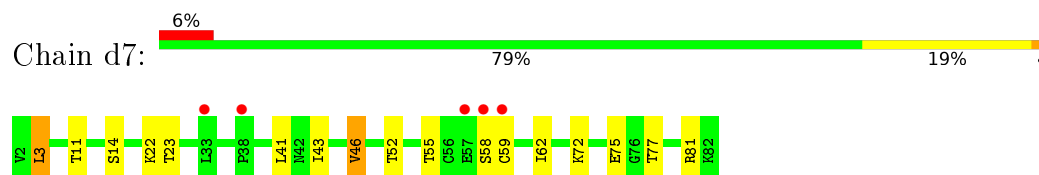
- Molecule 28: 40S ribosomal protein S26-A



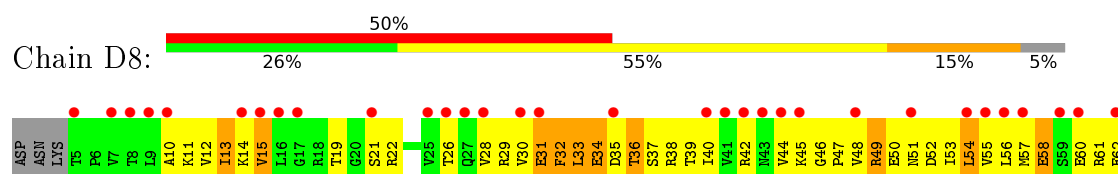
- Molecule 29: 40S ribosomal protein S27-A

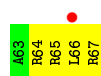


- Molecule 29: 40S ribosomal protein S27-A

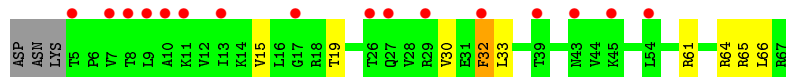
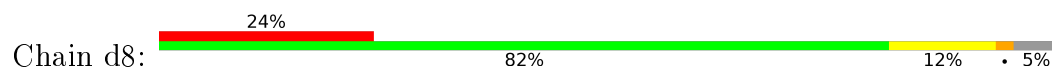


- Molecule 30: 40S ribosomal protein S28-A

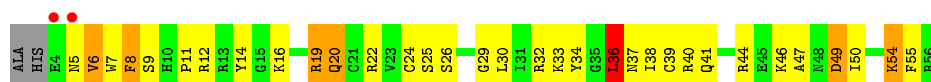




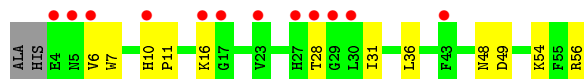
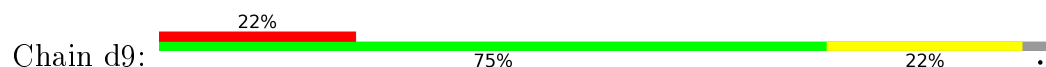
- Molecule 30: 40S ribosomal protein S28-A



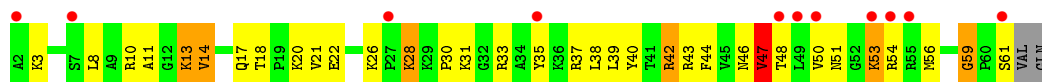
- Molecule 31: 40S ribosomal protein S29-A



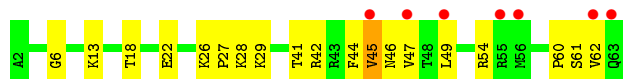
- Molecule 31: 40S ribosomal protein S29-A



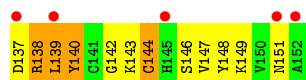
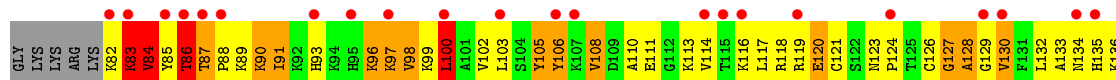
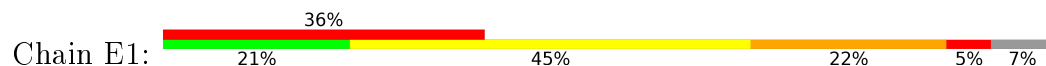
- Molecule 32: 40S ribosomal protein S30-A



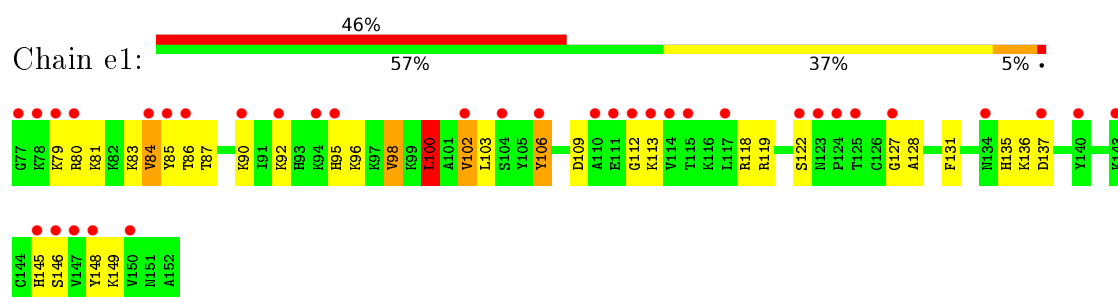
- Molecule 32: 40S ribosomal protein S30-A



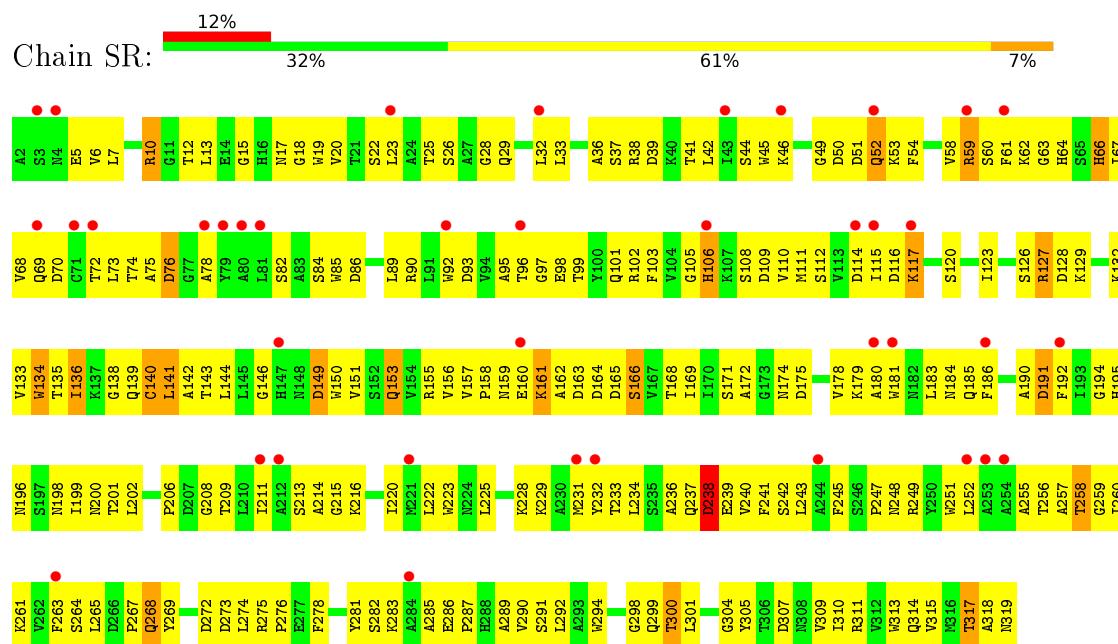
- Molecule 33: 40S ribosomal protein S31



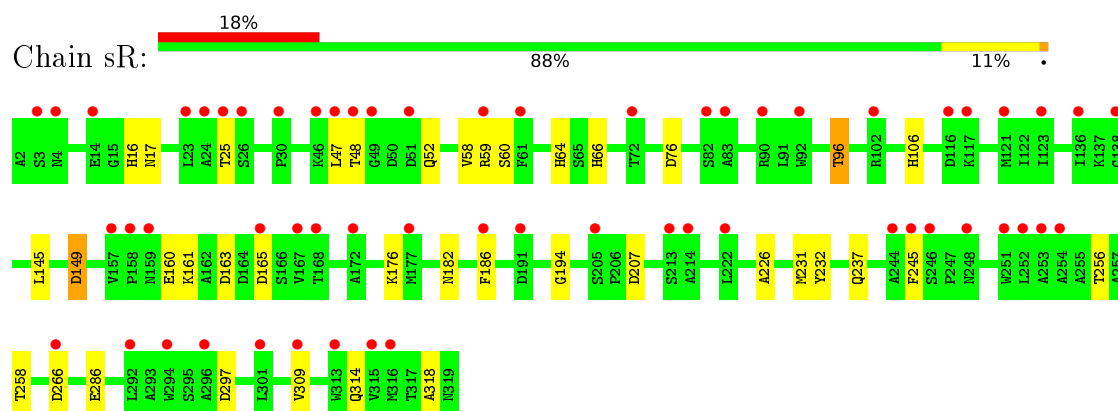
- Molecule 33: 40S ribosomal protein S31



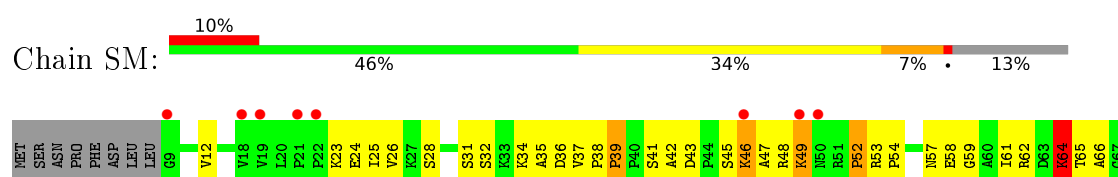
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

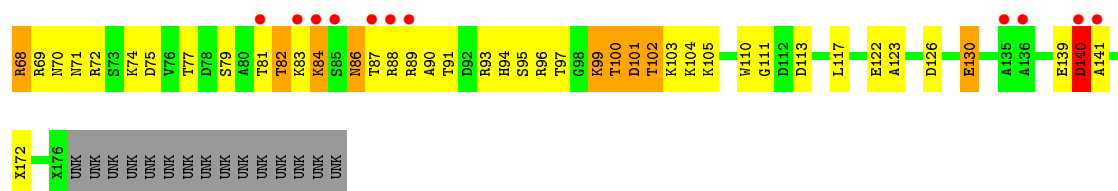


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

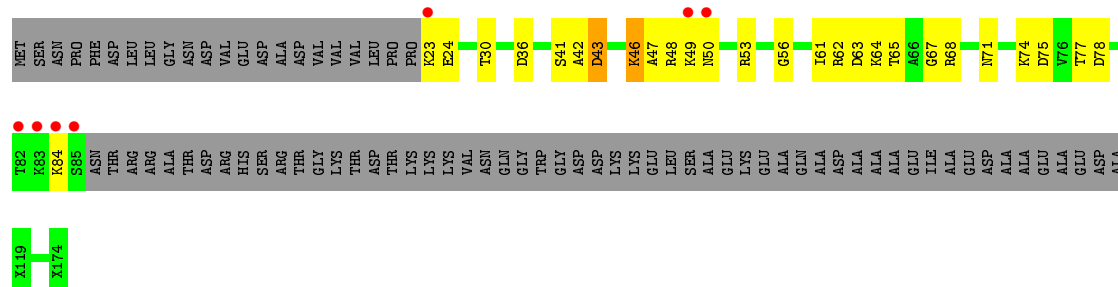
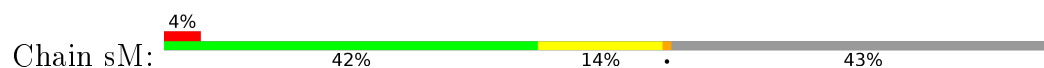


• Molecule 35: Suppressor protein STM1, Suppressor protein STM1

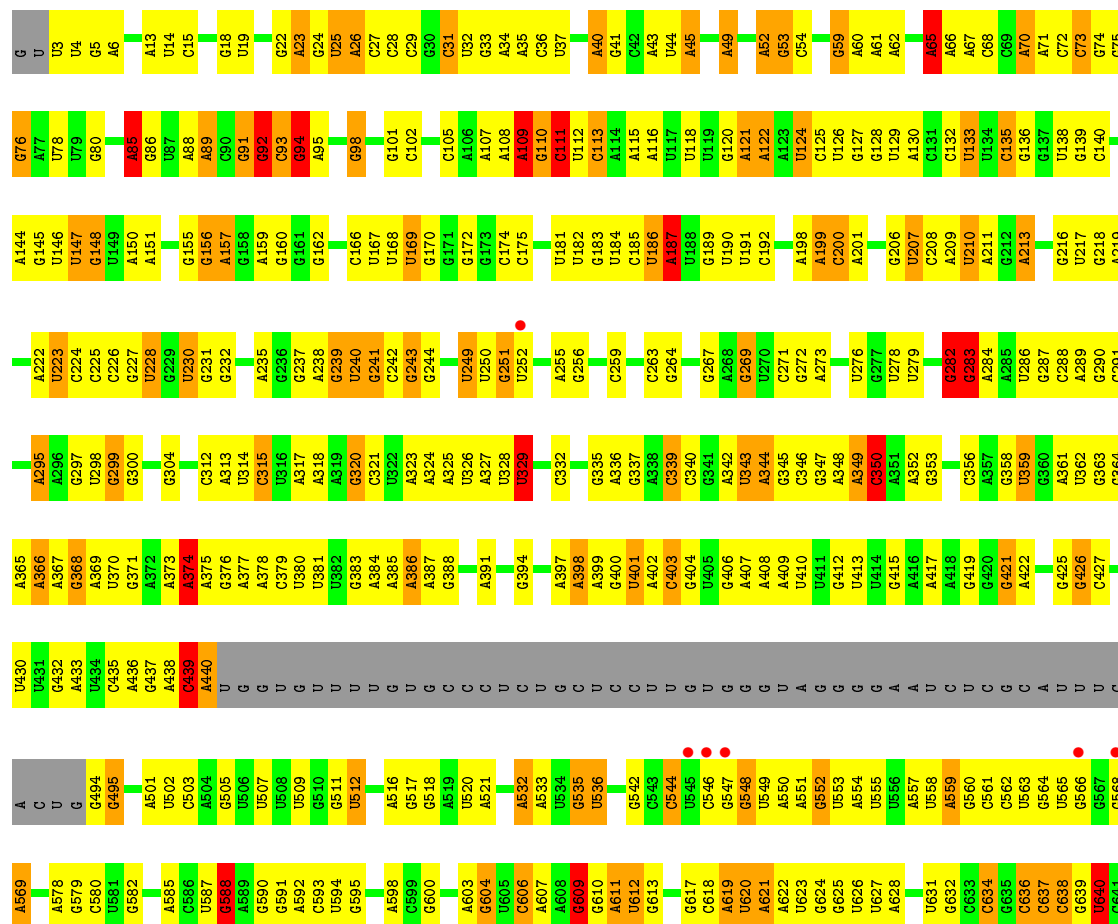




• Molecule 35: Suppressor protein STM1, Suppressor protein STM1

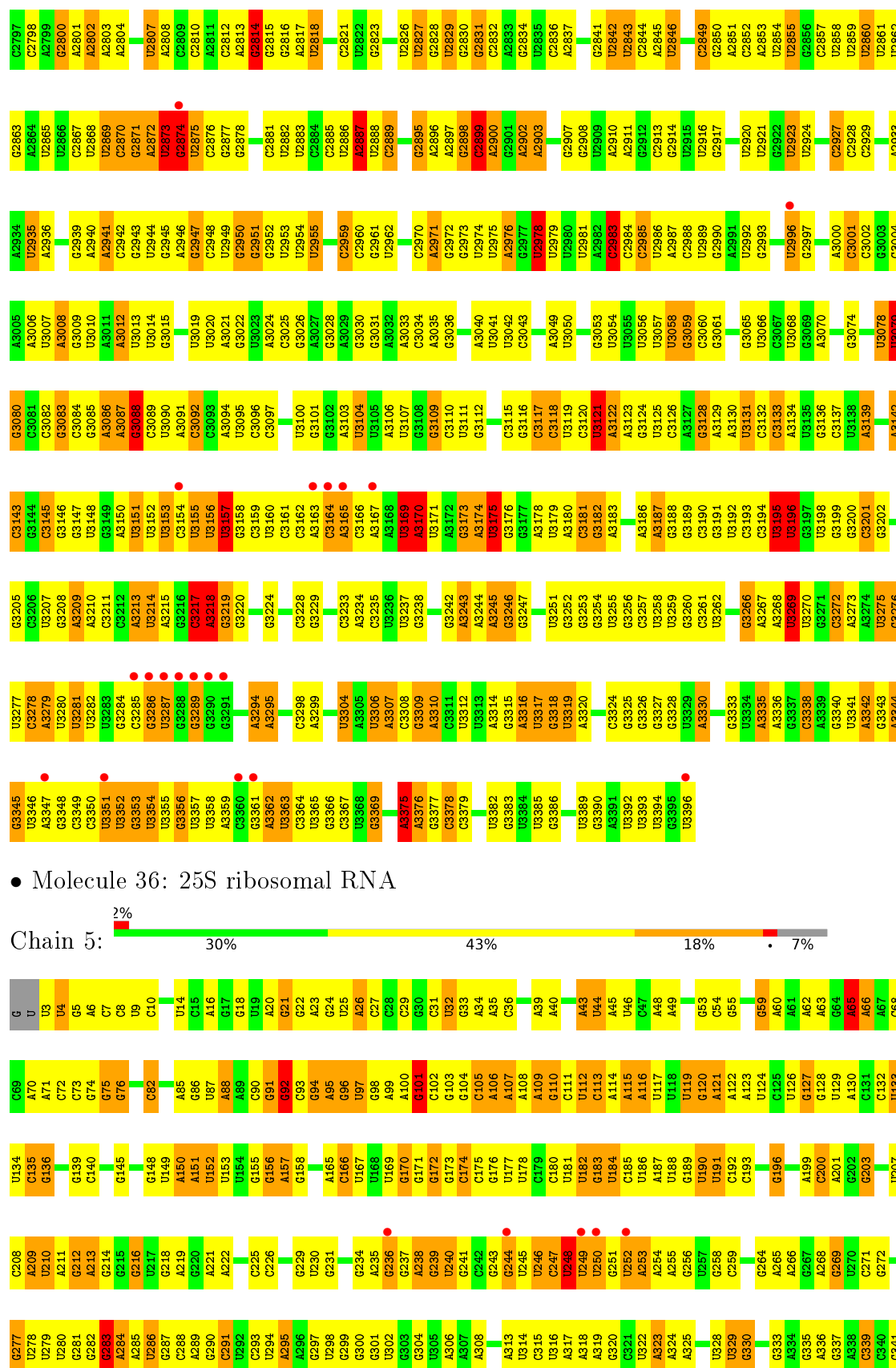


• Molecule 36: 25S ribosomal RNA



A1605	A1606	A1607	C1608	G1609	G1610	A1613	C1614	C1615	C1616	G1617	G1618	A1619	C1620	A1621	G1622	G1623	U1629	U1630	C1631	A1632	G1633	G1634	G1635	U1636	U1637	A1638	C1639	A1642	A1643	C1644	U1645	G1646	G1650	G1653	A1654	G1655	A1656	A1657	A1658	A1659	A1660	A1661	U1662	U1663	U1664	A1665	G1668	U1669	C670	U671	A672	C675	U676	A677	U678	C743	A744	U680	U681	U682	U683	U684	A751	U687	U688	U689	A690	A691	A692	A693	G694	C695	U696	U697	U698	U699	A837	U768	A699	C702	U703	U704	A705
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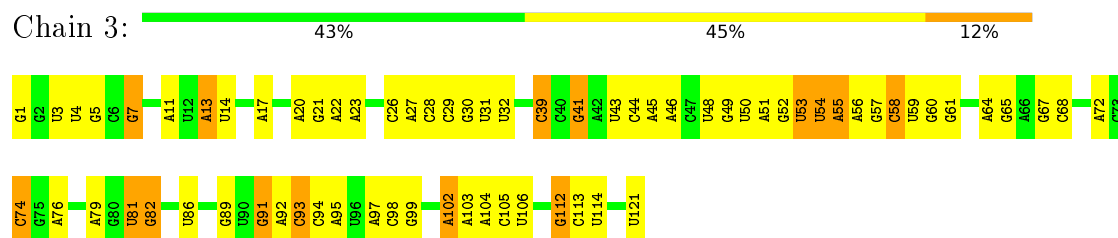


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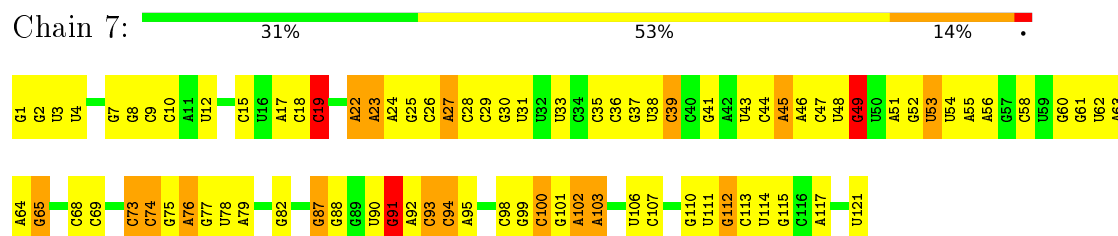


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												U3113	G2902	G2840	G2699	G2630	C
												A3114	A2903	G2841	U2701	U2631	C
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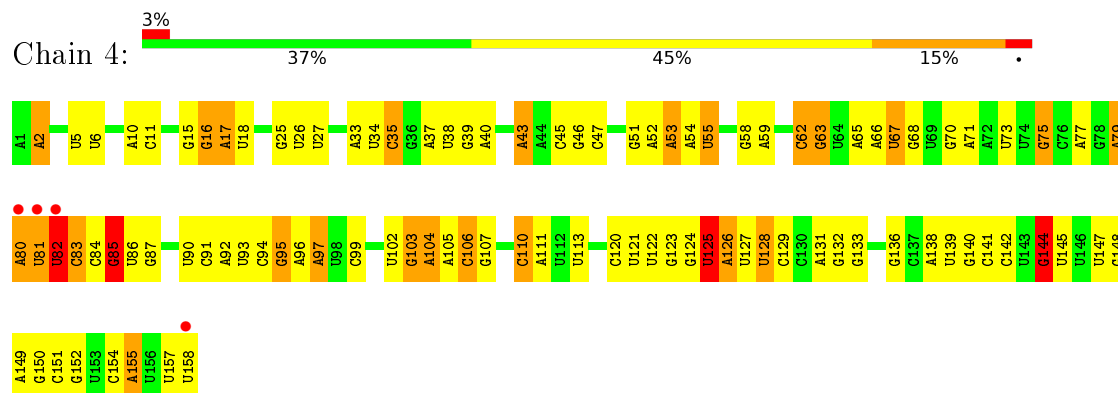
- Molecule 37: 5S ribosomal RNA



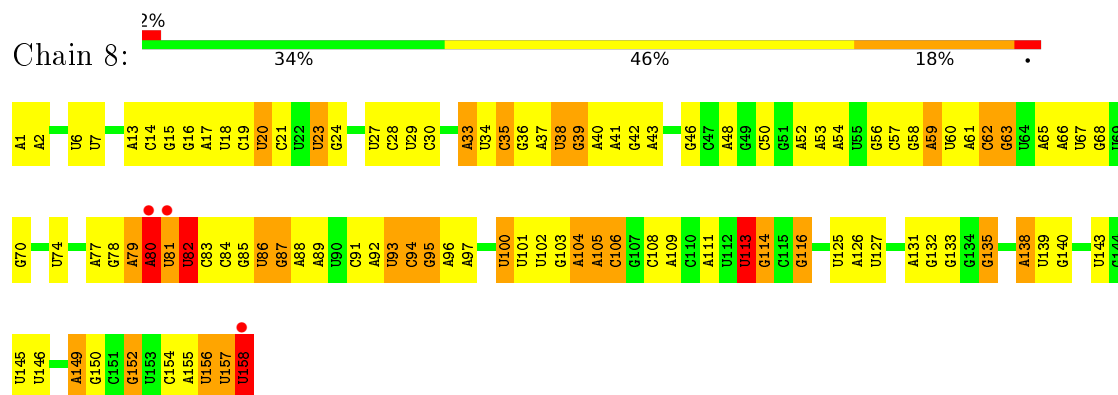
• Molecule 37: 5S ribosomal RNA



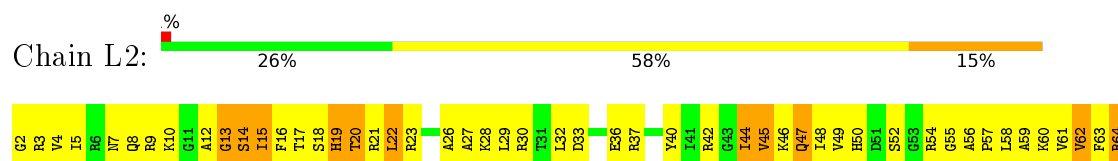
• Molecule 38: 5.8S ribosomal RNA

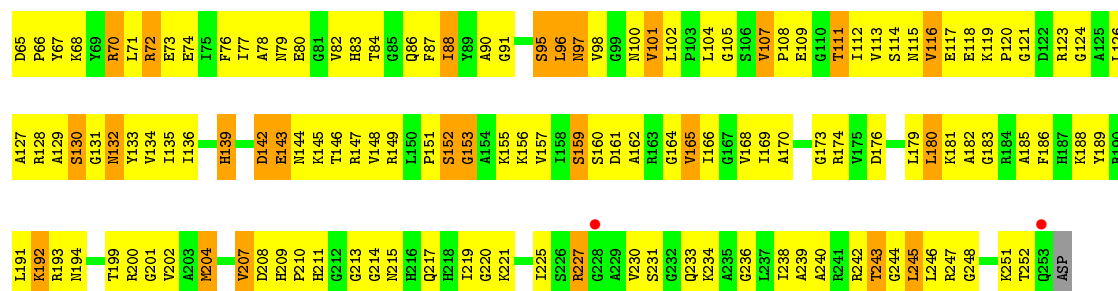


• Molecule 38: 5.8S ribosomal RNA

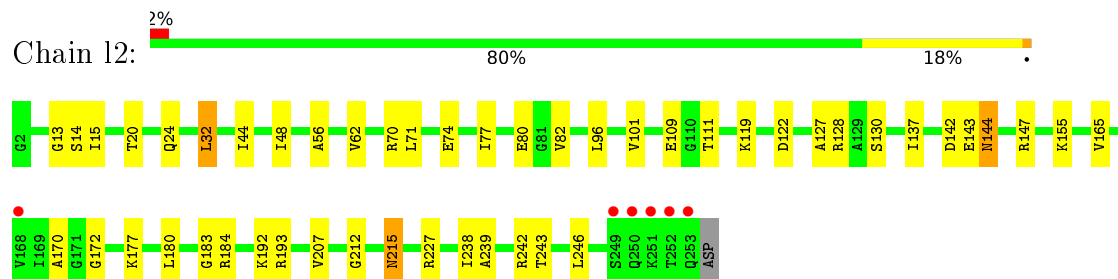


• Molecule 39: 60S ribosomal protein L2-A

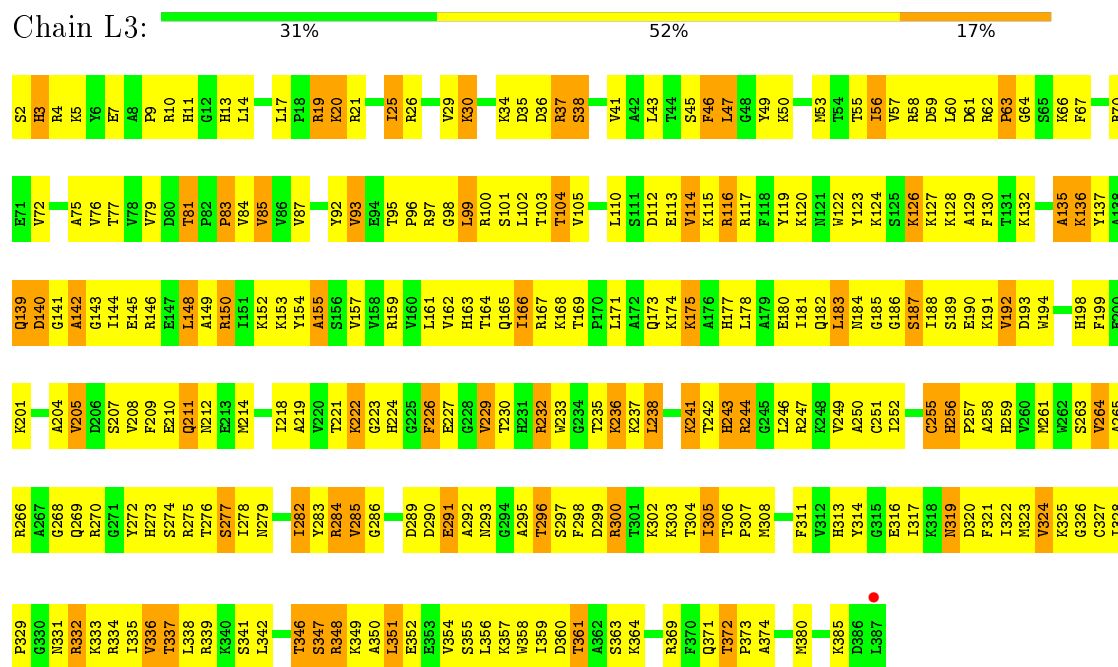




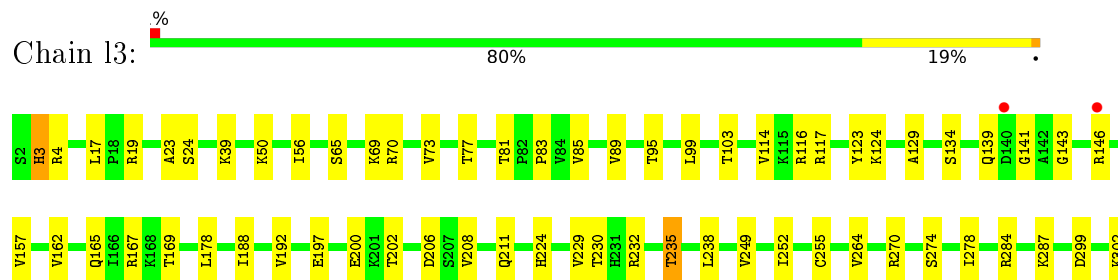
• Molecule 39: 60S ribosomal protein L2-A



• Molecule 40: 60S ribosomal protein L3

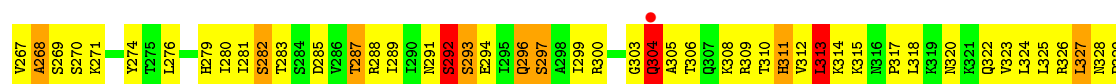
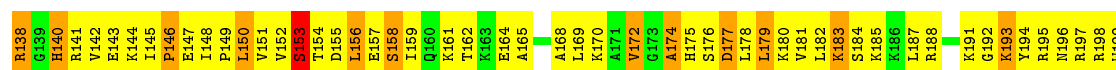
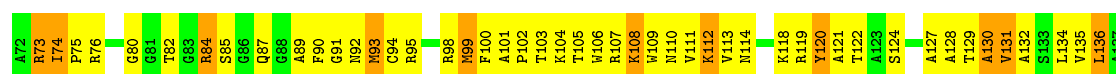


• Molecule 40: 60S ribosomal protein L3

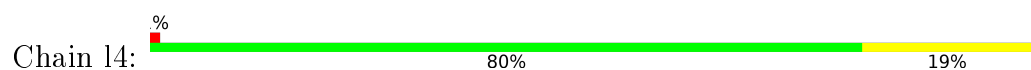




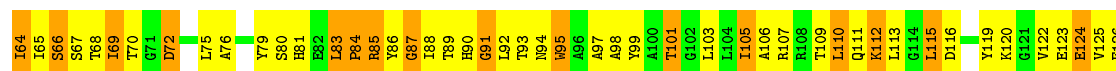
• Molecule 41: 60S ribosomal protein L4-A

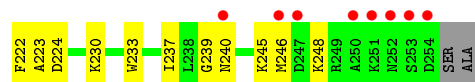


• Molecule 41: 60S ribosomal protein L4-A

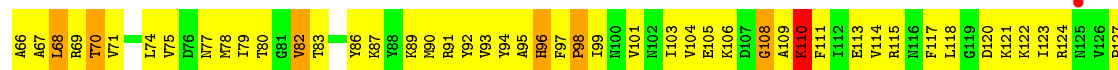
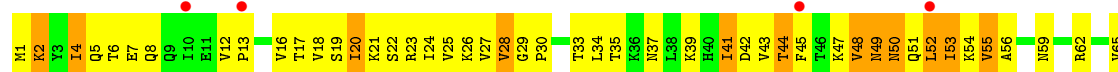


• Molecule 42: 60S ribosomal protein L5

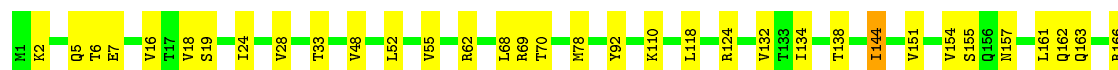
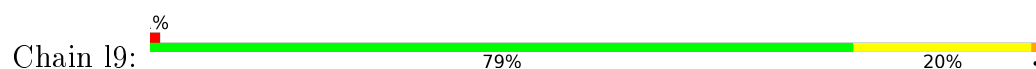




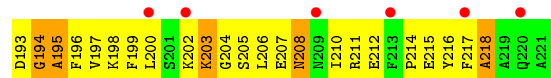
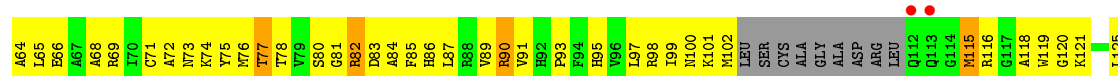
• Molecule 46: 60S ribosomal protein L9-A



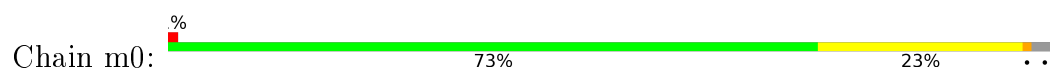
• Molecule 46: 60S ribosomal protein L9-A

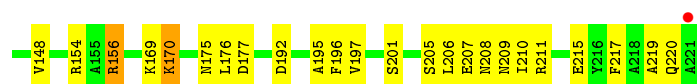


• Molecule 47: 60S ribosomal protein L10

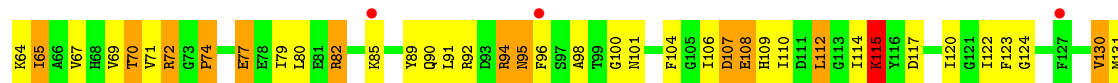
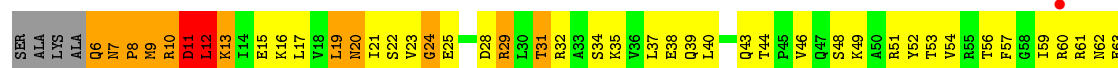


• Molecule 47: 60S ribosomal protein L10

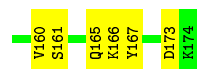
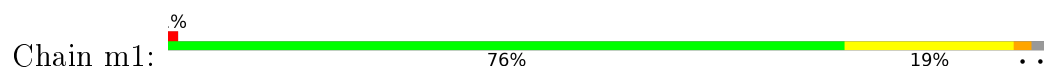




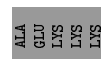
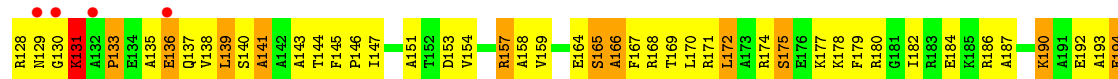
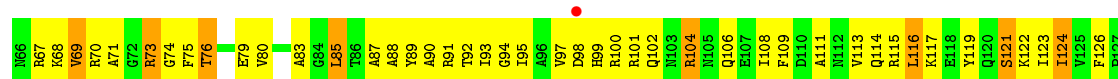
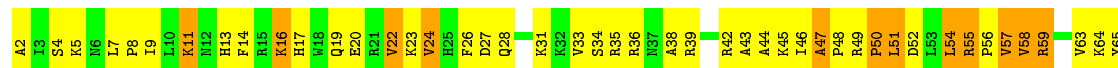
• Molecule 48: 60S ribosomal protein L11-A



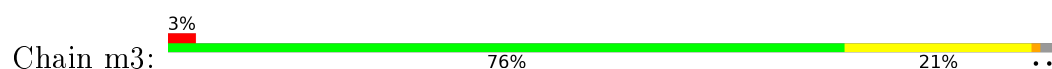
• Molecule 48: 60S ribosomal protein L11-A



• Molecule 49: 60S ribosomal protein L13-A

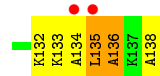


• Molecule 49: 60S ribosomal protein L13-A

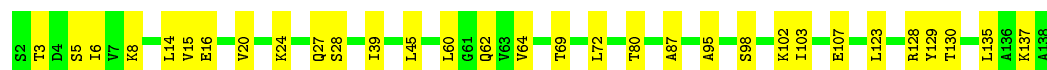
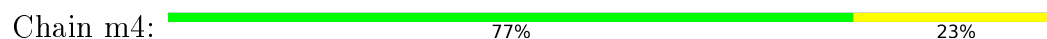




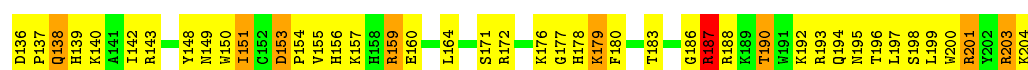
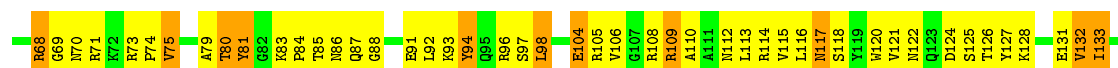
- Molecule 50: 60S ribosomal protein L14-A



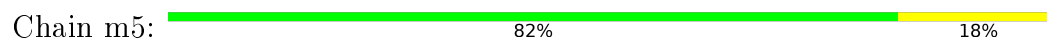
- Molecule 50: 60S ribosomal protein L14-A



- Molecule 51: 60S ribosomal protein L15-A



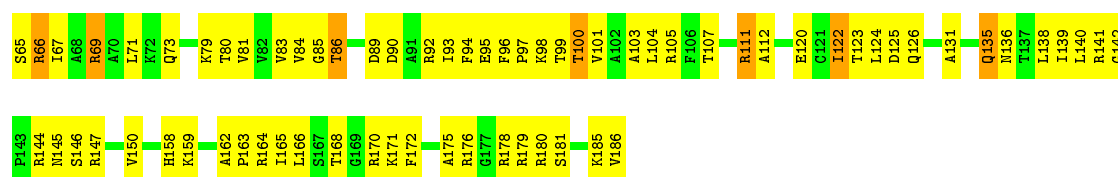
- Molecule 51: 60S ribosomal protein L15-A



- Molecule 52: 60S ribosomal protein L16-A







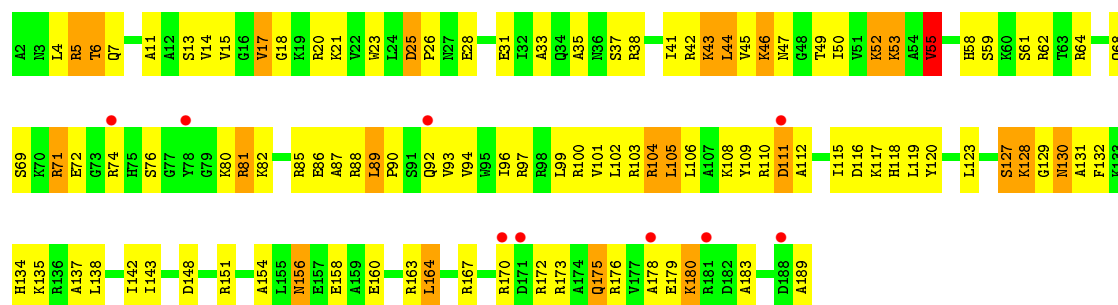
• Molecule 54: 60S ribosomal protein L18-A

Chain m8: 81% 18%



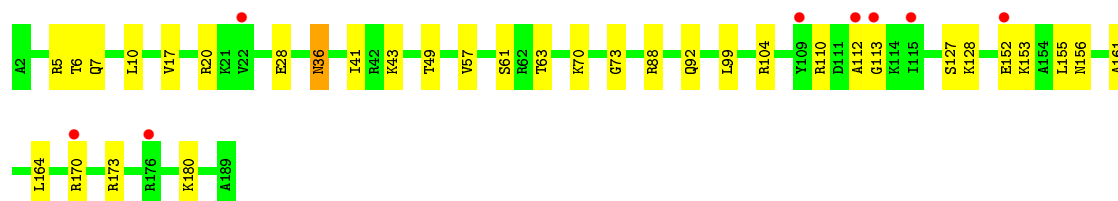
• Molecule 55: 60S ribosomal protein L19-A

Chain M9: 5% 42% 46% 12%



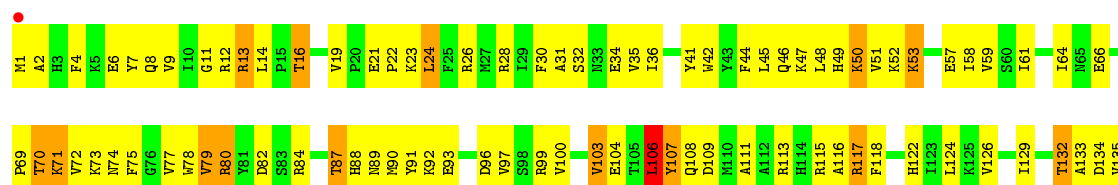
• Molecule 55: 60S ribosomal protein L19-A

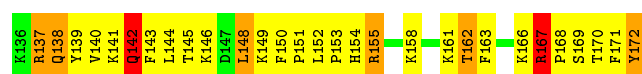
Chain m9: 4% 82% 18%



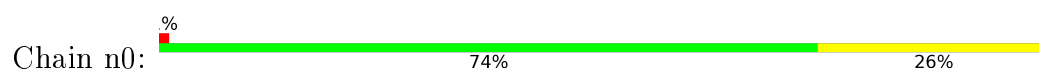
• Molecule 56: 60S ribosomal protein L20-A

Chain N0: 33% 54% 12%

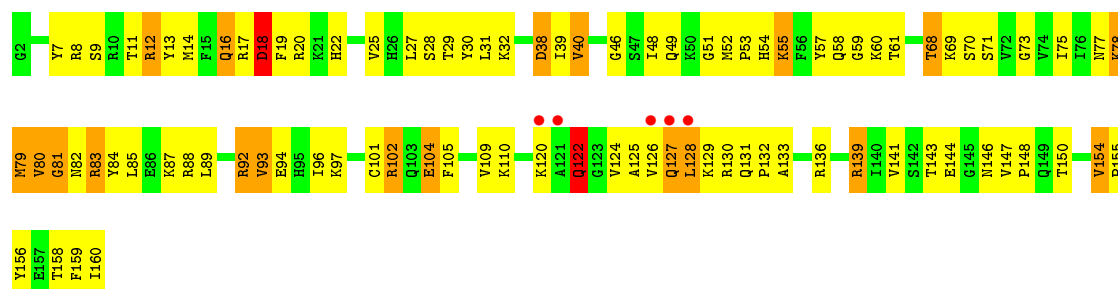




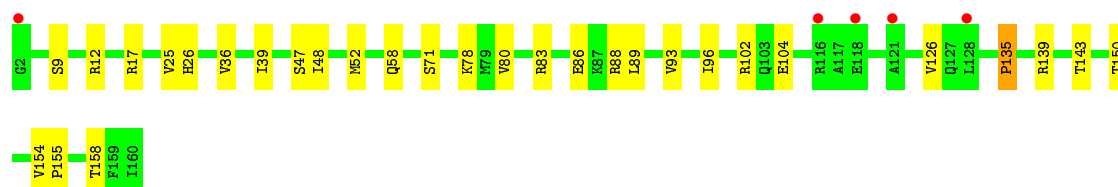
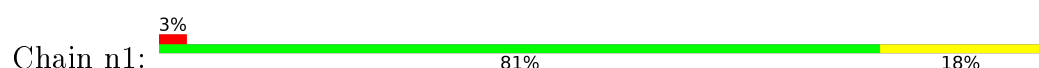
- Molecule 56: 60S ribosomal protein L20-A



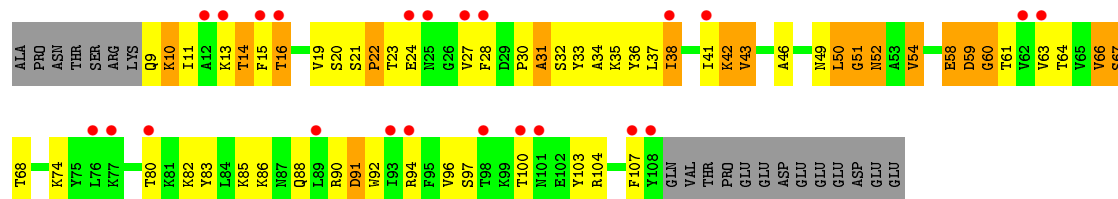
- Molecule 57: 60S ribosomal protein L21-A



