



wwPDB X-ray Structure Validation Summary Report i

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PDB ID : 4U4R
Title : Crystal structure of Lactimidomycin bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-24
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

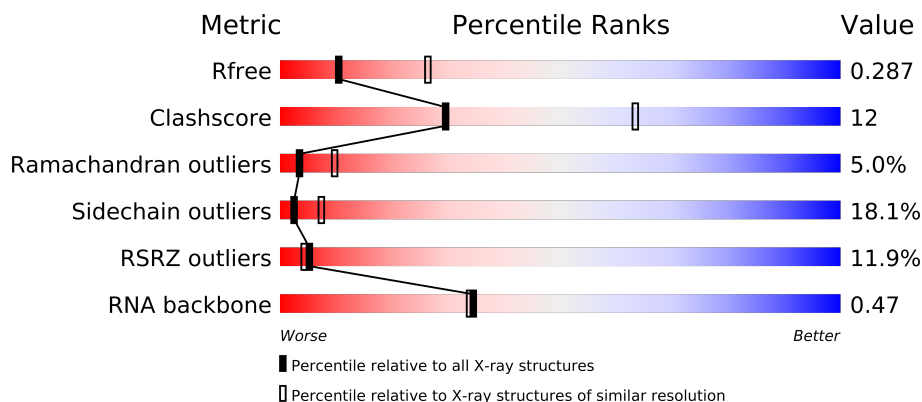
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable24037
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24037

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)
RNA backbone	1838	1076 (3.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	2	1800	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	

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Mol	Chain	Length	Quality of chain
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
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	

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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
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	

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Mol	Chain	Length	Quality of chain
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
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	
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	119	

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Mol	Chain	Length	Quality of chain
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	
80	e0	62	
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3401	-	X
85	MG	1	3402	-	X
85	MG	1	3404	-	X
85	MG	1	3405	-	X
85	MG	1	3408	-	X
85	MG	1	3409	-	X
85	MG	1	3410	-	X
85	MG	1	3412	-	X
85	MG	1	3413	-	X
85	MG	1	3417	-	X
85	MG	1	3418	-	X
85	MG	1	3419	-	X
85	MG	1	3423	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3429	-	X
85	MG	1	3431	-	X
85	MG	1	3439	-	X
85	MG	1	3444	-	X
85	MG	1	3447	-	X
85	MG	1	3450	-	X
85	MG	1	3451	-	X
85	MG	1	3454	-	X
85	MG	1	3456	-	X
85	MG	1	3458	-	X
85	MG	1	3460	-	X
85	MG	1	3462	-	X
85	MG	1	3463	-	X
85	MG	1	3466	-	X
85	MG	1	3469	-	X
85	MG	1	3470	-	X
85	MG	1	3471	-	X
85	MG	1	3472	-	X
85	MG	1	3474	-	X
85	MG	1	3475	-	X
85	MG	1	3479	-	X
85	MG	1	3481	-	X
85	MG	1	3482	-	X
85	MG	1	3484	-	X
85	MG	1	3485	-	X
85	MG	1	3487	-	X
85	MG	1	3493	-	X
85	MG	1	3494	-	X
85	MG	1	3495	-	X
85	MG	1	3496	-	X
85	MG	1	3502	-	X
85	MG	1	3504	-	X
85	MG	1	3505	-	X
85	MG	1	3506	-	X
85	MG	1	3507	-	X
85	MG	1	3508	-	X
85	MG	1	3509	-	X
85	MG	1	3510	-	X
85	MG	1	3512	-	X
85	MG	1	3513	-	X
85	MG	1	3515	-	X
85	MG	1	3516	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3517	-	X
85	MG	1	3518	-	X
85	MG	1	3519	-	X
85	MG	1	3521	-	X
85	MG	1	3522	-	X
85	MG	1	3523	-	X
85	MG	1	3525	-	X
85	MG	1	3526	-	X
85	MG	1	3527	-	X
85	MG	1	3528	-	X
85	MG	1	3529	-	X
85	MG	1	3530	-	X
85	MG	1	3531	-	X
85	MG	1	3532	-	X
85	MG	1	3533	-	X
85	MG	1	3535	-	X
85	MG	1	3536	-	X
85	MG	1	3537	-	X
85	MG	1	3538	-	X
85	MG	1	3539	-	X
85	MG	1	3540	-	X
85	MG	1	3541	-	X
85	MG	1	3542	-	X
85	MG	1	3543	-	X
85	MG	1	3544	-	X
85	MG	1	3545	-	X
85	MG	1	3546	-	X
85	MG	1	3548	-	X
85	MG	1	3549	-	X
85	MG	1	3550	-	X
85	MG	1	3551	-	X
85	MG	1	3552	-	X
85	MG	1	3556	-	X
85	MG	1	3559	-	X
85	MG	1	3560	-	X
85	MG	1	3561	-	X
85	MG	1	3562	-	X
85	MG	1	3566	-	X
85	MG	1	3568	-	X
85	MG	1	3569	-	X
85	MG	1	3571	-	X
85	MG	1	3572	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3573	-	X
85	MG	1	3574	-	X
85	MG	1	3575	-	X
85	MG	1	3576	-	X
85	MG	1	3578	-	X
85	MG	1	3579	-	X
85	MG	1	3580	-	X
85	MG	1	3583	-	X
85	MG	1	3585	-	X
85	MG	1	3586	-	X
85	MG	1	3587	-	X
85	MG	1	3588	-	X
85	MG	1	3589	-	X
85	MG	1	3590	-	X
85	MG	1	3591	-	X
85	MG	1	3592	-	X
85	MG	1	3593	-	X
85	MG	1	3594	-	X
85	MG	1	3595	-	X
85	MG	1	3596	-	X
85	MG	1	3597	-	X
85	MG	1	3598	-	X
85	MG	1	3599	-	X
85	MG	1	3600	-	X
85	MG	1	3604	-	X
85	MG	1	3607	-	X
85	MG	1	3609	-	X
85	MG	1	3610	-	X
85	MG	1	3614	-	X
85	MG	1	3615	-	X
85	MG	1	3618	-	X
85	MG	1	3622	-	X
85	MG	1	3623	-	X
85	MG	1	3624	-	X
85	MG	1	3625	-	X
85	MG	1	3629	-	X
85	MG	1	3630	-	X
85	MG	1	3631	-	X
85	MG	1	3634	-	X
85	MG	1	3637	-	X
85	MG	1	3643	-	X
85	MG	1	3646	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3647	-	X
85	MG	1	3652	-	X
85	MG	1	3653	-	X
85	MG	1	3655	-	X
85	MG	1	3658	-	X
85	MG	1	3660	-	X
85	MG	1	3663	-	X
85	MG	1	3667	-	X
85	MG	1	3669	-	X
85	MG	1	3670	-	X
85	MG	1	3674	-	X
85	MG	1	3677	-	X
85	MG	1	3679	-	X
85	MG	1	3684	-	X
85	MG	1	3685	-	X
85	MG	1	3687	-	X
85	MG	1	3694	-	X
85	MG	1	3700	-	X
85	MG	1	3702	-	X
85	MG	1	3704	-	X
85	MG	1	3707	-	X
85	MG	1	3708	-	X
85	MG	1	3709	-	X
85	MG	1	3713	-	X
85	MG	1	3716	-	X
85	MG	1	3718	-	X
85	MG	1	3720	-	X
85	MG	1	3721	-	X
85	MG	1	3722	-	X
85	MG	1	3726	-	X
85	MG	1	3728	-	X
85	MG	1	3730	-	X
85	MG	1	3733	-	X
85	MG	1	3734	-	X
85	MG	1	3735	-	X
85	MG	1	3739	-	X
85	MG	1	3742	-	X
85	MG	1	3743	-	X
85	MG	1	3747	-	X
85	MG	1	3748	-	X
85	MG	1	3749	-	X
85	MG	1	3751	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3752	-	X
85	MG	1	3757	-	X
85	MG	1	3761	-	X
85	MG	1	3762	-	X
85	MG	1	3766	-	X
85	MG	1	3769	-	X
85	MG	1	3773	-	X
85	MG	1	3774	-	X
85	MG	1	3776	-	X
85	MG	1	3785	-	X
85	MG	1	3786	-	X
85	MG	1	3789	-	X
85	MG	1	3791	-	X
85	MG	1	3796	-	X
85	MG	1	3799	-	X
85	MG	1	3801	-	X
85	MG	1	3804	-	X
85	MG	1	3805	-	X
85	MG	1	3806	-	X
85	MG	1	3808	-	X
85	MG	1	3809	-	X
85	MG	1	3810	-	X
85	MG	1	3813	-	X
85	MG	1	3814	-	X
85	MG	1	3815	-	X
85	MG	1	3817	-	X
85	MG	1	3818	-	X
85	MG	1	3820	-	X
85	MG	1	3821	-	X
85	MG	1	3826	-	X
85	MG	1	3827	-	X
85	MG	1	3834	-	X
85	MG	1	3835	-	X
85	MG	1	3836	-	X
85	MG	1	3839	-	X
85	MG	1	3843	-	X
85	MG	1	3844	-	X
85	MG	1	3847	-	X
85	MG	1	3848	-	X
85	MG	1	3850	-	X
85	MG	1	3853	-	X
85	MG	1	3854	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3856	-	X
85	MG	1	3858	-	X
85	MG	1	3859	-	X
85	MG	1	3860	-	X
85	MG	1	3861	-	X
85	MG	1	3862	-	X
85	MG	1	3863	-	X
85	MG	1	3865	-	X
85	MG	1	4217	-	X
85	MG	1	4219	-	X
85	MG	1	4224	-	X
85	MG	2	1901	-	X
85	MG	2	1903	-	X
85	MG	2	1904	-	X
85	MG	2	1905	-	X
85	MG	2	1906	-	X
85	MG	2	1907	-	X
85	MG	2	1909	-	X
85	MG	2	1910	-	X
85	MG	2	1911	-	X
85	MG	2	1913	-	X
85	MG	2	1914	-	X
85	MG	2	1915	-	X
85	MG	2	1917	-	X
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1921	-	X
85	MG	2	1923	-	X
85	MG	2	1924	-	X
85	MG	2	1925	-	X
85	MG	2	1926	-	X
85	MG	2	1928	-	X
85	MG	2	1929	-	X
85	MG	2	1930	-	X
85	MG	2	1931	-	X
85	MG	2	1932	-	X
85	MG	2	1933	-	X
85	MG	2	1934	-	X
85	MG	2	1935	-	X
85	MG	2	1936	-	X
85	MG	2	1937	-	X
85	MG	2	1938	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1939	-	X
85	MG	2	1943	-	X
85	MG	2	1944	-	X
85	MG	2	1946	-	X
85	MG	2	1950	-	X
85	MG	2	1951	-	X
85	MG	2	1952	-	X
85	MG	2	1953	-	X
85	MG	2	1955	-	X
85	MG	2	1957	-	X
85	MG	2	1958	-	X
85	MG	2	1959	-	X
85	MG	2	1960	-	X
85	MG	2	1961	-	X
85	MG	2	1962	-	X
85	MG	2	1963	-	X
85	MG	2	1965	-	X
85	MG	2	1967	-	X
85	MG	2	1968	-	X
85	MG	2	1969	-	X
85	MG	2	1971	-	X
85	MG	2	1972	-	X
85	MG	2	1974	-	X
85	MG	2	1975	-	X
85	MG	2	1977	-	X
85	MG	2	1978	-	X
85	MG	2	1979	-	X
85	MG	2	1981	-	X
85	MG	2	1983	-	X
85	MG	2	1984	-	X
85	MG	2	1986	-	X
85	MG	2	1989	-	X
85	MG	2	1990	-	X
85	MG	2	1995	-	X
85	MG	2	1997	-	X
85	MG	2	1998	-	X
85	MG	2	2003	-	X
85	MG	2	2007	-	X
85	MG	2	2008	-	X
85	MG	2	2009	-	X
85	MG	2	2010	-	X
85	MG	2	2011	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	2012	-	X
85	MG	2	2013	-	X
85	MG	2	2014	-	X
85	MG	2	2015	-	X
85	MG	2	2017	-	X
85	MG	2	2018	-	X
85	MG	2	2019	-	X
85	MG	2	2020	-	X
85	MG	2	2023	-	X
85	MG	2	2183	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	203	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	206	-	X
85	MG	3	207	-	X
85	MG	3	209	-	X
85	MG	3	210	-	X
85	MG	3	212	-	X
85	MG	3	213	-	X
85	MG	3	214	-	X
85	MG	4	203	-	X
85	MG	4	205	-	X
85	MG	4	206	-	X
85	MG	4	211	-	X
85	MG	4	214	-	X
85	MG	4	220	-	X
85	MG	4	221	-	X
85	MG	5	3401	-	X
85	MG	5	3403	-	X
85	MG	5	3409	-	X
85	MG	5	3410	-	X
85	MG	5	3411	-	X
85	MG	5	3412	-	X
85	MG	5	3413	-	X
85	MG	5	3415	-	X
85	MG	5	3416	-	X
85	MG	5	3419	-	X
85	MG	5	3422	-	X
85	MG	5	3423	-	X
85	MG	5	3424	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3426	-	X
85	MG	5	3427	-	X
85	MG	5	3429	-	X
85	MG	5	3431	-	X
85	MG	5	3432	-	X
85	MG	5	3433	-	X
85	MG	5	3438	-	X
85	MG	5	3439	-	X
85	MG	5	3441	-	X
85	MG	5	3442	-	X
85	MG	5	3443	-	X
85	MG	5	3445	-	X
85	MG	5	3446	-	X
85	MG	5	3448	-	X
85	MG	5	3449	-	X
85	MG	5	3453	-	X
85	MG	5	3456	-	X
85	MG	5	3457	-	X
85	MG	5	3458	-	X
85	MG	5	3462	-	X
85	MG	5	3463	-	X
85	MG	5	3465	-	X
85	MG	5	3466	-	X
85	MG	5	3467	-	X
85	MG	5	3468	-	X
85	MG	5	3469	-	X
85	MG	5	3470	-	X
85	MG	5	3472	-	X
85	MG	5	3473	-	X
85	MG	5	3474	-	X
85	MG	5	3475	-	X
85	MG	5	3476	-	X
85	MG	5	3477	-	X
85	MG	5	3479	-	X
85	MG	5	3481	-	X
85	MG	5	3482	-	X
85	MG	5	3490	-	X
85	MG	5	3498	-	X
85	MG	5	3499	-	X
85	MG	5	3502	-	X
85	MG	5	3503	-	X
85	MG	5	3505	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3506	-	X
85	MG	5	3507	-	X
85	MG	5	3508	-	X
85	MG	5	3511	-	X
85	MG	5	3512	-	X
85	MG	5	3514	-	X
85	MG	5	3515	-	X
85	MG	5	3516	-	X
85	MG	5	3517	-	X
85	MG	5	3518	-	X
85	MG	5	3519	-	X
85	MG	5	3520	-	X
85	MG	5	3521	-	X
85	MG	5	3522	-	X
85	MG	5	3523	-	X
85	MG	5	3524	-	X
85	MG	5	3525	-	X
85	MG	5	3526	-	X
85	MG	5	3528	-	X
85	MG	5	3529	-	X
85	MG	5	3530	-	X
85	MG	5	3531	-	X
85	MG	5	3533	-	X
85	MG	5	3534	-	X
85	MG	5	3535	-	X
85	MG	5	3537	-	X
85	MG	5	3538	-	X
85	MG	5	3539	-	X
85	MG	5	3540	-	X
85	MG	5	3541	-	X
85	MG	5	3542	-	X
85	MG	5	3544	-	X
85	MG	5	3546	-	X
85	MG	5	3547	-	X
85	MG	5	3548	-	X
85	MG	5	3549	-	X
85	MG	5	3551	-	X
85	MG	5	3553	-	X
85	MG	5	3555	-	X
85	MG	5	3557	-	X
85	MG	5	3558	-	X
85	MG	5	3559	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3560	-	X
85	MG	5	3561	-	X
85	MG	5	3562	-	X
85	MG	5	3563	-	X
85	MG	5	3564	-	X
85	MG	5	3565	-	X
85	MG	5	3566	-	X
85	MG	5	3567	-	X
85	MG	5	3568	-	X
85	MG	5	3569	-	X
85	MG	5	3570	-	X
85	MG	5	3571	-	X
85	MG	5	3572	-	X
85	MG	5	3573	-	X
85	MG	5	3574	-	X
85	MG	5	3575	-	X
85	MG	5	3576	-	X
85	MG	5	3577	-	X
85	MG	5	3578	-	X
85	MG	5	3579	-	X
85	MG	5	3580	-	X
85	MG	5	3581	-	X
85	MG	5	3582	-	X
85	MG	5	3583	-	X
85	MG	5	3584	-	X
85	MG	5	3585	-	X
85	MG	5	3586	-	X
85	MG	5	3587	-	X
85	MG	5	3588	-	X
85	MG	5	3590	-	X
85	MG	5	3591	-	X
85	MG	5	3592	-	X
85	MG	5	3593	-	X
85	MG	5	3594	-	X
85	MG	5	3595	-	X
85	MG	5	3596	-	X
85	MG	5	3598	-	X
85	MG	5	3605	-	X
85	MG	5	3606	-	X
85	MG	5	3610	-	X
85	MG	5	3612	-	X
85	MG	5	3613	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3618	-	X
85	MG	5	3619	-	X
85	MG	5	3622	-	X
85	MG	5	3623	-	X
85	MG	5	3626	-	X
85	MG	5	3629	-	X
85	MG	5	3630	-	X
85	MG	5	3633	-	X
85	MG	5	3634	-	X
85	MG	5	3638	-	X
85	MG	5	3639	-	X
85	MG	5	3643	-	X
85	MG	5	3644	-	X
85	MG	5	3646	-	X
85	MG	5	3647	-	X
85	MG	5	3648	-	X
85	MG	5	3649	-	X
85	MG	5	3652	-	X
85	MG	5	3655	-	X
85	MG	5	3659	-	X
85	MG	5	3661	-	X
85	MG	5	3662	-	X
85	MG	5	3665	-	X
85	MG	5	3667	-	X
85	MG	5	3670	-	X
85	MG	5	3671	-	X
85	MG	5	3672	-	X
85	MG	5	3673	-	X
85	MG	5	3676	-	X
85	MG	5	3677	-	X
85	MG	5	3680	-	X
85	MG	5	3681	-	X
85	MG	5	3683	-	X
85	MG	5	3693	-	X
85	MG	5	3695	-	X
85	MG	5	3697	-	X
85	MG	5	3700	-	X
85	MG	5	3706	-	X
85	MG	5	3707	-	X
85	MG	5	3710	-	X
85	MG	5	3717	-	X
85	MG	5	3721	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3726	-	X
85	MG	5	3727	-	X
85	MG	5	3730	-	X
85	MG	5	3731	-	X
85	MG	5	3732	-	X
85	MG	5	3734	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3743	-	X
85	MG	5	3746	-	X
85	MG	5	3748	-	X
85	MG	5	3751	-	X
85	MG	5	3755	-	X
85	MG	5	3756	-	X
85	MG	5	3757	-	X
85	MG	5	3763	-	X
85	MG	5	3764	-	X
85	MG	5	3766	-	X
85	MG	5	3770	-	X
85	MG	5	3772	-	X
85	MG	5	3776	-	X
85	MG	5	3780	-	X
85	MG	5	3783	-	X
85	MG	5	3785	-	X
85	MG	5	3786	-	X
85	MG	5	3790	-	X
85	MG	5	3793	-	X
85	MG	5	3796	-	X
85	MG	5	3802	-	X
85	MG	5	3803	-	X
85	MG	5	3807	-	X
85	MG	5	3813	-	X
85	MG	5	3815	-	X
85	MG	5	3821	-	X
85	MG	5	3823	-	X
85	MG	5	3825	-	X
85	MG	5	3827	-	X
85	MG	5	3828	-	X
85	MG	5	3832	-	X
85	MG	5	3833	-	X
85	MG	5	3841	-	X
85	MG	5	3844	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3846	-	X
85	MG	5	3847	-	X
85	MG	5	3848	-	X
85	MG	5	3853	-	X
85	MG	5	3855	-	X
85	MG	5	3856	-	X
85	MG	5	3858	-	X
85	MG	5	3864	-	X
85	MG	5	3867	-	X
85	MG	5	3868	-	X
85	MG	5	3869	-	X
85	MG	5	3871	-	X
85	MG	5	3872	-	X
85	MG	5	3874	-	X
85	MG	5	3875	-	X
85	MG	5	3877	-	X
85	MG	5	3880	-	X
85	MG	5	3881	-	X
85	MG	5	3882	-	X
85	MG	5	3884	-	X
85	MG	5	3887	-	X
85	MG	5	3892	-	X
85	MG	5	3894	-	X
85	MG	5	3896	-	X
85	MG	5	4253	-	X
85	MG	5	4254	-	X
85	MG	5	4255	-	X
85	MG	5	4257	-	X
85	MG	6	1901	-	X
85	MG	6	1903	-	X
85	MG	6	1904	-	X
85	MG	6	1906	-	X
85	MG	6	1907	-	X
85	MG	6	1908	-	X
85	MG	6	1909	-	X
85	MG	6	1910	-	X
85	MG	6	1911	-	X
85	MG	6	1912	-	X
85	MG	6	1913	-	X
85	MG	6	1914	-	X
85	MG	6	1916	-	X
85	MG	6	1917	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1918	-	X
85	MG	6	1919	-	X
85	MG	6	1920	-	X
85	MG	6	1921	-	X
85	MG	6	1922	-	X
85	MG	6	1923	-	X
85	MG	6	1925	-	X
85	MG	6	1926	-	X
85	MG	6	1927	-	X
85	MG	6	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1931	-	X
85	MG	6	1933	-	X
85	MG	6	1934	-	X
85	MG	6	1935	-	X
85	MG	6	1936	-	X
85	MG	6	1937	-	X
85	MG	6	1939	-	X
85	MG	6	1940	-	X
85	MG	6	1942	-	X
85	MG	6	1943	-	X
85	MG	6	1944	-	X
85	MG	6	1945	-	X
85	MG	6	1946	-	X
85	MG	6	1947	-	X
85	MG	6	1948	-	X
85	MG	6	1949	-	X
85	MG	6	1950	-	X
85	MG	6	1951	-	X
85	MG	6	1952	-	X
85	MG	6	1954	-	X
85	MG	6	1955	-	X
85	MG	6	1956	-	X
85	MG	6	1957	-	X
85	MG	6	1958	-	X
85	MG	6	1959	-	X
85	MG	6	1960	-	X
85	MG	6	1961	-	X
85	MG	6	1963	-	X
85	MG	6	1964	-	X
85	MG	6	1965	-	X
85	MG	6	1966	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1968	-	X
85	MG	6	1971	-	X
85	MG	6	1975	-	X
85	MG	6	1977	-	X
85	MG	6	1980	-	X
85	MG	6	1983	-	X
85	MG	6	1985	-	X
85	MG	6	1987	-	X
85	MG	6	1991	-	X
85	MG	6	1997	-	X
85	MG	6	1998	-	X
85	MG	6	2000	-	X
85	MG	6	2005	-	X
85	MG	6	2011	-	X
85	MG	6	2012	-	X
85	MG	6	2013	-	X
85	MG	6	2015	-	X
85	MG	6	2018	-	X
85	MG	6	2019	-	X
85	MG	6	2020	-	X
85	MG	6	2021	-	X
85	MG	6	2027	-	X
85	MG	6	2028	-	X
85	MG	6	2029	-	X
85	MG	6	2030	-	X
85	MG	6	2035	-	X
85	MG	6	2038	-	X
85	MG	6	2039	-	X
85	MG	6	2040	-	X
85	MG	6	2042	-	X
85	MG	6	2043	-	X
85	MG	6	2046	-	X
85	MG	7	201	-	X
85	MG	7	202	-	X
85	MG	7	203	-	X
85	MG	7	204	-	X
85	MG	7	205	-	X
85	MG	7	206	-	X
85	MG	7	207	-	X
85	MG	7	209	-	X
85	MG	7	213	-	X
85	MG	7	215	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	8	201	-	X
85	MG	8	203	-	X
85	MG	8	206	-	X
85	MG	8	207	-	X
85	MG	8	213	-	X
85	MG	M3	202	-	X
85	MG	M7	201	-	X
85	MG	N3	201	-	X
85	MG	SM	301	-	X
85	MG	c7	201	-	X
85	MG	c8	201	-	X
85	MG	d3	201	-	X
85	MG	l3	401	-	X
85	MG	l5	301	-	X
85	MG	l7	301	-	X
85	MG	m1	201	-	X
85	MG	m4	201	-	X
85	MG	n3	201	-	X
85	MG	n8	203	-	X
85	MG	n8	204	-	X
85	MG	n9	3802	-	X
85	MG	o1	201	-	X
85	MG	o3	202	-	X
85	MG	o4	202	-	X
85	MG	s1	301	-	X
86	OHX	1	3868	-	X
86	OHX	1	3872	-	X
86	OHX	1	3874	-	X
86	OHX	1	3891	-	X
86	OHX	1	3915	-	X
86	OHX	1	3924	-	X
86	OHX	1	3982	-	X
86	OHX	1	4017	-	X
86	OHX	1	4023	-	X
86	OHX	1	4031	-	X
86	OHX	1	4049	-	X
86	OHX	1	4050	-	X
86	OHX	1	4061	-	X
86	OHX	1	4065	-	X
86	OHX	1	4066	-	X
86	OHX	1	4067	-	X
86	OHX	1	4071	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4073	-	X
86	OHX	1	4076	-	X
86	OHX	1	4081	-	X
86	OHX	1	4085	-	X
86	OHX	1	4086	-	X
86	OHX	1	4098	-	X
86	OHX	1	4102	-	X
86	OHX	1	4111	-	X
86	OHX	1	4113	-	X
86	OHX	1	4114	-	X
86	OHX	1	4116	-	X
86	OHX	1	4118	-	X
86	OHX	1	4122	-	X
86	OHX	1	4123	-	X
86	OHX	1	4124	-	X
86	OHX	1	4125	-	X
86	OHX	1	4128	-	X
86	OHX	1	4129	-	X
86	OHX	1	4130	-	X
86	OHX	1	4135	-	X
86	OHX	1	4136	-	X
86	OHX	1	4138	-	X
86	OHX	1	4140	-	X
86	OHX	1	4141	-	X
86	OHX	1	4142	-	X
86	OHX	1	4144	-	X
86	OHX	1	4145	-	X
86	OHX	1	4146	-	X
86	OHX	1	4148	-	X
86	OHX	1	4149	-	X
86	OHX	1	4150	-	X
86	OHX	1	4155	-	X
86	OHX	1	4156	-	X
86	OHX	1	4157	-	X
86	OHX	1	4160	-	X
86	OHX	1	4161	-	X
86	OHX	1	4162	-	X
86	OHX	1	4165	-	X
86	OHX	1	4166	-	X
86	OHX	1	4167	-	X
86	OHX	1	4169	-	X
86	OHX	1	4170	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4171	-	X
86	OHX	1	4172	-	X
86	OHX	1	4173	-	X
86	OHX	1	4174	-	X
86	OHX	1	4176	-	X
86	OHX	1	4177	-	X
86	OHX	1	4178	-	X
86	OHX	1	4179	-	X
86	OHX	1	4180	-	X
86	OHX	1	4183	-	X
86	OHX	1	4184	-	X
86	OHX	1	4185	-	X
86	OHX	1	4187	-	X
86	OHX	1	4188	-	X
86	OHX	1	4189	-	X
86	OHX	1	4191	-	X
86	OHX	1	4192	-	X
86	OHX	1	4193	-	X
86	OHX	1	4195	-	X
86	OHX	1	4197	-	X
86	OHX	1	4199	-	X
86	OHX	1	4201	-	X
86	OHX	1	4202	-	X
86	OHX	1	4203	-	X
86	OHX	1	4204	-	X
86	OHX	1	4205	-	X
86	OHX	1	4206	-	X
86	OHX	1	4208	-	X
86	OHX	1	4209	-	X
86	OHX	1	4210	-	X
86	OHX	1	4211	-	X
86	OHX	1	4212	-	X
86	OHX	1	4214	-	X
86	OHX	1	4215	-	X
86	OHX	2	2026	-	X
86	OHX	2	2031	-	X
86	OHX	2	2075	-	X
86	OHX	2	2080	-	X
86	OHX	2	2099	-	X
86	OHX	2	2103	-	X
86	OHX	2	2117	-	X
86	OHX	2	2119	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2123	-	X
86	OHX	2	2126	-	X
86	OHX	2	2134	-	X
86	OHX	2	2136	-	X
86	OHX	2	2137	-	X
86	OHX	2	2138	-	X
86	OHX	2	2144	-	X
86	OHX	2	2146	-	X
86	OHX	2	2147	-	X
86	OHX	2	2149	-	X
86	OHX	2	2154	-	X
86	OHX	2	2155	-	X
86	OHX	2	2156	-	X
86	OHX	2	2158	-	X
86	OHX	2	2160	-	X
86	OHX	2	2161	-	X
86	OHX	2	2163	-	X
86	OHX	2	2164	-	X
86	OHX	2	2165	-	X
86	OHX	2	2167	-	X
86	OHX	2	2170	-	X
86	OHX	2	2172	-	X
86	OHX	2	2173	-	X
86	OHX	2	2174	-	X
86	OHX	2	2176	-	X
86	OHX	2	2177	-	X
86	OHX	2	2179	-	X
86	OHX	2	2180	-	X
86	OHX	3	223	-	X
86	OHX	3	225	-	X
86	OHX	4	227	-	X
86	OHX	4	232	-	X
86	OHX	4	233	-	X
86	OHX	4	235	-	X
86	OHX	4	236	-	X
86	OHX	5	3899	-	X
86	OHX	5	3900	-	X
86	OHX	5	3903	-	X
86	OHX	5	3909	-	X
86	OHX	5	3912	-	X
86	OHX	5	3913	-	X
86	OHX	5	3951	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4027	-	X
86	OHX	5	4039	-	X
86	OHX	5	4044	-	X
86	OHX	5	4089	-	X
86	OHX	5	4092	-	X
86	OHX	5	4099	-	X
86	OHX	5	4105	-	X
86	OHX	5	4108	-	X
86	OHX	5	4110	-	X
86	OHX	5	4112	-	X
86	OHX	5	4114	-	X
86	OHX	5	4125	-	X
86	OHX	5	4126	-	X
86	OHX	5	4127	-	X
86	OHX	5	4132	-	X
86	OHX	5	4134	-	X
86	OHX	5	4136	-	X
86	OHX	5	4137	-	X
86	OHX	5	4139	-	X
86	OHX	5	4140	-	X
86	OHX	5	4141	-	X
86	OHX	5	4142	-	X
86	OHX	5	4144	-	X
86	OHX	5	4145	-	X
86	OHX	5	4146	-	X
86	OHX	5	4147	-	X
86	OHX	5	4148	-	X
86	OHX	5	4149	-	X
86	OHX	5	4150	-	X
86	OHX	5	4151	-	X
86	OHX	5	4152	-	X
86	OHX	5	4154	-	X
86	OHX	5	4156	-	X
86	OHX	5	4157	-	X
86	OHX	5	4158	-	X
86	OHX	5	4159	-	X
86	OHX	5	4160	-	X
86	OHX	5	4161	-	X
86	OHX	5	4163	-	X
86	OHX	5	4164	-	X
86	OHX	5	4170	-	X
86	OHX	5	4171	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4172	-	X
86	OHX	5	4173	-	X
86	OHX	5	4175	-	X
86	OHX	5	4176	-	X
86	OHX	5	4177	-	X
86	OHX	5	4179	-	X
86	OHX	5	4181	-	X
86	OHX	5	4182	-	X
86	OHX	5	4183	-	X
86	OHX	5	4184	-	X
86	OHX	5	4185	-	X
86	OHX	5	4188	-	X
86	OHX	5	4189	-	X
86	OHX	5	4190	-	X
86	OHX	5	4191	-	X
86	OHX	5	4193	-	X
86	OHX	5	4194	-	X
86	OHX	5	4195	-	X
86	OHX	5	4199	-	X
86	OHX	5	4200	-	X
86	OHX	5	4201	-	X
86	OHX	5	4202	-	X
86	OHX	5	4203	-	X
86	OHX	5	4208	-	X
86	OHX	5	4210	-	X
86	OHX	5	4211	-	X
86	OHX	5	4212	-	X
86	OHX	5	4214	-	X
86	OHX	5	4216	-	X
86	OHX	5	4217	-	X
86	OHX	5	4218	-	X
86	OHX	5	4219	-	X
86	OHX	5	4220	-	X
86	OHX	5	4221	-	X
86	OHX	5	4225	-	X
86	OHX	5	4227	-	X
86	OHX	5	4228	-	X
86	OHX	5	4229	-	X
86	OHX	5	4230	-	X
86	OHX	5	4233	-	X
86	OHX	5	4234	-	X
86	OHX	5	4235	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4236	-	X
86	OHX	5	4238	-	X
86	OHX	5	4239	-	X
86	OHX	5	4244	-	X
86	OHX	5	4245	-	X
86	OHX	5	4246	-	X
86	OHX	5	4247	-	X
86	OHX	5	4248	-	X
86	OHX	6	2048	-	X
86	OHX	6	2053	-	X
86	OHX	6	2055	-	X
86	OHX	6	2126	-	X
86	OHX	6	2127	-	X
86	OHX	6	2144	-	X
86	OHX	6	2147	-	X
86	OHX	6	2157	-	X
86	OHX	6	2160	-	X
86	OHX	6	2161	-	X
86	OHX	6	2162	-	X
86	OHX	6	2163	-	X
86	OHX	6	2165	-	X
86	OHX	6	2168	-	X
86	OHX	6	2169	-	X
86	OHX	6	2171	-	X
86	OHX	6	2174	-	X
86	OHX	6	2176	-	X
86	OHX	6	2177	-	X
86	OHX	6	2178	-	X
86	OHX	6	2180	-	X
86	OHX	6	2181	-	X
86	OHX	6	2183	-	X
86	OHX	6	2184	-	X
86	OHX	6	2186	-	X
86	OHX	6	2187	-	X
86	OHX	6	2188	-	X
86	OHX	6	2189	-	X
86	OHX	6	2190	-	X
86	OHX	6	2191	-	X
86	OHX	6	2194	-	X
86	OHX	6	2195	-	X
86	OHX	6	2196	-	X
86	OHX	6	2197	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2198	-	X
86	OHX	6	2199	-	X
86	OHX	6	2200	-	X
86	OHX	6	2203	-	X
86	OHX	6	2204	-	X
86	OHX	7	225	-	X
86	OHX	7	227	-	X
86	OHX	8	219	-	X
86	OHX	8	224	-	X
86	OHX	8	225	-	X
86	OHX	8	227	-	X
86	OHX	8	228	-	X
86	OHX	8	229	-	X
86	OHX	M7	207	-	X
86	OHX	M9	202	-	X
86	OHX	O9	101	-	X
86	OHX	l4	403	-	X
86	OHX	m7	206	-	X
86	OHX	s9	201	-	X
87	ZN	d7	101	-	X
88	3H3	1	4216	-	X

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411226 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1750	Total	C	N	O	P	0	0	0
			37283	16668	6591	12274	1750			
1	6	1795	Total	C	N	O	P	0	0	0
			38238	17095	6758	12590	1795			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			773	500	126	145	2			
12	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745
c0	89	ALA	GLY	conflict	UNP Q08745

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47
c1	147	ALA	GLY	conflict	UNP P0CX47

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			
35	sM	104	Total	C	N	O	0	0	0
			680	403	140	137			

- Molecule 36 is a RNA chain called *Saccharomyces cerevisiae* chromosome XII cosmid 9634.

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

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

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 *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 S30-A.

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

- Molecule 81 is a protein called Unknown protein m2.

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 Unknown protein p1.

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 Unknown protein p2.

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

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	2	Total 2	Mg 2	0	0
85	m7	5	Total 5	Mg 5	0	0
85	n8	4	Total 4	Mg 4	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	147	Total 147	Mg 147	0	0
85	sM	2	Total 2	Mg 2	0	0
85	O4	1	Total 1	Mg 1	0	0
85	m5	1	Total 1	Mg 1	0	0
85	l3	1	Total 1	Mg 1	0	0
85	M1	1	Total 1	Mg 1	0	0
85	n0	2	Total 2	Mg 2	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	126	Total 126	Mg 126	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	3	Total 3	Mg 3	0	0
85	l7	1	Total 1	Mg 1	0	0
85	M5	2	Total 2	Mg 2	0	0
85	l4	1	Total 1	Mg 1	0	0
85	L8	1	Total 1	Mg 1	0	0
85	o4	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	504	Total 504	Mg 504	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	n9	2	Total 2	Mg 2	0	0
85	1	475	Total 475	Mg 475	0	0
85	d2	1	Total 1	Mg 1	0	0
85	n6	2	Total 2	Mg 2	0	0
85	S8	1	Total 1	Mg 1	0	0
85	m1	2	Total 2	Mg 2	0	0
85	d3	1	Total 1	Mg 1	0	0
85	q3	1	Total 1	Mg 1	0	0
85	o3	2	Total 2	Mg 2	0	0
85	M3	4	Total 4	Mg 4	0	0

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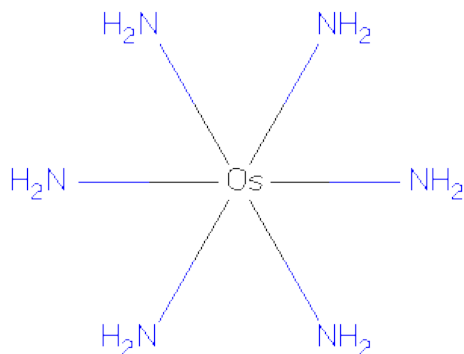
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N3	3	Total 3	Mg 3	0	0
85	N8	2	Total 2	Mg 2	0	0
85	4	21	Total 21	Mg 21	0	0
85	L2	1	Total 1	Mg 1	0	0
85	l5	3	Total 3	Mg 3	0	0
85	C3	1	Total 1	Mg 1	0	0
85	M7	6	Total 6	Mg 6	0	0
85	m4	1	Total 1	Mg 1	0	0
85	L6	1	Total 1	Mg 1	0	0
85	s1	1	Total 1	Mg 1	0	0
85	m6	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	15	Total 15	Mg 15	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	2	Total 2	Mg 2	0	0
85	l2	2	Total 2	Mg 2	0	0
85	8	13	Total 13	Mg 13	0	0
85	M6	1	Total 1	Mg 1	0	0
85	N0	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	3	14	Total	Mg	0	0
			14	14		

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	4	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	L6	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M6	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O2	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	Q2	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	s1	1	Total 7	N 6	Os 1	0	0
86	s1	1	Total 7	N 6	Os 1	0	0
86	s4	1	Total 7	N 6	Os 1	0	0
86	s8	1	Total 7	N 6	Os 1	0	0
86	s9	1	Total 7	N 6	Os 1	0	0
86	c1	1	Total 7	N 6	Os 1	0	0
86	c3	1	Total 7	N 6	Os 1	0	0
86	c5	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	c8	1	Total	N	Os	0	0
			7	6	1		
86	d4	1	Total	N	Os	0	0
			7	6	1		
86	d9	1	Total	N	Os	0	0
			7	6	1		
86	sR	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
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86	19	1	Total	N	Os	0	0
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86	m0	1	Total	N	Os	0	0
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86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m6	1	Total	N	Os	0	0
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86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	o4	1	Total	N	Os	0	0
			7	6	1		
86	o7	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

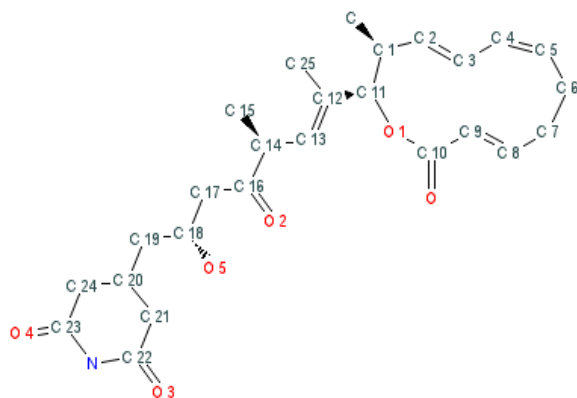
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q3	1	Total	Zn	0	0
			1	1		
87	d9	1	Total	Zn	0	0
			1	1		
87	D7	1	Total	Zn	0	0
			1	1		
87	d6	1	Total	Zn	0	0
			1	1		
87	o7	1	Total	Zn	0	0
			1	1		
87	O7	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		

- Molecule 88 is 4-{(2R,5S,6E)-2-hydroxy-5-methyl-7-[(2R,3S,4E,6Z,10E)-3-methyl-12-oxooxacyclododeca-4,6,10-trien-2-yl]-4-oxooct-6-en-1-yl}piperidine-2,6-dione (three-letter code: 3H3) (formula: C₂₆H₃₅NO₆).