- Molecule 57: 60S ribosomal protein L21-A

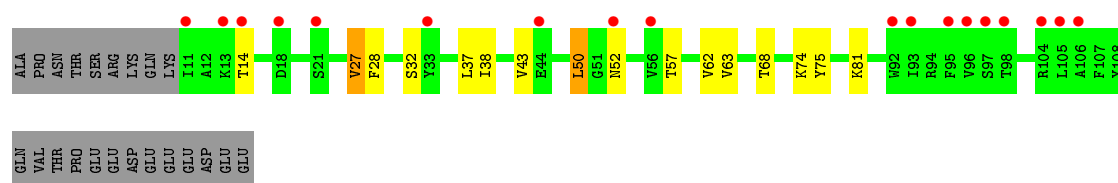


- Molecule 58: 60S ribosomal protein L22-A

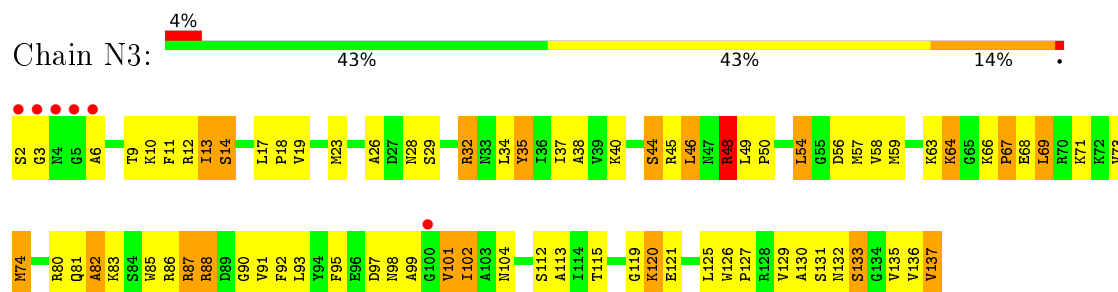


- Molecule 58: 60S ribosomal protein L22-A

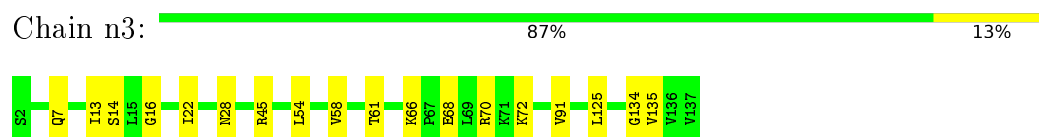




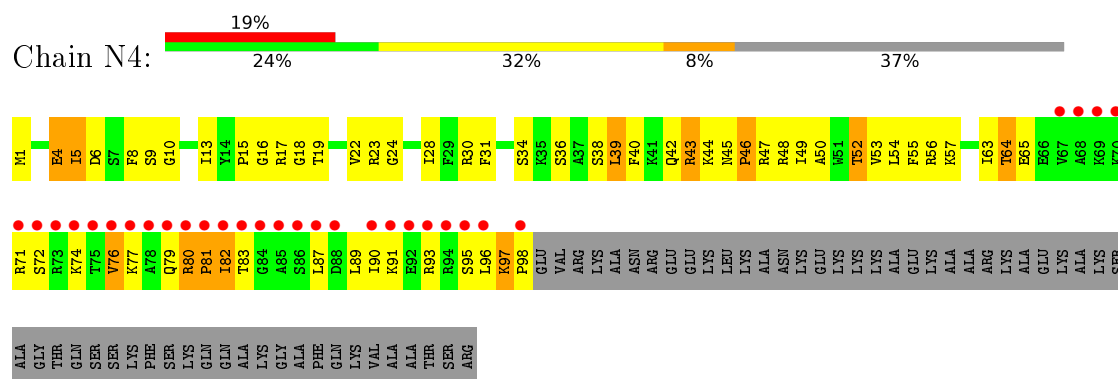
- Molecule 59: 60S ribosomal protein L23-A



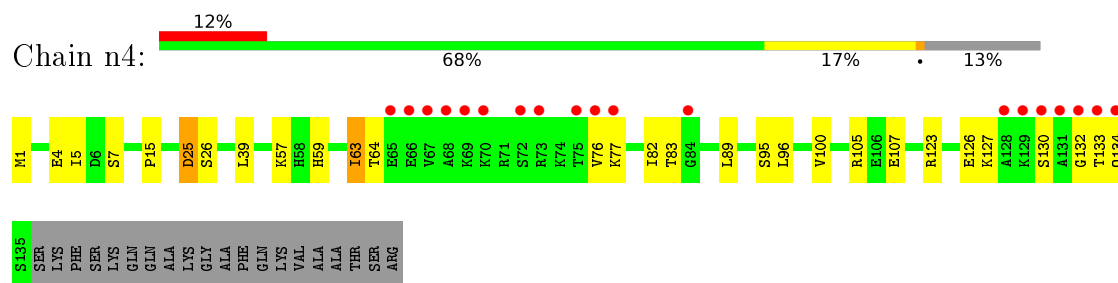
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 60: 60S ribosomal protein L24-A



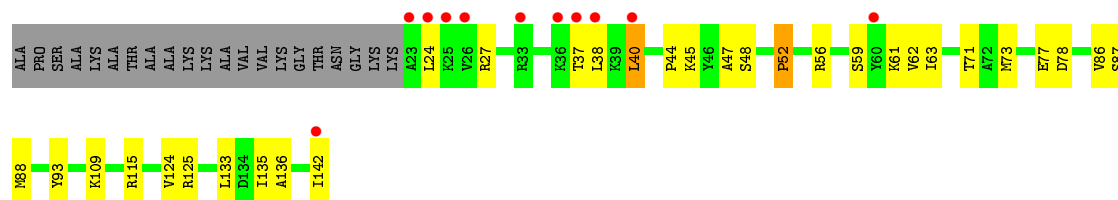
- Molecule 60: 60S ribosomal protein L24-A



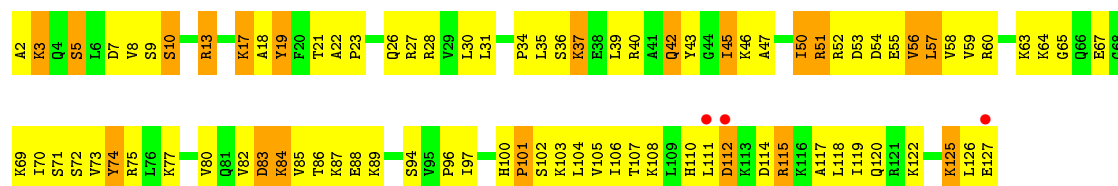
- Molecule 61: 60S ribosomal protein L25



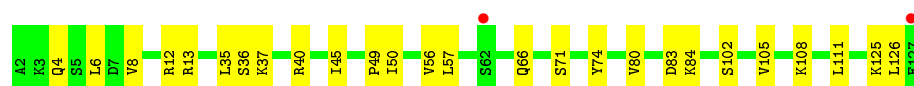
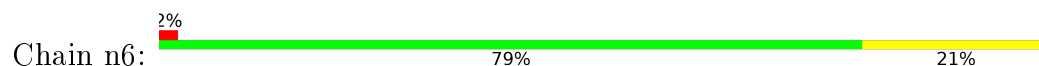
- Molecule 61: 60S ribosomal protein L25



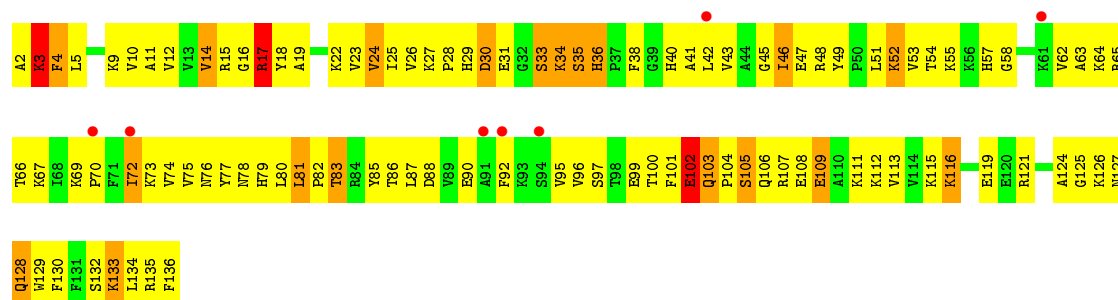
- Molecule 62: 60S ribosomal protein L26-A



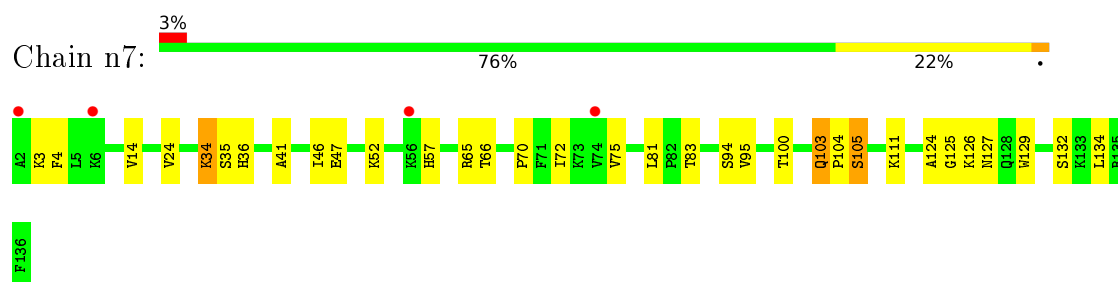
- Molecule 62: 60S ribosomal protein L26-A



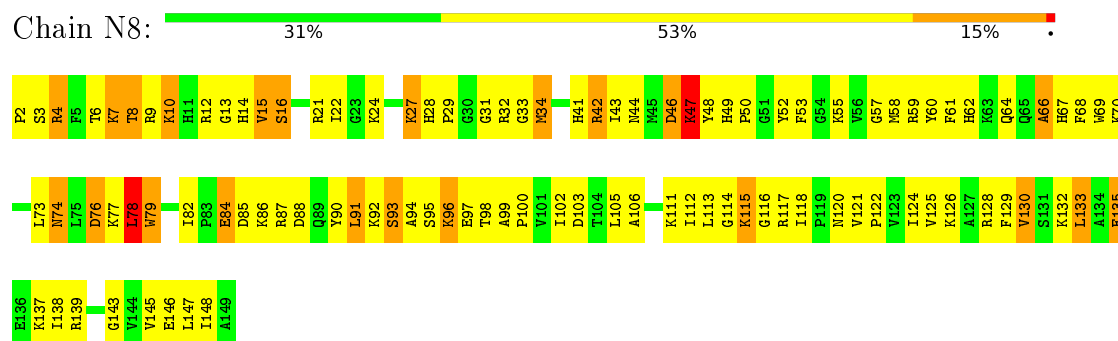
- Molecule 63: 60S ribosomal protein L27-A



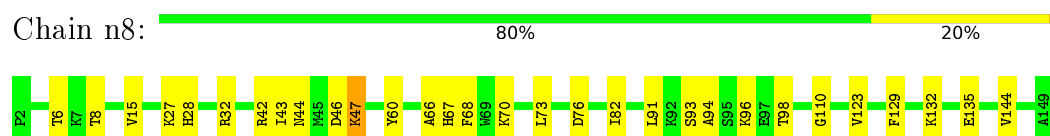
• Molecule 63: 60S ribosomal protein L27-A



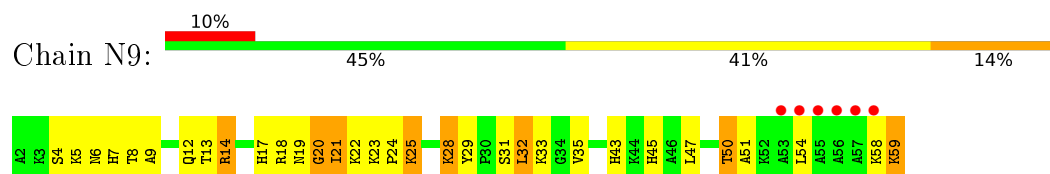
• Molecule 64: 60S ribosomal protein L28



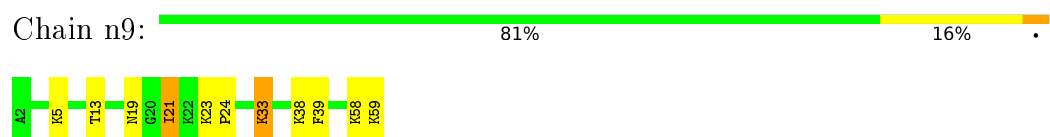
• Molecule 64: 60S ribosomal protein L28



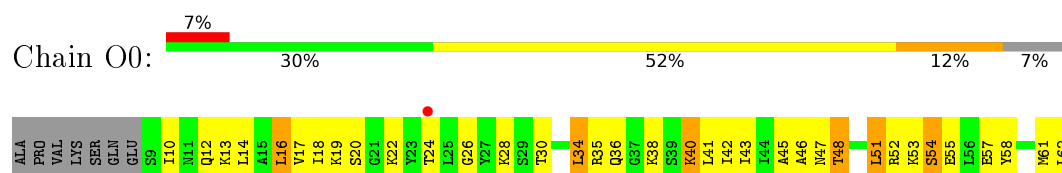
• Molecule 65: 60S ribosomal protein L29

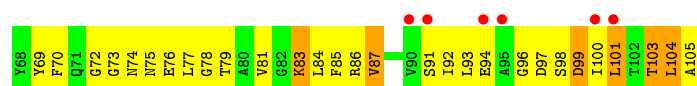


• Molecule 65: 60S ribosomal protein L29

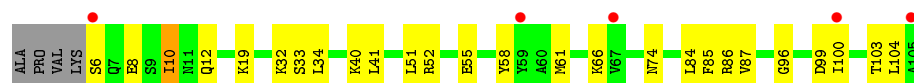
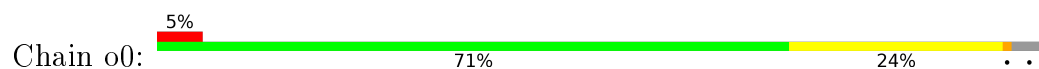


• Molecule 66: 60S ribosomal protein L30

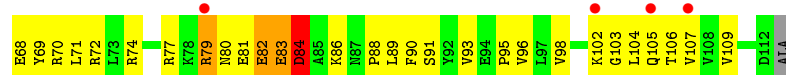




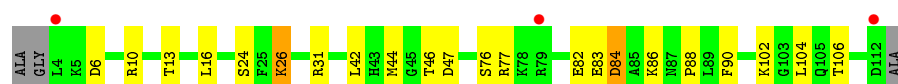
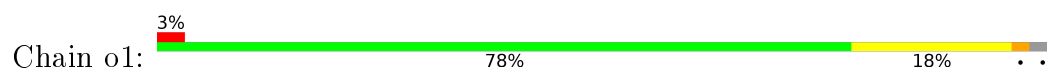
- Molecule 66: 60S ribosomal protein L30



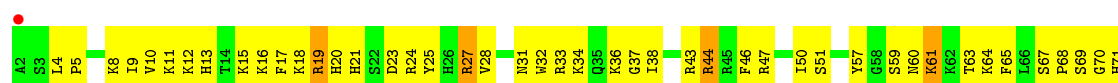
- Molecule 67: 60S ribosomal protein L31-A



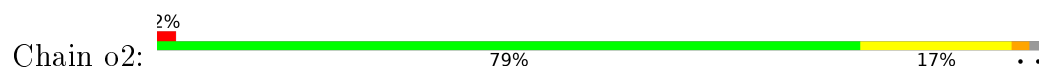
- Molecule 67: 60S ribosomal protein L31-A



- Molecule 68: 60S ribosomal protein L32

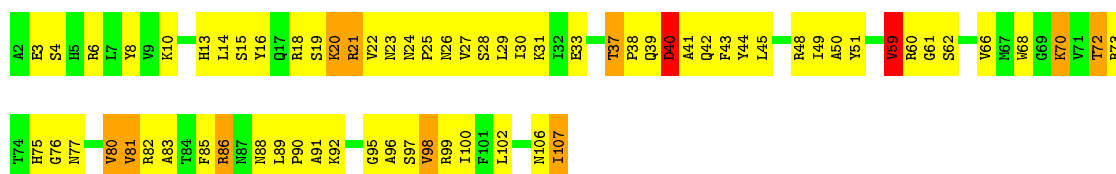


- Molecule 68: 60S ribosomal protein L32



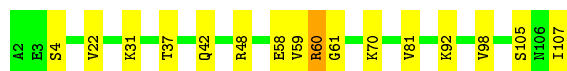
- Molecule 69: 60S ribosomal protein L33-A





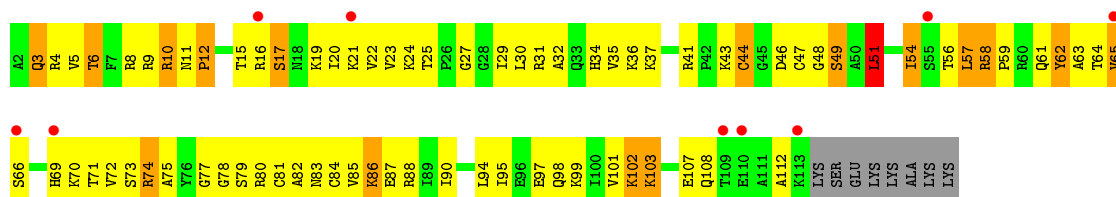
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 85% 14% .



- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 8% 28% 51% 13% 7% .



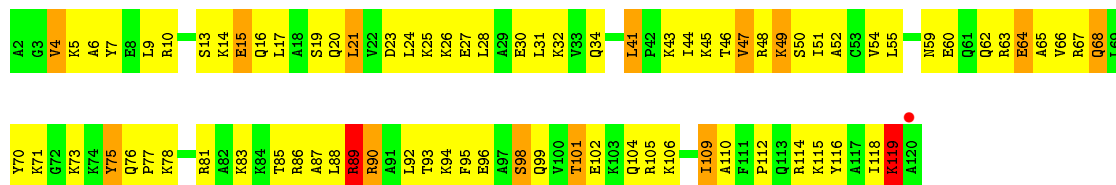
- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 6% 77% 16% 7% .



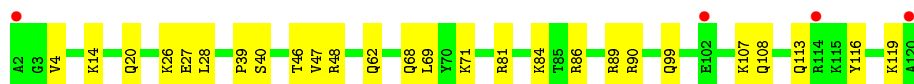
- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 32% 55% 11% .

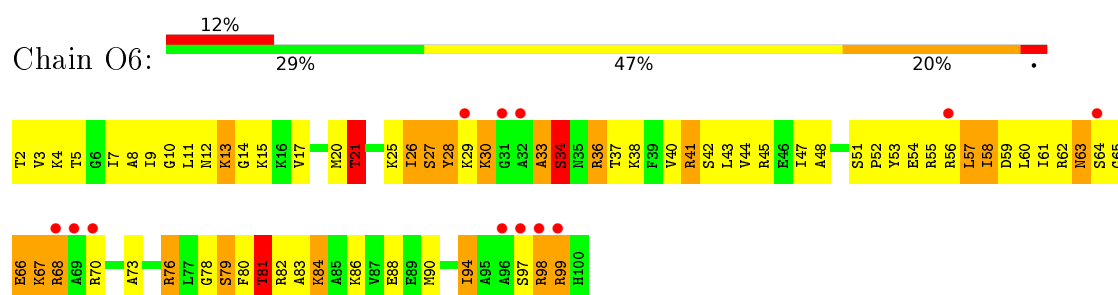


- Molecule 71: 60S ribosomal protein L35-A

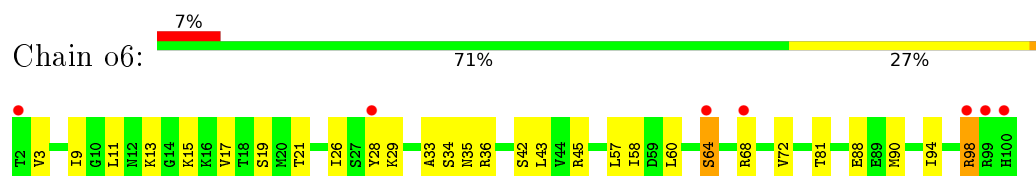
Chain o5: 3% 78% 22% .



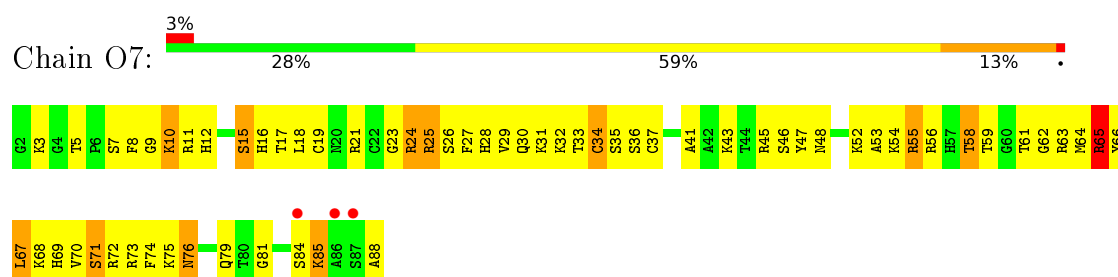
- Molecule 72: 60S ribosomal protein L36-A



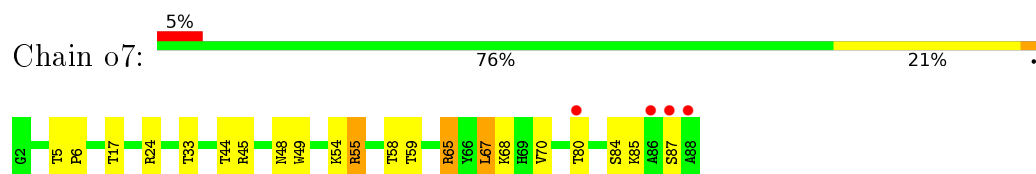
- Molecule 72: 60S ribosomal protein L36-A



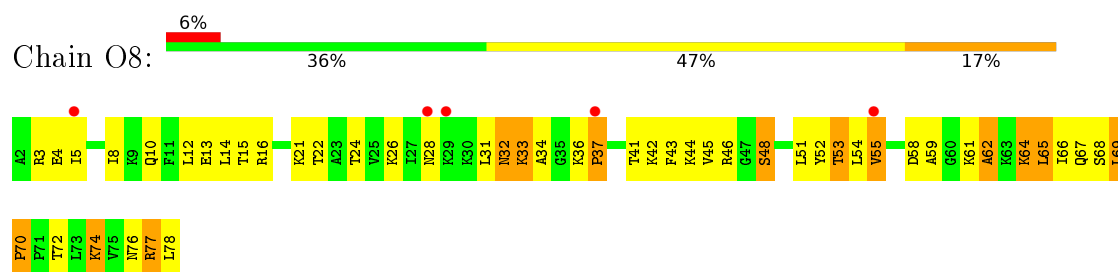
- Molecule 73: 60S ribosomal protein L37-A



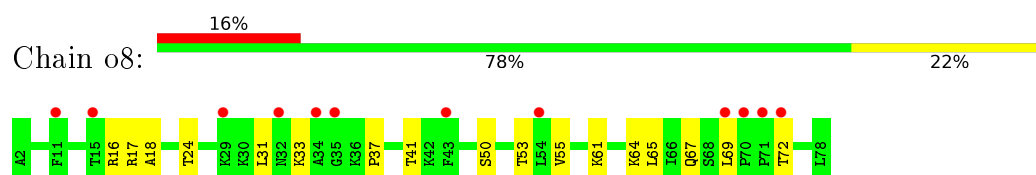
- Molecule 73: 60S ribosomal protein L37-A



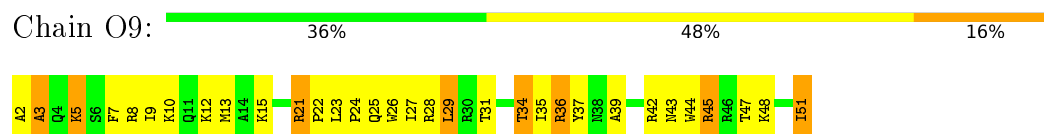
- Molecule 74: 60S ribosomal protein L38



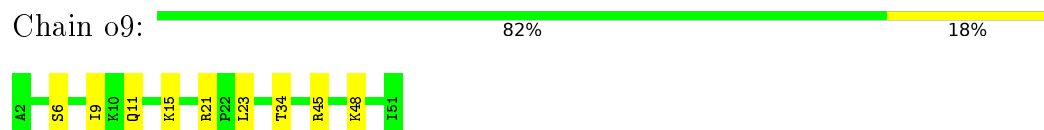
- Molecule 74: 60S ribosomal protein L38



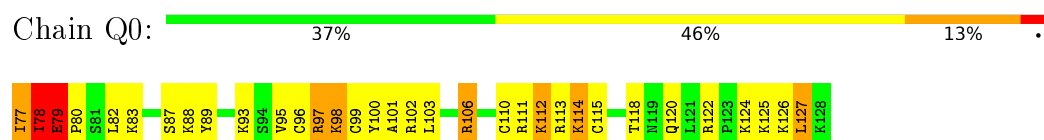
- Molecule 75: 60S ribosomal protein L39



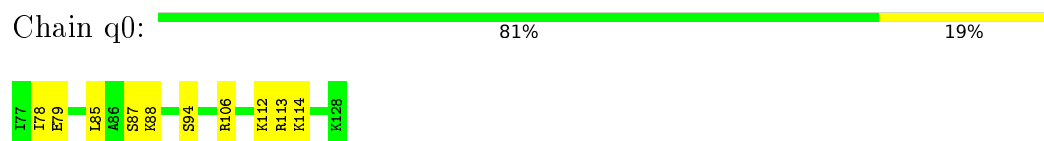
- Molecule 75: 60S ribosomal protein L39



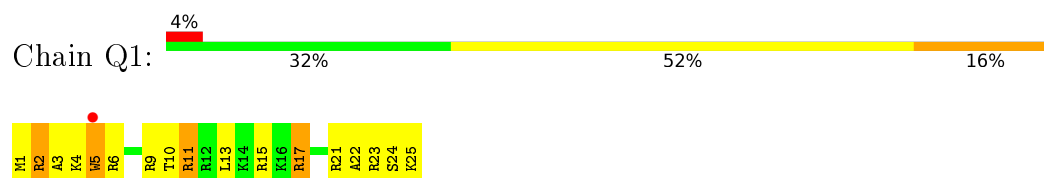
- Molecule 76: Ubiquitin-60S ribosomal protein L40



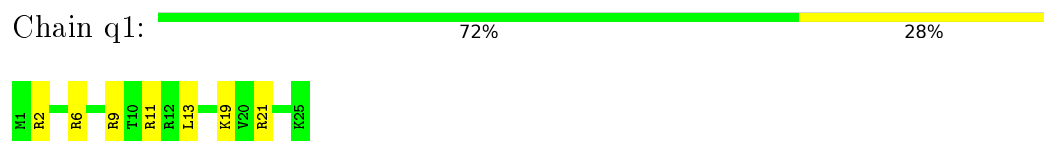
- Molecule 76: Ubiquitin-60S ribosomal protein L40



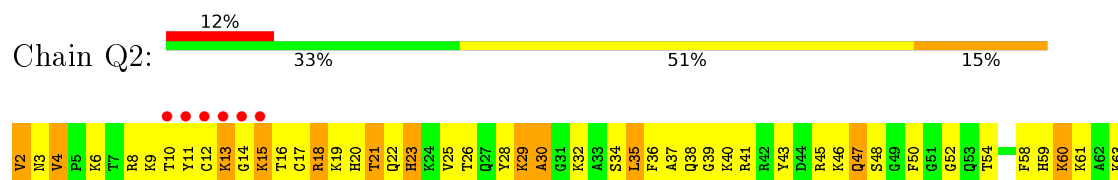
- Molecule 77: 60S ribosomal protein L41-A

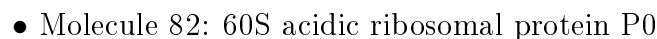


- Molecule 77: 60S ribosomal protein L41-A



- Molecule 78: 60S ribosomal protein L42-A





Y196	K221	SER	ILE	SER	LEU	ALA	ILE	GLY	PRO	TYR	THR	LEU	PRO	SER	VAL	GLY	HIS	THR	LEU	ILE	ASN	ASN	TYR	LYS	ASP	LEU	LEU	ALA	VAL	ALA	ILE	ALA	ALA	SER	TYR	HIS	TYR	PRO	GLU	ILE	GLU	ASP	LEU	VAL	ASP	ARG	ILE	GLU	ASN	PRO	GLU	LYS	TYR	ALA	ALA	ALA	PRO
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ALA	ALA	THR	SER	ALA	ALA	SER	GLY	ASP	ILE	ALA	ALA	PRO	ALA	GLU	GLU	ALA	ALA	ALA	GLU	GLU	GLU	GLU	GLU	SER	ASP	ASP	ASP	MET	GLY	PHE	GLY	GLY	LEU	PHE	ASP
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- Molecule 83: 60S ribosomal protein P1 alpha

Chain p1:

100%

There are no outlier residues recorded for this chain.

- Molecule 84: 60S ribosomal protein P2 beta

Chain p2:

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	435.45Å 287.66Å 303.76Å 90.00° 98.92° 90.00°	Depositor
Resolution (Å)	49.99 – 3.40 49.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.99-3.40) 84.7 (49.99-3.40)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.284 0.233 , 0.283	Depositor DCC
R_{free} test set	20186 reflections (2.31%)	DCC
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	411776	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.57	0/42468	1.13	127/66173 (0.2%)
1	6	0.68	1/42790 (0.0%)	1.19	169/66673 (0.3%)
2	S0	0.35	0/1653	0.57	0/2261
2	s0	0.39	0/1653	0.60	0/2261
3	S1	0.33	0/1735	0.60	2/2335 (0.1%)
3	s1	0.42	0/1748	0.61	0/2352
4	S2	0.40	0/1665	0.61	0/2263
4	s2	0.48	0/1665	0.67	0/2263
5	S3	0.40	0/1759	0.59	0/2368
5	s3	0.38	0/1759	0.58	0/2368
6	S4	0.39	0/2109	0.64	1/2839 (0.0%)
6	s4	0.45	0/2109	0.67	1/2839 (0.0%)
7	S5	0.36	0/1629	0.58	0/2202
7	s5	0.38	0/1629	0.59	0/2202
8	S6	0.35	0/1844	0.54	0/2464
8	s6	0.47	0/1779	0.63	0/2379
9	S7	0.40	0/1506	0.63	0/2028
9	s7	0.39	0/1517	0.62	0/2044
10	S8	0.43	0/1514	0.61	0/2021
10	s8	0.47	0/1514	0.62	0/2021
11	S9	0.38	0/1519	0.59	0/2035
11	s9	0.44	0/1519	0.62	0/2035
12	C0	0.38	0/789	0.61	1/1067 (0.1%)
13	C1	0.45	0/1194	0.60	0/1610
13	c1	0.52	0/1194	0.66	0/1610
14	C2	0.37	0/824	0.60	0/1116
14	c2	0.27	0/824	0.54	0/1116
15	C3	0.43	0/1215	0.59	1/1638 (0.1%)
15	c3	0.42	0/1215	0.59	0/1638
16	C4	0.33	0/901	0.61	0/1217
16	c4	0.41	0/960	0.64	0/1290
17	C5	0.39	0/998	0.63	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	c5	0.44	0/1060	0.64	0/1426
18	C6	0.40	0/1125	0.63	1/1510 (0.1%)
18	c6	0.38	0/1131	0.62	0/1518
19	C7	0.38	0/974	0.58	0/1304
19	c7	0.37	0/953	0.58	0/1275
20	C8	0.41	0/1211	0.61	1/1628 (0.1%)
20	c8	0.43	0/1211	0.63	1/1628 (0.1%)
21	C9	0.37	0/1130	0.57	0/1517
21	c9	0.40	0/1130	0.59	0/1517
22	D0	0.40	0/865	0.60	0/1169
22	d0	0.40	0/892	0.58	0/1205
23	D1	0.36	0/693	0.58	0/935
23	d1	0.40	0/693	0.56	0/935
24	D2	0.41	0/1038	0.67	2/1395 (0.1%)
24	d2	0.52	0/1038	0.69	1/1395 (0.1%)
25	D3	0.50	0/1139	0.67	0/1518
25	d3	0.56	0/1139	0.69	0/1518
26	D4	0.39	0/1087	0.56	0/1449
26	d4	0.43	0/1087	0.67	0/1449
27	D5	0.37	0/571	0.71	0/768
27	d5	0.37	0/566	0.58	0/761
28	D6	0.37	0/782	0.59	0/1047
28	d6	0.46	0/782	0.60	0/1047
29	D7	0.37	0/620	0.61	0/838
29	d7	0.41	0/620	0.63	0/838
30	D8	0.34	0/499	0.56	0/670
30	d8	0.38	0/499	0.62	0/670
31	D9	0.44	0/453	0.63	1/602 (0.2%)
31	d9	0.46	0/453	0.53	0/602
32	E0	0.37	0/483	0.57	0/643
32	e0	0.46	0/499	0.65	0/665
33	E1	0.38	0/577	0.69	0/770
33	e1	0.36	0/619	0.69	1/822 (0.1%)
34	SR	0.33	0/2494	0.56	0/3394
34	sR	0.33	0/2498	0.53	0/3398
35	SM	0.43	0/984	0.63	0/1323
35	sM	0.46	0/480	0.65	0/642
36	1	0.85	14/75394 (0.0%)	1.36	645/117545 (0.5%)
36	5	0.91	26/75418 (0.0%)	1.40	755/117583 (0.6%)
37	3	0.77	0/2883	1.23	10/4491 (0.2%)
37	7	0.85	0/2883	1.36	23/4491 (0.5%)
38	4	0.82	0/3746	1.32	18/5832 (0.3%)
38	8	0.78	0/3746	1.28	17/5832 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.56	0/1952	0.69	0/2622
39	l2	0.54	0/1952	0.73	0/2622
40	L3	0.56	0/3142	0.68	0/4224
40	l3	0.63	1/3142 (0.0%)	0.71	0/4224
41	L4	0.59	0/2801	0.75	1/3792 (0.0%)
41	l4	0.59	0/2801	0.73	1/3792 (0.0%)
42	L5	0.47	0/2425	0.65	0/3271
42	l5	0.58	0/2408	0.71	0/3248
43	L6	0.58	0/1260	0.72	0/1694
43	l6	0.58	0/1269	0.71	0/1705
44	L7	0.63	0/1821	0.72	0/2451
44	l7	0.66	0/1828	0.75	2/2461 (0.1%)
45	L8	0.43	0/1849	0.59	0/2495
45	l8	0.46	0/1795	0.61	0/2429
46	L9	0.54	0/1539	0.67	0/2073
46	l9	0.59	0/1539	0.69	0/2073
47	M0	0.57	0/1753	0.68	0/2350
47	m0	0.62	0/1769	0.74	0/2372
48	M1	0.44	0/1374	0.61	0/1842
48	m1	0.55	0/1374	0.68	1/1842 (0.1%)
49	M3	0.56	0/1568	0.74	1/2106 (0.0%)
49	m3	0.54	0/1573	0.73	0/2113
50	M4	0.60	0/1068	0.71	0/1438
50	m4	0.61	0/1074	0.71	0/1446
51	M5	0.56	0/1757	0.70	0/2354
51	m5	0.50	0/1757	0.64	0/2354
52	M6	0.66	0/1585	0.72	0/2128
52	m6	0.73	0/1585	0.75	0/2128
53	M7	0.55	0/1465	0.67	0/1968
53	m7	0.68	0/1250	0.76	1/1683 (0.1%)
54	M8	0.59	0/1465	0.75	1/1965 (0.1%)
54	m8	0.59	0/1465	0.75	1/1965 (0.1%)
55	M9	0.45	0/1538	0.56	0/2050
55	m9	0.50	0/1538	0.62	0/2050
56	N0	0.61	0/1481	0.73	0/1990
56	n0	0.67	0/1481	0.71	0/1990
57	N1	0.58	0/1300	0.66	0/1743
57	n1	0.61	0/1300	0.69	0/1743
58	N2	0.39	0/812	0.54	0/1099
58	n2	0.43	0/794	0.63	0/1076
59	N3	0.56	0/1018	0.71	1/1369 (0.1%)
59	n3	0.67	0/1018	0.76	0/1369
60	N4	0.43	0/814	0.65	0/1081

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.50	0/1103	0.65	0/1458
61	N5	0.49	0/983	0.72	2/1325 (0.2%)
61	n5	0.50	0/974	0.70	0/1314
62	N6	0.50	0/1004	0.70	0/1341
62	n6	0.53	0/1004	0.74	0/1341
63	N7	0.44	0/1118	0.60	0/1497
63	n7	0.40	0/1118	0.59	0/1497
64	N8	0.55	0/1204	0.75	0/1612
64	n8	0.56	0/1204	0.71	0/1612
65	N9	0.52	0/473	0.72	1/629 (0.2%)
65	n9	0.57	0/473	0.79	0/629
66	O0	0.39	0/751	0.56	0/1008
66	o0	0.43	0/775	0.65	0/1040
67	O1	0.51	0/904	0.65	0/1213
67	o1	0.60	0/904	0.70	0/1213
68	O2	0.63	0/1041	0.70	0/1394
68	o2	0.61	0/1041	0.73	0/1394
69	O3	0.68	0/868	0.72	0/1168
69	o3	0.65	0/868	0.73	0/1168
70	O4	0.47	0/891	0.62	1/1191 (0.1%)
70	o4	0.47	0/891	0.73	1/1191 (0.1%)
71	O5	0.51	0/978	0.69	1/1301 (0.1%)
71	o5	0.49	0/978	0.59	0/1301
72	O6	0.50	0/778	0.67	0/1034
72	o6	0.49	0/778	0.62	0/1034
73	O7	0.53	0/696	0.75	1/923 (0.1%)
73	o7	0.57	0/696	0.83	1/923 (0.1%)
74	O8	0.44	0/618	0.61	0/826
74	o8	0.39	0/618	0.57	0/826
75	O9	0.56	0/443	0.77	0/588
75	o9	0.54	0/443	0.65	0/588
76	Q0	0.54	0/423	0.71	0/562
76	q0	0.67	0/423	0.76	0/562
77	Q1	0.45	0/234	0.66	0/300
77	q1	0.50	0/234	0.65	0/300
78	Q2	0.63	1/860 (0.1%)	0.69	0/1136
78	q2	0.67	1/860 (0.1%)	0.69	2/1136 (0.2%)
79	Q3	0.56	0/701	0.72	0/934
79	q3	0.59	0/701	0.68	0/934
80	c0	0.34	0/718	0.60	1/968 (0.1%)
82	p0	0.42	0/977	0.60	0/1313
All	All	0.69	44/430590 (0.0%)	1.10	1799/632148 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	s5	0	1
9	S7	0	1
9	s7	0	1
18	c6	0	1
19	C7	0	1
22	d0	0	1
26	d4	0	1
27	D5	0	1
39	L2	0	2
42	l5	0	1
44	L7	0	1
44	l7	0	2
52	M6	0	1
56	n0	0	1
64	N8	0	1
64	n8	0	1
65	N9	0	1
All	All	0	19

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	11.01	2.00	1.82
78	Q2	17	CYS	CB-SG	10.91	2.00	1.82
36	5	1152	G	N9-C4	-7.21	1.32	1.38
36	5	706	A	N9-C4	-6.86	1.33	1.37
36	5	2214	A	N9-C4	-6.78	1.33	1.37

The worst 5 of 1799 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-14.54	117.27	126.00
36	5	1152	G	N3-C4-C5	13.47	135.34	128.60
36	5	1152	G	C2-N3-C4	-13.26	105.27	111.90
36	1	2874	G	C4-N9-C1'	-11.98	110.93	126.50
36	1	2618	G	N1-C6-O6	-11.78	112.83	119.90

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
39	L2	142	ASP	Peptide
39	L2	19	HIS	Peptide
9	S7	131	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37970	0	19104	1050	1
1	6	38260	0	19250	978	0
2	S0	1612	0	1623	152	0
2	s0	1612	0	1623	0	0
3	S1	1709	0	1784	156	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	1817	133	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	169	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	167	0
7	s5	1609	0	1675	0	0
8	S6	1820	0	1917	129	0
8	s6	1755	0	1845	0	0
9	S7	1481	0	1572	147	0
9	s7	1492	0	1581	0	0
10	S8	1489	0	1525	132	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	143	0
11	s9	1494	0	1573	0	0
12	C0	772	0	727	55	0
13	C1	1213	0	1242	99	0
13	c1	1168	0	1233	0	0
14	C2	892	0	874	57	0
14	c2	892	0	872	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C3	1192	0	1255	87	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	106	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	100	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	114	0
18	c6	1111	0	1171	0	0
19	C7	965	0	1026	97	0
19	c7	944	0	1006	0	0
20	C8	1192	0	1222	127	0
20	c8	1192	0	1221	0	0
21	C9	1112	0	1123	126	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	82	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	104	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	102	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	91	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	63	0
27	d5	558	0	598	0	0
28	D6	769	0	814	89	0
28	d6	769	0	814	0	0
29	D7	610	0	631	42	0
29	d7	610	0	631	0	0
30	D8	497	0	535	49	0
30	d8	497	0	535	0	0
31	D9	443	0	431	28	0
31	d9	443	0	432	0	0
32	E0	475	0	525	33	0
32	e0	491	0	542	0	0
33	E1	566	0	601	52	0
33	e1	608	0	657	0	0
34	SR	2441	0	2390	184	0
34	sR	2445	0	2401	0	0
35	SM	1104	0	971	80	0
35	sM	680	0	539	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	1	67355	0	33844	1644	0
36	5	67377	0	33851	1635	2
37	3	2579	0	1303	65	0
37	7	2579	0	1303	75	0
38	4	3353	0	1695	101	0
38	8	3353	0	1695	105	0
39	L2	1918	0	1987	204	0
39	l2	1918	0	1987	0	0
40	L3	3073	0	3160	282	0
40	l3	3073	0	3160	0	0
41	L4	2749	0	2863	267	0
41	l4	2749	0	2863	0	0
42	L5	2375	0	2325	225	0
42	l5	2359	0	2310	0	0
43	L6	1239	0	1326	112	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	172	0
44	l7	1791	0	1869	0	0
45	L8	1817	0	1908	151	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	151	0
46	l9	1518	0	1587	0	0
47	M0	1717	0	1754	176	0
47	m0	1733	0	1776	0	0
48	M1	1353	0	1383	116	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	162	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	114	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	162	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	135	0
52	m6	1555	0	1658	0	0
53	M7	1442	0	1485	121	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	121	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	114	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	137	0
56	n0	1445	0	1487	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	N1	1276	0	1323	113	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	51	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	72	0
59	n3	1003	0	1048	0	0
60	N4	800	0	865	61	0
60	n4	1089	0	1183	0	0
61	N5	968	0	1036	86	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	88	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	126	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1214	134	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	37	0
65	n9	462	0	491	0	0
66	O0	743	0	797	70	0
66	o0	767	0	816	0	0
67	O1	890	0	937	61	0
67	o1	890	0	938	0	0
68	O2	1020	0	1090	88	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	77	0
69	o3	850	0	880	0	0
70	O4	881	0	949	87	0
70	o4	881	0	949	0	0
71	O5	969	0	1078	100	0
71	o5	969	0	1078	0	0
72	O6	771	0	849	73	0
72	o6	771	0	849	0	0
73	O7	681	0	682	69	0
73	o7	681	0	682	0	0
74	O8	612	0	682	41	0
74	o8	612	0	682	0	0
75	O9	436	0	475	37	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	38	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	19	0
77	q1	233	0	284	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
78	Q2	847	0	917	76	0
78	q2	847	0	916	0	0
79	Q3	694	0	734	68	0
79	q3	694	0	734	0	0
80	c0	762	0	690	0	0
81	m2	750	0	175	0	0
82	p0	1077	0	1012	0	0
83	p1	235	0	50	0	0
84	p2	230	0	49	0	0
85	1	2359	0	0	274	0
85	2	1001	0	0	117	0
85	3	70	0	0	5	0
85	4	98	0	0	10	0
85	5	2422	0	0	280	0
85	6	1050	0	0	108	0
85	7	84	0	0	14	0
85	8	126	0	0	18	0
85	C3	7	0	0	0	0
85	C5	7	0	0	3	0
85	C8	7	0	0	0	0
85	D9	7	0	0	2	0
85	L3	14	0	0	3	0
85	L4	7	0	0	5	0
85	M0	7	0	0	2	0
85	M5	14	0	0	1	0
85	M7	14	0	0	3	0
85	M9	7	0	0	0	0
85	N1	7	0	0	2	0
85	N9	7	0	0	0	0
85	O3	7	0	0	3	0
85	O4	7	0	0	1	0
85	O7	14	0	0	3	0
85	Q2	7	0	0	7	0
85	S6	7	0	0	0	0
85	S8	7	0	0	0	0
85	S9	7	0	0	4	0
85	SR	7	0	0	0	0
85	c1	7	0	0	0	0
85	c3	7	0	0	0	0
85	c5	7	0	0	0	0
85	c8	7	0	0	0	0
85	d4	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	d9	7	0	0	0	0
85	l3	14	0	0	0	0
85	l4	14	0	0	0	0
85	l5	28	0	0	0	0
85	l9	7	0	0	0	0
85	m0	21	0	0	0	0
85	m1	7	0	0	0	0
85	m4	7	0	0	0	0
85	m5	7	0	0	0	0
85	n3	7	0	0	0	0
85	n5	7	0	0	0	0
85	n9	7	0	0	0	0
85	o2	7	0	0	0	0
85	o3	7	0	0	0	0
85	o4	7	0	0	0	0
85	o7	7	0	0	0	0
85	q2	7	0	0	0	0
85	s1	14	0	0	0	0
85	s4	7	0	0	0	0
85	s8	7	0	0	0	0
85	s9	7	0	0	0	0
85	sR	7	0	0	0	0
86	1	395	0	0	0	0
86	2	92	0	0	0	0
86	3	8	0	0	0	0
86	4	16	0	0	0	0
86	5	428	0	0	0	1
86	6	136	0	0	0	0
86	7	11	0	0	0	0
86	8	10	0	0	0	0
86	C2	7	0	0	0	0
86	C9	1	0	0	0	0
86	D1	1	0	0	0	0
86	D3	1	0	0	0	0
86	D9	2	0	0	0	0
86	L2	2	0	0	0	0
86	L3	2	0	0	0	0
86	L4	2	0	0	0	0
86	L5	1	0	0	0	0
86	L7	1	0	0	0	0
86	L9	1	0	0	0	0
86	M0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	M1	1	0	0	0	0
86	M3	1	0	0	0	0
86	M4	1	0	0	0	0
86	M5	1	0	0	0	0
86	M6	2	0	0	0	0
86	M7	6	0	0	0	0
86	M8	1	0	0	0	0
86	M9	1	0	0	0	0
86	MG	6	0	0	0	0
86	N0	1	0	0	0	0
86	N3	2	0	0	0	0
86	N4	1	0	0	0	0
86	N6	1	0	0	0	0
86	N8	1	0	0	0	0
86	N9	1	0	0	0	0
86	O1	1	0	0	0	0
86	O2	1	0	0	0	0
86	O5	1	0	0	0	0
86	O7	2	0	0	0	0
86	Q1	1	0	0	0	0
86	Q2	2	0	0	0	0
86	S4	1	0	0	0	0
86	S8	1	0	0	0	0
86	SM	1	0	0	0	0
86	c1	1	0	0	0	0
86	c8	1	0	0	0	0
86	l3	5	0	0	0	0
86	l4	1	0	0	0	0
86	l7	1	0	0	0	0
86	l9	1	0	0	0	0
86	m0	2	0	0	0	0
86	m1	1	0	0	0	0
86	m3	1	0	0	0	0
86	m4	1	0	0	0	0
86	m6	4	0	0	0	0
86	m7	1	0	0	0	0
86	n0	4	0	0	0	0
86	n3	1	0	0	0	0
86	n6	2	0	0	0	0
86	n8	1	0	0	0	0
86	n9	2	0	0	0	0
86	o1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	o2	1	0	0	0	0
86	o3	1	0	0	0	0
86	o4	1	0	0	0	0
86	p0	1	0	0	0	0
86	q0	1	0	0	0	0
86	q1	1	0	0	0	0
86	s1	1	0	0	0	0
86	s4	1	0	0	0	0
86	s6	1	0	0	0	0
86	sM	2	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	0	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
All	All	411776	0	298391	11926	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 11926 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)
36:1:1639:C:OP2	70:O4:74:ARG:NH2	1.96	0.98
1:2:992:A:H2	1:2:1012:U:H3	1.06	0.98
36:1:3272:C:OP2	43:L6:78:ARG:NH1	1.96	0.97
36:1:1466:G:O6	85:1:3415:OHX:N4	1.99	0.96
36:1:1222:G:HO2'	36:1:1285:G:H1	0.98	0.96

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5:2130:G:O4'	86:5:4174:MG:MG[1_656]	1.40	0.80
1:2:1353:U:O2'	36:5:3165:A:OP1[2_546]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	151 (74%)	32 (16%)	21 (10%)	1	7
2	s0	204/251 (81%)	148 (72%)	36 (18%)	20 (10%)	1	8
3	S1	212/254 (84%)	145 (68%)	39 (18%)	28 (13%)	0	4
3	s1	214/254 (84%)	162 (76%)	36 (17%)	16 (8%)	1	13
4	S2	215/253 (85%)	182 (85%)	16 (7%)	17 (8%)	1	12
4	s2	215/253 (85%)	169 (79%)	35 (16%)	11 (5%)	2	24
5	S3	221/239 (92%)	174 (79%)	36 (16%)	11 (5%)	3	24
5	s3	221/239 (92%)	168 (76%)	36 (16%)	17 (8%)	1	12
6	S4	258/260 (99%)	199 (77%)	49 (19%)	10 (4%)	4	32
6	s4	258/260 (99%)	200 (78%)	35 (14%)	23 (9%)	1	9
7	S5	204/224 (91%)	156 (76%)	34 (17%)	14 (7%)	1	15
7	s5	204/224 (91%)	140 (69%)	50 (24%)	14 (7%)	1	15
8	S6	224/236 (95%)	185 (83%)	26 (12%)	13 (6%)	2	20
8	s6	216/236 (92%)	179 (83%)	21 (10%)	16 (7%)	1	14
9	S7	182/189 (96%)	131 (72%)	35 (19%)	16 (9%)	1	10
9	s7	184/189 (97%)	135 (73%)	34 (18%)	15 (8%)	1	11
10	S8	184/200 (92%)	153 (83%)	21 (11%)	10 (5%)	2	22
10	s8	184/200 (92%)	155 (84%)	18 (10%)	11 (6%)	2	19
11	S9	183/196 (93%)	138 (75%)	29 (16%)	16 (9%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	s9	183/196 (93%)	133 (73%)	41 (22%)	9 (5%)	3	25
12	C0	94/105 (90%)	68 (72%)	16 (17%)	10 (11%)	0	6
13	C1	145/155 (94%)	117 (81%)	18 (12%)	10 (7%)	1	15
13	c1	144/155 (93%)	116 (81%)	21 (15%)	7 (5%)	3	25
14	C2	108/142 (76%)	67 (62%)	28 (26%)	13 (12%)	0	5
14	c2	108/142 (76%)	66 (61%)	29 (27%)	13 (12%)	0	5
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	3	30
15	c3	148/150 (99%)	108 (73%)	29 (20%)	11 (7%)	1	14
16	C4	125/136 (92%)	88 (70%)	22 (18%)	15 (12%)	0	5
16	c4	126/136 (93%)	96 (76%)	19 (15%)	11 (9%)	1	10
17	C5	122/141 (86%)	93 (76%)	19 (16%)	10 (8%)	1	11
17	c5	133/141 (94%)	93 (70%)	23 (17%)	17 (13%)	0	4
18	C6	139/142 (98%)	110 (79%)	22 (16%)	7 (5%)	3	24
18	c6	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	2	20
19	C7	116/136 (85%)	91 (78%)	17 (15%)	8 (7%)	1	15
19	c7	113/136 (83%)	91 (80%)	16 (14%)	6 (5%)	2	22
20	C8	143/145 (99%)	110 (77%)	24 (17%)	9 (6%)	2	18
20	c8	143/145 (99%)	111 (78%)	21 (15%)	11 (8%)	1	12
21	C9	141/143 (99%)	114 (81%)	19 (14%)	8 (6%)	2	20
21	c9	141/143 (99%)	117 (83%)	18 (13%)	6 (4%)	3	29
22	D0	105/120 (88%)	88 (84%)	13 (12%)	4 (4%)	4	32
22	d0	108/120 (90%)	83 (77%)	17 (16%)	8 (7%)	1	14
23	D1	85/87 (98%)	56 (66%)	19 (22%)	10 (12%)	0	5
23	d1	85/87 (98%)	66 (78%)	16 (19%)	3 (4%)	4	35
24	D2	127/129 (98%)	108 (85%)	12 (9%)	7 (6%)	2	21
24	d2	127/129 (98%)	99 (78%)	25 (20%)	3 (2%)	7	44
25	D3	142/144 (99%)	105 (74%)	26 (18%)	11 (8%)	1	12
25	d3	142/144 (99%)	120 (84%)	17 (12%)	5 (4%)	4	35
26	D4	132/134 (98%)	103 (78%)	18 (14%)	11 (8%)	1	11
26	d4	132/134 (98%)	103 (78%)	19 (14%)	10 (8%)	1	13
27	D5	68/107 (64%)	45 (66%)	13 (19%)	10 (15%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	d5	67/107 (63%)	54 (81%)	7 (10%)	6 (9%)	1	9
28	D6	95/97 (98%)	58 (61%)	19 (20%)	18 (19%)	0	1
28	d6	95/97 (98%)	71 (75%)	18 (19%)	6 (6%)	2	18
29	D7	79/81 (98%)	59 (75%)	15 (19%)	5 (6%)	2	18
29	d7	79/81 (98%)	61 (77%)	12 (15%)	6 (8%)	1	13
30	D8	61/66 (92%)	47 (77%)	13 (21%)	1 (2%)	12	53
30	d8	61/66 (92%)	46 (75%)	13 (21%)	2 (3%)	5	37
31	D9	51/55 (93%)	36 (71%)	11 (22%)	4 (8%)	1	12
31	d9	51/55 (93%)	44 (86%)	4 (8%)	3 (6%)	2	19
32	E0	58/62 (94%)	47 (81%)	7 (12%)	4 (7%)	1	15
32	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	1	7
33	E1	69/76 (91%)	35 (51%)	13 (19%)	21 (30%)	0	0
33	e1	74/76 (97%)	35 (47%)	18 (24%)	21 (28%)	0	0
34	SR	316/318 (99%)	261 (83%)	44 (14%)	11 (4%)	4	35
34	sR	316/318 (99%)	260 (82%)	40 (13%)	16 (5%)	2	24
35	SM	131/182 (72%)	95 (72%)	18 (14%)	18 (14%)	0	3
35	sM	61/182 (34%)	34 (56%)	15 (25%)	12 (20%)	0	1
39	L2	250/253 (99%)	203 (81%)	36 (14%)	11 (4%)	3	28
39	l2	250/253 (99%)	204 (82%)	28 (11%)	18 (7%)	1	14
40	L3	384/386 (100%)	311 (81%)	54 (14%)	19 (5%)	3	25
40	l3	384/386 (100%)	331 (86%)	39 (10%)	14 (4%)	4	34
41	L4	359/361 (99%)	286 (80%)	49 (14%)	24 (7%)	1	16
41	l4	359/361 (99%)	280 (78%)	54 (15%)	25 (7%)	1	15
42	L5	294/296 (99%)	225 (76%)	37 (13%)	32 (11%)	0	6
42	l5	292/296 (99%)	235 (80%)	40 (14%)	17 (6%)	2	20
43	L6	152/175 (87%)	132 (87%)	16 (10%)	4 (3%)	7	42
43	l6	153/175 (87%)	116 (76%)	29 (19%)	8 (5%)	2	23
44	L7	220/243 (90%)	186 (84%)	24 (11%)	10 (4%)	3	27
44	l7	221/243 (91%)	183 (83%)	28 (13%)	10 (4%)	3	27
45	L8	231/255 (91%)	183 (79%)	37 (16%)	11 (5%)	3	25
45	l8	229/255 (90%)	171 (75%)	37 (16%)	21 (9%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	L9	189/191 (99%)	151 (80%)	28 (15%)	10 (5%)	2	22
46	l9	189/191 (99%)	162 (86%)	22 (12%)	5 (3%)	7	42
47	M0	207/220 (94%)	165 (80%)	34 (16%)	8 (4%)	4	32
47	m0	209/220 (95%)	168 (80%)	26 (12%)	15 (7%)	1	14
48	M1	167/173 (96%)	125 (75%)	24 (14%)	18 (11%)	0	6
48	m1	167/173 (96%)	136 (81%)	15 (9%)	16 (10%)	1	8
49	M3	191/198 (96%)	136 (71%)	40 (21%)	15 (8%)	1	12
49	m3	192/198 (97%)	146 (76%)	31 (16%)	15 (8%)	1	12
50	M4	134/137 (98%)	111 (83%)	13 (10%)	10 (8%)	1	13
50	m4	135/137 (98%)	109 (81%)	20 (15%)	6 (4%)	3	28
51	M5	201/203 (99%)	172 (86%)	21 (10%)	8 (4%)	4	31
51	m5	201/203 (99%)	169 (84%)	25 (12%)	7 (4%)	4	35
52	M6	195/198 (98%)	172 (88%)	18 (9%)	5 (3%)	7	42
52	m6	195/198 (98%)	180 (92%)	9 (5%)	6 (3%)	5	39
53	M7	181/183 (99%)	137 (76%)	34 (19%)	10 (6%)	2	21
53	m7	153/183 (84%)	125 (82%)	24 (16%)	4 (3%)	7	42
54	M8	183/185 (99%)	151 (82%)	30 (16%)	2 (1%)	17	61
54	m8	183/185 (99%)	148 (81%)	25 (14%)	10 (6%)	2	21
55	M9	186/188 (99%)	157 (84%)	24 (13%)	5 (3%)	6	41
55	m9	186/188 (99%)	157 (84%)	21 (11%)	8 (4%)	3	29
56	N0	170/172 (99%)	147 (86%)	18 (11%)	5 (3%)	6	40
56	n0	170/172 (99%)	153 (90%)	14 (8%)	3 (2%)	11	50
57	N1	157/159 (99%)	127 (81%)	23 (15%)	7 (4%)	3	27
57	n1	157/159 (99%)	134 (85%)	20 (13%)	3 (2%)	10	49
58	N2	98/120 (82%)	74 (76%)	17 (17%)	7 (7%)	1	15
58	n2	96/120 (80%)	77 (80%)	17 (18%)	2 (2%)	9	47
59	N3	134/136 (98%)	114 (85%)	17 (13%)	3 (2%)	8	46
59	n3	134/136 (98%)	120 (90%)	10 (8%)	4 (3%)	5	39
60	N4	96/155 (62%)	77 (80%)	12 (12%)	7 (7%)	1	14
60	n4	133/155 (86%)	94 (71%)	28 (21%)	11 (8%)	1	11
61	N5	119/141 (84%)	101 (85%)	17 (14%)	1 (1%)	24	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	n5	118/141 (84%)	83 (70%)	24 (20%)	11 (9%)	1	9
62	N6	124/126 (98%)	105 (85%)	14 (11%)	5 (4%)	4	31
62	n6	124/126 (98%)	106 (86%)	12 (10%)	6 (5%)	3	25
63	N7	133/135 (98%)	101 (76%)	19 (14%)	13 (10%)	1	8
63	n7	133/135 (98%)	101 (76%)	18 (14%)	14 (10%)	1	7
64	N8	146/148 (99%)	110 (75%)	25 (17%)	11 (8%)	1	13
64	n8	146/148 (99%)	114 (78%)	26 (18%)	6 (4%)	3	30
65	N9	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	2	22
65	n9	56/58 (97%)	42 (75%)	9 (16%)	5 (9%)	1	9
66	O0	95/104 (91%)	84 (88%)	11 (12%)	0	100	100
66	o0	98/104 (94%)	78 (80%)	12 (12%)	8 (8%)	1	11
67	O1	107/112 (96%)	92 (86%)	11 (10%)	4 (4%)	4	33
67	o1	107/112 (96%)	82 (77%)	18 (17%)	7 (6%)	1	17
68	O2	125/129 (97%)	109 (87%)	15 (12%)	1 (1%)	24	67
68	o2	125/129 (97%)	106 (85%)	13 (10%)	6 (5%)	3	25
69	O3	104/106 (98%)	93 (89%)	8 (8%)	3 (3%)	6	40
69	o3	104/106 (98%)	88 (85%)	13 (12%)	3 (3%)	6	40
70	O4	110/120 (92%)	94 (86%)	12 (11%)	4 (4%)	4	34
70	o4	110/120 (92%)	93 (84%)	11 (10%)	6 (6%)	2	21
71	O5	117/119 (98%)	99 (85%)	13 (11%)	5 (4%)	3	29
71	o5	117/119 (98%)	94 (80%)	18 (15%)	5 (4%)	3	29
72	O6	97/99 (98%)	65 (67%)	20 (21%)	12 (12%)	0	4
72	o6	97/99 (98%)	79 (81%)	13 (13%)	5 (5%)	2	23
73	O7	85/87 (98%)	64 (75%)	19 (22%)	2 (2%)	7	44
73	o7	85/87 (98%)	61 (72%)	16 (19%)	8 (9%)	1	8
74	O8	75/77 (97%)	59 (79%)	11 (15%)	5 (7%)	1	16
74	o8	75/77 (97%)	56 (75%)	16 (21%)	3 (4%)	4	31
75	O9	48/50 (96%)	40 (83%)	6 (12%)	2 (4%)	3	29
75	o9	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
76	Q0	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	2	19
76	q0	50/52 (96%)	43 (86%)	6 (12%)	1 (2%)	9	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	78 (76%)	19 (18%)	6 (6%)	2	20
78	q2	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	10	49
79	Q3	89/91 (98%)	74 (83%)	12 (14%)	3 (3%)	5	36
79	q3	89/91 (98%)	64 (72%)	21 (24%)	4 (4%)	3	27
80	c0	82/96 (85%)	62 (76%)	10 (12%)	10 (12%)	0	5
82	p0	117/311 (38%)	96 (82%)	16 (14%)	5 (4%)	3	29
All	All	22204/23954 (93%)	17573 (79%)	3238 (15%)	1393 (6%)	2	18

5 of 1393 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	36	TYR
2	S0	158	VAL
3	S1	37	THR
3	S1	49	ASN

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	173/209 (83%)	143 (83%)	30 (17%)	2	13
2	s0	173/209 (83%)	139 (80%)	34 (20%)	1	8
3	S1	191/223 (86%)	159 (83%)	32 (17%)	2	14
3	s1	192/223 (86%)	150 (78%)	42 (22%)	1	6
4	S2	176/204 (86%)	140 (80%)	36 (20%)	1	7
4	s2	176/204 (86%)	133 (76%)	43 (24%)	1	4
5	S3	182/194 (94%)	145 (80%)	37 (20%)	1	7
5	s3	182/194 (94%)	154 (85%)	28 (15%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S4	221/221 (100%)	179 (81%)	42 (19%)	2	9
6	s4	221/221 (100%)	186 (84%)	35 (16%)	3	17
7	S5	173/190 (91%)	146 (84%)	27 (16%)	3	18
7	s5	173/190 (91%)	147 (85%)	26 (15%)	3	20
8	S6	193/201 (96%)	163 (84%)	30 (16%)	3	18
8	s6	187/201 (93%)	152 (81%)	35 (19%)	2	10
9	S7	165/169 (98%)	140 (85%)	25 (15%)	3	19
9	s7	166/169 (98%)	136 (82%)	30 (18%)	2	11
10	S8	150/161 (93%)	128 (85%)	22 (15%)	4	20
10	s8	150/161 (93%)	130 (87%)	20 (13%)	5	24
11	S9	158/165 (96%)	127 (80%)	31 (20%)	1	8
11	s9	158/165 (96%)	132 (84%)	26 (16%)	3	15
12	C0	77/98 (79%)	67 (87%)	10 (13%)	5	25
13	C1	129/129 (100%)	114 (88%)	15 (12%)	7	31
13	c1	129/129 (100%)	109 (84%)	20 (16%)	3	18
14	C2	88/106 (83%)	70 (80%)	18 (20%)	1	7
14	c2	88/106 (83%)	70 (80%)	18 (20%)	1	7
15	C3	127/127 (100%)	108 (85%)	19 (15%)	3	20
15	c3	127/127 (100%)	98 (77%)	29 (23%)	1	5
16	C4	81/104 (78%)	63 (78%)	18 (22%)	1	5
16	c4	97/104 (93%)	79 (81%)	18 (19%)	2	10
17	C5	101/117 (86%)	80 (79%)	21 (21%)	1	6
17	c5	103/117 (88%)	81 (79%)	22 (21%)	1	6
18	C6	117/118 (99%)	98 (84%)	19 (16%)	3	16
18	c6	118/118 (100%)	96 (81%)	22 (19%)	2	10
19	C7	109/124 (88%)	84 (77%)	25 (23%)	1	5
19	c7	106/124 (86%)	89 (84%)	17 (16%)	3	16
20	C8	128/128 (100%)	104 (81%)	24 (19%)	2	9
20	c8	128/128 (100%)	108 (84%)	20 (16%)	3	18
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1	5
21	c9	115/115 (100%)	96 (84%)	19 (16%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	D0	100/113 (88%)	86 (86%)	14 (14%)	4	23
22	d0	103/113 (91%)	79 (77%)	24 (23%)	1	4
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	12
23	d1	74/74 (100%)	59 (80%)	15 (20%)	1	7
24	D2	110/110 (100%)	86 (78%)	24 (22%)	1	6
24	d2	110/110 (100%)	90 (82%)	20 (18%)	2	11
25	D3	119/119 (100%)	94 (79%)	25 (21%)	1	6
25	d3	119/119 (100%)	94 (79%)	25 (21%)	1	6
26	D4	112/112 (100%)	94 (84%)	18 (16%)	3	16
26	d4	112/112 (100%)	94 (84%)	18 (16%)	3	16
27	D5	61/88 (69%)	46 (75%)	15 (25%)	1	4
27	d5	61/88 (69%)	51 (84%)	10 (16%)	3	15
28	D6	83/83 (100%)	62 (75%)	21 (25%)	1	3
28	d6	83/83 (100%)	66 (80%)	17 (20%)	1	7
29	D7	70/70 (100%)	61 (87%)	9 (13%)	5	26
29	d7	70/70 (100%)	57 (81%)	13 (19%)	2	10
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	6
30	d8	56/59 (95%)	48 (86%)	8 (14%)	4	22
31	D9	47/48 (98%)	41 (87%)	6 (13%)	5	26
31	d9	47/48 (98%)	38 (81%)	9 (19%)	2	9
32	E0	51/53 (96%)	41 (80%)	10 (20%)	1	8
32	e0	53/53 (100%)	39 (74%)	14 (26%)	0	3
33	E1	62/66 (94%)	49 (79%)	13 (21%)	1	6
33	e1	66/66 (100%)	49 (74%)	17 (26%)	0	3
34	SR	260/261 (100%)	230 (88%)	30 (12%)	7	31
34	sR	261/261 (100%)	237 (91%)	24 (9%)	11	43
35	SM	97/115 (84%)	80 (82%)	17 (18%)	2	13
35	sM	54/115 (47%)	37 (68%)	17 (32%)	0	2
39	L2	194/195 (100%)	155 (80%)	39 (20%)	1	7
39	l2	194/195 (100%)	160 (82%)	34 (18%)	2	13
40	L3	322/322 (100%)	246 (76%)	76 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	l3	322/322 (100%)	258 (80%)	64 (20%)	1	8
41	L4	288/288 (100%)	240 (83%)	48 (17%)	3	14
41	l4	288/288 (100%)	235 (82%)	53 (18%)	2	10
42	L5	244/244 (100%)	199 (82%)	45 (18%)	2	10
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	6
43	L6	134/152 (88%)	113 (84%)	21 (16%)	3	18
43	l6	135/152 (89%)	113 (84%)	22 (16%)	3	16
44	L7	186/204 (91%)	166 (89%)	20 (11%)	8	35
44	l7	187/204 (92%)	158 (84%)	29 (16%)	3	18
45	L8	191/207 (92%)	157 (82%)	34 (18%)	2	12
45	l8	177/207 (86%)	140 (79%)	37 (21%)	1	6
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	6
46	l9	171/171 (100%)	133 (78%)	38 (22%)	1	5
47	M0	180/186 (97%)	147 (82%)	33 (18%)	2	10
47	m0	182/186 (98%)	141 (78%)	41 (22%)	1	5
48	M1	147/149 (99%)	114 (78%)	33 (22%)	1	5
48	m1	147/149 (99%)	123 (84%)	24 (16%)	3	16
49	M3	154/158 (98%)	122 (79%)	32 (21%)	1	6
49	m3	154/158 (98%)	123 (80%)	31 (20%)	1	7
50	M4	107/108 (99%)	89 (83%)	18 (17%)	2	14
50	m4	108/108 (100%)	83 (77%)	25 (23%)	1	4
51	M5	175/175 (100%)	148 (85%)	27 (15%)	3	18
51	m5	175/175 (100%)	145 (83%)	30 (17%)	2	14
52	M6	160/161 (99%)	135 (84%)	25 (16%)	3	18
52	m6	160/161 (99%)	128 (80%)	32 (20%)	1	8
53	M7	145/145 (100%)	110 (76%)	35 (24%)	1	4
53	m7	125/145 (86%)	98 (78%)	27 (22%)	1	6
54	M8	150/150 (100%)	129 (86%)	21 (14%)	4	23
54	m8	150/150 (100%)	125 (83%)	25 (17%)	3	14
55	M9	153/153 (100%)	127 (83%)	26 (17%)	2	14
55	m9	153/153 (100%)	126 (82%)	27 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	N0	156/156 (100%)	129 (83%)	27 (17%)	2	13
56	n0	156/156 (100%)	116 (74%)	40 (26%)	0	3
57	N1	136/136 (100%)	108 (79%)	28 (21%)	1	7
57	n1	136/136 (100%)	108 (79%)	28 (21%)	1	7
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2	13
58	n2	85/106 (80%)	69 (81%)	16 (19%)	2	9
59	N3	104/104 (100%)	76 (73%)	28 (27%)	0	3
59	n3	104/104 (100%)	90 (86%)	14 (14%)	5	24
60	N4	86/129 (67%)	72 (84%)	14 (16%)	3	16
60	n4	114/129 (88%)	94 (82%)	20 (18%)	2	13
61	N5	105/117 (90%)	77 (73%)	28 (27%)	0	3
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	6
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	13
62	n6	109/109 (100%)	89 (82%)	20 (18%)	2	10
63	N7	115/115 (100%)	95 (83%)	20 (17%)	2	13
63	n7	115/115 (100%)	93 (81%)	22 (19%)	2	9
64	N8	118/118 (100%)	94 (80%)	24 (20%)	1	7
64	n8	118/118 (100%)	94 (80%)	24 (20%)	1	7
65	N9	46/46 (100%)	39 (85%)	7 (15%)	3	19
65	n9	46/46 (100%)	38 (83%)	8 (17%)	2	13
66	O0	81/87 (93%)	64 (79%)	17 (21%)	1	6
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1	5
67	O1	96/96 (100%)	78 (81%)	18 (19%)	2	9
67	o1	96/96 (100%)	79 (82%)	17 (18%)	2	12
68	O2	109/110 (99%)	94 (86%)	15 (14%)	4	23
68	o2	109/110 (99%)	87 (80%)	22 (20%)	1	7
69	O3	90/90 (100%)	72 (80%)	18 (20%)	1	8
69	o3	90/90 (100%)	76 (84%)	14 (16%)	3	18
70	O4	95/102 (93%)	77 (81%)	18 (19%)	2	9
70	o4	95/102 (93%)	81 (85%)	14 (15%)	4	20
71	O5	104/104 (100%)	89 (86%)	15 (14%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	o5	104/104 (100%)	83 (80%)	21 (20%)	1	7
72	O6	81/81 (100%)	58 (72%)	23 (28%)	0	2
72	o6	81/81 (100%)	55 (68%)	26 (32%)	0	2
73	O7	70/70 (100%)	54 (77%)	16 (23%)	1	5
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	6
74	O8	68/68 (100%)	55 (81%)	13 (19%)	2	9
74	o8	68/68 (100%)	54 (79%)	14 (21%)	1	7
75	O9	45/45 (100%)	38 (84%)	7 (16%)	3	18
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1	8
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	2	9
76	q0	47/47 (100%)	38 (81%)	9 (19%)	2	9
77	Q1	23/23 (100%)	18 (78%)	5 (22%)	1	6
77	q1	23/23 (100%)	16 (70%)	7 (30%)	0	2
78	Q2	90/90 (100%)	72 (80%)	18 (20%)	1	8
78	q2	90/90 (100%)	71 (79%)	19 (21%)	1	6
79	Q3	71/71 (100%)	63 (89%)	8 (11%)	7	32
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1	5
80	c0	73/78 (94%)	64 (88%)	9 (12%)	6	28
82	p0	105/232 (45%)	88 (84%)	17 (16%)	3	16
All	All	18856/19936 (95%)	15356 (81%)	3500 (19%)	2	10

5 of 3500 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	10	ARG
9	s7	28	GLU
64	n8	42	ARG
72	O6	67	LYS
3	s1	184	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
78	Q2	102	GLN

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Mol	Chain	Res	Type
9	s7	71	HIS
60	n4	104	ASN
2	s0	131	GLN
3	s1	209	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1777/1800 (98%)	519 (29%)	56 (3%)
1	6	1792/1800 (99%)	472 (26%)	47 (2%)
36	1	3145/3396 (92%)	710 (22%)	70 (2%)
36	5	3146/3396 (92%)	753 (23%)	72 (2%)
37	3	120/121 (99%)	18 (15%)	1 (0%)
37	7	120/121 (99%)	23 (19%)	1 (0%)
38	4	157/158 (99%)	37 (23%)	2 (1%)
38	8	157/158 (99%)	37 (23%)	1 (0%)
All	All	10414/10950 (95%)	2569 (24%)	250 (2%)

5 of 2569 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	13	C
1	2	25	C

5 of 250 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	1	3121	U
1	6	217	A
36	5	2682	C
36	1	3218	A
37	3	52	G

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2303 ligands modelled in this entry, 1214 are monoatomic - leaving 1089 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	$\# Z > 2$
85	OHX	1	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3427	-	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
85	OHX	1	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3439	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3470	-	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
85	OHX	1	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3482	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3513	-	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
85	OHX	1	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3525	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3556	-	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
85	OHX	1	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3568	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3599	-	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
85	OHX	1	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3611	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3642	-	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
85	OHX	1	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3654	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3685	-	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
85	OHX	1	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3696	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3697	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3716	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3722	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3723	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3725	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3727	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3728	-	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
85	OHX	1	3729	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3730	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3731	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3732	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3733	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3734	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3735	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3736	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	1	3737	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1934	-	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
85	OHX	2	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1937	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1938	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1939	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1940	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1941	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1942	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1943	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1944	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1945	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1946	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1947	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1948	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1949	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1950	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1951	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1952	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1953	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1954	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1955	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1956	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1957	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1958	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1959	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1960	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1961	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1962	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1963	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1964	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1965	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1966	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1967	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1968	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1969	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1970	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1971	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1972	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1973	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1974	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1975	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1976	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1977	-	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
85	OHX	2	1978	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1979	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1980	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1981	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1982	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1983	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1984	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1985	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1986	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1987	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1988	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1989	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1990	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1991	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1992	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1993	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1994	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1995	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1996	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1997	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1998	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	1999	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2000	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2001	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2002	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2003	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2004	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2005	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2006	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2007	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2008	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2009	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2010	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2011	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2012	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2013	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2014	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2015	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2016	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2017	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2018	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2019	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2020	-	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
85	OHX	2	2021	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	205	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	206	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	207	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	208	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	209	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	210	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	3	211	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	204	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	205	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	206	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	207	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	208	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	209	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	210	-	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
85	OHX	4	211	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	212	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	213	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	4	214	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3401	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3402	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3403	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3404	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3405	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3406	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3407	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3408	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3409	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3410	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3411	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3412	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3413	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3414	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3415	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3416	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3417	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3418	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3419	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3420	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3421	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3422	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3423	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3424	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3425	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3426	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3427	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3428	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3429	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3430	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3431	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3432	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3433	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3434	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3435	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3436	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3437	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3438	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3439	-	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
85	OHX	5	3440	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3441	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3442	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3443	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3444	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3445	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3446	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3447	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3448	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3449	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3450	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3451	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3452	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3453	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3454	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3455	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3456	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3457	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3458	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3459	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3460	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3461	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3462	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3463	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3464	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3465	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3466	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3467	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3468	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3469	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3470	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3471	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3472	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3473	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3474	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3475	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3476	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3477	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3478	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3479	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3480	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3481	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3482	-	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
85	OHX	5	3483	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3484	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3485	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3486	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3487	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3488	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3489	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3490	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3491	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3492	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3493	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3494	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3495	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3496	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3497	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3498	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3499	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3500	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3501	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3502	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3503	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3504	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3505	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3506	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3507	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3508	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3509	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3510	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3511	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3512	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3513	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3514	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3515	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3516	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3517	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3518	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3519	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3520	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3521	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3522	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3523	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3524	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3525	-	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
85	OHX	5	3526	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3527	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3528	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3529	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3530	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3531	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3532	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3533	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3534	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3535	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3536	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3537	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3538	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3539	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3540	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3541	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3542	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3543	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3544	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3545	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3546	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3547	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3548	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3549	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3550	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3551	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3552	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3553	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3554	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3555	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3556	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3557	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3558	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3559	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3560	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3561	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3562	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3563	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3564	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3565	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3566	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3567	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3568	-	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
85	OHX	5	3569	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3570	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3571	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3572	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3573	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3574	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3575	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3576	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3577	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3578	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3579	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3580	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3581	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3582	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3583	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3584	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3585	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3586	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3587	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3588	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3589	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3590	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3591	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3592	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3593	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3594	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3595	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3596	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3597	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3598	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3599	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3600	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3601	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3602	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3603	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3604	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3605	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3606	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3607	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3608	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3609	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3610	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3611	-	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
85	OHX	5	3612	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3613	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3614	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3615	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3616	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3617	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3618	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3619	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3620	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3621	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3622	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3623	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3624	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3625	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3626	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3627	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3628	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3629	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3630	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3631	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3632	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3633	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3634	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3635	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3636	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3637	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3638	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3639	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3640	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3641	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3642	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3643	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3644	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3645	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3646	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3647	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3648	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3649	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3650	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3651	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3652	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3653	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3654	-	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
85	OHX	5	3655	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3656	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3657	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3658	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3659	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3660	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3661	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3662	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3663	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3664	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3665	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3666	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3667	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3668	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3669	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3670	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3671	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3672	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3673	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3674	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3675	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3676	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3677	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3678	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3679	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3680	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3681	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3682	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3683	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3684	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3685	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3686	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3687	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3688	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3689	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3690	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3691	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3692	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3693	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3694	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3695	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3696	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3697	-	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
85	OHX	5	3698	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3699	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3700	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3701	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3702	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3703	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3704	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3705	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3706	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3707	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3708	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3709	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3710	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3711	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3712	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3713	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3714	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3715	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3716	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3717	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3718	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3719	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3720	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3721	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3722	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3723	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3724	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3725	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3726	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3727	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3728	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3729	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3730	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3731	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3732	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3733	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3734	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3735	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3736	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3737	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3738	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3739	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3740	-	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
85	OHX	5	3741	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3742	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3743	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3744	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3745	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	5	3746	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1901	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1902	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1903	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1904	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1905	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1906	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1907	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1908	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1909	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1910	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1911	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1912	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1913	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1914	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1915	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1916	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1917	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1918	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1919	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1920	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1921	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1922	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1923	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1924	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1925	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1926	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1927	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1928	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1929	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1930	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1931	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1932	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1933	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1934	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1935	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1936	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	1937	-	0,6,6	0.00	-	0,15,15	0.00	-

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	OHX	6	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	202	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	203	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	204	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	209	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	210	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	211	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	7	212	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	204	-	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
85	OHX	8	205	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	206	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	207	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	208	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	209	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	210	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	211	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	212	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	213	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	L3	401	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	L3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	L4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	M0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	M5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	M7	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	M7	202	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	M9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	N9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	O4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	O7	102	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	Q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	S6	301	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	S8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	S9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	c1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	c8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	d4	201	-	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
85	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l3	401	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l4	401	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l5	301	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	l9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	m0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	m1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	m5	501	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	n3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	n5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	o3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	o4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	s8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
85	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
85	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
85	OHX	1	3401	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3402	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3403	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3404	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3405	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3406	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	1	3407	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3408	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3409	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3410	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3411	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3412	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3413	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3414	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3415	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3416	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3417	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3418	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3419	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3420	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3421	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3422	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3423	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3424	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3425	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3426	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3427	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3428	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3429	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3430	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3431	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3432	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3433	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3434	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3435	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3436	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3437	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3438	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3439	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3440	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3441	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3442	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3443	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3444	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3445	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3446	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3447	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3448	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	1	3449	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3450	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3451	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3452	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3453	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3454	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3455	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3456	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3457	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3458	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3459	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3460	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3461	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3462	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3463	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3464	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3465	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3466	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3467	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3468	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3469	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3470	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3471	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3472	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3473	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3474	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3475	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3476	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3477	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3478	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3479	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3480	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3481	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3482	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3483	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3484	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3485	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3486	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3487	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3488	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3489	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3490	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	1	3491	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3492	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3493	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3494	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3495	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3496	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3497	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3498	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3499	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3500	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3501	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3502	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3503	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3504	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3505	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3506	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3507	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3508	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3509	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3510	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3511	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3512	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3513	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3514	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3515	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3516	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3517	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3518	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3519	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3520	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3521	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3522	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3523	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3524	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3525	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3526	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3527	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3528	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3529	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3530	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3531	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3532	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	1	3533	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3534	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3535	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3536	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3537	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3538	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3539	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3540	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3541	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3542	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3543	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3544	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3545	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3546	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3547	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3548	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3549	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3550	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3551	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3552	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3553	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3554	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3555	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3556	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3557	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3558	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3559	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3560	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3561	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3562	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3563	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3564	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3565	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3566	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3567	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3568	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3569	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3570	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3571	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3572	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3573	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3574	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	1	3575	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3576	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3577	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3578	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3579	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3580	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3581	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3582	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3583	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3584	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3585	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3586	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3587	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3588	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3589	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3590	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3591	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3592	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3593	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3594	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3595	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3596	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3597	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3598	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3599	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3600	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3601	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3602	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3603	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3604	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3605	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3606	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3607	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3608	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3609	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3610	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3611	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3612	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3613	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3614	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3615	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3616	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	1	3617	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3618	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3619	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3620	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3621	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3622	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3623	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3624	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3625	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3626	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3627	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3628	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3629	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3630	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3631	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3632	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3633	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3634	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3635	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3636	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3637	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3638	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3639	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3640	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3641	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3642	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3643	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3644	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3645	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3646	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3647	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3648	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3649	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3650	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3651	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3652	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3653	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3654	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3655	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3656	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3657	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3658	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	1	3659	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3660	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3661	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3662	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3663	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3664	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3665	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3666	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3667	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3668	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3669	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3670	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3671	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3672	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3673	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3674	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3675	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3676	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3677	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3678	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3679	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3680	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3681	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3682	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3683	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3684	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3685	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3686	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3687	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3688	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3689	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3690	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3691	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3692	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3693	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3694	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3695	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3696	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3697	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3698	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3699	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3700	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	1	3701	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3702	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3703	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3704	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3705	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3706	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3707	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3708	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3709	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3710	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3711	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3712	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3713	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3714	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3715	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3716	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3717	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3718	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3719	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3720	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3721	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3722	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3723	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3724	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3725	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3726	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3727	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3728	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3729	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3730	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3731	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3732	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3733	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3734	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3735	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3736	-	-	0/0/0/0	0/0/0/0
85	OHX	1	3737	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1901	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1902	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1903	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1904	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1905	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	2	1906	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1907	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1908	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1909	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1910	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1911	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1912	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1913	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1914	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1915	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1916	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1917	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1918	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1919	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1920	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1921	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1922	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1923	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1924	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1925	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1926	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1927	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1928	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1929	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1930	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1931	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1932	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1933	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1934	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1935	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1936	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1937	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1938	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1939	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1940	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1941	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1942	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1943	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1944	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1945	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1946	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1947	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	2	1948	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1949	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1950	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1951	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1952	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1953	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1954	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1955	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1956	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1957	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1958	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1959	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1960	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1961	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1962	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1963	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1964	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1965	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1966	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1967	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1968	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1969	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1970	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1971	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1972	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1973	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1974	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1975	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1976	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1977	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1978	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1979	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1980	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1981	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1982	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1983	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1984	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1985	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1986	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1987	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1988	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1989	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	2	1990	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1991	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1992	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1993	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1994	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1995	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1996	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1997	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1998	-	-	0/0/0/0	0/0/0/0
85	OHX	2	1999	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2000	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2001	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2002	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2003	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2004	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2005	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2006	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2007	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2008	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2009	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2010	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2011	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2012	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2013	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2014	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2015	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2016	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2017	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2018	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2019	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2020	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2021	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2031	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
85	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
85	OHX	3	202	-	-	0/0/0/0	0/0/0/0
85	OHX	3	203	-	-	0/0/0/0	0/0/0/0
85	OHX	3	204	-	-	0/0/0/0	0/0/0/0
85	OHX	3	205	-	-	0/0/0/0	0/0/0/0
85	OHX	3	206	-	-	0/0/0/0	0/0/0/0
85	OHX	3	207	-	-	0/0/0/0	0/0/0/0
85	OHX	3	208	-	-	0/0/0/0	0/0/0/0
85	OHX	3	209	-	-	0/0/0/0	0/0/0/0
85	OHX	3	210	-	-	0/0/0/0	0/0/0/0
85	OHX	3	211	-	-	0/0/0/0	0/0/0/0
85	OHX	4	201	-	-	0/0/0/0	0/0/0/0
85	OHX	4	202	-	-	0/0/0/0	0/0/0/0
85	OHX	4	203	-	-	0/0/0/0	0/0/0/0
85	OHX	4	204	-	-	0/0/0/0	0/0/0/0
85	OHX	4	205	-	-	0/0/0/0	0/0/0/0
85	OHX	4	206	-	-	0/0/0/0	0/0/0/0
85	OHX	4	207	-	-	0/0/0/0	0/0/0/0
85	OHX	4	208	-	-	0/0/0/0	0/0/0/0
85	OHX	4	209	-	-	0/0/0/0	0/0/0/0
85	OHX	4	210	-	-	0/0/0/0	0/0/0/0
85	OHX	4	211	-	-	0/0/0/0	0/0/0/0
85	OHX	4	212	-	-	0/0/0/0	0/0/0/0
85	OHX	4	213	-	-	0/0/0/0	0/0/0/0
85	OHX	4	214	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3401	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3402	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3403	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3404	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3405	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3406	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3407	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3408	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3409	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3410	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3411	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3412	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3413	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3414	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3415	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3416	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3417	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3418	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3419	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3420	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3421	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3422	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3423	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3424	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3425	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3426	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3427	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3428	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3429	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3430	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3431	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3432	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3433	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3434	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3435	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3436	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3437	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3438	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3439	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3440	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3441	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3442	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3443	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3444	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3445	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3446	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3447	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3448	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3449	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3450	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3451	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3452	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3453	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3454	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3455	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3456	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3457	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3458	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3459	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3460	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3461	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3462	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3463	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3464	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3465	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3466	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3467	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3468	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3469	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3470	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3471	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3472	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3473	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3474	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3475	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3476	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3477	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3478	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3479	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3480	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3481	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3482	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3483	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3484	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3485	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3486	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3487	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3488	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3489	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3490	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3491	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3492	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3493	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3494	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3495	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3496	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3497	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3498	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3499	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3500	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3501	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3502	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3503	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3504	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3505	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3506	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3507	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3508	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3509	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3510	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3511	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3512	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3513	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3514	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3515	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3516	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3517	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3518	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3519	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3520	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3521	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3522	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3523	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3524	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3525	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3526	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3527	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3528	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3529	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3530	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3531	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3532	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3533	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3534	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3535	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3536	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3537	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3538	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3539	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3540	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3541	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3542	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3543	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3544	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3545	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3546	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3547	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3548	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3549	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3550	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3551	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3552	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3553	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3554	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3555	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3556	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3557	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3558	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3559	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3560	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3561	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3562	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3563	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3564	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3565	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3566	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3567	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3568	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3569	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3570	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3571	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3572	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3573	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3574	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3575	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3576	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3577	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3578	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3579	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3580	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3581	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3582	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3583	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3584	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3585	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3586	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3587	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3588	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3589	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3590	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3591	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3592	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3593	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3594	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3595	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3596	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3597	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3598	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3599	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3600	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3601	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3602	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3603	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3604	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3605	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3606	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3607	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3608	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3609	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3610	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3611	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3612	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3613	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3614	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3615	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3616	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3617	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3618	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3619	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3620	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3621	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3622	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3623	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3624	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3625	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3626	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3627	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3628	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3629	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3630	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3631	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3632	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3633	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3634	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3635	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3636	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3637	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3638	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3639	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3640	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3641	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3642	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3643	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3644	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3645	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3646	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3647	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3648	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3649	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3650	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3651	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3652	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3653	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3654	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3655	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3656	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3657	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3658	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3659	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3660	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3661	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3662	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3663	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3664	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3665	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3666	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3667	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3668	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3669	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3670	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3671	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3672	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3673	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3674	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3675	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3676	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3677	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3678	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3679	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3680	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3681	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3682	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3683	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3684	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3685	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3686	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3687	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3688	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3689	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3690	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3691	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3692	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3693	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3694	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3695	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3696	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3697	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3698	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3699	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3700	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3701	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3702	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3703	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3704	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3705	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3706	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3707	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3708	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3709	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3710	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3711	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3712	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3713	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3714	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3715	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3716	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3717	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3718	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3719	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3720	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3721	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3722	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3723	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3724	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3725	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3726	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3727	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3728	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3729	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3730	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3731	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3732	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3733	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3734	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3735	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3736	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3737	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3738	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3739	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3740	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3741	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3742	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	5	3743	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3744	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3745	-	-	0/0/0/0	0/0/0/0
85	OHX	5	3746	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1901	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1902	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1903	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1904	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1905	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1906	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1907	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1908	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1909	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1910	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1911	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1912	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1913	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1914	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1915	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1916	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1917	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1918	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1919	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1920	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1921	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1922	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1923	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1924	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1925	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1926	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1927	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1928	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1929	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1930	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1931	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1932	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1933	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1934	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1935	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1936	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1937	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1938	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	6	1939	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1940	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1941	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1942	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1943	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1944	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1945	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1946	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1947	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1948	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1949	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1950	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1951	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1952	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1953	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1954	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1955	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1956	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1957	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1958	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1959	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1960	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1961	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1962	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1963	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1964	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1965	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1966	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1967	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1968	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1969	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1970	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1971	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1972	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1973	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1974	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1975	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1976	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1977	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1978	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1979	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1980	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	6	1981	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1982	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1983	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1984	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1985	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1986	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1987	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1988	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1989	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1990	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1991	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1992	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1993	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1994	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1995	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1996	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1997	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1998	-	-	0/0/0/0	0/0/0/0
85	OHX	6	1999	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2000	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2001	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2002	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2003	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2004	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2005	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2006	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2007	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2008	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2009	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2010	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2011	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2012	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2013	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2014	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2015	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2016	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2017	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2018	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2019	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2020	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2021	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2022	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	6	2023	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2024	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2025	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2026	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2027	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2028	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2029	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2030	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2031	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2032	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2033	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2034	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2035	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2036	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2037	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2038	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2039	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2040	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2041	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2042	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2043	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
85	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
85	OHX	7	201	-	-	0/0/0/0	0/0/0/0
85	OHX	7	202	-	-	0/0/0/0	0/0/0/0
85	OHX	7	203	-	-	0/0/0/0	0/0/0/0
85	OHX	7	204	-	-	0/0/0/0	0/0/0/0
85	OHX	7	205	-	-	0/0/0/0	0/0/0/0
85	OHX	7	206	-	-	0/0/0/0	0/0/0/0
85	OHX	7	207	-	-	0/0/0/0	0/0/0/0
85	OHX	7	208	-	-	0/0/0/0	0/0/0/0
85	OHX	7	209	-	-	0/0/0/0	0/0/0/0
85	OHX	7	210	-	-	0/0/0/0	0/0/0/0
85	OHX	7	211	-	-	0/0/0/0	0/0/0/0
85	OHX	7	212	-	-	0/0/0/0	0/0/0/0
85	OHX	8	201	-	-	0/0/0/0	0/0/0/0
85	OHX	8	202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	8	203	-	-	0/0/0/0	0/0/0/0
85	OHX	8	204	-	-	0/0/0/0	0/0/0/0
85	OHX	8	205	-	-	0/0/0/0	0/0/0/0
85	OHX	8	206	-	-	0/0/0/0	0/0/0/0
85	OHX	8	207	-	-	0/0/0/0	0/0/0/0
85	OHX	8	208	-	-	0/0/0/0	0/0/0/0
85	OHX	8	209	-	-	0/0/0/0	0/0/0/0
85	OHX	8	210	-	-	0/0/0/0	0/0/0/0
85	OHX	8	211	-	-	0/0/0/0	0/0/0/0
85	OHX	8	212	-	-	0/0/0/0	0/0/0/0
85	OHX	8	213	-	-	0/0/0/0	0/0/0/0
85	OHX	8	214	-	-	0/0/0/0	0/0/0/0
85	OHX	8	215	-	-	0/0/0/0	0/0/0/0
85	OHX	8	216	-	-	0/0/0/0	0/0/0/0
85	OHX	8	217	-	-	0/0/0/0	0/0/0/0
85	OHX	8	218	-	-	0/0/0/0	0/0/0/0
85	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
85	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
85	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
85	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
85	OHX	L3	401	-	-	0/0/0/0	0/0/0/0
85	OHX	L3	402	-	-	0/0/0/0	0/0/0/0
85	OHX	L4	401	-	-	0/0/0/0	0/0/0/0
85	OHX	M0	301	-	-	0/0/0/0	0/0/0/0
85	OHX	M5	302	-	-	0/0/0/0	0/0/0/0
85	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
85	OHX	M7	201	-	-	0/0/0/0	0/0/0/0
85	OHX	M7	202	-	-	0/0/0/0	0/0/0/0
85	OHX	M9	201	-	-	0/0/0/0	0/0/0/0
85	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
85	OHX	N9	102	-	-	0/0/0/0	0/0/0/0
85	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
85	OHX	O4	201	-	-	0/0/0/0	0/0/0/0
85	OHX	O7	102	-	-	0/0/0/0	0/0/0/0
85	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
85	OHX	Q2	502	-	-	0/0/0/0	0/0/0/0
85	OHX	S6	301	-	-	0/0/0/0	0/0/0/0
85	OHX	S8	301	-	-	0/0/0/0	0/0/0/0
85	OHX	S9	201	-	-	0/0/0/0	0/0/0/0
85	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
85	OHX	c1	201	-	-	0/0/0/0	0/0/0/0
85	OHX	c3	201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
85	OHX	c8	201	-	-	0/0/0/0	0/0/0/0
85	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
85	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
85	OHX	l3	401	-	-	0/0/0/0	0/0/0/0
85	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
85	OHX	l4	401	-	-	0/0/0/0	0/0/0/0
85	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
85	OHX	l5	301	-	-	0/0/0/0	0/0/0/0
85	OHX	l5	302	-	-	0/0/0/0	0/0/0/0
85	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
85	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
85	OHX	l9	201	-	-	0/0/0/0	0/0/0/0
85	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
85	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
85	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
85	OHX	m1	201	-	-	0/0/0/0	0/0/0/0
85	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
85	OHX	m5	501	-	-	0/0/0/0	0/0/0/0
85	OHX	n3	201	-	-	0/0/0/0	0/0/0/0
85	OHX	n5	201	-	-	0/0/0/0	0/0/0/0
85	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
85	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
85	OHX	o3	201	-	-	0/0/0/0	0/0/0/0
85	OHX	o4	201	-	-	0/0/0/0	0/0/0/0
85	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
85	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
85	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
85	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
85	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
85	OHX	s8	301	-	-	0/0/0/0	0/0/0/0
85	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
85	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.