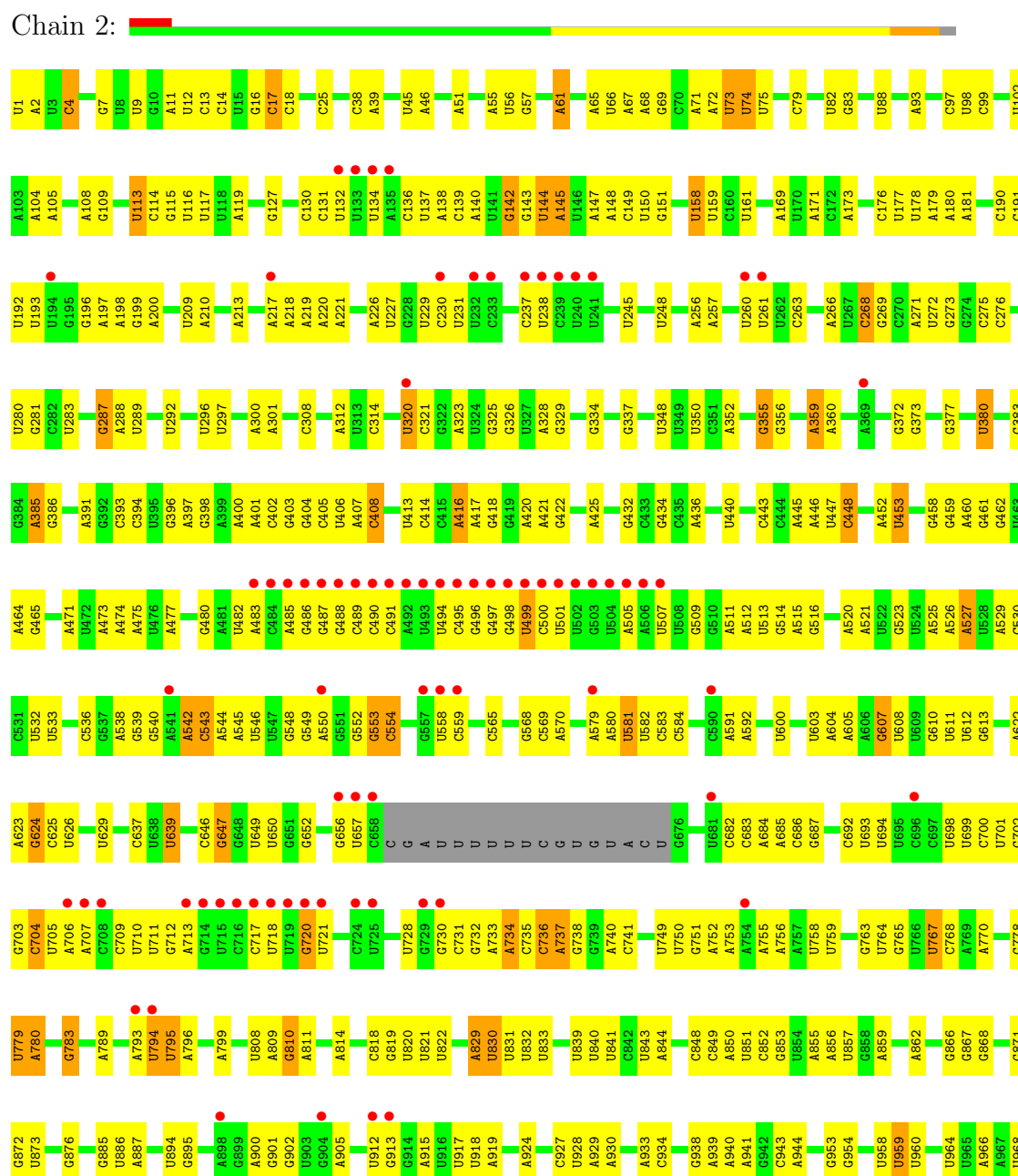


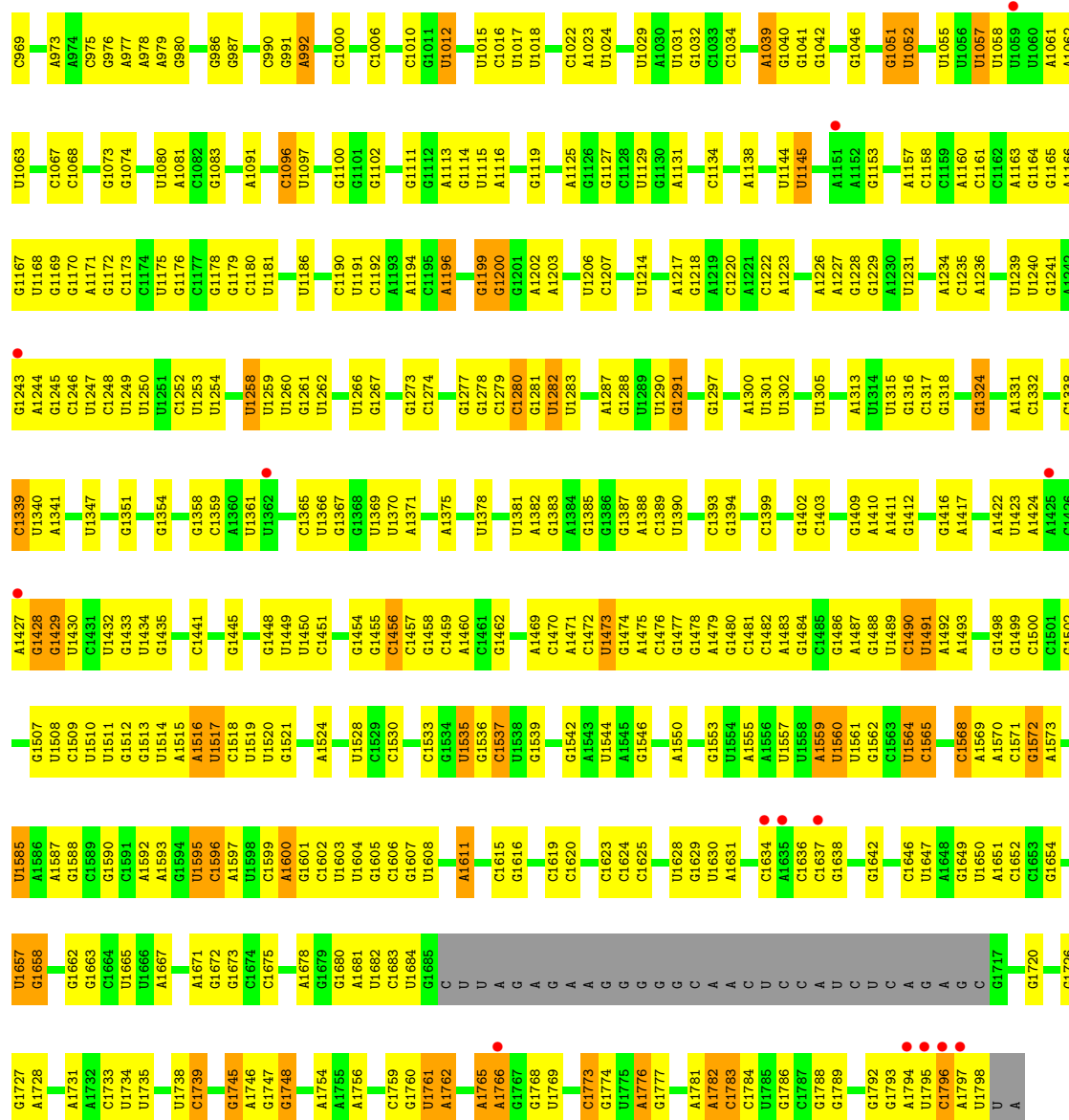
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			33	26	1	6		
88	5	1	Total	C	N	O	0	0
			33	26	1	6		

3 Residue-property plots

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

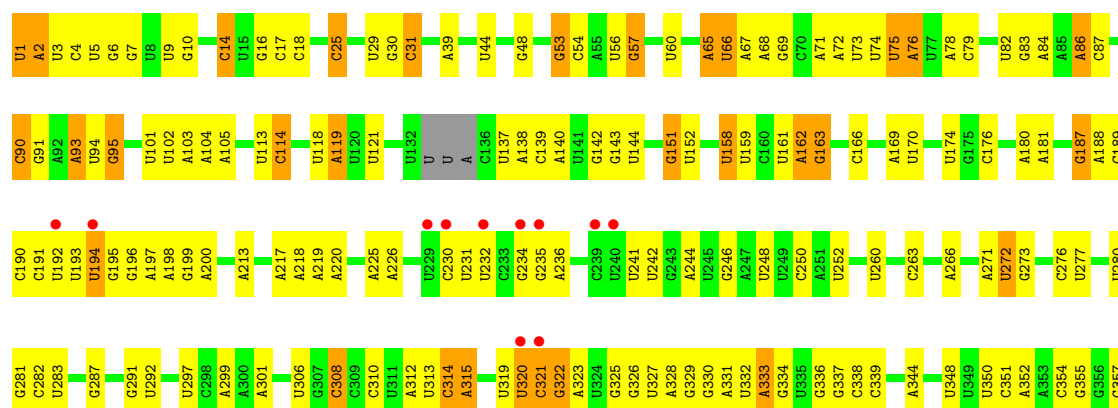
• Molecule 1: 18S rRNA



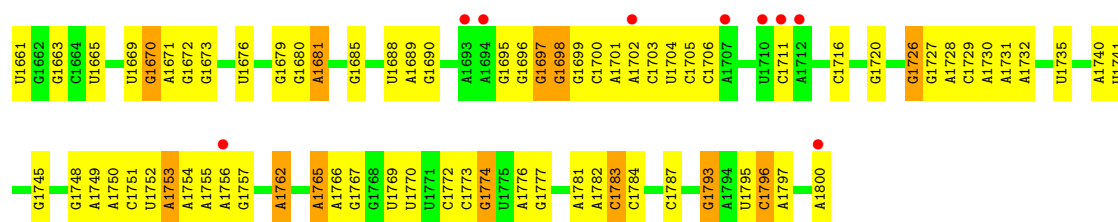


• Molecule 1: 18S rRNA

Chain 6:

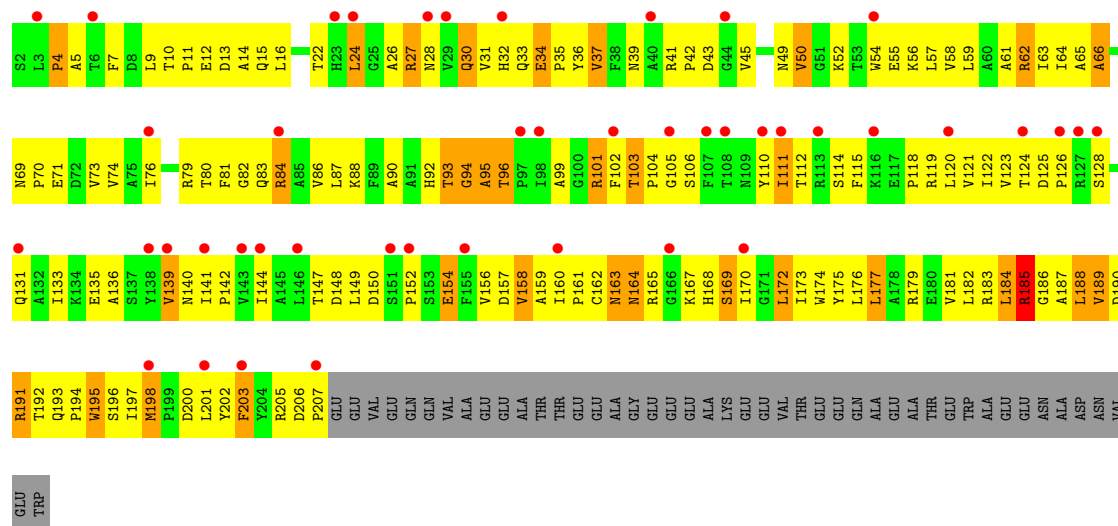


U1579	G1502	A1417	G1318	C1216	A1133	G1048	U965	U857	G765	U675	G597	A521	A437	U358
G1584	A1503	G1418	A1321	A1217	C1134	U1049	A956	G858	U766	G677	U600	G523	C443	A359
G1504	A1506	A1426	G1330	A1219	A1138	G1050	U968	A859	U767	A678	U603	G523	C449	A360
A1586	U1508	A1425	A1331	A1227	U1144	G1063	A970	A862	A770	U679	U604	A529	C448	G362
G1588	C1332	A1427	C1332	A1228	U1145	U1068	A973	A863	G775	U680	U607	U532	U453	A369
C1589	U1510	G1428	C1333	G1229	U1146	U1059	A978	U864	G778	C682	U608	U533	U454	A370
G1590	U1511	U1430	U1335	A1230	C1148	G1064	A979	G871	U782	C683	U609	C536	U455	U374
C1591	G1512	C1431	A1336	U1239	U1149	A1065	G980	U872	U783	U687	U610	G537	U456	U375
A1592	G1513	U1432	C1340	C1234	G1150	C1068	G986	G873	U788	U689	G613	A538	U457	C376
U1595	U1514	G1433	U1340	A1235	A1151	A1088	G987	C874	U789	U694	G614	G539	C459	G377
C1586	A1515	U1434	A1341	A1236	A1152	A1089	G988	C875	A788	U695	G615	G540	A470	G378
A1597	U1516	G1435	A1344	A1237	A1153	C1070	G989	G876	U793	C696	A615	A541	A471	U379
U1598	U1517	A1436	A1344	A1238	G1154	U1071	U989	U879	U794	U698	A623	C543	U474	U380
C1599	C1518	U1437	A1345	U1239	G1154	U1072	G990	G879	U795	U699	G624	A544	U475	C381
A1600	U1521	C1441	U1350	U1240	A1157	G1073	G991	G880	U800	C700	G625	A545	U476	C382
G1601	G1524	U1442	G1351	G1241	A1160	G1074	A992	U894	U801	U701	G629	A546	U477	A387
G1605	A1524	U1443	G1354	A1242	C1161	C1078	A993	G895	G801	G703	A630	U547	U478	G388
U1608	A1525	A1444	G1354	G1243	C1162	U1080	A994	U902	A804	U704	U633	U548	U481	G389
A1611	C1529	U1445	A1357	G1245	A1163	U1081	A995	A900	A805	U705	U634	A550	U482	G390
G1614	U1534	G1446	G1358	U1246	A1166	C1082	G1000	G901	A806	A706	U635	C554	A483	C393
C1615	U1535	U1447	C1359	C1248	G1167	C1083	A1001	U903	U813	U713	A636	C557	A484	C394
G1616	U1536	G1448	A1360	U1249	C1167	A1084	A1002	U904	G814	U714	U637	U558	A485	A397
C1617	C1537	C1456	U1361	U1250	A1171	G1085	A1003	G913	G815	U715	U638	U559	A486	G398
U1619	U1538	C1457	U1362	U1251	C1172	A1088	C1006	G914	G816	C716	U639	U560	A487	A399
C1620	G1539	G1458	G1364	U1253	U1175	U1095	C1007	U915	A817	C717	U640	U561	A488	A400
U1621	U1540	C1459	G1365	U1254	G1176	A1091	C1010	U916	C818	U718	C646	U562	A489	A401
G1622	U1541	C1461	U1366	G1255	C1177	A1092	G1011	U917	G819	U719	C647	C565	A490	C402
U1628	G1542	G1462	U1370	U1257	G1178	U1096	G1012	U918	U820	U720	C648	C566	A491	G403
G1629	A1543	C1463	A1371	U1258	G1179	U1097	G1013	U919	U821	U721	U649	C567	A492	G404
U1630	U1544	G1464	C1379	U1259	C1180	U1098	C1014	U920	U822	U722	U650	C568	A493	C405
A1631	C1549	U1465	G1382	G1263	A1183	U1099	C1015	G922	G823	G723	C652	C569	A494	C406
C1634	U1552	A1471	A1382	G1264	C1192	G1100	C1016	A923	G824	U727	C653	A570	A495	U406
G1635	G1553	U1472	G1385	U1265	A1193	G1101	C1017	A926	U825	U728	C654	C571	A496	U407
C1637	U1558	G1477	A1388	U1269	C1194	G1102	A1026	C931	C826	G729	C655	C572	A497	C408
G1638	A1559	A1478	C1389	C1274	A1196	U1103	C1027	C934	U829	U730	C656	C577	A498	C409
C1639	U1560	A1479	U1392	C1279	C1197	G1107	A1028	C934	U830	C658	C659	U578	A501	A410
G1645	U1561	G1480	C1393	G1280	G1198	G1108	U1029	A944	U831	A734	C660	C583	U502	A416
U1649	G1562	C1481	G1394	G1281	G1199	U1109	U1030	U945	U832	G737	U662	C584	U503	A417
U1650	U1563	C1482	G1395	U1282	G1200	G1201	U1031	U946	U833	U738	U663	A585	A504	G418
A1651	C1564	A1483	U1396	U1283	G1201	U1120	G1032	U947	G837	C747	U664	C586	A505	A421
G1654	U1565	G1484	U1397	U1293	A1202	U1121	C1033	A951	G838	U739	U665	C587	U506	G422
C1655	U1566	U1485	U1398	U1294	A1203	C1121	G1034	C956	U843	G751	U666	C588	U507	A425
U1656	C1568	C1490	C1399	G1299	C1207	G1122	A1035	G957	U844	A752	U667	C589	A511	G429
A1659	U1569	U1491	A1400	C1309	A1208	C1123	A1036	U958	G846	G669	C668	C590	A512	C430
U1657	G1572	A1492	A1401	U1312	C1209	A1125	A1039	U959	A847	A754	U670	A591	U513	C431
A1659	A1573	C1494	G1402	A1312	C1210	G1126	G1040	U960	C848	A755	G	A592	G514	G432
G1660	U1574	G1498	G1408	C1317	A1211	U1129	G1041	U964	C849	A756	U	A593	A515	G433
					C1212	G1130	C1045		A856	A757	C674	G595	G516	C434
					G1213					U758		C596	A518	



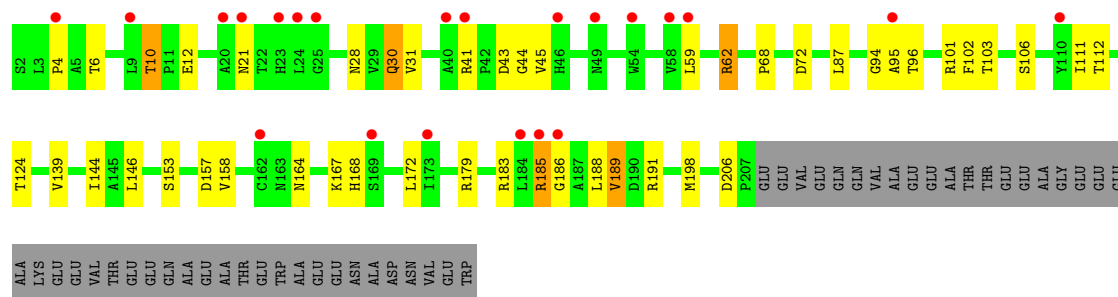
• Molecule 2: 40S ribosomal protein S0-A

Chain S0:



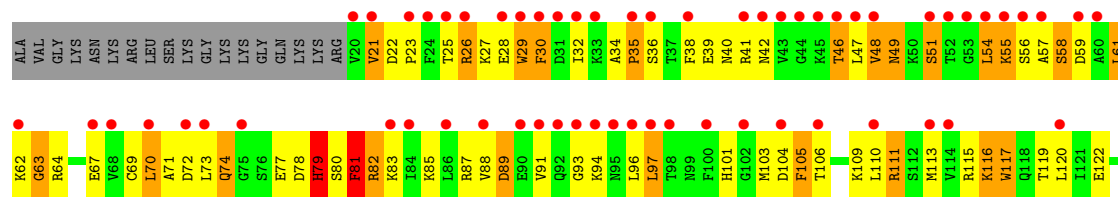
• Molecule 2: 40S ribosomal protein S0-A

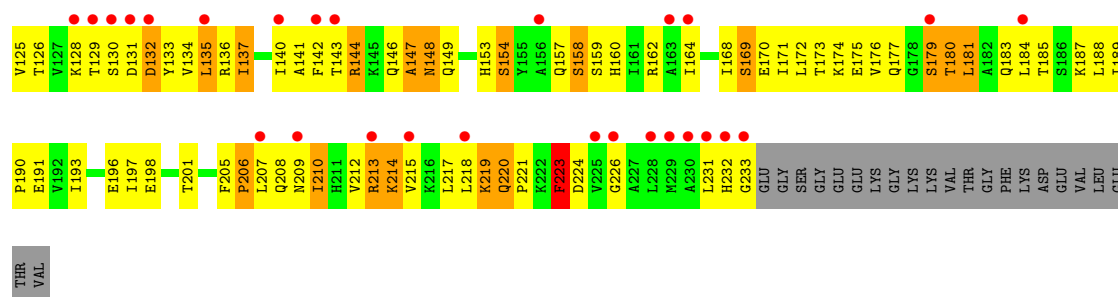
Chain s0:



• Molecule 3: 40S ribosomal protein S1-A

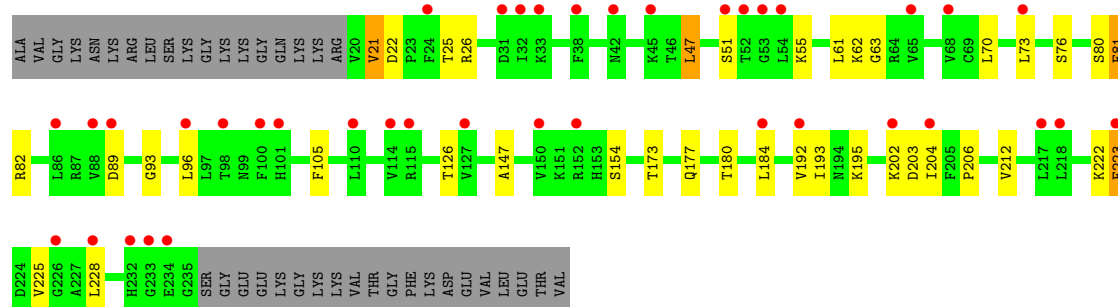
Chain S1:





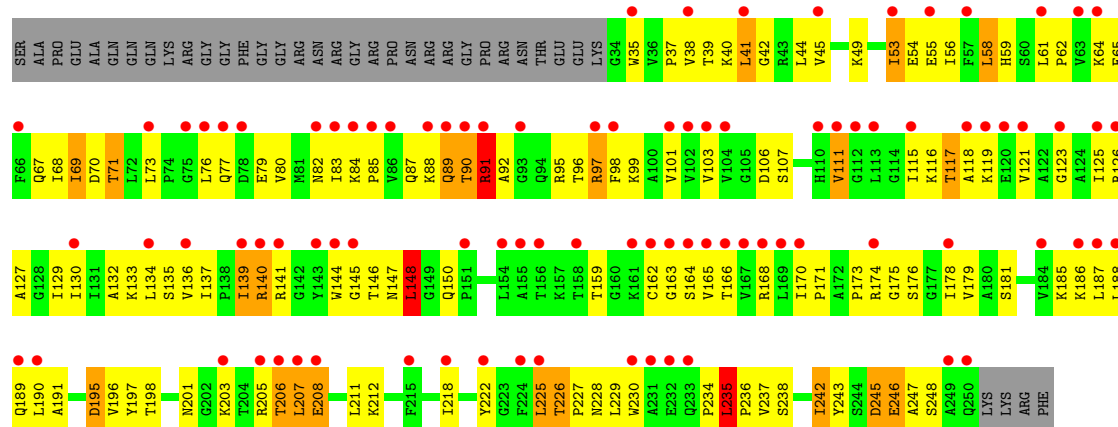
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



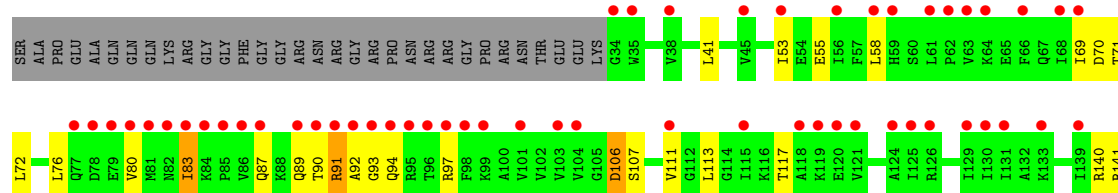
• Molecule 4: 40S ribosomal protein S2

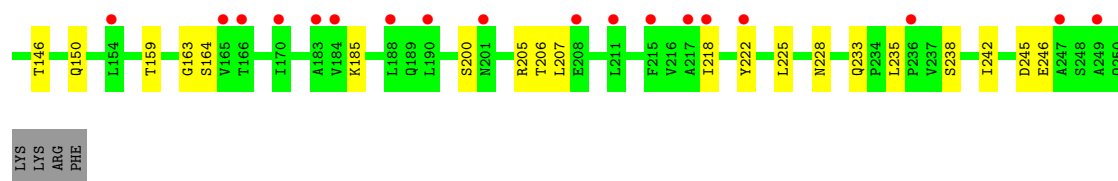
Chain S2:



• Molecule 4: 40S ribosomal protein S2

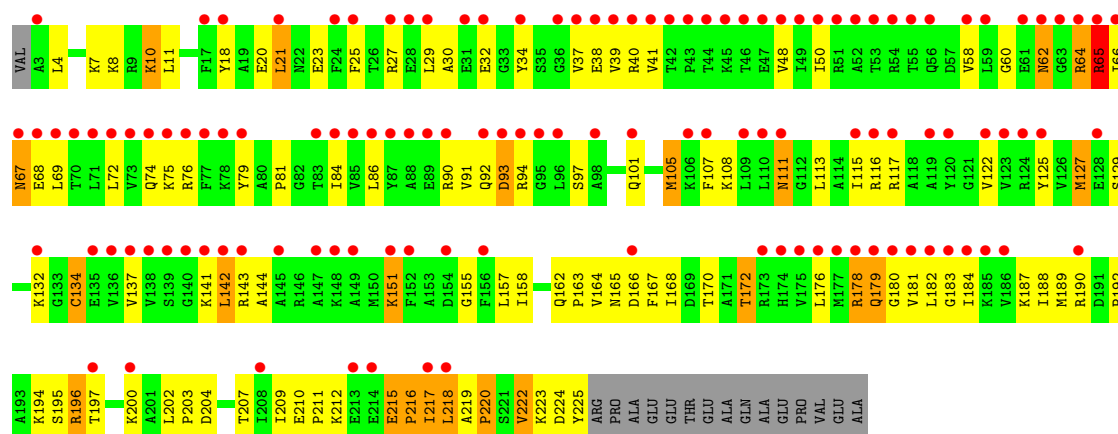
Chain s2:





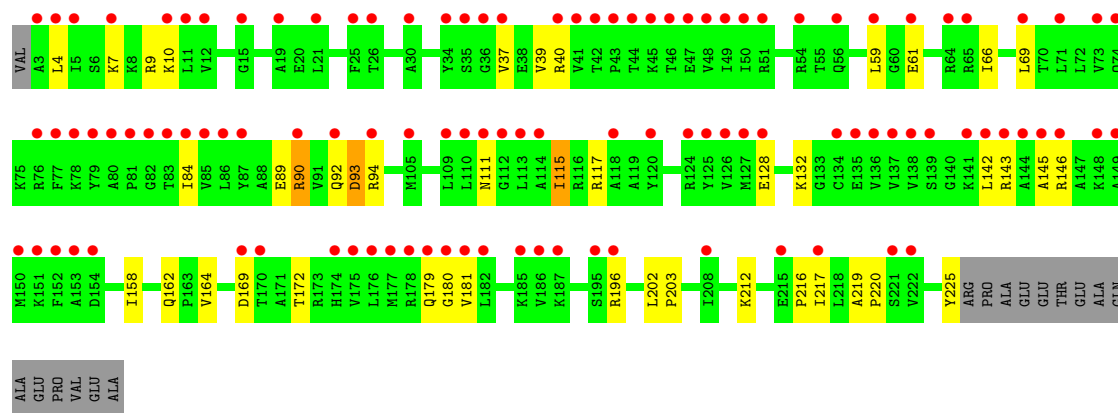
• Molecule 5: 40S ribosomal protein S3

Chain S3:



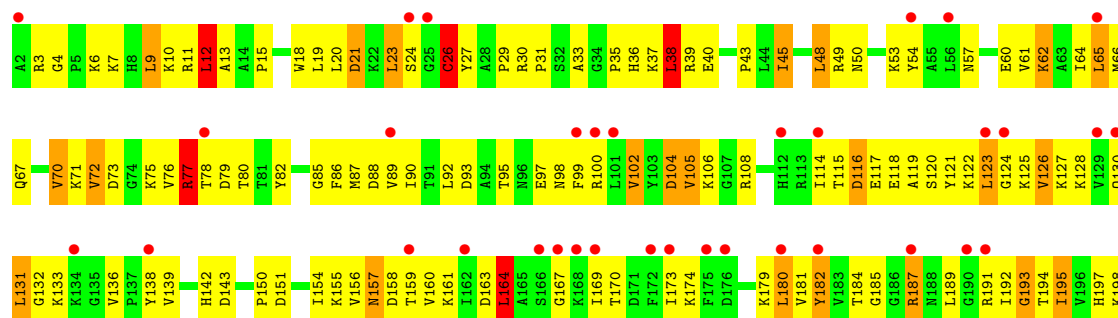
• Molecule 5: 40S ribosomal protein S3

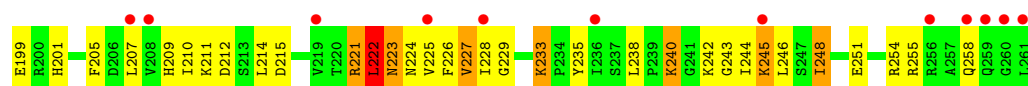
Chain s3:



• Molecule 6: 40S ribosomal protein S4-A

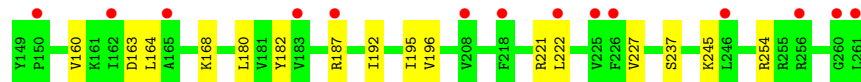
Chain S4:





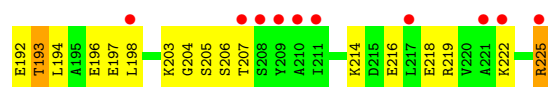
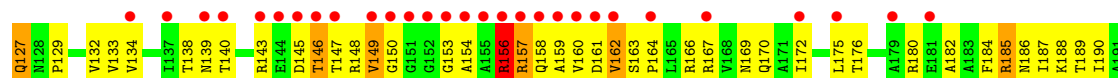
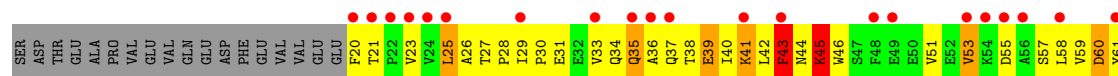
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



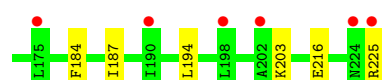
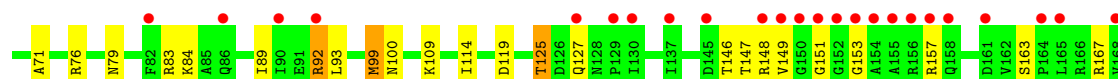
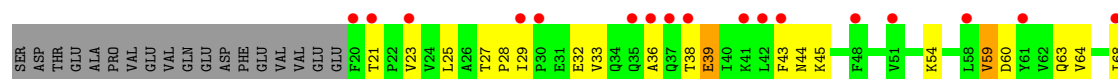
• Molecule 7: 40S ribosomal protein S5

Chain S5:



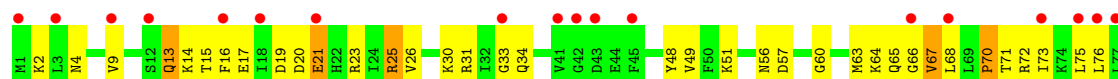
• Molecule 7: 40S ribosomal protein S5

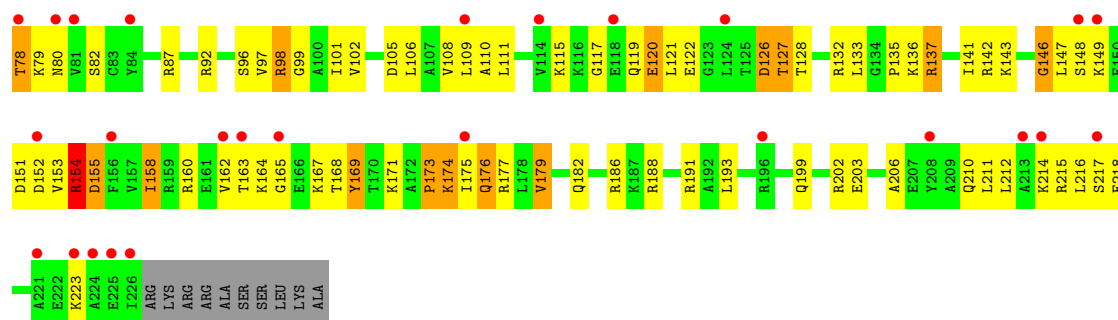
Chain s5:



• Molecule 8: 40S ribosomal protein S6-A

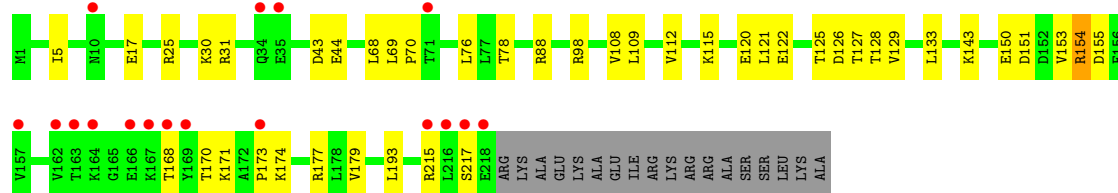
Chain S6:





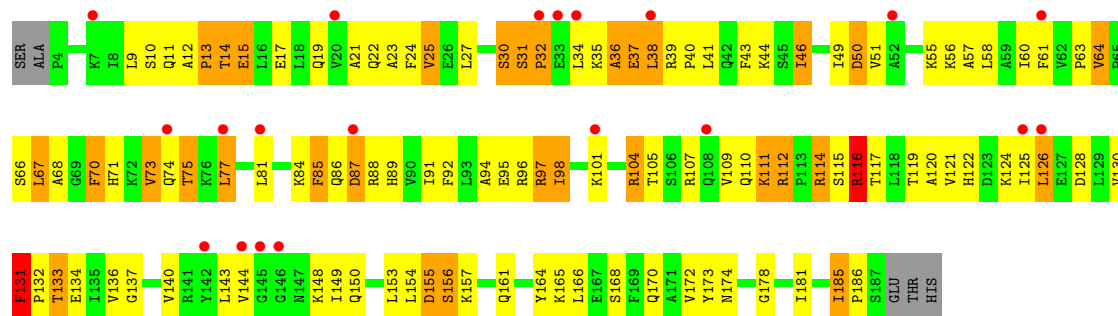
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



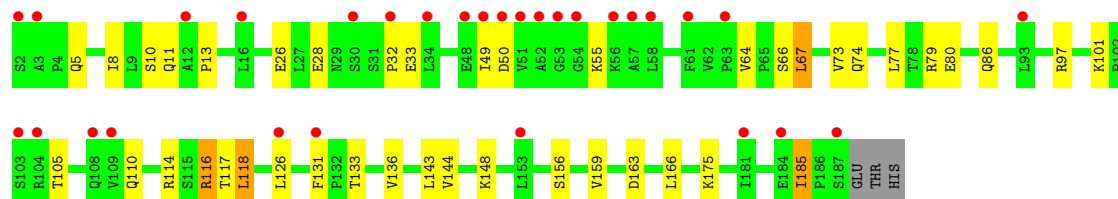
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



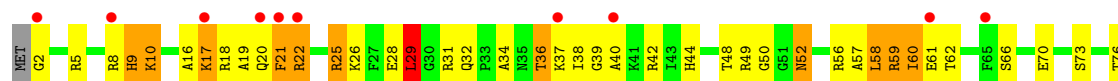
• Molecule 9: 40S ribosomal protein S7-A

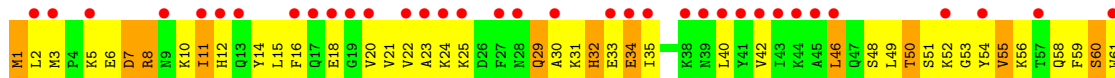
Chain s7:

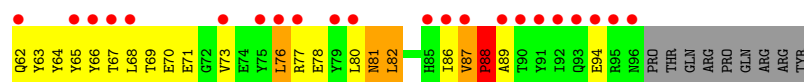


• Molecule 10: 40S ribosomal protein S8-A

Chain S8:

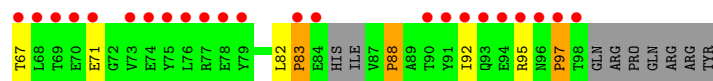
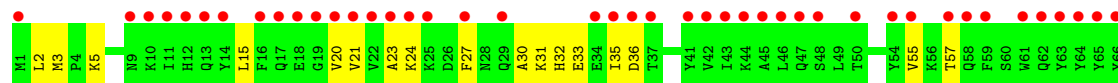






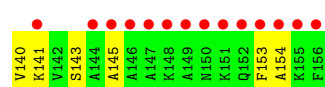
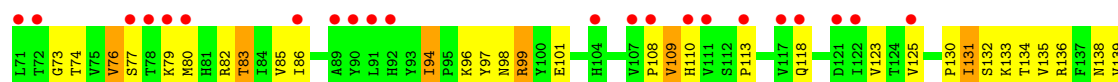
• Molecule 12: 40S ribosomal protein S10-A

Chain c0:



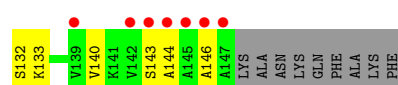
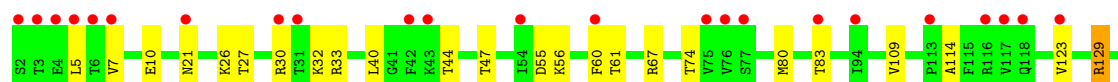
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:



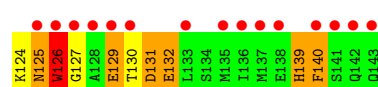
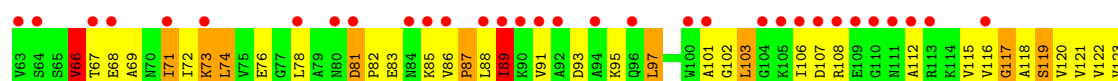
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



• Molecule 14: 40S ribosomal protein S12

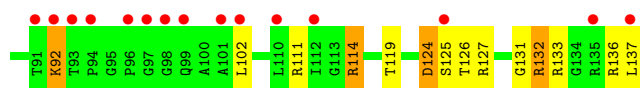
Chain C2:



• Molecule 14: 40S ribosomal protein S12

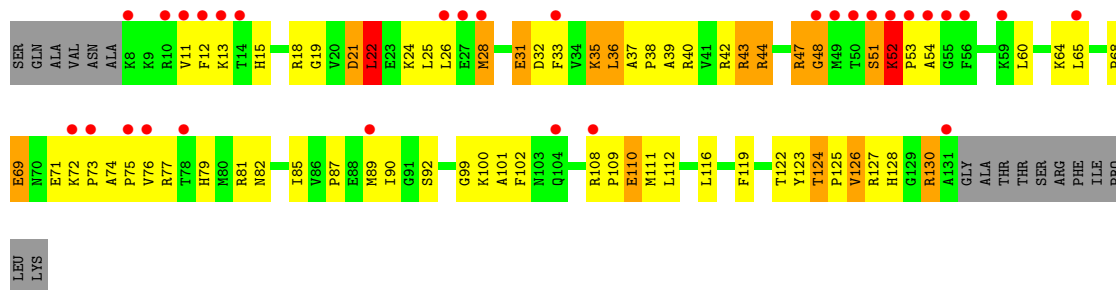
Group	Very satisfied (%)
All respondents	65
Those who have been in the U.S. for 10 years or more	55





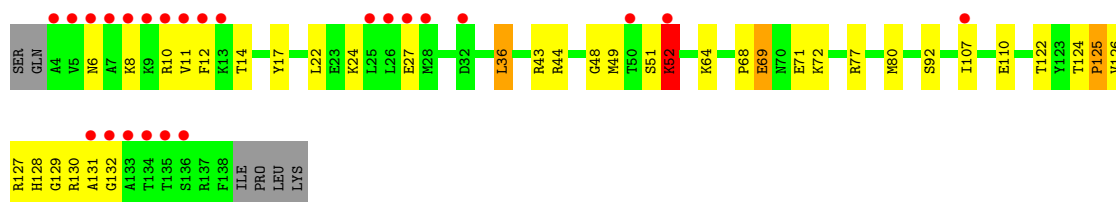
- Molecule 17: 40S ribosomal protein S15

Chain C5:



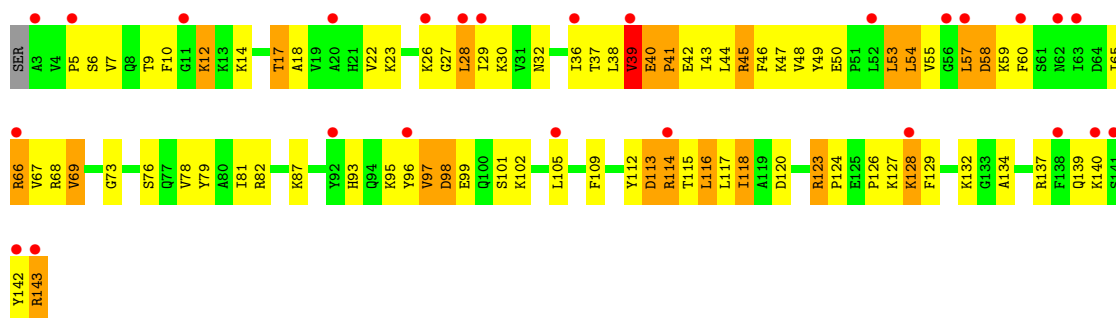
- Molecule 17: 40S ribosomal protein S15

Chain c5:



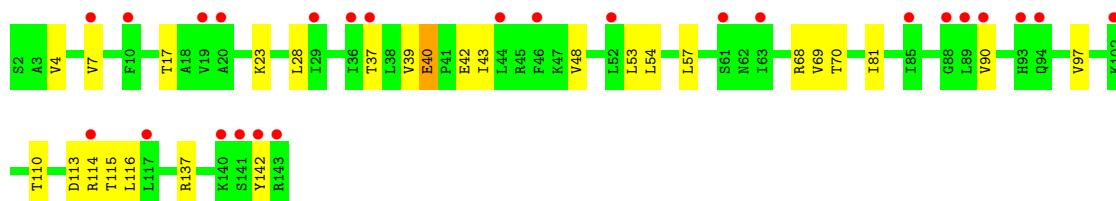
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



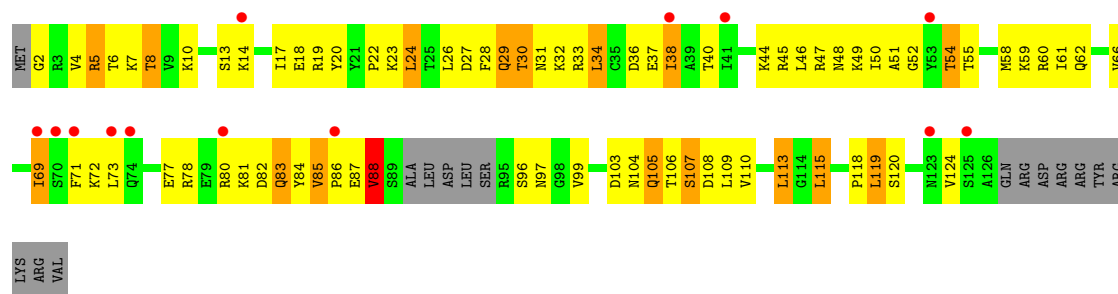
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:



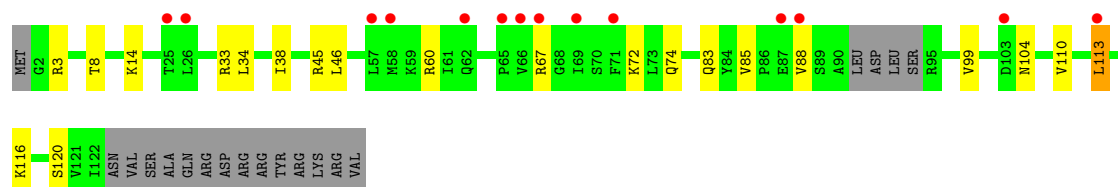
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:



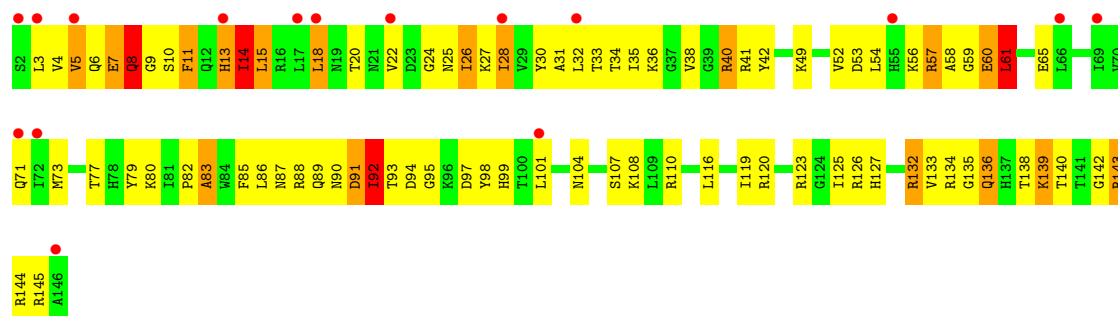
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:



- Molecule 20: 40S ribosomal protein S18-A

Chain C8:



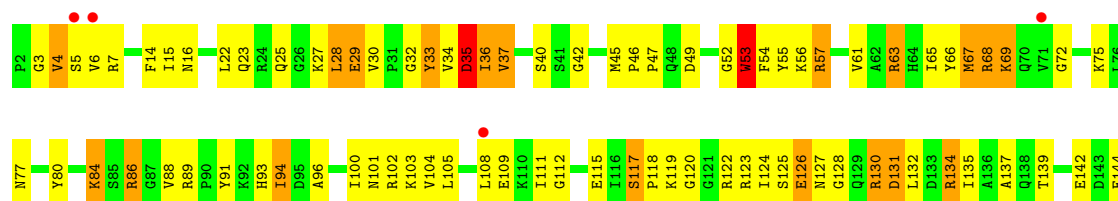
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



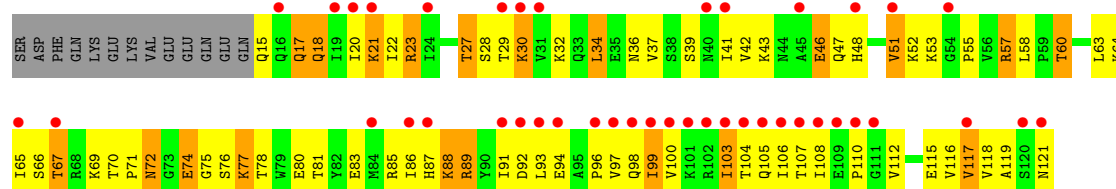
- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 



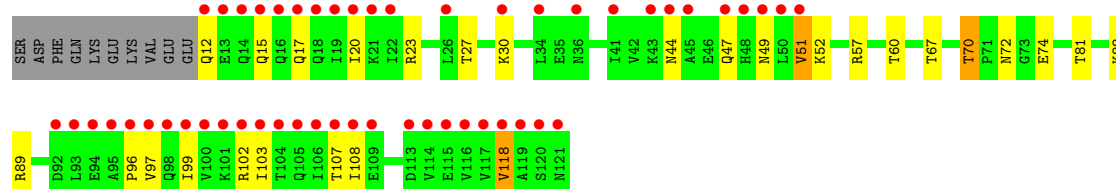
- Molecule 22: 40S ribosomal protein S20

Chain D0: 



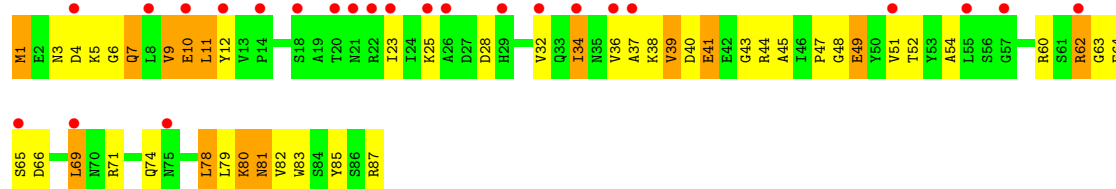
- Molecule 22: 40S ribosomal protein S20

Chain d0: 



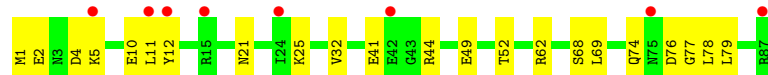
- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 



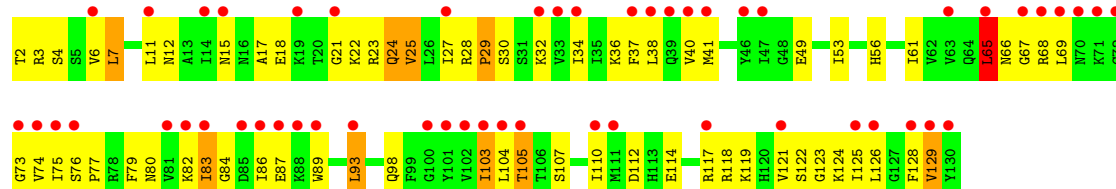
- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 

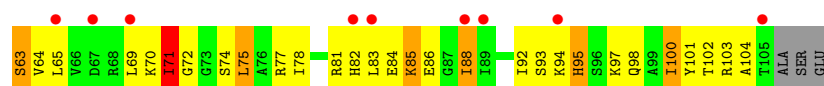


- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 

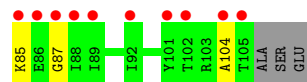
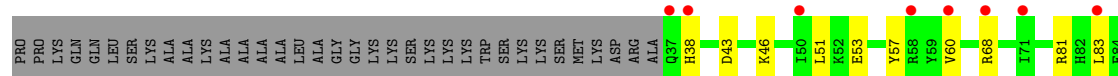


- [illegible]



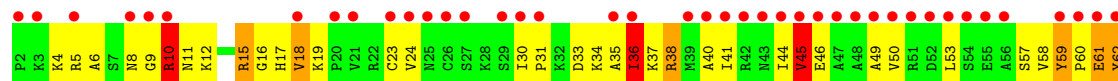
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



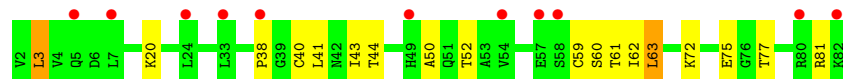
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