533 monomers are involved in 864 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3401	OHX	1	0
85	1	3403	OHX	1	0
85	1	3404	OHX	1	0
85	1	3405	OHX	3	0
85	1	3406	OHX	3	0
85	1	3408	OHX	1	0
85	1	3409	OHX	2	0
85	1	3410	OHX	2	0
85	1	3411	OHX	1	0
85	1	3412	OHX	1	0
85	1	3415	OHX	2	0
85	1	3416	OHX	1	0
85	1	3417	OHX	1	0
85	1	3419	OHX	1	0
85	1	3420	OHX	2	0
85	1	3421	OHX	1	0
85	1	3423	OHX	2	0
85	1	3425	OHX	1	0
85	1	3426	OHX	1	0
85	1	3427	OHX	1	0
85	1	3428	OHX	1	0
85	1	3429	OHX	2	0
85	1	3430	OHX	1	0
85	1	3434	OHX	1	0
85	1	3436	OHX	1	0
85	1	3437	OHX	2	0
85	1	3440	OHX	1	0
85	1	3442	OHX	1	0
85	1	3445	OHX	1	0
85	1	3448	OHX	4	0
85	1	3450	OHX	1	0
85	1	3451	OHX	1	0
85	1	3454	OHX	1	0
85	1	3457	OHX	1	0
85	1	3458	OHX	1	0
85	1	3460	OHX	1	0
85	1	3461	OHX	1	0
85	1	3462	OHX	1	0
85	1	3463	OHX	1	0
85	1	3464	OHX	1	0
85	1	3467	OHX	1	0
85	1	3469	OHX	1	0
85	1	3470	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3473	OHX	1	0
85	1	3475	OHX	6	0
85	1	3476	OHX	1	0
85	1	3477	OHX	1	0
85	1	3483	OHX	6	0
85	1	3485	OHX	1	0
85	1	3489	OHX	1	0
85	1	3491	OHX	1	0
85	1	3493	OHX	1	0
85	1	3495	OHX	6	0
85	1	3496	OHX	1	0
85	1	3497	OHX	4	0
85	1	3499	OHX	1	0
85	1	3500	OHX	1	0
85	1	3502	OHX	1	0
85	1	3504	OHX	1	0
85	1	3509	OHX	6	0
85	1	3510	OHX	2	0
85	1	3511	OHX	1	0
85	1	3512	OHX	1	0
85	1	3513	OHX	4	0
85	1	3515	OHX	2	0
85	1	3517	OHX	2	0
85	1	3518	OHX	2	0
85	1	3519	OHX	2	0
85	1	3520	OHX	2	0
85	1	3521	OHX	1	0
85	1	3529	OHX	1	0
85	1	3532	OHX	1	0
85	1	3534	OHX	2	0
85	1	3535	OHX	1	0
85	1	3536	OHX	1	0
85	1	3538	OHX	2	0
85	1	3540	OHX	6	0
85	1	3542	OHX	1	0
85	1	3543	OHX	1	0
85	1	3544	OHX	1	0
85	1	3545	OHX	1	0
85	1	3550	OHX	1	0
85	1	3554	OHX	1	0
85	1	3556	OHX	4	0
85	1	3561	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3565	OHX	6	0
85	1	3567	OHX	2	0
85	1	3569	OHX	6	0
85	1	3571	OHX	1	0
85	1	3573	OHX	1	0
85	1	3575	OHX	2	0
85	1	3576	OHX	3	0
85	1	3577	OHX	1	0
85	1	3578	OHX	2	0
85	1	3580	OHX	1	0
85	1	3581	OHX	3	0
85	1	3582	OHX	7	0
85	1	3583	OHX	1	0
85	1	3584	OHX	2	0
85	1	3586	OHX	1	0
85	1	3587	OHX	1	0
85	1	3592	OHX	6	0
85	1	3593	OHX	4	0
85	1	3594	OHX	4	0
85	1	3595	OHX	2	0
85	1	3597	OHX	1	0
85	1	3598	OHX	1	0
85	1	3600	OHX	1	0
85	1	3602	OHX	1	0
85	1	3603	OHX	2	0
85	1	3607	OHX	1	0
85	1	3611	OHX	1	0
85	1	3616	OHX	5	0
85	1	3620	OHX	1	0
85	1	3621	OHX	2	0
85	1	3624	OHX	1	0
85	1	3626	OHX	1	0
85	1	3631	OHX	1	0
85	1	3632	OHX	1	0
85	1	3635	OHX	1	0
85	1	3642	OHX	1	0
85	1	3643	OHX	1	0
85	1	3644	OHX	2	0
85	1	3645	OHX	1	0
85	1	3646	OHX	1	0
85	1	3647	OHX	2	0
85	1	3650	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3651	OHX	1	0
85	1	3652	OHX	1	0
85	1	3655	OHX	1	0
85	1	3656	OHX	8	0
85	1	3657	OHX	1	0
85	1	3658	OHX	1	0
85	1	3660	OHX	2	0
85	1	3663	OHX	1	0
85	1	3666	OHX	1	0
85	1	3670	OHX	1	0
85	1	3672	OHX	1	0
85	1	3673	OHX	1	0
85	1	3676	OHX	2	0
85	1	3677	OHX	4	0
85	1	3678	OHX	3	0
85	1	3679	OHX	2	0
85	1	3680	OHX	1	0
85	1	3681	OHX	1	0
85	1	3682	OHX	2	0
85	1	3685	OHX	6	0
85	1	3688	OHX	2	0
85	1	3689	OHX	3	0
85	1	3694	OHX	4	0
85	1	3695	OHX	6	0
85	1	3697	OHX	1	0
85	1	3699	OHX	1	0
85	1	3702	OHX	6	0
85	1	3703	OHX	1	0
85	1	3704	OHX	1	0
85	1	3706	OHX	1	0
85	1	3707	OHX	3	0
85	1	3708	OHX	1	0
85	1	3711	OHX	7	0
85	1	3717	OHX	1	0
85	1	3719	OHX	1	0
85	1	3720	OHX	5	0
85	1	3723	OHX	1	0
85	1	3727	OHX	3	0
85	1	3731	OHX	1	0
85	1	3733	OHX	1	0
85	1	3734	OHX	1	0
85	1	3735	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	1	3737	OHX	7	0
85	2	1901	OHX	1	0
85	2	1902	OHX	1	0
85	2	1904	OHX	2	0
85	2	1907	OHX	1	0
85	2	1909	OHX	7	0
85	2	1910	OHX	1	0
85	2	1912	OHX	1	0
85	2	1914	OHX	3	0
85	2	1916	OHX	1	0
85	2	1917	OHX	2	0
85	2	1919	OHX	1	0
85	2	1920	OHX	2	0
85	2	1922	OHX	8	0
85	2	1923	OHX	1	0
85	2	1924	OHX	1	0
85	2	1925	OHX	1	0
85	2	1927	OHX	1	0
85	2	1928	OHX	1	0
85	2	1929	OHX	1	0
85	2	1932	OHX	1	0
85	2	1936	OHX	1	0
85	2	1937	OHX	1	0
85	2	1938	OHX	1	0
85	2	1939	OHX	1	0
85	2	1940	OHX	2	0
85	2	1942	OHX	1	0
85	2	1943	OHX	2	0
85	2	1944	OHX	1	0
85	2	1948	OHX	2	0
85	2	1949	OHX	1	0
85	2	1951	OHX	2	0
85	2	1952	OHX	1	0
85	2	1953	OHX	4	0
85	2	1954	OHX	1	0
85	2	1956	OHX	1	0
85	2	1960	OHX	2	0
85	2	1961	OHX	2	0
85	2	1963	OHX	2	0
85	2	1967	OHX	3	0
85	2	1968	OHX	5	0
85	2	1970	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	2	1971	OHX	1	0
85	2	1972	OHX	1	0
85	2	1974	OHX	1	0
85	2	1976	OHX	1	0
85	2	1977	OHX	7	0
85	2	1978	OHX	1	0
85	2	1983	OHX	1	0
85	2	1984	OHX	1	0
85	2	1986	OHX	1	0
85	2	1987	OHX	1	0
85	2	1988	OHX	1	0
85	2	1989	OHX	4	0
85	2	1993	OHX	1	0
85	2	1999	OHX	3	0
85	2	2001	OHX	1	0
85	2	2004	OHX	1	0
85	2	2005	OHX	1	0
85	2	2006	OHX	1	0
85	2	2008	OHX	2	0
85	2	2009	OHX	2	0
85	2	2010	OHX	6	0
85	2	2011	OHX	1	0
85	2	2017	OHX	1	0
85	2	2024	OHX	1	0
85	2	2025	OHX	6	0
85	2	2028	OHX	1	0
85	2	2029	OHX	1	0
85	2	2031	OHX	1	0
85	2	2033	OHX	2	0
85	2	2034	OHX	1	0
85	2	2035	OHX	1	0
85	2	2036	OHX	1	0
85	2	2038	OHX	1	0
85	2	2039	OHX	2	0
85	2	2040	OHX	4	0
85	2	2043	OHX	1	0
85	3	205	OHX	2	0
85	3	207	OHX	1	0
85	3	208	OHX	2	0
85	4	203	OHX	1	0
85	4	204	OHX	1	0
85	4	205	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	4	206	OHX	2	0
85	4	207	OHX	1	0
85	4	210	OHX	1	0
85	4	211	OHX	2	0
85	4	214	OHX	1	0
85	5	3401	OHX	3	0
85	5	3402	OHX	1	0
85	5	3403	OHX	3	0
85	5	3405	OHX	1	0
85	5	3407	OHX	2	0
85	5	3408	OHX	1	0
85	5	3409	OHX	1	0
85	5	3410	OHX	1	0
85	5	3411	OHX	1	0
85	5	3412	OHX	1	0
85	5	3413	OHX	3	0
85	5	3414	OHX	1	0
85	5	3415	OHX	2	0
85	5	3417	OHX	1	0
85	5	3418	OHX	3	0
85	5	3419	OHX	1	0
85	5	3420	OHX	1	0
85	5	3425	OHX	1	0
85	5	3427	OHX	3	0
85	5	3428	OHX	1	0
85	5	3430	OHX	1	0
85	5	3437	OHX	1	0
85	5	3438	OHX	1	0
85	5	3439	OHX	1	0
85	5	3441	OHX	1	0
85	5	3443	OHX	1	0
85	5	3444	OHX	8	0
85	5	3446	OHX	1	0
85	5	3447	OHX	2	0
85	5	3450	OHX	1	0
85	5	3452	OHX	1	0
85	5	3454	OHX	1	0
85	5	3455	OHX	1	0
85	5	3456	OHX	1	0
85	5	3458	OHX	2	0
85	5	3459	OHX	3	0
85	5	3461	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	3462	OHX	1	0
85	5	3464	OHX	2	0
85	5	3466	OHX	1	0
85	5	3471	OHX	1	0
85	5	3480	OHX	8	0
85	5	3486	OHX	3	0
85	5	3487	OHX	1	0
85	5	3488	OHX	1	0
85	5	3489	OHX	1	0
85	5	3494	OHX	1	0
85	5	3499	OHX	1	0
85	5	3504	OHX	7	0
85	5	3505	OHX	5	0
85	5	3506	OHX	1	0
85	5	3508	OHX	2	0
85	5	3510	OHX	1	0
85	5	3511	OHX	1	0
85	5	3512	OHX	1	0
85	5	3513	OHX	1	0
85	5	3514	OHX	6	0
85	5	3516	OHX	2	0
85	5	3517	OHX	1	0
85	5	3518	OHX	1	0
85	5	3521	OHX	1	0
85	5	3524	OHX	6	0
85	5	3526	OHX	1	0
85	5	3527	OHX	1	0
85	5	3528	OHX	2	0
85	5	3530	OHX	1	0
85	5	3531	OHX	1	0
85	5	3532	OHX	1	0
85	5	3533	OHX	1	0
85	5	3534	OHX	1	0
85	5	3535	OHX	1	0
85	5	3537	OHX	5	0
85	5	3539	OHX	7	0
85	5	3541	OHX	1	0
85	5	3543	OHX	1	0
85	5	3545	OHX	1	0
85	5	3546	OHX	1	0
85	5	3549	OHX	1	0
85	5	3550	OHX	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	3553	OHX	1	0
85	5	3555	OHX	1	0
85	5	3558	OHX	1	0
85	5	3559	OHX	6	0
85	5	3568	OHX	1	0
85	5	3570	OHX	8	0
85	5	3578	OHX	1	0
85	5	3579	OHX	1	0
85	5	3582	OHX	1	0
85	5	3583	OHX	1	0
85	5	3584	OHX	1	0
85	5	3585	OHX	5	0
85	5	3586	OHX	1	0
85	5	3588	OHX	1	0
85	5	3591	OHX	1	0
85	5	3592	OHX	1	0
85	5	3594	OHX	8	0
85	5	3595	OHX	2	0
85	5	3596	OHX	2	0
85	5	3597	OHX	3	0
85	5	3600	OHX	1	0
85	5	3601	OHX	2	0
85	5	3604	OHX	1	0
85	5	3605	OHX	1	0
85	5	3606	OHX	5	0
85	5	3609	OHX	1	0
85	5	3610	OHX	1	0
85	5	3611	OHX	2	0
85	5	3614	OHX	1	0
85	5	3615	OHX	1	0
85	5	3623	OHX	1	0
85	5	3629	OHX	1	0
85	5	3631	OHX	1	0
85	5	3633	OHX	1	0
85	5	3634	OHX	1	0
85	5	3635	OHX	2	0
85	5	3636	OHX	1	0
85	5	3641	OHX	1	0
85	5	3644	OHX	1	0
85	5	3645	OHX	1	0
85	5	3647	OHX	6	0
85	5	3648	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	3649	OHX	1	0
85	5	3651	OHX	1	0
85	5	3652	OHX	1	0
85	5	3657	OHX	1	0
85	5	3658	OHX	1	0
85	5	3660	OHX	1	0
85	5	3663	OHX	2	0
85	5	3664	OHX	1	0
85	5	3666	OHX	1	0
85	5	3667	OHX	2	0
85	5	3672	OHX	1	0
85	5	3673	OHX	1	0
85	5	3676	OHX	2	0
85	5	3677	OHX	1	0
85	5	3681	OHX	1	0
85	5	3683	OHX	1	0
85	5	3684	OHX	2	0
85	5	3686	OHX	1	0
85	5	3688	OHX	1	0
85	5	3689	OHX	1	0
85	5	3691	OHX	1	0
85	5	3693	OHX	4	0
85	5	3695	OHX	3	0
85	5	3697	OHX	2	0
85	5	3698	OHX	1	0
85	5	3699	OHX	1	0
85	5	3702	OHX	1	0
85	5	3703	OHX	11	0
85	5	3704	OHX	7	0
85	5	3705	OHX	7	0
85	5	3706	OHX	4	0
85	5	3707	OHX	1	0
85	5	3708	OHX	1	0
85	5	3709	OHX	1	0
85	5	3715	OHX	1	0
85	5	3718	OHX	3	0
85	5	3720	OHX	1	0
85	5	3721	OHX	7	0
85	5	3723	OHX	1	0
85	5	3725	OHX	1	0
85	5	3728	OHX	3	0
85	5	3731	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	5	3732	OHX	1	0
85	5	3733	OHX	1	0
85	5	3735	OHX	1	0
85	5	3737	OHX	1	0
85	5	3739	OHX	6	0
85	5	3740	OHX	1	0
85	5	3742	OHX	7	0
85	5	3743	OHX	4	0
85	6	1903	OHX	1	0
85	6	1904	OHX	2	0
85	6	1908	OHX	1	0
85	6	1910	OHX	1	0
85	6	1911	OHX	2	0
85	6	1912	OHX	1	0
85	6	1913	OHX	1	0
85	6	1914	OHX	8	0
85	6	1915	OHX	1	0
85	6	1916	OHX	1	0
85	6	1920	OHX	1	0
85	6	1922	OHX	1	0
85	6	1923	OHX	1	0
85	6	1925	OHX	1	0
85	6	1926	OHX	2	0
85	6	1929	OHX	1	0
85	6	1930	OHX	1	0
85	6	1932	OHX	1	0
85	6	1934	OHX	1	0
85	6	1936	OHX	1	0
85	6	1938	OHX	2	0
85	6	1940	OHX	1	0
85	6	1941	OHX	1	0
85	6	1943	OHX	1	0
85	6	1947	OHX	1	0
85	6	1950	OHX	1	0
85	6	1951	OHX	3	0
85	6	1955	OHX	2	0
85	6	1956	OHX	1	0
85	6	1957	OHX	1	0
85	6	1958	OHX	1	0
85	6	1960	OHX	1	0
85	6	1962	OHX	1	0
85	6	1966	OHX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	6	1967	OHX	2	0
85	6	1969	OHX	1	0
85	6	1972	OHX	1	0
85	6	1975	OHX	7	0
85	6	1976	OHX	1	0
85	6	1977	OHX	1	0
85	6	1978	OHX	2	0
85	6	1980	OHX	3	0
85	6	1984	OHX	1	0
85	6	1989	OHX	1	0
85	6	1990	OHX	1	0
85	6	1991	OHX	2	0
85	6	1992	OHX	1	0
85	6	1994	OHX	1	0
85	6	1997	OHX	1	0
85	6	1998	OHX	2	0
85	6	2000	OHX	1	0
85	6	2001	OHX	8	0
85	6	2003	OHX	1	0
85	6	2004	OHX	2	0
85	6	2007	OHX	1	0
85	6	2008	OHX	1	0
85	6	2009	OHX	1	0
85	6	2010	OHX	1	0
85	6	2014	OHX	1	0
85	6	2017	OHX	1	0
85	6	2022	OHX	1	0
85	6	2025	OHX	8	0
85	6	2029	OHX	1	0
85	6	2032	OHX	1	0
85	6	2034	OHX	1	0
85	6	2036	OHX	2	0
85	6	2037	OHX	1	0
85	6	2038	OHX	2	0
85	6	2041	OHX	1	0
85	6	2042	OHX	1	0
85	6	2043	OHX	2	0
85	6	2044	OHX	1	0
85	6	2046	OHX	1	0
85	6	2048	OHX	1	0
85	7	203	OHX	7	0
85	7	204	OHX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	7	206	OHX	2	0
85	7	209	OHX	4	0
85	7	211	OHX	7	0
85	8	201	OHX	2	0
85	8	203	OHX	9	0
85	8	204	OHX	1	0
85	8	205	OHX	2	0
85	8	207	OHX	1	0
85	8	211	OHX	6	0
85	8	212	OHX	1	0
85	8	215	OHX	1	0
85	8	217	OHX	1	0
85	C5	201	OHX	3	0
85	D9	102	OHX	2	0
85	L3	401	OHX	1	0
85	L3	402	OHX	2	0
85	L4	401	OHX	5	0
85	M0	301	OHX	2	0
85	M5	302	OHX	1	0
85	M7	201	OHX	2	0
85	M7	202	OHX	1	0
85	N1	201	OHX	2	0
85	O3	201	OHX	3	0
85	O4	201	OHX	1	0
85	O7	102	OHX	2	0
85	O7	103	OHX	1	0
85	Q2	502	OHX	7	0
85	S9	201	OHX	4	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
81	m2	2
35	sM	1
80	c0	1

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Mol	Chain	Number of breaks
1	2	1
35	SM	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	139:UNK	C	155:UNK	N	37.65
1	SM	141:ALA	C	151:UNK	N	26.56
1	c0	84:GLU	C	87:UNK	N	8.21
1	2	1716:C	O3'	1717:G	P	4.60
1	m2	23:UNK	C	28:UNK	N	4.05

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%)	0.66	155 (8%) 13 12	61, 97, 186, 235	0
1	6	1795/1800 (99%)	0.45	122 (6%) 20 19	48, 82, 168, 218	0
2	S0	206/251 (82%)	0.91	27 (13%) 5 4	108, 147, 226, 316	0
2	s0	206/251 (82%)	0.34	8 (3%) 43 38	81, 112, 176, 255	0
3	S1	214/254 (84%)	1.36	49 (22%) 1 1	111, 136, 156, 161	0
3	s1	216/254 (85%)	0.52	20 (9%) 11 11	74, 87, 104, 112	0
4	S2	217/253 (85%)	0.28	7 (3%) 51 47	81, 93, 115, 123	0
4	s2	217/253 (85%)	0.35	12 (5%) 29 26	62, 74, 89, 98	0
5	S3	223/239 (93%)	0.48	16 (7%) 18 17	81, 94, 124, 132	0
5	s3	223/239 (93%)	0.56	18 (8%) 15 14	85, 109, 132, 140	0
6	S4	260/260 (100%)	0.66	23 (8%) 12 12	72, 98, 110, 122	0
6	s4	260/260 (100%)	0.20	7 (2%) 58 53	53, 79, 92, 115	0
7	S5	206/224 (91%)	0.68	24 (11%) 6 6	101, 117, 125, 131	0
7	s5	206/224 (91%)	0.58	13 (6%) 23 22	81, 101, 114, 117	0
8	S6	226/236 (95%)	0.77	25 (11%) 7 7	72, 126, 220, 365	0
8	s6	218/236 (92%)	0.56	7 (3%) 51 47	54, 87, 104, 115	0
9	S7	184/189 (97%)	0.83	26 (14%) 4 4	91, 117, 133, 136	0
9	s7	186/189 (98%)	0.59	17 (9%) 11 11	72, 103, 131, 195	0
10	S8	188/200 (94%)	0.65	14 (7%) 17 17	65, 84, 127, 136	0
10	s8	188/200 (94%)	0.56	10 (5%) 30 27	49, 74, 126, 145	0
11	S9	185/196 (94%)	0.81	22 (11%) 6 6	88, 103, 128, 145	0
11	s9	185/196 (94%)	0.43	8 (4%) 39 34	67, 85, 114, 132	0
12	C0	96/105 (91%)	0.52	7 (7%) 18 17	87, 106, 124, 135	0
13	C1	146/155 (94%)	0.38	9 (6%) 24 22	68, 82, 105, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	c1	146/155 (94%)	0.39	9 (6%) 24 22	55, 69, 111, 187	0
14	C2	109/142 (76%)	1.89	47 (43%) 0 0	139, 144, 148, 151	0
14	c2	109/142 (76%)	2.81	59 (54%) 0 0	184, 196, 200, 201	0
15	C3	150/150 (100%)	0.36	3 (2%) 68 62	73, 92, 108, 111	0
15	c3	150/150 (100%)	0.22	2 (1%) 79 74	60, 77, 92, 103	0
16	C4	127/136 (93%)	1.24	28 (22%) 1 1	82, 139, 149, 152	0
16	c4	128/136 (94%)	0.34	3 (2%) 64 58	60, 88, 93, 97	0
17	C5	124/141 (87%)	0.40	6 (4%) 34 31	79, 96, 120, 131	0
17	c5	135/141 (95%)	0.73	18 (13%) 4 4	71, 98, 118, 128	0
18	C6	141/142 (99%)	0.83	14 (9%) 9 10	86, 109, 113, 116	0
18	c6	142/142 (100%)	0.90	20 (14%) 4 4	75, 97, 114, 131	0
19	C7	120/136 (88%)	1.26	22 (18%) 2 2	99, 112, 309, 332	0
19	c7	117/136 (86%)	1.21	32 (27%) 1 1	88, 102, 310, 364	0
20	C8	145/145 (100%)	1.14	37 (25%) 1 1	78, 103, 123, 127	0
20	c8	145/145 (100%)	0.63	10 (6%) 20 19	73, 92, 109, 115	0
21	C9	143/143 (100%)	0.74	14 (9%) 10 10	95, 103, 117, 124	0
21	c9	143/143 (100%)	0.25	2 (1%) 78 73	76, 88, 102, 109	0
22	D0	107/120 (89%)	1.35	27 (25%) 1 1	81, 109, 125, 128	0
22	d0	110/120 (91%)	1.53	35 (31%) 1 1	79, 113, 136, 142	0
23	D1	87/87 (100%)	0.39	1 (1%) 82 77	102, 112, 163, 190	0
23	d1	87/87 (100%)	0.08	0 100 100	74, 85, 129, 145	0
24	D2	129/129 (100%)	0.36	4 (3%) 52 48	76, 90, 98, 109	0
24	d2	129/129 (100%)	0.04	1 (0%) 87 83	58, 70, 79, 92	0
25	D3	144/144 (100%)	0.45	12 (8%) 14 13	63, 69, 77, 86	0
25	d3	144/144 (100%)	0.08	0 100 100	48, 54, 64, 71	0
26	D4	134/134 (100%)	0.96	26 (19%) 1 2	86, 104, 115, 117	0
26	d4	134/134 (100%)	0.55	14 (10%) 8 8	62, 84, 97, 116	0
27	D5	70/107 (65%)	0.82	9 (12%) 5 4	116, 124, 128, 128	0
27	d5	69/107 (64%)	0.74	9 (13%) 5 4	92, 109, 115, 117	0
28	D6	97/97 (100%)	1.41	26 (26%) 1 1	85, 101, 146, 147	0
28	d6	97/97 (100%)	0.29	3 (3%) 52 48	63, 78, 96, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	D7	81/81 (100%)	0.49	6 (7%) 17 17	93, 109, 126, 129	0
29	d7	81/81 (100%)	0.37	5 (6%) 24 22	74, 89, 114, 118	0
30	D8	63/66 (95%)	2.25	33 (52%) 0 0	108, 122, 128, 130	0
30	d8	63/66 (95%)	1.50	16 (25%) 1 1	96, 107, 115, 118	0
31	D9	53/55 (96%)	0.43	2 (3%) 44 39	84, 89, 106, 110	0
31	d9	53/55 (96%)	1.18	12 (22%) 1 1	82, 94, 123, 130	0
32	E0	60/62 (96%)	1.30	11 (18%) 2 2	69, 99, 123, 125	0
32	e0	62/62 (100%)	0.84	7 (11%) 7 7	57, 82, 104, 111	0
33	E1	71/76 (93%)	1.76	27 (38%) 0 1	96, 137, 146, 147	0
33	e1	76/76 (100%)	2.52	35 (46%) 0 0	111, 170, 193, 197	0
34	SR	318/318 (100%)	0.86	39 (12%) 5 5	110, 123, 140, 202	0
34	sR	318/318 (100%)	1.07	58 (18%) 2 2	112, 128, 142, 186	0
35	SM	133/182 (73%)	0.82	19 (14%) 4 3	57, 87, 146, 161	0
35	sM	63/182 (34%)	0.61	7 (11%) 7 7	45, 97, 104, 108	0
36	1	3149/3396 (92%)	0.10	110 (3%) 48 42	31, 57, 131, 226	0
36	5	3150/3396 (92%)	0.05	73 (2%) 64 58	30, 54, 119, 190	0
37	3	121/121 (100%)	-0.01	0 100 100	41, 71, 88, 91	0
37	7	121/121 (100%)	-0.13	0 100 100	36, 55, 70, 74	0
38	4	158/158 (100%)	-0.02	4 (2%) 61 55	37, 60, 97, 140	0
38	8	158/158 (100%)	-0.02	3 (1%) 70 64	41, 63, 100, 119	0
39	L2	252/253 (99%)	0.14	2 (0%) 87 83	41, 56, 73, 147	0
39	l2	252/253 (99%)	0.06	6 (2%) 62 57	39, 57, 78, 146	0
40	L3	386/386 (100%)	-0.11	1 (0%) 94 92	36, 58, 75, 93	0
40	l3	386/386 (100%)	-0.21	4 (1%) 84 79	30, 44, 62, 97	0
41	L4	361/361 (100%)	-0.20	2 (0%) 90 86	34, 48, 64, 76	0
41	l4	361/361 (100%)	-0.14	3 (0%) 87 83	36, 50, 68, 80	0
42	L5	296/296 (100%)	0.21	7 (2%) 62 57	52, 75, 96, 113	0
42	l5	294/296 (99%)	0.05	5 (1%) 73 67	40, 58, 85, 120	0
43	L6	156/175 (89%)	-0.19	0 100 100	43, 50, 67, 83	0
43	l6	157/175 (89%)	-0.12	2 (1%) 79 74	41, 50, 70, 79	0
44	L7	222/243 (91%)	-0.35	1 (0%) 91 89	36, 42, 65, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	-0.30	2 (0%) 85 81	33, 41, 72, 98	0
45	L8	233/255 (91%)	0.46	19 (8%) 14 13	61, 81, 173, 291	0
45	l8	231/255 (90%)	0.80	30 (12%) 5 4	68, 83, 110, 115	0
46	L9	191/191 (100%)	0.31	5 (2%) 59 54	48, 61, 73, 82	0
46	l9	191/191 (100%)	-0.04	1 (0%) 91 89	40, 49, 64, 73	0
47	M0	211/220 (95%)	-0.03	8 (3%) 44 39	40, 50, 87, 161	0
47	m0	213/220 (96%)	0.02	3 (1%) 78 73	35, 48, 82, 172	0
48	M1	169/173 (97%)	0.30	5 (2%) 54 49	65, 81, 94, 100	0
48	m1	169/173 (97%)	0.05	1 (0%) 90 86	46, 61, 70, 82	0
49	M3	193/198 (97%)	0.16	5 (2%) 59 54	37, 59, 96, 119	0
49	m3	194/198 (97%)	0.16	5 (2%) 59 54	38, 64, 96, 112	0
50	M4	136/137 (99%)	-0.12	3 (2%) 65 60	45, 50, 63, 71	0
50	m4	137/137 (100%)	-0.30	0 100 100	39, 45, 68, 80	0
51	M5	203/203 (100%)	-0.15	0 100 100	37, 53, 63, 68	0
51	m5	203/203 (100%)	0.01	0 100 100	41, 58, 69, 73	0
52	M6	197/198 (99%)	-0.24	2 (1%) 84 79	35, 41, 60, 63	0
52	m6	197/198 (99%)	-0.30	4 (2%) 68 62	31, 35, 58, 62	0
53	M7	183/183 (100%)	0.21	15 (8%) 14 13	39, 50, 170, 329	0
53	m7	155/183 (84%)	-0.07	0 100 100	35, 42, 53, 67	0
54	M8	185/185 (100%)	-0.18	0 100 100	38, 50, 66, 85	0
54	m8	185/185 (100%)	-0.17	0 100 100	36, 52, 64, 70	0
55	M9	188/188 (100%)	0.48	9 (4%) 34 31	64, 76, 138, 144	0
55	m9	188/188 (100%)	0.33	8 (4%) 39 34	55, 64, 120, 135	0
56	N0	172/172 (100%)	-0.21	1 (0%) 90 86	39, 48, 61, 64	0
56	n0	172/172 (100%)	-0.22	1 (0%) 90 86	35, 40, 51, 61	0
57	N1	159/159 (100%)	-0.06	5 (3%) 52 48	41, 51, 87, 91	0
57	n1	159/159 (100%)	-0.04	5 (3%) 52 48	38, 44, 80, 85	0
58	N2	100/120 (83%)	1.10	23 (23%) 1 1	91, 102, 109, 112	0
58	n2	98/120 (81%)	0.99	18 (18%) 2 2	75, 84, 92, 95	0
59	N3	136/136 (100%)	0.33	6 (4%) 38 34	43, 52, 61, 68	0
59	n3	136/136 (100%)	-0.18	0 100 100	31, 41, 54, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	2.22	30 (30%) 1 1	52, 74, 448, 489	0
60	n4	135/155 (87%)	0.79	19 (14%) 4 4	41, 94, 307, 436	0
61	N5	121/141 (85%)	0.32	7 (5%) 26 24	52, 64, 84, 149	0
61	n5	120/141 (85%)	0.48	11 (9%) 11 11	51, 67, 87, 95	0
62	N6	126/126 (100%)	0.07	3 (2%) 62 57	43, 59, 70, 76	0
62	n6	126/126 (100%)	0.13	2 (1%) 74 69	45, 60, 78, 83	0
63	N7	135/135 (100%)	0.64	7 (5%) 31 28	77, 89, 107, 114	0
63	n7	135/135 (100%)	0.30	4 (2%) 54 49	79, 90, 109, 117	0
64	N8	148/148 (100%)	-0.15	0 100 100	31, 52, 72, 81	0
64	n8	148/148 (100%)	-0.21	0 100 100	31, 53, 66, 70	0
65	N9	58/58 (100%)	0.39	6 (10%) 9 8	37, 56, 94, 104	0
65	n9	58/58 (100%)	0.20	0 100 100	35, 53, 76, 80	0
66	O0	97/104 (93%)	0.62	7 (7%) 18 17	75, 83, 96, 98	0
66	o0	100/104 (96%)	0.29	5 (5%) 32 29	72, 80, 98, 105	0
67	O1	109/112 (97%)	0.53	6 (5%) 29 26	54, 72, 123, 237	0
67	o1	109/112 (97%)	0.27	3 (2%) 56 52	46, 58, 93, 168	0
68	O2	127/129 (98%)	-0.10	3 (2%) 62 57	31, 48, 57, 70	0
68	o2	127/129 (98%)	-0.14	2 (1%) 74 69	31, 50, 60, 70	0
69	O3	106/106 (100%)	-0.22	0 100 100	36, 43, 68, 83	0
69	o3	106/106 (100%)	-0.17	0 100 100	35, 40, 65, 72	0
70	O4	112/120 (93%)	0.55	9 (8%) 15 14	55, 74, 101, 106	0
70	o4	112/120 (93%)	0.54	7 (6%) 23 22	53, 71, 100, 105	0
71	O5	119/119 (100%)	0.25	1 (0%) 87 83	51, 67, 75, 81	0
71	o5	119/119 (100%)	0.25	4 (3%) 49 44	58, 68, 82, 90	0
72	O6	99/99 (100%)	0.62	12 (12%) 6 6	57, 66, 91, 98	0
72	o6	99/99 (100%)	0.19	7 (7%) 19 18	61, 72, 86, 100	0
73	O7	87/87 (100%)	0.30	3 (3%) 49 44	39, 46, 70, 86	0
73	o7	87/87 (100%)	0.23	4 (4%) 36 32	38, 47, 81, 114	0
74	O8	77/77 (100%)	0.47	5 (6%) 22 21	84, 91, 99, 101	0
74	o8	77/77 (100%)	0.86	12 (15%) 3 3	83, 91, 111, 122	0
75	O9	50/50 (100%)	-0.30	0 100 100	48, 52, 60, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	0.00	0 100 100	48, 51, 61, 77	0
76	Q0	52/52 (100%)	-0.01	0 100 100	48, 55, 66, 71	0
76	q0	52/52 (100%)	-0.21	0 100 100	38, 41, 48, 54	0
77	Q1	25/25 (100%)	0.61	1 (4%) 42 37	67, 68, 72, 73	0
77	q1	25/25 (100%)	0.14	0 100 100	54, 57, 67, 72	0
78	Q2	105/105 (100%)	0.65	13 (12%) 5 5	44, 63, 74, 88	0
78	q2	105/105 (100%)	0.78	10 (9%) 10 10	44, 56, 70, 88	0
79	Q3	91/91 (100%)	0.05	0 100 100	48, 58, 72, 82	0
79	q3	91/91 (100%)	-0.05	2 (2%) 65 60	46, 55, 71, 78	0
80	c0	84/96 (87%)	0.91	11 (13%) 5 4	107, 133, 141, 144	0
81	m2	0/150	-	-	-	-
82	p0	120/311 (38%)	0.38	4 (3%) 50 45	86, 103, 118, 125	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	32953/35147 (93%)	0.34	2043 (6%) 24 22	30, 72, 139, 489	0

The worst 5 of 2043 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	75	THR	20.0
14	c2	30	VAL	13.5
19	C7	125	SER	13.0
60	N4	76	VAL	12.9
16	C4	15	GLY	12.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	MG	6	2073	1/1	0.86	0.65	57.83	53,53,53,53	0
86	MG	1	3830	1/1	0.84	0.61	49.63	29,29,29,29	0
86	MG	5	3862	1/1	0.95	0.62	49.23	54,54,54,54	0
86	MG	1	4057	1/1	0.98	0.52	47.69	39,39,39,39	0
86	MG	1	4062	1/1	0.96	0.89	46.28	37,37,37,37	0
86	MG	n0	204	1/1	0.30	1.48	43.58	42,42,42,42	0
86	MG	5	3880	1/1	0.95	0.65	39.58	54,54,54,54	0
86	MG	1	3845	1/1	0.91	0.42	37.60	59,59,59,59	0
86	MG	5	3919	1/1	0.97	0.56	36.21	33,33,33,33	0
86	MG	5	3832	1/1	0.89	0.79	34.07	54,54,54,54	0
86	MG	5	3929	1/1	0.88	0.66	33.19	40,40,40,40	0
86	MG	1	3907	1/1	0.97	0.66	32.62	28,28,28,28	0
86	MG	1	3981	1/1	0.93	0.56	31.54	41,41,41,41	0
86	MG	1	3878	1/1	0.97	0.48	31.10	31,31,31,31	0
86	MG	6	2064	1/1	0.85	1.28	31.10	75,75,75,75	0
86	MG	5	3751	1/1	0.89	0.38	30.58	44,44,44,44	0
86	MG	1	3865	1/1	0.97	0.56	29.95	39,39,39,39	0
86	MG	5	3928	1/1	0.94	0.57	29.80	24,24,24,24	0
86	MG	1	3881	1/1	0.92	0.47	29.68	31,31,31,31	0
86	MG	5	3908	1/1	0.93	0.77	29.51	41,41,41,41	0
86	MG	1	3836	1/1	0.98	0.68	28.98	30,30,30,30	0
86	MG	5	4087	1/1	0.81	0.97	28.69	50,50,50,50	0
86	MG	5	3763	1/1	0.90	0.65	28.55	28,28,28,28	0
86	MG	1	3897	1/1	0.92	1.01	28.00	57,57,57,57	0
86	MG	5	3866	1/1	0.95	0.52	27.76	22,22,22,22	0
86	MG	5	3993	1/1	0.89	0.61	27.60	39,39,39,39	0
86	MG	1	3902	1/1	0.96	0.99	27.49	51,51,51,51	0
86	MG	1	3910	1/1	0.92	0.47	26.67	17,17,17,17	0
86	MG	5	4090	1/1	0.84	0.63	25.43	37,37,37,37	0
86	MG	5	3885	1/1	0.88	0.88	25.41	49,49,49,49	0
86	MG	5	3894	1/1	0.96	0.67	25.24	36,36,36,36	0
86	MG	1	3796	1/1	0.93	0.59	25.15	31,31,31,31	0
86	MG	6	2101	1/1	0.78	0.68	24.81	53,53,53,53	0
86	MG	1	3993	1/1	0.56	0.74	24.44	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	O2	201	1/1	0.59	0.84	24.12	48,48,48,48	0
86	MG	1	3743	1/1	0.83	0.62	24.09	47,47,47,47	0
86	MG	6	2128	1/1	0.76	0.79	23.85	81,81,81,81	0
86	MG	5	4067	1/1	0.91	0.91	23.69	39,39,39,39	0
86	MG	1	3858	1/1	0.94	0.50	23.63	45,45,45,45	0
86	MG	2	2078	1/1	0.48	0.87	22.93	77,77,77,77	0
86	MG	5	3903	1/1	0.94	0.55	22.53	37,37,37,37	0
86	MG	1	3885	1/1	0.94	0.58	22.53	30,30,30,30	0
86	MG	1	4094	1/1	0.88	0.76	21.69	68,68,68,68	0
86	MG	1	3866	1/1	0.72	0.63	21.68	47,47,47,47	0
86	MG	1	3886	1/1	0.93	0.60	21.66	41,41,41,41	0
86	MG	5	4125	1/1	0.97	0.36	21.41	35,35,35,35	0
86	MG	8	222	1/1	0.77	0.56	21.22	53,53,53,53	0
86	MG	5	3927	1/1	0.98	0.65	20.69	46,46,46,46	0
86	MG	1	3908	1/1	0.96	0.42	19.81	30,30,30,30	0
86	MG	5	3861	1/1	0.91	0.45	19.77	33,33,33,33	0
86	MG	1	3839	1/1	0.94	0.44	19.60	39,39,39,39	0
86	MG	2	2075	1/1	0.82	0.56	19.50	72,72,72,72	0
85	OHX	5	3590	7/7	0.95	0.29	18.90	124,124,124,124	0
86	MG	1	3887	1/1	0.93	0.45	18.73	27,27,27,27	0
86	MG	5	3950	1/1	0.67	0.49	18.47	38,38,38,38	0
86	MG	1	3898	1/1	0.94	1.01	18.26	53,53,53,53	0
86	MG	5	3756	1/1	0.92	0.65	18.19	46,46,46,46	0
86	MG	5	3895	1/1	0.96	0.55	17.90	36,36,36,36	0
86	MG	1	4109	1/1	0.92	0.47	17.59	36,36,36,36	0
85	OHX	1	3656	7/7	0.95	0.33	17.50	99,99,99,99	0
85	OHX	1	3727	7/7	0.95	0.39	17.44	119,119,119,119	0
86	MG	1	3896	1/1	0.94	0.71	17.44	47,47,47,47	0
86	MG	1	4037	1/1	0.61	0.64	17.35	104,104,104,104	0
85	OHX	5	3657	7/7	0.95	0.50	17.34	113,113,113,113	0
85	OHX	1	3734	7/7	0.91	0.51	17.30	136,136,136,136	0
86	MG	1	4049	1/1	0.78	0.63	17.04	41,41,41,41	0
86	MG	5	4107	1/1	0.84	0.48	17.00	40,40,40,40	0
86	MG	5	3846	1/1	0.91	0.76	16.94	38,38,38,38	0
86	MG	1	3890	1/1	0.96	0.51	16.76	26,26,26,26	0
86	MG	5	3815	1/1	0.95	0.41	16.42	29,29,29,29	0
86	MG	5	4063	1/1	0.91	0.73	16.41	37,37,37,37	0
85	OHX	1	3705	7/7	0.95	0.30	16.24	109,109,109,109	0
86	MG	1	3844	1/1	0.94	0.49	16.17	33,33,33,33	0
86	MG	5	3851	1/1	0.77	0.59	16.14	48,48,48,48	0
85	OHX	1	3710	7/7	0.96	0.48	16.10	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3833	1/1	0.78	0.63	15.74	70,70,70,70	0
86	MG	1	3946	1/1	0.84	0.35	15.59	52,52,52,52	0
85	OHX	1	3716	7/7	0.95	0.38	15.53	113,113,113,113	0
86	MG	2	2071	1/1	0.79	0.59	15.25	74,74,74,74	0
86	MG	5	4062	1/1	0.89	0.90	15.17	51,51,51,51	0
86	MG	5	3926	1/1	0.94	0.43	15.16	30,30,30,30	0
86	MG	1	3990	1/1	0.86	0.42	14.78	47,47,47,47	0
85	OHX	1	3649	7/7	0.90	0.50	14.70	118,118,118,118	0
86	MG	1	3818	1/1	0.91	0.30	14.61	38,38,38,38	0
86	MG	5	3845	1/1	0.89	0.68	14.55	44,44,44,44	0
86	MG	MG	2224	1/1	-0.19	3.24	14.53	243,243,243,243	0
86	MG	6	2091	1/1	0.98	0.51	14.31	77,77,77,77	0
86	MG	5	3972	1/1	0.79	0.37	14.28	41,41,41,41	0
85	OHX	1	3542	7/7	0.95	0.34	14.14	120,120,120,120	0
86	MG	2	2081	1/1	0.51	0.93	14.11	77,77,77,77	0
86	MG	6	2072	1/1	0.90	0.49	14.07	42,42,42,42	0
85	OHX	1	3680	7/7	0.94	0.35	14.06	114,114,114,114	0
86	MG	6	2109	1/1	0.86	0.52	13.85	65,65,65,65	0
86	MG	5	3844	1/1	0.94	0.62	13.84	38,38,38,38	0
86	MG	1	3786	1/1	0.85	0.47	13.54	37,37,37,37	0
86	MG	5	3782	1/1	0.90	0.32	13.52	41,41,41,41	0
86	MG	5	3804	1/1	0.90	0.42	13.49	39,39,39,39	0
86	MG	2	2051	1/1	0.81	0.52	13.41	80,80,80,80	0
85	OHX	4	208	7/7	0.97	0.33	13.34	99,99,99,99	0
85	OHX	5	3701	7/7	0.91	0.36	13.33	126,126,126,126	0
86	MG	2	2100	1/1	0.90	0.74	13.18	69,69,69,69	0
86	MG	2	2097	1/1	0.53	0.56	13.06	82,82,82,82	0
86	MG	N3	201	1/1	0.90	0.36	13.04	38,38,38,38	0
86	MG	2	2047	1/1	0.94	0.44	13.03	65,65,65,65	0
86	MG	4	219	1/1	0.97	0.44	12.97	38,38,38,38	0
86	MG	1	3740	1/1	0.79	0.28	12.89	41,41,41,41	0
85	OHX	1	3663	7/7	0.95	0.35	12.77	107,107,107,107	0
86	MG	2	2074	1/1	0.94	0.44	12.76	66,66,66,66	0
86	MG	5	3774	1/1	0.90	0.26	12.74	31,31,31,31	0
86	MG	5	3884	1/1	0.89	0.64	12.71	47,47,47,47	0
86	MG	n3	202	1/1	0.94	0.46	12.70	27,27,27,27	0
86	MG	1	4118	1/1	0.89	0.42	12.61	54,54,54,54	0
85	OHX	5	3710	7/7	0.92	0.42	12.60	137,137,137,137	0
85	OHX	5	3604	7/7	0.97	0.29	12.33	128,128,128,128	0
86	MG	2	2095	1/1	0.80	0.82	12.30	72,72,72,72	0
86	MG	6	2061	1/1	0.94	0.35	12.25	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3668	7/7	0.96	0.31	12.25	148,148,148,148	0
86	MG	1	3768	1/1	0.93	0.37	12.21	37,37,37,37	0
86	MG	5	3968	1/1	0.93	0.49	12.20	42,42,42,42	0
86	MG	1	4003	1/1	0.94	0.39	12.01	34,34,34,34	0
86	MG	1	4132	1/1	0.82	0.82	11.97	53,53,53,53	0
86	MG	1	4041	1/1	0.70	0.70	11.86	45,45,45,45	0
86	MG	5	3930	1/1	0.91	0.41	11.86	32,32,32,32	0
86	MG	1	3942	1/1	0.70	0.47	11.83	38,38,38,38	0
85	OHX	5	3690	7/7	0.96	0.32	11.72	120,120,120,120	0
86	MG	1	3795	1/1	0.87	0.33	11.72	39,39,39,39	0
86	MG	5	4166	1/1	0.76	0.32	11.72	51,51,51,51	0
85	OHX	5	3696	7/7	0.91	0.39	11.72	114,114,114,114	0
86	MG	6	2054	1/1	0.88	0.58	11.71	58,58,58,58	0
85	OHX	5	3593	7/7	0.96	0.37	11.66	106,106,106,106	0
85	OHX	1	3651	7/7	0.97	0.31	11.52	119,119,119,119	0
85	OHX	5	3615	7/7	0.94	0.38	11.45	130,130,130,130	0
86	MG	5	3876	1/1	0.92	0.46	11.41	34,34,34,34	0
86	MG	1	3826	1/1	0.92	0.53	11.32	24,24,24,24	0
86	MG	6	2070	1/1	0.97	0.37	11.16	59,59,59,59	0
86	MG	6	2076	1/1	0.83	0.33	11.10	58,58,58,58	0
86	MG	5	3792	1/1	0.66	0.39	11.07	52,52,52,52	0
86	MG	5	3850	1/1	0.94	0.52	11.02	27,27,27,27	0
86	MG	6	2085	1/1	0.93	0.46	10.85	74,74,74,74	0
86	MG	5	3837	1/1	0.96	0.36	10.80	35,35,35,35	0
85	OHX	8	215	7/7	0.96	0.36	10.77	112,112,112,112	0
86	MG	5	3920	1/1	0.97	0.52	10.76	24,24,24,24	0
86	MG	5	3983	1/1	0.89	0.36	10.71	36,36,36,36	0
86	MG	1	3808	1/1	0.78	0.33	10.67	54,54,54,54	0
86	MG	5	3907	1/1	0.94	0.44	10.66	33,33,33,33	0
85	OHX	6	2034	7/7	0.94	0.39	10.61	129,129,129,129	0
85	OHX	1	3691	7/7	0.94	0.36	10.61	129,129,129,129	0
85	OHX	1	3692	7/7	0.97	0.29	10.59	125,125,125,125	0
86	MG	1	4084	1/1	0.99	0.24	10.53	35,35,35,35	0
85	OHX	5	3667	7/7	0.98	0.27	10.47	100,100,100,100	0
85	OHX	5	3664	7/7	0.92	0.40	10.47	125,125,125,125	0
86	MG	5	4137	1/1	0.92	0.38	10.40	36,36,36,36	0
86	MG	1	4105	1/1	0.76	0.52	10.37	62,62,62,62	0
86	MG	5	3788	1/1	0.95	0.32	10.36	31,31,31,31	0
86	MG	5	4108	1/1	0.96	0.38	10.35	29,29,29,29	0
85	OHX	1	3673	7/7	0.93	0.33	10.34	116,116,116,116	0
85	OHX	1	3698	7/7	0.95	0.44	10.32	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	l3	403	1/1	0.98	0.43	10.29	27,27,27,27	0
86	MG	o1	201	1/1	0.88	0.70	10.29	51,51,51,51	0
86	MG	2	2076	1/1	0.96	0.35	10.20	75,75,75,75	0
86	MG	5	3979	1/1	0.90	0.34	10.17	36,36,36,36	0
86	MG	L4	403	1/1	0.92	0.87	10.17	39,39,39,39	0
86	MG	5	4165	1/1	0.98	0.36	10.14	33,33,33,33	0
86	MG	l3	404	1/1	0.91	0.73	10.12	49,49,49,49	0
85	OHX	5	3577	7/7	0.98	0.27	10.08	105,105,105,105	0
85	OHX	5	3700	7/7	0.93	0.30	9.98	136,136,136,136	0
85	OHX	2	2022	7/7	0.92	0.57	9.97	127,127,127,127	0
86	MG	1	3912	1/1	0.90	0.38	9.96	34,34,34,34	0
86	MG	5	3918	1/1	0.95	0.43	9.78	29,29,29,29	0
86	MG	C2	201	1/1	0.11	1.07	9.78	78,78,78,78	0
86	MG	1	3905	1/1	0.92	0.50	9.76	33,33,33,33	0
86	MG	1	3782	1/1	0.80	0.38	9.75	35,35,35,35	0
86	MG	1	3921	1/1	0.84	0.35	9.67	50,50,50,50	0
85	OHX	5	3720	7/7	0.96	0.40	9.63	128,128,128,128	0
85	OHX	1	3672	7/7	0.93	0.35	9.62	113,113,113,113	0
86	MG	5	3847	1/1	0.98	0.48	9.59	27,27,27,27	0
85	OHX	1	3609	7/7	0.96	0.36	9.58	91,91,91,91	0
86	MG	5	3883	1/1	0.87	0.35	9.56	48,48,48,48	0
86	MG	5	3915	1/1	0.95	0.45	9.53	38,38,38,38	0
86	MG	5	3800	1/1	0.96	0.26	9.33	27,27,27,27	0
85	OHX	5	3702	7/7	0.95	0.34	9.33	107,107,107,107	0
86	MG	2	2054	1/1	0.88	0.42	9.31	70,70,70,70	0
86	MG	1	3835	1/1	0.93	0.49	9.22	38,38,38,38	0
86	MG	6	2060	1/1	0.91	0.36	9.21	54,54,54,54	0
85	OHX	5	3650	7/7	0.95	0.30	9.17	117,117,117,117	0
86	MG	5	3925	1/1	0.89	0.43	9.17	26,26,26,26	0
86	MG	1	3929	1/1	0.80	0.35	9.16	42,42,42,42	0
86	MG	5	4038	1/1	0.77	0.38	9.13	37,37,37,37	0
86	MG	5	4010	1/1	0.90	0.46	9.10	40,40,40,40	0
86	MG	5	3948	1/1	0.97	0.35	9.04	50,50,50,50	0
86	MG	1	3851	1/1	0.96	0.37	9.04	48,48,48,48	0
86	MG	6	2119	1/1	0.83	0.31	9.00	76,76,76,76	0
86	MG	1	3787	1/1	0.89	0.28	8.98	35,35,35,35	0
86	MG	M1	201	1/1	0.77	0.50	8.94	74,74,74,74	0
86	MG	5	3986	1/1	0.78	0.32	8.92	35,35,35,35	0
85	OHX	2	2015	7/7	0.95	0.37	8.86	128,128,128,128	0
85	OHX	6	1990	7/7	0.91	0.31	8.80	129,129,129,129	0
86	MG	1	3913	1/1	0.95	0.42	8.77	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3594	7/7	0.96	0.33	8.67	109,109,109,109	0
86	MG	5	4146	1/1	0.91	0.39	8.66	31,31,31,31	0
86	MG	1	4033	1/1	0.97	0.36	8.65	42,42,42,42	0
86	MG	5	4170	1/1	0.89	0.47	8.64	55,55,55,55	0
86	MG	S4	301	1/1	0.78	0.68	8.64	82,82,82,82	0
86	MG	5	4113	1/1	0.84	0.33	8.63	44,44,44,44	0
85	OHX	1	3645	7/7	0.95	0.32	8.61	119,119,119,119	0
86	MG	1	3819	1/1	0.92	0.42	8.55	33,33,33,33	0
86	MG	2	2055	1/1	0.90	0.54	8.54	77,77,77,77	0
86	MG	5	3899	1/1	0.94	0.40	8.51	33,33,33,33	0
86	MG	2	2112	1/1	0.71	0.45	8.50	80,80,80,80	0
86	MG	2	2064	1/1	0.84	0.56	8.50	83,83,83,83	0
86	MG	l3	406	1/1	0.94	0.37	8.43	44,44,44,44	0
85	OHX	5	3646	7/7	0.96	0.43	8.38	123,123,123,123	0
85	OHX	5	3728	7/7	0.94	0.27	8.27	115,115,115,115	0
85	OHX	1	3598	7/7	0.93	0.43	8.26	142,142,142,142	0
86	MG	1	4040	1/1	0.90	0.50	8.19	61,61,61,61	0
85	OHX	5	3546	7/7	0.96	0.22	8.19	122,122,122,122	0
85	OHX	M7	201	7/7	0.96	0.45	8.14	100,100,100,100	0
85	OHX	4	213	7/7	0.93	0.37	8.13	137,137,137,137	0
85	OHX	1	3537	7/7	0.96	0.32	8.10	108,108,108,108	0
86	MG	2	2110	1/1	0.92	0.49	8.10	91,91,91,91	0
85	OHX	1	3666	7/7	0.95	0.30	8.10	115,115,115,115	0
85	OHX	5	3630	7/7	0.97	0.35	7.95	132,132,132,132	0
86	MG	1	3977	1/1	0.86	0.33	7.90	48,48,48,48	0
86	MG	6	2099	1/1	0.87	0.35	7.90	57,57,57,57	0
86	MG	5	4066	1/1	0.92	0.32	7.88	64,64,64,64	0
86	MG	1	3882	1/1	0.90	0.40	7.82	31,31,31,31	0
86	MG	5	3922	1/1	0.99	0.44	7.79	23,23,23,23	0
85	OHX	6	2028	7/7	0.94	0.36	7.78	116,116,116,116	0
85	OHX	5	3663	7/7	0.95	0.32	7.77	99,99,99,99	0
86	MG	1	3812	1/1	0.90	0.36	7.76	40,40,40,40	0
85	OHX	5	3688	7/7	0.95	0.36	7.70	111,111,111,111	0
85	OHX	4	212	7/7	0.84	0.51	7.68	135,135,135,135	0
85	OHX	1	3564	7/7	0.94	0.33	7.65	107,107,107,107	0
86	MG	2	2089	1/1	0.83	0.52	7.58	102,102,102,102	0
86	MG	1	3864	1/1	0.91	0.46	7.57	53,53,53,53	0
86	MG	6	2081	1/1	0.96	0.46	7.55	85,85,85,85	0
86	MG	1	3834	1/1	0.90	0.45	7.52	43,43,43,43	0
85	OHX	1	3630	7/7	0.93	0.35	7.52	126,126,126,126	0
85	OHX	5	3691	7/7	0.92	0.42	7.51	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	4076	1/1	0.85	0.34	7.48	36,36,36,36	0
86	MG	5	4089	1/1	0.91	0.38	7.44	67,67,67,67	0
85	OHX	1	3714	7/7	0.98	0.33	7.42	95,95,95,95	0
86	MG	5	3814	1/1	0.95	0.37	7.38	45,45,45,45	0
86	MG	6	2056	1/1	0.85	0.35	7.38	82,82,82,82	0
85	OHX	1	3721	7/7	0.92	0.39	7.37	137,137,137,137	0
85	OHX	5	3596	7/7	0.96	0.31	7.27	102,102,102,102	0
85	OHX	5	3617	7/7	0.97	0.35	7.21	102,102,102,102	0
86	MG	5	3835	1/1	0.98	0.28	7.21	37,37,37,37	0
86	MG	1	3813	1/1	0.93	0.32	7.16	33,33,33,33	0
86	MG	1	3752	1/1	0.85	0.41	7.15	41,41,41,41	0
86	MG	5	3947	1/1	0.85	0.41	7.12	38,38,38,38	0
86	MG	2	2104	1/1	0.86	0.34	7.12	68,68,68,68	0
86	MG	s1	301	1/1	0.28	1.37	7.10	88,88,88,88	0
85	OHX	5	3642	7/7	0.95	0.33	7.09	126,126,126,126	0
85	OHX	6	1987	7/7	0.88	0.39	7.03	156,156,156,156	0
85	OHX	5	3737	7/7	0.96	0.42	7.02	118,118,118,118	0
86	MG	1	3995	1/1	0.86	0.33	6.97	39,39,39,39	0
86	MG	1	3843	1/1	0.97	0.25	6.95	30,30,30,30	0
85	OHX	S9	201	7/7	0.94	0.49	6.94	127,127,127,127	0
85	OHX	1	3677	7/7	0.94	0.41	6.91	104,104,104,104	0
86	MG	1	3738	1/1	0.86	0.47	6.88	50,50,50,50	0
85	OHX	2	2027	7/7	0.96	0.32	6.86	117,117,117,117	0
85	OHX	1	3707	7/7	0.94	0.30	6.82	113,113,113,113	0
85	OHX	2	1991	7/7	0.97	0.29	6.82	136,136,136,136	0
86	MG	1	3744	1/1	0.89	0.28	6.80	36,36,36,36	0
85	OHX	1	3657	7/7	0.96	0.34	6.74	110,110,110,110	0
86	MG	n6	201	1/1	0.62	0.57	6.72	58,58,58,58	0
86	MG	1	4013	1/1	0.98	0.29	6.71	34,34,34,34	0
86	MG	6	2094	1/1	0.70	0.64	6.66	52,52,52,52	0
85	OHX	6	2045	7/7	0.94	0.34	6.64	154,154,154,154	0
86	MG	5	4050	1/1	0.96	0.34	6.64	52,52,52,52	0
86	MG	1	4104	1/1	0.92	0.40	6.61	46,46,46,46	0
85	OHX	1	3697	7/7	0.95	0.29	6.56	126,126,126,126	0
86	MG	6	2067	1/1	0.95	0.41	6.50	42,42,42,42	0
85	OHX	5	3682	7/7	0.97	0.42	6.45	103,103,103,103	0
86	MG	1	3825	1/1	0.90	0.30	6.41	38,38,38,38	0
86	MG	1	3758	1/1	0.94	0.35	6.39	57,57,57,57	0
85	OHX	1	3713	7/7	0.93	0.41	6.37	140,140,140,140	0
86	MG	5	3892	1/1	0.94	0.37	6.34	29,29,29,29	0
86	MG	5	3900	1/1	0.98	0.25	6.33	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	5	3644	7/7	0.97	0.33	6.33	90,90,90,90	0
85	OHX	3	210	7/7	0.96	0.29	6.30	107,107,107,107	0
86	MG	5	3966	1/1	0.94	0.32	6.28	38,38,38,38	0
86	MG	5	3760	1/1	0.93	0.38	6.27	56,56,56,56	0
85	OHX	5	3718	7/7	0.97	0.26	6.24	109,109,109,109	0
86	MG	1	3827	1/1	0.94	0.24	6.23	46,46,46,46	0
86	MG	s4	302	1/1	0.87	0.52	6.23	62,62,62,62	0
86	MG	5	4110	1/1	0.84	0.31	6.20	34,34,34,34	0
86	MG	5	4135	1/1	0.92	0.34	6.18	83,83,83,83	0
86	MG	6	2147	1/1	0.79	0.50	6.14	62,62,62,62	0
85	OHX	1	3593	7/7	0.97	0.25	6.14	88,88,88,88	0
86	MG	4	223	1/1	0.85	0.29	6.12	65,65,65,65	0
86	MG	1	4030	1/1	0.94	0.43	6.11	43,43,43,43	0
86	MG	1	4053	1/1	0.91	0.41	6.09	45,45,45,45	0
86	MG	5	3803	1/1	0.84	0.38	6.09	44,44,44,44	0
86	MG	2	2053	1/1	0.93	0.27	6.06	72,72,72,72	0
85	OHX	4	211	7/7	0.91	0.31	6.06	111,111,111,111	0
85	OHX	5	3738	7/7	0.88	0.27	6.06	160,160,160,160	0
85	OHX	5	3631	7/7	0.96	0.35	6.00	113,113,113,113	0
86	MG	1	3857	1/1	0.97	0.32	5.94	36,36,36,36	0
86	MG	1	4068	1/1	0.96	0.37	5.92	34,34,34,34	0
85	OHX	6	2043	7/7	0.91	0.32	5.88	138,138,138,138	0
85	OHX	5	3707	7/7	0.93	0.36	5.87	135,135,135,135	0
85	OHX	5	3553	7/7	0.97	0.22	5.86	95,95,95,95	0
85	OHX	1	3627	7/7	0.97	0.31	5.84	108,108,108,108	0
85	OHX	1	3570	7/7	0.98	0.29	5.83	99,99,99,99	0
86	MG	6	2053	1/1	0.94	0.43	5.72	79,79,79,79	0
85	OHX	5	3639	7/7	0.97	0.30	5.72	106,106,106,106	0
85	OHX	1	3646	7/7	0.96	0.40	5.70	129,129,129,129	0
86	MG	5	3858	1/1	0.97	0.32	5.69	39,39,39,39	0
85	OHX	1	3676	7/7	0.95	0.33	5.69	128,128,128,128	0
86	MG	n9	103	1/1	0.76	0.46	5.67	40,40,40,40	0
86	MG	1	4014	1/1	0.97	0.27	5.62	32,32,32,32	0
86	MG	2	2109	1/1	0.87	0.59	5.62	73,73,73,73	0
86	MG	6	2114	1/1	0.64	0.30	5.59	78,78,78,78	0
85	OHX	6	2011	7/7	0.95	0.32	5.58	136,136,136,136	0
86	MG	1	4060	1/1	0.90	0.26	5.38	35,35,35,35	0
86	MG	5	3869	1/1	0.86	0.24	5.38	52,52,52,52	0
86	MG	1	3855	1/1	0.84	0.31	5.37	29,29,29,29	0
86	MG	5	4115	1/1	0.74	0.40	5.34	47,47,47,47	0
85	OHX	5	3660	7/7	0.91	0.40	5.27	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2132	1/1	0.41	0.29	5.26	65,65,65,65	0
86	MG	1	3901	1/1	0.92	0.26	5.21	34,34,34,34	0
86	MG	1	3871	1/1	0.96	0.28	5.20	31,31,31,31	0
85	OHX	5	3530	7/7	0.98	0.22	5.18	92,92,92,92	0
86	MG	1	3801	1/1	0.90	0.36	5.15	43,43,43,43	0
86	MG	5	3764	1/1	0.95	0.34	5.14	38,38,38,38	0
86	MG	1	3870	1/1	0.96	0.33	4.99	43,43,43,43	0
85	OHX	1	3515	7/7	0.98	0.29	4.97	86,86,86,86	0
85	OHX	2	1953	7/7	0.95	0.36	4.95	141,141,141,141	0
86	MG	5	4091	1/1	0.87	0.45	4.94	73,73,73,73	0
85	OHX	2	2036	7/7	0.95	0.37	4.90	112,112,112,112	0
85	OHX	5	3697	7/7	0.97	0.29	4.90	111,111,111,111	0
86	MG	5	4104	1/1	0.87	0.41	4.88	32,32,32,32	0
85	OHX	2	2004	7/7	0.97	0.30	4.86	126,126,126,126	0
85	OHX	5	3695	7/7	0.95	0.30	4.86	117,117,117,117	0
85	OHX	1	3544	7/7	0.97	0.22	4.85	101,101,101,101	0
86	MG	2	2060	1/1	0.69	0.67	4.83	75,75,75,75	0
85	OHX	2	1981	7/7	0.94	0.27	4.82	146,146,146,146	0
85	OHX	6	2031	7/7	0.95	0.36	4.82	106,106,106,106	0
85	OHX	2	1995	7/7	0.93	0.37	4.78	139,139,139,139	0
85	OHX	1	3490	7/7	0.94	0.20	4.77	94,94,94,94	0
85	OHX	1	3583	7/7	0.97	0.30	4.77	107,107,107,107	0
85	OHX	6	2015	7/7	0.97	0.29	4.77	119,119,119,119	0
86	MG	6	2092	1/1	0.86	0.33	4.76	58,58,58,58	0
85	OHX	1	3584	7/7	0.95	0.29	4.74	127,127,127,127	0
85	OHX	1	3731	7/7	0.93	0.43	4.73	144,144,144,144	0
86	MG	5	3839	1/1	0.93	0.27	4.72	47,47,47,47	0
86	MG	5	3958	1/1	0.86	0.30	4.71	56,56,56,56	0
86	MG	2	2091	1/1	0.98	0.27	4.70	74,74,74,74	0
85	OHX	1	3624	7/7	0.98	0.28	4.66	83,83,83,83	0
86	MG	1	4114	1/1	0.52	0.35	4.55	41,41,41,41	0
85	OHX	6	1981	7/7	0.97	0.26	4.51	114,114,114,114	0
85	OHX	5	3689	7/7	0.97	0.32	4.51	114,114,114,114	0
86	MG	1	4131	1/1	0.97	0.30	4.49	34,34,34,34	0
86	MG	1	4061	1/1	0.98	0.34	4.48	43,43,43,43	0
86	MG	6	2051	1/1	0.97	0.26	4.48	52,52,52,52	0
86	MG	1	4066	1/1	0.86	0.25	4.46	41,41,41,41	0
86	MG	5	3878	1/1	0.86	0.29	4.45	37,37,37,37	0
85	OHX	5	3610	7/7	0.97	0.24	4.41	103,103,103,103	0
85	OHX	6	2005	7/7	0.93	0.33	4.39	117,117,117,117	0
85	OHX	5	3496	7/7	0.96	0.28	4.39	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3969	1/1	0.50	0.26	4.38	64,64,64,64	0
85	OHX	1	3591	7/7	0.97	0.25	4.35	100,100,100,100	0
86	MG	n6	202	1/1	0.69	0.55	4.34	44,44,44,44	0
85	OHX	5	3609	7/7	0.97	0.28	4.30	99,99,99,99	0
85	OHX	2	2034	7/7	0.93	0.26	4.30	135,135,135,135	0
86	MG	5	3887	1/1	0.84	0.32	4.26	49,49,49,49	0
86	MG	5	3810	1/1	0.93	0.36	4.24	39,39,39,39	0
86	MG	6	2181	1/1	0.80	0.33	4.22	62,62,62,62	0
86	MG	5	3902	1/1	0.88	0.24	4.20	33,33,33,33	0
85	OHX	7	209	7/7	0.96	0.24	4.18	102,102,102,102	0
85	OHX	5	3740	7/7	0.96	0.36	4.16	134,134,134,134	0
85	OHX	5	3665	7/7	0.95	0.32	4.15	114,114,114,114	0
85	OHX	8	208	7/7	0.97	0.24	4.09	108,108,108,108	0
86	MG	5	3904	1/1	0.93	0.31	4.09	35,35,35,35	0
85	OHX	1	3522	7/7	0.97	0.29	4.06	98,98,98,98	0
86	MG	1	4063	1/1	0.94	0.48	4.06	33,33,33,33	0
86	MG	5	4055	1/1	0.91	0.46	4.05	47,47,47,47	0
86	MG	n0	202	1/1	0.83	0.28	4.05	36,36,36,36	0
85	OHX	8	213	7/7	0.91	0.31	3.99	124,124,124,124	0
86	MG	5	3941	1/1	0.89	0.30	3.99	40,40,40,40	0
85	OHX	5	3606	7/7	0.96	0.24	3.98	91,91,91,91	0
86	MG	5	4119	1/1	0.92	0.27	3.98	33,33,33,33	0
86	MG	6	2058	1/1	0.95	0.39	3.97	109,109,109,109	0
86	MG	1	3888	1/1	0.90	0.36	3.93	31,31,31,31	0
85	OHX	6	1995	7/7	0.94	0.23	3.92	162,162,162,162	0
85	OHX	7	212	7/7	0.94	0.27	3.92	138,138,138,138	0
85	OHX	6	1988	7/7	0.96	0.23	3.91	124,124,124,124	0
85	OHX	1	3558	7/7	0.96	0.21	3.89	111,111,111,111	0
86	MG	5	4075	1/1	0.95	0.30	3.88	37,37,37,37	0
85	OHX	5	3611	7/7	0.94	0.31	3.86	110,110,110,110	0
86	MG	n0	203	1/1	0.93	0.24	3.86	40,40,40,40	0
85	OHX	2	2013	7/7	0.94	0.29	3.85	136,136,136,136	0
85	OHX	4	207	7/7	0.96	0.21	3.84	117,117,117,117	0
86	MG	sM	402	1/1	0.88	0.64	3.77	44,44,44,44	0
86	MG	1	3954	1/1	0.88	0.30	3.77	58,58,58,58	0
86	MG	1	3750	1/1	0.90	0.45	3.76	39,39,39,39	0
85	OHX	5	3699	7/7	0.97	0.32	3.76	115,115,115,115	0
86	MG	1	3753	1/1	0.94	0.33	3.73	49,49,49,49	0
85	OHX	m0	303	7/7	0.95	0.32	3.72	119,119,119,119	0
85	OHX	1	3687	7/7	0.97	0.28	3.71	140,140,140,140	0
86	MG	6	2059	1/1	0.93	0.44	3.70	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2145	1/1	0.98	0.22	3.69	92,92,92,92	0
85	OHX	6	2022	7/7	0.93	0.35	3.66	116,116,116,116	0
86	MG	1	3920	1/1	0.94	0.55	3.58	70,70,70,70	0
86	MG	5	3768	1/1	0.93	0.21	3.57	43,43,43,43	0
85	OHX	6	2032	7/7	0.94	0.29	3.53	140,140,140,140	0
85	OHX	1	3723	7/7	0.92	0.41	3.53	115,115,115,115	0
86	MG	2	2093	1/1	0.89	0.59	3.52	125,125,125,125	0
86	MG	5	3906	1/1	0.97	0.36	3.51	45,45,45,45	0
85	OHX	1	3648	7/7	0.96	0.35	3.51	137,137,137,137	0
85	OHX	6	1964	7/7	0.98	0.22	3.48	110,110,110,110	0
86	MG	5	3852	1/1	0.97	0.25	3.47	32,32,32,32	0
85	OHX	1	3689	7/7	0.98	0.31	3.46	108,108,108,108	0
86	MG	m0	305	1/1	0.89	0.29	3.44	39,39,39,39	0
85	OHX	5	3637	7/7	0.97	0.33	3.40	111,111,111,111	0
85	OHX	1	3719	7/7	0.95	0.28	3.38	127,127,127,127	0
85	OHX	1	3603	7/7	0.97	0.31	3.38	103,103,103,103	0
85	OHX	5	3709	7/7	0.92	0.35	3.37	128,128,128,128	0
85	OHX	5	3583	7/7	0.97	0.20	3.37	113,113,113,113	0
86	MG	l7	301	1/1	0.91	0.23	3.36	35,35,35,35	0
85	OHX	1	3652	7/7	0.94	0.30	3.33	111,111,111,111	0
86	MG	m6	203	1/1	0.95	0.27	3.33	37,37,37,37	0
86	MG	5	3749	1/1	0.67	0.28	3.32	52,52,52,52	0
85	OHX	8	212	7/7	0.96	0.23	3.28	125,125,125,125	0
85	OHX	5	3658	7/7	0.96	0.36	3.25	97,97,97,97	0
85	OHX	5	3625	7/7	0.96	0.31	3.25	146,146,146,146	0
86	MG	5	4154	1/1	0.89	0.24	3.25	40,40,40,40	0
85	OHX	5	3648	7/7	0.97	0.28	3.25	102,102,102,102	0
85	OHX	5	3556	7/7	0.97	0.27	3.20	94,94,94,94	0
86	MG	1	3973	1/1	0.84	0.23	3.16	55,55,55,55	0
86	MG	6	2086	1/1	0.98	0.30	3.14	61,61,61,61	0
85	OHX	6	1971	7/7	0.94	0.36	3.13	138,138,138,138	0
86	MG	5	3830	1/1	0.95	0.30	3.12	32,32,32,32	0
85	OHX	5	3721	7/7	0.96	0.23	3.12	95,95,95,95	0
86	MG	L3	404	1/1	0.74	0.52	3.07	71,71,71,71	0
85	OHX	5	3624	7/7	0.96	0.27	3.07	119,119,119,119	0
85	OHX	1	3670	7/7	0.96	0.24	3.02	110,110,110,110	0
85	OHX	1	3510	7/7	0.97	0.20	2.99	104,104,104,104	0
85	OHX	5	3558	7/7	0.96	0.26	2.97	107,107,107,107	0
86	MG	8	219	1/1	0.91	0.23	2.97	42,42,42,42	0
85	OHX	1	3736	7/7	0.96	0.32	2.93	119,119,119,119	0
86	MG	1	4130	1/1	0.90	0.32	2.93	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	6	2019	7/7	0.96	0.27	2.92	139,139,139,139	0
85	OHX	6	2030	7/7	0.96	0.24	2.92	98,98,98,98	0
85	OHX	6	1966	7/7	0.97	0.21	2.92	122,122,122,122	0
85	OHX	6	2038	7/7	0.95	0.43	2.91	127,127,127,127	0
85	OHX	5	3678	7/7	0.97	0.24	2.89	110,110,110,110	0
85	OHX	1	3633	7/7	0.95	0.33	2.87	138,138,138,138	0
86	MG	1	3746	1/1	0.93	0.44	2.86	53,53,53,53	0
85	OHX	1	3527	7/7	0.98	0.23	2.84	109,109,109,109	0
85	OHX	5	3676	7/7	0.94	0.33	2.83	90,90,90,90	0
85	OHX	1	3528	7/7	0.97	0.25	2.83	102,102,102,102	0
86	MG	6	2130	1/1	0.89	0.37	2.80	82,82,82,82	0
86	MG	5	3757	1/1	0.94	0.24	2.80	29,29,29,29	0
86	MG	5	3889	1/1	0.98	0.31	2.78	33,33,33,33	0
85	OHX	2	1942	7/7	0.98	0.28	2.77	115,115,115,115	0
85	OHX	5	3527	7/7	0.97	0.23	2.76	102,102,102,102	0
85	OHX	5	3715	7/7	0.97	0.24	2.75	92,92,92,92	0
86	MG	5	3772	1/1	0.97	0.35	2.73	39,39,39,39	0
86	MG	2	2083	1/1	0.68	0.32	2.73	73,73,73,73	0
86	MG	6	2170	1/1	0.90	0.24	2.70	62,62,62,62	0
85	OHX	6	2001	7/7	0.94	0.20	2.69	101,101,101,101	0
86	MG	1	4031	1/1	0.78	0.39	2.68	121,121,121,121	0
85	OHX	s9	201	7/7	0.90	0.47	2.65	126,126,126,126	0
86	MG	6	2164	1/1	0.58	0.27	2.64	90,90,90,90	0
85	OHX	1	3724	7/7	0.94	0.41	2.64	136,136,136,136	0
85	OHX	1	3611	7/7	0.98	0.30	2.63	113,113,113,113	0
86	MG	5	4140	1/1	0.84	0.25	2.58	34,34,34,34	0
86	MG	M8	201	1/1	0.96	0.30	2.57	43,43,43,43	0
86	MG	1	3815	1/1	0.89	0.23	2.55	54,54,54,54	0
85	OHX	1	3612	7/7	0.97	0.25	2.54	117,117,117,117	0
85	OHX	6	1979	7/7	0.94	0.31	2.53	134,134,134,134	0
85	OHX	2	1964	7/7	0.96	0.28	2.52	120,120,120,120	0
86	MG	m7	201	1/1	0.94	0.33	2.48	32,32,32,32	0
86	MG	N0	201	1/1	0.95	0.27	2.47	47,47,47,47	0
85	OHX	1	3634	7/7	0.97	0.30	2.46	112,112,112,112	0
86	MG	n8	201	1/1	0.90	0.25	2.46	49,49,49,49	0
85	OHX	7	211	7/7	0.95	0.22	2.41	104,104,104,104	0
86	MG	5	4069	1/1	0.81	0.30	2.40	49,49,49,49	0
85	OHX	o7	502	7/7	0.96	0.34	2.39	116,116,116,116	0
86	MG	5	3999	1/1	0.87	0.26	2.37	42,42,42,42	0
86	MG	2	2085	1/1	0.81	0.46	2.36	97,97,97,97	0
85	OHX	5	3668	7/7	0.97	0.22	2.35	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3914	1/1	0.90	0.22	2.35	43,43,43,43	0
85	OHX	5	3505	7/7	0.98	0.27	2.35	71,71,71,71	0
85	OHX	5	3622	7/7	0.96	0.22	2.34	132,132,132,132	0
85	OHX	6	1967	7/7	0.98	0.25	2.34	102,102,102,102	0
86	MG	5	4163	1/1	0.86	0.27	2.34	54,54,54,54	0
86	MG	5	4051	1/1	0.93	0.28	2.33	67,67,67,67	0
85	OHX	1	3635	7/7	0.97	0.25	2.31	111,111,111,111	0
85	OHX	1	3647	7/7	0.96	0.30	2.31	101,101,101,101	0
85	OHX	D9	102	7/7	0.93	0.36	2.30	140,140,140,140	0
85	OHX	5	3694	7/7	0.95	0.34	2.30	135,135,135,135	0
85	OHX	O4	201	7/7	0.94	0.51	2.28	135,135,135,135	0
86	MG	1	3961	1/1	0.86	0.20	2.27	36,36,36,36	0
86	MG	1	3814	1/1	0.96	0.22	2.27	50,50,50,50	0
86	MG	1	3983	1/1	0.84	0.31	2.24	80,80,80,80	0
86	MG	c1	202	1/1	0.89	0.34	2.24	52,52,52,52	0
86	MG	5	3769	1/1	0.97	0.40	2.19	59,59,59,59	0
85	OHX	5	3616	7/7	0.97	0.25	2.15	111,111,111,111	0
85	OHX	6	2002	7/7	0.95	0.24	2.13	125,125,125,125	0
85	OHX	6	2029	7/7	0.87	0.35	2.11	159,159,159,159	0
85	OHX	6	2049	7/7	0.95	0.34	2.09	157,157,157,157	0
85	OHX	2	2024	7/7	0.83	0.32	2.08	154,154,154,154	0
85	OHX	6	2039	7/7	0.90	0.30	2.08	166,166,166,166	0
86	MG	1	3872	1/1	0.97	0.24	2.08	42,42,42,42	0
85	OHX	1	3625	7/7	0.96	0.25	2.05	125,125,125,125	0
85	OHX	2	1947	7/7	0.96	0.25	2.04	111,111,111,111	0
85	OHX	6	1980	7/7	0.96	0.29	2.04	99,99,99,99	0
85	OHX	1	3671	7/7	0.96	0.25	2.03	128,128,128,128	0
86	MG	6	2126	1/1	0.80	0.23	1.99	82,82,82,82	0
86	MG	5	4027	1/1	0.92	0.24	1.99	45,45,45,45	0
85	OHX	1	3703	7/7	0.97	0.32	1.97	121,121,121,121	0
85	OHX	5	3711	7/7	0.89	0.38	1.95	134,134,134,134	0
85	OHX	8	218	7/7	0.95	0.36	1.95	123,123,123,123	0
85	OHX	1	3659	7/7	0.94	0.26	1.94	145,145,145,145	0
86	MG	1	4072	1/1	0.87	0.25	1.92	44,44,44,44	0
85	OHX	1	3535	7/7	0.96	0.23	1.90	106,106,106,106	0
86	MG	1	3994	1/1	0.98	0.19	1.89	43,43,43,43	0
86	MG	5	4072	1/1	0.74	0.30	1.88	60,60,60,60	0
85	OHX	5	3536	7/7	0.98	0.24	1.87	104,104,104,104	0
85	OHX	2	1966	7/7	0.97	0.24	1.87	124,124,124,124	0
85	OHX	M5	303	7/7	0.96	0.30	1.86	114,114,114,114	0
85	OHX	5	3499	7/7	0.98	0.24	1.84	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	5	3595	7/7	0.98	0.25	1.84	99,99,99,99	0
86	MG	C9	201	1/1	0.27	0.68	1.83	95,95,95,95	0
86	MG	1	3797	1/1	0.98	0.23	1.83	38,38,38,38	0
85	OHX	6	2033	7/7	0.93	0.24	1.82	156,156,156,156	0
85	OHX	2	2041	7/7	0.92	0.28	1.81	159,159,159,159	0
86	MG	2	2068	1/1	0.87	0.27	1.81	74,74,74,74	0
85	OHX	5	3651	7/7	0.96	0.26	1.80	100,100,100,100	0
85	OHX	6	2027	7/7	0.96	0.36	1.79	143,143,143,143	0
86	MG	1	3982	1/1	0.97	0.21	1.78	32,32,32,32	0
86	MG	5	3761	1/1	0.86	0.28	1.78	36,36,36,36	0
86	MG	5	3767	1/1	0.89	0.30	1.77	39,39,39,39	0
86	MG	6	2082	1/1	0.88	0.26	1.73	70,70,70,70	0
85	OHX	2	2031	7/7	0.86	0.40	1.73	147,147,147,147	0
86	MG	1	3880	1/1	0.80	0.29	1.71	36,36,36,36	0
85	OHX	2	1998	7/7	0.94	0.24	1.70	138,138,138,138	0
86	MG	2	2073	1/1	0.97	0.25	1.69	60,60,60,60	0
85	OHX	5	3569	7/7	0.98	0.22	1.67	106,106,106,106	0
85	OHX	5	3673	7/7	0.89	0.29	1.65	130,130,130,130	0
86	MG	L7	301	1/1	0.92	0.23	1.63	39,39,39,39	0
85	OHX	6	2025	7/7	0.97	0.33	1.62	107,107,107,107	0
85	OHX	1	3682	7/7	0.95	0.22	1.60	109,109,109,109	0
86	MG	1	3868	1/1	0.94	0.29	1.60	37,37,37,37	0
85	OHX	1	3586	7/7	0.98	0.20	1.60	98,98,98,98	0
85	OHX	1	3605	7/7	0.95	0.22	1.58	117,117,117,117	0
85	OHX	5	3533	7/7	0.95	0.22	1.57	84,84,84,84	0
86	MG	5	3963	1/1	0.96	0.20	1.56	52,52,52,52	0
86	MG	5	3971	1/1	0.96	0.20	1.54	38,38,38,38	0
85	OHX	o4	201	7/7	0.91	0.41	1.54	126,126,126,126	0
85	OHX	5	3550	7/7	0.98	0.22	1.53	94,94,94,94	0
86	MG	1	3971	1/1	0.72	0.29	1.52	46,46,46,46	0