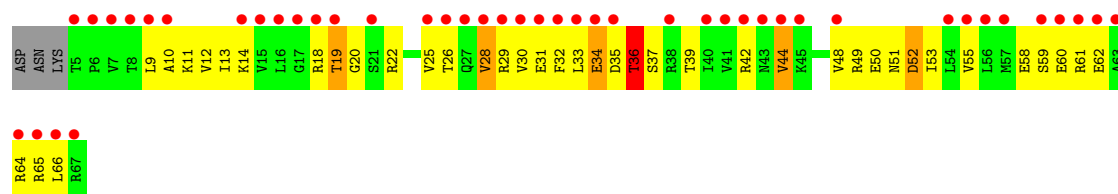
- Molecule 29: 40S ribosomal protein S27-A

Chain d7:



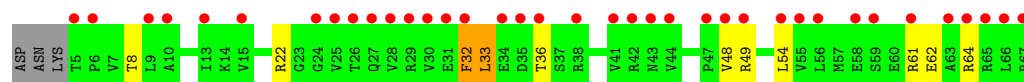
- Molecule 30: 40S ribosomal protein S28-A

Chain D8:



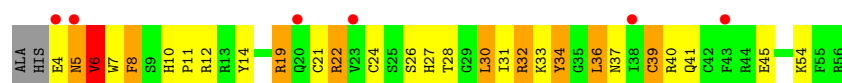
- Molecule 30: 40S ribosomal protein S28-A

Chain d8:



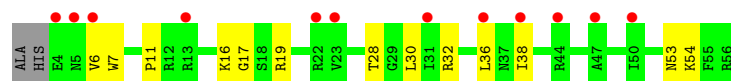
- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



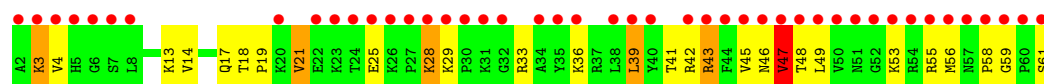
- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



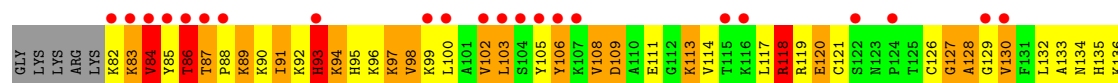
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



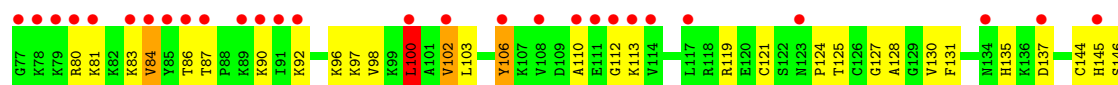
- Molecule 33: Ubiquitin-40S ribosomal protein S31

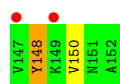
Chain E1:



- Molecule 33: Ubiquitin-40S ribosomal protein S31

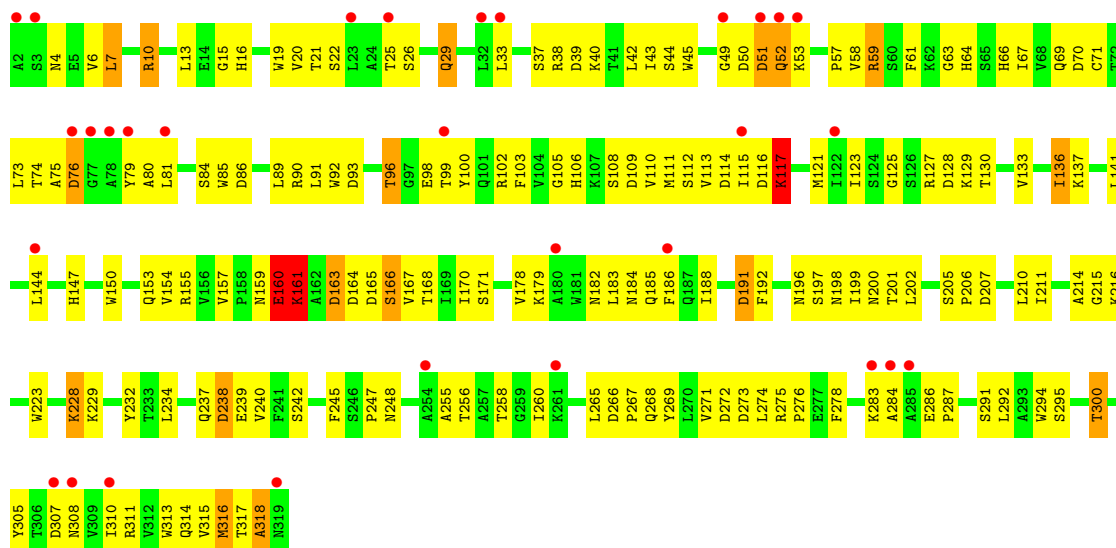
Chain e1:





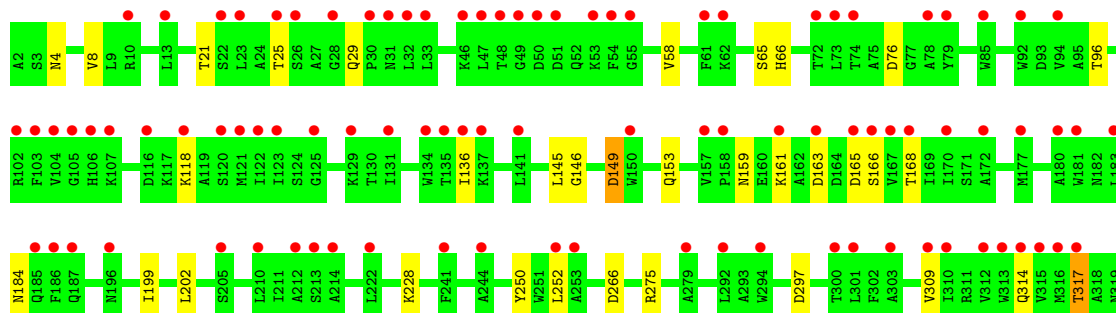
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



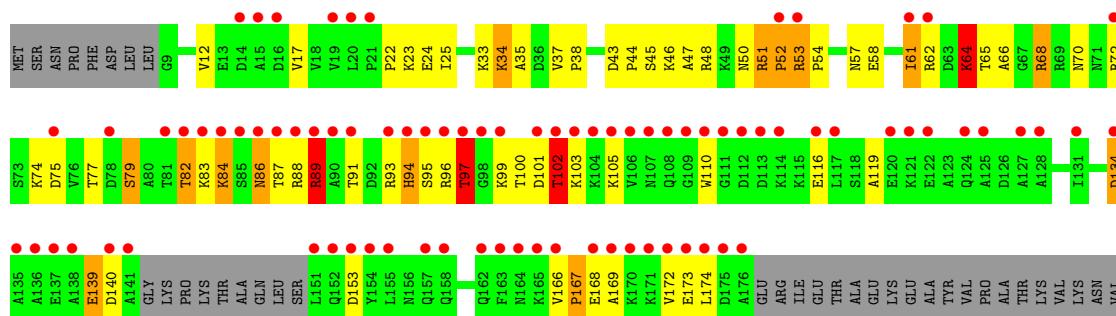
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



- Molecule 35: Suppressor protein STM1

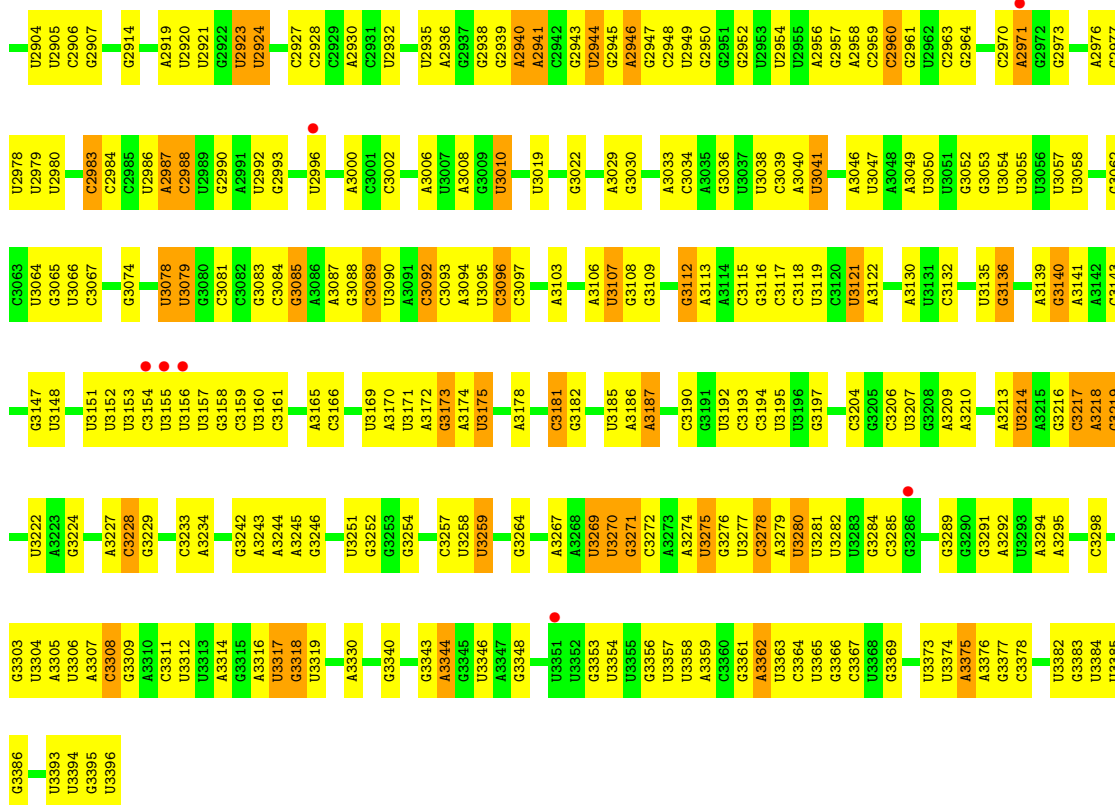
Chain SM:





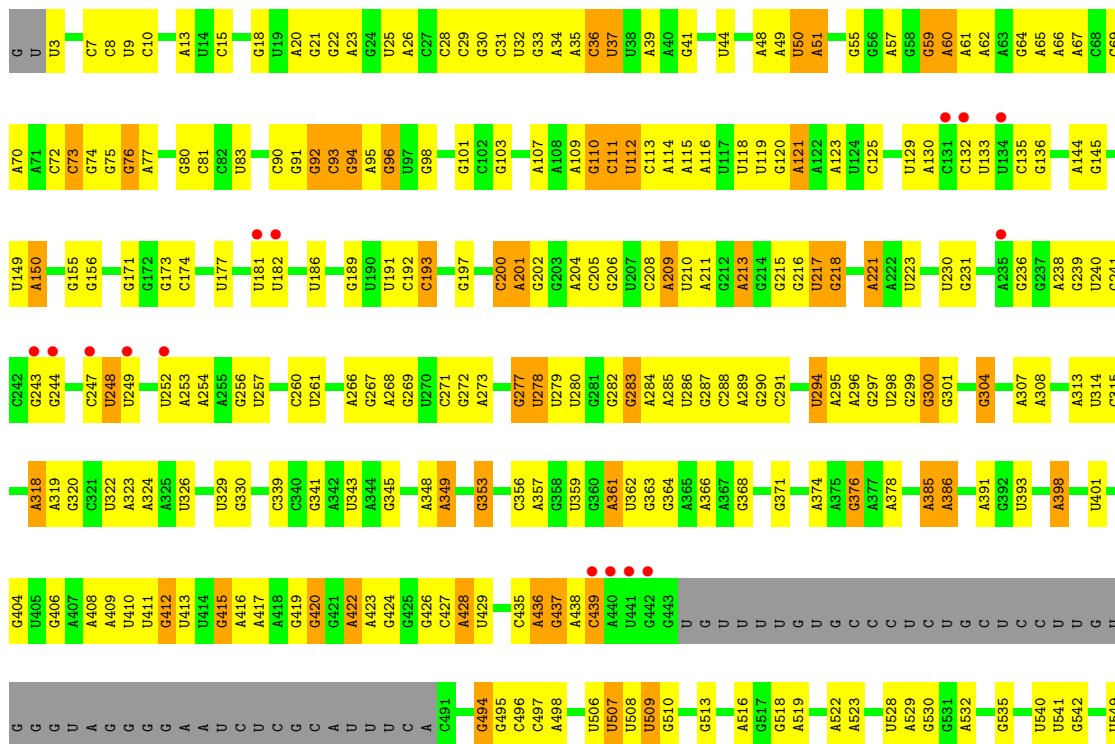
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C1709	U1606	G1528	U1455	C1320	G1242	A1159	G1097	C1000	A926	A858	A781	A690	U626
G1713	C1608	G1536	A1456	G1321	G1243	G1160	U1100		C927	A859	G782	A691	U627
A1714	C1609			U1322	A1244	G1161	A1103	U1004	A929	A860	A783	A692	U629
A1715	G1610	U1540	C1459	G1323	G1245	U1162	G1104	G1005	U930	C861	A784	A693	A630
U1716	G1611	G1541	A1461	U1325	G1246	A1163	A1106	A1006	C931	U862	A785	A694	U631
U1717	A1612			A1326	U1247	G1164	G1106	U1007	U932	C863	A786	A695	G632
G1718	A1613	A1546	A1467	C1327	A1252	A1165	A1107	U1008	U933	G864	G787	A696	G633
G1719	C1614	G1547	A1468	U1328	C1255	U1166	G1108	A1009	A934	A867	C788	A697	G634
U1720	C1615	C1548	A1469	C1329	G1256	U1167	U1108	C1107	U935	G868	A789	A698	G635
U1721	U1616	U1549	U1471	U1330	G1256	A1169	U1109	U1109	A936	G869	U790	C702	G636
U1722			U1472	U1331	A1260	A1170	U1110	U1014	A937	G870	U791		G637
A1723	A1621	G1551	G1473	U1334	G1261	G1171	U1111	U1015	C938	C871	G792	U707	C638
U1724	U1622	U1474	A1474	U1335	G1262	C1175	A1112	C1016		U871	C793	G708	G639
C1725	A1475	A1475	U1405	U1336	A1263	G1176	U1114	G1113	U942	U872	U794	A709	U640
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A1741	C1631	C1555	A1477	C1338	G1265	G1178	U1116	G1024	C944	U874	U796	A711	U642
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G1743	U1636	A1559	U1479	C1340	U1269	A1180	C1118	U1028	G947	G878	A801	G714	G644
G1744	A1637	G1560	A1481	G1341	U1270	U1181	C1119	G1029	C948	A882	C802	A715	A646
A1638	A1638	G1561	A1482	C1342	A1271	U1182	A1120	A1030	C949	A883	C803	A716	A647
C1639	C1639	G1413	G1483	U1345	C1272	A1184	U1121	G1035	U954	A884	C804	G717	C648
			U1484				U1122	A1036	U955	U885	A806	U719	C650
U1645	U1645	U1564	G1485	G1346	U1276	C1189	U1123	U1086	U956	C886	A807	A720	G651
G1646		G1486	G1486	U1348	C1277		U1124	C1043	U957	A888	C808	G721	G652
G1653	A1653	A1566	G1487	G1349	A1278	C1192	U1125	U1048	C958	U889	A810	G722	
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U1765	G1658	U1572	U1495	U1355	G1284	C1201	C1132	A1054	C964	A896	A816	G737	A660
G1766	U1659	G1573	U1496	U1356	G1285	A1202	A1133	U1060	U965	U897	C817		A661
C1767	C1660	C1574	A1497	G1357	A1286	A1207	G1134	U1061	U966	U898	C818	G742	C663
U1768	G1661	U1497	U1427		A1287		A1135	A1061	A967	U899	U819	G743	A664
G1769				G1362			A1136	A1062	G968	G900			A665
	G1664	U1576	A1498	A1363	U1293	U1211	C1137	G1063	C969	U903	U824	U748	C670
G1778	C1665	G1577	C1429	C1364	A1294	A1212	U1138	A1064	A970	A904	G826	G749	U671
C1779		U1500	U1430	G1365	G1295	A1213	G1139	A1065	C971	U905	U829	G750	A672
G1780	G1668	A1580	G1431	C1366	C1296	G1213	U1140	U1070	A972	G907	A830	G760	C673
U1785	C1669	C1581	A1433	U1367	C1297	A1221	C1141	G1066	A973	A906	U829	G764	C675
G1786	C1670	C1582	G1434	A1368	A1301	G1222	G1142	C1069	G974	G907	A831	U764	A676
A1787	C1671		A1435	A1369	A1302	G1227	U1143	U1070	C975	G908	G832	C765	A677
C1788	U1672	G1586	U1436	G1370	A1303	C1228	G1144	A1070	U976	G909	G833	U766	C678
G1789	G1673	A1587	C1437	U1371	A1304	G1229	G1145	U1074	C977	G910	U834	U767	U679
U1790	C1674	A1588	U1438	G1372	U1305	G1230	G1146	A1075	G978	G912	U835	C768	G680
G1791		G1590	G1441	G1374	G1306	A1231	G1147	U1078	U979	A913	A836	G769	U681
C1792	A1683	G1591	U1442		G1307	C1232	G1148	A1079	U981	A837	C837	G769	U682
G1793	U1686	G1592	G1443	G1379	A1308	G1233	G1149	A1080	C982	G916	C839	A771	U683
G1794	U1687	A1593	G1444	G1380	U1309	G1234	U1150	U1081	C983	A917	C840	U772	G684
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A1695	U1695	C1597	G1447	G1383	C1313	G1237	A1154	A1084	U989	C923	A847	U777	G688
U1798		G1598	G1450	G1387	C1314	C1238	C1155	U1095	G993	G924			
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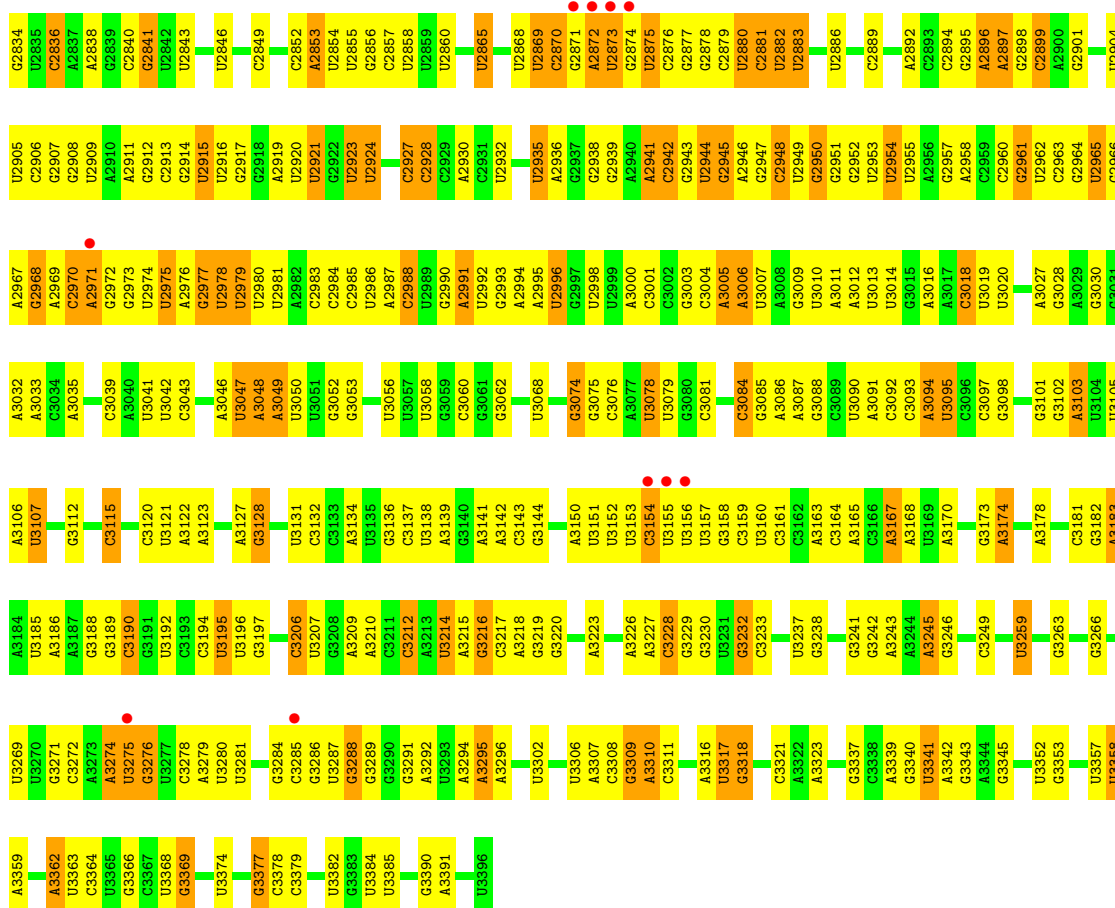
● Molecule 36: *Saccharomyces cerevisiae* chromosome XII cosmid 9634

Chain 5:



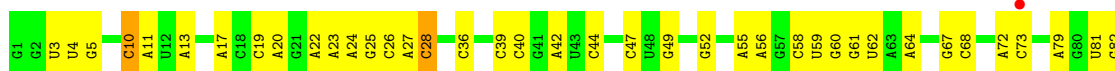
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U1555	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527																									
C1391	G1392	A1393	A1394	C1395	C1396	C1397	U1398	A1399	C1402	G1403	G1404	U1405	A1406	A1407	G1408	G1409	U1410	G1411	G1412	G1413	G1414	U1415	G1416	G1417	A1418	A1419	C1420	G1421	C1426	U1427	G1428	G1429	U1430	G1431	C1432	A1433	G1434	A1435	U1436	C1437	U1438	U1439	U1445	A1446	U1447	U1448	A1449	G1450	C1451	A1452	A1456	C1461	U1464															
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A850	A851	G852	U853	A854	C855	G856	A857	C858	A859	G860	C861	A862	A863	C864	U865	A866	A867	C868	U869	A870	C871	A872	U873	U875	U876	C877	A878	U879	C880	U881	U882	C883	G884	C885	U886	U887	C888	U889	A890	A891	C892	C893	U894	U895	U896	U897	G898	A899	C900	C901	C902	A806	A807															
A822	A823	C824	U825	G826	A827	C828	U829	A830	G831	A832	C833	U834	A835	A836	C837	A838	A839	C840	G841	U842	A843	C844	A845	A847	A848	U849	U850	C851	U852	C853	G854	C855	U856	U857	C858	U859	A860	U861	C862	C863	U864	A865	U866	A867	C868	A869	C870	U871	C872	A873	A874	C875	A876	C877	U878	A879												
A637	U640	G641	U642	G643	U644	A645	A646	A647	A648	A649	C652	A653	C654	U655	A656	A657	C658	A659	A660	G661	U662	C663	U666	U667	C668	U669	A670	C671	U672	U673	U675	U676	U677	U678	U679	A680	U681	C682	A683	U684	A685	U686	A687	C688	A689	C690	A691	C692	A693	U698	A699	C700	U623	G624	G701	C702	U626	U627	A628	U629	A630	U631	A715	C632	C633	G634	U635	C636
A550	A551	G556	C641	G567	G568	A569	A570	G575	C577	A578	C579	C580	G583	G584	A585	C586	U594	G595	C596	U597	A598	G599	C599	G600	A603	G604	A608	U609	G610	A611	U612	C618	A619	U620	A621	A622	U623	G624	C625	U626	U627	A628	U629	A630	U631	A715	C632	C633	G634	U635	C636																	





• Molecule 37: Yeast 5S rRNA gene

Chain 3:



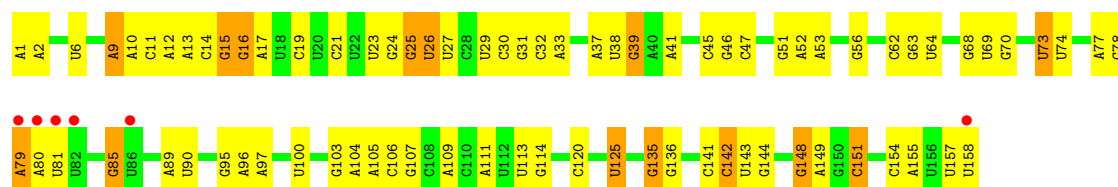
• Molecule 37: Yeast 5S rRNA gene

Chain 7:



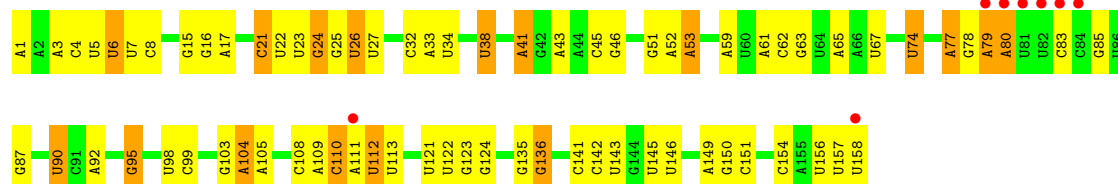
• Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



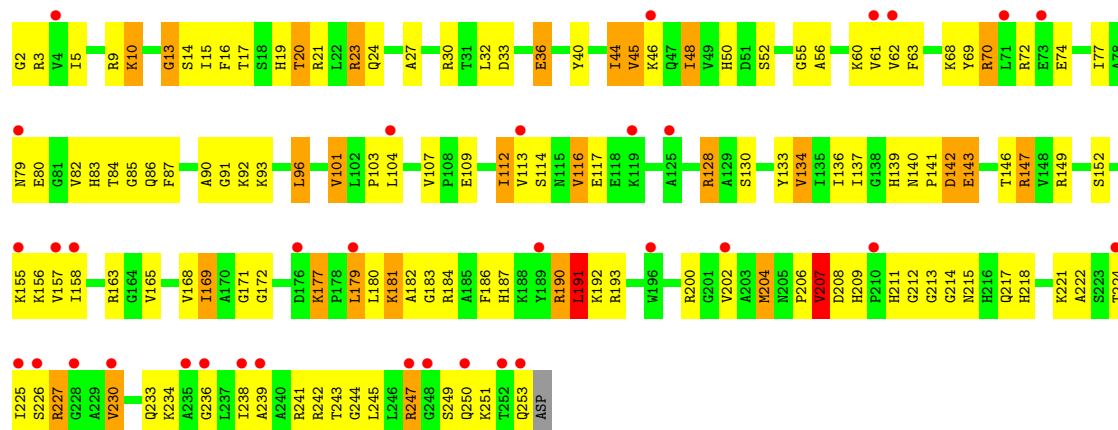
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 8:



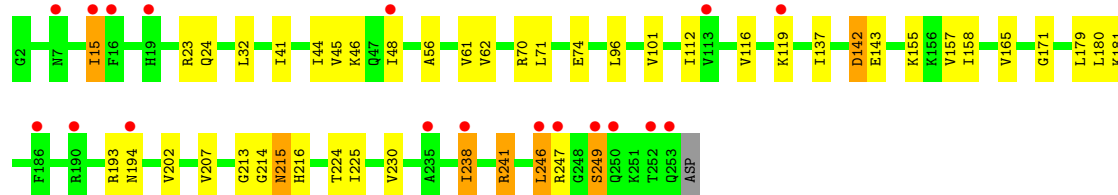
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



- Molecule 39: 60S ribosomal protein L2-A

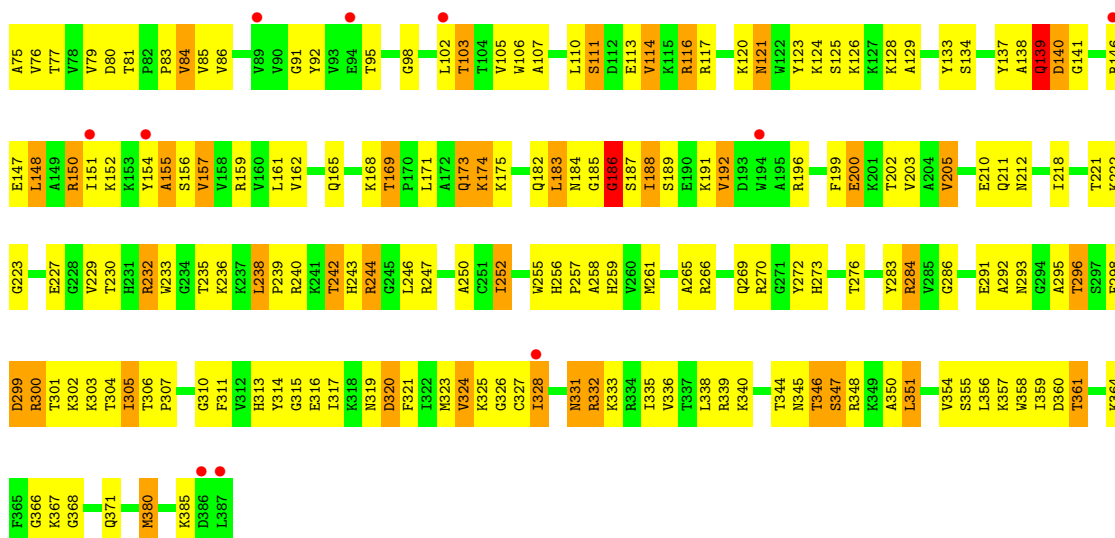
Chain L2:



- Molecule 40: 60S ribosomal protein L3

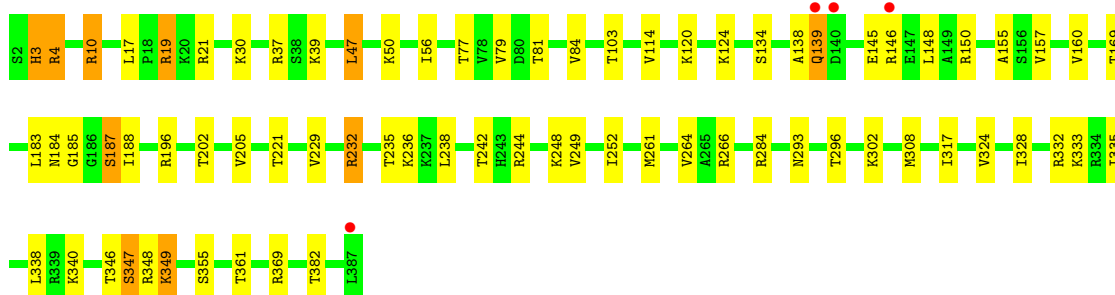
Chain L3:





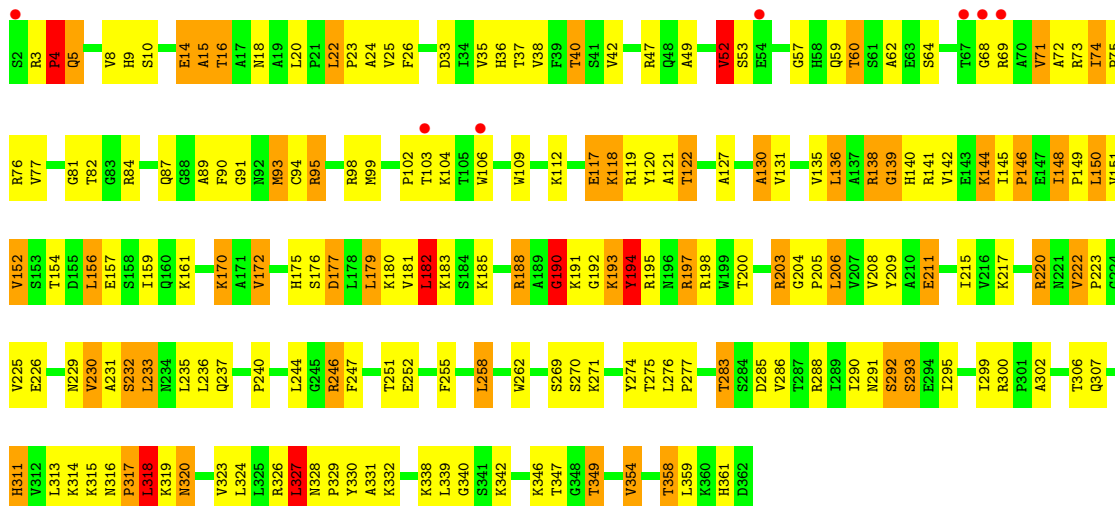
• Molecule 40: 60S ribosomal protein L3

Chain 13:



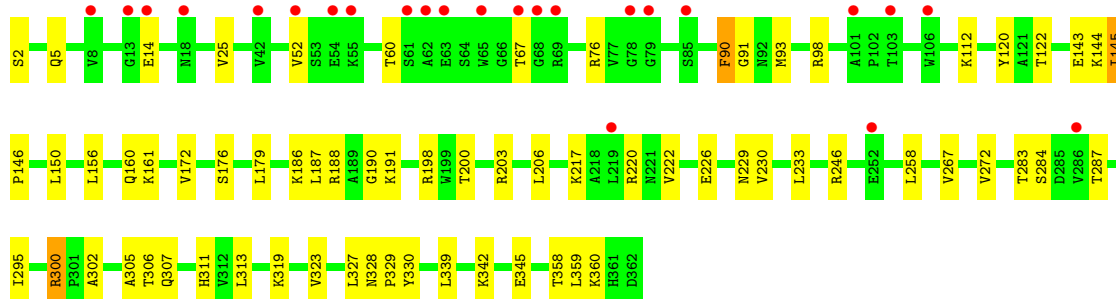
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



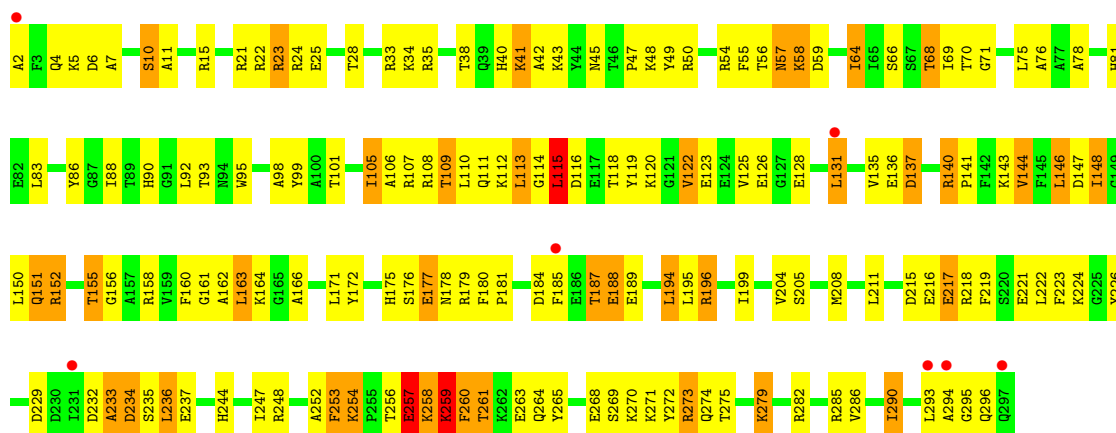
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



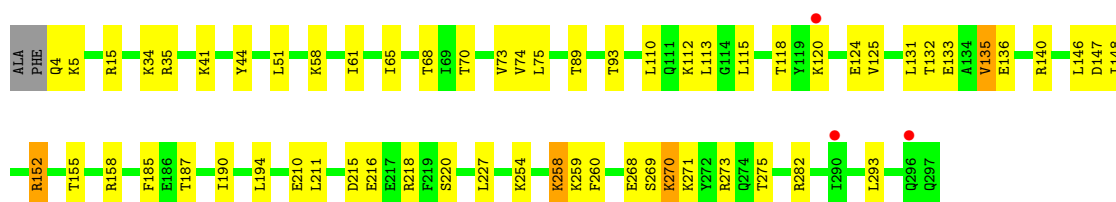
- Molecule 42: 60S ribosomal protein L5

Chain L5:



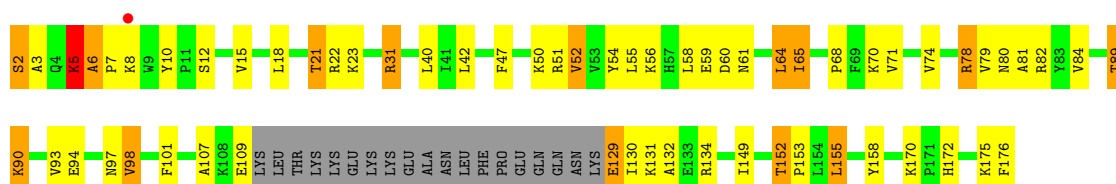
- Molecule 42: 60S ribosomal protein L5

Chain l5:



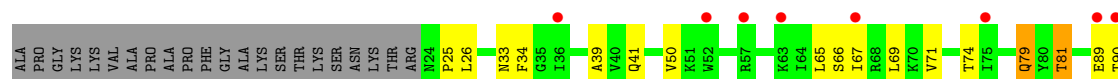
- Molecule 43: 60S ribosomal protein L6-A

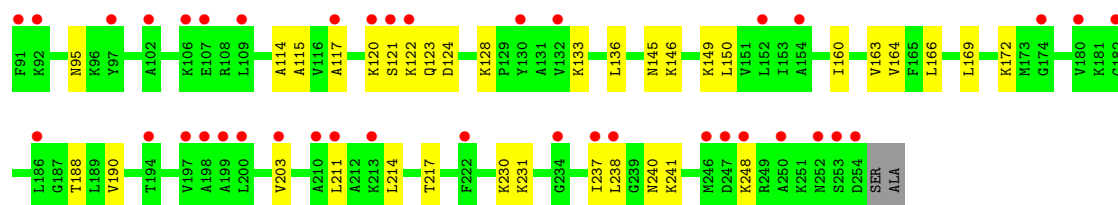
Chain L6:



- Molecule 43: 60S ribosomal protein L6-A

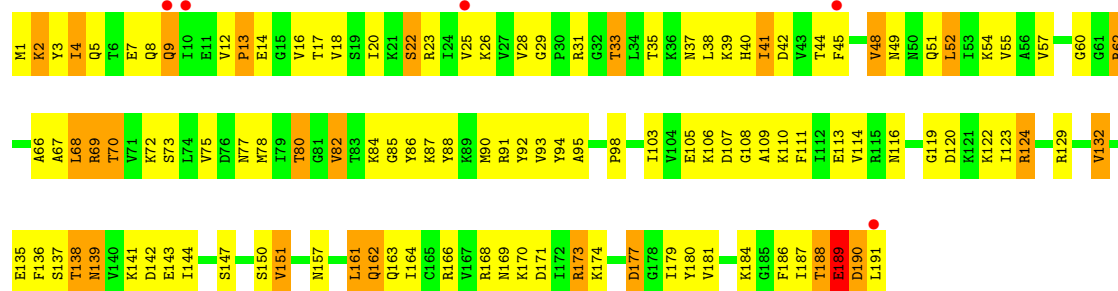
Chain l6:





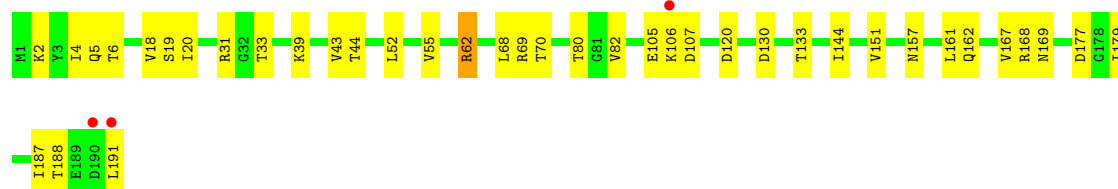
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



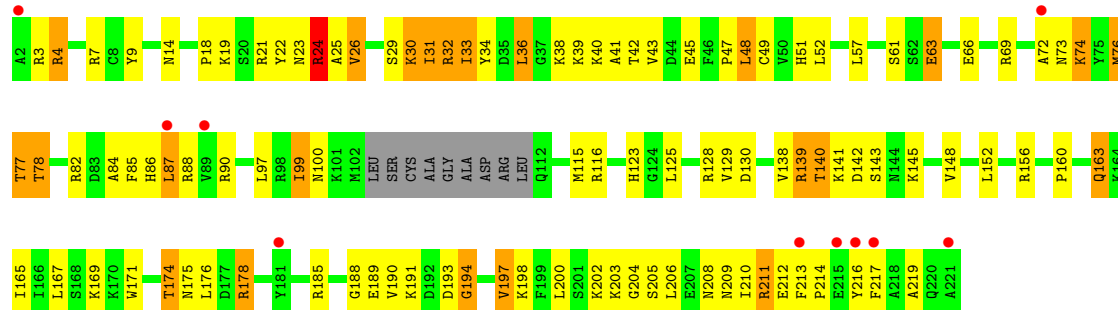
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



• Molecule 47: 60S ribosomal protein L10

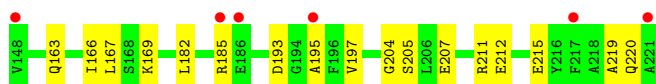
Chain M0:



• Molecule 47: 60S ribosomal protein L10

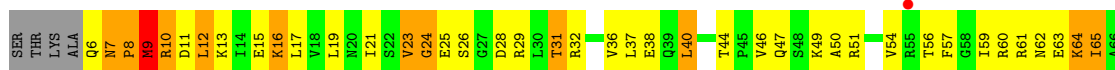
Chain m0:





• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



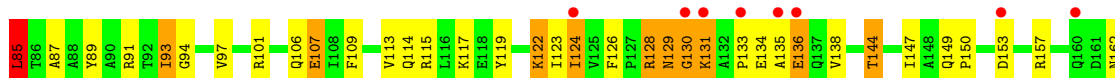
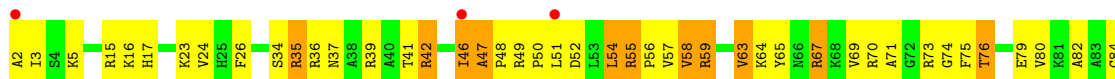
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



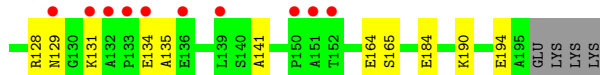
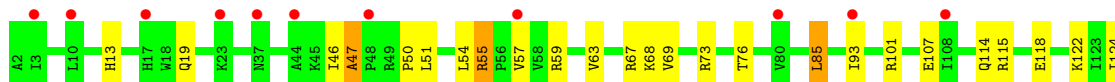
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



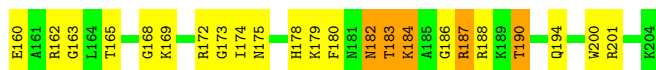
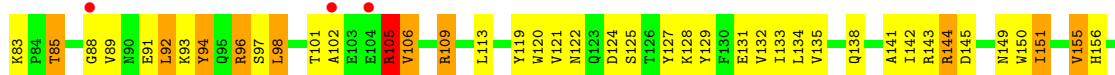
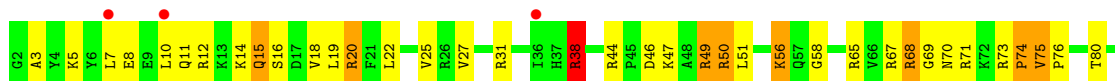
- Molecule 50: 60S ribosomal protein L14-A

Chain m4:



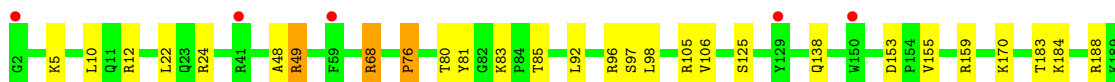
- Molecule 51: 60S ribosomal protein L15-A

Chain M5:



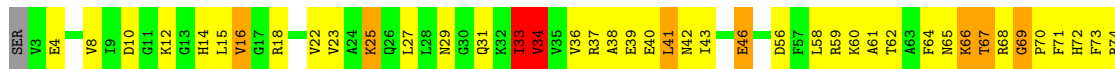
- Molecule 51: 60S ribosomal protein L15-A

Chain m5:



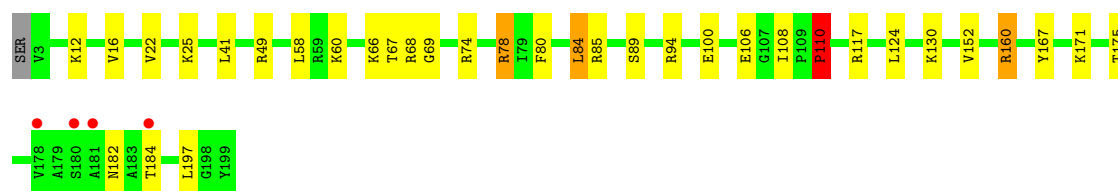
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



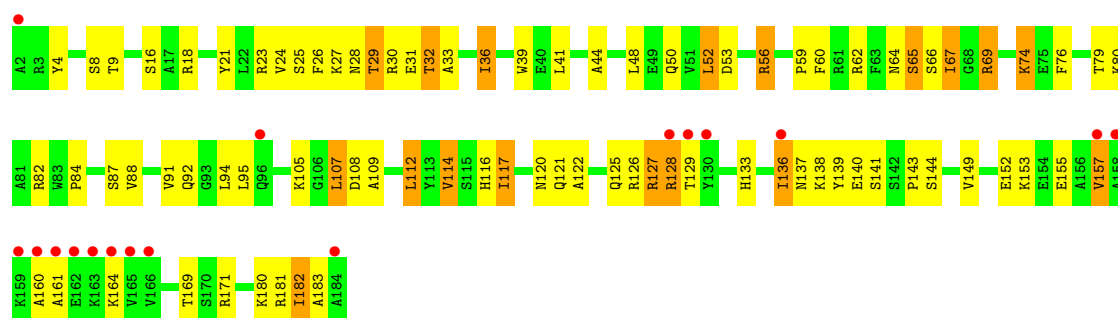
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



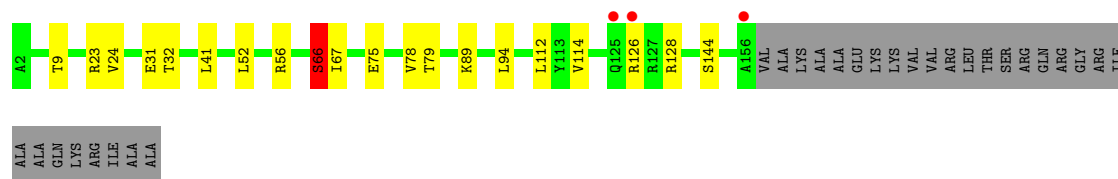
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:



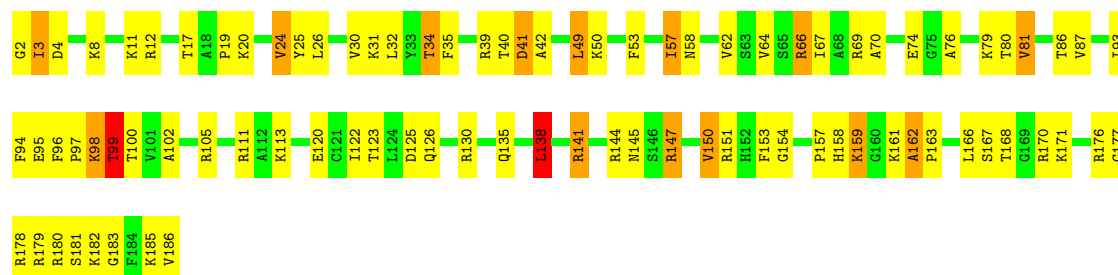
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



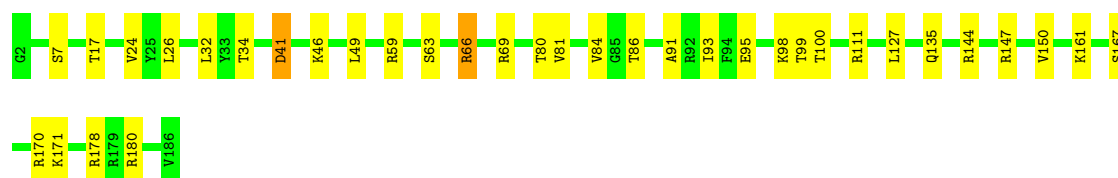
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



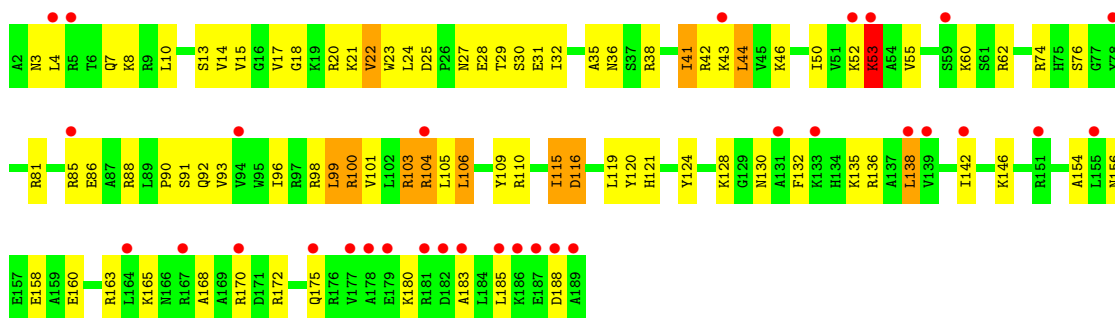
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



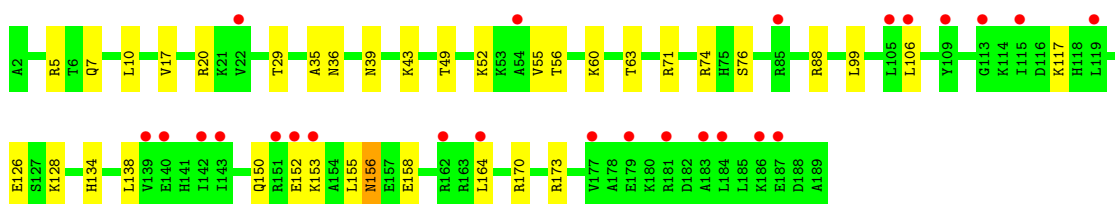
- Molecule 55: 60S ribosomal protein L19-A

Chain M9: 



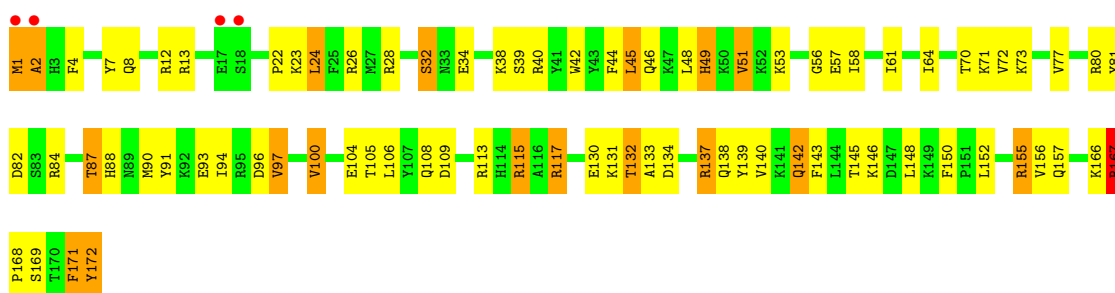
- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 



- Molecule 56: 60S ribosomal protein L20-A

Chain N0: 



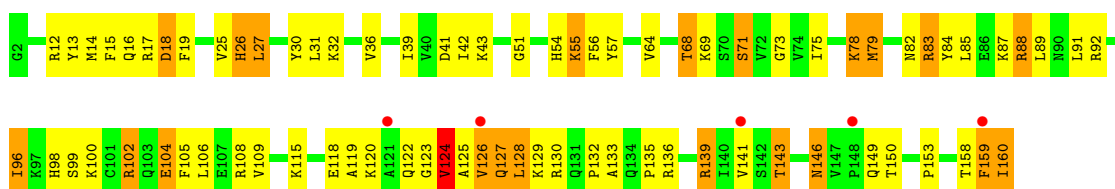
- Molecule 56: 60S ribosomal protein L20-A

Chain n0: 



- Molecule 57: 60S ribosomal protein L21-A

Chain N1: 



- Molecule 57: 60S ribosomal protein L21-A

Chain n1:

- Molecule 58: 60S ribosomal protein L22-A

Chain N2:

- Molecule 58: 60S ribosomal protein L22-A

Chain n2:

ALA
LYS
GLY
ALA
PHE
GLN
LYS
VAL
ALA
ALA
THR
SER
ARG

- Molecule 60: 60S ribosomal protein L24-A

Chain n4:

M1 K2 I5 S26 L39 R43 L54 T63 T64 E65 E66 V67 A68 K69 K70 R71 S72 L73 K74 T75 V76 K77 T83 L87 L96 E99 V100 K127 G132 S135 SER LYS PHE LYS GLN GLN ALA GLY PHE GLN LYS VAL ALA

THR
SER
ARG

- Molecule 61: 60S ribosomal protein L25

Chain N5:

ALA PRO SER ALA LYS THR ALA ALA LYS VAL VAL LYS THR ASN GLY LYS K22 A23 L24 K25 V26 R27 K36 T37 L38 K39 R40 A41 P44 K45 Y46 A47 S48 K49 A50 V51 R56 L57 D58 S59 Y60 K61 V62 I63 T67 T68 T71 A72 N73 V76

E77 D78 G79 N80 I81 L82 V83 F84 Q85 V86 N91 K92 Y83 Q94 K100 E101 L102 Y103 E104 V105 D106 L108 K109 V110 L113 V114 R115 P116 N117 G118 T119 K120 K121 A122 Y123 V124 R125 L126 T127 Y130 D131 A132 L133 D134 I135 A136 N137 R138 I139 G140 Y141 I142

- Molecule 61: 60S ribosomal protein L25

Chain n5:

ALA PRO SER ALA LYS THR ALA ALA LYS VAL VAL LYS THR ASN GLY LYS A23 L24 K25 V26 R27 F32 R33 L34 T37 L38 K39 L40 P44 K45 Y46 A47 P52 R56 L57 D58 S59 Y60 K61 V62 I63 E64 Q65 T71 F84 Q85 V86 S87

N88 T96 K96 K97 E101 Y102 E104 V105 D106 L108 K109 L113 V114 R115 P116 N117 G118 T119 V124 R125 L126 L133 D134 I135 A136 N137 I142

- Molecule 62: 60S ribosomal protein L26-A

Chain N6:

A2 K3 Q4 S5 L6 D7 V8 R12 R13 R16 S24 S25 Q26 K37 F38 L39 Q42 Y43 G44 I45 K46 A47 I50 R51 R52 D53 E55 V56 L57 V58 V59 R60 K64 E67 T70 Y74 R75 L76 K77 F78 A79 V80 Q81 V82 D83 K84 V85 E88

N91 G92 A93 S94 T97 N98 S102 K103 L104 V105 K108 L109 H110 L111 D112 R115 I119 Q120 R121 K122 K125 L126 R127 E127

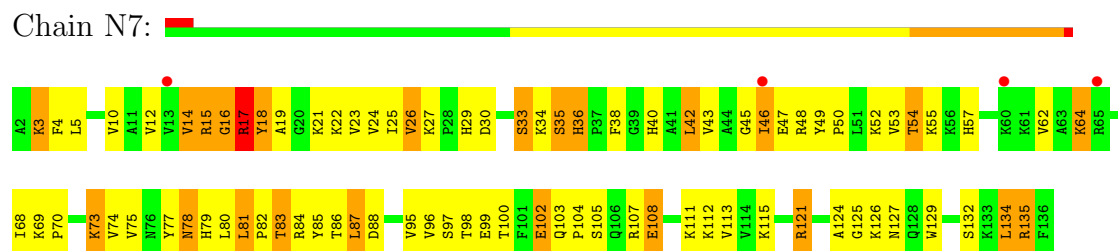
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:

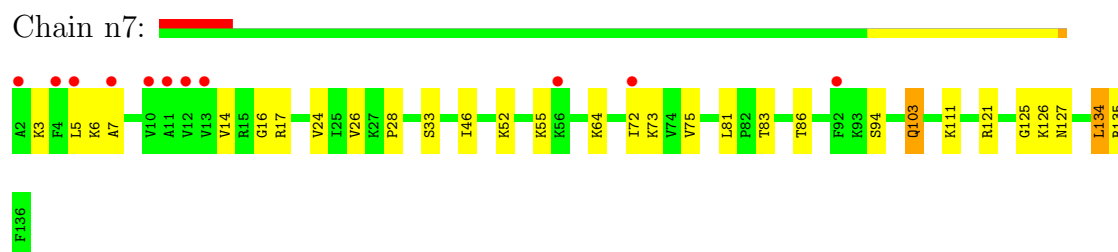
A2 S9 S10 D11 R12 R13 A18 L35 S36 K37 E38 L39 R40 Y43 G44 I45 I50 R51 R52 D53 E55 V56 L57 S62 Q66 K69 I70 S71 S72 Y73 Y74 L76 V80 D83 K84 K87 E88 K89 V90 N91 G92 A93 S94 I97 N98

L104 V105 I106 T107 K108 L109 H110 L111 D112 K113 R115 S116 A117 L118 I119 Q120 R121 K125 L126 E127

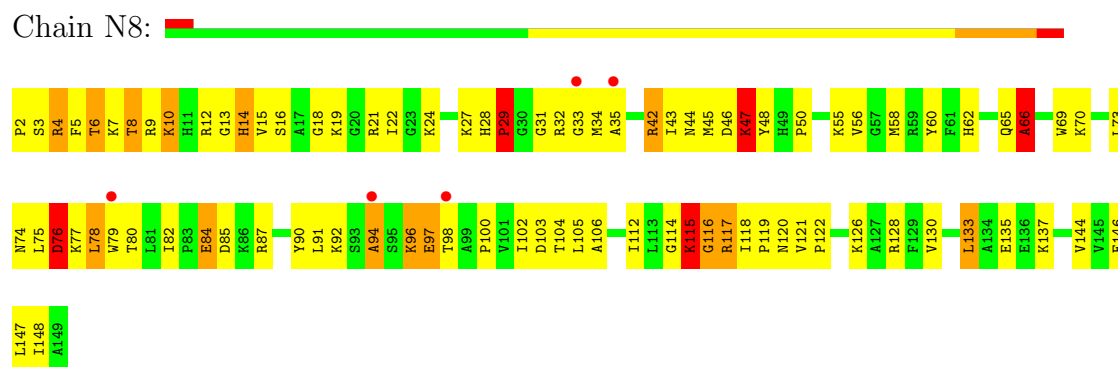
- Molecule 63: 60S ribosomal protein L27-A



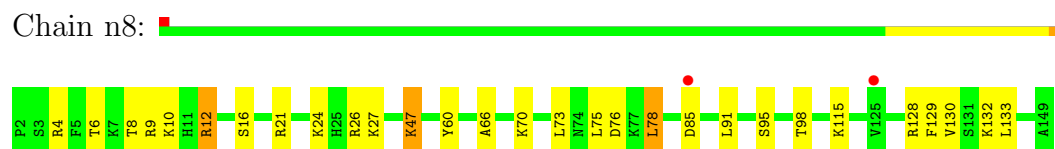
- Molecule 63: 60S ribosomal protein L27-A



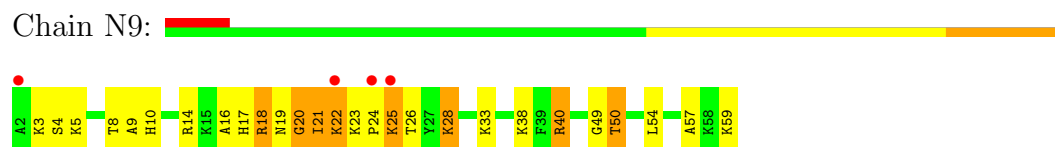
- Molecule 64: 60S ribosomal protein L28



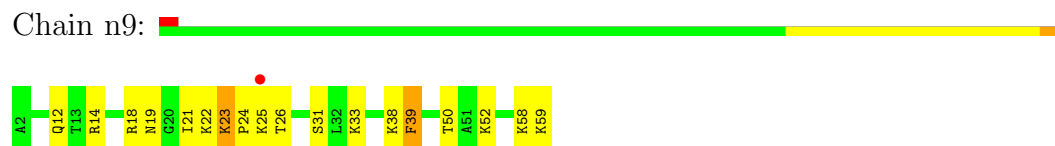
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29

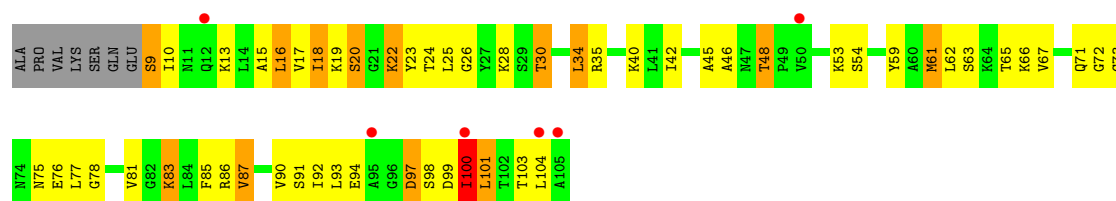


- Molecule 65: 60S ribosomal protein L29



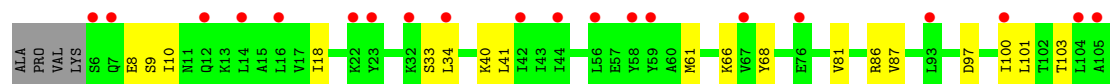
- Molecule 66: 60S ribosomal protein L30

Chain O0:



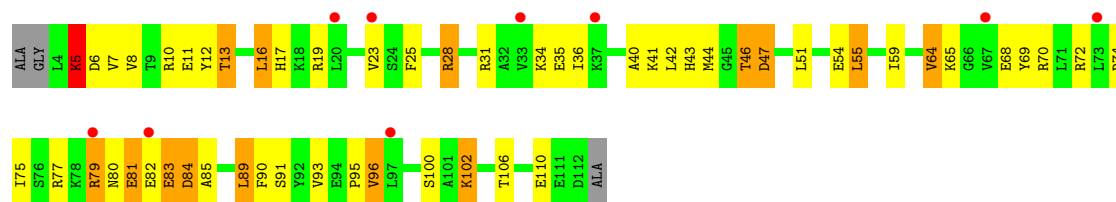
- Molecule 66: 60S ribosomal protein L30

Chain o0:



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



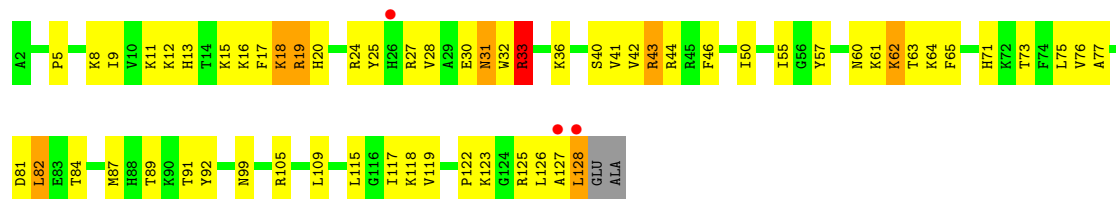
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



- Molecule 68: 60S ribosomal protein L32

Chain O2:



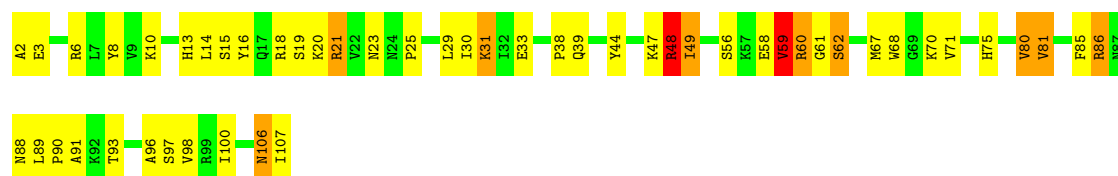
- Molecule 68: 60S ribosomal protein L32

Chain o2:



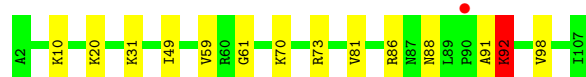
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



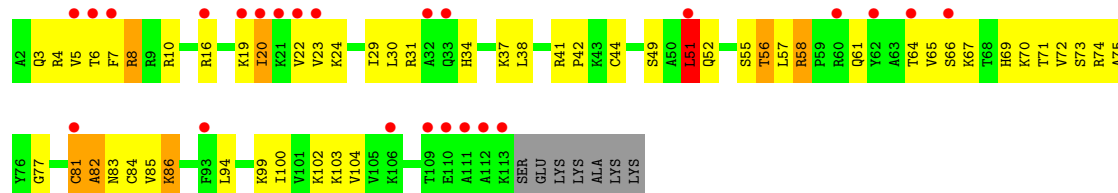
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



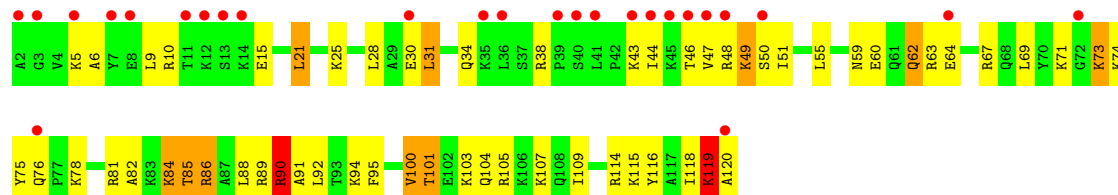
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



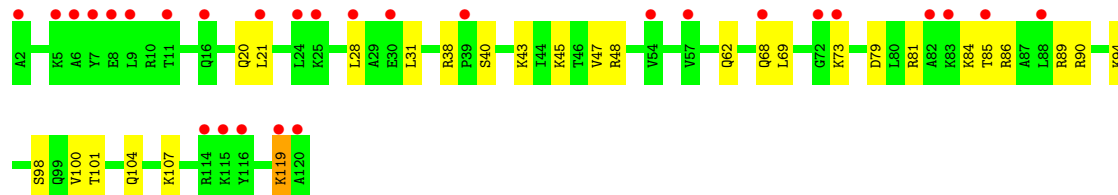
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



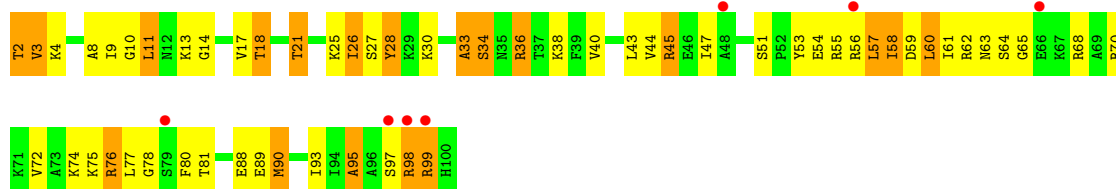
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



- Molecule 72: 60S ribosomal protein L36-A

Chain O6: 



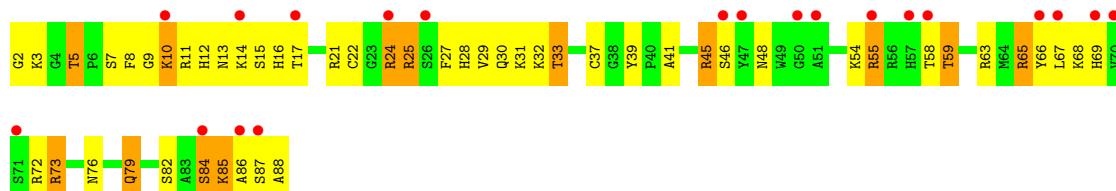
- Molecule 72: 60S ribosomal protein L36-A

Chain o6: 



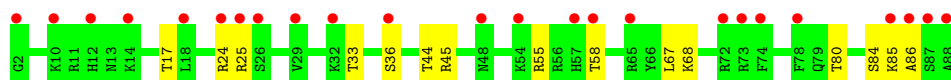
- Molecule 73: 60S ribosomal protein L37-A

Chain O7: 



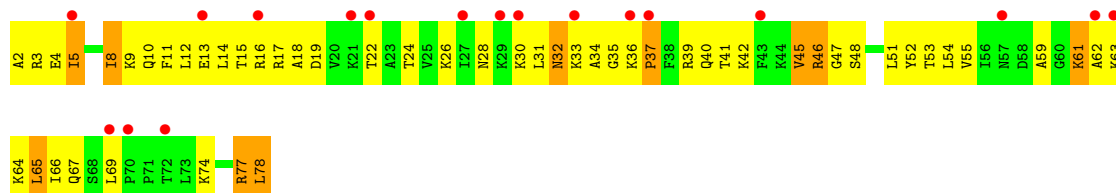
- Molecule 73: 60S ribosomal protein L37-A

Chain o7: 



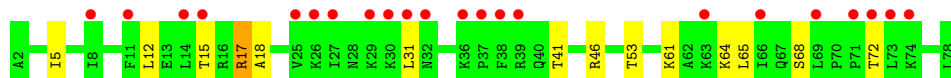
- Molecule 74: 60S ribosomal protein L38

Chain O8: 



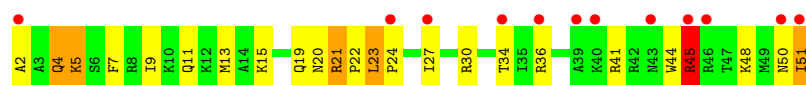
- Molecule 74: 60S ribosomal protein L38

Chain o8: 



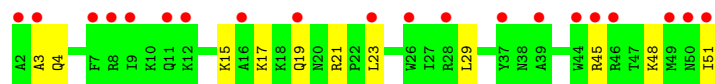
- Molecule 75: 60S ribosomal protein L39

Chain O9: 



- Molecule 75: 60S ribosomal protein L39

Chain o9: 



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0: 



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0: 



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1: 



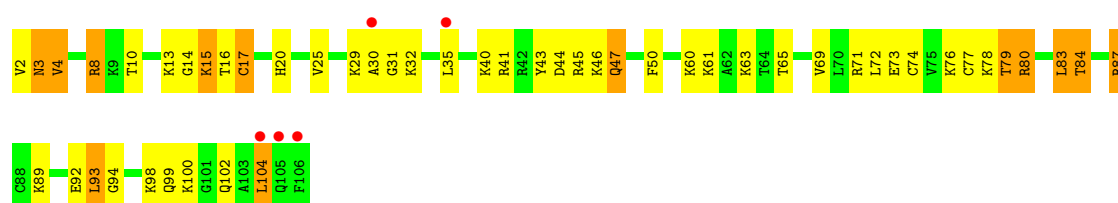
- Molecule 77: 60S ribosomal protein L41-A

Chain q1: 



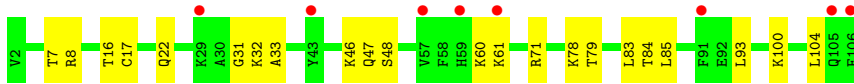
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2: 



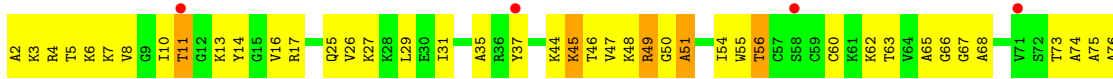
- Molecule 78: 60S ribosomal protein L42-A

Chain q2: 



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



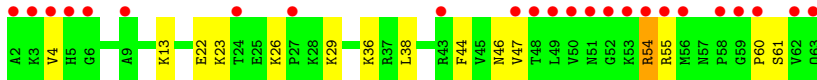
- Molecule 79: 60S ribosomal protein L43-A

Chain q3: 



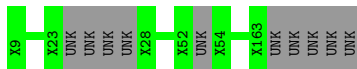
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:



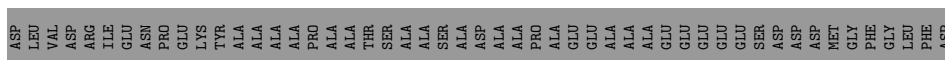
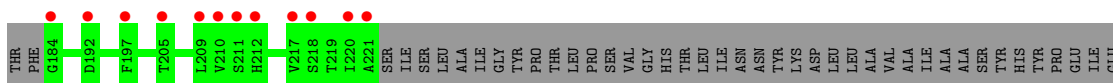
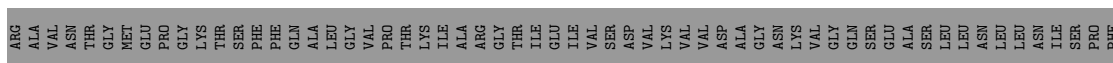
- Molecule 81: Unknown protein m2

Chain m2: 



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0:



- Molecule 83: Unknown protein p1

Chain p1: 

There are no outlier residues recorded for this chain.

- Molecule 84: Unknown protein p2

Chain p2: 

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	436.64Å 287.69Å 304.39Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	300.66 – 2.80 300.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (300.66-2.80) 99.5 (300.66-2.80)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.208 , 0.246 0.253 , 0.287	Depositor DCC
R_{free} test set	26295 reflections (1.46%)	DCC
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 1805319 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	411226	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3H3, 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	0.75	5/41698 (0.0%)	1.30	337/64972 (0.5%)
1	6	0.87	23/42765 (0.1%)	1.40	490/66634 (0.7%)
2	S0	0.47	0/1617	0.67	0/2215
2	s0	0.53	0/1623	0.76	2/2222 (0.1%)
3	S1	0.37	0/1735	0.62	0/2335
3	s1	0.52	0/1748	0.71	1/2352 (0.0%)
4	S2	0.51	0/1665	0.67	0/2263
4	s2	0.61	0/1665	0.79	0/2263
5	S3	0.50	0/1759	0.65	0/2368
5	s3	0.48	0/1759	0.62	0/2368
6	S4	0.51	0/2109	0.74	2/2839 (0.1%)
6	s4	0.57	0/2109	0.79	1/2839 (0.0%)
7	S5	0.43	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.66	1/2202 (0.0%)
8	S6	0.48	0/1823	0.65	0/2439
8	s6	0.58	0/1779	0.72	1/2379 (0.0%)
9	S7	0.46	0/1506	0.65	0/2028
9	s7	0.54	0/1516	0.70	1/2043 (0.0%)
10	S8	0.58	0/1514	0.79	3/2021 (0.1%)
10	s8	0.64	0/1514	0.77	1/2021 (0.0%)
11	S9	0.50	0/1519	0.69	0/2035
11	s9	0.59	0/1519	0.74	0/2035
12	C0	0.45	0/790	0.69	1/1069 (0.1%)
12	c0	0.40	0/777	0.63	3/1049 (0.3%)
13	C1	0.59	0/1240	0.71	0/1675
13	c1	0.66	0/1194	0.86	0/1610
14	C2	0.37	0/898	0.62	0/1220
14	c2	0.31	0/898	0.58	1/1220 (0.1%)
15	C3	0.50	0/1215	0.71	2/1638 (0.1%)
15	c3	0.61	0/1215	0.77	0/1638
16	C4	0.38	0/901	0.65	0/1217
16	c4	0.54	0/960	0.77	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.50	0/998	0.67	0/1341
17	c5	0.51	0/1060	0.68	1/1426 (0.1%)
18	C6	0.47	0/1125	0.74	3/1510 (0.2%)
18	c6	0.50	0/1131	0.69	0/1518
19	C7	0.46	0/935	0.65	0/1254
19	c7	0.50	0/914	0.70	0/1224
20	C8	0.49	0/1211	0.67	0/1628
20	c8	0.51	0/1211	0.73	1/1628 (0.1%)
21	C9	0.48	0/1130	0.68	0/1517
21	c9	0.51	0/1130	0.71	0/1517
22	D0	0.48	0/865	0.66	0/1169
22	d0	0.49	0/892	0.68	0/1205
23	D1	0.47	0/693	0.66	0/935
23	d1	0.57	0/693	0.80	0/935
24	D2	0.55	0/1038	0.75	1/1395 (0.1%)
24	d2	0.68	0/1038	0.75	0/1395
25	D3	0.63	0/1139	0.79	1/1518 (0.1%)
25	d3	0.73	0/1139	0.83	3/1518 (0.2%)
26	D4	0.48	0/1087	0.63	0/1449
26	d4	0.53	0/1087	0.72	0/1449
27	D5	0.42	0/571	0.71	0/768
27	d5	0.45	0/566	0.63	0/761
28	D6	0.47	0/782	0.67	0/1047
28	d6	0.59	0/782	0.75	0/1047
29	D7	0.46	0/620	0.68	1/838 (0.1%)
29	d7	0.52	0/620	0.73	0/838
30	D8	0.36	0/499	0.56	0/670
30	d8	0.44	0/499	0.67	0/670
31	D9	0.56	0/452	0.82	1/600 (0.2%)
31	d9	0.58	0/452	0.72	0/600
32	E0	0.49	0/483	0.65	0/643
33	E1	0.49	0/577	0.83	0/770
33	e1	0.43	0/619	0.75	1/822 (0.1%)
34	SR	1.06	2/2494 (0.1%)	1.50	6/3393 (0.2%)
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.55	0/1113	0.71	2/1502 (0.1%)
35	sM	0.51	0/683	0.68	1/923 (0.1%)
36	1	1.16	152/75394 (0.2%)	1.67	1955/117545 (1.7%)
36	5	1.20	176/75414 (0.2%)	1.69	1938/117575 (1.6%)
37	3	0.96	4/2883 (0.1%)	1.42	33/4491 (0.7%)
37	7	1.13	7/2883 (0.2%)	1.63	50/4491 (1.1%)
38	4	1.11	2/3746 (0.1%)	1.60	70/5832 (1.2%)
38	8	1.00	5/3746 (0.1%)	1.51	46/5832 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	L2	0.75	0/1948	0.87	2/2617 (0.1%)
39	l2	0.82	1/1946 (0.1%)	0.95	5/2614 (0.2%)
40	L3	0.77	2/3146 (0.1%)	0.88	2/4228 (0.0%)
40	l3	0.85	1/3146 (0.0%)	0.96	11/4228 (0.3%)
41	L4	0.86	3/2800 (0.1%)	1.02	10/3790 (0.3%)
41	l4	0.79	0/2800	0.94	6/3790 (0.2%)
42	L5	0.59	0/2425	0.72	0/3271
42	l5	0.78	0/2408	0.83	3/3248 (0.1%)
43	L6	0.77	0/1260	0.85	3/1694 (0.2%)
43	l6	0.78	0/1269	0.85	0/1705
44	L7	0.85	1/1821 (0.1%)	0.90	0/2451
44	l7	0.86	1/1828 (0.1%)	0.91	5/2461 (0.2%)
45	L8	0.59	0/1836	0.69	1/2481 (0.0%)
45	l8	0.57	0/1795	0.69	0/2429
46	L9	0.70	0/1539	0.79	0/2073
46	l9	0.80	0/1539	0.85	0/2073
47	M0	0.76	0/1741	0.88	3/2335 (0.1%)
47	m0	0.82	0/1758	0.89	0/2358
48	M1	0.55	0/1374	0.74	1/1842 (0.1%)
48	m1	0.67	0/1374	0.83	2/1842 (0.1%)
49	M3	0.77	0/1568	0.91	3/2106 (0.1%)
49	m3	0.75	0/1573	0.89	4/2113 (0.2%)
50	M4	0.79	0/1068	0.87	2/1438 (0.1%)
50	m4	0.81	0/1074	0.84	1/1446 (0.1%)
51	M5	0.78	0/1757	0.97	3/2354 (0.1%)
51	m5	0.72	0/1757	0.83	0/2354
52	M6	0.93	3/1585 (0.2%)	1.00	7/2128 (0.3%)
52	m6	1.06	2/1585 (0.1%)	1.04	9/2128 (0.4%)
53	M7	0.84	0/1443	0.87	0/1944
53	m7	0.93	1/1250 (0.1%)	0.89	0/1683
54	M8	0.84	0/1465	0.95	4/1965 (0.2%)
54	m8	0.76	0/1465	0.94	2/1965 (0.1%)
55	M9	0.58	0/1538	0.68	0/2050
55	m9	0.65	0/1538	0.72	0/2050
56	N0	0.81	0/1481	0.87	3/1990 (0.2%)
56	n0	0.84	0/1481	0.92	1/1990 (0.1%)
57	N1	0.81	0/1300	0.86	0/1743
57	n1	0.86	1/1300 (0.1%)	0.86	0/1743
58	N2	0.46	0/812	0.61	0/1099
58	n2	0.53	0/794	0.66	0/1076
59	N3	0.78	0/1018	0.94	5/1369 (0.4%)
59	n3	0.85	0/1018	0.93	4/1369 (0.3%)
60	N4	0.61	0/712	0.69	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	n4	0.68	0/1052	0.72	0/1398
61	N5	0.65	0/979	0.82	1/1321 (0.1%)
61	n5	0.68	0/974	0.84	0/1314
62	N6	0.76	0/1004	0.94	4/1341 (0.3%)
62	n6	0.68	0/1004	0.82	0/1341
63	N7	0.54	0/1118	0.72	0/1497
63	n7	0.52	0/1118	0.66	0/1497
64	N8	0.86	0/1204	0.97	4/1612 (0.2%)
64	n8	0.84	0/1204	0.97	4/1612 (0.2%)
65	N9	0.85	0/473	0.81	1/629 (0.2%)
65	n9	0.90	0/473	0.93	2/629 (0.3%)
66	O0	0.53	0/751	0.68	0/1008
66	o0	0.55	0/775	0.67	0/1040
67	O1	0.68	0/890	0.75	0/1196
67	o1	0.85	1/897 (0.1%)	0.86	0/1205
68	O2	0.87	0/1041	0.95	4/1394 (0.3%)
68	o2	0.89	0/1041	1.02	5/1394 (0.4%)
69	O3	0.92	0/868	0.90	3/1168 (0.3%)
69	o3	0.98	1/868 (0.1%)	0.92	2/1168 (0.2%)
70	O4	0.62	0/890	0.80	1/1189 (0.1%)
70	o4	0.67	0/890	0.74	0/1189
71	O5	0.71	1/978 (0.1%)	0.84	2/1301 (0.2%)
71	o5	0.62	0/974	0.71	0/1297
72	O6	0.68	0/778	0.84	0/1034
72	o6	0.60	0/777	0.74	0/1033
73	O7	0.89	1/696 (0.1%)	1.00	2/923 (0.2%)
73	o7	0.75	0/696	0.88	1/923 (0.1%)
74	O8	0.52	0/618	0.64	0/826
74	o8	0.49	0/614	0.67	0/822
75	O9	0.89	1/443 (0.2%)	0.96	1/588 (0.2%)
75	o9	0.81	0/443	0.95	0/588
76	Q0	0.73	0/423	0.90	1/562 (0.2%)
76	q0	0.89	0/423	0.92	1/562 (0.2%)
77	Q1	0.70	0/234	0.93	0/300
77	q1	0.94	0/234	1.05	1/300 (0.3%)
78	Q2	1.00	1/860 (0.1%)	0.99	2/1136 (0.2%)
78	q2	0.83	2/860 (0.2%)	0.87	0/1136
79	Q3	0.73	0/701	0.84	0/934
79	q3	0.78	0/701	0.88	0/934
80	e0	0.58	0/499	0.77	0/665
82	p0	0.46	0/1092	0.62	0/1474
All	All	0.92	400/430070 (0.1%)	1.33	5106/631356 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S0	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	1
22	d0	0	1
25	D3	0	1
25	d3	0	1
26	d4	0	2
27	D5	0	1
28	D6	0	3
31	d9	0	1
33	E1	0	1
34	SR	0	2
39	L2	0	1
39	l2	0	2
40	l3	0	2
41	L4	0	2
41	l4	0	1
42	L5	0	1
42	l5	0	2
43	l6	0	1
44	L7	0	1
44	l7	0	2
51	M5	0	1
52	M6	0	2
52	m6	0	1
53	M7	0	1
53	m7	0	1
57	N1	0	1
59	n3	0	1
62	n6	0	1
63	N7	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
67	O1	0	1
67	o1	0	1
72	O6	0	1
All	All	0	57

The worst 5 of 400 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-38.52	0.45	1.34
34	SR	161	LYS	C-N	-29.42	0.66	1.34
78	Q2	17	CYS	CB-SG	16.03	2.09	1.82
36	5	1152	G	N9-C4	-13.26	1.27	1.38
39	l2	213	GLY	C-O	9.71	1.39	1.23

The worst 5 of 5106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	SR	161	LYS	O-C-N	-48.73	44.74	122.70
34	SR	160	GLU	C-N-CA	-43.07	14.02	121.70
34	SR	160	GLU	CA-C-N	-38.98	31.43	117.20
36	5	1152	G	N3-C4-C5	26.73	141.96	128.60
36	5	1152	G	N3-C4-N9	-24.27	111.44	126.00

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
2	S0	188	LEU	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	748	0
1	6	38238	0	19241	711	0
2	S0	1577	0	1567	139	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	145	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	111	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	93	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	146	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	130	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	106	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	106	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	98	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	116	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	58	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	59	0
13	c1	1168	0	1231	0	0
14	C2	890	0	887	64	0
14	c2	890	0	887	0	0
15	C3	1192	0	1255	76	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	91	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	74	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	90	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	68	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	89	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	84	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	d0	882	0	939	0	0
23	D1	684	0	672	54	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	65	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	72	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	70	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	52	0
27	d5	558	0	598	0	0
28	D6	769	0	814	84	0
28	d6	769	0	814	0	0
29	D7	610	0	631	49	0
29	d7	610	0	631	0	0
30	D8	497	0	535	34	0
30	d8	497	0	535	0	0
31	D9	442	0	428	33	0
31	d9	442	0	428	0	0
32	E0	475	0	525	25	0
33	E1	566	0	602	63	0
33	e1	608	0	657	0	0
34	SR	2441	0	2395	133	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	67	0
35	sM	680	0	607	0	0
36	1	67355	0	33840	1037	0
36	5	67376	0	33857	1042	0
37	3	2579	0	1304	39	0
37	7	2579	0	1304	39	0
38	4	3353	0	1695	51	0
38	8	3353	0	1695	58	0
39	L2	1914	0	1981	137	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	218	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	173	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	169	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	61	0
43	l6	1248	0	1339	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	L7	1784	0	1862	74	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	114	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	106	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	107	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	84	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	94	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	54	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	118	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	83	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	81	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	87	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	77	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	71	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	72	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	29	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	62	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	18	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	65	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	51	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	80	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	94	0
64	n8	1173	0	1215	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	N9	462	0	491	28	0
65	n9	462	0	491	0	0
66	O0	743	0	797	52	0
66	o0	767	0	816	0	0
67	O1	876	0	912	40	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	48	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	45	0
69	o3	850	0	880	0	0
70	O4	880	0	945	53	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	61	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	55	0
72	o6	770	0	846	0	0
73	O7	681	0	683	55	0
73	o7	681	0	683	0	0
74	O8	612	0	682	46	0
74	o8	608	0	671	0	0
75	O9	436	0	475	31	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	26	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	25	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	51	0
78	q2	847	0	914	0	0
79	Q3	694	0	734	44	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	175	0	0
82	p0	1077	0	1041	0	0
83	p1	235	0	51	0	0
84	p2	230	0	50	0	0
85	1	475	0	0	0	0
85	2	126	0	0	0	0
85	3	14	0	0	0	0
85	4	21	0	0	0	0
85	5	504	0	0	0	0
85	6	147	0	0	0	0
85	7	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	8	13	0	0	0	0
85	C3	1	0	0	0	0
85	L2	1	0	0	0	0
85	L3	2	0	0	0	0
85	L4	3	0	0	0	0
85	L5	1	0	0	0	0
85	L6	1	0	0	0	0
85	L7	2	0	0	0	0
85	L8	1	0	0	0	0
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	4	0	0	0	0
85	M5	2	0	0	0	0
85	M6	1	0	0	0	0
85	M7	6	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N8	2	0	0	0	0
85	O3	1	0	0	0	0
85	O4	1	0	0	0	0
85	O7	1	0	0	0	0
85	Q2	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	2	0	0	0	0
85	d2	1	0	0	0	0
85	d3	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	2	0	0	0	0
85	l3	1	0	0	0	0
85	l4	1	0	0	0	0
85	l5	3	0	0	0	0
85	l7	1	0	0	0	0
85	m1	2	0	0	0	0
85	m4	1	0	0	0	0
85	m5	1	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n0	2	0	0	0	0
85	n3	2	0	0	0	0
85	n6	2	0	0	0	0
85	n8	4	0	0	0	0
85	n9	2	0	0	0	0
85	o1	1	0	0	0	0
85	o3	2	0	0	0	0
85	o4	2	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	1	0	0	0	0
85	s1	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2436	0	0	247	0
86	2	1106	0	0	132	0
86	3	84	0	0	5	0
86	4	105	0	0	5	0
86	5	2471	0	0	233	0
86	6	1106	0	0	97	0
86	7	84	0	0	12	0
86	8	112	0	0	21	0
86	C1	7	0	0	7	0
86	C3	7	0	0	1	0
86	C5	7	0	0	4	0
86	C8	7	0	0	1	0
86	D9	7	0	0	1	0
86	L3	14	0	0	1	0
86	L4	7	0	0	2	0
86	L6	7	0	0	0	0
86	M0	7	0	0	0	0
86	M5	14	0	0	2	0
86	M6	7	0	0	1	0
86	M7	14	0	0	1	0
86	M9	7	0	0	1	0
86	N9	7	0	0	1	0
86	O2	7	0	0	0	0
86	O3	7	0	0	0	0
86	O7	14	0	0	6	0
86	O9	7	0	0	4	0
86	Q2	7	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	S8	7	0	0	1	0
86	SR	7	0	0	0	0
86	c1	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	21	0	0	0	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	n3	7	0	0	0	0
86	n9	7	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	o4	7	0	0	0	0
86	o7	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	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	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
88	1	33	0	0	0	0
88	5	33	0	0	1	0
All	All	411226	0	297271	8412	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 8412 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
52:M6:66:LYS:NZ	52:M6:66:LYS:CE	1.48	1.54
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.09	1.40
78:Q2:17:CYS:CB	87:Q2:501:ZN:ZN	1.31	1.09
40:L3:296:THR:HG22	40:L3:298:PHE:H	1.82	1.07
36:5:2403:G:N2	36:5:2404:A:N7	2.03	1.03

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	154 (76%)	27 (13%)	23 (11%)	1	1
2	s0	204/251 (81%)	161 (79%)	27 (13%)	16 (8%)	1	3
3	S1	212/254 (84%)	152 (72%)	31 (15%)	29 (14%)	0	1
3	s1	214/254 (84%)	179 (84%)	23 (11%)	12 (6%)	3	7
4	S2	215/253 (85%)	181 (84%)	25 (12%)	9 (4%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	s2	215/253 (85%)	187 (87%)	16 (7%)	12 (6%)	3	7
5	S3	221/239 (92%)	198 (90%)	14 (6%)	9 (4%)	4	14
5	s3	221/239 (92%)	193 (87%)	15 (7%)	13 (6%)	2	6
6	S4	258/260 (99%)	219 (85%)	27 (10%)	12 (5%)	4	11
6	s4	258/260 (99%)	223 (86%)	23 (9%)	12 (5%)	4	11
7	S5	204/224 (91%)	162 (79%)	21 (10%)	21 (10%)	1	1
7	s5	204/224 (91%)	164 (80%)	23 (11%)	17 (8%)	1	3
8	S6	224/236 (95%)	195 (87%)	21 (9%)	8 (4%)	5	17
8	s6	216/236 (92%)	194 (90%)	14 (6%)	8 (4%)	5	16
9	S7	182/189 (96%)	143 (79%)	21 (12%)	18 (10%)	1	2
9	s7	184/189 (97%)	148 (80%)	22 (12%)	14 (8%)	2	3
10	S8	184/200 (92%)	159 (86%)	12 (6%)	13 (7%)	2	4
10	s8	184/200 (92%)	164 (89%)	11 (6%)	9 (5%)	3	10
11	S9	183/196 (93%)	159 (87%)	15 (8%)	9 (5%)	3	10
11	s9	183/196 (93%)	148 (81%)	23 (13%)	12 (7%)	2	5
12	C0	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	2	5
12	c0	92/105 (88%)	63 (68%)	16 (17%)	13 (14%)	0	1
13	C1	153/155 (99%)	125 (82%)	18 (12%)	10 (6%)	2	5
13	c1	144/155 (93%)	117 (81%)	18 (12%)	9 (6%)	2	5
14	C2	122/142 (86%)	70 (57%)	26 (21%)	26 (21%)	0	0
14	c2	122/142 (86%)	71 (58%)	29 (24%)	22 (18%)	0	0
15	C3	148/150 (99%)	132 (89%)	13 (9%)	3 (2%)	11	35
15	c3	148/150 (99%)	123 (83%)	16 (11%)	9 (6%)	2	6
16	C4	125/136 (92%)	97 (78%)	16 (13%)	12 (10%)	1	2
16	c4	126/136 (93%)	101 (80%)	15 (12%)	10 (8%)	1	3
17	C5	122/141 (86%)	95 (78%)	16 (13%)	11 (9%)	1	2
17	c5	133/141 (94%)	97 (73%)	16 (12%)	20 (15%)	0	1
18	C6	139/142 (98%)	121 (87%)	13 (9%)	5 (4%)	5	17
18	c6	140/142 (99%)	121 (86%)	11 (8%)	8 (6%)	3	7
19	C7	116/136 (85%)	87 (75%)	22 (19%)	7 (6%)	2	6
19	c7	113/136 (83%)	96 (85%)	11 (10%)	6 (5%)	3	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	C8	143/145 (99%)	121 (85%)	11 (8%)	11 (8%)	1	3
20	c8	143/145 (99%)	115 (80%)	21 (15%)	7 (5%)	3	10
21	C9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	6	18
21	c9	141/143 (99%)	122 (86%)	14 (10%)	5 (4%)	6	18
22	D0	105/120 (88%)	88 (84%)	15 (14%)	2 (2%)	12	37
22	d0	108/120 (90%)	85 (79%)	15 (14%)	8 (7%)	2	3
23	D1	85/87 (98%)	69 (81%)	10 (12%)	6 (7%)	2	4
23	d1	85/87 (98%)	75 (88%)	5 (6%)	5 (6%)	2	6
24	D2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	27	65
24	d2	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	27	65
25	D3	142/144 (99%)	117 (82%)	14 (10%)	11 (8%)	1	3
25	d3	142/144 (99%)	131 (92%)	10 (7%)	1 (1%)	30	69
26	D4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	2	6
26	d4	132/134 (98%)	106 (80%)	15 (11%)	11 (8%)	1	3
27	D5	68/107 (64%)	51 (75%)	9 (13%)	8 (12%)	1	1
27	d5	67/107 (63%)	48 (72%)	13 (19%)	6 (9%)	1	2
28	D6	95/97 (98%)	69 (73%)	12 (13%)	14 (15%)	0	1
28	d6	95/97 (98%)	73 (77%)	14 (15%)	8 (8%)	1	3
29	D7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	2	5
29	d7	79/81 (98%)	60 (76%)	10 (13%)	9 (11%)	1	1
30	D8	61/66 (92%)	51 (84%)	7 (12%)	3 (5%)	3	10
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	1	3
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	6
31	d9	51/55 (93%)	42 (82%)	5 (10%)	4 (8%)	1	3
32	E0	58/60 (97%)	45 (78%)	12 (21%)	1 (2%)	14	42
33	E1	69/76 (91%)	36 (52%)	14 (20%)	19 (28%)	0	0
33	e1	74/76 (97%)	38 (51%)	16 (22%)	20 (27%)	0	0
34	SR	316/318 (99%)	274 (87%)	29 (9%)	13 (4%)	4	14
34	sR	316/318 (99%)	268 (85%)	40 (13%)	8 (2%)	9	28
35	SM	155/273 (57%)	109 (70%)	26 (17%)	20 (13%)	0	1
35	sM	98/273 (36%)	61 (62%)	24 (24%)	13 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	L2	250/253 (99%)	226 (90%)	20 (8%)	4 (2%)	14	44
39	l2	250/253 (99%)	214 (86%)	27 (11%)	9 (4%)	5	17
40	L3	384/386 (100%)	340 (88%)	31 (8%)	13 (3%)	6	19
40	l3	384/386 (100%)	350 (91%)	25 (6%)	9 (2%)	10	31
41	L4	359/361 (99%)	315 (88%)	23 (6%)	21 (6%)	3	7
41	l4	359/361 (99%)	308 (86%)	38 (11%)	13 (4%)	5	17
42	L5	294/296 (99%)	253 (86%)	23 (8%)	18 (6%)	2	6
42	l5	292/296 (99%)	262 (90%)	21 (7%)	9 (3%)	7	21
43	L6	152/175 (87%)	141 (93%)	8 (5%)	3 (2%)	11	35
43	l6	153/175 (87%)	132 (86%)	17 (11%)	4 (3%)	8	26
44	L7	220/243 (90%)	205 (93%)	6 (3%)	9 (4%)	4	14
44	l7	221/243 (91%)	203 (92%)	15 (7%)	3 (1%)	16	49
45	L8	231/255 (91%)	193 (84%)	30 (13%)	8 (4%)	6	18
45	l8	229/255 (90%)	184 (80%)	25 (11%)	20 (9%)	1	2
46	L9	189/191 (99%)	170 (90%)	14 (7%)	5 (3%)	8	26
46	l9	189/191 (99%)	173 (92%)	10 (5%)	6 (3%)	6	20
47	M0	207/220 (94%)	185 (89%)	17 (8%)	5 (2%)	9	29
47	m0	209/220 (95%)	181 (87%)	20 (10%)	8 (4%)	5	15
48	M1	167/173 (96%)	133 (80%)	20 (12%)	14 (8%)	1	3
48	m1	167/173 (96%)	146 (87%)	11 (7%)	10 (6%)	2	6
49	M3	191/198 (96%)	164 (86%)	19 (10%)	8 (4%)	4	13
49	m3	192/198 (97%)	164 (85%)	17 (9%)	11 (6%)	3	7
50	M4	134/137 (98%)	118 (88%)	11 (8%)	5 (4%)	5	16
50	m4	135/137 (98%)	127 (94%)	6 (4%)	2 (2%)	15	46
51	M5	201/203 (99%)	188 (94%)	7 (4%)	6 (3%)	7	22
51	m5	201/203 (99%)	180 (90%)	14 (7%)	7 (4%)	6	18
52	M6	195/198 (98%)	185 (95%)	6 (3%)	4 (2%)	11	33
52	m6	195/198 (98%)	185 (95%)	8 (4%)	2 (1%)	22	60
53	M7	181/183 (99%)	159 (88%)	16 (9%)	6 (3%)	6	19
53	m7	153/183 (84%)	140 (92%)	10 (6%)	3 (2%)	11	35
54	M8	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	10	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	m8	183/185 (99%)	165 (90%)	11 (6%)	7 (4%)	5	15
55	M9	186/188 (99%)	173 (93%)	12 (6%)	1 (0%)	38	76
55	m9	186/188 (99%)	175 (94%)	8 (4%)	3 (2%)	14	44
56	N0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	19	54
56	n0	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	13	39
57	N1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	6	20
57	n1	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	9	28
58	N2	98/120 (82%)	79 (81%)	15 (15%)	4 (4%)	4	14
58	n2	96/120 (80%)	84 (88%)	9 (9%)	3 (3%)	7	21
59	N3	134/136 (98%)	126 (94%)	7 (5%)	1 (1%)	30	69
59	n3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	30	69
60	N4	96/155 (62%)	77 (80%)	14 (15%)	5 (5%)	3	9
60	n4	133/155 (86%)	113 (85%)	12 (9%)	8 (6%)	2	6
61	N5	119/141 (84%)	110 (92%)	8 (7%)	1 (1%)	27	65
61	n5	118/141 (84%)	100 (85%)	13 (11%)	5 (4%)	4	13
62	N6	124/126 (98%)	114 (92%)	6 (5%)	4 (3%)	6	20
62	n6	124/126 (98%)	113 (91%)	6 (5%)	5 (4%)	5	14
63	N7	133/135 (98%)	111 (84%)	12 (9%)	10 (8%)	2	3
63	n7	133/135 (98%)	111 (84%)	14 (10%)	8 (6%)	2	6
64	N8	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	3	8
64	n8	146/148 (99%)	126 (86%)	16 (11%)	4 (3%)	8	25
65	N9	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	5	17
65	n9	56/58 (97%)	43 (77%)	9 (16%)	4 (7%)	2	4
66	O0	95/104 (91%)	87 (92%)	6 (6%)	2 (2%)	11	33
66	o0	98/104 (94%)	89 (91%)	7 (7%)	2 (2%)	11	35
67	O1	107/112 (96%)	95 (89%)	7 (6%)	5 (5%)	4	11
67	o1	107/112 (96%)	98 (92%)	5 (5%)	4 (4%)	5	16
68	O2	125/129 (97%)	116 (93%)	8 (6%)	1 (1%)	27	65
68	o2	125/129 (97%)	111 (89%)	11 (9%)	3 (2%)	9	29
69	O3	104/106 (98%)	101 (97%)	2 (2%)	1 (1%)	22	60
69	o3	104/106 (98%)	92 (88%)	7 (7%)	5 (5%)	4	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	O4	110/119 (92%)	103 (94%)	4 (4%)	3 (3%)	8	25
70	o4	110/119 (92%)	100 (91%)	8 (7%)	2 (2%)	13	39
71	O5	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	6	19
71	o5	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	14	42
72	O6	97/99 (98%)	78 (80%)	11 (11%)	8 (8%)	1	3
72	o6	97/99 (98%)	81 (84%)	9 (9%)	7 (7%)	2	4
73	O7	85/87 (98%)	76 (89%)	6 (7%)	3 (4%)	6	18
73	o7	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	6	18
74	O8	75/77 (97%)	62 (83%)	10 (13%)	3 (4%)	5	14
74	o8	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	5	14
75	O9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
75	o9	48/50 (96%)	44 (92%)	3 (6%)	1 (2%)	11	33
76	Q0	50/52 (96%)	48 (96%)	0	2 (4%)	5	14
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	11	35
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	23 (100%)	0	0	100	100
78	Q2	103/105 (98%)	90 (87%)	10 (10%)	3 (3%)	7	23
78	q2	103/105 (98%)	92 (89%)	8 (8%)	3 (3%)	7	23
79	Q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	10	32
79	q3	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	21	57
80	e0	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	2	5
82	p0	139/311 (45%)	117 (84%)	19 (14%)	3 (2%)	10	32
All	All	22333/24141 (92%)	19119 (86%)	2092 (9%)	1122 (5%)	3	10

5 of 1122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	66	ALA
2	S0	103	THR
2	S0	158	VAL
2	S0	163	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	164/209 (78%)	134 (82%)	30 (18%)	2	7
2	s0	165/209 (79%)	131 (79%)	34 (21%)	2	5
3	S1	191/223 (86%)	162 (85%)	29 (15%)	4	12
3	s1	192/223 (86%)	162 (84%)	30 (16%)	4	11
4	S2	176/204 (86%)	137 (78%)	39 (22%)	1	4
4	s2	176/204 (86%)	139 (79%)	37 (21%)	1	5
5	S3	182/194 (94%)	149 (82%)	33 (18%)	2	7
5	s3	182/194 (94%)	149 (82%)	33 (18%)	2	7
6	S4	221/221 (100%)	182 (82%)	39 (18%)	3	8
6	s4	221/221 (100%)	187 (85%)	34 (15%)	4	12
7	S5	173/190 (91%)	140 (81%)	33 (19%)	2	6
7	s5	173/190 (91%)	138 (80%)	35 (20%)	2	5
8	S6	188/201 (94%)	155 (82%)	33 (18%)	3	8
8	s6	187/201 (93%)	152 (81%)	35 (19%)	2	7
9	S7	165/169 (98%)	140 (85%)	25 (15%)	4	12
9	s7	165/169 (98%)	134 (81%)	31 (19%)	2	7
10	S8	150/161 (93%)	128 (85%)	22 (15%)	4	13
10	s8	150/161 (93%)	129 (86%)	21 (14%)	5	15
11	S9	158/165 (96%)	123 (78%)	35 (22%)	1	4
11	s9	158/165 (96%)	128 (81%)	30 (19%)	2	6
12	C0	77/98 (79%)	58 (75%)	19 (25%)	1	2
12	c0	73/98 (74%)	61 (84%)	12 (16%)	3	10
13	C1	129/136 (95%)	104 (81%)	25 (19%)	2	6
13	c1	129/136 (95%)	107 (83%)	22 (17%)	3	8
14	C2	88/118 (75%)	68 (77%)	20 (23%)	1	3
14	c2	88/118 (75%)	65 (74%)	23 (26%)	1	2
15	C3	127/127 (100%)	101 (80%)	26 (20%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	c3	127/127 (100%)	105 (83%)	22 (17%)	3	8
16	C4	81/104 (78%)	61 (75%)	20 (25%)	1	2
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	3
17	C5	101/117 (86%)	86 (85%)	15 (15%)	4	12
17	c5	103/117 (88%)	83 (81%)	20 (19%)	2	6
18	C6	117/118 (99%)	94 (80%)	23 (20%)	2	6
18	c6	118/118 (100%)	98 (83%)	20 (17%)	3	9
19	C7	94/124 (76%)	70 (74%)	24 (26%)	1	2
19	c7	92/124 (74%)	76 (83%)	16 (17%)	3	8
20	C8	128/128 (100%)	102 (80%)	26 (20%)	2	5
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	4
21	C9	115/115 (100%)	93 (81%)	22 (19%)	2	6
21	c9	115/115 (100%)	95 (83%)	20 (17%)	3	8
22	D0	100/113 (88%)	74 (74%)	26 (26%)	1	2
22	d0	103/113 (91%)	80 (78%)	23 (22%)	1	4
23	D1	74/74 (100%)	60 (81%)	14 (19%)	2	7
23	d1	74/74 (100%)	57 (77%)	17 (23%)	1	3
24	D2	110/110 (100%)	94 (86%)	16 (14%)	5	13
24	d2	110/110 (100%)	96 (87%)	14 (13%)	6	19
25	D3	119/119 (100%)	97 (82%)	22 (18%)	2	7
25	d3	119/119 (100%)	104 (87%)	15 (13%)	7	19
26	D4	112/112 (100%)	93 (83%)	19 (17%)	3	9
26	d4	112/112 (100%)	99 (88%)	13 (12%)	8	23
27	D5	61/88 (69%)	43 (70%)	18 (30%)	0	1
27	d5	61/88 (69%)	54 (88%)	7 (12%)	8	23
28	D6	83/83 (100%)	66 (80%)	17 (20%)	2	5
28	d6	83/83 (100%)	69 (83%)	14 (17%)	3	9
29	D7	70/70 (100%)	57 (81%)	13 (19%)	2	7
29	d7	70/70 (100%)	59 (84%)	11 (16%)	4	11
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1	4
30	d8	56/59 (95%)	48 (86%)	8 (14%)	5	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D9	47/48 (98%)	38 (81%)	9 (19%)	2	6
31	d9	47/48 (98%)	39 (83%)	8 (17%)	3	9
32	E0	51/51 (100%)	41 (80%)	10 (20%)	2	6
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	3
33	e1	66/66 (100%)	48 (73%)	18 (27%)	0	2
34	SR	260/261 (100%)	237 (91%)	23 (9%)	14	38
34	sR	260/261 (100%)	232 (89%)	28 (11%)	9	26
35	SM	97/228 (42%)	79 (81%)	18 (19%)	2	7
35	sM	54/228 (24%)	47 (87%)	7 (13%)	6	17
39	L2	193/195 (99%)	157 (81%)	36 (19%)	2	7
39	l2	192/195 (98%)	155 (81%)	37 (19%)	2	6
40	L3	321/322 (100%)	258 (80%)	63 (20%)	2	6
40	l3	320/322 (99%)	255 (80%)	65 (20%)	2	5
41	L4	288/288 (100%)	239 (83%)	49 (17%)	3	9
41	l4	288/288 (100%)	235 (82%)	53 (18%)	2	7
42	L5	244/244 (100%)	194 (80%)	50 (20%)	2	5
42	l5	243/244 (100%)	192 (79%)	51 (21%)	1	5
43	L6	134/152 (88%)	115 (86%)	19 (14%)	5	14
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	8
44	L7	186/204 (91%)	162 (87%)	24 (13%)	6	18
44	l7	187/204 (92%)	159 (85%)	28 (15%)	4	12
45	L8	187/207 (90%)	154 (82%)	33 (18%)	3	8
45	l8	177/207 (86%)	143 (81%)	34 (19%)	2	6
46	L9	171/171 (100%)	139 (81%)	32 (19%)	2	7
46	l9	171/171 (100%)	137 (80%)	34 (20%)	2	6
47	M0	177/186 (95%)	144 (81%)	33 (19%)	2	7
47	m0	179/186 (96%)	142 (79%)	37 (21%)	2	5
48	M1	147/150 (98%)	119 (81%)	28 (19%)	2	6
48	m1	147/150 (98%)	125 (85%)	22 (15%)	4	12
49	M3	154/158 (98%)	126 (82%)	28 (18%)	2	7
49	m3	154/158 (98%)	130 (84%)	24 (16%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	M4	107/108 (99%)	86 (80%)	21 (20%)	2	6
50	m4	108/108 (100%)	90 (83%)	18 (17%)	3	9
51	M5	175/175 (100%)	146 (83%)	29 (17%)	3	9
51	m5	175/175 (100%)	148 (85%)	27 (15%)	4	12
52	M6	160/161 (99%)	137 (86%)	23 (14%)	5	13
52	m6	160/161 (99%)	132 (82%)	28 (18%)	3	8
53	M7	140/145 (97%)	113 (81%)	27 (19%)	2	6
53	m7	125/145 (86%)	108 (86%)	17 (14%)	5	16
54	M8	150/150 (100%)	125 (83%)	25 (17%)	3	9
54	m8	150/150 (100%)	122 (81%)	28 (19%)	2	7
55	M9	153/153 (100%)	133 (87%)	20 (13%)	6	17
55	m9	153/153 (100%)	119 (78%)	34 (22%)	1	4
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	7
56	n0	156/156 (100%)	132 (85%)	24 (15%)	4	12
57	N1	136/136 (100%)	108 (79%)	28 (21%)	2	5
57	n1	136/136 (100%)	116 (85%)	20 (15%)	4	13
58	N2	87/106 (82%)	76 (87%)	11 (13%)	7	19
58	n2	85/106 (80%)	73 (86%)	12 (14%)	5	14
59	N3	104/104 (100%)	90 (86%)	14 (14%)	6	16
59	n3	104/104 (100%)	95 (91%)	9 (9%)	15	39
60	N4	57/129 (44%)	52 (91%)	5 (9%)	14	38
60	n4	100/129 (78%)	88 (88%)	12 (12%)	7	21
61	N5	104/117 (89%)	79 (76%)	25 (24%)	1	3
61	n5	104/117 (89%)	80 (77%)	24 (23%)	1	3
62	N6	109/109 (100%)	88 (81%)	21 (19%)	2	6
62	n6	109/109 (100%)	84 (77%)	25 (23%)	1	3
63	N7	115/115 (100%)	91 (79%)	24 (21%)	1	5
63	n7	115/115 (100%)	92 (80%)	23 (20%)	2	6
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	8
64	n8	118/118 (100%)	95 (80%)	23 (20%)	2	6
65	N9	46/46 (100%)	38 (83%)	8 (17%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	n9	46/46 (100%)	35 (76%)	11 (24%)	1	3
66	O0	81/87 (93%)	66 (82%)	15 (18%)	2	7
66	o0	84/87 (97%)	68 (81%)	16 (19%)	2	6
67	O1	92/96 (96%)	72 (78%)	20 (22%)	1	4
67	o1	94/96 (98%)	77 (82%)	17 (18%)	2	7
68	O2	109/110 (99%)	94 (86%)	15 (14%)	5	15
68	o2	109/110 (99%)	92 (84%)	17 (16%)	4	11
69	O3	90/90 (100%)	76 (84%)	14 (16%)	4	11
69	o3	90/90 (100%)	82 (91%)	8 (9%)	14	38
70	O4	95/101 (94%)	78 (82%)	17 (18%)	2	7
70	o4	95/101 (94%)	81 (85%)	14 (15%)	4	13
71	O5	104/104 (100%)	83 (80%)	21 (20%)	2	5
71	o5	103/104 (99%)	76 (74%)	27 (26%)	1	2
72	O6	81/81 (100%)	60 (74%)	21 (26%)	1	2
72	o6	80/81 (99%)	52 (65%)	28 (35%)	0	0
73	O7	70/70 (100%)	58 (83%)	12 (17%)	3	8
73	o7	70/70 (100%)	59 (84%)	11 (16%)	4	11
74	O8	68/68 (100%)	55 (81%)	13 (19%)	2	6
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	7
75	O9	45/45 (100%)	36 (80%)	9 (20%)	2	6
75	o9	45/45 (100%)	35 (78%)	10 (22%)	1	4
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	4	12
76	q0	47/47 (100%)	40 (85%)	7 (15%)	4	12
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	76 (84%)	14 (16%)	4	11
78	q2	90/90 (100%)	73 (81%)	17 (19%)	2	7
79	Q3	71/71 (100%)	61 (86%)	10 (14%)	5	14
79	q3	71/71 (100%)	58 (82%)	13 (18%)	2	7
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1	3
82	p0	105/253 (42%)	84 (80%)	21 (20%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	18729/20239 (92%)	15348 (82%)	3381 (18%)	2 7

5 of 3381 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
67	O1	110	GLU
7	s5	216	GLU
64	n8	10	LYS
70	O4	86	LYS
2	s0	172	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
48	M1	95	ASN
61	N5	80	ASN
61	n5	111	ASN
53	M7	125	GLN
59	N3	81	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	0/1800	-	-
1	6	0/1800	-	-
36	1	0/3396	-	-
36	5	0/3396	-	-
37	3	0/121	-	-
37	7	0/121	-	-
38	4	0/158	-	-
38	8	0/158	-	-
All	All	0/10950	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 2559 ligands modelled in this entry, 1424 are monoatomic - leaving 1135 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3H3	1	4216	-	34,34,34	1.01	3 (8%)	45,45,45	1.77	8 (17%)
86	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2032	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2147	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3942	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	86	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3H3	5	4251	-	34,34,34	1.13	2 (5%)	45,45,45	1.38	5 (11%)
86	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	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
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	3803	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o4	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3869	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3911	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3953	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3995	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4037	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4079	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4121	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4163	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
88	3H3	1	4216	-	-	0/39/51/51	0/1/2/2
86	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2032	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2054	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2096	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2138	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	86	-	0/0/0/0	0/0/0/0
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2180	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	3	225	-	-	0/0/0/0	0/0/0/0
86	OHX	3	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	222	-	-	0/0/0/0	0/0/0/0
86	OHX	4	223	-	-	0/0/0/0	0/0/0/0
86	OHX	4	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	4	236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3942	86	-	0/0/0/0	0/0/0/0
86	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3995	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4037	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4079	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4121	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4163	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4205	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	86	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4247	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
88	3H3	5	4251	-	-	0/39/51/51	0/1/2/2
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
86	OHX	7	216	-	-	0/0/0/0	0/0/0/0
86	OHX	7	217	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	214	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	C1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	M6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	208	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	103	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
86	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	3803	-	-	0/0/0/0	0/0/0/0
86	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o4	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	4251	3H3	C14-C16	5.04	1.56	1.52
88	1	4216	3H3	C3-C2	3.25	1.47	1.33
88	5	4251	3H3	C15-C14	-2.47	1.50	1.53
88	1	4216	3H3	C15-C14	-2.47	1.50	1.53
88	1	4216	3H3	C14-C16	2.45	1.54	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4216	3H3	C-C1-C11	5.41	119.56	111.11
88	1	4216	3H3	C1-C11-C12	4.79	122.64	113.80
88	5	4251	3H3	C15-C14-C16	4.11	116.50	109.83
88	1	4216	3H3	C15-C14-C16	4.07	116.44	109.83
88	1	4216	3H3	C11-C1-C2	4.04	118.12	110.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	SR	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SR	161:LYS	C	162:ALA	N	0.66
1	SR	160:GLU	C	161:LYS	N	0.45

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	1750/1800 (97%)	0.52	92 (5%) 25 26	40, 69, 136, 230	0
1	6	1795/1800 (99%)	0.50	82 (4%) 31 31	30, 58, 149, 237	0
2	S0	206/251 (82%)	1.13	44 (21%) 1 1	73, 88, 101, 127	0
2	s0	206/251 (82%)	0.67	22 (10%) 6 6	54, 71, 86, 92	0
3	S1	214/254 (84%)	2.28	87 (40%) 1 0	79, 109, 140, 148	0
3	s1	216/254 (85%)	1.00	39 (18%) 2 2	53, 65, 88, 95	0
4	S2	217/253 (85%)	1.76	92 (42%) 1 0	54, 68, 83, 96	0
4	s2	217/253 (85%)	1.58	72 (33%) 1 1	42, 56, 69, 78	0
5	S3	223/239 (93%)	2.60	125 (56%) 0 0	59, 72, 92, 108	0
5	s3	223/239 (93%)	2.23	108 (48%) 1 0	55, 76, 98, 104	0
6	S4	260/260 (100%)	1.02	46 (17%) 2 2	47, 69, 80, 108	0
6	s4	260/260 (100%)	0.67	18 (6%) 17 15	37, 58, 69, 100	0
7	S5	206/224 (91%)	1.56	67 (32%) 1 1	73, 92, 107, 120	0
7	s5	206/224 (91%)	1.21	47 (22%) 1 1	56, 77, 101, 113	0
8	S6	226/236 (95%)	1.02	44 (19%) 2 1	49, 82, 98, 126	0
8	s6	218/236 (92%)	0.61	17 (7%) 13 11	38, 66, 87, 107	0
9	S7	184/189 (97%)	0.74	20 (10%) 6 5	65, 92, 123, 131	0
9	s7	186/189 (98%)	1.25	30 (16%) 2 2	49, 78, 112, 122	0
10	S8	188/200 (94%)	0.96	34 (18%) 2 2	40, 55, 89, 104	0
10	s8	188/200 (94%)	1.05	32 (17%) 2 2	33, 52, 95, 111	0
11	S9	185/196 (94%)	2.38	94 (50%) 0 0	64, 77, 113, 146	0
11	s9	185/196 (94%)	0.69	14 (7%) 14 12	49, 62, 99, 125	0
12	C0	96/105 (91%)	2.77	57 (59%) 0 0	63, 83, 110, 128	0
12	c0	96/105 (91%)	3.57	66 (68%) 0 0	69, 99, 122, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	2.23	59 (38%)	1	0	43, 53, 103, 117	0
13	c1	146/155 (94%)	1.48	30 (20%)	1	1	34, 48, 76, 96	0
14	C2	124/142 (87%)	3.56	77 (62%)	0	0	105, 118, 138, 151	0
14	c2	124/142 (87%)	5.19	99 (79%)	0	0	139, 159, 175, 184	0
15	C3	150/150 (100%)	0.64	12 (8%)	12	11	50, 67, 80, 86	0
15	c3	150/150 (100%)	0.58	9 (6%)	21	21	40, 55, 71, 85	0
16	C4	127/136 (93%)	2.47	64 (50%)	0	0	54, 113, 128, 131	0
16	c4	128/136 (94%)	1.68	43 (33%)	1	1	38, 71, 80, 83	0
17	C5	124/141 (87%)	1.28	30 (24%)	1	1	58, 72, 108, 128	0
17	c5	135/141 (95%)	1.11	24 (17%)	2	2	58, 74, 98, 120	0
18	C6	141/142 (99%)	1.06	26 (18%)	2	2	62, 82, 87, 89	0
18	c6	142/142 (100%)	0.86	25 (17%)	2	2	50, 71, 84, 105	0
19	C7	120/136 (88%)	0.50	13 (10%)	6	5	68, 85, 111, 113	0
19	c7	117/136 (86%)	0.65	14 (11%)	5	4	59, 72, 98, 109	0
20	C8	145/145 (100%)	0.56	16 (11%)	6	5	58, 80, 105, 114	0
20	c8	145/145 (100%)	0.09	5 (3%)	43	44	55, 65, 90, 103	0
21	C9	143/143 (100%)	0.16	4 (2%)	50	52	66, 80, 94, 105	0
21	c9	143/143 (100%)	0.27	6 (4%)	35	35	51, 64, 82, 98	0
22	D0	107/120 (89%)	2.01	42 (39%)	1	0	56, 87, 118, 129	0
22	d0	110/120 (91%)	3.45	51 (46%)	1	0	50, 82, 120, 132	0
23	D1	87/87 (100%)	1.29	24 (27%)	1	1	69, 75, 92, 99	0
23	d1	87/87 (100%)	0.75	8 (9%)	9	7	53, 59, 77, 88	0
24	D2	129/129 (100%)	1.78	53 (41%)	1	0	52, 62, 68, 78	0
24	d2	129/129 (100%)	0.68	6 (4%)	30	30	37, 47, 53, 61	0
25	D3	144/144 (100%)	1.78	52 (36%)	1	1	43, 49, 59, 73	0
25	d3	144/144 (100%)	1.03	18 (12%)	5	4	33, 38, 52, 65	0
26	D4	134/134 (100%)	0.86	23 (17%)	2	2	59, 82, 97, 105	0
26	d4	134/134 (100%)	0.20	5 (3%)	39	39	46, 66, 81, 100	0
27	D5	70/107 (65%)	1.42	18 (25%)	1	1	87, 103, 115, 121	0
27	d5	69/107 (64%)	1.14	18 (26%)	1	1	66, 87, 99, 101	0
28	D6	97/97 (100%)	3.25	64 (65%)	0	0	59, 74, 129, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	d6	97/97 (100%)	1.77	33 (34%) 1 1	43, 55, 84, 93	0
29	D7	81/81 (100%)	0.75	8 (9%) 8 6	64, 79, 113, 123	0
29	d7	81/81 (100%)	1.09	11 (13%) 4 3	49, 66, 106, 109	0
30	D8	63/66 (95%)	3.90	45 (71%) 0 0	89, 104, 118, 130	0
30	d8	63/66 (95%)	2.42	37 (58%) 0 0	74, 89, 103, 112	0
31	D9	53/55 (96%)	0.83	6 (11%) 6 5	56, 60, 80, 89	0
31	d9	53/55 (96%)	1.08	12 (22%) 1 1	52, 58, 95, 109	0
32	E0	60/60 (100%)	4.86	45 (75%) 0 0	47, 79, 115, 121	0
33	E1	71/76 (93%)	1.84	27 (38%) 1 0	91, 102, 113, 115	0
33	e1	76/76 (100%)	2.10	30 (39%) 1 0	117, 130, 148, 153	0
34	SR	318/318 (100%)	0.47	30 (9%) 9 7	55, 87, 106, 129	0
34	sR	318/318 (100%)	1.34	93 (29%) 1 1	73, 91, 107, 124	0
35	SM	159/273 (58%)	2.69	83 (52%) 0 0	51, 73, 118, 120	0
35	sM	104/273 (38%)	1.62	32 (30%) 1 1	40, 75, 155, 158	0
36	1	3149/3396 (92%)	0.48	89 (2%) 50 52	17, 37, 108, 219	0
36	5	3150/3396 (92%)	0.48	91 (2%) 49 50	17, 36, 101, 220	0
37	3	121/121 (100%)	0.21	1 (0%) 83 83	28, 53, 70, 75	0
37	7	121/121 (100%)	0.29	0 100 100	24, 40, 51, 59	0
38	4	158/158 (100%)	0.62	6 (3%) 38 38	22, 40, 74, 105	0
38	8	158/158 (100%)	0.72	8 (5%) 27 27	27, 46, 80, 102	0
39	L2	252/253 (99%)	0.95	34 (13%) 4 3	20, 35, 50, 58	0
39	l2	252/253 (99%)	0.69	18 (7%) 16 14	21, 37, 55, 62	0
40	L3	386/386 (100%)	0.36	13 (3%) 43 44	23, 41, 54, 87	0
40	l3	386/386 (100%)	0.17	4 (1%) 79 79	17, 30, 42, 73	0
41	L4	361/361 (100%)	0.06	7 (1%) 64 64	19, 33, 49, 57	0
41	l4	361/361 (100%)	0.37	24 (6%) 18 16	21, 38, 55, 62	0
42	L5	296/296 (100%)	0.10	7 (2%) 56 57	37, 59, 77, 103	0
42	l5	294/296 (99%)	0.01	3 (1%) 79 79	29, 43, 66, 101	0
43	L6	156/175 (89%)	-0.08	1 (0%) 86 88	28, 35, 53, 69	0
43	l6	157/175 (89%)	-0.00	5 (3%) 45 46	30, 38, 56, 68	0
44	L7	222/243 (91%)	0.02	1 (0%) 88 90	21, 29, 54, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	l7	223/243 (91%)	0.06	4 (1%) 65 66	20, 28, 65, 105	0
45	L8	233/255 (91%)	0.79	33 (14%) 3 3	42, 54, 88, 105	0
45	l8	231/255 (90%)	1.13	47 (20%) 1 1	51, 63, 88, 93	0
46	L9	191/191 (100%)	0.25	5 (2%) 53 54	37, 48, 60, 76	0
46	l9	191/191 (100%)	0.15	3 (1%) 68 69	27, 35, 54, 75	0
47	M0	211/220 (95%)	0.32	10 (4%) 30 30	24, 38, 72, 91	0
47	m0	213/220 (96%)	0.59	13 (6%) 21 20	25, 41, 64, 83	0
48	M1	169/173 (97%)	0.22	7 (4%) 35 36	45, 63, 76, 84	0
48	m1	169/173 (97%)	0.11	2 (1%) 75 76	32, 48, 60, 71	0
49	M3	193/198 (97%)	0.54	11 (5%) 23 23	21, 39, 73, 98	0
49	m3	194/198 (97%)	0.66	21 (10%) 6 5	27, 47, 80, 102	0
50	M4	136/137 (99%)	-0.01	4 (2%) 49 50	31, 38, 51, 59	0
50	m4	137/137 (100%)	-0.06	3 (2%) 59 60	28, 33, 51, 62	0
51	M5	203/203 (100%)	0.51	6 (2%) 48 49	20, 34, 42, 49	0
51	m5	203/203 (100%)	0.59	5 (2%) 54 55	25, 41, 51, 56	0
52	M6	197/198 (99%)	0.13	2 (1%) 79 79	22, 29, 48, 54	0
52	m6	197/198 (99%)	0.09	4 (2%) 62 63	18, 23, 47, 53	0
53	M7	183/183 (100%)	0.83	17 (9%) 9 7	25, 32, 82, 114	0
53	m7	155/183 (84%)	0.45	3 (1%) 64 64	21, 28, 40, 64	0
54	M8	185/185 (100%)	0.02	0 100 100	22, 31, 44, 56	0
54	m8	185/185 (100%)	0.30	0 100 100	26, 37, 46, 52	0
55	M9	188/188 (100%)	0.90	32 (17%) 2 2	38, 51, 127, 140	0
55	m9	188/188 (100%)	0.71	25 (13%) 4 3	34, 45, 105, 122	0
56	N0	172/172 (100%)	0.28	4 (2%) 57 58	29, 36, 48, 54	0
56	n0	172/172 (100%)	0.09	3 (1%) 67 68	23, 30, 40, 48	0
57	N1	159/159 (100%)	0.18	5 (3%) 47 47	25, 35, 71, 78	0
57	n1	159/159 (100%)	0.19	4 (2%) 54 55	25, 31, 64, 70	0
58	N2	100/120 (83%)	0.38	11 (11%) 6 5	67, 81, 92, 101	0
58	n2	98/120 (81%)	1.00	20 (20%) 1 1	58, 70, 80, 81	0
59	N3	136/136 (100%)	0.64	13 (9%) 8 7	27, 37, 50, 57	0
59	n3	136/136 (100%)	0.86	11 (8%) 12 10	19, 28, 42, 45	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
60	N4	98/155 (63%)	2.88	34 (34%)	1 1	37, 48, 127, 130	0
60	n4	135/155 (87%)	0.99	13 (9%)	8 7	28, 74, 108, 124	0
61	N5	121/141 (85%)	1.04	20 (16%)	2 2	34, 46, 61, 83	0
61	n5	120/141 (85%)	1.25	30 (25%)	1 1	36, 49, 67, 72	0
62	N6	126/126 (100%)	0.66	11 (8%)	10 9	27, 42, 53, 61	0
62	n6	126/126 (100%)	1.70	42 (33%)	1 1	32, 45, 60, 65	0
63	N7	135/135 (100%)	0.24	4 (2%)	48 49	53, 66, 80, 88	0
63	n7	135/135 (100%)	0.35	11 (8%)	12 10	57, 72, 91, 99	0
64	N8	148/148 (100%)	0.36	5 (3%)	43 44	18, 32, 54, 63	0
64	n8	148/148 (100%)	0.43	2 (1%)	72 72	19, 39, 56, 58	0
65	N9	58/58 (100%)	0.27	4 (6%)	17 15	19, 39, 79, 90	0
65	n9	58/58 (100%)	0.16	1 (1%)	67 68	19, 40, 59, 70	0
66	O0	97/104 (93%)	0.39	6 (6%)	20 19	51, 60, 81, 85	0
66	o0	100/104 (96%)	1.09	20 (20%)	2 1	54, 63, 88, 100	0
67	O1	109/112 (97%)	0.54	9 (8%)	11 10	35, 48, 77, 91	0
67	o1	109/112 (97%)	0.31	5 (4%)	31 31	28, 39, 72, 90	0
68	O2	127/129 (98%)	0.24	3 (2%)	56 57	18, 30, 40, 56	0
68	o2	127/129 (98%)	0.70	6 (4%)	30 30	19, 34, 46, 65	0
69	O3	106/106 (100%)	-0.11	0	100 100	23, 28, 47, 56	0
69	o3	106/106 (100%)	0.10	1 (0%)	81 81	20, 27, 51, 60	0
70	O4	112/119 (94%)	0.97	24 (21%)	1 1	34, 49, 87, 100	0
70	o4	112/119 (94%)	0.42	6 (5%)	25 25	34, 49, 85, 93	0
71	O5	119/119 (100%)	1.32	26 (21%)	1 1	32, 49, 55, 58	0
71	o5	119/119 (100%)	1.45	28 (23%)	1 1	40, 54, 62, 68	0
72	O6	99/99 (100%)	0.60	7 (7%)	16 14	36, 45, 72, 86	0
72	o6	99/99 (100%)	0.58	9 (9%)	9 8	45, 55, 74, 90	0
73	O7	87/87 (100%)	1.40	20 (22%)	1 1	23, 28, 50, 71	0
73	o7	87/87 (100%)	1.69	24 (27%)	1 1	24, 30, 60, 95	0
74	O8	77/77 (100%)	1.45	18 (23%)	1 1	57, 69, 90, 98	0
74	o8	77/77 (100%)	1.13	22 (28%)	1 1	57, 69, 87, 91	0
75	O9	50/50 (100%)	1.56	12 (24%)	1 1	32, 35, 44, 49	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	o9	50/50 (100%)	2.02	20 (40%) 1 0	35, 38, 48, 52	0
76	Q0	52/52 (100%)	0.09	1 (1%) 64 64	33, 38, 53, 64	0
76	q0	52/52 (100%)	0.03	2 (3%) 38 38	23, 26, 38, 44	0
77	Q1	25/25 (100%)	1.58	9 (36%) 1 1	41, 43, 47, 52	0
77	q1	25/25 (100%)	0.70	2 (8%) 12 11	31, 35, 44, 50	0
78	Q2	105/105 (100%)	0.40	5 (4%) 29 30	22, 38, 56, 82	0
78	q2	105/105 (100%)	0.61	8 (7%) 14 12	26, 38, 51, 78	0
79	Q3	91/91 (100%)	0.74	6 (6%) 18 16	28, 38, 53, 66	0
79	q3	91/91 (100%)	0.59	5 (5%) 24 24	27, 38, 51, 59	0
80	e0	62/62 (100%)	2.38	24 (38%) 1 0	46, 64, 97, 99	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	0.74	15 (10%) 7 6	72, 90, 159, 170	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	0.78	3939 (11%) 5 4	17, 52, 109, 237	0

The worst 5 of 3939 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	c2	20	ALA	41.0
60	N4	76	VAL	34.4
12	c0	98	THR	26.5
32	E0	53	LYS	21.3
32	E0	54	ARG	20.3