85	OHX	6	1994	7/7	0.98	0.26	1.52	127,127,127,127	0
85	OHX	2	2039	7/7	0.90	0.48	1.51	153,153,153,153	0
86	MG	5	3784	1/1	0.95	0.18	1.50	31,31,31,31	0
85	OHX	1	3601	7/7	0.95	0.26	1.49	97,97,97,97	0
85	OHX	5	3580	7/7	0.97	0.27	1.49	119,119,119,119	0
85	OHX	5	3727	7/7	0.93	0.32	1.48	136,136,136,136	0
85	OHX	5	3560	7/7	0.97	0.21	1.47	101,101,101,101	0
85	OHX	1	3521	7/7	0.97	0.20	1.43	86,86,86,86	0
85	OHX	6	1978	7/7	0.98	0.20	1.41	98,98,98,98	0
86	MG	5	4109	1/1	0.96	0.20	1.41	31,31,31,31	0
85	OHX	2	2014	7/7	0.96	0.23	1.38	125,125,125,125	0
86	MG	D9	104	1/1	0.93	0.32	1.36	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3567	7/7	0.96	0.27	1.36	104,104,104,104	0
85	OHX	M7	202	7/7	0.94	0.32	1.35	127,127,127,127	0
86	MG	5	4173	1/1	0.69	0.37	1.35	43,43,43,43	0
85	OHX	5	3597	7/7	0.98	0.26	1.34	107,107,107,107	0
86	MG	N8	201	1/1	0.83	0.32	1.30	48,48,48,48	0
85	OHX	5	3705	7/7	0.97	0.27	1.29	114,114,114,114	0
86	MG	8	224	1/1	0.90	0.25	1.29	61,61,61,61	0
86	MG	5	3939	1/1	0.91	0.33	1.25	41,41,41,41	0
85	OHX	1	3660	7/7	0.97	0.30	1.25	98,98,98,98	0
85	OHX	5	3706	7/7	0.98	0.26	1.24	106,106,106,106	0
86	MG	M6	202	1/1	0.94	0.25	1.23	42,42,42,42	0
86	MG	5	4003	1/1	0.85	0.23	1.21	33,33,33,33	0
85	OHX	6	1986	7/7	0.96	0.30	1.20	127,127,127,127	0
86	MG	19	202	1/1	0.88	0.33	1.20	46,46,46,46	0
86	MG	6	2121	1/1	0.96	0.25	1.20	68,68,68,68	0
85	OHX	5	3672	7/7	0.96	0.20	1.18	143,143,143,143	0
85	OHX	15	303	7/7	0.93	0.38	1.18	136,136,136,136	0
85	OHX	8	209	7/7	0.96	0.16	1.18	114,114,114,114	0
85	OHX	2	2029	7/7	0.92	0.36	1.18	167,167,167,167	0
86	MG	M7	205	1/1	0.97	0.26	1.17	34,34,34,34	0
86	MG	M5	301	1/1	0.92	0.23	1.16	42,42,42,42	0
86	MG	5	3770	1/1	0.95	0.17	1.16	37,37,37,37	0
86	MG	2	2103	1/1	0.93	0.30	1.16	93,93,93,93	0
86	MG	6	2135	1/1	0.95	0.22	1.15	76,76,76,76	0
85	OHX	1	3587	7/7	0.97	0.23	1.14	104,104,104,104	0
85	OHX	1	3699	7/7	0.90	0.37	1.12	147,147,147,147	0
85	OHX	5	3635	7/7	0.98	0.20	1.12	103,103,103,103	0
85	OHX	5	3621	7/7	0.97	0.26	1.12	99,99,99,99	0
85	OHX	5	3693	7/7	0.96	0.41	1.09	116,116,116,116	0
85	OHX	1	3592	7/7	0.95	0.24	1.07	144,144,144,144	0
86	MG	8	225	1/1	0.92	0.27	1.06	66,66,66,66	0
85	OHX	2	2010	7/7	0.90	0.38	1.06	134,134,134,134	0
85	OHX	5	3623	7/7	0.96	0.26	1.06	110,110,110,110	0
85	OHX	6	1970	7/7	0.96	0.21	1.03	130,130,130,130	0
85	OHX	1	3643	7/7	0.98	0.25	1.03	106,106,106,106	0
86	MG	O1	201	1/1	0.98	0.45	1.02	75,75,75,75	0
86	MG	1	3955	1/1	0.93	0.26	1.01	42,42,42,42	0
85	OHX	1	3688	7/7	0.91	0.37	1.00	146,146,146,146	0
85	OHX	2	1983	7/7	0.97	0.25	0.99	116,116,116,116	0
85	OHX	5	3561	7/7	0.98	0.23	0.99	123,123,123,123	0
85	OHX	5	3548	7/7	0.98	0.20	0.98	86,86,86,86	0
85	OHX	5	3692	7/7	0.93	0.23	0.97	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	2	1957	7/7	0.97	0.26	0.94	117,117,117,117	0
85	OHX	1	3576	7/7	0.98	0.30	0.94	110,110,110,110	0
85	OHX	6	2050	7/7	0.87	0.27	0.94	173,173,173,173	0
85	OHX	5	3486	7/7	0.98	0.20	0.93	99,99,99,99	0
86	MG	1	3931	1/1	0.96	0.25	0.92	49,49,49,49	0
86	MG	N9	101	1/1	0.78	0.33	0.92	38,38,38,38	0
85	OHX	2	1987	7/7	0.96	0.23	0.92	147,147,147,147	0
86	MG	6	2116	1/1	0.93	0.22	0.91	57,57,57,57	0
86	MG	5	4172	1/1	0.89	0.34	0.90	70,70,70,70	0
85	OHX	6	1926	7/7	0.99	0.20	0.89	87,87,87,87	0
85	OHX	1	3616	7/7	0.97	0.42	0.89	111,111,111,111	0
85	OHX	1	3693	7/7	0.94	0.27	0.86	123,123,123,123	0
86	MG	6	2097	1/1	0.93	0.31	0.84	76,76,76,76	0
86	MG	D1	101	1/1	0.95	0.27	0.84	109,109,109,109	0
86	MG	5	4124	1/1	0.87	0.45	0.83	86,86,86,86	0
86	MG	5	3752	1/1	0.86	0.19	0.83	46,46,46,46	0
86	MG	5	4036	1/1	0.86	0.19	0.82	41,41,41,41	0
86	MG	1	3951	1/1	0.95	0.23	0.77	40,40,40,40	0
85	OHX	6	1993	7/7	0.97	0.20	0.76	142,142,142,142	0
85	OHX	c1	201	7/7	0.93	0.26	0.75	137,137,137,137	0
85	OHX	5	3515	7/7	0.98	0.21	0.75	102,102,102,102	0
85	OHX	1	3575	7/7	0.95	0.26	0.74	110,110,110,110	0
85	OHX	5	3729	7/7	0.96	0.24	0.74	135,135,135,135	0
85	OHX	5	3541	7/7	0.95	0.20	0.73	114,114,114,114	0
86	MG	4	226	1/1	0.96	0.21	0.72	56,56,56,56	0
85	OHX	2	2000	7/7	0.97	0.27	0.71	140,140,140,140	0
86	MG	1	3807	1/1	0.96	0.26	0.68	59,59,59,59	0
85	OHX	5	3543	7/7	0.98	0.22	0.67	80,80,80,80	0
85	OHX	1	3546	7/7	0.98	0.19	0.66	117,117,117,117	0
85	OHX	2	1978	7/7	0.92	0.28	0.66	153,153,153,153	0
86	MG	5	3786	1/1	0.88	0.21	0.66	37,37,37,37	0
86	MG	6	2057	1/1	0.90	0.19	0.66	49,49,49,49	0
85	OHX	6	1997	7/7	0.95	0.29	0.65	142,142,142,142	0
87	ZN	d7	101	1/1	0.85	0.41	0.64	133,133,133,133	0
85	OHX	6	2013	7/7	0.97	0.23	0.64	103,103,103,103	0
86	MG	6	2125	1/1	0.90	0.29	0.62	51,51,51,51	0
86	MG	l3	405	1/1	0.69	0.26	0.62	39,39,39,39	0
85	OHX	s1	303	7/7	0.90	0.31	0.60	154,154,154,154	0
86	MG	5	3747	1/1	0.91	0.26	0.55	34,34,34,34	0
85	OHX	6	2036	7/7	0.92	0.38	0.55	128,128,128,128	0
85	OHX	5	3731	7/7	0.90	0.29	0.55	146,146,146,146	0
85	OHX	2	2003	7/7	0.91	0.32	0.55	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3540	7/7	0.97	0.19	0.55	101,101,101,101	0
85	OHX	5	3579	7/7	0.93	0.31	0.54	122,122,122,122	0
85	OHX	4	214	7/7	0.94	0.25	0.54	130,130,130,130	0
85	OHX	3	209	7/7	0.96	0.20	0.52	132,132,132,132	0
85	OHX	d9	102	7/7	0.96	0.35	0.52	153,153,153,153	0
85	OHX	1	3580	7/7	0.97	0.20	0.50	96,96,96,96	0
85	OHX	2	1956	7/7	0.95	0.22	0.49	138,138,138,138	0
85	OHX	5	3487	7/7	0.98	0.20	0.48	89,89,89,89	0
85	OHX	5	3649	7/7	0.95	0.23	0.47	129,129,129,129	0
86	MG	N6	201	1/1	0.95	0.25	0.44	45,45,45,45	0
86	MG	5	4122	1/1	0.87	0.26	0.44	53,53,53,53	0
85	OHX	5	3495	7/7	0.97	0.16	0.44	103,103,103,103	0
85	OHX	5	3526	7/7	0.97	0.18	0.43	109,109,109,109	0
85	OHX	5	3713	7/7	0.97	0.25	0.42	107,107,107,107	0
86	MG	1	3943	1/1	0.78	0.23	0.40	73,73,73,73	0
86	MG	4	220	1/1	0.96	0.21	0.38	36,36,36,36	0
85	OHX	5	3504	7/7	0.97	0.28	0.38	98,98,98,98	0
85	OHX	1	3640	7/7	0.96	0.20	0.36	122,122,122,122	0
86	MG	M0	302	1/1	0.81	0.21	0.36	40,40,40,40	0
85	OHX	5	3559	7/7	0.96	0.20	0.35	98,98,98,98	0
86	MG	1	3934	1/1	0.88	0.20	0.35	44,44,44,44	0
85	OHX	6	1996	7/7	0.98	0.29	0.34	125,125,125,125	0
85	OHX	O3	201	7/7	0.97	0.26	0.34	105,105,105,105	0
85	OHX	2	2019	7/7	0.91	0.23	0.33	156,156,156,156	0
85	OHX	1	3711	7/7	0.97	0.19	0.33	100,100,100,100	0
85	OHX	5	3677	7/7	0.99	0.18	0.32	74,74,74,74	0
85	OHX	2	1961	7/7	0.96	0.20	0.32	135,135,135,135	0
85	OHX	5	3626	7/7	0.95	0.25	0.30	136,136,136,136	0
86	MG	1	4088	1/1	0.92	0.26	0.30	52,52,52,52	0
85	OHX	1	3720	7/7	0.95	0.22	0.29	96,96,96,96	0
85	OHX	5	3594	7/7	0.97	0.23	0.29	93,93,93,93	0
85	OHX	6	2003	7/7	0.97	0.21	0.28	103,103,103,103	0
85	OHX	2	1932	7/7	0.95	0.21	0.28	128,128,128,128	0
85	OHX	5	3517	7/7	0.97	0.21	0.27	90,90,90,90	0
85	OHX	1	3504	7/7	0.98	0.17	0.27	88,88,88,88	0
85	OHX	l5	302	7/7	0.94	0.32	0.25	134,134,134,134	0
86	MG	1	4067	1/1	0.90	0.32	0.25	58,58,58,58	0
85	OHX	1	3610	7/7	0.96	0.20	0.25	114,114,114,114	0
85	OHX	6	2009	7/7	0.96	0.20	0.24	103,103,103,103	0
86	MG	o4	202	1/1	0.89	0.30	0.23	61,61,61,61	0
85	OHX	6	1972	7/7	0.97	0.21	0.22	101,101,101,101	0
86	MG	5	4023	1/1	0.78	0.20	0.22	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	6	2016	7/7	0.95	0.29	0.22	117,117,117,117	0
85	OHX	1	3607	7/7	0.97	0.22	0.21	130,130,130,130	0
85	OHX	5	3539	7/7	0.96	0.24	0.19	117,117,117,117	0
85	OHX	1	3566	7/7	0.96	0.24	0.18	133,133,133,133	0
85	OHX	1	3509	7/7	0.97	0.20	0.18	94,94,94,94	0
85	OHX	5	3572	7/7	0.97	0.24	0.18	99,99,99,99	0
85	OHX	1	3552	7/7	0.98	0.17	0.17	104,104,104,104	0
85	OHX	l3	402	7/7	0.92	0.42	0.17	145,145,145,145	0
85	OHX	3	203	7/7	0.97	0.18	0.16	112,112,112,112	0
86	MG	2	2119	1/1	0.84	0.30	0.16	81,81,81,81	0
86	MG	2	2122	1/1	0.95	0.33	0.15	74,74,74,74	0
85	OHX	5	3686	7/7	0.97	0.28	0.15	133,133,133,133	0
85	OHX	1	3636	7/7	0.96	0.25	0.14	147,147,147,147	0
85	OHX	5	3522	7/7	0.98	0.19	0.13	93,93,93,93	0
85	OHX	L4	401	7/7	0.97	0.23	0.12	121,121,121,121	0
85	OHX	1	3555	7/7	0.94	0.23	0.08	135,135,135,135	0
85	OHX	d4	201	7/7	0.93	0.29	0.07	142,142,142,142	0
85	OHX	1	3619	7/7	0.92	0.23	0.07	146,146,146,146	0
85	OHX	1	3695	7/7	0.96	0.21	0.05	101,101,101,101	0
85	OHX	2	2007	7/7	0.97	0.20	0.05	150,150,150,150	0
85	OHX	6	1961	7/7	0.97	0.21	0.04	125,125,125,125	0
85	OHX	1	3623	7/7	0.94	0.22	0.03	120,120,120,120	0
85	OHX	1	3683	7/7	0.90	0.25	0.03	153,153,153,153	0
85	OHX	1	3543	7/7	0.96	0.20	0.02	97,97,97,97	0
85	OHX	2	1999	7/7	0.95	0.29	0.01	144,144,144,144	0
85	OHX	6	2000	7/7	0.94	0.24	0.01	131,131,131,131	0
85	OHX	1	3526	7/7	0.98	0.19	-0.03	96,96,96,96	0
86	MG	2	2134	1/1	0.75	0.27	-0.03	116,116,116,116	0
86	MG	6	2117	1/1	0.98	0.19	-0.05	50,50,50,50	0
85	OHX	6	2046	7/7	0.95	0.30	-0.06	142,142,142,142	0
85	OHX	1	3520	7/7	0.97	0.23	-0.08	102,102,102,102	0
85	OHX	1	3595	7/7	0.96	0.20	-0.09	159,159,159,159	0
86	MG	5	4001	1/1	0.63	0.19	-0.10	38,38,38,38	0
85	OHX	6	1991	7/7	0.96	0.28	-0.10	118,118,118,118	0
86	MG	1	3751	1/1	0.89	0.23	-0.11	59,59,59,59	0
86	MG	1	3774	1/1	0.92	0.18	-0.15	53,53,53,53	0
86	MG	5	4008	1/1	0.89	0.19	-0.15	42,42,42,42	0
86	MG	5	3997	1/1	0.85	0.20	-0.16	76,76,76,76	0
85	OHX	1	3569	7/7	0.99	0.20	-0.18	98,98,98,98	0
86	MG	2	2116	1/1	0.86	0.28	-0.18	82,82,82,82	0
86	MG	4	227	1/1	0.97	0.15	-0.20	47,47,47,47	0
85	OHX	1	3641	7/7	0.97	0.24	-0.20	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	4	203	7/7	0.97	0.18	-0.21	95,95,95,95	0
86	MG	1	3947	1/1	0.96	0.17	-0.21	34,34,34,34	0
85	OHX	5	3524	7/7	0.98	0.19	-0.21	91,91,91,91	0
87	ZN	q2	501	1/1	0.88	0.33	-0.21	83,83,83,83	0
85	OHX	1	3514	7/7	0.98	0.16	-0.24	83,83,83,83	0
85	OHX	S6	301	7/7	0.92	0.33	-0.25	167,167,167,167	0
86	MG	1	3804	1/1	0.93	0.14	-0.25	38,38,38,38	0
85	OHX	2	1935	7/7	0.98	0.19	-0.27	134,134,134,134	0
86	MG	5	3821	1/1	0.88	0.23	-0.27	72,72,72,72	0
85	OHX	2	1980	7/7	0.96	0.20	-0.27	141,141,141,141	0
85	OHX	6	1963	7/7	0.97	0.17	-0.27	116,116,116,116	0
85	OHX	6	2012	7/7	0.97	0.19	-0.28	139,139,139,139	0
85	OHX	4	205	7/7	0.99	0.20	-0.28	121,121,121,121	0
85	OHX	2	2005	7/7	0.94	0.22	-0.30	136,136,136,136	0
85	OHX	5	3585	7/7	0.98	0.18	-0.30	96,96,96,96	0
85	OHX	5	3531	7/7	0.97	0.16	-0.31	94,94,94,94	0
85	OHX	1	3669	7/7	0.86	0.34	-0.32	161,161,161,161	0
85	OHX	1	3589	7/7	0.97	0.21	-0.32	137,137,137,137	0
85	OHX	1	3585	7/7	0.96	0.18	-0.32	129,129,129,129	0
85	OHX	2	2002	7/7	0.93	0.24	-0.33	149,149,149,149	0
85	OHX	3	206	7/7	0.98	0.20	-0.33	112,112,112,112	0
85	OHX	5	3537	7/7	0.98	0.18	-0.34	92,92,92,92	0
85	OHX	5	3514	7/7	0.97	0.18	-0.35	102,102,102,102	0
85	OHX	5	3608	7/7	0.93	0.23	-0.35	127,127,127,127	0
86	MG	1	3917	1/1	0.95	0.17	-0.37	63,63,63,63	0
85	OHX	L3	402	7/7	0.97	0.21	-0.37	116,116,116,116	0
85	OHX	1	3572	7/7	0.98	0.18	-0.39	85,85,85,85	0
85	OHX	1	3516	7/7	0.97	0.16	-0.40	106,106,106,106	0
85	OHX	6	1960	7/7	0.97	0.20	-0.42	109,109,109,109	0
85	OHX	5	3508	7/7	0.99	0.19	-0.42	93,93,93,93	0
86	MG	l3	407	1/1	0.96	0.19	-0.43	31,31,31,31	0
85	OHX	5	3614	7/7	0.99	0.16	-0.43	81,81,81,81	0
85	OHX	6	1999	7/7	0.96	0.20	-0.43	125,125,125,125	0
87	ZN	Q2	501	1/1	0.96	0.30	-0.43	83,83,83,83	0
86	MG	1	3959	1/1	0.90	0.15	-0.45	74,74,74,74	0
86	MG	1	3764	1/1	0.93	0.16	-0.46	37,37,37,37	0
85	OHX	1	3579	7/7	0.97	0.19	-0.47	117,117,117,117	0
85	OHX	1	3737	7/7	0.95	0.14	-0.48	118,118,118,118	0
85	OHX	2	1967	7/7	0.95	0.24	-0.49	113,113,113,113	0
86	MG	6	2162	1/1	0.91	0.21	-0.49	71,71,71,71	0
85	OHX	5	3567	7/7	0.95	0.17	-0.51	119,119,119,119	0
86	MG	O7	105	1/1	0.91	0.21	-0.52	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	S8	301	7/7	0.93	0.23	-0.53	165,165,165,165	0
85	OHX	2	2025	7/7	0.97	0.18	-0.55	126,126,126,126	0
85	OHX	5	3402	7/7	1.00	0.15	-0.55	43,43,43,43	0
85	OHX	2	1985	7/7	0.98	0.17	-0.55	110,110,110,110	0
85	OHX	2	1963	7/7	0.96	0.20	-0.55	142,142,142,142	0
85	OHX	8	211	7/7	0.93	0.25	-0.55	120,120,120,120	0
85	OHX	6	1962	7/7	0.97	0.18	-0.56	97,97,97,97	0
85	OHX	1	3539	7/7	0.96	0.20	-0.57	119,119,119,119	0
86	MG	4	221	1/1	0.96	0.19	-0.57	41,41,41,41	0
86	MG	1	3810	1/1	0.89	0.17	-0.57	41,41,41,41	0
85	OHX	3	208	7/7	0.96	0.14	-0.57	120,120,120,120	0
85	OHX	7	208	7/7	0.96	0.14	-0.59	125,125,125,125	0
85	OHX	1	3578	7/7	0.97	0.20	-0.60	134,134,134,134	0
85	OHX	6	1949	7/7	0.96	0.17	-0.60	122,122,122,122	0
85	OHX	5	3698	7/7	0.93	0.27	-0.60	164,164,164,164	0
85	OHX	1	3549	7/7	0.92	0.18	-0.61	139,139,139,139	0
85	OHX	14	401	7/7	0.94	0.23	-0.61	127,127,127,127	0
85	OHX	6	2007	7/7	0.97	0.18	-0.62	130,130,130,130	0
85	OHX	5	3562	7/7	0.96	0.19	-0.62	130,130,130,130	0
85	OHX	2	1962	7/7	0.98	0.18	-0.63	114,114,114,114	0
85	OHX	1	3483	7/7	0.98	0.17	-0.63	89,89,89,89	0
85	OHX	6	1982	7/7	0.97	0.20	-0.64	137,137,137,137	0
85	OHX	4	210	7/7	0.97	0.17	-0.64	131,131,131,131	0
85	OHX	5	3467	7/7	0.99	0.16	-0.65	92,92,92,92	0
85	OHX	s8	301	7/7	0.91	0.30	-0.66	155,155,155,155	0
85	OHX	5	3475	7/7	0.97	0.12	-0.66	80,80,80,80	0
85	OHX	2	1974	7/7	0.97	0.20	-0.67	140,140,140,140	0
85	OHX	5	3401	7/7	0.99	0.17	-0.69	48,48,48,48	0
85	OHX	2	2017	7/7	0.95	0.20	-0.69	139,139,139,139	0
85	OHX	o2	201	7/7	0.99	0.16	-0.69	86,86,86,86	0
85	OHX	5	3525	7/7	0.98	0.12	-0.71	108,108,108,108	0
85	OHX	1	3492	7/7	0.99	0.16	-0.72	87,87,87,87	0
85	OHX	5	3544	7/7	0.98	0.18	-0.73	114,114,114,114	0
85	OHX	2	1988	7/7	0.98	0.14	-0.73	138,138,138,138	0
85	OHX	2	1943	7/7	0.97	0.18	-0.76	104,104,104,104	0
85	OHX	2	1971	7/7	0.94	0.17	-0.80	151,151,151,151	0
85	OHX	2	1945	7/7	0.94	0.16	-0.81	144,144,144,144	0
85	OHX	1	3536	7/7	0.99	0.14	-0.82	83,83,83,83	0
85	OHX	2	1933	7/7	0.97	0.15	-0.83	112,112,112,112	0
85	OHX	m5	501	7/7	0.99	0.21	-0.84	117,117,117,117	0
85	OHX	2	1993	7/7	0.97	0.21	-0.84	119,119,119,119	0
85	OHX	1	3475	7/7	0.96	0.12	-0.84	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	sR	401	7/7	0.96	0.16	-0.84	156,156,156,156	0
85	OHX	1	3694	7/7	0.96	0.18	-0.86	98,98,98,98	0
85	OHX	5	3534	7/7	0.97	0.14	-0.87	110,110,110,110	0
85	OHX	5	3587	7/7	0.97	0.17	-0.87	108,108,108,108	0
85	OHX	1	3484	7/7	0.96	0.14	-0.88	114,114,114,114	0
85	OHX	1	3446	7/7	0.97	0.18	-0.89	88,88,88,88	0
85	OHX	6	1973	7/7	0.95	0.17	-0.91	138,138,138,138	0
85	OHX	1	3590	7/7	0.96	0.16	-0.94	131,131,131,131	0
85	OHX	1	3577	7/7	0.97	0.19	-0.95	102,102,102,102	0
85	OHX	1	3508	7/7	0.97	0.16	-0.95	111,111,111,111	0
85	OHX	2	1938	7/7	0.99	0.18	-0.96	104,104,104,104	0
85	OHX	5	3412	7/7	0.99	0.16	-0.97	68,68,68,68	0
85	OHX	o3	201	7/7	0.97	0.16	-0.97	101,101,101,101	0
85	OHX	2	2043	7/7	0.91	0.23	-0.98	179,179,179,179	0
85	OHX	1	3479	7/7	0.99	0.17	-0.98	85,85,85,85	0
85	OHX	5	3489	7/7	0.99	0.14	-0.98	86,86,86,86	0
85	OHX	6	1922	7/7	0.98	0.16	-0.99	90,90,90,90	0
86	MG	L2	301	1/1	0.96	0.17	-0.99	41,41,41,41	0
85	OHX	M5	302	7/7	0.98	0.19	-0.99	107,107,107,107	0
85	OHX	1	3405	7/7	0.99	0.17	-1.02	58,58,58,58	0
85	OHX	1	3556	7/7	0.98	0.17	-1.02	105,105,105,105	0
86	MG	4	230	1/1	0.96	0.16	-1.06	51,51,51,51	0
85	OHX	2	2009	7/7	0.96	0.20	-1.06	112,112,112,112	0
85	OHX	8	206	7/7	0.97	0.12	-1.07	115,115,115,115	0
85	OHX	5	3565	7/7	0.99	0.16	-1.08	97,97,97,97	0
86	MG	1	4129	1/1	0.97	0.15	-1.09	70,70,70,70	0
85	OHX	8	203	7/7	0.95	0.11	-1.10	114,114,114,114	0
85	OHX	2	1946	7/7	0.91	0.25	-1.11	170,170,170,170	0
85	OHX	2	2020	7/7	0.92	0.20	-1.11	172,172,172,172	0
85	OHX	1	3495	7/7	0.98	0.15	-1.12	71,71,71,71	0
85	OHX	6	1924	7/7	0.98	0.16	-1.12	91,91,91,91	0
85	OHX	2	1970	7/7	0.98	0.15	-1.12	107,107,107,107	0
85	OHX	m0	302	7/7	0.97	0.20	-1.13	116,116,116,116	0
85	OHX	6	1901	7/7	0.99	0.15	-1.14	61,61,61,61	0
86	MG	6	2186	1/1	0.72	0.17	-1.14	87,87,87,87	0
85	OHX	2	1901	7/7	0.99	0.16	-1.15	79,79,79,79	0
85	OHX	1	3452	7/7	0.97	0.13	-1.15	87,87,87,87	0
85	OHX	5	3481	7/7	0.98	0.12	-1.16	87,87,87,87	0
86	MG	5	3808	1/1	0.86	0.22	-1.17	114,114,114,114	0
85	OHX	1	3471	7/7	0.96	0.12	-1.18	97,97,97,97	0
85	OHX	6	1921	7/7	0.99	0.12	-1.19	86,86,86,86	0
85	OHX	7	207	7/7	0.97	0.11	-1.19	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	M0	301	7/7	0.94	0.16	-1.20	104,104,104,104	0
86	MG	sM	401	1/1	0.96	0.12	-1.21	44,44,44,44	0
85	OHX	Q2	502	7/7	0.98	0.14	-1.22	71,71,71,71	0
85	OHX	5	3405	7/7	0.99	0.16	-1.22	55,55,55,55	0
85	OHX	1	3532	7/7	0.98	0.18	-1.22	99,99,99,99	0
85	OHX	O7	102	7/7	0.98	0.09	-1.24	94,94,94,94	0
85	OHX	5	3739	7/7	0.97	0.16	-1.25	97,97,97,97	0
86	MG	5	4094	1/1	0.94	0.15	-1.25	35,35,35,35	0
85	OHX	5	3484	7/7	0.97	0.15	-1.27	91,91,91,91	0
86	MG	2	2080	1/1	0.95	0.15	-1.29	78,78,78,78	0
85	OHX	5	3703	7/7	0.97	0.16	-1.31	83,83,83,83	0
85	OHX	1	3466	7/7	0.98	0.14	-1.31	95,95,95,95	0
85	OHX	O7	103	7/7	0.96	0.16	-1.31	92,92,92,92	0
85	OHX	5	3483	7/7	0.97	0.13	-1.32	103,103,103,103	0
85	OHX	1	3548	7/7	0.97	0.16	-1.33	117,117,117,117	0
85	OHX	1	3445	7/7	0.98	0.12	-1.33	76,76,76,76	0
85	OHX	5	3602	7/7	0.95	0.15	-1.34	123,123,123,123	0
86	MG	6	2171	1/1	0.75	0.19	-1.35	92,92,92,92	0
85	OHX	1	3494	7/7	0.97	0.16	-1.35	93,93,93,93	0
85	OHX	l9	201	7/7	0.97	0.17	-1.35	103,103,103,103	0
85	OHX	6	1989	7/7	0.95	0.18	-1.35	137,137,137,137	0
86	MG	1	4128	1/1	0.91	0.15	-1.36	41,41,41,41	0
85	OHX	1	3485	7/7	0.98	0.11	-1.36	99,99,99,99	0
85	OHX	1	3487	7/7	0.95	0.13	-1.37	118,118,118,118	0
85	OHX	1	3426	7/7	0.98	0.13	-1.38	82,82,82,82	0
85	OHX	5	3480	7/7	0.97	0.16	-1.38	84,84,84,84	0
85	OHX	C8	201	7/7	0.97	0.09	-1.39	112,112,112,112	0
86	MG	6	2136	1/1	0.98	0.12	-1.39	76,76,76,76	0
85	OHX	5	3477	7/7	0.97	0.12	-1.40	90,90,90,90	0
85	OHX	1	3401	7/7	1.00	0.14	-1.42	44,44,44,44	0
86	MG	1	3756	1/1	0.89	0.13	-1.42	37,37,37,37	0
86	MG	p0	401	1/1	0.88	0.15	-1.44	89,89,89,89	0
85	OHX	5	3488	7/7	0.99	0.13	-1.45	83,83,83,83	0
85	OHX	c5	201	7/7	0.94	0.27	-1.45	151,151,151,151	0
85	OHX	5	3540	7/7	0.96	0.14	-1.46	123,123,123,123	0
85	OHX	5	3618	7/7	0.98	0.17	-1.46	103,103,103,103	0
85	OHX	5	3502	7/7	0.96	0.13	-1.47	112,112,112,112	0
85	OHX	1	3529	7/7	0.97	0.17	-1.47	133,133,133,133	0
85	OHX	1	3443	7/7	0.99	0.12	-1.47	81,81,81,81	0
87	ZN	d9	101	1/1	0.95	0.08	-1.48	97,97,97,97	0
85	OHX	6	1983	7/7	0.97	0.13	-1.48	136,136,136,136	0
85	OHX	1	3404	7/7	0.99	0.13	-1.49	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	2135	1/1	0.91	0.11	-1.51	101,101,101,101	0
85	OHX	1	3513	7/7	0.98	0.17	-1.52	101,101,101,101	0
85	OHX	2	1950	7/7	0.99	0.17	-1.54	115,115,115,115	0
85	OHX	1	3491	7/7	0.98	0.15	-1.54	95,95,95,95	0
87	ZN	e1	501	1/1	0.94	0.16	-1.54	173,173,173,173	0
85	OHX	5	3429	7/7	0.99	0.13	-1.55	70,70,70,70	0
85	OHX	1	3642	7/7	0.94	0.22	-1.55	208,208,208,208	0
85	OHX	5	3518	7/7	0.98	0.15	-1.56	103,103,103,103	0
86	MG	2	2062	1/1	0.93	0.19	-1.57	74,74,74,74	0
86	MG	1	4044	1/1	0.98	0.17	-1.57	77,77,77,77	0
85	OHX	6	1902	7/7	0.99	0.19	-1.58	79,79,79,79	0
85	OHX	6	1992	7/7	0.98	0.17	-1.59	117,117,117,117	0
85	OHX	2	1976	7/7	0.94	0.14	-1.59	148,148,148,148	0
85	OHX	6	1943	7/7	0.97	0.14	-1.60	125,125,125,125	0
85	OHX	6	1951	7/7	0.94	0.18	-1.60	161,161,161,161	0
85	OHX	1	3620	7/7	0.97	0.15	-1.61	124,124,124,124	0
85	OHX	5	3528	7/7	0.98	0.12	-1.62	117,117,117,117	0
85	OHX	2	1949	7/7	0.97	0.18	-1.63	127,127,127,127	0
85	OHX	4	201	7/7	0.99	0.13	-1.63	57,57,57,57	0
85	OHX	2	1973	7/7	0.96	0.16	-1.64	146,146,146,146	0
85	OHX	1	3690	7/7	0.97	0.16	-1.65	125,125,125,125	0
85	OHX	1	3581	7/7	0.99	0.16	-1.66	101,101,101,101	0
85	OHX	2	1914	7/7	0.99	0.09	-1.66	97,97,97,97	0
85	OHX	6	1965	7/7	0.97	0.18	-1.67	125,125,125,125	0
85	OHX	1	3531	7/7	0.98	0.12	-1.67	129,129,129,129	0
85	OHX	1	3409	7/7	0.99	0.12	-1.68	64,64,64,64	0
86	MG	5	3753	1/1	0.96	0.12	-1.69	35,35,35,35	0
85	OHX	1	3530	7/7	0.97	0.15	-1.69	124,124,124,124	0
85	OHX	5	3471	7/7	0.98	0.10	-1.69	91,91,91,91	0
85	OHX	5	3578	7/7	0.98	0.14	-1.70	109,109,109,109	0
85	OHX	n3	201	7/7	0.98	0.10	-1.70	85,85,85,85	0
85	OHX	1	3407	7/7	0.99	0.14	-1.70	64,64,64,64	0
85	OHX	5	3509	7/7	0.96	0.14	-1.72	107,107,107,107	0
85	OHX	6	1952	7/7	0.97	0.13	-1.72	114,114,114,114	0
85	OHX	SR	401	7/7	0.94	0.15	-1.72	168,168,168,168	0
85	OHX	5	3419	7/7	0.98	0.12	-1.75	61,61,61,61	0
85	OHX	2	1909	7/7	0.98	0.16	-1.80	119,119,119,119	0
85	OHX	l5	301	7/7	0.96	0.16	-1.82	127,127,127,127	0
85	OHX	2	1965	7/7	0.96	0.17	-1.82	126,126,126,126	0
85	OHX	1	3573	7/7	0.97	0.17	-1.84	110,110,110,110	0
85	OHX	C5	201	7/7	0.96	0.20	-1.84	153,153,153,153	0
85	OHX	1	3538	7/7	0.97	0.16	-1.85	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	5	3424	7/7	0.98	0.10	-1.86	66,66,66,66	0
87	ZN	Q0	201	1/1	0.99	0.09	-1.86	49,49,49,49	0
85	OHX	8	204	7/7	0.99	0.10	-1.86	97,97,97,97	0
85	OHX	5	3634	7/7	0.97	0.14	-1.87	139,139,139,139	0
85	OHX	8	205	7/7	0.97	0.16	-1.88	101,101,101,101	0
85	OHX	6	1944	7/7	0.98	0.14	-1.88	108,108,108,108	0
85	OHX	1	3456	7/7	0.95	0.13	-1.90	112,112,112,112	0
85	OHX	q2	502	7/7	0.99	0.09	-1.90	73,73,73,73	0
85	OHX	5	3408	7/7	0.99	0.14	-1.93	59,59,59,59	0
85	OHX	m0	301	7/7	0.98	0.09	-1.94	118,118,118,118	0
85	OHX	6	1918	7/7	0.97	0.12	-1.94	95,95,95,95	0
85	OHX	2	1936	7/7	0.97	0.13	-1.94	107,107,107,107	0
85	OHX	1	3460	7/7	0.98	0.09	-1.95	88,88,88,88	0
85	OHX	1	3497	7/7	0.99	0.14	-1.97	102,102,102,102	0
85	OHX	5	3516	7/7	0.97	0.08	-1.99	141,141,141,141	0
85	OHX	2	1910	7/7	0.99	0.10	-2.01	100,100,100,100	0
85	OHX	N9	102	7/7	0.99	0.11	-2.01	63,63,63,63	0
85	OHX	5	3535	7/7	0.95	0.14	-2.02	132,132,132,132	0
85	OHX	1	3432	7/7	0.98	0.14	-2.03	77,77,77,77	0
85	OHX	5	3435	7/7	0.98	0.12	-2.04	90,90,90,90	0
85	OHX	1	3482	7/7	0.96	0.10	-2.04	114,114,114,114	0
85	OHX	1	3403	7/7	0.99	0.10	-2.06	45,45,45,45	0
85	OHX	1	3459	7/7	0.98	0.10	-2.06	79,79,79,79	0
85	OHX	5	3410	7/7	0.99	0.12	-2.07	59,59,59,59	0
85	OHX	4	202	7/7	0.99	0.11	-2.07	77,77,77,77	0
85	OHX	5	3500	7/7	0.97	0.11	-2.09	117,117,117,117	0
85	OHX	5	3605	7/7	0.95	0.16	-2.10	141,141,141,141	0
86	MG	5	4046	1/1	0.98	0.13	-2.10	33,33,33,33	0
85	OHX	2	1917	7/7	0.99	0.10	-2.11	95,95,95,95	0
85	OHX	5	3497	7/7	0.99	0.14	-2.13	116,116,116,116	0
85	OHX	5	3547	7/7	0.97	0.15	-2.13	101,101,101,101	0
85	OHX	5	3459	7/7	0.98	0.11	-2.14	80,80,80,80	0
85	OHX	1	3517	7/7	0.97	0.13	-2.15	95,95,95,95	0
85	OHX	n9	101	7/7	0.99	0.12	-2.16	64,64,64,64	0
85	OHX	7	203	7/7	0.97	0.14	-2.16	95,95,95,95	0
85	OHX	5	3490	7/7	0.98	0.13	-2.17	91,91,91,91	0
85	OHX	3	205	7/7	0.98	0.15	-2.19	90,90,90,90	0
85	OHX	2	1955	7/7	0.97	0.14	-2.20	119,119,119,119	0
85	OHX	2	1915	7/7	0.96	0.11	-2.20	142,142,142,142	0
85	OHX	1	3423	7/7	0.99	0.17	-2.20	71,71,71,71	0
85	OHX	5	3557	7/7	0.98	0.15	-2.21	91,91,91,91	0
85	OHX	1	3525	7/7	0.98	0.11	-2.23	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	2094	1/1	0.94	0.16	-2.23	75,75,75,75	0
85	OHX	s1	302	7/7	0.99	0.12	-2.25	81,81,81,81	0
85	OHX	2	1975	7/7	0.95	0.11	-2.26	161,161,161,161	0
87	ZN	d6	500	1/1	0.92	0.08	-2.26	71,71,71,71	0
86	MG	1	4056	1/1	0.98	0.08	-2.30	38,38,38,38	0
85	OHX	5	3520	7/7	0.93	0.13	-2.30	131,131,131,131	0
85	OHX	1	3419	7/7	0.99	0.12	-2.32	70,70,70,70	0
85	OHX	2	1921	7/7	0.97	0.12	-2.32	112,112,112,112	0
85	OHX	1	3418	7/7	0.99	0.12	-2.33	72,72,72,72	0
85	OHX	5	3457	7/7	0.98	0.15	-2.33	88,88,88,88	0
85	OHX	6	1977	7/7	0.96	0.14	-2.33	138,138,138,138	0
85	OHX	5	3592	7/7	0.98	0.17	-2.34	96,96,96,96	0
85	OHX	2	1911	7/7	0.97	0.13	-2.34	116,116,116,116	0
85	OHX	6	1928	7/7	0.97	0.10	-2.36	136,136,136,136	0
85	OHX	5	3474	7/7	0.97	0.15	-2.36	80,80,80,80	0
85	OHX	5	3493	7/7	0.97	0.13	-2.37	99,99,99,99	0
85	OHX	6	1912	7/7	0.98	0.11	-2.37	87,87,87,87	0
85	OHX	1	3519	7/7	0.97	0.12	-2.37	120,120,120,120	0
85	OHX	1	3499	7/7	0.97	0.11	-2.40	119,119,119,119	0
85	OHX	1	3534	7/7	0.97	0.10	-2.41	146,146,146,146	0
85	OHX	2	1940	7/7	0.97	0.16	-2.41	120,120,120,120	0
85	OHX	1	3518	7/7	0.98	0.14	-2.41	76,76,76,76	0
87	ZN	Q3	501	1/1	0.97	0.06	-2.43	68,68,68,68	0
85	OHX	6	1954	7/7	0.95	0.11	-2.45	164,164,164,164	0
85	OHX	1	3502	7/7	0.98	0.14	-2.46	98,98,98,98	0
85	OHX	5	3439	7/7	0.99	0.10	-2.50	69,69,69,69	0
86	MG	5	3942	1/1	0.95	0.13	-2.51	31,31,31,31	0
85	OHX	6	1910	7/7	0.99	0.11	-2.51	73,73,73,73	0
85	OHX	2	1907	7/7	0.98	0.09	-2.51	101,101,101,101	0
85	OHX	6	1909	7/7	0.98	0.10	-2.52	96,96,96,96	0
85	OHX	1	3402	7/7	0.99	0.10	-2.53	53,53,53,53	0
85	OHX	1	3473	7/7	0.97	0.11	-2.53	89,89,89,89	0
85	OHX	2	1903	7/7	0.97	0.16	-2.53	89,89,89,89	0
85	OHX	6	1946	7/7	0.97	0.11	-2.55	113,113,113,113	0
87	ZN	E1	501	1/1	0.86	0.05	-2.56	134,134,134,134	0
85	OHX	6	1953	7/7	0.93	0.14	-2.57	155,155,155,155	0
85	OHX	5	3445	7/7	0.99	0.08	-2.58	79,79,79,79	0
85	OHX	7	201	7/7	0.99	0.09	-2.59	80,80,80,80	0
85	OHX	6	1955	7/7	0.97	0.07	-2.61	167,167,167,167	0
85	OHX	5	3403	7/7	0.99	0.11	-2.61	42,42,42,42	0
86	MG	1	3765	1/1	0.97	0.11	-2.61	51,51,51,51	0
85	OHX	1	3416	7/7	0.98	0.13	-2.61	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	5	3420	7/7	0.99	0.10	-2.62	62,62,62,62	0
87	ZN	D9	101	1/1	0.98	0.09	-2.64	89,89,89,89	0
85	OHX	5	3512	7/7	0.98	0.13	-2.65	90,90,90,90	0
85	OHX	5	3482	7/7	0.98	0.10	-2.65	93,93,93,93	0
85	OHX	1	3448	7/7	0.99	0.07	-2.65	86,86,86,86	0
85	OHX	2	1918	7/7	0.98	0.09	-2.66	99,99,99,99	0
85	OHX	5	3440	7/7	0.99	0.11	-2.66	83,83,83,83	0
85	OHX	5	3449	7/7	0.98	0.10	-2.66	88,88,88,88	0
87	ZN	O7	101	1/1	0.98	0.04	-2.70	45,45,45,45	0
85	OHX	5	3510	7/7	0.98	0.09	-2.72	122,122,122,122	0
85	OHX	5	3409	7/7	0.99	0.13	-2.72	58,58,58,58	0
85	OHX	1	3469	7/7	0.97	0.09	-2.75	100,100,100,100	0
85	OHX	6	1908	7/7	0.99	0.14	-2.77	80,80,80,80	0
85	OHX	5	3416	7/7	0.99	0.11	-2.77	65,65,65,65	0
86	MG	5	3762	1/1	0.95	0.12	-2.77	34,34,34,34	0
85	OHX	1	3427	7/7	0.98	0.11	-2.78	70,70,70,70	0
85	OHX	7	205	7/7	0.98	0.14	-2.79	93,93,93,93	0
85	OHX	6	1929	7/7	0.99	0.11	-2.80	81,81,81,81	0
85	OHX	8	202	7/7	0.99	0.08	-2.81	74,74,74,74	0
85	OHX	2	1941	7/7	0.98	0.10	-2.81	135,135,135,135	0
85	OHX	5	3415	7/7	0.99	0.09	-2.82	65,65,65,65	0
85	OHX	5	3485	7/7	0.99	0.09	-2.85	75,75,75,75	0
85	OHX	1	3412	7/7	0.99	0.11	-2.86	67,67,67,67	0
85	OHX	5	3501	7/7	0.98	0.11	-2.88	106,106,106,106	0
85	OHX	1	3732	7/7	0.95	0.10	-2.91	158,158,158,158	0
85	OHX	1	3421	7/7	1.00	0.09	-2.91	74,74,74,74	0
85	OHX	6	1906	7/7	0.99	0.12	-2.92	71,71,71,71	0
85	OHX	5	3433	7/7	0.99	0.10	-2.93	64,64,64,64	0
87	ZN	q0	201	1/1	0.98	0.07	-2.93	37,37,37,37	0
85	OHX	1	3464	7/7	0.96	0.12	-2.95	102,102,102,102	0
85	OHX	2	2035	7/7	0.84	0.19	-3.01	223,223,223,223	0
85	OHX	1	3411	7/7	0.99	0.12	-3.01	59,59,59,59	0
85	OHX	5	3581	7/7	0.97	0.08	-3.02	150,150,150,150	0
85	OHX	7	206	7/7	0.98	0.11	-3.05	100,100,100,100	0
85	OHX	1	3574	7/7	0.97	0.13	-3.09	137,137,137,137	0
85	OHX	5	3426	7/7	0.99	0.12	-3.11	70,70,70,70	0
85	OHX	5	3468	7/7	0.98	0.09	-3.13	99,99,99,99	0
85	OHX	1	3461	7/7	0.98	0.11	-3.14	80,80,80,80	0
85	OHX	1	3414	7/7	0.99	0.11	-3.15	65,65,65,65	0
85	OHX	5	3450	7/7	0.99	0.05	-3.18	91,91,91,91	0
85	OHX	6	1932	7/7	0.98	0.10	-3.19	90,90,90,90	0
85	OHX	2	1925	7/7	0.98	0.14	-3.19	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	5	3460	7/7	0.97	0.10	-3.20	89,89,89,89	0
85	OHX	7	204	7/7	0.96	0.14	-3.24	86,86,86,86	0
85	OHX	5	3545	7/7	0.97	0.07	-3.26	148,148,148,148	0
85	OHX	5	3404	7/7	0.99	0.09	-3.26	51,51,51,51	0
85	OHX	1	3465	7/7	0.98	0.10	-3.27	98,98,98,98	0
85	OHX	2	1905	7/7	0.99	0.09	-3.28	86,86,86,86	0
85	OHX	5	3417	7/7	0.99	0.10	-3.30	57,57,57,57	0
85	OHX	5	3473	7/7	0.98	0.13	-3.31	85,85,85,85	0
87	ZN	D6	500	1/1	0.95	0.04	-3.35	93,93,93,93	0
85	OHX	5	3503	7/7	0.99	0.09	-3.35	102,102,102,102	0
85	OHX	1	3500	7/7	0.97	0.15	-3.37	85,85,85,85	0
85	OHX	1	3433	7/7	0.98	0.12	-3.37	77,77,77,77	0
85	OHX	1	3406	7/7	0.99	0.10	-3.37	54,54,54,54	0
85	OHX	3	204	7/7	0.98	0.10	-3.39	99,99,99,99	0
85	OHX	6	1907	7/7	0.99	0.11	-3.41	82,82,82,82	0
85	OHX	5	3452	7/7	0.98	0.11	-3.43	84,84,84,84	0
87	ZN	o7	501	1/1	0.98	0.05	-3.44	46,46,46,46	0
85	OHX	6	1903	7/7	0.99	0.10	-3.45	70,70,70,70	0
85	OHX	5	3532	7/7	0.98	0.13	-3.46	79,79,79,79	0
85	OHX	5	3584	7/7	0.97	0.12	-3.46	116,116,116,116	0
85	OHX	5	3464	7/7	0.99	0.07	-3.46	87,87,87,87	0
85	OHX	l3	401	7/7	0.98	0.12	-3.48	95,95,95,95	0
85	OHX	5	3422	7/7	0.99	0.10	-3.49	70,70,70,70	0
85	OHX	5	3442	7/7	0.98	0.10	-3.52	82,82,82,82	0
85	OHX	1	3486	7/7	0.95	0.12	-3.52	117,117,117,117	0
85	OHX	5	3443	7/7	0.98	0.09	-3.52	81,81,81,81	0
85	OHX	1	3470	7/7	0.99	0.07	-3.53	77,77,77,77	0
85	OHX	1	3478	7/7	0.98	0.12	-3.54	96,96,96,96	0
85	OHX	5	3444	7/7	0.98	0.12	-3.54	95,95,95,95	0
85	OHX	6	1945	7/7	0.96	0.14	-3.56	110,110,110,110	0