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	1	3624	1/1	0.49	657.00	69,69,69,69	0
85	MG	1	3865	1/1	0.45	617.00	67,67,67,67	0
85	MG	6	1945	1/1	0.43	288.00	43,43,43,43	0
85	MG	6	1933	1/1	0.32	281.00	53,53,53,53	0
85	MG	6	2020	1/1	0.51	261.92	40,40,40,40	0
85	MG	2	1989	1/1	0.23	151.00	65,65,65,65	0
85	MG	5	3655	1/1	0.30	144.00	45,45,45,45	0
85	MG	5	3481	1/1	0.38	143.67	57,57,57,57	0
85	MG	2	1983	1/1	0.28	122.00	62,62,62,62	0
85	MG	4	211	1/1	0.28	115.00	52,52,52,52	0
85	MG	1	3419	1/1	0.36	108.00	74,74,74,74	0
85	MG	1	3827	1/1	0.44	107.40	33,33,33,33	0
85	MG	5	3707	1/1	0.40	104.60	75,75,75,75	0
85	MG	1	3761	1/1	0.26	102.00	42,42,42,42	0
85	MG	1	3861	1/1	0.96	97.00	65,65,65,65	0
85	MG	1	3634	1/1	0.33	87.28	60,60,60,60	0
85	MG	2	2003	1/1	0.52	80.56	96,96,96,96	0
85	MG	1	3548	1/1	0.30	80.50	42,42,42,42	0
85	MG	8	213	1/1	0.36	77.80	31,31,31,31	0
85	MG	6	1944	1/1	0.46	73.44	50,50,50,50	0
85	MG	2	1959	1/1	0.41	71.75	66,66,66,66	0
85	MG	1	3687	1/1	0.19	71.00	69,69,69,69	0
86	OHX	5	4236	7/7	0.32	70.89	125,125,125,125	0
85	MG	6	2019	1/1	0.26	59.67	48,48,48,48	0
85	MG	1	3590	1/1	0.40	54.53	34,34,34,34	0
85	MG	1	3583	1/1	0.26	54.50	31,31,31,31	0
85	MG	2	2017	1/1	0.39	54.11	58,58,58,58	0
85	MG	1	3789	1/1	0.56	53.27	26,26,26,26	0
85	MG	1	3529	1/1	0.39	52.23	29,29,29,29	0
85	MG	2	1946	1/1	0.38	52.20	64,64,64,64	0
86	OHX	1	4144	7/7	0.41	50.47	112,112,112,112	0
85	MG	1	3409	1/1	0.35	49.93	30,30,30,30	0
85	MG	5	3661	1/1	0.43	49.82	59,59,59,59	0
85	MG	5	3756	1/1	0.28	49.50	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	3	204	1/1	0.58	49.10	51,51,51,51	0
86	OHX	5	4227	7/7	0.38	47.91	96,96,96,96	0
85	MG	5	3466	1/1	0.56	46.89	88,88,88,88	0
85	MG	6	1918	1/1	0.44	45.55	57,57,57,57	0
85	MG	5	3594	1/1	0.45	44.51	26,26,26,26	0
85	MG	6	1983	1/1	0.51	44.50	38,38,38,38	0
85	MG	1	3546	1/1	0.39	44.49	52,52,52,52	0
86	OHX	5	4212	7/7	0.42	42.31	98,98,98,98	0
85	MG	5	3573	1/1	0.29	41.52	26,26,26,26	0
85	MG	5	3856	1/1	0.47	40.50	68,68,68,68	0
85	MG	6	2029	1/1	0.55	40.11	68,68,68,68	0
85	MG	1	3579	1/1	0.47	39.16	33,33,33,33	0
85	MG	4	221	1/1	0.56	38.79	45,45,45,45	0
85	MG	N3	201	1/1	0.30	38.58	25,25,25,25	0
85	MG	5	3575	1/1	0.36	38.16	33,33,33,33	0
85	MG	5	3872	1/1	0.29	37.68	34,34,34,34	0
85	MG	2	1913	1/1	0.49	37.63	64,64,64,64	0
85	MG	2	2020	1/1	0.35	37.60	59,59,59,59	0
85	MG	6	1959	1/1	0.41	37.33	52,52,52,52	0
85	MG	1	3444	1/1	0.36	37.00	49,49,49,49	0
85	MG	2	1904	1/1	0.49	36.56	62,62,62,62	0
85	MG	6	2040	1/1	0.50	35.97	82,82,82,82	0
85	MG	1	3493	1/1	0.30	34.54	69,69,69,69	0
85	MG	1	3573	1/1	0.47	34.23	32,32,32,32	0
85	MG	5	3630	1/1	0.47	34.10	75,75,75,75	0
85	MG	5	3874	1/1	0.51	33.21	41,41,41,41	0
85	MG	2	1967	1/1	0.40	32.87	70,70,70,70	0
85	MG	1	3552	1/1	0.43	32.35	32,32,32,32	0
85	MG	5	3540	1/1	0.38	31.75	28,28,28,28	0
85	MG	6	1961	1/1	0.38	31.63	60,60,60,60	0
85	MG	7	209	1/1	0.39	31.35	35,35,35,35	0
85	MG	1	3817	1/1	0.35	31.15	40,40,40,40	0
85	MG	7	204	1/1	0.43	31.13	61,61,61,61	0
85	MG	5	3673	1/1	0.34	31.00	37,37,37,37	0
85	MG	7	215	1/1	0.34	31.00	48,48,48,48	0
85	MG	5	3887	1/1	0.35	30.96	53,53,53,53	0
85	MG	2	1975	1/1	0.48	30.57	71,71,71,71	0
85	MG	6	2013	1/1	0.51	29.92	42,42,42,42	0
85	MG	1	3728	1/1	0.48	29.90	27,27,27,27	0
85	MG	2	1981	1/1	0.31	29.76	52,52,52,52	0
85	MG	5	3403	1/1	0.41	29.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3847	1/1	0.26	28.75	51,51,51,51	0
85	MG	1	3860	1/1	0.35	27.67	43,43,43,43	0
85	MG	1	3528	1/1	0.31	27.59	37,37,37,37	0
85	MG	1	3412	1/1	0.36	27.21	37,37,37,37	0
86	OHX	6	2181	7/7	0.40	27.19	113,113,113,113	0
85	MG	1	3809	1/1	0.78	27.18	162,162,162,162	0
85	MG	2	1984	1/1	0.34	26.87	60,60,60,60	0
85	MG	1	3463	1/1	0.32	26.82	19,19,19,19	0
85	MG	5	3477	1/1	0.32	26.69	59,59,59,59	0
85	MG	6	2046	1/1	0.47	26.12	66,66,66,66	0
85	MG	5	3683	1/1	0.28	25.78	51,51,51,51	0
85	MG	1	3646	1/1	0.22	25.78	30,30,30,30	0
85	MG	3	207	1/1	0.41	25.74	55,55,55,55	0
85	MG	5	3731	1/1	0.20	25.67	37,37,37,37	0
85	MG	1	3820	1/1	0.52	25.59	84,84,84,84	0
85	MG	1	3469	1/1	0.31	25.37	56,56,56,56	0
85	MG	1	3854	1/1	0.44	25.28	52,52,52,52	0
85	MG	1	3667	1/1	0.40	25.20	62,62,62,62	0
85	MG	1	3408	1/1	0.28	24.96	27,27,27,27	0
85	MG	1	3566	1/1	0.43	24.91	33,33,33,33	0
85	MG	5	3574	1/1	0.38	24.74	40,40,40,40	0
85	MG	5	3633	1/1	0.51	24.50	71,71,71,71	0
85	MG	1	3721	1/1	0.33	24.46	44,44,44,44	0
85	MG	5	3737	1/1	0.26	24.31	36,36,36,36	0
85	MG	5	3582	1/1	0.41	24.31	27,27,27,27	0
86	OHX	5	4151	7/7	0.33	23.98	92,92,92,92	0
85	MG	6	2027	1/1	0.31	23.91	61,61,61,61	0
85	MG	5	3511	1/1	0.38	23.89	45,45,45,45	0
85	MG	1	3537	1/1	0.47	23.87	25,25,25,25	0
85	MG	1	3591	1/1	0.34	23.68	34,34,34,34	0
85	MG	6	1946	1/1	0.39	23.64	52,52,52,52	0
85	MG	6	2039	1/1	0.42	23.50	67,67,67,67	0
85	MG	6	1956	1/1	0.43	23.39	38,38,38,38	0
85	MG	2	1960	1/1	0.45	22.91	87,87,87,87	0
85	MG	6	2011	1/1	0.34	22.86	54,54,54,54	0
85	MG	5	3646	1/1	0.25	22.65	35,35,35,35	0
85	MG	6	1943	1/1	0.38	22.56	32,32,32,32	0
85	MG	1	3405	1/1	0.70	22.25	95,95,95,95	0
86	OHX	1	4205	7/7	0.39	22.23	108,108,108,108	0
85	MG	6	1927	1/1	0.34	22.22	39,39,39,39	0
85	MG	5	3438	1/1	0.36	22.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	2	1929	1/1	0.38	22.20	51,51,51,51	0
85	MG	5	3634	1/1	0.34	22.06	33,33,33,33	0
85	MG	5	3647	1/1	0.18	22.00	41,41,41,41	0
85	MG	1	3423	1/1	0.21	21.98	28,28,28,28	0
85	MG	5	3515	1/1	0.30	21.97	28,28,28,28	0
85	MG	1	3730	1/1	0.39	21.91	23,23,23,23	0
86	OHX	1	4142	7/7	0.40	21.56	89,89,89,89	0
85	MG	6	1951	1/1	0.39	21.34	55,55,55,55	0
86	OHX	5	4219	7/7	0.36	21.23	111,111,111,111	0
85	MG	5	3410	1/1	0.34	21.07	47,47,47,47	0
85	MG	2	2014	1/1	0.42	20.94	61,61,61,61	0
85	MG	2	1951	1/1	0.49	20.94	68,68,68,68	0
85	MG	1	3713	1/1	0.52	20.93	73,73,73,73	0
86	OHX	1	4179	7/7	0.43	20.82	101,101,101,101	0
86	OHX	1	4180	7/7	0.31	20.82	120,120,120,120	0
85	MG	2	2010	1/1	0.39	20.77	62,62,62,62	0
85	MG	5	3821	1/1	0.42	20.58	32,32,32,32	0
85	MG	6	1955	1/1	0.46	20.54	32,32,32,32	0
85	MG	2	2018	1/1	0.34	20.47	62,62,62,62	0
85	MG	5	3535	1/1	0.38	20.43	32,32,32,32	0
85	MG	6	1935	1/1	0.34	20.38	46,46,46,46	0
85	MG	5	3618	1/1	0.24	20.25	37,37,37,37	0
86	OHX	1	4192	7/7	0.44	20.22	98,98,98,98	0
86	OHX	1	4071	7/7	0.24	20.21	99,99,99,99	0
86	OHX	5	4217	7/7	0.31	20.16	106,106,106,106	0
85	MG	5	3547	1/1	0.41	20.06	32,32,32,32	0
86	OHX	6	2147	7/7	0.31	20.05	90,90,90,90	0
86	OHX	1	4174	7/7	0.33	20.04	112,112,112,112	0
85	MG	2	1914	1/1	0.42	19.97	55,55,55,55	0
85	MG	5	3786	1/1	0.28	19.95	70,70,70,70	0
85	MG	n3	201	1/1	0.42	19.92	21,21,21,21	0
86	OHX	M9	202	7/7	0.24	19.89	130,130,130,130	0
85	MG	1	3540	1/1	0.34	19.70	48,48,48,48	0
86	OHX	6	2190	7/7	0.39	19.62	110,110,110,110	0
85	MG	1	3504	1/1	0.38	19.55	39,39,39,39	0
85	MG	5	3871	1/1	0.51	19.54	47,47,47,47	0
85	MG	3	201	1/1	0.46	19.28	59,59,59,59	0
85	MG	1	3858	1/1	0.33	19.12	36,36,36,36	0
85	MG	1	3684	1/1	0.24	19.00	41,41,41,41	0
86	OHX	5	4193	7/7	0.40	18.96	107,107,107,107	0
85	MG	2	2008	1/1	0.40	18.91	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4184	7/7	0.28	18.88	98,98,98,98	0
85	MG	6	2028	1/1	0.39	18.83	56,56,56,56	0
85	MG	5	3453	1/1	0.34	18.81	34,34,34,34	0
86	OHX	6	2174	7/7	0.41	18.76	101,101,101,101	0
86	OHX	1	4208	7/7	0.46	18.68	100,100,100,100	0
85	MG	3	209	1/1	0.38	18.67	50,50,50,50	0
85	MG	1	3580	1/1	0.32	18.46	34,34,34,34	0
85	MG	1	3844	1/1	0.27	18.33	40,40,40,40	0
86	OHX	1	4191	7/7	0.31	18.29	104,104,104,104	0
85	MG	3	213	1/1	0.44	18.20	49,49,49,49	0
86	OHX	5	4173	7/7	0.32	18.20	110,110,110,110	0
86	OHX	5	4190	7/7	0.36	18.19	98,98,98,98	0
85	MG	1	3515	1/1	0.45	18.12	29,29,29,29	0
85	MG	2	1921	1/1	0.36	18.12	44,44,44,44	0
85	MG	5	3832	1/1	0.26	18.12	37,37,37,37	0
85	MG	6	1919	1/1	0.35	17.92	34,34,34,34	0
85	MG	5	3580	1/1	0.31	17.71	36,36,36,36	0
85	MG	5	3412	1/1	0.31	17.69	26,26,26,26	0
85	MG	2	1924	1/1	0.32	17.68	65,65,65,65	0
85	MG	6	1931	1/1	0.40	17.58	54,54,54,54	0
86	OHX	1	4166	7/7	0.20	17.57	130,130,130,130	0
86	OHX	2	2160	7/7	0.44	17.46	117,117,117,117	0
85	MG	5	3780	1/1	0.34	17.46	70,70,70,70	0
85	MG	1	3663	1/1	0.42	17.46	31,31,31,31	0
85	MG	1	3516	1/1	0.33	17.44	28,28,28,28	0
85	MG	5	3522	1/1	0.30	17.10	31,31,31,31	0
85	MG	1	3562	1/1	0.33	17.10	22,22,22,22	0
85	MG	6	2038	1/1	0.49	17.09	48,48,48,48	0
85	MG	5	3581	1/1	0.29	17.06	36,36,36,36	0
85	MG	5	3473	1/1	0.28	17.00	44,44,44,44	0
85	MG	3	214	1/1	0.33	16.94	50,50,50,50	0
85	MG	6	1907	1/1	0.35	16.90	53,53,53,53	0
85	MG	5	3570	1/1	0.34	16.89	30,30,30,30	0
86	OHX	5	4185	7/7	0.43	16.75	94,94,94,94	0
85	MG	1	3674	1/1	0.31	16.75	50,50,50,50	0
85	MG	1	3843	1/1	0.30	16.67	46,46,46,46	0
85	MG	1	3834	1/1	0.32	16.50	16,16,16,16	0
86	OHX	5	4149	7/7	0.27	16.47	96,96,96,96	0
85	MG	7	201	1/1	0.46	16.39	36,36,36,36	0
85	MG	8	201	1/1	0.38	16.27	31,31,31,31	0
85	MG	5	3783	1/1	0.31	16.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3793	1/1	0.46	16.25	36,36,36,36	0
85	MG	5	3755	1/1	0.25	16.19	47,47,47,47	0
85	MG	6	2021	1/1	0.29	16.18	93,93,93,93	0
86	OHX	6	2163	7/7	0.28	16.16	106,106,106,106	0
85	MG	6	1916	1/1	0.40	16.13	54,54,54,54	0
85	MG	6	1925	1/1	0.37	16.10	34,34,34,34	0
85	MG	5	3572	1/1	0.40	16.08	34,34,34,34	0
85	MG	6	1971	1/1	0.33	16.07	54,54,54,54	0
85	MG	1	3574	1/1	0.35	15.96	30,30,30,30	0
85	MG	7	205	1/1	0.30	15.81	23,23,23,23	0
85	MG	5	3566	1/1	0.35	15.80	24,24,24,24	0
85	MG	6	1934	1/1	0.39	15.77	62,62,62,62	0
85	MG	5	3644	1/1	0.30	15.69	29,29,29,29	0
85	MG	1	3456	1/1	0.38	15.69	50,50,50,50	0
85	MG	6	1909	1/1	0.41	15.68	79,79,79,79	0
85	MG	1	3592	1/1	0.43	15.64	43,43,43,43	0
85	MG	6	1975	1/1	0.28	15.62	53,53,53,53	0
86	OHX	1	4195	7/7	0.28	15.62	116,116,116,116	0
85	MG	2	1965	1/1	0.35	15.60	74,74,74,74	0
85	MG	5	3578	1/1	0.29	15.58	28,28,28,28	0
85	MG	4	220	1/1	0.44	15.58	77,77,77,77	0
86	OHX	1	4165	7/7	0.35	15.54	123,123,123,123	0
85	MG	1	3526	1/1	0.27	15.34	21,21,21,21	0
85	MG	5	3517	1/1	0.32	15.25	18,18,18,18	0
85	MG	1	3585	1/1	0.41	15.19	40,40,40,40	0
85	MG	1	3509	1/1	0.28	15.15	34,34,34,34	0
86	OHX	5	4179	7/7	0.23	15.12	113,113,113,113	0
85	MG	2	1936	1/1	0.35	15.05	42,42,42,42	0
85	MG	5	3588	1/1	0.34	15.01	30,30,30,30	0
85	MG	2	2011	1/1	0.23	15.00	59,59,59,59	0
85	MG	6	1926	1/1	0.29	14.97	40,40,40,40	0
85	MG	1	3607	1/1	0.36	14.91	45,45,45,45	0
85	MG	5	3734	1/1	0.28	14.90	58,58,58,58	0
85	MG	5	3571	1/1	0.33	14.88	27,27,27,27	0
85	MG	2	1997	1/1	0.23	14.87	80,80,80,80	0
85	MG	5	3833	1/1	0.31	14.83	26,26,26,26	0
85	MG	1	3677	1/1	0.35	14.81	60,60,60,60	0
85	MG	5	3730	1/1	0.24	14.78	41,41,41,41	0
85	MG	6	1921	1/1	0.34	14.73	36,36,36,36	0
85	MG	n9	3802	1/1	0.48	14.72	31,31,31,31	0
85	MG	5	3521	1/1	0.37	14.63	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3475	1/1	0.24	14.60	64,64,64,64	0
85	MG	5	3593	1/1	0.39	14.57	34,34,34,34	0
86	OHX	5	4230	7/7	0.36	14.54	99,99,99,99	0
85	MG	8	206	1/1	0.74	14.53	44,44,44,44	0
85	MG	6	1960	1/1	0.34	14.50	38,38,38,38	0
85	MG	5	3751	1/1	0.30	14.44	49,49,49,49	0
85	MG	6	2015	1/1	0.56	14.27	104,104,104,104	0
85	MG	6	1914	1/1	0.30	14.24	29,29,29,29	0
85	MG	6	1928	1/1	0.30	14.19	54,54,54,54	0
85	MG	5	3880	1/1	0.33	14.18	45,45,45,45	0
85	MG	5	3652	1/1	0.28	13.95	55,55,55,55	0
85	MG	1	3859	1/1	0.47	13.95	54,54,54,54	0
85	MG	1	3799	1/1	0.40	13.87	21,21,21,21	0
86	OHX	1	4073	7/7	0.31	13.71	94,94,94,94	0
85	MG	5	3551	1/1	0.34	13.69	39,39,39,39	0
85	MG	5	3721	1/1	0.24	13.67	46,46,46,46	0
85	MG	5	3413	1/1	0.27	13.65	25,25,25,25	0
86	OHX	1	4187	7/7	0.45	13.63	105,105,105,105	0
86	OHX	5	4160	7/7	0.30	13.61	93,93,93,93	0
85	MG	5	3498	1/1	0.34	13.44	27,27,27,27	0
85	MG	5	3531	1/1	0.29	13.43	31,31,31,31	0
86	OHX	2	2144	7/7	0.33	13.40	105,105,105,105	0
86	OHX	2	2172	7/7	0.26	13.38	119,119,119,119	0
85	MG	5	3505	1/1	0.30	13.35	30,30,30,30	0
85	MG	6	1939	1/1	0.37	13.31	51,51,51,51	0
85	MG	5	3530	1/1	0.35	13.28	40,40,40,40	0
85	MG	1	3484	1/1	0.39	13.28	38,38,38,38	0
86	OHX	5	4159	7/7	0.22	13.28	101,101,101,101	0
85	MG	6	1958	1/1	0.35	13.27	46,46,46,46	0
85	MG	6	1911	1/1	0.24	13.25	38,38,38,38	0
85	MG	5	3595	1/1	0.33	13.19	27,27,27,27	0
85	MG	1	3614	1/1	0.26	13.17	29,29,29,29	0
85	MG	5	3738	1/1	0.38	13.15	61,61,61,61	0
85	MG	1	3510	1/1	0.32	13.14	25,25,25,25	0
85	MG	6	1903	1/1	0.27	13.12	36,36,36,36	0
85	MG	5	3606	1/1	0.30	13.10	18,18,18,18	0
85	MG	5	3562	1/1	0.32	13.08	24,24,24,24	0
85	MG	5	3884	1/1	0.41	13.05	55,55,55,55	0
85	MG	5	3548	1/1	0.39	13.00	44,44,44,44	0
85	MG	6	1947	1/1	0.45	12.90	50,50,50,50	0
85	MG	5	3560	1/1	0.35	12.88	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3881	1/1	0.49	12.88	81,81,81,81	0
85	MG	1	3587	1/1	0.38	12.77	26,26,26,26	0
86	OHX	6	2194	7/7	0.21	12.75	140,140,140,140	0
85	MG	3	206	1/1	0.35	12.74	29,29,29,29	0
86	OHX	2	2123	7/7	0.20	12.68	114,114,114,114	0
86	OHX	1	4145	7/7	0.27	12.65	110,110,110,110	0
85	MG	5	3770	1/1	0.29	12.53	70,70,70,70	0
86	OHX	1	4162	7/7	0.28	12.50	121,121,121,121	0
86	OHX	6	2168	7/7	0.29	12.50	97,97,97,97	0
85	MG	6	1904	1/1	0.40	12.48	56,56,56,56	0
85	MG	2	2013	1/1	0.19	12.43	44,44,44,44	0
85	MG	1	3543	1/1	0.31	12.35	29,29,29,29	0
85	MG	5	3841	1/1	0.28	12.33	37,37,37,37	0
85	MG	5	3727	1/1	0.22	12.23	85,85,85,85	0
85	MG	1	3766	1/1	0.41	12.22	32,32,32,32	0
85	MG	1	3853	1/1	0.22	12.20	35,35,35,35	0
85	MG	4	214	1/1	0.49	12.15	43,43,43,43	0
85	MG	5	3623	1/1	0.23	12.04	33,33,33,33	0
86	OHX	6	2183	7/7	0.46	11.94	118,118,118,118	0
85	MG	5	3523	1/1	0.31	11.92	23,23,23,23	0
86	OHX	8	227	7/7	0.31	11.86	108,108,108,108	0
85	MG	5	3869	1/1	0.26	11.86	28,28,28,28	0
85	MG	5	3858	1/1	0.21	11.86	70,70,70,70	0
85	MG	5	3643	1/1	0.35	11.81	37,37,37,37	0
85	MG	5	3596	1/1	0.36	11.79	25,25,25,25	0
85	MG	1	3749	1/1	0.23	11.76	43,43,43,43	0
85	MG	1	3506	1/1	0.31	11.70	37,37,37,37	0
85	MG	5	3569	1/1	0.32	11.66	20,20,20,20	0
85	MG	5	3896	1/1	0.23	11.60	82,82,82,82	0
85	MG	SM	301	1/1	0.23	11.51	38,38,38,38	0
85	MG	5	3467	1/1	0.28	11.48	31,31,31,31	0
85	MG	1	3410	1/1	0.27	11.47	36,36,36,36	0
85	MG	6	1937	1/1	0.34	11.47	36,36,36,36	0
86	OHX	14	403	7/7	0.37	11.45	111,111,111,111	0
85	MG	6	1917	1/1	0.34	11.44	44,44,44,44	0
85	MG	1	3485	1/1	0.27	11.43	35,35,35,35	0
85	MG	5	3431	1/1	0.34	11.30	37,37,37,37	0
85	MG	5	3748	1/1	0.28	11.29	29,29,29,29	0
85	MG	5	3426	1/1	0.30	11.28	37,37,37,37	0
86	OHX	5	4200	7/7	0.29	11.22	114,114,114,114	0
85	MG	6	1922	1/1	0.34	11.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3670	1/1	0.35	11.12	65,65,65,65	0
85	MG	5	3565	1/1	0.32	11.08	22,22,22,22	0
86	OHX	M7	207	7/7	0.43	11.01	83,83,83,83	0
85	MG	5	4254	1/1	0.60	11.00	19,19,19,19	0
85	MG	1	3623	1/1	0.19	10.97	42,42,42,42	0
85	MG	5	3518	1/1	0.40	10.97	32,32,32,32	0
85	MG	2	1915	1/1	0.40	10.96	53,53,53,53	0
85	MG	5	3508	1/1	0.34	10.96	24,24,24,24	0
85	MG	5	3579	1/1	0.29	10.95	28,28,28,28	0
86	OHX	3	225	7/7	0.27	10.94	103,103,103,103	0
85	MG	2	1995	1/1	0.30	10.93	75,75,75,75	0
85	MG	1	3716	1/1	0.44	10.92	39,39,39,39	0
85	MG	5	3520	1/1	0.27	10.90	24,24,24,24	0
85	MG	5	3855	1/1	0.28	10.83	42,42,42,42	0
85	MG	5	3544	1/1	0.36	10.77	41,41,41,41	0
85	MG	1	3556	1/1	0.34	10.76	30,30,30,30	0
86	OHX	2	2149	7/7	0.29	10.75	96,96,96,96	0
86	OHX	5	4214	7/7	0.38	10.74	110,110,110,110	0
85	MG	1	3401	1/1	0.34	10.73	33,33,33,33	0
85	MG	1	3575	1/1	0.32	10.71	22,22,22,22	0
86	OHX	5	4244	7/7	0.35	10.66	122,122,122,122	0
85	MG	5	3813	1/1	0.38	10.66	47,47,47,47	0
85	MG	1	3599	1/1	0.42	10.66	20,20,20,20	0
85	MG	1	3718	1/1	0.56	10.61	33,33,33,33	0
85	MG	5	3449	1/1	0.41	10.58	53,53,53,53	0
86	OHX	5	4234	7/7	0.34	10.58	111,111,111,111	0
85	MG	5	3559	1/1	0.28	10.52	21,21,21,21	0
85	MG	1	3522	1/1	0.34	10.50	27,27,27,27	0
85	MG	6	1940	1/1	0.58	10.49	70,70,70,70	0
86	OHX	1	4189	7/7	0.33	10.45	145,145,145,145	0
85	MG	1	3808	1/1	0.29	10.44	30,30,30,30	0
85	MG	5	3672	1/1	0.20	10.42	57,57,57,57	0
86	OHX	5	4164	7/7	0.27	10.39	111,111,111,111	0
85	MG	5	3502	1/1	0.33	10.38	28,28,28,28	0
86	OHX	1	4065	7/7	0.31	10.32	113,113,113,113	0
85	MG	1	3847	1/1	0.27	10.29	49,49,49,49	0
85	MG	2	1934	1/1	0.38	10.29	58,58,58,58	0
85	MG	2	1933	1/1	0.27	10.29	57,57,57,57	0
85	MG	1	3536	1/1	0.28	10.28	42,42,42,42	0
86	OHX	1	4049	7/7	0.23	10.27	87,87,87,87	0
85	MG	6	1929	1/1	0.25	10.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3561	1/1	0.47	10.19	31,31,31,31	0
85	MG	1	3796	1/1	0.74	10.15	31,31,31,31	0
85	MG	1	3742	1/1	0.34	10.14	53,53,53,53	0
86	OHX	5	4152	7/7	0.36	10.13	95,95,95,95	0
85	MG	5	3846	1/1	0.26	10.01	50,50,50,50	0
86	OHX	1	4116	7/7	0.34	10.00	91,91,91,91	0
85	MG	5	3598	1/1	0.27	9.96	30,30,30,30	0
85	MG	5	3499	1/1	0.27	9.96	24,24,24,24	0
85	MG	6	2043	1/1	0.25	9.88	39,39,39,39	0
85	MG	6	1980	1/1	0.28	9.88	60,60,60,60	0
85	MG	2	1907	1/1	0.37	9.87	46,46,46,46	0
85	MG	5	3576	1/1	0.38	9.87	36,36,36,36	0
85	MG	1	4219	1/1	0.30	9.85	24,24,24,24	0
86	OHX	5	4208	7/7	0.26	9.80	110,110,110,110	0
85	MG	5	3848	1/1	0.28	9.80	34,34,34,34	0
85	MG	6	1963	1/1	0.28	9.74	67,67,67,67	0
85	MG	1	3776	1/1	0.25	9.73	53,53,53,53	0
86	OHX	1	4123	7/7	0.32	9.71	94,94,94,94	0
85	MG	1	3479	1/1	0.34	9.67	70,70,70,70	0
85	MG	5	3796	1/1	0.24	9.64	27,27,27,27	0
86	OHX	1	4173	7/7	0.37	9.64	132,132,132,132	0
85	MG	5	3670	1/1	0.25	9.63	44,44,44,44	0
85	MG	1	3560	1/1	0.29	9.59	28,28,28,28	0
85	MG	1	3593	1/1	0.33	9.56	59,59,59,59	0
85	MG	5	3892	1/1	0.27	9.50	38,38,38,38	0
85	MG	7	206	1/1	0.20	9.50	36,36,36,36	0
85	MG	5	3558	1/1	0.26	9.49	24,24,24,24	0
86	OHX	5	4238	7/7	0.37	9.48	117,117,117,117	0
86	OHX	5	4140	7/7	0.27	9.42	101,101,101,101	0
85	MG	5	3807	1/1	0.24	9.41	29,29,29,29	0
85	MG	1	3709	1/1	0.25	9.36	28,28,28,28	0
86	OHX	8	228	7/7	0.30	9.33	101,101,101,101	0
85	MG	2	1926	1/1	0.39	9.33	77,77,77,77	0
86	OHX	1	4031	7/7	0.22	9.32	88,88,88,88	0
85	MG	1	3815	1/1	0.24	9.31	26,26,26,26	0
85	MG	5	3680	1/1	0.40	9.25	68,68,68,68	0
86	OHX	6	2186	7/7	0.35	9.25	113,113,113,113	0
86	OHX	6	2180	7/7	0.32	9.24	106,106,106,106	0
86	OHX	6	2165	7/7	0.26	9.23	119,119,119,119	0
85	MG	5	3519	1/1	0.24	9.20	35,35,35,35	0
85	MG	5	3875	1/1	0.28	9.19	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	2	2019	1/1	0.36	9.16	61,61,61,61	0
86	OHX	1	4130	7/7	0.30	9.14	120,120,120,120	0
85	MG	1	3734	1/1	0.29	9.14	68,68,68,68	0
86	OHX	1	4185	7/7	0.25	9.10	111,111,111,111	0
85	MG	1	3527	1/1	0.34	9.10	27,27,27,27	0
85	MG	1	3402	1/1	0.33	9.02	51,51,51,51	0
85	MG	6	1991	1/1	0.29	9.02	56,56,56,56	0
85	MG	1	3561	1/1	0.27	9.01	30,30,30,30	0
85	MG	2	2012	1/1	0.20	9.00	57,57,57,57	0
85	MG	1	3679	1/1	0.23	8.97	38,38,38,38	0
86	OHX	1	4085	7/7	0.25	8.97	114,114,114,114	0
85	MG	1	3594	1/1	0.29	8.96	22,22,22,22	0
85	MG	6	1901	1/1	0.28	8.91	37,37,37,37	0
86	OHX	8	225	7/7	0.33	8.89	103,103,103,103	0
86	OHX	5	4228	7/7	0.25	8.89	141,141,141,141	0
85	MG	6	1913	1/1	0.33	8.86	46,46,46,46	0
85	MG	1	3502	1/1	0.31	8.86	35,35,35,35	0
86	OHX	1	4140	7/7	0.27	8.85	100,100,100,100	0
86	OHX	5	4195	7/7	0.28	8.83	95,95,95,95	0
85	MG	6	1952	1/1	0.37	8.83	53,53,53,53	0
85	MG	5	3506	1/1	0.29	8.83	23,23,23,23	0
86	OHX	1	4199	7/7	0.28	8.80	107,107,107,107	0
85	MG	2	1958	1/1	0.23	8.78	62,62,62,62	0
85	MG	1	3637	1/1	0.32	8.73	41,41,41,41	0
85	MG	5	3462	1/1	0.29	8.73	27,27,27,27	0
85	MG	5	3746	1/1	0.25	8.72	51,51,51,51	0
86	OHX	2	2179	7/7	0.23	8.70	137,137,137,137	0
85	MG	2	1932	1/1	0.34	8.69	48,48,48,48	0
86	OHX	6	2187	7/7	0.32	8.66	136,136,136,136	0
85	MG	5	3537	1/1	0.22	8.65	33,33,33,33	0
86	OHX	4	236	7/7	0.32	8.60	105,105,105,105	0
86	OHX	1	4118	7/7	0.26	8.55	95,95,95,95	0
85	MG	5	3825	1/1	0.32	8.51	31,31,31,31	0
85	MG	1	3739	1/1	0.30	8.50	53,53,53,53	0
85	MG	5	3479	1/1	0.26	8.46	56,56,56,56	0
85	MG	2	2015	1/1	0.26	8.45	59,59,59,59	0
85	MG	1	3466	1/1	0.23	8.40	49,49,49,49	0
85	MG	7	203	1/1	0.28	8.39	43,43,43,43	0
85	MG	6	1954	1/1	0.32	8.39	33,33,33,33	0
85	MG	3	203	1/1	0.21	8.38	75,75,75,75	0
85	MG	5	3528	1/1	0.33	8.36	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3577	1/1	0.28	8.36	23,23,23,23	0
86	OHX	5	4089	7/7	0.24	8.35	84,84,84,84	0
86	OHX	2	2170	7/7	0.29	8.33	126,126,126,126	0
85	MG	1	3596	1/1	0.36	8.33	20,20,20,20	0
85	MG	1	3404	1/1	0.31	8.31	46,46,46,46	0
86	OHX	6	2171	7/7	0.30	8.30	90,90,90,90	0
86	OHX	1	4193	7/7	0.28	8.27	110,110,110,110	0
86	OHX	6	2160	7/7	0.45	8.26	103,103,103,103	0
85	MG	1	3451	1/1	0.30	8.26	34,34,34,34	0
86	OHX	5	4158	7/7	0.29	8.20	110,110,110,110	0
86	OHX	8	224	7/7	0.33	8.19	108,108,108,108	0
85	MG	1	3513	1/1	0.31	8.14	18,18,18,18	0
85	MG	6	2035	1/1	0.35	8.13	74,74,74,74	0
86	OHX	5	4176	7/7	0.40	8.11	86,86,86,86	0
85	MG	5	3583	1/1	0.39	8.09	27,27,27,27	0
85	MG	2	1943	1/1	0.25	8.08	55,55,55,55	0
85	MG	5	3693	1/1	0.24	8.08	59,59,59,59	0
86	OHX	2	2117	7/7	0.20	8.07	110,110,110,110	0
86	OHX	1	4178	7/7	0.29	8.04	126,126,126,126	0
85	MG	5	3546	1/1	0.30	8.02	39,39,39,39	0
85	MG	5	3463	1/1	0.31	8.01	44,44,44,44	0
85	MG	3	202	1/1	0.25	7.99	39,39,39,39	0
86	OHX	2	2137	7/7	0.32	7.97	104,104,104,104	0
85	MG	1	3848	1/1	0.21	7.95	45,45,45,45	0
85	MG	6	1964	1/1	0.24	7.89	44,44,44,44	0
85	MG	1	3532	1/1	0.32	7.88	34,34,34,34	0
85	MG	2	1969	1/1	0.24	7.88	79,79,79,79	0
85	MG	5	3823	1/1	0.30	7.88	51,51,51,51	0
86	OHX	2	2136	7/7	0.32	7.86	107,107,107,107	0
85	MG	1	3525	1/1	0.21	7.85	20,20,20,20	0
85	MG	1	3647	1/1	0.27	7.84	28,28,28,28	0
85	MG	1	3814	1/1	0.21	7.80	38,38,38,38	0
85	MG	5	3677	1/1	0.26	7.79	34,34,34,34	0
85	MG	1	3533	1/1	0.23	7.75	24,24,24,24	0
86	OHX	1	4128	7/7	0.27	7.74	96,96,96,96	0
85	MG	5	3529	1/1	0.31	7.73	25,25,25,25	0
85	MG	5	3415	1/1	0.25	7.73	19,19,19,19	0
85	MG	5	3648	1/1	0.23	7.71	72,72,72,72	0
85	MG	1	3542	1/1	0.34	7.69	27,27,27,27	0
85	MG	1	3512	1/1	0.29	7.69	22,22,22,22	0
85	MG	5	3458	1/1	0.24	7.67	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4066	7/7	0.27	7.66	106,106,106,106	0
86	OHX	5	4248	7/7	0.24	7.66	126,126,126,126	0
85	MG	2	1928	1/1	0.32	7.66	69,69,69,69	0
85	MG	2	1957	1/1	0.29	7.64	47,47,47,47	0
85	MG	5	3586	1/1	0.47	7.62	52,52,52,52	0
85	MG	2	1917	1/1	0.36	7.60	46,46,46,46	0
86	OHX	5	3951	7/7	0.23	7.58	95,95,95,95	0
85	MG	5	3726	1/1	0.23	7.58	31,31,31,31	0
85	MG	n8	204	1/1	0.51	7.54	25,25,25,25	0
85	MG	1	3786	1/1	0.48	7.54	25,25,25,25	0
85	MG	6	1948	1/1	0.27	7.52	37,37,37,37	0
85	MG	1	3839	1/1	0.33	7.47	28,28,28,28	0
85	MG	2	1931	1/1	0.35	7.45	60,60,60,60	0
85	MG	5	3864	1/1	0.23	7.44	52,52,52,52	0
85	MG	1	4224	1/1	0.36	7.42	19,19,19,19	0
85	MG	1	3821	1/1	0.26	7.40	37,37,37,37	0
85	MG	2	1909	1/1	0.25	7.39	59,59,59,59	0
86	OHX	5	4136	7/7	0.27	7.32	103,103,103,103	0
85	MG	5	3638	1/1	0.24	7.27	29,29,29,29	0
86	OHX	4	232	7/7	0.29	7.26	93,93,93,93	0
85	MG	1	3773	1/1	0.25	7.25	37,37,37,37	0
85	MG	5	3766	1/1	0.24	7.25	35,35,35,35	0
86	OHX	5	4154	7/7	0.27	7.23	106,106,106,106	0
86	OHX	1	4201	7/7	0.24	7.23	100,100,100,100	0
85	MG	15	301	1/1	0.30	7.21	36,36,36,36	0
85	MG	7	213	1/1	0.28	7.20	44,44,44,44	0
85	MG	1	3774	1/1	0.21	7.20	45,45,45,45	0
85	MG	5	3563	1/1	0.25	7.20	17,17,17,17	0
85	MG	1	3653	1/1	0.20	7.19	49,49,49,49	0
85	MG	5	3503	1/1	0.27	7.18	45,45,45,45	0
85	MG	5	3475	1/1	0.27	7.12	25,25,25,25	0
85	MG	5	3422	1/1	0.24	7.12	47,47,47,47	0
86	OHX	1	4212	7/7	0.29	7.07	98,98,98,98	0
86	OHX	5	4112	7/7	0.26	7.06	79,79,79,79	0
85	MG	1	3551	1/1	0.30	7.04	25,25,25,25	0
86	OHX	2	2163	7/7	0.26	7.02	138,138,138,138	0
85	MG	5	3416	1/1	0.27	7.01	21,21,21,21	0
86	OHX	1	4209	7/7	0.33	7.00	104,104,104,104	0
86	OHX	1	4215	7/7	0.32	7.00	118,118,118,118	0
86	OHX	1	4169	7/7	0.27	6.99	90,90,90,90	0
86	OHX	5	4235	7/7	0.24	6.94	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	6	1968	1/1	0.30	6.93	65,65,65,65	0
86	OHX	5	4147	7/7	0.28	6.91	104,104,104,104	0
86	OHX	2	2165	7/7	0.36	6.89	125,125,125,125	0
86	OHX	5	4177	7/7	0.28	6.88	110,110,110,110	0
85	MG	5	3409	1/1	0.31	6.84	39,39,39,39	0
85	MG	1	3418	1/1	0.25	6.84	41,41,41,41	0
85	MG	1	3417	1/1	0.27	6.83	34,34,34,34	0
85	MG	5	3443	1/1	0.28	6.83	20,20,20,20	0
86	OHX	1	4176	7/7	0.21	6.81	133,133,133,133	0
85	MG	5	3662	1/1	0.23	6.79	54,54,54,54	0
85	MG	5	3533	1/1	0.25	6.79	29,29,29,29	0
86	OHX	1	4148	7/7	0.22	6.70	118,118,118,118	0
86	OHX	1	4138	7/7	0.25	6.70	91,91,91,91	0
85	MG	5	3568	1/1	0.33	6.68	23,23,23,23	0
85	MG	1	3523	1/1	0.28	6.68	22,22,22,22	0
86	OHX	5	4134	7/7	0.28	6.68	99,99,99,99	0
85	MG	5	3706	1/1	0.24	6.66	42,42,42,42	0
85	MG	5	3764	1/1	0.25	6.65	30,30,30,30	0
85	MG	5	4255	1/1	0.40	6.63	23,23,23,23	0
85	MG	1	3494	1/1	0.24	6.63	30,30,30,30	0
85	MG	1	3450	1/1	0.25	6.63	35,35,35,35	0
86	OHX	1	4188	7/7	0.29	6.63	115,115,115,115	0
86	OHX	1	4067	7/7	0.24	6.60	100,100,100,100	0
85	MG	5	3470	1/1	0.28	6.56	25,25,25,25	0
85	MG	1	3569	1/1	0.32	6.56	21,21,21,21	0
85	MG	4	206	1/1	0.30	6.53	28,28,28,28	0
86	OHX	5	4233	7/7	0.36	6.52	118,118,118,118	0
85	MG	5	3894	1/1	0.25	6.49	45,45,45,45	0
85	MG	5	3584	1/1	0.38	6.49	19,19,19,19	0
86	OHX	1	4141	7/7	0.31	6.48	113,113,113,113	0
85	MG	6	2042	1/1	0.39	6.48	65,65,65,65	0
86	OHX	5	4216	7/7	0.23	6.46	113,113,113,113	0
86	OHX	5	4191	7/7	0.25	6.46	97,97,97,97	0
85	MG	5	3469	1/1	0.29	6.44	101,101,101,101	0
86	OHX	5	4220	7/7	0.29	6.43	133,133,133,133	0
85	MG	1	3460	1/1	0.26	6.41	26,26,26,26	0
85	MG	5	3785	1/1	0.23	6.40	31,31,31,31	0
85	MG	5	3619	1/1	0.23	6.38	34,34,34,34	0
86	OHX	2	2119	7/7	0.19	6.37	110,110,110,110	0
85	MG	5	3743	1/1	0.27	6.35	22,22,22,22	0
86	OHX	5	4181	7/7	0.28	6.34	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	6	2204	7/7	0.28	6.31	118,118,118,118	0
85	MG	1	3519	1/1	0.29	6.31	31,31,31,31	0
85	MG	2	1972	1/1	0.33	6.30	66,66,66,66	0
85	MG	5	3710	1/1	0.27	6.30	28,28,28,28	0
85	MG	6	1949	1/1	0.27	6.30	40,40,40,40	0
86	OHX	5	4142	7/7	0.19	6.29	96,96,96,96	0
85	MG	m1	201	1/1	0.24	6.26	51,51,51,51	0
85	MG	6	2000	1/1	0.58	6.26	42,42,42,42	0
85	MG	2	1901	1/1	0.48	6.24	57,57,57,57	0
86	OHX	1	4171	7/7	0.30	6.24	91,91,91,91	0
85	MG	1	3559	1/1	0.26	6.21	18,18,18,18	0
85	MG	1	3482	1/1	0.30	6.18	22,22,22,22	0
85	MG	1	3747	1/1	0.23	6.18	22,22,22,22	0
85	MG	6	1985	1/1	0.26	6.17	59,59,59,59	0
86	OHX	1	4210	7/7	0.34	6.15	100,100,100,100	0
85	MG	5	3433	1/1	0.34	6.13	64,64,64,64	0
85	MG	5	3697	1/1	0.31	6.12	26,26,26,26	0
86	OHX	5	4137	7/7	0.31	6.12	101,101,101,101	0
86	OHX	1	4177	7/7	0.26	6.09	114,114,114,114	0
85	MG	2	1938	1/1	0.33	6.07	48,48,48,48	0
86	OHX	1	4172	7/7	0.24	6.05	123,123,123,123	0
85	MG	5	3507	1/1	0.27	6.03	33,33,33,33	0
86	OHX	6	2126	7/7	0.32	6.03	81,81,81,81	0
85	MG	5	3649	1/1	0.38	6.03	59,59,59,59	0
85	MG	6	1908	1/1	0.29	6.03	41,41,41,41	0
85	MG	5	3882	1/1	0.23	6.02	19,19,19,19	0
85	MG	5	3772	1/1	0.22	6.01	23,23,23,23	0
85	MG	5	3592	1/1	0.25	5.99	29,29,29,29	0
85	MG	2	1905	1/1	0.36	5.97	51,51,51,51	0
85	MG	6	2018	1/1	0.26	5.96	44,44,44,44	0
85	MG	2	1968	1/1	0.55	5.95	97,97,97,97	0
85	MG	5	3456	1/1	0.25	5.95	21,21,21,21	0
85	MG	1	3694	1/1	0.21	5.94	27,27,27,27	0
85	MG	5	3732	1/1	0.26	5.93	65,65,65,65	0
85	MG	3	212	1/1	0.21	5.93	63,63,63,63	0
85	MG	l3	401	1/1	0.37	5.93	22,22,22,22	0
85	MG	5	3626	1/1	0.19	5.92	42,42,42,42	0
85	MG	6	1957	1/1	0.49	5.90	48,48,48,48	0
85	MG	6	2030	1/1	0.19	5.89	83,83,83,83	0
85	MG	2	1955	1/1	0.27	5.87	79,79,79,79	0
86	OHX	1	4125	7/7	0.23	5.86	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	4	233	7/7	0.29	5.84	121,121,121,121	0
85	MG	2	1944	1/1	0.22	5.81	53,53,53,53	0
85	MG	5	3439	1/1	0.20	5.81	24,24,24,24	0
86	OHX	5	4171	7/7	0.28	5.81	73,73,73,73	0
85	MG	6	2012	1/1	0.23	5.77	41,41,41,41	0
86	OHX	2	2138	7/7	0.21	5.77	132,132,132,132	0
85	MG	1	3454	1/1	0.26	5.76	30,30,30,30	0
85	MG	4	205	1/1	0.24	5.74	41,41,41,41	0
85	MG	6	1923	1/1	0.32	5.74	56,56,56,56	0
88	3H3	1	4216	33/33	0.40	5.73	26,26,26,26	0
86	OHX	5	4225	7/7	0.28	5.72	105,105,105,105	0
85	MG	o1	201	1/1	0.54	5.72	76,76,76,76	0
85	MG	1	3589	1/1	0.32	5.71	25,25,25,25	0
85	MG	1	3431	1/1	0.23	5.71	41,41,41,41	0
86	OHX	5	4105	7/7	0.29	5.70	87,87,87,87	0
85	MG	1	3413	1/1	0.26	5.67	52,52,52,52	0