85	OHX	5	3494	7/7	0.98	0.12	-3.59	86,86,86,86	0
85	OHX	5	3507	7/7	0.98	0.11	-3.60	87,87,87,87	0
86	MG	M7	208	1/1	0.97	0.06	-3.60	50,50,50,50	0
85	OHX	5	3414	7/7	0.99	0.11	-3.62	61,61,61,61	0
85	OHX	2	1923	7/7	0.98	0.10	-3.63	101,101,101,101	0
85	OHX	6	1920	7/7	0.97	0.11	-3.67	124,124,124,124	0
85	OHX	5	3554	7/7	0.98	0.10	-3.69	130,130,130,130	0
85	OHX	1	3415	7/7	0.99	0.07	-3.69	68,68,68,68	0
85	OHX	2	1928	7/7	0.98	0.13	-3.71	114,114,114,114	0
85	OHX	1	3501	7/7	0.99	0.10	-3.73	70,70,70,70	0
85	OHX	2	1908	7/7	0.98	0.12	-3.77	108,108,108,108	0
85	OHX	1	3429	7/7	0.99	0.09	-3.80	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	5	3511	7/7	0.99	0.10	-3.81	63,63,63,63	0
85	OHX	6	1956	7/7	0.98	0.13	-3.83	112,112,112,112	0
85	OHX	5	3582	7/7	0.98	0.14	-3.84	85,85,85,85	0
85	OHX	2	1916	7/7	0.98	0.10	-3.84	107,107,107,107	0
85	OHX	1	3424	7/7	0.99	0.11	-3.85	76,76,76,76	0
85	OHX	8	201	7/7	0.99	0.12	-3.86	57,57,57,57	0
85	OHX	1	3410	7/7	0.99	0.09	-3.87	63,63,63,63	0
85	OHX	2	1937	7/7	0.97	0.11	-3.88	123,123,123,123	0
85	OHX	5	3438	7/7	0.99	0.09	-3.91	76,76,76,76	0
85	OHX	1	3422	7/7	0.99	0.10	-3.97	73,73,73,73	0
85	OHX	6	1947	7/7	0.98	0.10	-4.00	102,102,102,102	0
85	OHX	1	3430	7/7	0.99	0.09	-4.02	75,75,75,75	0
85	OHX	6	1917	7/7	0.98	0.10	-4.03	86,86,86,86	0
85	OHX	1	3481	7/7	0.99	0.09	-4.03	89,89,89,89	0
85	OHX	5	3430	7/7	0.99	0.07	-4.04	77,77,77,77	0
85	OHX	6	1939	7/7	0.97	0.09	-4.04	135,135,135,135	0
85	OHX	5	3453	7/7	0.98	0.11	-4.06	111,111,111,111	0
85	OHX	6	1923	7/7	0.98	0.10	-4.07	99,99,99,99	0
85	OHX	2	1922	7/7	0.98	0.09	-4.08	99,99,99,99	0
85	OHX	5	3413	7/7	0.99	0.09	-4.08	57,57,57,57	0
85	OHX	N1	201	7/7	0.99	0.09	-4.12	68,68,68,68	0
85	OHX	2	1919	7/7	0.99	0.07	-4.12	94,94,94,94	0
85	OHX	6	1904	7/7	0.99	0.09	-4.17	70,70,70,70	0
85	OHX	2	1927	7/7	0.97	0.12	-4.26	129,129,129,129	0
85	OHX	1	3462	7/7	0.96	0.12	-4.31	121,121,121,121	0
85	OHX	1	3621	7/7	0.94	0.12	-4.34	193,193,193,193	0
85	OHX	1	3488	7/7	0.98	0.11	-4.49	98,98,98,98	0
85	OHX	5	3455	7/7	0.99	0.08	-4.50	65,65,65,65	0
85	OHX	2	1982	7/7	0.91	0.18	-4.51	193,193,193,193	0
85	OHX	1	3428	7/7	0.99	0.10	-4.54	68,68,68,68	0
85	OHX	1	3454	7/7	0.97	0.12	-4.58	99,99,99,99	0
85	OHX	1	3447	7/7	0.99	0.09	-4.61	87,87,87,87	0
86	MG	5	4071	1/1	1.00	0.07	-4.64	53,53,53,53	0
85	OHX	2	1913	7/7	0.98	0.09	-4.65	106,106,106,106	0
85	OHX	1	3425	7/7	0.99	0.11	-4.69	77,77,77,77	0
85	OHX	1	3413	7/7	1.00	0.04	-4.71	66,66,66,66	0
85	OHX	5	3472	7/7	0.98	0.09	-4.72	99,99,99,99	0
85	OHX	6	1911	7/7	0.99	0.08	-4.74	78,78,78,78	0
85	OHX	1	3442	7/7	0.99	0.10	-4.79	85,85,85,85	0
85	OHX	5	3428	7/7	0.99	0.08	-4.79	60,60,60,60	0
85	OHX	5	3418	7/7	0.99	0.08	-4.80	69,69,69,69	0
85	OHX	5	3498	7/7	0.97	0.12	-4.82	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3468	7/7	0.98	0.10	-4.83	100,100,100,100	0
85	OHX	6	1933	7/7	0.98	0.10	-4.87	112,112,112,112	0
85	OHX	5	3406	7/7	0.99	0.07	-4.88	55,55,55,55	0
85	OHX	5	3461	7/7	0.98	0.10	-4.92	74,74,74,74	0
85	OHX	2	1948	7/7	0.97	0.09	-4.97	124,124,124,124	0
85	OHX	6	1941	7/7	0.99	0.13	-5.06	111,111,111,111	0
85	OHX	1	3450	7/7	0.99	0.07	-5.08	90,90,90,90	0
85	OHX	5	3462	7/7	0.99	0.07	-5.12	73,73,73,73	0
85	OHX	5	3425	7/7	0.99	0.08	-5.13	71,71,71,71	0
85	OHX	1	3417	7/7	0.99	0.07	-5.16	65,65,65,65	0
86	MG	1	4007	1/1	0.98	0.09	-5.30	51,51,51,51	0
85	OHX	1	3437	7/7	0.99	0.07	-5.34	67,67,67,67	0
85	OHX	5	3441	7/7	0.99	0.06	-5.36	87,87,87,87	0
85	OHX	1	3489	7/7	0.96	0.10	-5.65	109,109,109,109	0
85	OHX	1	3438	7/7	0.99	0.07	-5.69	76,76,76,76	0
85	OHX	1	3451	7/7	0.98	0.09	-5.70	99,99,99,99	0
85	OHX	5	3456	7/7	0.98	0.08	-5.72	91,91,91,91	0
85	OHX	2	1944	7/7	0.97	0.11	-5.76	142,142,142,142	0
85	OHX	5	3538	7/7	0.98	0.10	-5.97	108,108,108,108	0
85	OHX	5	3479	7/7	0.99	0.08	-6.06	83,83,83,83	0
85	OHX	2	1904	7/7	0.98	0.08	-6.07	89,89,89,89	0
85	OHX	1	3431	7/7	0.99	0.08	-6.23	70,70,70,70	0
85	OHX	2	1902	7/7	0.99	0.09	-6.29	86,86,86,86	0
85	OHX	6	1931	7/7	0.96	0.12	-6.41	109,109,109,109	0
85	OHX	6	1915	7/7	0.99	0.08	-6.44	84,84,84,84	0
85	OHX	2	1920	7/7	0.98	0.09	-6.49	101,101,101,101	0
85	OHX	1	3440	7/7	0.99	0.06	-6.63	68,68,68,68	0
85	OHX	1	3434	7/7	0.99	0.06	-7.24	82,82,82,82	0
85	OHX	6	1919	7/7	0.99	0.08	-7.31	108,108,108,108	0
85	OHX	6	1927	7/7	0.97	0.09	-7.34	128,128,128,128	0
85	OHX	5	3437	7/7	0.99	0.08	-7.51	74,74,74,74	0
85	OHX	5	3492	7/7	0.99	0.05	-7.53	73,73,73,73	0
85	OHX	5	3529	7/7	0.98	0.10	-7.61	102,102,102,102	0
85	OHX	6	1914	7/7	0.98	0.08	-7.71	83,83,83,83	0
85	OHX	5	3427	7/7	0.99	0.06	-7.82	69,69,69,69	0
85	OHX	5	3431	7/7	0.99	0.06	-7.83	73,73,73,73	0
85	OHX	2	1924	7/7	0.98	0.11	-7.97	117,117,117,117	0
85	OHX	5	3466	7/7	0.98	0.13	-8.00	84,84,84,84	0
85	OHX	5	3432	7/7	0.99	0.08	-8.77	67,67,67,67	0
85	OHX	6	1958	7/7	0.98	0.12	-9.98	120,120,120,120	0
85	OHX	5	3465	7/7	0.98	0.10	-10.22	90,90,90,90	0
85	OHX	7	202	7/7	0.98	0.10	-11.28	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3420	7/7	0.99	0.07	-12.52	63,63,63,63	0
85	OHX	6	1916	7/7	0.99	0.07	-14.76	88,88,88,88	0
86	MG	1	3932	1/1	0.68	0.19	-	78,78,78,78	0
85	OHX	1	3728	7/7	0.96	0.36	-	111,111,111,111	0
85	OHX	8	210	7/7	0.97	0.11	-	139,139,139,139	0
85	OHX	5	3743	7/7	0.93	0.20	-	129,129,129,129	0
86	MG	4	228	1/1	0.87	0.26	-	36,36,36,36	0
85	OHX	1	3596	7/7	0.93	0.23	-	120,120,120,120	0
86	MG	1	4097	1/1	-0.36	2.34	-	70,70,70,70	0
85	OHX	6	2041	7/7	0.94	0.34	-	153,153,153,153	0
86	MG	6	2065	1/1	0.84	0.67	-	60,60,60,60	0
86	MG	5	4034	1/1	0.85	0.26	-	51,51,51,51	0
86	MG	1	4077	1/1	0.75	0.22	-	88,88,88,88	0
86	MG	5	3855	1/1	0.95	0.38	-	28,28,28,28	0
86	MG	5	4093	1/1	0.66	0.41	-	49,49,49,49	0
86	MG	5	3955	1/1	0.83	0.24	-	46,46,46,46	0
86	MG	5	3954	1/1	0.90	0.20	-	46,46,46,46	0
86	MG	c8	202	1/1	0.67	0.31	-	94,94,94,94	0
86	MG	5	4161	1/1	0.94	0.19	-	113,113,113,113	0
86	MG	1	4117	1/1	0.97	0.43	-	36,36,36,36	0
86	MG	5	4039	1/1	0.49	0.39	-	52,52,52,52	0
86	MG	6	2175	1/1	0.65	0.39	-	84,84,84,84	0
86	MG	3	214	1/1	0.90	0.68	-	68,68,68,68	0
85	OHX	1	3588	7/7	0.97	0.25	-	135,135,135,135	0
85	OHX	5	3641	7/7	0.98	0.29	-	119,119,119,119	0
85	OHX	1	3408	7/7	0.99	0.09	-	50,50,50,50	0
86	MG	1	3966	1/1	0.87	0.51	-	64,64,64,64	0
85	OHX	1	3582	7/7	0.99	0.21	-	101,101,101,101	0
86	MG	5	3868	1/1	0.97	0.49	-	31,31,31,31	0
86	MG	1	3800	1/1	0.93	0.59	-	51,51,51,51	0
86	MG	2	2125	1/1	0.76	0.23	-	123,123,123,123	0
86	MG	o2	202	1/1	0.93	0.28	-	38,38,38,38	0
85	OHX	n5	201	7/7	0.84	0.28	-	193,193,193,193	0
86	MG	3	201	1/1	0.96	0.51	-	33,33,33,33	0
85	OHX	1	3650	7/7	0.94	0.20	-	158,158,158,158	0
85	OHX	1	3467	7/7	0.98	0.09	-	87,87,87,87	0
86	MG	Q2	504	1/1	0.95	0.31	-	52,52,52,52	0
86	MG	5	3916	1/1	0.85	0.91	-	52,52,52,52	0
85	OHX	6	2020	7/7	0.95	0.30	-	146,146,146,146	0
86	MG	1	4065	1/1	0.64	0.44	-	47,47,47,47	0
86	MG	1	3841	1/1	0.65	0.45	-	42,42,42,42	0
86	MG	1	3972	1/1	0.69	0.35	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	7	215	1/1	0.93	0.39	-	61,61,61,61	0
85	OHX	5	3684	7/7	0.94	0.25	-	150,150,150,150	0
86	MG	5	3964	1/1	0.69	0.33	-	57,57,57,57	0
86	MG	1	3770	1/1	0.97	0.43	-	36,36,36,36	0
86	MG	6	2122	1/1	0.70	0.52	-	105,105,105,105	0
86	MG	1	4000	1/1	0.94	0.30	-	58,58,58,58	0
85	OHX	5	3717	7/7	0.94	0.28	-	143,143,143,143	0
86	MG	4	229	1/1	0.87	0.45	-	51,51,51,51	0
86	MG	5	4019	1/1	0.77	0.25	-	68,68,68,68	0
86	MG	5	3820	1/1	0.93	0.34	-	28,28,28,28	0
85	OHX	3	202	7/7	0.98	0.09	-	90,90,90,90	0
86	MG	2	2129	1/1	0.94	0.76	-	80,80,80,80	0
85	OHX	2	1951	7/7	0.97	0.14	-	148,148,148,148	0
86	MG	8	223	1/1	0.86	0.46	-	50,50,50,50	0
85	OHX	6	2017	7/7	0.96	0.30	-	122,122,122,122	0
86	MG	1	4026	1/1	0.79	0.40	-	69,69,69,69	0
85	OHX	7	210	7/7	0.91	0.30	-	140,140,140,140	0
85	OHX	1	3700	7/7	0.95	0.22	-	136,136,136,136	0
86	MG	1	3874	1/1	0.85	0.37	-	29,29,29,29	0
86	MG	6	2123	1/1	0.82	0.58	-	83,83,83,83	0
86	MG	4	224	1/1	0.77	0.34	-	50,50,50,50	0
86	MG	1	4102	1/1	0.60	0.49	-	77,77,77,77	0
85	OHX	2	2006	7/7	0.96	0.34	-	135,135,135,135	0
86	MG	1	3979	1/1	0.94	0.26	-	43,43,43,43	0
86	MG	5	3945	1/1	0.93	0.23	-	32,32,32,32	0
86	MG	1	3915	1/1	0.93	0.25	-	45,45,45,45	0
85	OHX	5	3640	7/7	0.95	0.24	-	123,123,123,123	0
86	MG	6	2139	1/1	0.97	0.31	-	112,112,112,112	0
86	MG	m1	202	1/1	0.88	0.23	-	59,59,59,59	0
86	MG	1	3984	1/1	0.45	0.60	-	75,75,75,75	0
86	MG	5	4160	1/1	0.96	0.29	-	70,70,70,70	0
85	OHX	1	3726	7/7	0.87	0.35	-	140,140,140,140	0
86	MG	6	2110	1/1	0.76	0.21	-	85,85,85,85	0
86	MG	5	4149	1/1	0.49	0.72	-	51,51,51,51	0
86	MG	5	3773	1/1	0.87	0.83	-	47,47,47,47	0
86	MG	6	2120	1/1	0.62	0.69	-	62,62,62,62	0
86	MG	1	3785	1/1	0.93	0.33	-	46,46,46,46	0
86	MG	2	2059	1/1	0.72	0.63	-	70,70,70,70	0
85	OHX	6	2047	7/7	0.94	0.32	-	168,168,168,168	0
86	MG	1	4080	1/1	0.80	0.30	-	46,46,46,46	0
86	MG	1	4028	1/1	0.97	0.16	-	87,87,87,87	0
85	OHX	5	3458	7/7	0.98	0.10	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	4127	1/1	0.68	0.36	-	113,113,113,113	0
85	OHX	1	3439	7/7	0.99	0.10	-	75,75,75,75	0
86	MG	5	4126	1/1	0.97	0.45	-	49,49,49,49	0
86	MG	1	3854	1/1	0.96	0.37	-	43,43,43,43	0
86	MG	2	2107	1/1	0.90	0.72	-	65,65,65,65	0
86	MG	1	4124	1/1	0.85	0.35	-	59,59,59,59	0
85	OHX	5	3542	7/7	0.96	0.12	-	127,127,127,127	0
86	MG	5	4077	1/1	0.79	0.20	-	79,79,79,79	0
86	MG	5	3812	1/1	0.42	0.51	-	57,57,57,57	0
86	MG	5	3794	1/1	0.87	0.31	-	56,56,56,56	0
85	OHX	1	3512	7/7	0.97	0.15	-	100,100,100,100	0
86	MG	6	2127	1/1	0.57	0.57	-	57,57,57,57	0
86	MG	6	2153	1/1	0.98	0.20	-	97,97,97,97	0
86	MG	1	3748	1/1	0.86	0.34	-	40,40,40,40	0
86	MG	1	3879	1/1	0.92	0.50	-	30,30,30,30	0
85	OHX	1	3597	7/7	0.94	0.14	-	144,144,144,144	0
85	OHX	5	3722	7/7	0.95	0.30	-	131,131,131,131	0
86	MG	5	3848	1/1	0.97	0.11	-	38,38,38,38	0
86	MG	5	4015	1/1	0.73	0.22	-	51,51,51,51	0
86	MG	5	4012	1/1	0.86	0.23	-	69,69,69,69	0
86	MG	1	3924	1/1	0.92	0.17	-	79,79,79,79	0
86	MG	5	3809	1/1	0.92	0.53	-	38,38,38,38	0
86	MG	5	3951	1/1	0.95	0.14	-	41,41,41,41	0
86	MG	5	3857	1/1	0.85	0.57	-	37,37,37,37	0
85	OHX	1	3561	7/7	0.98	0.20	-	97,97,97,97	0
86	MG	L5	301	1/1	0.07	0.53	-	110,110,110,110	0
85	OHX	6	1957	7/7	0.95	0.19	-	104,104,104,104	0
85	OHX	6	1925	7/7	0.97	0.11	-	105,105,105,105	0
86	MG	5	3973	1/1	0.81	0.26	-	65,65,65,65	0
86	MG	1	3962	1/1	0.98	0.13	-	46,46,46,46	0
85	OHX	2	1997	7/7	0.95	0.26	-	138,138,138,138	0
86	MG	5	4043	1/1	0.95	0.21	-	40,40,40,40	0
86	MG	1	4005	1/1	0.74	0.40	-	69,69,69,69	0
86	MG	6	2137	1/1	0.92	0.48	-	66,66,66,66	0
86	MG	1	4082	1/1	0.52	0.63	-	53,53,53,53	0
86	MG	1	4046	1/1	0.89	0.57	-	55,55,55,55	0
86	MG	1	4048	1/1	0.62	0.49	-	67,67,67,67	0
85	OHX	5	3613	7/7	0.95	0.30	-	113,113,113,113	0
86	MG	5	3807	1/1	0.63	0.32	-	102,102,102,102	0
85	OHX	6	1934	7/7	0.98	0.14	-	101,101,101,101	0
86	MG	1	4038	1/1	0.91	0.26	-	60,60,60,60	0
86	MG	1	3867	1/1	0.84	0.28	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	2	1934	7/7	0.96	0.15	-	124,124,124,124	0
86	MG	1	3850	1/1	0.81	0.45	-	35,35,35,35	0
86	MG	5	3960	1/1	0.90	0.35	-	45,45,45,45	0
86	MG	1	3840	1/1	0.88	0.38	-	34,34,34,34	0
86	MG	8	221	1/1	0.96	0.13	-	56,56,56,56	0
86	MG	2	2105	1/1	0.85	0.36	-	90,90,90,90	0
86	MG	1	4083	1/1	0.83	0.22	-	46,46,46,46	0
86	MG	1	4110	1/1	0.86	0.24	-	32,32,32,32	0
86	MG	1	3789	1/1	0.93	0.28	-	30,30,30,30	0
86	MG	n9	102	1/1	0.76	0.39	-	34,34,34,34	0
86	MG	5	4153	1/1	0.68	0.32	-	38,38,38,38	0
86	MG	5	3823	1/1	0.89	0.48	-	50,50,50,50	0
86	MG	5	3822	1/1	0.94	0.30	-	50,50,50,50	0
86	MG	5	3888	1/1	0.92	0.53	-	43,43,43,43	0
85	OHX	5	3588	7/7	0.97	0.13	-	127,127,127,127	0
86	MG	6	2180	1/1	0.52	0.39	-	88,88,88,88	0
85	OHX	5	3628	7/7	0.98	0.18	-	139,139,139,139	0
85	OHX	2	1939	7/7	0.97	0.11	-	123,123,123,123	0
86	MG	5	4013	1/1	0.90	0.24	-	48,48,48,48	0
85	OHX	1	3449	7/7	0.98	0.08	-	82,82,82,82	0
86	MG	L2	302	1/1	0.05	0.49	-	73,73,73,73	0
86	MG	5	3849	1/1	0.85	0.69	-	62,62,62,62	0
86	MG	5	3754	1/1	0.97	0.28	-	47,47,47,47	0
86	MG	6	2083	1/1	0.94	0.46	-	43,43,43,43	0
86	MG	6	2071	1/1	0.91	0.30	-	73,73,73,73	0
86	MG	5	3840	1/1	0.73	0.53	-	34,34,34,34	0
86	MG	5	3755	1/1	0.87	0.16	-	52,52,52,52	0
86	MG	M7	206	1/1	0.77	0.53	-	37,37,37,37	0
85	OHX	L3	401	7/7	0.98	0.29	-	117,117,117,117	0
86	MG	1	4054	1/1	0.50	0.66	-	86,86,86,86	0
86	MG	4	216	1/1	0.83	0.55	-	55,55,55,55	0
86	MG	5	3875	1/1	0.94	0.33	-	20,20,20,20	0
85	OHX	2	1926	7/7	0.96	0.14	-	119,119,119,119	0
86	MG	5	3817	1/1	0.78	0.29	-	66,66,66,66	0
85	OHX	1	3712	7/7	0.93	0.28	-	170,170,170,170	0
86	MG	5	4014	1/1	0.68	0.33	-	66,66,66,66	0
86	MG	5	3990	1/1	0.92	0.14	-	36,36,36,36	0
86	MG	5	3819	1/1	0.91	0.16	-	49,49,49,49	0
86	MG	D9	103	1/1	0.89	0.33	-	88,88,88,88	0
86	MG	5	3910	1/1	0.97	0.53	-	40,40,40,40	0
86	MG	5	3975	1/1	0.87	0.20	-	40,40,40,40	0
86	MG	1	3911	1/1	0.97	0.22	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3909	1/1	0.89	0.52	-	36,36,36,36	0
86	MG	1	3761	1/1	0.71	0.38	-	47,47,47,47	0
85	OHX	5	3633	7/7	0.94	0.28	-	141,141,141,141	0
86	MG	1	3831	1/1	0.89	0.50	-	30,30,30,30	0
85	OHX	6	1985	7/7	0.95	0.21	-	143,143,143,143	0
85	OHX	1	3679	7/7	0.94	0.40	-	122,122,122,122	0
86	MG	MG	2222	1/1	0.36	1.31	-	136,136,136,136	0
86	MG	1	3997	1/1	0.85	0.35	-	58,58,58,58	0
85	OHX	6	1968	7/7	0.97	0.14	-	123,123,123,123	0
86	MG	1	3763	1/1	0.96	0.59	-	44,44,44,44	0
85	OHX	1	3709	7/7	0.94	0.41	-	166,166,166,166	0
85	OHX	2	1954	7/7	0.95	0.18	-	115,115,115,115	0
86	MG	5	3898	1/1	0.93	0.76	-	30,30,30,30	0
86	MG	1	3953	1/1	0.89	0.22	-	57,57,57,57	0
86	MG	6	2062	1/1	0.95	0.58	-	46,46,46,46	0
86	MG	1	4023	1/1	0.91	0.35	-	47,47,47,47	0
86	MG	1	3838	1/1	0.96	0.20	-	38,38,38,38	0
85	OHX	2	1912	7/7	0.98	0.09	-	110,110,110,110	0
86	MG	6	2063	1/1	0.96	0.39	-	42,42,42,42	0
86	MG	5	4086	1/1	0.86	0.20	-	92,92,92,92	0
86	MG	1	3869	1/1	0.96	0.41	-	31,31,31,31	0
86	MG	6	2074	1/1	0.60	0.75	-	76,76,76,76	0
86	MG	5	3932	1/1	0.82	0.22	-	42,42,42,42	0
86	MG	5	3799	1/1	0.83	0.39	-	43,43,43,43	0
86	MG	1	3767	1/1	0.95	0.25	-	61,61,61,61	0
86	MG	6	2134	1/1	0.86	0.55	-	56,56,56,56	0
86	MG	6	2111	1/1	0.96	0.38	-	86,86,86,86	0
85	OHX	5	3549	7/7	0.97	0.24	-	109,109,109,109	0
86	MG	2	2049	1/1	0.84	0.53	-	58,58,58,58	0
86	MG	1	3999	1/1	0.87	0.25	-	66,66,66,66	0
86	MG	5	4021	1/1	0.90	0.36	-	54,54,54,54	0
86	MG	1	3842	1/1	0.94	0.41	-	33,33,33,33	0
86	MG	6	2100	1/1	0.83	0.81	-	42,42,42,42	0
86	MG	1	3944	1/1	0.76	0.31	-	59,59,59,59	0
86	MG	5	3913	1/1	0.97	0.33	-	27,27,27,27	0
86	MG	2	2057	1/1	0.98	0.46	-	57,57,57,57	0
85	OHX	2	2001	7/7	0.96	0.24	-	141,141,141,141	0
86	MG	1	4076	1/1	0.67	0.50	-	45,45,45,45	0
86	MG	1	3967	1/1	0.89	0.47	-	42,42,42,42	0
86	MG	5	3797	1/1	0.80	0.59	-	52,52,52,52	0
85	OHX	2	2021	7/7	0.94	0.19	-	133,133,133,133	0
85	OHX	1	3733	7/7	0.96	0.42	-	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2182	1/1	0.84	0.37	-	76,76,76,76	0
85	OHX	2	1979	7/7	0.95	0.15	-	156,156,156,156	0
86	MG	1	3969	1/1	0.86	0.28	-	35,35,35,35	0
86	MG	5	3977	1/1	0.89	0.29	-	45,45,45,45	0
86	MG	1	4075	1/1	0.98	0.17	-	54,54,54,54	0
86	MG	5	4060	1/1	0.77	0.14	-	44,44,44,44	0
85	OHX	1	3559	7/7	0.96	0.19	-	143,143,143,143	0
86	MG	5	4097	1/1	0.64	0.67	-	75,75,75,75	0
86	MG	5	4095	1/1	0.77	0.29	-	59,59,59,59	0
86	MG	1	3893	1/1	0.94	0.50	-	52,52,52,52	0
85	OHX	5	3669	7/7	0.87	0.28	-	192,192,192,192	0
86	MG	5	3864	1/1	0.88	0.22	-	34,34,34,34	0
86	MG	6	2108	1/1	0.83	0.64	-	77,77,77,77	0
85	OHX	m1	201	7/7	0.95	0.25	-	135,135,135,135	0
86	MG	2	2118	1/1	0.89	0.57	-	51,51,51,51	0
86	MG	6	2166	1/1	0.71	0.32	-	72,72,72,72	0
85	OHX	1	3735	7/7	0.94	0.42	-	153,153,153,153	0
86	MG	1	3794	1/1	0.96	0.28	-	29,29,29,29	0
86	MG	5	3981	1/1	0.93	0.72	-	58,58,58,58	0
86	MG	5	4148	1/1	0.93	0.21	-	52,52,52,52	0
85	OHX	1	3496	7/7	0.98	0.11	-	108,108,108,108	0
86	MG	2	2092	1/1	0.83	0.75	-	98,98,98,98	0
86	MG	5	4025	1/1	0.42	0.49	-	56,56,56,56	0
86	MG	5	4102	1/1	0.83	0.45	-	42,42,42,42	0
85	OHX	1	3608	7/7	0.94	0.26	-	135,135,135,135	0
85	OHX	6	2048	7/7	0.90	0.31	-	171,171,171,171	0
86	MG	6	2106	1/1	0.77	0.46	-	87,87,87,87	0
85	OHX	2	1929	7/7	0.98	0.20	-	116,116,116,116	0
86	MG	5	3834	1/1	0.95	0.19	-	39,39,39,39	0
86	MG	5	3912	1/1	0.94	1.00	-	43,43,43,43	0
85	OHX	2	2040	7/7	0.97	0.22	-	147,147,147,147	0
86	MG	1	3745	1/1	0.89	0.59	-	32,32,32,32	0
86	MG	5	3778	1/1	0.88	0.53	-	53,53,53,53	0
85	OHX	5	3730	7/7	0.84	0.35	-	158,158,158,158	0
86	MG	5	3853	1/1	0.95	0.35	-	43,43,43,43	0
86	MG	1	4018	1/1	0.70	0.40	-	40,40,40,40	0
85	OHX	1	3599	7/7	0.92	0.42	-	126,126,126,126	0
86	MG	1	3975	1/1	0.65	0.42	-	58,58,58,58	0
86	MG	2	2046	1/1	0.84	0.81	-	84,84,84,84	0
86	MG	5	4139	1/1	0.76	0.40	-	52,52,52,52	0
85	OHX	6	2042	7/7	0.94	0.32	-	139,139,139,139	0
85	OHX	5	3679	7/7	0.96	0.39	-	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3725	7/7	0.90	0.38	-	178,178,178,178	0
86	MG	1	4096	1/1	0.94	0.12	-	56,56,56,56	0
86	MG	3	218	1/1	0.87	0.51	-	81,81,81,81	0
86	MG	2	2077	1/1	0.86	0.55	-	71,71,71,71	0
86	MG	5	3867	1/1	0.93	0.21	-	45,45,45,45	0
86	MG	5	4130	1/1	0.88	0.31	-	46,46,46,46	0
86	MG	1	3922	1/1	0.95	0.48	-	55,55,55,55	0
85	OHX	2	2038	7/7	0.96	0.40	-	143,143,143,143	0
85	OHX	c8	201	7/7	0.98	0.10	-	132,132,132,132	0
85	OHX	5	3423	7/7	0.99	0.08	-	67,67,67,67	0
85	OHX	l5	304	7/7	0.87	0.43	-	134,134,134,134	0
85	OHX	5	3627	7/7	0.96	0.24	-	127,127,127,127	0
86	MG	4	218	1/1	0.59	0.63	-	49,49,49,49	0
85	OHX	2	1972	7/7	0.94	0.12	-	151,151,151,151	0
86	MG	1	4081	1/1	0.95	0.42	-	53,53,53,53	0
85	OHX	1	3600	7/7	0.96	0.28	-	118,118,118,118	0
85	OHX	1	3533	7/7	0.95	0.09	-	155,155,155,155	0
86	MG	5	4040	1/1	0.93	0.23	-	46,46,46,46	0
86	MG	5	4120	1/1	0.68	0.29	-	52,52,52,52	0
86	MG	MG	2217	1/1	0.48	0.39	-	77,77,77,77	0
86	MG	6	2185	1/1	0.78	0.36	-	71,71,71,71	0
86	MG	1	4009	1/1	0.87	0.26	-	65,65,65,65	0
86	MG	6	2158	1/1	0.69	0.42	-	46,46,46,46	0
86	MG	6	2160	1/1	0.80	0.24	-	71,71,71,71	0
86	MG	5	4081	1/1	0.89	0.24	-	49,49,49,49	0
85	OHX	1	3702	7/7	0.94	0.29	-	157,157,157,157	0
86	MG	2	2099	1/1	0.77	0.72	-	62,62,62,62	0
85	OHX	5	3600	7/7	0.95	0.23	-	147,147,147,147	0
86	MG	1	3832	1/1	0.95	0.30	-	40,40,40,40	0
85	OHX	1	3715	7/7	0.90	0.38	-	147,147,147,147	0
86	MG	5	3890	1/1	0.89	0.58	-	49,49,49,49	0
86	MG	1	3985	1/1	0.81	0.74	-	61,61,61,61	0
86	MG	5	4084	1/1	0.94	0.12	-	143,143,143,143	0
86	MG	1	4015	1/1	0.91	0.24	-	41,41,41,41	0
86	MG	1	3904	1/1	0.92	0.36	-	51,51,51,51	0
86	MG	5	4070	1/1	0.88	0.26	-	68,68,68,68	0
85	OHX	5	3666	7/7	0.97	0.42	-	104,104,104,104	0
86	MG	1	4042	1/1	0.76	0.18	-	79,79,79,79	0
85	OHX	5	3575	7/7	0.96	0.25	-	119,119,119,119	0
86	MG	3	213	1/1	0.85	0.56	-	44,44,44,44	0
86	MG	2	2117	1/1	0.50	0.31	-	68,68,68,68	0
85	OHX	1	3547	7/7	0.97	0.24	-	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3861	1/1	0.72	0.14	-	65,65,65,65	0
86	MG	6	2183	1/1	0.82	0.76	-	64,64,64,64	0
85	OHX	1	3606	7/7	0.97	0.26	-	106,106,106,106	0
86	MG	5	3924	1/1	0.71	0.37	-	49,49,49,49	0
86	MG	6	2098	1/1	0.62	0.41	-	69,69,69,69	0
85	OHX	1	3615	7/7	0.99	0.17	-	119,119,119,119	0
86	MG	1	4112	1/1	0.83	0.24	-	54,54,54,54	0
85	OHX	5	3674	7/7	0.86	0.20	-	178,178,178,178	0
85	OHX	5	3683	7/7	0.94	0.40	-	133,133,133,133	0
86	MG	2	2130	1/1	0.76	0.71	-	70,70,70,70	0
86	MG	2	2123	1/1	0.40	0.36	-	97,97,97,97	0
85	OHX	1	3523	7/7	0.99	0.21	-	117,117,117,117	0
85	OHX	5	3685	7/7	0.94	0.38	-	133,133,133,133	0
85	OHX	2	1986	7/7	0.96	0.32	-	131,131,131,131	0
86	MG	1	3805	1/1	0.40	0.44	-	97,97,97,97	0
86	MG	5	4037	1/1	0.87	0.38	-	39,39,39,39	0
86	MG	1	3980	1/1	0.84	0.27	-	58,58,58,58	0
85	OHX	5	3724	7/7	0.94	0.43	-	175,175,175,175	0
86	MG	N3	202	1/1	0.65	0.21	-	59,59,59,59	0
86	MG	1	3863	1/1	0.84	0.26	-	30,30,30,30	0
86	MG	1	4095	1/1	0.18	0.47	-	70,70,70,70	0
85	OHX	1	3701	7/7	0.94	0.37	-	144,144,144,144	0
86	MG	5	3882	1/1	0.85	0.27	-	44,44,44,44	0
86	MG	7	222	1/1	0.93	0.21	-	48,48,48,48	0
85	OHX	1	3441	7/7	0.97	0.11	-	87,87,87,87	0
86	MG	5	3824	1/1	0.85	0.32	-	51,51,51,51	0
86	MG	1	3846	1/1	0.96	0.92	-	31,31,31,31	0
86	MG	1	3991	1/1	0.81	0.30	-	48,48,48,48	0
85	OHX	5	3745	7/7	0.95	0.37	-	139,139,139,139	0
86	MG	M7	203	1/1	0.83	0.73	-	65,65,65,65	0
86	MG	1	4123	1/1	0.71	0.35	-	47,47,47,47	0
86	MG	1	4122	1/1	0.93	0.32	-	46,46,46,46	0
86	MG	1	4121	1/1	0.60	0.71	-	56,56,56,56	0
85	OHX	2	1960	7/7	0.96	0.10	-	149,149,149,149	0
86	MG	1	3856	1/1	0.96	0.47	-	32,32,32,32	0
86	MG	1	3989	1/1	0.59	0.37	-	47,47,47,47	0
86	MG	1	3772	1/1	0.93	0.24	-	32,32,32,32	0
86	MG	6	2131	1/1	0.70	0.20	-	102,102,102,102	0
86	MG	1	3933	1/1	0.90	0.20	-	43,43,43,43	0
85	OHX	8	216	7/7	0.94	0.31	-	134,134,134,134	0
86	MG	2	2087	1/1	0.93	0.82	-	95,95,95,95	0
86	MG	5	3779	1/1	0.86	0.23	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2141	1/1	0.82	0.81	-	59,59,59,59	0
86	MG	5	3750	1/1	0.77	0.36	-	34,34,34,34	0
85	OHX	6	1905	7/7	0.98	0.14	-	80,80,80,80	0
86	MG	5	3836	1/1	0.92	0.36	-	40,40,40,40	0
85	OHX	5	3725	7/7	0.93	0.39	-	125,125,125,125	0
85	OHX	2	2023	7/7	0.90	0.40	-	166,166,166,166	0
86	MG	5	4157	1/1	0.85	0.26	-	48,48,48,48	0
85	OHX	1	3551	7/7	0.96	0.22	-	128,128,128,128	0
86	MG	5	3831	1/1	0.89	0.50	-	32,32,32,32	0
86	MG	1	3803	1/1	0.92	0.45	-	47,47,47,47	0
86	MG	6	2112	1/1	0.88	0.53	-	71,71,71,71	0
85	OHX	8	207	7/7	0.96	0.12	-	114,114,114,114	0
86	MG	1	4126	1/1	0.56	1.03	-	87,87,87,87	0
86	MG	1	3978	1/1	0.68	0.65	-	51,51,51,51	0
86	MG	2	2101	1/1	0.67	0.84	-	126,126,126,126	0
86	MG	6	2133	1/1	0.91	0.66	-	84,84,84,84	0
86	MG	1	3760	1/1	0.93	0.36	-	47,47,47,47	0
86	MG	6	2090	1/1	0.97	0.46	-	32,32,32,32	0
86	MG	5	4159	1/1	0.95	0.45	-	52,52,52,52	0
86	MG	1	3970	1/1	0.94	0.24	-	44,44,44,44	0
86	MG	1	4059	1/1	0.94	0.22	-	62,62,62,62	0
86	MG	6	2151	1/1	0.70	0.25	-	140,140,140,140	0
86	MG	1	3769	1/1	0.88	0.77	-	56,56,56,56	0
86	MG	1	3820	1/1	0.94	1.07	-	54,54,54,54	0
86	MG	1	3941	1/1	0.96	0.51	-	34,34,34,34	0
85	OHX	5	3454	7/7	0.98	0.07	-	98,98,98,98	0
85	OHX	1	3632	7/7	0.97	0.24	-	136,136,136,136	0
86	MG	1	4116	1/1	0.71	0.46	-	67,67,67,67	0
85	OHX	m4	201	7/7	0.90	0.41	-	181,181,181,181	0
85	OHX	5	3607	7/7	0.92	0.18	-	144,144,144,144	0
86	MG	6	2184	1/1	0.83	0.45	-	58,58,58,58	0
86	MG	m4	202	1/1	0.85	0.24	-	42,42,42,42	0
86	MG	1	4047	1/1	0.87	0.18	-	75,75,75,75	0
86	MG	1	3956	1/1	0.89	0.46	-	81,81,81,81	0
86	MG	5	4064	1/1	0.90	0.26	-	47,47,47,47	0
85	OHX	5	3519	7/7	0.97	0.16	-	105,105,105,105	0
86	MG	n0	201	1/1	0.94	0.21	-	38,38,38,38	0
86	MG	5	4111	1/1	0.73	0.35	-	42,42,42,42	0
86	MG	5	3891	1/1	0.97	0.45	-	31,31,31,31	0
86	MG	5	4009	1/1	0.83	0.20	-	49,49,49,49	0
86	MG	5	3838	1/1	0.83	0.29	-	35,35,35,35	0
85	OHX	6	2021	7/7	0.90	0.30	-	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3817	1/1	0.85	0.39	-	53,53,53,53	0
86	MG	5	4022	1/1	0.84	0.33	-	41,41,41,41	0
86	MG	5	3959	1/1	0.96	0.31	-	54,54,54,54	0
86	MG	5	3982	1/1	0.66	0.57	-	36,36,36,36	0
86	MG	1	4055	1/1	0.61	0.31	-	78,78,78,78	0
86	MG	7	214	1/1	0.71	0.46	-	27,27,27,27	0
85	OHX	6	1976	7/7	0.96	0.17	-	147,147,147,147	0
86	MG	4	222	1/1	0.82	0.36	-	43,43,43,43	0
86	MG	5	4098	1/1	0.87	0.69	-	54,54,54,54	0
85	OHX	5	3434	7/7	0.98	0.09	-	68,68,68,68	0
86	MG	1	3771	1/1	0.93	0.34	-	37,37,37,37	0
86	MG	q0	202	1/1	0.83	0.26	-	43,43,43,43	0
86	MG	2	2065	1/1	0.62	0.41	-	50,50,50,50	0
86	MG	5	3970	1/1	0.72	0.43	-	49,49,49,49	0
85	OHX	5	3570	7/7	0.97	0.17	-	104,104,104,104	0
86	MG	2	2124	1/1	0.18	0.84	-	113,113,113,113	0
86	MG	6	2093	1/1	0.93	0.48	-	42,42,42,42	0
86	MG	1	3988	1/1	0.76	0.48	-	58,58,58,58	0
86	MG	5	3854	1/1	0.93	0.45	-	25,25,25,25	0
86	MG	5	4152	1/1	0.80	0.32	-	48,48,48,48	0
85	OHX	2	1996	7/7	0.94	0.16	-	144,144,144,144	0
86	MG	1	3837	1/1	0.89	0.31	-	37,37,37,37	0
86	MG	1	4106	1/1	0.73	0.43	-	55,55,55,55	0
86	MG	1	4087	1/1	0.16	0.97	-	84,84,84,84	0
86	MG	2	2050	1/1	0.87	0.35	-	87,87,87,87	0
85	OHX	5	3632	7/7	0.97	0.32	-	132,132,132,132	0
86	MG	1	4025	1/1	0.79	0.18	-	55,55,55,55	0
85	OHX	6	2044	7/7	0.94	0.33	-	123,123,123,123	0
86	MG	5	3946	1/1	0.90	0.19	-	39,39,39,39	0
85	OHX	5	3589	7/7	0.97	0.20	-	115,115,115,115	0
85	OHX	14	402	7/7	0.93	0.47	-	134,134,134,134	0
86	MG	5	4156	1/1	0.92	0.25	-	55,55,55,55	0
86	MG	6	2144	1/1	0.90	0.34	-	75,75,75,75	0
86	MG	1	3775	1/1	0.80	0.44	-	39,39,39,39	0
86	MG	2	2128	1/1	0.52	0.70	-	56,56,56,56	0
85	OHX	8	217	7/7	0.97	0.38	-	113,113,113,113	0
86	MG	5	3771	1/1	0.84	0.39	-	50,50,50,50	0
85	OHX	5	3734	7/7	0.98	0.25	-	97,97,97,97	0
86	MG	6	2150	1/1	0.94	0.73	-	113,113,113,113	0
86	MG	7	221	1/1	0.81	0.57	-	51,51,51,51	0
85	OHX	1	3665	7/7	0.95	0.41	-	138,138,138,138	0
86	MG	1	3777	1/1	0.80	0.18	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3506	7/7	0.97	0.16	-	107,107,107,107	0
85	OHX	5	3598	7/7	0.95	0.32	-	130,130,130,130	0
86	MG	6	2146	1/1	0.72	0.50	-	55,55,55,55	0
86	MG	q1	101	1/1	0.86	0.45	-	52,52,52,52	0
86	MG	6	2155	1/1	0.93	0.52	-	108,108,108,108	0
86	MG	5	3935	1/1	0.92	0.32	-	37,37,37,37	0
86	MG	5	3917	1/1	0.90	0.48	-	41,41,41,41	0
86	MG	1	4035	1/1	0.93	0.16	-	49,49,49,49	0
86	MG	1	3876	1/1	0.92	0.23	-	48,48,48,48	0
86	MG	7	213	1/1	0.73	0.80	-	49,49,49,49	0
86	MG	5	3785	1/1	0.95	0.28	-	39,39,39,39	0
86	MG	1	3903	1/1	0.91	0.73	-	43,43,43,43	0
85	OHX	5	3551	7/7	0.96	0.18	-	117,117,117,117	0
86	MG	5	4127	1/1	0.98	0.17	-	61,61,61,61	0
86	MG	5	4045	1/1	0.83	0.27	-	42,42,42,42	0
85	OHX	1	3553	7/7	0.96	0.10	-	141,141,141,141	0
86	MG	1	4108	1/1	0.52	0.92	-	66,66,66,66	0
86	MG	6	2115	1/1	0.87	0.33	-	56,56,56,56	0
86	MG	1	4050	1/1	0.35	0.25	-	92,92,92,92	0
86	MG	1	4022	1/1	0.90	0.28	-	56,56,56,56	0
86	MG	6	2149	1/1	0.85	0.68	-	52,52,52,52	0
85	OHX	5	3521	7/7	0.98	0.09	-	119,119,119,119	0
85	OHX	5	3563	7/7	0.98	0.19	-	103,103,103,103	0
86	MG	5	4002	1/1	0.84	0.27	-	38,38,38,38	0
86	MG	5	3859	1/1	0.97	0.50	-	37,37,37,37	0
85	OHX	1	3629	7/7	0.95	0.19	-	144,144,144,144	0
85	OHX	2	1984	7/7	0.94	0.21	-	133,133,133,133	0
86	MG	1	3974	1/1	0.84	0.17	-	52,52,52,52	0
86	MG	2	2084	1/1	0.86	0.83	-	59,59,59,59	0
86	MG	6	2089	1/1	0.92	0.73	-	84,84,84,84	0
85	OHX	5	3653	7/7	0.97	0.35	-	126,126,126,126	0
85	OHX	6	1913	7/7	0.99	0.09	-	94,94,94,94	0
86	MG	5	4047	1/1	0.85	0.26	-	35,35,35,35	0
85	OHX	1	3667	7/7	0.93	0.29	-	154,154,154,154	0
86	MG	5	3944	1/1	0.91	0.26	-	39,39,39,39	0
85	OHX	2	1969	7/7	0.97	0.26	-	136,136,136,136	0
86	MG	5	4092	1/1	0.88	0.34	-	58,58,58,58	0
86	MG	1	3755	1/1	0.96	0.41	-	40,40,40,40	0
85	OHX	1	3550	7/7	0.97	0.21	-	119,119,119,119	0
85	OHX	1	3545	7/7	0.97	0.17	-	115,115,115,115	0
85	OHX	6	2014	7/7	0.97	0.34	-	119,119,119,119	0
85	OHX	5	3681	7/7	0.96	0.23	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	5	3576	7/7	0.97	0.28	-	117,117,117,117	0
85	OHX	1	3503	7/7	0.98	0.10	-	109,109,109,109	0
86	MG	2	2121	1/1	0.91	0.35	-	88,88,88,88	0
86	MG	5	4162	1/1	0.71	0.52	-	76,76,76,76	0
86	MG	2	2127	1/1	0.79	0.78	-	60,60,60,60	0
85	OHX	1	3477	7/7	0.98	0.12	-	95,95,95,95	0
86	MG	5	4011	1/1	0.90	0.38	-	42,42,42,42	0
86	MG	5	4061	1/1	0.97	0.30	-	62,62,62,62	0
86	MG	5	3991	1/1	0.87	0.25	-	47,47,47,47	0
86	MG	o3	202	1/1	0.89	0.47	-	40,40,40,40	0
86	MG	5	4101	1/1	0.73	0.73	-	34,34,34,34	0
86	MG	1	3759	1/1	0.67	0.53	-	47,47,47,47	0
86	MG	1	4078	1/1	0.94	0.17	-	84,84,84,84	0
86	MG	5	3877	1/1	0.96	0.46	-	36,36,36,36	0
86	MG	6	2068	1/1	0.79	0.38	-	45,45,45,45	0
86	MG	8	226	1/1	0.80	0.37	-	55,55,55,55	0
86	MG	1	3828	1/1	0.91	0.36	-	35,35,35,35	0
86	MG	2	2082	1/1	0.94	0.99	-	104,104,104,104	0
86	MG	1	3822	1/1	0.96	0.33	-	56,56,56,56	0
86	MG	1	3790	1/1	0.89	0.18	-	41,41,41,41	0
86	MG	1	4008	1/1	0.83	0.43	-	49,49,49,49	0
86	MG	5	4079	1/1	0.93	0.22	-	41,41,41,41	0
85	OHX	5	3675	7/7	0.92	0.25	-	149,149,149,149	0
85	OHX	5	3407	7/7	1.00	0.08	-	59,59,59,59	0
86	MG	1	3773	1/1	0.72	0.44	-	64,64,64,64	0
86	MG	2	2045	1/1	0.89	0.72	-	53,53,53,53	0
86	MG	5	3765	1/1	0.91	0.36	-	68,68,68,68	0
85	OHX	6	2006	7/7	0.95	0.26	-	141,141,141,141	0
86	MG	5	4020	1/1	0.91	0.24	-	62,62,62,62	0
85	OHX	1	3654	7/7	0.97	0.20	-	116,116,116,116	0
86	MG	5	4105	1/1	0.96	0.13	-	47,47,47,47	0
86	MG	C2	203	1/1	-0.21	1.11	-	132,132,132,132	0
86	MG	5	4123	1/1	0.84	0.32	-	49,49,49,49	0
85	OHX	5	3552	7/7	0.97	0.18	-	108,108,108,108	0
85	OHX	1	3498	7/7	0.99	0.15	-	94,94,94,94	0
86	MG	5	3881	1/1	0.60	0.38	-	49,49,49,49	0
86	MG	5	3825	1/1	0.94	0.46	-	30,30,30,30	0
86	MG	6	2173	1/1	0.74	0.47	-	58,58,58,58	0
86	MG	5	4085	1/1	0.90	0.13	-	36,36,36,36	0