85	MG	5	3432	1/1	0.22	5.62	49,49,49,49	0
86	OHX	1	4111	7/7	0.27	5.61	110,110,110,110	0
85	MG	1	3610	1/1	0.21	5.60	34,34,34,34	0
86	OHX	6	2203	7/7	0.27	5.58	117,117,117,117	0
85	MG	1	3850	1/1	0.26	5.58	41,41,41,41	0
86	OHX	1	4214	7/7	0.29	5.57	103,103,103,103	0
86	OHX	2	2158	7/7	0.34	5.55	93,93,93,93	0
85	MG	1	3470	1/1	0.20	5.52	37,37,37,37	0
86	OHX	1	4146	7/7	0.32	5.51	94,94,94,94	0
85	MG	2	1923	1/1	0.26	5.50	53,53,53,53	0
85	MG	1	3733	1/1	0.28	5.46	46,46,46,46	0
85	MG	7	202	1/1	0.26	5.44	27,27,27,27	0
86	OHX	5	4157	7/7	0.22	5.44	87,87,87,87	0
86	OHX	6	2162	7/7	0.28	5.43	96,96,96,96	0
85	MG	1	3471	1/1	0.19	5.42	35,35,35,35	0
85	MG	5	3776	1/1	0.20	5.42	56,56,56,56	0
85	MG	1	3720	1/1	0.30	5.38	42,42,42,42	0
85	MG	5	3553	1/1	0.31	5.38	37,37,37,37	0
85	MG	8	207	1/1	0.21	5.37	53,53,53,53	0
85	MG	5	3468	1/1	0.20	5.37	29,29,29,29	0
86	OHX	1	4081	7/7	0.26	5.35	96,96,96,96	0
85	MG	5	3877	1/1	0.28	5.34	14,14,14,14	0
85	MG	1	3535	1/1	0.27	5.33	41,41,41,41	0
85	MG	4	203	1/1	0.32	5.33	44,44,44,44	0
85	MG	5	3671	1/1	0.34	5.30	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	3	205	1/1	0.23	5.30	28,28,28,28	0
86	OHX	5	4246	7/7	0.34	5.27	122,122,122,122	0
86	OHX	6	2189	7/7	0.37	5.27	115,115,115,115	0
85	MG	5	3629	1/1	0.24	5.26	37,37,37,37	0
86	OHX	1	4203	7/7	0.26	5.26	108,108,108,108	0
86	OHX	2	2026	7/7	0.22	5.23	69,69,69,69	0
85	MG	1	3804	1/1	0.18	5.22	45,45,45,45	0
86	OHX	5	4175	7/7	0.22	5.21	105,105,105,105	0
85	MG	5	3516	1/1	0.39	5.21	20,20,20,20	0
85	MG	2	1971	1/1	0.28	5.20	56,56,56,56	0
85	MG	1	3538	1/1	0.20	5.18	31,31,31,31	0
86	OHX	1	4086	7/7	0.24	5.18	101,101,101,101	0
85	MG	1	3751	1/1	0.20	5.17	34,34,34,34	0
85	MG	1	3549	1/1	0.24	5.13	27,27,27,27	0
85	MG	5	3490	1/1	0.25	5.12	53,53,53,53	0
86	OHX	5	4163	7/7	0.24	5.12	145,145,145,145	0
85	MG	1	3630	1/1	0.19	5.11	21,21,21,21	0
85	MG	1	3743	1/1	0.21	5.11	36,36,36,36	0
85	MG	m4	201	1/1	0.23	5.11	46,46,46,46	0
85	MG	5	3542	1/1	0.26	5.08	53,53,53,53	0
85	MG	1	3572	1/1	0.26	5.08	24,24,24,24	0
85	MG	1	3652	1/1	0.42	5.08	84,84,84,84	0
86	OHX	1	4098	7/7	0.23	5.07	103,103,103,103	0
85	MG	6	1912	1/1	0.32	5.03	60,60,60,60	0
86	OHX	4	235	7/7	0.33	5.02	108,108,108,108	0
86	OHX	1	4076	7/7	0.31	5.00	81,81,81,81	0
85	MG	5	3605	1/1	0.24	4.98	46,46,46,46	0
85	MG	5	3427	1/1	0.25	4.95	23,23,23,23	0
86	OHX	1	4050	7/7	0.23	4.92	92,92,92,92	0
85	MG	2	1925	1/1	0.25	4.91	60,60,60,60	0
85	MG	6	1920	1/1	0.27	4.90	58,58,58,58	0
85	MG	5	3419	1/1	0.18	4.89	91,91,91,91	0
85	MG	5	4253	1/1	0.49	4.87	28,28,28,28	0
86	OHX	6	2176	7/7	0.23	4.87	87,87,87,87	0
85	MG	6	1966	1/1	0.34	4.86	73,73,73,73	0
85	MG	1	3631	1/1	0.33	4.85	62,62,62,62	0
86	OHX	5	4189	7/7	0.21	4.85	100,100,100,100	0
85	MG	5	3514	1/1	0.26	4.83	22,22,22,22	0
85	MG	1	3863	1/1	0.24	4.82	118,118,118,118	0
85	MG	1	3600	1/1	0.23	4.81	25,25,25,25	0
85	MG	5	3555	1/1	0.28	4.80	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4061	7/7	0.23	4.77	97,97,97,97	0
85	MG	1	3576	1/1	0.28	4.76	21,21,21,21	0
85	MG	1	3856	1/1	0.21	4.75	22,22,22,22	0
85	MG	2	1990	1/1	0.20	4.74	51,51,51,51	0
85	MG	1	3474	1/1	0.24	4.73	20,20,20,20	0
86	OHX	5	3900	7/7	0.20	4.73	35,35,35,35	0
86	OHX	5	4245	7/7	0.24	4.73	119,119,119,119	0
86	OHX	1	4170	7/7	0.22	4.72	95,95,95,95	0
86	OHX	5	4210	7/7	0.21	4.70	109,109,109,109	0
86	OHX	2	2031	7/7	0.19	4.69	80,80,80,80	0
85	MG	5	3534	1/1	0.34	4.68	24,24,24,24	0
85	MG	1	3810	1/1	0.44	4.67	26,26,26,26	0
85	MG	5	3457	1/1	0.20	4.66	35,35,35,35	0
85	MG	1	3472	1/1	0.41	4.64	29,29,29,29	0
85	MG	1	3785	1/1	0.25	4.64	55,55,55,55	0
86	OHX	5	4239	7/7	0.30	4.64	149,149,149,149	0
85	MG	5	3828	1/1	0.25	4.63	50,50,50,50	0
85	MG	M7	201	1/1	0.41	4.62	52,52,52,52	0
85	MG	5	3564	1/1	0.36	4.61	38,38,38,38	0
85	MG	5	3790	1/1	0.24	4.61	41,41,41,41	0
86	OHX	5	4229	7/7	0.30	4.60	131,131,131,131	0
85	MG	1	3818	1/1	0.20	4.60	48,48,48,48	0
85	MG	1	3505	1/1	0.24	4.58	25,25,25,25	0
85	MG	5	3557	1/1	0.24	4.57	21,21,21,21	0
85	MG	2	1953	1/1	0.24	4.56	76,76,76,76	0
85	MG	1	3507	1/1	0.28	4.55	22,22,22,22	0
85	MG	2	1911	1/1	0.33	4.53	50,50,50,50	0
85	MG	5	3524	1/1	0.22	4.50	36,36,36,36	0
86	OHX	5	4148	7/7	0.32	4.49	119,119,119,119	0
85	MG	5	3441	1/1	0.32	4.49	26,26,26,26	0
86	OHX	5	4211	7/7	0.19	4.49	118,118,118,118	0
85	MG	5	3610	1/1	0.21	4.47	40,40,40,40	0
86	OHX	5	4125	7/7	0.20	4.47	113,113,113,113	0
85	MG	c7	201	1/1	0.34	4.46	63,63,63,63	0
85	MG	5	3585	1/1	0.24	4.43	20,20,20,20	0
86	OHX	5	3913	7/7	0.20	4.43	54,54,54,54	0
85	MG	1	3429	1/1	0.21	4.42	36,36,36,36	0
86	OHX	2	2180	7/7	0.24	4.42	116,116,116,116	0
85	MG	2	1937	1/1	0.29	4.41	46,46,46,46	0
85	MG	1	3707	1/1	0.20	4.40	46,46,46,46	0
85	MG	1	3748	1/1	0.21	4.39	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	7	207	1/1	0.21	4.39	43,43,43,43	0
85	MG	2	1952	1/1	0.37	4.39	75,75,75,75	0
86	OHX	4	227	7/7	0.22	4.38	86,86,86,86	0
85	MG	5	3445	1/1	0.20	4.38	33,33,33,33	0
86	OHX	1	4124	7/7	0.21	4.37	104,104,104,104	0
85	MG	1	3518	1/1	0.30	4.37	19,19,19,19	0
85	MG	1	3702	1/1	0.18	4.36	39,39,39,39	0
86	OHX	6	2191	7/7	0.25	4.35	131,131,131,131	0
85	MG	1	3735	1/1	0.25	4.34	55,55,55,55	0
85	MG	1	3862	1/1	0.32	4.33	41,41,41,41	0
85	MG	6	1997	1/1	0.26	4.32	43,43,43,43	0
85	MG	5	3525	1/1	0.26	4.32	30,30,30,30	0
85	MG	2	1910	1/1	0.22	4.31	48,48,48,48	0
86	OHX	1	4202	7/7	0.24	4.29	110,110,110,110	0
86	OHX	1	4135	7/7	0.25	4.28	95,95,95,95	0
86	OHX	5	4247	7/7	0.30	4.27	102,102,102,102	0
86	OHX	1	4184	7/7	0.26	4.27	86,86,86,86	0
85	MG	1	3625	1/1	0.21	4.25	27,27,27,27	0
86	OHX	6	2184	7/7	0.23	4.24	108,108,108,108	0
85	MG	3	210	1/1	0.24	4.22	50,50,50,50	0
86	OHX	5	4139	7/7	0.25	4.20	105,105,105,105	0
85	MG	5	3539	1/1	0.37	4.19	19,19,19,19	0
85	MG	1	3571	1/1	0.27	4.19	35,35,35,35	0
86	OHX	1	3982	7/7	0.28	4.17	69,69,69,69	0
86	OHX	5	4144	7/7	0.24	4.16	97,97,97,97	0
85	MG	5	3442	1/1	0.22	4.14	27,27,27,27	0
85	MG	5	3512	1/1	0.32	4.12	20,20,20,20	0
85	MG	1	3447	1/1	0.37	4.11	44,44,44,44	0
86	OHX	6	2127	7/7	0.25	4.10	98,98,98,98	0
85	MG	1	3813	1/1	0.26	4.09	26,26,26,26	0
85	MG	1	3604	1/1	0.20	4.05	27,27,27,27	0
85	MG	5	3474	1/1	0.28	4.05	64,64,64,64	0
86	OHX	6	2178	7/7	0.23	4.03	114,114,114,114	0
86	OHX	2	2164	7/7	0.22	4.02	140,140,140,140	0
85	MG	2	1962	1/1	0.25	3.99	44,44,44,44	0
85	MG	2	1978	1/1	0.21	3.99	80,80,80,80	0
86	OHX	2	2173	7/7	0.46	3.99	121,121,121,121	0
85	MG	5	3476	1/1	0.22	3.98	19,19,19,19	0
85	MG	1	3462	1/1	0.22	3.98	23,23,23,23	0
86	OHX	2	2099	7/7	0.21	3.97	94,94,94,94	0
85	MG	o4	202	1/1	0.29	3.96	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3465	1/1	0.20	3.94	48,48,48,48	0
85	MG	5	4257	1/1	0.35	3.93	22,22,22,22	0
86	OHX	6	2055	7/7	0.19	3.93	70,70,70,70	0
86	OHX	1	4197	7/7	0.21	3.92	117,117,117,117	0
86	OHX	1	4211	7/7	0.29	3.88	106,106,106,106	0
85	MG	2	2007	1/1	0.50	3.88	52,52,52,52	0
85	MG	1	3598	1/1	0.28	3.88	33,33,33,33	0
85	MG	1	3439	1/1	0.24	3.87	34,34,34,34	0
86	OHX	2	2146	7/7	0.30	3.86	115,115,115,115	0
86	OHX	6	2197	7/7	0.29	3.85	113,113,113,113	0
85	MG	1	3660	1/1	0.24	3.83	40,40,40,40	0
85	MG	1	3541	1/1	0.24	3.83	19,19,19,19	0
85	MG	1	3669	1/1	0.22	3.81	37,37,37,37	0
85	MG	5	3482	1/1	0.34	3.80	30,30,30,30	0
85	MG	1	3545	1/1	0.22	3.77	37,37,37,37	0
85	MG	5	3844	1/1	0.23	3.76	22,22,22,22	0
85	MG	2	1974	1/1	0.30	3.74	59,59,59,59	0
86	OHX	5	4172	7/7	0.25	3.72	102,102,102,102	0
85	MG	5	3757	1/1	0.21	3.72	49,49,49,49	0
86	OHX	2	2134	7/7	0.21	3.72	127,127,127,127	0
86	OHX	1	4136	7/7	0.25	3.71	106,106,106,106	0
85	MG	17	301	1/1	0.24	3.71	32,32,32,32	0
85	MG	5	3612	1/1	0.20	3.70	26,26,26,26	0
85	MG	5	3424	1/1	0.20	3.68	34,34,34,34	0
85	MG	s1	301	1/1	0.32	3.65	62,62,62,62	0
86	OHX	2	2147	7/7	0.20	3.63	105,105,105,105	0
86	OHX	2	2177	7/7	0.24	3.58	113,113,113,113	0
86	OHX	7	227	7/7	0.22	3.58	127,127,127,127	0
85	MG	1	3517	1/1	0.28	3.58	22,22,22,22	0
86	OHX	1	3872	7/7	0.22	3.57	46,46,46,46	0
85	MG	1	3586	1/1	0.34	3.53	38,38,38,38	0
86	OHX	5	4202	7/7	0.25	3.53	112,112,112,112	0
85	MG	5	3667	1/1	0.20	3.52	31,31,31,31	0
85	MG	6	1906	1/1	0.25	3.50	43,43,43,43	0
86	OHX	1	4122	7/7	0.38	3.48	103,103,103,103	0
85	MG	1	3588	1/1	0.24	3.48	21,21,21,21	0
85	MG	5	3448	1/1	0.24	3.46	54,54,54,54	0
86	OHX	5	4150	7/7	0.25	3.46	113,113,113,113	0
85	MG	5	3763	1/1	0.26	3.46	26,26,26,26	0
85	MG	1	3826	1/1	0.18	3.45	59,59,59,59	0
86	OHX	5	4161	7/7	0.20	3.44	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4127	7/7	0.20	3.44	100,100,100,100	0
86	OHX	2	2161	7/7	0.42	3.43	109,109,109,109	0
87	ZN	d7	101	1/1	0.42	3.43	119,119,119,119	0
85	MG	2	2023	1/1	0.22	3.43	101,101,101,101	0
85	MG	2	1961	1/1	0.22	3.42	54,54,54,54	0
86	OHX	1	4167	7/7	0.22	3.41	103,103,103,103	0
86	OHX	6	2053	7/7	0.18	3.41	61,61,61,61	0
86	OHX	1	4156	7/7	0.20	3.40	105,105,105,105	0
86	OHX	1	3874	7/7	0.20	3.40	48,48,48,48	0
86	OHX	6	2161	7/7	0.23	3.40	101,101,101,101	0
85	MG	5	3472	1/1	0.23	3.40	23,23,23,23	0
86	OHX	1	4157	7/7	0.26	3.39	105,105,105,105	0
85	MG	5	3639	1/1	0.27	3.39	40,40,40,40	0
86	OHX	1	4150	7/7	0.29	3.38	111,111,111,111	0
85	MG	1	3496	1/1	0.22	3.38	26,26,26,26	0
86	OHX	5	4108	7/7	0.25	3.38	95,95,95,95	0
85	MG	M3	202	1/1	0.38	3.37	34,34,34,34	0
86	OHX	5	3912	7/7	0.17	3.37	49,49,49,49	0
85	MG	2	1903	1/1	0.30	3.35	40,40,40,40	0
86	OHX	1	4204	7/7	0.31	3.33	109,109,109,109	0
85	MG	2	1998	1/1	0.20	3.33	60,60,60,60	0
85	MG	2	1918	1/1	0.30	3.33	46,46,46,46	0
86	OHX	5	3909	7/7	0.22	3.32	53,53,53,53	0
86	OHX	5	4114	7/7	0.27	3.32	95,95,95,95	0
85	MG	1	3806	1/1	0.23	3.31	48,48,48,48	0
85	MG	1	3458	1/1	0.20	3.30	30,30,30,30	0
86	OHX	5	4203	7/7	0.31	3.29	110,110,110,110	0
86	OHX	1	4160	7/7	0.22	3.28	114,114,114,114	0
86	OHX	2	2103	7/7	0.21	3.27	112,112,112,112	0
85	MG	o3	202	1/1	0.26	3.26	24,24,24,24	0
86	OHX	5	4027	7/7	0.20	3.26	83,83,83,83	0
86	OHX	6	2157	7/7	0.18	3.25	110,110,110,110	0
86	OHX	5	4145	7/7	0.23	3.23	93,93,93,93	0
85	MG	2	1986	1/1	0.30	3.23	50,50,50,50	0
85	MG	6	1950	1/1	0.22	3.22	35,35,35,35	0
86	OHX	6	2199	7/7	0.25	3.21	110,110,110,110	0
85	MG	5	3681	1/1	0.19	3.21	29,29,29,29	0
85	MG	2	1950	1/1	0.22	3.20	47,47,47,47	0
85	MG	8	203	1/1	0.24	3.19	37,37,37,37	0
85	MG	1	3700	1/1	0.21	3.19	31,31,31,31	0
86	OHX	1	4023	7/7	0.22	3.16	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2177	7/7	0.22	3.16	97,97,97,97	0
85	MG	1	3550	1/1	0.25	3.15	31,31,31,31	0
86	OHX	5	4199	7/7	0.23	3.14	98,98,98,98	0
85	MG	n8	203	1/1	0.21	3.14	38,38,38,38	0
86	OHX	5	4110	7/7	0.19	3.13	103,103,103,103	0
85	MG	1	3726	1/1	0.21	3.11	33,33,33,33	0
85	MG	1	3530	1/1	0.25	3.10	52,52,52,52	0
85	MG	1	3618	1/1	0.27	3.08	48,48,48,48	0
86	OHX	5	4092	7/7	0.22	3.08	93,93,93,93	0
85	MG	1	3487	1/1	0.22	3.08	27,27,27,27	0
86	OHX	6	2048	7/7	0.19	3.08	60,60,60,60	0
85	MG	2	1977	1/1	0.27	3.07	73,73,73,73	0
85	MG	1	3769	1/1	0.23	3.02	53,53,53,53	0
86	OHX	6	2195	7/7	0.24	3.01	127,127,127,127	0
85	MG	1	3791	1/1	0.30	3.00	19,19,19,19	0
85	MG	1	3704	1/1	0.19	3.00	53,53,53,53	0
86	OHX	O9	101	7/7	0.45	2.99	88,88,88,88	0
85	MG	5	3695	1/1	0.19	2.99	46,46,46,46	0
86	OHX	5	4194	7/7	0.27	2.99	116,116,116,116	0
85	MG	1	3595	1/1	0.29	2.94	22,22,22,22	0
85	MG	1	3658	1/1	0.21	2.93	36,36,36,36	0
86	OHX	6	2144	7/7	0.25	2.91	105,105,105,105	0
85	MG	6	1998	1/1	0.25	2.90	49,49,49,49	0
86	OHX	5	4218	7/7	0.18	2.90	141,141,141,141	0
86	OHX	6	2198	7/7	0.28	2.87	117,117,117,117	0
85	MG	5	3827	1/1	0.21	2.86	20,20,20,20	0
85	MG	5	3867	1/1	0.52	2.85	31,31,31,31	0
85	MG	6	1977	1/1	0.26	2.85	40,40,40,40	0
86	OHX	2	2080	7/7	0.23	2.82	98,98,98,98	0
86	OHX	1	3891	7/7	0.18	2.81	65,65,65,65	0
86	OHX	2	2075	7/7	0.28	2.81	95,95,95,95	0
86	OHX	5	4188	7/7	0.20	2.80	111,111,111,111	0
85	MG	1	3762	1/1	0.20	2.80	24,24,24,24	0
85	MG	1	3521	1/1	0.27	2.75	60,60,60,60	0
85	MG	5	3541	1/1	0.22	2.73	22,22,22,22	0
86	OHX	5	4201	7/7	0.47	2.73	104,104,104,104	0
85	MG	1	3836	1/1	0.24	2.72	23,23,23,23	0
85	MG	6	2005	1/1	0.21	2.72	81,81,81,81	0
86	OHX	5	4221	7/7	0.27	2.71	113,113,113,113	0
86	OHX	7	225	7/7	0.18	2.71	118,118,118,118	0
86	OHX	1	4161	7/7	0.20	2.70	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4183	7/7	0.22	2.69	100,100,100,100	0
85	MG	1	3805	1/1	0.40	2.68	49,49,49,49	0
85	MG	1	3757	1/1	0.21	2.65	35,35,35,35	0
86	OHX	1	3924	7/7	0.21	2.65	94,94,94,94	0
85	MG	5	3700	1/1	0.47	2.64	47,47,47,47	0
85	MG	2	2183	1/1	0.21	2.63	73,73,73,73	0
85	MG	2	1906	1/1	0.20	2.63	39,39,39,39	0
86	OHX	1	4114	7/7	0.25	2.62	87,87,87,87	0
86	OHX	2	2167	7/7	0.22	2.59	132,132,132,132	0
85	MG	1	3722	1/1	0.21	2.58	34,34,34,34	0
86	OHX	1	3915	7/7	0.20	2.55	73,73,73,73	0
85	MG	1	3615	1/1	0.22	2.55	31,31,31,31	0
86	OHX	1	4102	7/7	0.28	2.55	90,90,90,90	0
86	OHX	6	2188	7/7	0.19	2.54	120,120,120,120	0
85	MG	c8	201	1/1	0.25	2.54	57,57,57,57	0
85	MG	5	3549	1/1	0.30	2.54	24,24,24,24	0
85	MG	6	1965	1/1	0.23	2.54	52,52,52,52	0
85	MG	5	3429	1/1	0.23	2.52	59,59,59,59	0
86	OHX	s9	201	7/7	0.31	2.52	102,102,102,102	0
86	OHX	3	223	7/7	0.23	2.52	96,96,96,96	0
85	MG	1	3481	1/1	0.23	2.51	31,31,31,31	0
85	MG	1	3708	1/1	0.18	2.50	34,34,34,34	0
85	MG	5	3446	1/1	0.19	2.50	30,30,30,30	0
85	MG	5	3717	1/1	0.18	2.48	58,58,58,58	0
85	MG	1	3539	1/1	0.25	2.48	17,17,17,17	0
85	MG	5	3567	1/1	0.24	2.48	26,26,26,26	0
86	OHX	m7	206	7/7	0.40	2.47	99,99,99,99	0
86	OHX	5	4039	7/7	0.28	2.46	67,67,67,67	0
85	MG	5	3665	1/1	0.21	2.45	19,19,19,19	0
85	MG	1	3752	1/1	0.22	2.45	48,48,48,48	0
85	MG	5	3659	1/1	0.24	2.43	22,22,22,22	0
85	MG	5	3423	1/1	0.24	2.42	36,36,36,36	0
86	OHX	8	229	7/7	0.25	2.41	108,108,108,108	0
86	OHX	5	4141	7/7	0.18	2.41	108,108,108,108	0
86	OHX	5	4156	7/7	0.20	2.40	107,107,107,107	0
85	MG	1	3622	1/1	0.20	2.40	42,42,42,42	0
86	OHX	5	3903	7/7	0.20	2.39	43,43,43,43	0
85	MG	5	3411	1/1	0.22	2.38	30,30,30,30	0
86	OHX	8	219	7/7	0.24	2.38	91,91,91,91	0
85	MG	1	3597	1/1	0.25	2.38	22,22,22,22	0
86	OHX	1	4113	7/7	0.21	2.37	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	2	2156	7/7	0.24	2.36	114,114,114,114	0
85	MG	1	3609	1/1	0.30	2.35	54,54,54,54	0
86	OHX	2	2174	7/7	0.22	2.35	115,115,115,115	0
85	MG	5	3853	1/1	0.33	2.35	34,34,34,34	0
86	OHX	1	4183	7/7	0.33	2.34	110,110,110,110	0
86	OHX	1	4155	7/7	0.21	2.34	115,115,115,115	0
85	MG	1	3629	1/1	0.21	2.34	30,30,30,30	0
85	MG	5	3538	1/1	0.28	2.34	19,19,19,19	0
85	MG	2	1935	1/1	0.28	2.31	60,60,60,60	0
86	OHX	2	2126	7/7	0.22	2.31	103,103,103,103	0
85	MG	1	3835	1/1	0.20	2.31	46,46,46,46	0
85	MG	2	2009	1/1	0.21	2.31	46,46,46,46	0
85	MG	2	1939	1/1	0.30	2.30	57,57,57,57	0
85	MG	5	3802	1/1	0.24	2.30	40,40,40,40	0
85	MG	1	3568	1/1	0.26	2.28	19,19,19,19	0
86	OHX	6	2200	7/7	0.23	2.28	115,115,115,115	0
86	OHX	2	2154	7/7	0.18	2.27	131,131,131,131	0
86	OHX	1	4129	7/7	0.18	2.27	118,118,118,118	0
86	OHX	5	4182	7/7	0.23	2.26	98,98,98,98	0
85	MG	5	3401	1/1	0.26	2.26	36,36,36,36	0
85	MG	2	1979	1/1	0.28	2.25	45,45,45,45	0
85	MG	5	3591	1/1	0.23	2.24	26,26,26,26	0
86	OHX	5	4099	7/7	0.20	2.23	94,94,94,94	0
86	OHX	6	2196	7/7	0.19	2.23	142,142,142,142	0
85	MG	1	3508	1/1	0.27	2.22	19,19,19,19	0
85	MG	5	3587	1/1	0.29	2.22	21,21,21,21	0
86	OHX	1	4206	7/7	0.20	2.22	106,106,106,106	0
85	MG	5	3815	1/1	0.22	2.21	36,36,36,36	0
85	MG	6	1942	1/1	0.22	2.21	30,30,30,30	0
86	OHX	2	2176	7/7	0.29	2.20	125,125,125,125	0
85	MG	2	1963	1/1	0.28	2.19	65,65,65,65	0
85	MG	1	3531	1/1	0.23	2.18	19,19,19,19	0
85	MG	d3	201	1/1	0.39	2.18	39,39,39,39	0
86	OHX	5	4126	7/7	0.19	2.17	103,103,103,103	0
85	MG	1	4217	1/1	0.21	2.17	19,19,19,19	0
85	MG	2	1930	1/1	0.23	2.16	53,53,53,53	0
86	OHX	5	4170	7/7	0.26	2.15	81,81,81,81	0
86	OHX	5	3899	7/7	0.19	2.15	34,34,34,34	0
85	MG	1	3578	1/1	0.27	2.14	20,20,20,20	0
85	MG	1	3801	1/1	0.25	2.13	41,41,41,41	0
85	MG	1	3655	1/1	0.26	2.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3526	1/1	0.30	2.13	42,42,42,42	0
85	MG	2	1919	1/1	0.37	2.12	62,62,62,62	0
86	OHX	5	4146	7/7	0.25	2.12	100,100,100,100	0
86	OHX	1	3868	7/7	0.20	2.10	35,35,35,35	0
85	MG	6	1910	1/1	0.22	2.08	54,54,54,54	0
85	MG	6	1987	1/1	0.18	2.08	54,54,54,54	0
86	OHX	6	2169	7/7	0.16	2.08	124,124,124,124	0
85	MG	5	3676	1/1	0.27	2.07	81,81,81,81	0
85	MG	5	3590	1/1	0.31	2.07	21,21,21,21	0
85	MG	1	3495	1/1	0.22	2.07	36,36,36,36	0
85	MG	5	3622	1/1	0.23	2.07	29,29,29,29	0
85	MG	1	3643	1/1	0.21	2.06	39,39,39,39	0
85	MG	5	3613	1/1	0.22	2.05	36,36,36,36	0
85	MG	6	1936	1/1	0.24	2.05	57,57,57,57	0
86	OHX	5	4132	7/7	0.24	2.05	96,96,96,96	0
85	MG	5	3803	1/1	0.21	2.04	132,132,132,132	0
86	OHX	1	4149	7/7	0.20	2.04	105,105,105,105	0
86	OHX	5	4044	7/7	0.22	2.03	77,77,77,77	0
85	MG	1	3544	1/1	0.22	2.02	32,32,32,32	0
86	OHX	2	2155	7/7	0.19	2.02	114,114,114,114	0
85	MG	1	3685	1/1	0.20	2.02	45,45,45,45	0
86	OHX	1	4017	7/7	0.20	2.01	97,97,97,97	0
86	OHX	5	4093	7/7	0.22	2.00	97,97,97,97	0
86	OHX	4	231	7/7	0.23	1.99	115,115,115,115	0
86	OHX	5	3898	7/7	0.20	1.99	37,37,37,37	0
85	MG	1	3619	1/1	0.17	1.98	53,53,53,53	0
85	MG	1	3825	1/1	0.35	1.97	31,31,31,31	0
85	MG	1	3711	1/1	0.18	1.97	52,52,52,52	0
85	MG	1	3420	1/1	0.43	1.96	57,57,57,57	0
86	OHX	5	4186	7/7	0.31	1.96	120,120,120,120	0
86	OHX	5	4209	7/7	0.24	1.95	91,91,91,91	0
85	MG	q0	202	1/1	0.20	1.95	34,34,34,34	0
86	OHX	m4	202	7/7	0.19	1.95	190,190,190,190	0
85	MG	5	3625	1/1	0.17	1.93	53,53,53,53	0
85	MG	5	3608	1/1	0.22	1.93	29,29,29,29	0
86	OHX	2	2175	7/7	0.24	1.93	128,128,128,128	0
86	OHX	2	2109	7/7	0.17	1.93	123,123,123,123	0
86	OHX	1	3883	7/7	0.19	1.92	52,52,52,52	0
85	MG	s6	301	1/1	0.31	1.92	59,59,59,59	0
85	MG	5	3729	1/1	0.31	1.91	61,61,61,61	0
86	OHX	6	2151	7/7	0.20	1.90	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3436	1/1	0.21	1.90	35,35,35,35	0
86	OHX	1	3900	7/7	0.19	1.89	65,65,65,65	0
86	OHX	2	2153	7/7	0.20	1.87	118,118,118,118	0
85	MG	N0	201	1/1	0.26	1.87	42,42,42,42	0
86	OHX	m8	201	7/7	0.29	1.86	111,111,111,111	0
86	OHX	L6	202	7/7	0.29	1.85	112,112,112,112	0
85	MG	1	3644	1/1	0.19	1.84	50,50,50,50	0
86	OHX	1	4115	7/7	0.22	1.83	106,106,106,106	0
85	MG	6	2037	1/1	0.19	1.83	52,52,52,52	0
85	MG	1	3654	1/1	0.19	1.83	33,33,33,33	0
86	OHX	5	3907	7/7	0.18	1.83	44,44,44,44	0
85	MG	5	3607	1/1	0.21	1.83	20,20,20,20	0
85	MG	5	3814	1/1	0.17	1.82	53,53,53,53	0
85	MG	1	3680	1/1	0.19	1.81	30,30,30,30	0
85	MG	6	2022	1/1	0.20	1.80	71,71,71,71	0
85	MG	1	3798	1/1	0.18	1.80	39,39,39,39	0
85	MG	1	3784	1/1	0.29	1.78	29,29,29,29	0
85	MG	1	3790	1/1	0.20	1.78	33,33,33,33	0
86	OHX	5	4169	7/7	0.20	1.77	130,130,130,130	0
85	MG	1	3432	1/1	0.22	1.77	36,36,36,36	0
85	MG	1	3414	1/1	0.23	1.76	28,28,28,28	0
86	OHX	1	4133	7/7	0.21	1.76	121,121,121,121	0
85	MG	5	3640	1/1	0.21	1.75	32,32,32,32	0
85	MG	7	208	1/1	0.20	1.74	42,42,42,42	0
86	OHX	5	4062	7/7	0.21	1.74	99,99,99,99	0
85	MG	2	1949	1/1	0.26	1.73	68,68,68,68	0
86	OHX	6	2121	7/7	0.19	1.73	89,89,89,89	0
86	OHX	8	214	7/7	0.18	1.72	47,47,47,47	0
86	OHX	5	4115	7/7	0.16	1.70	118,118,118,118	0
86	OHX	5	4222	7/7	0.31	1.70	101,101,101,101	0
85	MG	L7	302	1/1	0.20	1.69	29,29,29,29	0
86	OHX	1	4132	7/7	0.17	1.69	129,129,129,129	0
86	OHX	6	2113	7/7	0.20	1.69	87,87,87,87	0
86	OHX	6	2175	7/7	0.28	1.68	122,122,122,122	0
86	OHX	4	226	7/7	0.28	1.68	91,91,91,91	0
85	MG	L5	301	1/1	0.38	1.67	50,50,50,50	0
88	3H3	5	4251	33/33	0.35	1.67	29,29,29,29	0
86	OHX	5	3938	7/7	0.18	1.65	71,71,71,71	0
86	OHX	6	2136	7/7	0.19	1.65	105,105,105,105	0
85	MG	2	1956	1/1	0.20	1.64	53,53,53,53	0
86	OHX	6	2193	7/7	0.28	1.64	142,142,142,142	0
86	OHX	1	4053	7/7	0.22	1.63	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	3877	7/7	0.18	1.63	46,46,46,46	0
85	MG	1	3514	1/1	0.19	1.62	29,29,29,29	0
85	MG	1	3673	1/1	0.33	1.61	56,56,56,56	0
85	MG	1	3849	1/1	0.23	1.60	33,33,33,33	0
85	MG	6	1938	1/1	0.23	1.59	35,35,35,35	0
85	MG	5	3627	1/1	0.22	1.57	52,52,52,52	0
86	OHX	2	2035	7/7	0.17	1.57	82,82,82,82	0
85	MG	2	1927	1/1	0.28	1.56	46,46,46,46	0
85	MG	1	3459	1/1	0.21	1.55	55,55,55,55	0
86	OHX	1	4103	7/7	0.22	1.55	98,98,98,98	0
86	OHX	o4	203	7/7	0.31	1.54	104,104,104,104	0
87	ZN	D7	101	1/1	0.34	1.54	133,133,133,133	0
85	MG	1	3648	1/1	0.18	1.52	35,35,35,35	0
85	MG	5	3532	1/1	0.17	1.51	39,39,39,39	0
86	OHX	2	2034	7/7	0.19	1.51	88,88,88,88	0
85	MG	5	3589	1/1	0.20	1.49	33,33,33,33	0
86	OHX	5	4243	7/7	0.26	1.49	109,109,109,109	0
85	MG	1	3767	1/1	0.19	1.48	50,50,50,50	0
86	OHX	1	4079	7/7	0.19	1.48	99,99,99,99	0
85	MG	6	2031	1/1	0.20	1.48	59,59,59,59	0
85	MG	6	1953	1/1	0.38	1.48	55,55,55,55	0
85	MG	5	3509	1/1	0.25	1.47	22,22,22,22	0
85	MG	5	3811	1/1	0.18	1.47	29,29,29,29	0
85	MG	5	3414	1/1	0.19	1.46	39,39,39,39	0
86	OHX	1	3876	7/7	0.17	1.46	50,50,50,50	0
86	OHX	5	3940	7/7	0.18	1.44	69,69,69,69	0
85	MG	1	3768	1/1	0.16	1.44	45,45,45,45	0
85	MG	3	211	1/1	0.22	1.44	62,62,62,62	0
85	MG	5	3709	1/1	0.22	1.44	74,74,74,74	0
85	MG	1	3661	1/1	0.25	1.43	30,30,30,30	0
86	OHX	6	2185	7/7	0.16	1.41	143,143,143,143	0
85	MG	2	1993	1/1	0.27	1.41	46,46,46,46	0
85	MG	1	3736	1/1	0.19	1.41	32,32,32,32	0
85	MG	6	2014	1/1	0.20	1.40	53,53,53,53	0
85	MG	5	3493	1/1	0.22	1.40	21,21,21,21	0
86	OHX	5	4207	7/7	0.42	1.39	89,89,89,89	0
85	MG	5	3762	1/1	0.17	1.39	34,34,34,34	0
85	MG	8	209	1/1	0.18	1.38	56,56,56,56	0
85	MG	5	3842	1/1	0.23	1.38	42,42,42,42	0
86	OHX	5	4204	7/7	0.42	1.38	111,111,111,111	0
85	MG	1	3553	1/1	0.21	1.37	46,46,46,46	0
86	OHX	1	4182	7/7	0.35	1.37	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2087	7/7	0.22	1.36	93,93,93,93	0
86	OHX	1	4152	7/7	0.21	1.36	124,124,124,124	0
86	OHX	2	2166	7/7	0.14	1.35	144,144,144,144	0
86	OHX	15	306	7/7	0.24	1.34	114,114,114,114	0
85	MG	5	3713	1/1	0.18	1.33	41,41,41,41	0
86	OHX	1	4060	7/7	0.21	1.33	77,77,77,77	0
86	OHX	2	2113	7/7	0.26	1.32	108,108,108,108	0
85	MG	5	3405	1/1	0.19	1.32	18,18,18,18	0
85	MG	2	2004	1/1	0.17	1.32	67,67,67,67	0
85	MG	m7	204	1/1	0.22	1.32	36,36,36,36	0
86	OHX	6	2133	7/7	0.21	1.31	126,126,126,126	0
86	OHX	5	3999	7/7	0.17	1.31	91,91,91,91	0
85	MG	1	3612	1/1	0.16	1.30	37,37,37,37	0
85	MG	2	2001	1/1	0.18	1.30	63,63,63,63	0
86	OHX	5	4053	7/7	0.19	1.29	80,80,80,80	0
86	OHX	M7	208	7/7	0.36	1.29	109,109,109,109	0
86	OHX	7	224	7/7	0.19	1.27	92,92,92,92	0
85	MG	2	1912	1/1	0.21	1.27	53,53,53,53	0
86	OHX	1	4190	7/7	0.22	1.26	115,115,115,115	0
85	MG	5	3868	1/1	0.66	1.26	32,32,32,32	0
86	OHX	1	4198	7/7	0.24	1.25	125,125,125,125	0
85	MG	1	3832	1/1	0.39	1.25	31,31,31,31	0
86	OHX	5	4205	7/7	0.26	1.24	113,113,113,113	0
85	MG	1	3555	1/1	0.30	1.23	25,25,25,25	0
86	OHX	1	4151	7/7	0.18	1.22	113,113,113,113	0
86	OHX	1	3894	7/7	0.18	1.20	64,64,64,64	0
85	MG	5	3478	1/1	0.28	1.19	50,50,50,50	0
86	OHX	5	4155	7/7	0.19	1.18	111,111,111,111	0
86	OHX	5	4082	7/7	0.19	1.17	85,85,85,85	0
85	MG	6	1996	1/1	0.24	1.17	62,62,62,62	0
86	OHX	1	4046	7/7	0.21	1.17	75,75,75,75	0
85	MG	1	3842	1/1	0.22	1.16	22,22,22,22	0
86	OHX	6	2059	7/7	0.16	1.16	81,81,81,81	0
86	OHX	1	3897	7/7	0.17	1.15	60,60,60,60	0
86	OHX	5	4250	7/7	0.19	1.14	128,128,128,128	0
86	OHX	2	2108	7/7	0.19	1.14	110,110,110,110	0
85	MG	1	3797	1/1	0.20	1.14	16,16,16,16	0
85	MG	5	3656	1/1	0.17	1.14	35,35,35,35	0
86	OHX	1	4131	7/7	0.17	1.13	102,102,102,102	0
86	OHX	1	3903	7/7	0.16	1.13	68,68,68,68	0
85	MG	C3	201	1/1	0.32	1.13	56,56,56,56	0
86	OHX	6	2156	7/7	0.31	1.12	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4200	7/7	0.29	1.12	112,112,112,112	0
85	MG	2	1945	1/1	0.18	1.12	51,51,51,51	0
86	OHX	2	2116	7/7	0.26	1.12	111,111,111,111	0
86	OHX	1	4163	7/7	0.18	1.11	118,118,118,118	0
85	MG	2	1922	1/1	0.22	1.11	55,55,55,55	0
85	MG	L7	301	1/1	0.20	1.08	29,29,29,29	0
86	OHX	1	4104	7/7	0.16	1.08	119,119,119,119	0
85	MG	5	3434	1/1	0.21	1.07	24,24,24,24	0
85	MG	2	1987	1/1	0.24	1.07	91,91,91,91	0
86	OHX	1	4025	7/7	0.20	1.07	91,91,91,91	0
85	MG	5	3421	1/1	0.17	1.07	33,33,33,33	0
86	OHX	2	2092	7/7	0.21	1.05	103,103,103,103	0
85	MG	5	3805	1/1	0.19	1.05	87,87,87,87	0
86	OHX	1	3953	7/7	0.16	1.04	105,105,105,105	0
86	OHX	6	2173	7/7	0.22	1.02	116,116,116,116	0
85	MG	1	3699	1/1	0.21	1.02	31,31,31,31	0
85	MG	N5	201	1/1	0.21	1.00	61,61,61,61	0
85	MG	5	3545	1/1	0.21	1.00	42,42,42,42	0
85	MG	m1	202	1/1	0.18	1.00	49,49,49,49	0
86	OHX	6	2140	7/7	0.16	0.99	111,111,111,111	0
86	OHX	5	4059	7/7	0.18	0.98	96,96,96,96	0
85	MG	2	1970	1/1	0.22	0.98	60,60,60,60	0
86	OHX	1	4070	7/7	0.24	0.97	88,88,88,88	0
86	OHX	1	4082	7/7	0.17	0.96	93,93,93,93	0
85	MG	6	1932	1/1	0.18	0.96	37,37,37,37	0
86	OHX	5	4075	7/7	0.25	0.95	91,91,91,91	0
86	OHX	1	4194	7/7	0.20	0.95	114,114,114,114	0
86	OHX	5	4056	7/7	0.20	0.94	87,87,87,87	0
85	MG	1	3563	1/1	0.19	0.94	38,38,38,38	0
85	MG	6	1976	1/1	0.20	0.94	33,33,33,33	0
85	MG	5	3834	1/1	0.18	0.94	31,31,31,31	0
85	MG	1	3448	1/1	0.20	0.93	32,32,32,32	0
86	OHX	5	3939	7/7	0.18	0.92	76,76,76,76	0
85	MG	1	3838	1/1	0.23	0.92	43,43,43,43	0
86	OHX	1	4034	7/7	0.21	0.91	86,86,86,86	0
85	MG	1	3635	1/1	0.28	0.91	55,55,55,55	0
85	MG	2	1976	1/1	0.23	0.91	43,43,43,43	0
86	OHX	2	2122	7/7	0.18	0.90	116,116,116,116	0
86	OHX	2	2169	7/7	0.21	0.90	96,96,96,96	0
85	MG	6	2009	1/1	0.18	0.90	40,40,40,40	0
85	MG	1	3457	1/1	0.20	0.90	21,21,21,21	0
86	OHX	7	226	7/7	0.18	0.89	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4223	7/7	0.30	0.88	117,117,117,117	0
86	OHX	6	2050	7/7	0.18	0.87	60,60,60,60	0
85	MG	c8	202	1/1	0.30	0.87	54,54,54,54	0
85	MG	8	205	1/1	0.21	0.86	59,59,59,59	0
85	MG	5	3851	1/1	0.20	0.85	46,46,46,46	0
86	OHX	6	2051	7/7	0.17	0.84	60,60,60,60	0
85	MG	1	3781	1/1	0.18	0.84	39,39,39,39	0
86	OHX	1	4039	7/7	0.19	0.83	98,98,98,98	0
85	MG	5	3614	1/1	0.19	0.83	32,32,32,32	0
86	OHX	5	4107	7/7	0.23	0.83	103,103,103,103	0
85	MG	4	219	1/1	0.18	0.82	45,45,45,45	0
86	OHX	5	4072	7/7	0.16	0.82	96,96,96,96	0
85	MG	5	3420	1/1	0.24	0.82	29,29,29,29	0
86	OHX	5	4106	7/7	0.20	0.82	88,88,88,88	0
86	OHX	5	4187	7/7	0.21	0.81	97,97,97,97	0
85	MG	6	1941	1/1	0.21	0.81	41,41,41,41	0
85	MG	1	3701	1/1	0.19	0.80	34,34,34,34	0
86	OHX	2	2085	7/7	0.19	0.80	95,95,95,95	0
86	OHX	2	2041	7/7	0.17	0.78	85,85,85,85	0
86	OHX	5	3914	7/7	0.18	0.78	53,53,53,53	0
86	OHX	2	2135	7/7	0.23	0.78	108,108,108,108	0
86	OHX	1	4037	7/7	0.20	0.78	86,86,86,86	0
86	OHX	2	2141	7/7	0.17	0.77	133,133,133,133	0
85	MG	1	3755	1/1	0.18	0.77	18,18,18,18	0
86	OHX	5	3901	7/7	0.18	0.77	37,37,37,37	0
85	MG	5	3889	1/1	0.18	0.77	31,31,31,31	0
86	OHX	1	4084	7/7	0.21	0.76	89,89,89,89	0
86	OHX	5	4076	7/7	0.20	0.76	99,99,99,99	0
85	MG	2	1902	1/1	0.20	0.76	34,34,34,34	0
85	MG	5	3784	1/1	0.20	0.76	22,22,22,22	0
85	MG	4	204	1/1	0.35	0.76	60,60,60,60	0
85	MG	15	302	1/1	0.29	0.75	54,54,54,54	0
86	OHX	2	2127	7/7	0.17	0.74	115,115,115,115	0
85	MG	2	1920	1/1	0.31	0.74	48,48,48,48	0
86	OHX	4	234	7/7	0.29	0.74	116,116,116,116	0
86	OHX	1	4083	7/7	0.24	0.72	100,100,100,100	0
85	MG	5	3798	1/1	0.18	0.72	62,62,62,62	0
85	MG	1	3557	1/1	0.18	0.72	38,38,38,38	0
85	MG	1	3778	1/1	0.21	0.70	41,41,41,41	0
85	MG	m7	203	1/1	0.24	0.70	26,26,26,26	0
86	OHX	5	3926	7/7	0.19	0.69	59,59,59,59	0
86	OHX	1	4092	7/7	0.39	0.67	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2124	7/7	0.17	0.67	87,87,87,87	0
85	MG	m7	202	1/1	0.26	0.66	25,25,25,25	0
85	MG	5	3879	1/1	0.18	0.65	26,26,26,26	0
86	OHX	6	2170	7/7	0.19	0.64	117,117,117,117	0
85	MG	5	3552	1/1	0.26	0.63	23,23,23,23	0
85	MG	1	3800	1/1	0.19	0.63	42,42,42,42	0
85	MG	d2	201	1/1	0.23	0.63	55,55,55,55	0
85	MG	5	3742	1/1	0.35	0.62	32,32,32,32	0
85	MG	5	3768	1/1	0.26	0.62	36,36,36,36	0
85	MG	5	3504	1/1	0.21	0.61	26,26,26,26	0
86	OHX	5	4226	7/7	0.23	0.61	130,130,130,130	0
85	MG	1	3758	1/1	0.23	0.60	23,23,23,23	0
85	MG	5	3487	1/1	0.21	0.59	23,23,23,23	0
86	OHX	5	4162	7/7	0.17	0.59	115,115,115,115	0
86	OHX	2	2105	7/7	0.21	0.59	97,97,97,97	0
85	MG	5	3775	1/1	0.18	0.59	21,21,21,21	0
86	OHX	1	3870	7/7	0.18	0.59	35,35,35,35	0
85	MG	5	3604	1/1	0.17	0.59	33,33,33,33	0
86	OHX	2	2128	7/7	0.32	0.58	107,107,107,107	0
85	MG	5	3497	1/1	0.20	0.58	21,21,21,21	0
85	MG	5	3658	1/1	0.17	0.58	38,38,38,38	0
85	MG	1	3443	1/1	0.20	0.58	65,65,65,65	0