85	OHX	1	3493	7/7	0.98	0.11	-	102,102,102,102	0
85	OHX	5	3470	7/7	0.99	0.08	-	87,87,87,87	0
86	MG	1	4045	1/1	0.55	0.36	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3949	1/1	0.86	0.40	-	41,41,41,41	0
86	MG	5	3783	1/1	0.88	0.37	-	57,57,57,57	0
86	MG	5	4057	1/1	0.87	0.14	-	115,115,115,115	0
85	OHX	5	3643	7/7	0.92	0.22	-	133,133,133,133	0
86	MG	1	3847	1/1	0.96	0.19	-	71,71,71,71	0
85	OHX	1	3436	7/7	0.99	0.07	-	83,83,83,83	0
86	MG	5	4088	1/1	0.98	0.19	-	35,35,35,35	0
86	MG	2	2052	1/1	0.86	0.40	-	64,64,64,64	0
86	MG	1	4090	1/1	0.09	0.73	-	129,129,129,129	0
86	MG	6	2159	1/1	0.90	0.26	-	81,81,81,81	0
86	MG	5	4035	1/1	0.58	0.60	-	66,66,66,66	0
86	MG	5	4112	1/1	0.90	0.10	-	103,103,103,103	0
86	MG	5	4168	1/1	0.95	0.62	-	38,38,38,38	0
86	MG	1	3821	1/1	0.96	0.40	-	33,33,33,33	0
86	MG	8	220	1/1	0.96	0.19	-	41,41,41,41	0
86	MG	5	4005	1/1	0.89	0.23	-	61,61,61,61	0
85	OHX	5	3599	7/7	0.95	0.24	-	123,123,123,123	0
86	MG	m6	201	1/1	0.84	0.28	-	40,40,40,40	0
86	MG	5	3897	1/1	0.97	0.69	-	25,25,25,25	0
85	OHX	5	3662	7/7	0.96	0.31	-	129,129,129,129	0
85	OHX	1	3511	7/7	0.96	0.12	-	122,122,122,122	0
86	MG	7	220	1/1	0.94	0.64	-	44,44,44,44	0
86	MG	1	3778	1/1	0.93	0.48	-	40,40,40,40	0
86	MG	O5	201	1/1	0.54	1.66	-	144,144,144,144	0
85	OHX	5	3723	7/7	0.96	0.34	-	128,128,128,128	0
86	MG	1	3925	1/1	0.65	0.46	-	73,73,73,73	0
86	MG	5	3871	1/1	0.88	0.65	-	35,35,35,35	0
86	MG	6	2179	1/1	0.70	0.81	-	55,55,55,55	0
85	OHX	1	3631	7/7	0.94	0.29	-	135,135,135,135	0
86	MG	8	228	1/1	0.90	0.37	-	44,44,44,44	0
86	MG	5	4118	1/1	0.91	0.34	-	52,52,52,52	0
85	OHX	6	1937	7/7	0.97	0.10	-	113,113,113,113	0
86	MG	5	3776	1/1	0.70	0.33	-	33,33,33,33	0
86	MG	5	4029	1/1	0.69	0.42	-	62,62,62,62	0
86	MG	1	4029	1/1	0.91	0.38	-	73,73,73,73	0
85	OHX	1	3565	7/7	0.93	0.26	-	138,138,138,138	0
86	MG	1	4074	1/1	0.87	0.22	-	48,48,48,48	0
85	OHX	6	2008	7/7	0.95	0.16	-	133,133,133,133	0
85	OHX	5	3735	7/7	0.96	0.27	-	158,158,158,158	0
85	OHX	5	3719	7/7	0.89	0.19	-	181,181,181,181	0
86	MG	1	3742	1/1	0.78	0.57	-	138,138,138,138	0
85	OHX	2	1990	7/7	0.96	0.20	-	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	6	1984	7/7	0.96	0.17	-	110,110,110,110	0
86	MG	1	3806	1/1	0.86	0.14	-	56,56,56,56	0
86	MG	1	3992	1/1	0.80	0.27	-	51,51,51,51	0
86	MG	3	215	1/1	0.95	0.29	-	39,39,39,39	0
86	MG	5	3758	1/1	0.95	0.31	-	37,37,37,37	0
86	MG	1	3894	1/1	0.90	0.32	-	42,42,42,42	0
85	OHX	2	1931	7/7	0.96	0.10	-	134,134,134,134	0
86	MG	5	3798	1/1	0.81	0.43	-	27,27,27,27	0
86	MG	1	4034	1/1	0.78	0.34	-	51,51,51,51	0
86	MG	5	4065	1/1	0.49	0.83	-	75,75,75,75	0
85	OHX	6	1948	7/7	0.96	0.11	-	131,131,131,131	0
85	OHX	6	1974	7/7	0.97	0.19	-	117,117,117,117	0
86	MG	5	3886	1/1	0.96	0.43	-	31,31,31,31	0
85	OHX	5	3612	7/7	0.97	0.30	-	129,129,129,129	0
86	MG	1	3987	1/1	0.80	0.22	-	70,70,70,70	0
85	OHX	5	3564	7/7	0.97	0.11	-	137,137,137,137	0
86	MG	5	3994	1/1	0.72	0.49	-	44,44,44,44	0
86	MG	2	2120	1/1	0.57	0.42	-	128,128,128,128	0
85	OHX	1	3674	7/7	0.97	0.12	-	102,102,102,102	0
86	MG	1	3968	1/1	0.91	0.50	-	47,47,47,47	0
86	MG	2	2131	1/1	0.62	0.72	-	80,80,80,80	0
86	MG	5	4024	1/1	0.98	0.09	-	33,33,33,33	0
85	OHX	5	3661	7/7	0.95	0.26	-	122,122,122,122	0
85	OHX	2	1989	7/7	0.97	0.18	-	109,109,109,109	0
86	MG	1	3754	1/1	0.87	0.13	-	89,89,89,89	0
86	MG	2	2063	1/1	0.49	0.45	-	70,70,70,70	0
85	OHX	5	3712	7/7	0.94	0.24	-	148,148,148,148	0
85	OHX	1	3696	7/7	0.95	0.44	-	139,139,139,139	0
85	OHX	5	3447	7/7	0.99	0.09	-	73,73,73,73	0
86	MG	5	4142	1/1	0.92	0.33	-	53,53,53,53	0
85	OHX	1	3658	7/7	0.97	0.22	-	124,124,124,124	0
86	MG	5	3873	1/1	0.94	0.38	-	36,36,36,36	0
85	OHX	2	1959	7/7	0.94	0.19	-	133,133,133,133	0
86	MG	2	2098	1/1	0.35	0.43	-	135,135,135,135	0
86	MG	O7	104	1/1	0.85	0.77	-	58,58,58,58	0
85	OHX	2	1977	7/7	0.96	0.14	-	113,113,113,113	0
85	OHX	6	1930	7/7	0.98	0.10	-	99,99,99,99	0
86	MG	2	2115	1/1	0.88	0.71	-	79,79,79,79	0
85	OHX	2	2042	7/7	0.96	0.36	-	130,130,130,130	0
86	MG	5	3976	1/1	0.90	0.19	-	42,42,42,42	0
86	MG	5	4004	1/1	0.83	0.21	-	53,53,53,53	0
86	MG	5	4147	1/1	0.63	0.52	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	7	217	1/1	0.97	0.57	-	28,28,28,28	0
86	MG	5	3989	1/1	0.79	0.37	-	50,50,50,50	0
86	MG	m6	204	1/1	0.88	0.14	-	43,43,43,43	0
85	OHX	2	2030	7/7	0.90	0.22	-	179,179,179,179	0
86	MG	1	3747	1/1	0.91	0.34	-	40,40,40,40	0
86	MG	1	4043	1/1	0.87	0.34	-	52,52,52,52	0
86	MG	1	3927	1/1	0.81	0.34	-	52,52,52,52	0
86	MG	1	4036	1/1	0.89	0.32	-	58,58,58,58	0
86	MG	5	4006	1/1	0.88	0.21	-	44,44,44,44	0
85	OHX	6	2040	7/7	0.93	0.29	-	137,137,137,137	0
86	MG	5	3893	1/1	0.90	0.34	-	48,48,48,48	0
85	OHX	C3	201	7/7	0.95	0.16	-	150,150,150,150	0
85	OHX	1	3560	7/7	0.93	0.19	-	145,145,145,145	0
85	OHX	5	3638	7/7	0.96	0.19	-	130,130,130,130	0
86	MG	7	223	1/1	0.89	0.12	-	71,71,71,71	0
86	MG	M3	201	1/1	0.68	0.48	-	94,94,94,94	0
86	MG	6	2075	1/1	0.97	0.46	-	61,61,61,61	0
86	MG	1	3784	1/1	0.97	0.31	-	32,32,32,32	0
85	OHX	2	2028	7/7	0.92	0.39	-	175,175,175,175	0
86	MG	2	2102	1/1	0.91	0.50	-	79,79,79,79	0
86	MG	5	4053	1/1	0.89	0.60	-	77,77,77,77	0
85	OHX	1	3602	7/7	0.95	0.14	-	137,137,137,137	0
86	MG	6	2172	1/1	0.98	0.32	-	74,74,74,74	0
85	OHX	5	3656	7/7	0.93	0.28	-	151,151,151,151	0
86	MG	2	2056	1/1	0.85	0.47	-	57,57,57,57	0
86	MG	5	3816	1/1	0.88	0.23	-	37,37,37,37	0
86	MG	L4	402	1/1	0.85	0.26	-	35,35,35,35	0
85	OHX	5	3476	7/7	0.96	0.10	-	104,104,104,104	0
86	MG	5	4150	1/1	0.96	0.16	-	79,79,79,79	0
86	MG	1	3809	1/1	0.88	0.40	-	41,41,41,41	0
86	MG	1	3739	1/1	0.93	0.48	-	52,52,52,52	0
86	MG	1	3965	1/1	0.95	0.15	-	44,44,44,44	0
86	MG	1	3899	1/1	0.96	0.64	-	43,43,43,43	0
86	MG	5	3967	1/1	0.91	0.22	-	54,54,54,54	0
86	MG	2	2090	1/1	0.76	0.50	-	72,72,72,72	0
86	MG	1	3824	1/1	0.91	0.47	-	40,40,40,40	0
85	OHX	1	3453	7/7	0.98	0.09	-	94,94,94,94	0
86	MG	1	4089	1/1	0.60	0.59	-	56,56,56,56	0
86	MG	1	3952	1/1	0.88	0.29	-	50,50,50,50	0
86	MG	5	3766	1/1	0.91	0.21	-	88,88,88,88	0
86	MG	5	4100	1/1	0.88	0.21	-	40,40,40,40	0
86	MG	6	2079	1/1	0.94	0.21	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3655	7/7	0.97	0.40	-	115,115,115,115	0
86	MG	1	3940	1/1	0.90	0.32	-	65,65,65,65	0
86	MG	6	2105	1/1	0.91	0.59	-	42,42,42,42	0
86	MG	5	4134	1/1	0.78	0.60	-	69,69,69,69	0
85	OHX	1	3704	7/7	0.83	0.30	-	190,190,190,190	0
86	MG	6	2088	1/1	0.96	0.26	-	45,45,45,45	0
86	MG	6	2177	1/1	0.90	0.27	-	99,99,99,99	0
86	MG	5	3980	1/1	0.66	0.44	-	46,46,46,46	0
86	MG	1	4079	1/1	0.55	0.26	-	82,82,82,82	0
85	OHX	5	3446	7/7	0.98	0.08	-	85,85,85,85	0
85	OHX	8	214	7/7	0.95	0.22	-	142,142,142,142	0
85	OHX	1	3444	7/7	0.98	0.08	-	92,92,92,92	0
86	MG	5	4068	1/1	0.89	0.35	-	36,36,36,36	0
86	MG	s6	301	1/1	0.92	0.43	-	105,105,105,105	0
86	MG	6	2077	1/1	0.85	0.26	-	62,62,62,62	0
86	MG	1	3906	1/1	0.93	0.41	-	24,24,24,24	0
85	OHX	2	2037	7/7	0.72	0.20	-	242,242,242,242	0
85	OHX	1	3678	7/7	0.96	0.27	-	116,116,116,116	0
86	MG	1	4092	1/1	0.93	0.45	-	44,44,44,44	0
86	MG	N4	201	1/1	-0.09	0.70	-	142,142,142,142	0
86	MG	6	2103	1/1	0.94	0.59	-	62,62,62,62	0
85	OHX	5	3726	7/7	0.94	0.39	-	151,151,151,151	0
85	OHX	1	3614	7/7	0.97	0.37	-	110,110,110,110	0
86	MG	1	3939	1/1	0.81	0.23	-	65,65,65,65	0
86	MG	M7	207	1/1	0.81	0.38	-	56,56,56,56	0
86	MG	1	3757	1/1	0.89	0.30	-	42,42,42,42	0
85	OHX	1	3681	7/7	0.97	0.40	-	131,131,131,131	0
86	MG	5	4136	1/1	0.72	1.05	-	55,55,55,55	0
86	MG	1	3958	1/1	0.95	0.56	-	42,42,42,42	0
86	MG	5	3870	1/1	0.93	0.43	-	43,43,43,43	0
86	MG	6	2156	1/1	0.60	0.45	-	81,81,81,81	0
85	OHX	1	3524	7/7	0.98	0.17	-	109,109,109,109	0
85	OHX	1	3637	7/7	0.98	0.21	-	132,132,132,132	0
86	MG	5	3818	1/1	0.97	0.39	-	51,51,51,51	0
85	OHX	4	206	7/7	0.96	0.27	-	103,103,103,103	0
86	MG	2	2067	1/1	0.95	0.55	-	71,71,71,71	0
86	MG	6	2163	1/1	0.78	0.54	-	79,79,79,79	0
86	MG	1	4119	1/1	0.98	0.36	-	31,31,31,31	0
86	MG	2	2108	1/1	0.78	0.60	-	73,73,73,73	0
86	MG	6	2167	1/1	0.90	0.28	-	60,60,60,60	0
86	MG	L9	201	1/1	0.83	0.40	-	57,57,57,57	0
86	MG	6	2095	1/1	0.92	0.32	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	4164	1/1	0.87	0.67	-	45,45,45,45	0
86	MG	1	3802	1/1	0.77	0.24	-	93,93,93,93	0
86	MG	5	3827	1/1	0.81	0.28	-	45,45,45,45	0
86	MG	D3	201	1/1	0.78	0.20	-	64,64,64,64	0
85	OHX	5	3491	7/7	0.99	0.11	-	118,118,118,118	0
86	MG	1	3923	1/1	0.95	0.33	-	40,40,40,40	0
85	OHX	5	3568	7/7	0.96	0.19	-	146,146,146,146	0
86	MG	5	3865	1/1	0.96	0.33	-	30,30,30,30	0
86	MG	5	4054	1/1	0.92	0.31	-	56,56,56,56	0
86	MG	6	2174	1/1	0.91	0.88	-	62,62,62,62	0
86	MG	1	3852	1/1	0.90	0.33	-	37,37,37,37	0
86	MG	1	3938	1/1	0.93	0.32	-	60,60,60,60	0
85	OHX	c3	201	7/7	0.96	0.24	-	144,144,144,144	0
85	OHX	1	3708	7/7	0.90	0.52	-	152,152,152,152	0
86	MG	1	3892	1/1	0.91	0.33	-	44,44,44,44	0
86	MG	1	4016	1/1	0.84	0.28	-	61,61,61,61	0
86	MG	1	4064	1/1	0.63	0.23	-	81,81,81,81	0
85	OHX	1	3622	7/7	0.97	0.29	-	119,119,119,119	0
85	OHX	5	3513	7/7	0.98	0.11	-	101,101,101,101	0
85	OHX	5	3619	7/7	0.97	0.26	-	109,109,109,109	0
85	OHX	5	3463	7/7	0.98	0.08	-	90,90,90,90	0
86	MG	5	4041	1/1	0.89	0.67	-	47,47,47,47	0
86	MG	5	3909	1/1	0.92	0.48	-	25,25,25,25	0
86	MG	1	3935	1/1	0.91	0.24	-	36,36,36,36	0
86	MG	14	403	1/1	0.37	0.62	-	52,52,52,52	0
85	OHX	5	3746	7/7	0.89	0.28	-	172,172,172,172	0
86	MG	1	3780	1/1	0.95	0.44	-	42,42,42,42	0
85	OHX	6	2024	7/7	0.93	0.33	-	142,142,142,142	0
85	OHX	5	3421	7/7	0.99	0.10	-	67,67,67,67	0
86	MG	1	3926	1/1	0.97	0.24	-	48,48,48,48	0
86	MG	5	4018	1/1	0.80	0.75	-	54,54,54,54	0
85	OHX	2	2033	7/7	0.93	0.27	-	138,138,138,138	0
85	OHX	4	209	7/7	0.96	0.13	-	140,140,140,140	0
86	MG	1	4086	1/1	0.87	0.57	-	55,55,55,55	0
86	MG	2	2132	1/1	0.68	0.43	-	70,70,70,70	0
85	OHX	5	3742	7/7	0.94	0.30	-	127,127,127,127	0
86	MG	3	216	1/1	0.93	0.32	-	71,71,71,71	0
85	OHX	5	3655	7/7	0.94	0.40	-	100,100,100,100	0
86	MG	5	4144	1/1	0.76	0.32	-	85,85,85,85	0
86	MG	6	2118	1/1	0.88	0.27	-	59,59,59,59	0
85	OHX	5	3436	7/7	0.99	0.09	-	66,66,66,66	0
86	MG	5	4145	1/1	0.93	0.17	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2124	1/1	0.91	0.34	-	54,54,54,54	0
86	MG	M9	202	1/1	0.87	0.33	-	74,74,74,74	0
85	OHX	5	3704	7/7	0.96	0.20	-	100,100,100,100	0
85	OHX	6	2035	7/7	0.93	0.41	-	144,144,144,144	0
86	MG	4	225	1/1	0.96	0.38	-	41,41,41,41	0
86	MG	5	3985	1/1	0.86	0.42	-	44,44,44,44	0
85	OHX	1	3554	7/7	0.97	0.18	-	109,109,109,109	0
86	MG	5	3777	1/1	0.85	0.17	-	44,44,44,44	0
85	OHX	M9	201	7/7	0.93	0.31	-	163,163,163,163	0
86	MG	1	3781	1/1	0.93	0.23	-	45,45,45,45	0
86	MG	5	3921	1/1	0.94	0.32	-	28,28,28,28	0
85	OHX	1	3638	7/7	0.97	0.16	-	126,126,126,126	0
86	MG	1	3964	1/1	0.92	0.36	-	51,51,51,51	0
85	OHX	5	3451	7/7	0.98	0.09	-	96,96,96,96	0
86	MG	1	3916	1/1	0.93	0.19	-	46,46,46,46	0
85	OHX	6	1959	7/7	0.96	0.15	-	110,110,110,110	0
86	MG	1	4002	1/1	0.99	0.10	-	43,43,43,43	0
86	MG	5	3943	1/1	0.88	0.18	-	65,65,65,65	0
86	MG	5	4078	1/1	0.87	0.28	-	32,32,32,32	0
86	MG	5	4074	1/1	0.88	0.37	-	51,51,51,51	0
86	MG	C2	206	1/1	-0.17	1.21	-	170,170,170,170	0
86	MG	5	4031	1/1	0.92	0.22	-	62,62,62,62	0
86	MG	1	3949	1/1	0.71	0.74	-	43,43,43,43	0
85	OHX	1	3618	7/7	0.96	0.24	-	125,125,125,125	0
86	MG	2	2066	1/1	0.94	0.73	-	98,98,98,98	0
86	MG	1	3996	1/1	0.86	0.24	-	47,47,47,47	0
86	MG	5	4169	1/1	0.95	0.30	-	34,34,34,34	0
86	MG	1	4103	1/1	0.64	0.41	-	51,51,51,51	0
86	MG	5	3860	1/1	0.94	0.19	-	37,37,37,37	0
86	MG	1	3749	1/1	0.79	0.49	-	66,66,66,66	0
86	MG	6	2055	1/1	0.89	0.50	-	51,51,51,51	0
85	OHX	2	1968	7/7	0.96	0.31	-	130,130,130,130	0
86	MG	6	2052	1/1	0.81	0.67	-	49,49,49,49	0
86	MG	5	4138	1/1	0.83	0.53	-	62,62,62,62	0
85	OHX	5	3574	7/7	0.98	0.18	-	110,110,110,110	0
86	MG	2	2088	1/1	0.96	0.54	-	101,101,101,101	0
86	MG	1	3798	1/1	0.90	0.34	-	41,41,41,41	0
86	MG	1	4021	1/1	0.19	0.32	-	77,77,77,77	0
86	MG	5	3992	1/1	0.94	0.16	-	29,29,29,29	0
86	MG	5	4042	1/1	0.64	0.76	-	35,35,35,35	0
85	OHX	5	3741	7/7	0.95	0.35	-	127,127,127,127	0
86	MG	5	3863	1/1	0.98	0.43	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	OHX	1	3463	7/7	0.98	0.10	-	84,84,84,84	0
86	MG	m0	304	1/1	0.88	0.26	-	88,88,88,88	0
86	MG	7	219	1/1	0.86	0.35	-	50,50,50,50	0
86	MG	5	4128	1/1	0.88	0.15	-	87,87,87,87	0
86	MG	5	4117	1/1	0.89	0.49	-	48,48,48,48	0
85	OHX	5	3469	7/7	0.98	0.12	-	92,92,92,92	0
86	MG	2	2069	1/1	0.89	0.41	-	67,67,67,67	0
85	OHX	1	3507	7/7	0.98	0.11	-	106,106,106,106	0
86	MG	5	3872	1/1	0.87	0.43	-	30,30,30,30	0
85	OHX	5	3523	7/7	0.98	0.22	-	116,116,116,116	0
85	OHX	5	3601	7/7	0.97	0.27	-	112,112,112,112	0
86	MG	5	3952	1/1	0.97	0.22	-	38,38,38,38	0
85	OHX	1	3644	7/7	0.94	0.28	-	126,126,126,126	0
86	MG	1	4011	1/1	0.76	0.30	-	41,41,41,41	0
86	MG	5	3998	1/1	0.81	0.43	-	76,76,76,76	0
85	OHX	6	2023	7/7	0.93	0.25	-	155,155,155,155	0
85	OHX	5	3629	7/7	0.96	0.18	-	135,135,135,135	0
86	MG	MG	2196	1/1	0.02	0.45	-	77,77,77,77	0
86	MG	5	3759	1/1	0.88	0.50	-	36,36,36,36	0
85	OHX	2	2011	7/7	0.94	0.18	-	161,161,161,161	0
85	OHX	1	3628	7/7	0.95	0.21	-	146,146,146,146	0
85	OHX	5	3680	7/7	0.95	0.26	-	132,132,132,132	0
86	MG	6	2107	1/1	0.95	0.19	-	48,48,48,48	0
85	OHX	5	3571	7/7	0.97	0.11	-	113,113,113,113	0
86	MG	1	4091	1/1	0.70	0.37	-	41,41,41,41	0
86	MG	6	2140	1/1	0.91	0.28	-	61,61,61,61	0
85	OHX	5	3652	7/7	0.92	0.27	-	126,126,126,126	0
86	MG	1	3848	1/1	0.92	0.18	-	32,32,32,32	0
86	MG	6	2129	1/1	0.94	0.32	-	54,54,54,54	0
86	MG	1	4125	1/1	0.88	0.37	-	64,64,64,64	0
86	MG	1	3883	1/1	0.96	0.57	-	51,51,51,51	0
85	OHX	5	3636	7/7	0.94	0.15	-	162,162,162,162	0
86	MG	5	3938	1/1	0.97	0.23	-	33,33,33,33	0
85	OHX	6	1942	7/7	0.97	0.12	-	112,112,112,112	0
86	MG	5	3974	1/1	0.69	0.49	-	58,58,58,58	0
86	MG	1	3889	1/1	0.90	0.23	-	36,36,36,36	0
85	OHX	6	1975	7/7	0.97	0.40	-	109,109,109,109	0
86	MG	6	2154	1/1	0.43	0.43	-	92,92,92,92	0
86	MG	4	215	1/1	0.91	0.55	-	51,51,51,51	0
85	OHX	5	3573	7/7	0.97	0.25	-	131,131,131,131	0
85	OHX	1	3729	7/7	0.95	0.26	-	134,134,134,134	0
86	MG	m3	201	1/1	0.88	0.26	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3931	1/1	0.95	0.20	-	48,48,48,48	0
86	MG	1	3793	1/1	0.89	0.47	-	46,46,46,46	0
85	OHX	1	3684	7/7	0.93	0.28	-	139,139,139,139	0
86	MG	1	3937	1/1	0.92	0.20	-	57,57,57,57	0
86	MG	5	3789	1/1	0.92	0.26	-	36,36,36,36	0
86	MG	1	3891	1/1	0.94	0.66	-	36,36,36,36	0
85	OHX	1	3457	7/7	0.98	0.12	-	91,91,91,91	0
86	MG	1	3957	1/1	0.80	0.44	-	55,55,55,55	0
85	OHX	1	3568	7/7	0.97	0.20	-	131,131,131,131	0
85	OHX	1	3718	7/7	0.81	0.26	-	204,204,204,204	0
86	MG	MG	2215	1/1	-0.32	0.43	-	126,126,126,126	0
85	OHX	1	3613	7/7	0.95	0.22	-	123,123,123,123	0
86	MG	5	3829	1/1	0.86	0.49	-	54,54,54,54	0
86	MG	5	4052	1/1	0.78	0.27	-	75,75,75,75	0
86	MG	1	3963	1/1	0.85	0.43	-	70,70,70,70	0
86	MG	6	2161	1/1	0.06	0.57	-	149,149,149,149	0
86	MG	5	3934	1/1	0.78	0.56	-	44,44,44,44	0
85	OHX	6	1969	7/7	0.97	0.25	-	120,120,120,120	0
86	MG	1	3930	1/1	0.95	0.36	-	51,51,51,51	0
86	MG	1	3986	1/1	0.82	0.37	-	42,42,42,42	0
85	OHX	5	3670	7/7	0.94	0.34	-	126,126,126,126	0
86	MG	1	3862	1/1	0.90	0.40	-	40,40,40,40	0
86	MG	5	3996	1/1	0.83	0.35	-	56,56,56,56	0
86	MG	2	2126	1/1	0.94	0.29	-	82,82,82,82	0
86	MG	5	4073	1/1	0.62	0.24	-	72,72,72,72	0
86	MG	1	3741	1/1	0.89	0.39	-	60,60,60,60	0
86	MG	1	4113	1/1	0.94	0.38	-	34,34,34,34	0
86	MG	6	2069	1/1	0.86	0.44	-	71,71,71,71	0
85	OHX	1	3472	7/7	0.99	0.10	-	92,92,92,92	0
86	MG	5	4141	1/1	0.85	0.34	-	28,28,28,28	0
86	MG	5	3813	1/1	0.88	0.76	-	48,48,48,48	0
85	OHX	4	204	7/7	0.98	0.11	-	108,108,108,108	0
86	MG	1	3860	1/1	0.92	0.26	-	45,45,45,45	0
85	OHX	5	3714	7/7	0.95	0.26	-	144,144,144,144	0
86	MG	2	2044	1/1	0.92	0.27	-	38,38,38,38	0
86	MG	1	4093	1/1	0.58	0.82	-	78,78,78,78	0
86	MG	1	4100	1/1	0.95	0.14	-	45,45,45,45	0
86	MG	5	4132	1/1	0.88	0.40	-	35,35,35,35	0
85	OHX	6	2010	7/7	0.95	0.30	-	146,146,146,146	0
86	MG	5	3806	1/1	0.79	0.44	-	57,57,57,57	0
86	MG	1	3875	1/1	0.97	0.34	-	54,54,54,54	0
86	MG	5	3995	1/1	0.70	0.39	-	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	ZN	D7	101	1/1	0.55	0.34	-	147,147,147,147	0
86	MG	L3	403	1/1	0.95	0.15	-	38,38,38,38	0
86	MG	M7	204	1/1	0.88	0.30	-	43,43,43,43	0
86	MG	1	4069	1/1	0.89	0.76	-	69,69,69,69	0
85	OHX	5	3733	7/7	0.95	0.29	-	148,148,148,148	0
85	OHX	6	2037	7/7	0.92	0.38	-	146,146,146,146	0
86	MG	C2	204	1/1	0.35	0.88	-	69,69,69,69	0
86	MG	5	3796	1/1	0.90	0.30	-	38,38,38,38	0
86	MG	1	4010	1/1	0.70	0.47	-	35,35,35,35	0
86	MG	5	4017	1/1	-0.34	0.33	-	131,131,131,131	0
86	MG	1	3823	1/1	0.94	0.14	-	40,40,40,40	0
86	MG	5	3781	1/1	0.97	0.39	-	30,30,30,30	0
86	MG	6	2096	1/1	0.79	0.80	-	73,73,73,73	0
86	MG	5	4044	1/1	0.61	0.42	-	46,46,46,46	0
86	MG	2	2086	1/1	0.97	0.11	-	65,65,65,65	0
86	MG	1	4098	1/1	0.69	0.28	-	106,106,106,106	0
86	MG	1	4058	1/1	0.63	0.59	-	70,70,70,70	0
85	OHX	1	3653	7/7	0.95	0.36	-	119,119,119,119	0
86	MG	3	217	1/1	0.38	0.72	-	66,66,66,66	0
86	MG	5	4158	1/1	0.68	0.61	-	52,52,52,52	0
86	MG	1	4107	1/1	0.46	0.48	-	44,44,44,44	0
86	MG	1	3859	1/1	0.81	0.35	-	48,48,48,48	0
86	MG	1	3816	1/1	0.88	0.24	-	40,40,40,40	0
86	MG	5	3843	1/1	0.88	0.69	-	37,37,37,37	0
86	MG	5	4049	1/1	0.87	0.46	-	54,54,54,54	0
86	MG	1	4073	1/1	0.74	0.32	-	47,47,47,47	0
86	MG	1	4006	1/1	0.93	0.23	-	48,48,48,48	0
85	OHX	1	3458	7/7	0.98	0.07	-	96,96,96,96	0
86	MG	1	3783	1/1	0.63	0.91	-	65,65,65,65	0
86	MG	1	4052	1/1	0.80	0.29	-	49,49,49,49	0
85	OHX	1	3455	7/7	0.98	0.12	-	91,91,91,91	0
86	MG	5	3795	1/1	0.93	0.28	-	36,36,36,36	0
86	MG	5	4106	1/1	0.86	0.20	-	64,64,64,64	0
86	MG	6	2168	1/1	0.92	0.28	-	44,44,44,44	0
85	OHX	1	3604	7/7	0.95	0.27	-	129,129,129,129	0
86	MG	2	2072	1/1	0.71	0.40	-	62,62,62,62	0
85	OHX	5	3555	7/7	0.96	0.41	-	104,104,104,104	0
86	MG	6	2157	1/1	0.90	0.57	-	49,49,49,49	0
86	MG	1	4051	1/1	0.85	0.42	-	44,44,44,44	0
85	OHX	5	3647	7/7	0.94	0.31	-	117,117,117,117	0
86	MG	5	3842	1/1	0.95	0.32	-	33,33,33,33	0
86	MG	1	3829	1/1	0.83	0.50	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3984	1/1	0.75	0.39	-	30,30,30,30	0
86	MG	2	2114	1/1	0.64	0.62	-	67,67,67,67	0
85	OHX	2	1958	7/7	0.93	0.25	-	170,170,170,170	0
85	OHX	6	1935	7/7	0.98	0.12	-	98,98,98,98	0
86	MG	5	3901	1/1	0.87	0.32	-	40,40,40,40	0
85	OHX	5	3603	7/7	0.93	0.37	-	134,134,134,134	0
86	MG	1	4111	1/1	-0.01	0.99	-	145,145,145,145	0
85	OHX	5	3620	7/7	0.96	0.26	-	138,138,138,138	0
86	MG	5	3811	1/1	0.84	0.23	-	39,39,39,39	0
85	OHX	6	2026	7/7	0.94	0.25	-	158,158,158,158	0
86	MG	6	2080	1/1	0.71	1.05	-	69,69,69,69	0
86	MG	1	3895	1/1	0.93	0.24	-	29,29,29,29	0
86	MG	C2	205	1/1	-0.68	1.56	-	170,170,170,170	0
85	OHX	5	3448	7/7	0.99	0.08	-	69,69,69,69	0
86	MG	2	2096	1/1	0.87	0.48	-	66,66,66,66	0
86	MG	5	4096	1/1	0.83	0.27	-	36,36,36,36	0
86	MG	1	3900	1/1	0.95	0.45	-	27,27,27,27	0
85	OHX	1	3541	7/7	0.95	0.24	-	119,119,119,119	0
86	MG	1	4020	1/1	0.93	0.53	-	39,39,39,39	0
86	MG	5	3957	1/1	0.86	0.30	-	83,83,83,83	0
86	MG	S8	302	1/1	0.45	0.53	-	69,69,69,69	0
85	OHX	2	1906	7/7	0.98	0.14	-	103,103,103,103	0
86	MG	1	3873	1/1	0.94	0.54	-	32,32,32,32	0
86	MG	5	4016	1/1	0.99	0.15	-	40,40,40,40	0
85	OHX	6	1936	7/7	0.99	0.09	-	112,112,112,112	0
86	MG	M4	201	1/1	0.94	0.24	-	49,49,49,49	0
86	MG	6	2165	1/1	0.93	0.60	-	70,70,70,70	0
86	MG	6	2102	1/1	0.86	1.71	-	68,68,68,68	0
85	OHX	6	1950	7/7	0.98	0.11	-	123,123,123,123	0
86	MG	2	2111	1/1	0.33	0.38	-	77,77,77,77	0
86	MG	1	3945	1/1	0.83	0.22	-	43,43,43,43	0
86	MG	2	2106	1/1	0.80	0.27	-	103,103,103,103	0
86	MG	5	3787	1/1	0.83	0.32	-	34,34,34,34	0
85	OHX	2	2032	7/7	0.91	0.27	-	168,168,168,168	0
86	MG	5	4059	1/1	0.65	0.47	-	74,74,74,74	0
85	OHX	6	1998	7/7	0.95	0.33	-	127,127,127,127	0
85	OHX	2	2016	7/7	0.95	0.21	-	149,149,149,149	0
86	MG	5	4056	1/1	0.75	0.20	-	57,57,57,57	0
85	OHX	5	3687	7/7	0.93	0.42	-	130,130,130,130	0
86	MG	2	2058	1/1	0.92	0.55	-	58,58,58,58	0
86	MG	5	4028	1/1	0.93	0.22	-	41,41,41,41	0
86	MG	6	2104	1/1	0.74	0.70	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	SM	301	1/1	0.67	0.42	-	57,57,57,57	0
86	MG	1	3918	1/1	0.94	0.59	-	47,47,47,47	0
86	MG	C2	202	1/1	0.47	0.79	-	88,88,88,88	0
86	MG	5	4083	1/1	0.91	0.23	-	44,44,44,44	0
86	MG	5	4114	1/1	0.69	0.23	-	59,59,59,59	0
86	MG	1	3792	1/1	0.99	0.34	-	60,60,60,60	0
86	MG	1	4019	1/1	0.66	0.26	-	51,51,51,51	0
86	MG	5	3953	1/1	0.73	0.41	-	43,43,43,43	0
86	MG	5	3965	1/1	0.80	0.47	-	56,56,56,56	0
85	OHX	1	3722	7/7	0.97	0.30	-	139,139,139,139	0
86	MG	2	2070	1/1	0.83	0.54	-	62,62,62,62	0
85	OHX	5	3411	7/7	0.99	0.12	-	44,44,44,44	0
86	MG	1	3799	1/1	0.81	0.31	-	50,50,50,50	0
85	OHX	5	3566	7/7	0.95	0.27	-	121,121,121,121	0
86	MG	1	3849	1/1	0.94	0.40	-	42,42,42,42	0
85	OHX	5	3659	7/7	0.98	0.17	-	112,112,112,112	0
85	OHX	2	2026	7/7	0.92	0.23	-	168,168,168,168	0
86	MG	5	3841	1/1	0.83	0.29	-	53,53,53,53	0
85	OHX	5	3654	7/7	0.94	0.40	-	134,134,134,134	0
86	MG	5	4048	1/1	0.65	0.12	-	106,106,106,106	0
86	MG	5	3879	1/1	0.97	0.14	-	37,37,37,37	0
86	MG	5	3961	1/1	0.89	0.23	-	38,38,38,38	0
86	MG	5	3933	1/1	0.88	0.28	-	61,61,61,61	0
86	MG	5	3936	1/1	0.93	0.55	-	55,55,55,55	0
86	MG	5	3956	1/1	0.83	0.30	-	34,34,34,34	0
85	OHX	6	1938	7/7	0.98	0.09	-	110,110,110,110	0
86	MG	1	3928	1/1	0.86	0.38	-	44,44,44,44	0
86	MG	5	3802	1/1	0.93	0.24	-	31,31,31,31	0
86	MG	M6	201	1/1	0.80	0.17	-	39,39,39,39	0
86	MG	1	4071	1/1	0.84	0.34	-	38,38,38,38	0
85	OHX	1	3662	7/7	0.95	0.17	-	146,146,146,146	0
86	MG	5	3940	1/1	0.95	0.27	-	48,48,48,48	0
85	OHX	5	3586	7/7	0.98	0.30	-	105,105,105,105	0
86	MG	6	2087	1/1	0.83	0.33	-	45,45,45,45	0
86	MG	1	3811	1/1	0.70	0.42	-	53,53,53,53	0
86	MG	1	3779	1/1	0.89	0.36	-	53,53,53,53	0
86	MG	5	3911	1/1	0.92	0.41	-	30,30,30,30	0
86	MG	Q2	503	1/1	0.93	0.28	-	68,68,68,68	0
86	MG	5	3791	1/1	0.91	0.59	-	29,29,29,29	0
86	MG	6	2169	1/1	0.69	0.41	-	70,70,70,70	0
85	OHX	3	211	7/7	0.93	0.32	-	165,165,165,165	0
85	OHX	5	3736	7/7	0.95	0.35	-	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2178	1/1	0.57	0.64	-	56,56,56,56	0
85	OHX	6	2018	7/7	0.93	0.24	-	174,174,174,174	0
86	MG	1	3948	1/1	0.94	0.31	-	41,41,41,41	0
86	MG	6	2084	1/1	0.99	0.40	-	48,48,48,48	0
85	OHX	2	2018	7/7	0.95	0.37	-	151,151,151,151	0
85	OHX	1	3626	7/7	0.95	0.28	-	152,152,152,152	0
86	MG	5	4026	1/1	0.63	0.41	-	54,54,54,54	0
86	MG	5	3914	1/1	0.94	0.33	-	31,31,31,31	0
86	MG	5	4131	1/1	0.85	1.00	-	86,86,86,86	0
86	MG	5	4129	1/1	0.84	0.49	-	66,66,66,66	0
85	OHX	2	1930	7/7	0.97	0.18	-	118,118,118,118	0
86	MG	1	3998	1/1	0.87	0.28	-	60,60,60,60	0
85	OHX	5	3744	7/7	0.92	0.17	-	134,134,134,134	0
86	MG	1	4115	1/1	0.91	0.51	-	29,29,29,29	0
86	MG	6	2066	1/1	0.84	0.58	-	66,66,66,66	0
86	MG	5	4151	1/1	0.94	0.13	-	99,99,99,99	0
86	MG	5	4116	1/1	0.63	0.44	-	67,67,67,67	0
85	OHX	1	3480	7/7	0.98	0.12	-	105,105,105,105	0
86	MG	MG	2207	1/1	0.31	1.19	-	109,109,109,109	0
86	MG	1	4085	1/1	0.87	0.31	-	47,47,47,47	0
86	MG	1	3950	1/1	0.79	0.45	-	71,71,71,71	0
86	MG	5	4058	1/1	0.87	0.19	-	35,35,35,35	0
85	OHX	1	3557	7/7	0.96	0.27	-	113,113,113,113	0
86	MG	5	3896	1/1	0.92	0.55	-	29,29,29,29	0
86	MG	6	2138	1/1	0.84	0.27	-	67,67,67,67	0
86	MG	1	3788	1/1	0.89	0.38	-	32,32,32,32	0
86	MG	5	3856	1/1	0.85	0.30	-	38,38,38,38	0
86	MG	6	2152	1/1	0.98	0.13	-	70,70,70,70	0
86	MG	5	4171	1/1	0.81	0.72	-	35,35,35,35	0
85	OHX	1	3617	7/7	0.97	0.38	-	129,129,129,129	0
86	MG	5	4082	1/1	0.73	0.44	-	66,66,66,66	0
86	MG	5	3923	1/1	0.93	0.35	-	36,36,36,36	0
86	MG	5	4121	1/1	0.87	0.69	-	44,44,44,44	0
86	MG	1	4099	1/1	0.83	0.13	-	52,52,52,52	0
86	MG	1	4039	1/1	0.84	0.26	-	44,44,44,44	0
85	OHX	3	207	7/7	0.97	0.17	-	118,118,118,118	0
86	MG	7	216	1/1	0.94	0.37	-	68,68,68,68	0
85	OHX	5	3732	7/7	0.95	0.32	-	127,127,127,127	0
86	MG	7	218	1/1	0.95	0.26	-	35,35,35,35	0
86	MG	5	3905	1/1	0.98	0.45	-	27,27,27,27	0
85	OHX	2	1994	7/7	0.94	0.34	-	152,152,152,152	0
85	OHX	1	3706	7/7	0.94	0.29	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2142	1/1	0.91	0.15	-	57,57,57,57	0
85	OHX	1	3563	7/7	0.98	0.14	-	119,119,119,119	0
86	MG	1	3877	1/1	0.80	0.46	-	35,35,35,35	0
86	MG	1	3919	1/1	0.64	1.09	-	67,67,67,67	0
86	MG	5	3937	1/1	0.94	0.38	-	34,34,34,34	0
85	OHX	5	3506	7/7	0.97	0.12	-	104,104,104,104	0
85	OHX	1	3505	7/7	0.98	0.08	-	124,124,124,124	0
86	MG	1	4001	1/1	0.89	0.17	-	51,51,51,51	0
85	OHX	2	1952	7/7	0.97	0.28	-	119,119,119,119	0
85	OHX	5	3478	7/7	0.98	0.11	-	96,96,96,96	0
86	MG	5	3962	1/1	0.92	0.46	-	42,42,42,42	0
86	MG	5	3978	1/1	0.88	0.34	-	30,30,30,30	0
86	MG	5	3988	1/1	0.72	0.24	-	68,68,68,68	0
86	MG	5	3793	1/1	0.78	0.35	-	46,46,46,46	0
85	OHX	1	3685	7/7	0.92	0.30	-	128,128,128,128	0
86	MG	2	2048	1/1	0.74	0.55	-	73,73,73,73	0
86	MG	1	3936	1/1	0.91	0.32	-	66,66,66,66	0
86	MG	5	3775	1/1	0.94	0.27	-	34,34,34,34	0
85	OHX	5	3591	7/7	0.99	0.22	-	118,118,118,118	0
86	MG	5	3826	1/1	0.85	0.48	-	51,51,51,51	0
86	MG	5	3790	1/1	0.94	0.32	-	37,37,37,37	0
85	OHX	1	3675	7/7	0.96	0.26	-	122,122,122,122	0
86	MG	1	4070	1/1	0.35	0.13	-	203,203,203,203	0
86	MG	1	4032	1/1	0.98	0.24	-	70,70,70,70	0
86	MG	5	4080	1/1	0.99	0.23	-	33,33,33,33	0
85	OHX	1	3474	7/7	0.98	0.11	-	87,87,87,87	0
86	MG	5	3748	1/1	0.92	0.57	-	43,43,43,43	0
86	MG	1	3853	1/1	0.94	0.83	-	38,38,38,38	0
86	MG	5	3801	1/1	0.78	0.39	-	35,35,35,35	0
86	MG	1	3776	1/1	0.89	0.30	-	34,34,34,34	0
85	OHX	1	3639	7/7	0.98	0.18	-	107,107,107,107	0
85	OHX	1	3571	7/7	0.97	0.13	-	143,143,143,143	0
86	MG	5	3874	1/1	0.93	0.47	-	43,43,43,43	0
86	MG	5	4030	1/1	0.78	0.29	-	47,47,47,47	0
87	ZN	q3	501	1/1	0.94	0.10	-	65,65,65,65	0
86	MG	1	3976	1/1	0.94	0.17	-	41,41,41,41	0
86	MG	5	3828	1/1	0.81	0.31	-	49,49,49,49	0
85	OHX	5	3708	7/7	0.96	0.41	-	122,122,122,122	0
86	MG	Q1	101	1/1	0.71	0.41	-	66,66,66,66	0
85	OHX	1	3730	7/7	0.94	0.26	-	150,150,150,150	0
86	MG	5	4143	1/1	0.11	1.08	-	55,55,55,55	0
86	MG	1	3791	1/1	0.92	0.42	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3762	1/1	0.87	0.43	-	44,44,44,44	0
85	OHX	1	3686	7/7	0.93	0.24	-	141,141,141,141	0
86	MG	1	4012	1/1	0.83	0.44	-	45,45,45,45	0
85	OHX	5	3671	7/7	0.96	0.24	-	114,114,114,114	0
85	OHX	1	3664	7/7	0.91	0.36	-	137,137,137,137	0
86	MG	1	4004	1/1	0.99	0.10	-	42,42,42,42	0
86	MG	6	2176	1/1	0.86	0.33	-	54,54,54,54	0
86	MG	5	4167	1/1	0.64	0.55	-	65,65,65,65	0
86	MG	2	2133	1/1	0.48	0.46	-	66,66,66,66	0
86	MG	1	4101	1/1	0.53	0.57	-	95,95,95,95	0
86	MG	1	3884	1/1	0.94	0.24	-	37,37,37,37	0
86	MG	5	4103	1/1	0.85	0.36	-	92,92,92,92	0
86	MG	5	4007	1/1	0.91	0.41	-	61,61,61,61	0
86	MG	1	3766	1/1	0.77	0.20	-	39,39,39,39	0
85	OHX	6	2004	7/7	0.94	0.19	-	141,141,141,141	0
86	MG	m6	202	1/1	0.89	0.30	-	35,35,35,35	0
86	MG	5	4033	1/1	0.88	0.66	-	41,41,41,41	0
86	MG	5	3780	1/1	0.94	0.17	-	41,41,41,41	0
86	MG	2	2061	1/1	0.92	0.40	-	59,59,59,59	0
86	MG	1	4017	1/1	0.68	0.45	-	50,50,50,50	0
86	MG	1	4024	1/1	0.83	0.29	-	57,57,57,57	0
86	MG	5	4032	1/1	0.64	0.61	-	70,70,70,70	0
86	MG	4	217	1/1	0.94	0.50	-	69,69,69,69	0
86	MG	6	2143	1/1	0.69	0.44	-	82,82,82,82	0
86	MG	5	4133	1/1	0.77	0.56	-	55,55,55,55	0
85	OHX	s4	301	7/7	0.94	0.22	-	139,139,139,139	0
86	MG	8	227	1/1	0.78	0.41	-	54,54,54,54	0
85	OHX	5	3645	7/7	0.94	0.22	-	119,119,119,119	0
86	MG	5	4099	1/1	0.85	0.36	-	63,63,63,63	0
85	OHX	1	3435	7/7	0.99	0.12	-	85,85,85,85	0
85	OHX	1	3476	7/7	0.98	0.08	-	98,98,98,98	0
86	MG	6	2078	1/1	0.63	0.59	-	70,70,70,70	0
85	OHX	2	2012	7/7	0.93	0.17	-	153,153,153,153	0
86	MG	6	2148	1/1	0.78	0.21	-	65,65,65,65	0
86	MG	1	4120	1/1	0.37	0.64	-	76,76,76,76	0
86	MG	5	4174	1/1	0.95	0.12	-	48,48,48,48	0
85	OHX	2	2008	7/7	0.91	0.26	-	185,185,185,185	0
86	MG	5	3805	1/1	0.96	0.34	-	41,41,41,41	0
85	OHX	6	1940	7/7	0.97	0.14	-	102,102,102,102	0
86	MG	1	4027	1/1	0.70	0.24	-	120,120,120,120	0
86	MG	1	3960	1/1	0.80	0.40	-	46,46,46,46	0
86	MG	5	4155	1/1	0.67	0.99	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	2079	1/1	0.86	0.37	-	154,154,154,154	0
86	MG	1	3833	1/1	0.95	0.44	-	39,39,39,39	0
85	OHX	5	3716	7/7	0.93	0.26	-	131,131,131,131	0
86	MG	C2	207	1/1	0.21	0.89	-	105,105,105,105	0
85	OHX	1	3717	7/7	0.94	0.33	-	132,132,132,132	0
86	MG	5	3987	1/1	0.97	0.44	-	53,53,53,53	0
86	MG	3	212	1/1	0.91	0.34	-	78,78,78,78	0
85	OHX	1	3661	7/7	0.92	0.25	-	132,132,132,132	0
86	MG	6	2113	1/1	0.89	0.68	-	50,50,50,50	0
86	MG	2	2113	1/1	0.92	0.34	-	105,105,105,105	0
85	OHX	1	3562	7/7	0.95	0.20	-	122,122,122,122	0
85	OHX	2	1992	7/7	0.96	0.22	-	153,153,153,153	0
86	MG	5	4000	1/1	0.67	0.55	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.