86	OHX	2	2120	7/7	0.20	0.57	111,111,111,111	0
85	MG	1	3488	1/1	0.23	0.57	42,42,42,42	0
86	OHX	5	4019	7/7	0.18	0.55	84,84,84,84	0
85	MG	1	3651	1/1	0.20	0.53	51,51,51,51	0
86	OHX	5	4113	7/7	0.19	0.51	92,92,92,92	0
85	MG	5	3501	1/1	0.19	0.51	30,30,30,30	0
87	ZN	q0	201	1/1	0.19	0.51	23,23,23,23	0
85	MG	6	2036	1/1	0.30	0.51	62,62,62,62	0
85	MG	2	1916	1/1	0.22	0.50	44,44,44,44	0
85	MG	1	3617	1/1	0.20	0.50	48,48,48,48	0
86	OHX	6	2201	7/7	0.25	0.50	116,116,116,116	0
85	MG	M7	202	1/1	0.26	0.48	26,26,26,26	0
86	OHX	5	4122	7/7	0.17	0.48	114,114,114,114	0
86	OHX	1	3901	7/7	0.17	0.48	65,65,65,65	0
85	MG	1	3668	1/1	0.18	0.48	43,43,43,43	0
85	MG	1	3697	1/1	0.19	0.47	45,45,45,45	0
86	OHX	2	2129	7/7	0.14	0.47	121,121,121,121	0
86	OHX	2	2140	7/7	0.16	0.47	125,125,125,125	0
86	OHX	1	3878	7/7	0.17	0.47	51,51,51,51	0
85	MG	2	2016	1/1	0.31	0.46	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4198	7/7	0.20	0.46	98,98,98,98	0
85	MG	6	2205	1/1	0.21	0.46	42,42,42,42	0
86	OHX	5	3931	7/7	0.17	0.45	60,60,60,60	0
85	MG	1	3511	1/1	0.19	0.45	21,21,21,21	0
86	OHX	8	226	7/7	0.14	0.45	115,115,115,115	0
86	OHX	s1	303	7/7	0.25	0.42	128,128,128,128	0
86	OHX	2	2038	7/7	0.15	0.39	97,97,97,97	0
85	MG	5	3550	1/1	0.23	0.39	36,36,36,36	0
85	MG	5	3451	1/1	0.19	0.38	25,25,25,25	0
85	MG	1	3582	1/1	0.28	0.38	30,30,30,30	0
85	MG	5	3556	1/1	0.20	0.36	36,36,36,36	0
86	OHX	2	2181	7/7	0.27	0.36	130,130,130,130	0
85	MG	2	1980	1/1	0.20	0.36	55,55,55,55	0
85	MG	5	3631	1/1	0.22	0.35	33,33,33,33	0
86	OHX	2	2152	7/7	0.14	0.34	145,145,145,145	0
85	MG	L4	401	1/1	0.17	0.34	32,32,32,32	0
86	OHX	5	4231	7/7	0.17	0.34	137,137,137,137	0
86	OHX	5	4102	7/7	0.17	0.34	82,82,82,82	0
85	MG	1	3693	1/1	0.21	0.34	36,36,36,36	0
85	MG	2	2006	1/1	0.20	0.33	45,45,45,45	0
85	MG	1	3473	1/1	0.21	0.33	18,18,18,18	0
85	MG	5	3722	1/1	0.18	0.33	39,39,39,39	0
86	OHX	2	2148	7/7	0.18	0.33	142,142,142,142	0
85	MG	6	1992	1/1	0.17	0.32	40,40,40,40	0
86	OHX	5	4167	7/7	0.21	0.31	108,108,108,108	0
86	OHX	1	4153	7/7	0.16	0.31	92,92,92,92	0
85	MG	5	3696	1/1	0.18	0.31	36,36,36,36	0
85	MG	6	2003	1/1	0.19	0.31	60,60,60,60	0
85	MG	5	3536	1/1	0.21	0.30	27,27,27,27	0
85	MG	5	3829	1/1	0.21	0.30	59,59,59,59	0
85	MG	5	3745	1/1	0.17	0.30	33,33,33,33	0
85	MG	1	3430	1/1	0.21	0.30	41,41,41,41	0
85	MG	5	3657	1/1	0.21	0.30	30,30,30,30	0
86	OHX	s1	302	7/7	0.18	0.29	67,67,67,67	0
86	OHX	6	2172	7/7	0.23	0.29	114,114,114,114	0
86	OHX	5	4249	7/7	0.17	0.28	109,109,109,109	0
86	OHX	6	2182	7/7	0.30	0.28	109,109,109,109	0
85	MG	5	3789	1/1	0.42	0.28	36,36,36,36	0
86	OHX	5	4143	7/7	0.20	0.27	106,106,106,106	0
85	MG	1	3656	1/1	0.19	0.27	39,39,39,39	0
86	OHX	1	4207	7/7	0.21	0.26	111,111,111,111	0
86	OHX	1	4091	7/7	0.22	0.26	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	N8	202	1/1	0.23	0.25	37,37,37,37	0
86	OHX	5	4174	7/7	0.21	0.25	109,109,109,109	0
86	OHX	5	4237	7/7	0.14	0.25	116,116,116,116	0
85	MG	1	3501	1/1	0.25	0.24	22,22,22,22	0
85	MG	1	3534	1/1	0.28	0.24	31,31,31,31	0
86	OHX	5	4091	7/7	0.19	0.23	92,92,92,92	0
85	MG	5	3495	1/1	0.19	0.23	26,26,26,26	0
85	MG	1	3696	1/1	0.15	0.23	35,35,35,35	0
85	MG	M3	203	1/1	0.36	0.23	79,79,79,79	0
85	MG	6	1967	1/1	0.19	0.23	59,59,59,59	0
87	ZN	Q0	500	1/1	0.18	0.23	35,35,35,35	0
85	MG	1	3411	1/1	0.21	0.22	33,33,33,33	0
86	OHX	2	2112	7/7	0.16	0.22	130,130,130,130	0
86	OHX	5	4232	7/7	0.18	0.22	82,82,82,82	0
86	OHX	5	4224	7/7	0.22	0.22	113,113,113,113	0
86	OHX	1	4094	7/7	0.17	0.21	129,129,129,129	0
86	OHX	1	4058	7/7	0.18	0.21	80,80,80,80	0
85	MG	6	1990	1/1	0.21	0.20	58,58,58,58	0
86	OHX	1	4068	7/7	0.23	0.20	78,78,78,78	0
86	OHX	1	4108	7/7	0.18	0.20	97,97,97,97	0
86	OHX	8	221	7/7	0.21	0.20	95,95,95,95	0
85	MG	5	3754	1/1	0.23	0.19	38,38,38,38	0
85	MG	1	3483	1/1	0.23	0.19	39,39,39,39	0
86	OHX	2	2162	7/7	0.21	0.19	126,126,126,126	0
86	OHX	1	3882	7/7	0.16	0.18	53,53,53,53	0
85	MG	1	3567	1/1	0.29	0.18	24,24,24,24	0
85	MG	1	3727	1/1	0.16	0.18	51,51,51,51	0
85	MG	2	1988	1/1	0.23	0.17	62,62,62,62	0
86	OHX	5	4049	7/7	0.20	0.16	83,83,83,83	0
86	OHX	6	2066	7/7	0.16	0.16	94,94,94,94	0
85	MG	1	3822	1/1	0.15	0.16	48,48,48,48	0
85	MG	1	3675	1/1	0.18	0.16	18,18,18,18	0
86	OHX	6	2145	7/7	0.22	0.14	110,110,110,110	0
85	MG	1	3421	1/1	0.23	0.14	37,37,37,37	0
85	MG	5	3402	1/1	0.18	0.13	16,16,16,16	0
85	MG	4	207	1/1	0.23	0.13	32,32,32,32	0
86	OHX	5	4121	7/7	0.17	0.12	111,111,111,111	0
86	OHX	s4	301	7/7	0.17	0.11	122,122,122,122	0
86	OHX	5	3932	7/7	0.18	0.11	77,77,77,77	0
86	OHX	6	2159	7/7	0.27	0.11	96,96,96,96	0
85	MG	1	3570	1/1	0.19	0.11	13,13,13,13	0
85	MG	1	3467	1/1	0.18	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3871	7/7	0.19	0.10	43,43,43,43	0
85	MG	6	2004	1/1	0.19	0.09	62,62,62,62	0
86	OHX	2	2100	7/7	0.16	0.08	115,115,115,115	0
86	OHX	1	4213	7/7	0.21	0.08	128,128,128,128	0
85	MG	6	1972	1/1	0.17	0.07	46,46,46,46	0
86	OHX	L3	404	7/7	0.28	0.07	128,128,128,128	0
86	OHX	5	3902	7/7	0.20	0.07	43,43,43,43	0
85	MG	5	3645	1/1	0.21	0.07	47,47,47,47	0
86	OHX	5	4242	7/7	0.19	0.07	124,124,124,124	0
86	OHX	O3	202	7/7	0.18	0.07	91,91,91,91	0
85	MG	2	2022	1/1	0.16	0.06	66,66,66,66	0
86	OHX	1	3957	7/7	0.16	0.06	80,80,80,80	0
86	OHX	5	4037	7/7	0.20	0.06	94,94,94,94	0
86	OHX	6	2148	7/7	0.17	0.06	108,108,108,108	0
85	MG	1	3415	1/1	0.24	0.05	36,36,36,36	0
85	MG	5	3822	1/1	0.23	0.05	78,78,78,78	0
86	OHX	2	2115	7/7	0.17	0.04	100,100,100,100	0
85	MG	5	3758	1/1	0.19	0.04	46,46,46,46	0
85	MG	5	3635	1/1	0.19	0.04	39,39,39,39	0
85	MG	1	3461	1/1	0.19	0.03	20,20,20,20	0
85	MG	2	1941	1/1	0.17	0.03	50,50,50,50	0
86	OHX	2	2093	7/7	0.21	0.02	94,94,94,94	0
86	OHX	5	3904	7/7	0.18	0.01	47,47,47,47	0
86	OHX	C8	201	7/7	0.16	0.01	91,91,91,91	0
86	OHX	d9	102	7/7	0.20	0.01	117,117,117,117	0
86	OHX	1	4020	7/7	0.14	0.00	127,127,127,127	0
85	MG	5	3728	1/1	0.19	-0.00	20,20,20,20	0
85	MG	1	3819	1/1	0.23	-0.01	42,42,42,42	0
85	MG	5	3885	1/1	0.24	-0.01	59,59,59,59	0
86	OHX	5	4241	7/7	0.34	-0.01	81,81,81,81	0
86	OHX	2	2139	7/7	0.16	-0.01	112,112,112,112	0
85	MG	1	3503	1/1	0.18	-0.02	17,17,17,17	0
85	MG	n0	202	1/1	0.18	-0.02	32,32,32,32	0
86	OHX	1	4186	7/7	0.16	-0.02	120,120,120,120	0
85	MG	Q2	502	1/1	0.17	-0.03	50,50,50,50	0
85	MG	1	3425	1/1	0.22	-0.05	21,21,21,21	0
86	OHX	S8	302	7/7	0.24	-0.05	126,126,126,126	0
86	OHX	5	4052	7/7	0.17	-0.07	83,83,83,83	0
86	OHX	2	2150	7/7	0.18	-0.07	134,134,134,134	0
85	MG	2	1992	1/1	0.35	-0.07	50,50,50,50	0
86	OHX	5	4074	7/7	0.18	-0.08	93,93,93,93	0
86	OHX	5	4042	7/7	0.17	-0.08	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4109	7/7	0.30	-0.09	93,93,93,93	0
86	OHX	L4	404	7/7	0.20	-0.11	103,103,103,103	0
85	MG	1	3688	1/1	0.16	-0.11	39,39,39,39	0
86	OHX	1	4105	7/7	0.29	-0.11	101,101,101,101	0
85	MG	5	3486	1/1	0.28	-0.11	28,28,28,28	0
86	OHX	1	4063	7/7	0.18	-0.11	102,102,102,102	0
85	MG	5	3602	1/1	0.19	-0.11	40,40,40,40	0
85	MG	1	3765	1/1	0.18	-0.13	40,40,40,40	0
85	MG	o3	201	1/1	0.19	-0.13	40,40,40,40	0
86	OHX	3	226	7/7	0.15	-0.13	113,113,113,113	0
86	OHX	1	4041	7/7	0.18	-0.14	85,85,85,85	0
85	MG	5	3723	1/1	0.18	-0.16	32,32,32,32	0
86	OHX	2	2171	7/7	0.15	-0.16	110,110,110,110	0
86	OHX	s8	303	7/7	0.28	-0.16	129,129,129,129	0
85	MG	5	3454	1/1	0.15	-0.16	37,37,37,37	0
86	OHX	2	2178	7/7	0.27	-0.16	141,141,141,141	0
86	OHX	2	2110	7/7	0.14	-0.17	113,113,113,113	0
86	OHX	1	4106	7/7	0.16	-0.17	113,113,113,113	0
85	MG	1	3437	1/1	0.19	-0.18	22,22,22,22	0
86	OHX	6	2117	7/7	0.17	-0.19	108,108,108,108	0
85	MG	5	3404	1/1	0.18	-0.20	32,32,32,32	0
85	MG	2	1966	1/1	0.20	-0.20	49,49,49,49	0
86	OHX	1	3996	7/7	0.22	-0.21	93,93,93,93	0
86	OHX	d4	201	7/7	0.20	-0.21	120,120,120,120	0
86	OHX	2	2168	7/7	0.15	-0.21	135,135,135,135	0
86	OHX	1	3932	7/7	0.16	-0.22	82,82,82,82	0
85	MG	5	3791	1/1	0.19	-0.23	74,74,74,74	0
86	OHX	6	2125	7/7	0.16	-0.23	106,106,106,106	0
85	MG	2	1991	1/1	0.28	-0.23	102,102,102,102	0
85	MG	1	3807	1/1	0.18	-0.23	26,26,26,26	0
86	OHX	6	2137	7/7	0.23	-0.24	101,101,101,101	0
86	OHX	2	2125	7/7	0.20	-0.24	120,120,120,120	0
86	OHX	l3	404	7/7	0.20	-0.24	112,112,112,112	0
86	OHX	1	3888	7/7	0.15	-0.25	56,56,56,56	0
86	OHX	m1	203	7/7	0.31	-0.25	124,124,124,124	0
86	OHX	m0	302	7/7	0.28	-0.26	96,96,96,96	0
85	MG	6	2023	1/1	0.15	-0.26	41,41,41,41	0
86	OHX	1	4143	7/7	0.16	-0.26	107,107,107,107	0
85	MG	2	1948	1/1	0.28	-0.27	57,57,57,57	0
85	MG	n9	3801	1/1	0.18	-0.27	24,24,24,24	0
85	MG	5	3690	1/1	0.16	-0.27	36,36,36,36	0
86	OHX	5	3997	7/7	0.15	-0.28	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3554	1/1	0.17	-0.28	31,31,31,31	0
86	OHX	5	3949	7/7	0.15	-0.28	84,84,84,84	0
86	OHX	6	2047	7/7	0.18	-0.29	47,47,47,47	0
86	OHX	5	4090	7/7	0.19	-0.31	79,79,79,79	0
86	OHX	1	4093	7/7	0.14	-0.31	109,109,109,109	0
86	OHX	2	2025	7/7	0.16	-0.31	66,66,66,66	0
86	OHX	1	4126	7/7	0.16	-0.31	110,110,110,110	0
85	MG	L8	301	1/1	0.31	-0.32	54,54,54,54	0
86	OHX	5	3988	7/7	0.13	-0.33	97,97,97,97	0
85	MG	4	209	1/1	0.19	-0.33	37,37,37,37	0
86	OHX	5	4081	7/7	0.18	-0.33	87,87,87,87	0
86	OHX	5	4117	7/7	0.17	-0.33	96,96,96,96	0
86	OHX	1	4090	7/7	0.17	-0.33	102,102,102,102	0
86	OHX	n9	3803	7/7	0.17	-0.33	52,52,52,52	0
86	OHX	6	2074	7/7	0.13	-0.34	103,103,103,103	0
85	MG	5	3460	1/1	0.19	-0.34	24,24,24,24	0
85	MG	6	1905	1/1	0.19	-0.36	49,49,49,49	0
85	MG	O4	201	1/1	0.20	-0.36	45,45,45,45	0
85	MG	1	3621	1/1	0.17	-0.37	32,32,32,32	0
85	MG	6	1988	1/1	0.17	-0.37	36,36,36,36	0
85	MG	1	3754	1/1	0.17	-0.37	29,29,29,29	0
85	MG	5	3609	1/1	0.20	-0.37	24,24,24,24	0
86	OHX	1	3988	7/7	0.17	-0.37	73,73,73,73	0
86	OHX	1	4134	7/7	0.17	-0.37	127,127,127,127	0
85	MG	1	3659	1/1	0.29	-0.38	49,49,49,49	0
85	MG	1	3689	1/1	0.20	-0.39	25,25,25,25	0
86	OHX	6	2192	7/7	0.16	-0.39	130,130,130,130	0
86	OHX	5	4029	7/7	0.18	-0.39	76,76,76,76	0
85	MG	1	3855	1/1	0.16	-0.40	41,41,41,41	0
86	OHX	6	2179	7/7	0.16	-0.40	123,123,123,123	0
86	OHX	6	2158	7/7	0.15	-0.41	112,112,112,112	0
85	MG	d6	102	1/1	0.25	-0.41	47,47,47,47	0
85	MG	q1	101	1/1	0.18	-0.41	39,39,39,39	0
86	OHX	5	3974	7/7	0.17	-0.42	89,89,89,89	0
86	OHX	5	4180	7/7	0.18	-0.42	120,120,120,120	0
86	OHX	5	4120	7/7	0.14	-0.42	118,118,118,118	0
85	MG	1	3867	1/1	0.18	-0.42	21,21,21,21	0
85	MG	5	3494	1/1	0.19	-0.42	23,23,23,23	0
86	OHX	1	4159	7/7	0.15	-0.43	92,92,92,92	0
86	OHX	6	2049	7/7	0.17	-0.43	51,51,51,51	0
86	OHX	5	4041	7/7	0.16	-0.43	126,126,126,126	0
86	OHX	1	3981	7/7	0.18	-0.43	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	D9	102	7/7	0.19	-0.43	109,109,109,109	0
85	MG	6	1981	1/1	0.23	-0.44	47,47,47,47	0
86	OHX	1	4005	7/7	0.20	-0.44	79,79,79,79	0
86	OHX	2	2132	7/7	0.15	-0.44	103,103,103,103	0
86	OHX	5	4178	7/7	0.12	-0.44	126,126,126,126	0
85	MG	2	1940	1/1	0.16	-0.45	53,53,53,53	0
85	MG	M1	201	1/1	0.19	-0.45	61,61,61,61	0
85	MG	n6	201	1/1	0.24	-0.45	52,52,52,52	0
85	MG	M7	203	1/1	0.21	-0.46	28,28,28,28	0
85	MG	1	3455	1/1	0.19	-0.46	45,45,45,45	0
85	MG	5	3406	1/1	0.17	-0.46	26,26,26,26	0
86	OHX	2	2070	7/7	0.18	-0.46	89,89,89,89	0
85	MG	8	211	1/1	0.17	-0.46	79,79,79,79	0
85	MG	m6	201	1/1	0.17	-0.46	25,25,25,25	0
86	OHX	1	3869	7/7	0.17	-0.46	38,38,38,38	0
85	MG	5	3675	1/1	0.16	-0.46	28,28,28,28	0
86	OHX	6	2146	7/7	0.17	-0.47	109,109,109,109	0
85	MG	s8	301	1/1	0.17	-0.47	45,45,45,45	0
85	MG	5	3810	1/1	0.21	-0.47	32,32,32,32	0
86	OHX	5	4079	7/7	0.19	-0.48	99,99,99,99	0
86	OHX	1	4147	7/7	0.20	-0.48	120,120,120,120	0
85	MG	1	3837	1/1	0.17	-0.49	30,30,30,30	0
86	OHX	1	4137	7/7	0.18	-0.50	89,89,89,89	0
85	MG	1	3641	1/1	0.16	-0.51	32,32,32,32	0
85	MG	2	1973	1/1	0.18	-0.52	57,57,57,57	0
85	MG	2	2000	1/1	0.16	-0.52	53,53,53,53	0
86	OHX	1	3909	7/7	0.15	-0.53	70,70,70,70	0
85	MG	1	3554	1/1	0.20	-0.53	21,21,21,21	0
85	MG	1	3698	1/1	0.17	-0.53	62,62,62,62	0
85	MG	L3	401	1/1	0.16	-0.54	28,28,28,28	0
86	OHX	5	4033	7/7	0.18	-0.54	85,85,85,85	0
85	MG	1	3824	1/1	0.14	-0.54	50,50,50,50	0
86	OHX	5	4078	7/7	0.18	-0.55	78,78,78,78	0
85	MG	5	3744	1/1	0.15	-0.55	25,25,25,25	0
86	OHX	C1	201	7/7	0.17	-0.55	101,101,101,101	0
86	OHX	1	4000	7/7	0.18	-0.56	82,82,82,82	0
85	MG	5	3491	1/1	0.15	-0.56	34,34,34,34	0
85	MG	5	3480	1/1	0.18	-0.56	29,29,29,29	0
86	OHX	5	3905	7/7	0.17	-0.56	45,45,45,45	0
86	OHX	5	4165	7/7	0.16	-0.57	102,102,102,102	0
86	OHX	6	2134	7/7	0.17	-0.57	101,101,101,101	0
85	MG	4	208	1/1	0.16	-0.57	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4127	7/7	0.15	-0.57	120,120,120,120	0
85	MG	q3	502	1/1	0.22	-0.57	45,45,45,45	0
86	OHX	2	2033	7/7	0.16	-0.58	75,75,75,75	0
86	OHX	6	2112	7/7	0.17	-0.58	99,99,99,99	0
85	MG	1	3788	1/1	0.17	-0.58	48,48,48,48	0
85	MG	M3	204	1/1	0.23	-0.59	24,24,24,24	0
85	MG	5	3865	1/1	0.17	-0.61	38,38,38,38	0
86	OHX	2	2086	7/7	0.13	-0.61	112,112,112,112	0
86	OHX	5	3973	7/7	0.12	-0.62	62,62,62,62	0
87	ZN	d9	101	1/1	0.13	-0.62	60,60,60,60	0
85	MG	M0	301	1/1	0.16	-0.62	25,25,25,25	0
86	OHX	6	2064	7/7	0.15	-0.63	80,80,80,80	0
85	MG	1	3683	1/1	0.16	-0.63	32,32,32,32	0
86	OHX	1	3922	7/7	0.14	-0.64	77,77,77,77	0
85	MG	5	3621	1/1	0.17	-0.64	46,46,46,46	0
85	MG	N8	201	1/1	0.16	-0.64	26,26,26,26	0
85	MG	5	3669	1/1	0.15	-0.64	26,26,26,26	0
85	MG	6	1993	1/1	0.16	-0.64	42,42,42,42	0
85	MG	5	3863	1/1	0.16	-0.65	44,44,44,44	0
86	OHX	19	600	7/7	0.15	-0.65	105,105,105,105	0
85	MG	5	3735	1/1	0.16	-0.65	31,31,31,31	0
86	OHX	1	4008	7/7	0.17	-0.65	99,99,99,99	0
86	OHX	15	305	7/7	0.18	-0.65	112,112,112,112	0
86	OHX	1	4120	7/7	0.16	-0.65	105,105,105,105	0
85	MG	5	3752	1/1	0.15	-0.66	36,36,36,36	0
85	MG	6	2006	1/1	0.15	-0.67	46,46,46,46	0
86	OHX	6	2139	7/7	0.14	-0.67	106,106,106,106	0
85	MG	5	3685	1/1	0.14	-0.68	37,37,37,37	0
85	MG	1	4222	1/1	0.14	-0.68	45,45,45,45	0
85	MG	5	4258	1/1	0.18	-0.68	29,29,29,29	0
85	MG	1	3489	1/1	0.17	-0.68	22,22,22,22	0
86	OHX	5	3948	7/7	0.14	-0.69	85,85,85,85	0
85	MG	5	3642	1/1	0.17	-0.70	27,27,27,27	0
86	OHX	6	2143	7/7	0.14	-0.70	117,117,117,117	0
86	OHX	5	4116	7/7	0.18	-0.71	82,82,82,82	0
85	MG	5	3797	1/1	0.18	-0.71	33,33,33,33	0
85	MG	S8	301	1/1	0.16	-0.71	51,51,51,51	0
86	OHX	5	4100	7/7	0.13	-0.71	100,100,100,100	0
86	OHX	2	2107	7/7	0.13	-0.72	96,96,96,96	0
85	MG	5	3866	1/1	0.14	-0.72	31,31,31,31	0
85	MG	L4	403	1/1	0.23	-0.72	25,25,25,25	0
86	OHX	1	3880	7/7	0.16	-0.72	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3873	7/7	0.18	-0.73	42,42,42,42	0
86	OHX	2	2101	7/7	0.12	-0.73	116,116,116,116	0
85	MG	1	3620	1/1	0.15	-0.73	55,55,55,55	0
86	OHX	1	4096	7/7	0.14	-0.74	123,123,123,123	0
86	OHX	sR	401	7/7	0.14	-0.74	135,135,135,135	0
86	OHX	1	4107	7/7	0.16	-0.74	98,98,98,98	0
86	OHX	6	2152	7/7	0.16	-0.74	126,126,126,126	0
85	MG	5	3418	1/1	0.17	-0.74	59,59,59,59	0
85	MG	2	1947	1/1	0.18	-0.75	50,50,50,50	0
86	OHX	1	3943	7/7	0.14	-0.75	92,92,92,92	0
86	OHX	2	2058	7/7	0.16	-0.75	103,103,103,103	0
86	OHX	1	4196	7/7	0.14	-0.75	149,149,149,149	0
86	OHX	2	2143	7/7	0.14	-0.75	113,113,113,113	0
85	MG	n0	201	1/1	0.17	-0.76	33,33,33,33	0
85	MG	5	3897	1/1	0.17	-0.78	44,44,44,44	0
85	MG	1	3403	1/1	0.17	-0.78	27,27,27,27	0
85	MG	1	3633	1/1	0.15	-0.78	35,35,35,35	0
85	MG	5	3691	1/1	0.14	-0.79	38,38,38,38	0
85	MG	L6	201	1/1	0.15	-0.79	35,35,35,35	0
85	MG	M6	201	1/1	0.18	-0.79	39,39,39,39	0
86	OHX	N9	101	7/7	0.17	-0.80	48,48,48,48	0
86	OHX	5	3921	7/7	0.16	-0.80	49,49,49,49	0
86	OHX	8	223	7/7	0.17	-0.81	99,99,99,99	0
85	MG	sM	302	1/1	0.16	-0.81	31,31,31,31	0
86	OHX	1	4072	7/7	0.14	-0.82	103,103,103,103	0
85	MG	5	3816	1/1	0.14	-0.82	37,37,37,37	0
86	OHX	1	3930	7/7	0.14	-0.82	90,90,90,90	0
85	MG	7	210	1/1	0.15	-0.82	28,28,28,28	0
85	MG	5	3753	1/1	0.16	-0.82	42,42,42,42	0
85	MG	5	3893	1/1	0.12	-0.83	95,95,95,95	0
86	OHX	2	2030	7/7	0.15	-0.83	80,80,80,80	0
85	MG	n6	202	1/1	0.17	-0.83	34,34,34,34	0
86	OHX	1	4042	7/7	0.14	-0.83	97,97,97,97	0
86	OHX	1	4047	7/7	0.13	-0.84	85,85,85,85	0
85	MG	l5	303	1/1	0.15	-0.84	51,51,51,51	0
86	OHX	6	2107	7/7	0.17	-0.84	96,96,96,96	0
85	MG	5	3705	1/1	0.16	-0.85	41,41,41,41	0
86	OHX	5	3965	7/7	0.15	-0.85	82,82,82,82	0
86	OHX	2	2145	7/7	0.13	-0.85	133,133,133,133	0
86	OHX	5	3917	7/7	0.16	-0.86	49,49,49,49	0
86	OHX	1	3954	7/7	0.13	-0.86	98,98,98,98	0
85	MG	2	1982	1/1	0.22	-0.87	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3921	7/7	0.15	-0.87	79,79,79,79	0
85	MG	1	3407	1/1	0.16	-0.87	34,34,34,34	0
86	OHX	7	216	7/7	0.16	-0.88	73,73,73,73	0
85	MG	1	3486	1/1	0.14	-0.89	39,39,39,39	0
85	MG	5	3716	1/1	0.16	-0.89	44,44,44,44	0
85	MG	1	3608	1/1	0.15	-0.89	50,50,50,50	0
86	OHX	6	2167	7/7	0.12	-0.90	140,140,140,140	0
86	OHX	5	3944	7/7	0.16	-0.90	71,71,71,71	0
85	MG	4	216	1/1	0.11	-0.90	55,55,55,55	0
86	OHX	1	4164	7/7	0.18	-0.91	108,108,108,108	0
86	OHX	1	3939	7/7	0.15	-0.91	84,84,84,84	0
86	OHX	1	3966	7/7	0.13	-0.91	98,98,98,98	0
85	MG	5	3684	1/1	0.14	-0.92	61,61,61,61	0
85	MG	1	3426	1/1	0.16	-0.92	44,44,44,44	0
85	MG	5	3778	1/1	0.16	-0.93	52,52,52,52	0
86	OHX	1	4033	7/7	0.17	-0.93	103,103,103,103	0
86	OHX	5	4192	7/7	0.13	-0.94	135,135,135,135	0
86	OHX	5	4061	7/7	0.16	-0.94	80,80,80,80	0
85	MG	5	3835	1/1	0.16	-0.94	46,46,46,46	0
85	MG	1	3452	1/1	0.18	-0.95	23,23,23,23	0
86	OHX	5	3906	7/7	0.17	-0.95	49,49,49,49	0
86	OHX	5	3966	7/7	0.14	-0.96	83,83,83,83	0
85	MG	5	3845	1/1	0.15	-0.96	44,44,44,44	0
85	MG	6	2033	1/1	0.19	-0.96	45,45,45,45	0
85	MG	s8	302	1/1	0.16	-0.96	40,40,40,40	0
86	OHX	5	4031	7/7	0.11	-0.96	110,110,110,110	0
86	OHX	6	2155	7/7	0.16	-0.97	93,93,93,93	0
85	MG	5	3714	1/1	0.16	-0.97	42,42,42,42	0
86	OHX	1	3937	7/7	0.12	-0.97	88,88,88,88	0
86	OHX	14	402	7/7	0.20	-0.97	103,103,103,103	0
85	MG	1	3650	1/1	0.16	-0.98	35,35,35,35	0
86	OHX	m0	301	7/7	0.10	-0.98	105,105,105,105	0
86	OHX	8	215	7/7	0.10	-0.98	90,90,90,90	0
85	MG	1	3416	1/1	0.20	-0.99	21,21,21,21	0
86	OHX	6	2154	7/7	0.12	-0.99	117,117,117,117	0
85	MG	5	3859	1/1	0.16	-1.00	44,44,44,44	0
85	MG	1	3719	1/1	0.15	-1.00	30,30,30,30	0
85	MG	1	3547	1/1	0.17	-1.00	32,32,32,32	0
85	MG	5	3617	1/1	0.13	-1.00	32,32,32,32	0
85	MG	1	3777	1/1	0.14	-1.01	55,55,55,55	0
86	OHX	4	222	7/7	0.16	-1.01	46,46,46,46	0
86	OHX	6	2109	7/7	0.14	-1.01	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3890	1/1	0.10	-1.02	21,21,21,21	0
86	OHX	5	4119	7/7	0.15	-1.02	99,99,99,99	0
85	MG	1	4221	1/1	0.16	-1.02	36,36,36,36	0
86	OHX	5	3919	7/7	0.15	-1.02	53,53,53,53	0
85	MG	1	3714	1/1	0.18	-1.02	25,25,25,25	0
86	OHX	5	3955	7/7	0.13	-1.03	79,79,79,79	0
85	MG	5	3435	1/1	0.16	-1.03	28,28,28,28	0
85	MG	6	1902	1/1	0.16	-1.04	47,47,47,47	0
85	MG	1	3577	1/1	0.18	-1.04	17,17,17,17	0
85	MG	5	3620	1/1	0.16	-1.04	25,25,25,25	0
85	MG	5	3689	1/1	0.15	-1.04	45,45,45,45	0
87	ZN	e1	501	1/1	0.09	-1.05	130,130,130,130	0
86	OHX	2	2090	7/7	0.13	-1.05	89,89,89,89	0
85	MG	1	3445	1/1	0.17	-1.05	39,39,39,39	0
86	OHX	2	2024	7/7	0.16	-1.05	62,62,62,62	0
85	MG	1	3520	1/1	0.15	-1.06	23,23,23,23	0
86	OHX	2	2048	7/7	0.08	-1.06	104,104,104,104	0
85	MG	5	3801	1/1	0.13	-1.06	50,50,50,50	0
85	MG	1	3759	1/1	0.14	-1.06	35,35,35,35	0
86	OHX	2	2142	7/7	0.10	-1.07	127,127,127,127	0
85	MG	1	3564	1/1	0.17	-1.08	35,35,35,35	0
86	OHX	O7	103	7/7	0.10	-1.08	77,77,77,77	0
86	OHX	8	216	7/7	0.15	-1.10	86,86,86,86	0
86	OHX	1	3919	7/7	0.13	-1.10	79,79,79,79	0
85	MG	1	3782	1/1	0.14	-1.10	46,46,46,46	0
85	MG	1	3717	1/1	0.14	-1.11	56,56,56,56	0
85	MG	5	3809	1/1	0.20	-1.11	62,62,62,62	0
87	ZN	D9	101	1/1	0.10	-1.11	60,60,60,60	0
85	MG	5	4252	1/1	0.15	-1.11	25,25,25,25	0
86	OHX	2	2151	7/7	0.14	-1.11	134,134,134,134	0
86	OHX	4	229	7/7	0.10	-1.13	121,121,121,121	0
86	OHX	4	230	7/7	0.11	-1.13	113,113,113,113	0
86	OHX	1	3944	7/7	0.14	-1.14	87,87,87,87	0
86	OHX	L3	403	7/7	0.16	-1.14	90,90,90,90	0
86	OHX	2	2036	7/7	0.14	-1.15	88,88,88,88	0
86	OHX	1	3931	7/7	0.10	-1.15	68,68,68,68	0
86	OHX	Q2	503	7/7	0.16	-1.17	64,64,64,64	0
86	OHX	5	4013	7/7	0.12	-1.17	129,129,129,129	0
86	OHX	2	2043	7/7	0.10	-1.17	80,80,80,80	0
85	MG	5	3852	1/1	0.18	-1.18	58,58,58,58	0
85	MG	5	3861	1/1	0.15	-1.18	30,30,30,30	0
86	OHX	6	2132	7/7	0.15	-1.18	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3771	1/1	0.19	-1.19	55,55,55,55	0
85	MG	L3	402	1/1	0.15	-1.20	43,43,43,43	0
86	OHX	1	4075	7/7	0.15	-1.20	113,113,113,113	0
85	MG	M7	204	1/1	0.17	-1.21	27,27,27,27	0
86	OHX	5	3956	7/7	0.15	-1.21	76,76,76,76	0
86	OHX	2	2049	7/7	0.10	-1.21	94,94,94,94	0
85	MG	1	3816	1/1	0.15	-1.21	38,38,38,38	0
86	OHX	5	4026	7/7	0.16	-1.21	83,83,83,83	0
86	OHX	6	2142	7/7	0.15	-1.21	108,108,108,108	0
85	MG	6	2026	1/1	0.10	-1.22	69,69,69,69	0
86	OHX	1	3893	7/7	0.15	-1.23	52,52,52,52	0
86	OHX	6	2057	7/7	0.14	-1.23	63,63,63,63	0
85	MG	M5	302	1/1	0.13	-1.23	46,46,46,46	0
86	OHX	1	4168	7/7	0.12	-1.23	161,161,161,161	0
85	MG	n8	201	1/1	0.14	-1.23	29,29,29,29	0
85	MG	1	3492	1/1	0.17	-1.24	42,42,42,42	0
86	OHX	1	3970	7/7	0.12	-1.24	94,94,94,94	0
87	ZN	q3	501	1/1	0.11	-1.25	50,50,50,50	0
85	MG	6	2002	1/1	0.15	-1.25	43,43,43,43	0
85	MG	1	3491	1/1	0.16	-1.25	23,23,23,23	0
85	MG	n3	202	1/1	0.14	-1.25	35,35,35,35	0
86	OHX	5	4118	7/7	0.15	-1.26	94,94,94,94	0
86	OHX	6	2120	7/7	0.12	-1.26	93,93,93,93	0
85	MG	5	3641	1/1	0.17	-1.26	47,47,47,47	0
86	OHX	6	2118	7/7	0.10	-1.26	89,89,89,89	0
85	MG	2	2005	1/1	0.10	-1.27	59,59,59,59	0
86	OHX	1	4117	7/7	0.12	-1.27	136,136,136,136	0
86	OHX	5	4094	7/7	0.15	-1.28	101,101,101,101	0
85	MG	6	1982	1/1	0.12	-1.29	31,31,31,31	0
85	MG	6	1969	1/1	0.13	-1.30	49,49,49,49	0
86	OHX	5	3947	7/7	0.14	-1.30	72,72,72,72	0
86	OHX	6	2073	7/7	0.13	-1.30	99,99,99,99	0
85	MG	5	3428	1/1	0.17	-1.30	21,21,21,21	0
85	MG	4	202	1/1	0.18	-1.31	48,48,48,48	0
85	MG	L4	402	1/1	0.18	-1.32	51,51,51,51	0
85	MG	M3	201	1/1	0.12	-1.33	37,37,37,37	0
86	OHX	3	219	7/7	0.07	-1.34	96,96,96,96	0
86	OHX	2	2118	7/7	0.16	-1.35	129,129,129,129	0
85	MG	2	1994	1/1	0.15	-1.35	60,60,60,60	0
85	MG	1	3682	1/1	0.16	-1.35	50,50,50,50	0
86	OHX	5	4009	7/7	0.16	-1.35	74,74,74,74	0
85	MG	o4	201	1/1	0.16	-1.36	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4166	7/7	0.12	-1.36	120,120,120,120	0
86	OHX	5	4001	7/7	0.15	-1.36	79,79,79,79	0
85	MG	1	3498	1/1	0.16	-1.36	20,20,20,20	0
86	OHX	C5	201	7/7	0.13	-1.37	136,136,136,136	0
86	OHX	2	2124	7/7	0.10	-1.37	116,116,116,116	0
86	OHX	1	4074	7/7	0.12	-1.37	105,105,105,105	0
86	OHX	5	3983	7/7	0.16	-1.37	77,77,77,77	0
86	OHX	5	3910	7/7	0.17	-1.37	48,48,48,48	0
86	OHX	5	3915	7/7	0.15	-1.37	53,53,53,53	0
85	MG	5	3663	1/1	0.14	-1.38	35,35,35,35	0
86	OHX	1	4027	7/7	0.09	-1.38	112,112,112,112	0
86	OHX	1	3889	7/7	0.14	-1.38	56,56,56,56	0
85	MG	1	4218	1/1	0.17	-1.38	17,17,17,17	0
85	MG	2	1908	1/1	0.17	-1.39	60,60,60,60	0
86	OHX	5	3987	7/7	0.10	-1.39	80,80,80,80	0
85	MG	5	3624	1/1	0.17	-1.39	18,18,18,18	0
85	MG	4	218	1/1	0.14	-1.40	34,34,34,34	0
85	MG	8	204	1/1	0.15	-1.40	42,42,42,42	0
86	OHX	5	3975	7/7	0.14	-1.40	75,75,75,75	0
85	MG	1	3626	1/1	0.16	-1.41	39,39,39,39	0
85	MG	1	3666	1/1	0.12	-1.41	30,30,30,30	0
86	OHX	2	2079	7/7	0.13	-1.41	107,107,107,107	0
86	OHX	l3	403	7/7	0.14	-1.42	87,87,87,87	0
85	MG	5	3543	1/1	0.16	-1.42	23,23,23,23	0
86	OHX	o2	201	7/7	0.11	-1.42	78,78,78,78	0
86	OHX	5	4005	7/7	0.12	-1.42	80,80,80,80	0
85	MG	1	3428	1/1	0.12	-1.43	41,41,41,41	0
86	OHX	2	2089	7/7	0.16	-1.43	100,100,100,100	0
86	OHX	5	4054	7/7	0.15	-1.43	86,86,86,86	0
85	MG	5	3782	1/1	0.11	-1.44	64,64,64,64	0
85	MG	5	3436	1/1	0.14	-1.44	36,36,36,36	0
85	MG	M9	201	1/1	0.14	-1.44	52,52,52,52	0
85	MG	5	3701	1/1	0.14	-1.44	56,56,56,56	0
86	OHX	1	4001	7/7	0.13	-1.44	133,133,133,133	0
85	MG	6	1995	1/1	0.15	-1.44	32,32,32,32	0
85	MG	1	3802	1/1	0.14	-1.44	74,74,74,74	0
85	MG	5	3777	1/1	0.11	-1.45	45,45,45,45	0
86	OHX	2	2068	7/7	0.07	-1.45	113,113,113,113	0
86	OHX	3	215	7/7	0.12	-1.46	79,79,79,79	0
85	MG	5	3819	1/1	0.17	-1.48	47,47,47,47	0
86	OHX	5	3929	7/7	0.14	-1.48	50,50,50,50	0
86	OHX	1	3875	7/7	0.15	-1.49	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	5	4124	7/7	0.12	-1.49	119,119,119,119	0
86	OHX	1	4054	7/7	0.14	-1.49	94,94,94,94	0
85	MG	6	1962	1/1	0.14	-1.50	37,37,37,37	0
86	OHX	5	4024	7/7	0.12	-1.50	95,95,95,95	0
85	MG	1	3581	1/1	0.16	-1.50	29,29,29,29	0
86	OHX	15	304	7/7	0.11	-1.51	116,116,116,116	0
86	OHX	6	2105	7/7	0.14	-1.51	97,97,97,97	0
85	MG	5	3489	1/1	0.16	-1.52	42,42,42,42	0
86	OHX	5	4018	7/7	0.10	-1.53	101,101,101,101	0
85	MG	5	3425	1/1	0.16	-1.53	30,30,30,30	0
86	OHX	1	4044	7/7	0.08	-1.53	109,109,109,109	0
86	OHX	5	3979	7/7	0.10	-1.54	76,76,76,76	0
86	OHX	1	4087	7/7	0.13	-1.54	120,120,120,120	0
85	MG	5	3870	1/1	0.12	-1.54	39,39,39,39	0
85	MG	M7	206	1/1	0.15	-1.54	42,42,42,42	0
85	MG	6	2024	1/1	0.15	-1.54	40,40,40,40	0
87	ZN	Q3	501	1/1	0.11	-1.54	47,47,47,47	0
86	OHX	5	4135	7/7	0.15	-1.55	109,109,109,109	0
86	OHX	2	2106	7/7	0.14	-1.55	111,111,111,111	0
86	OHX	c3	201	7/7	0.24	-1.55	122,122,122,122	0
85	MG	2	2184	1/1	0.11	-1.55	78,78,78,78	0
87	ZN	q2	501	1/1	0.06	-1.55	59,59,59,59	0
86	OHX	c5	201	7/7	0.17	-1.55	127,127,127,127	0
86	OHX	1	4097	7/7	0.12	-1.55	115,115,115,115	0
86	OHX	1	3995	7/7	0.14	-1.55	81,81,81,81	0
85	MG	5	3849	1/1	0.15	-1.56	40,40,40,40	0
85	MG	5	3660	1/1	0.12	-1.56	39,39,39,39	0
86	OHX	1	4004	7/7	0.17	-1.56	72,72,72,72	0
86	OHX	c1	202	7/7	0.15	-1.56	108,108,108,108	0
86	OHX	2	2037	7/7	0.09	-1.56	71,71,71,71	0
86	OHX	5	4240	7/7	0.16	-1.57	192,192,192,192	0
85	MG	sM	301	1/1	0.12	-1.57	33,33,33,33	0
86	OHX	1	3904	7/7	0.14	-1.57	70,70,70,70	0
87	ZN	O7	101	1/1	0.13	-1.57	25,25,25,25	0
86	OHX	2	2078	7/7	0.10	-1.57	100,100,100,100	0
86	OHX	1	3971	7/7	0.12	-1.58	75,75,75,75	0
86	OHX	1	4029	7/7	0.11	-1.58	102,102,102,102	0
85	MG	5	3455	1/1	0.16	-1.59	82,82,82,82	0
86	OHX	1	3986	7/7	0.05	-1.59	93,93,93,93	0
86	OHX	5	3918	7/7	0.14	-1.59	56,56,56,56	0
86	OHX	1	3928	7/7	0.12	-1.59	72,72,72,72	0
86	OHX	5	4077	7/7	0.09	-1.60	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	3978	7/7	0.09	-1.60	101,101,101,101	0
86	OHX	6	2202	7/7	0.06	-1.60	159,159,159,159	0
86	OHX	5	4104	7/7	0.12	-1.60	107,107,107,107	0
85	MG	5	3718	1/1	0.15	-1.61	49,49,49,49	0
87	ZN	E1	501	1/1	0.10	-1.61	100,100,100,100	0
85	MG	5	3818	1/1	0.07	-1.61	51,51,51,51	0
86	OHX	6	2054	7/7	0.15	-1.61	69,69,69,69	0
86	OHX	5	4046	7/7	0.17	-1.62	78,78,78,78	0
85	MG	5	3712	1/1	0.14	-1.62	38,38,38,38	0
86	OHX	5	4206	7/7	0.13	-1.62	121,121,121,121	0
86	OHX	1	3905	7/7	0.14	-1.63	52,52,52,52	0
86	OHX	6	2067	7/7	0.11	-1.64	70,70,70,70	0
86	OHX	5	4017	7/7	0.13	-1.64	128,128,128,128	0
86	OHX	O2	201	7/7	0.12	-1.65	74,74,74,74	0
85	MG	1	3449	1/1	0.13	-1.65	32,32,32,32	0
86	OHX	5	4138	7/7	0.13	-1.65	111,111,111,111	0
86	OHX	5	4040	7/7	0.13	-1.65	103,103,103,103	0
86	OHX	6	2141	7/7	0.09	-1.65	127,127,127,127	0
86	OHX	1	4121	7/7	0.16	-1.65	102,102,102,102	0
85	MG	5	3720	1/1	0.15	-1.65	31,31,31,31	0
86	OHX	6	2065	7/7	0.12	-1.66	78,78,78,78	0
86	OHX	2	2069	7/7	0.10	-1.67	125,125,125,125	0
86	OHX	2	2121	7/7	0.10	-1.67	116,116,116,116	0
85	MG	1	3499	1/1	0.17	-1.67	52,52,52,52	0
85	MG	5	3611	1/1	0.13	-1.68	22,22,22,22	0
86	OHX	1	3948	7/7	0.14	-1.69	90,90,90,90	0
86	OHX	5	3958	7/7	0.14	-1.69	71,71,71,71	0
85	MG	14	401	1/1	0.16	-1.69	28,28,28,28	0
86	OHX	1	4038	7/7	0.05	-1.70	119,119,119,119	0
85	MG	1	3686	1/1	0.11	-1.71	44,44,44,44	0
86	OHX	1	4110	7/7	0.14	-1.71	92,92,92,92	0
86	OHX	6	2101	7/7	0.10	-1.72	134,134,134,134	0
86	OHX	5	3933	7/7	0.13	-1.72	60,60,60,60	0
86	OHX	1	3885	7/7	0.15	-1.73	55,55,55,55	0
86	OHX	1	4045	7/7	0.12	-1.73	94,94,94,94	0
85	MG	1	3731	1/1	0.13	-1.73	40,40,40,40	0
86	OHX	1	3886	7/7	0.15	-1.74	53,53,53,53	0
85	MG	1	3771	1/1	0.07	-1.74	36,36,36,36	0
86	OHX	1	4016	7/7	0.08	-1.74	105,105,105,105	0
86	OHX	5	3908	7/7	0.15	-1.74	39,39,39,39	0
85	MG	1	3763	1/1	0.14	-1.74	38,38,38,38	0
87	ZN	o7	501	1/1	0.11	-1.74	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4100	7/7	0.11	-1.74	116,116,116,116	0
86	OHX	6	2100	7/7	0.12	-1.75	127,127,127,127	0
85	MG	1	3649	1/1	0.13	-1.76	19,19,19,19	0
86	OHX	2	2044	7/7	0.12	-1.76	96,96,96,96	0
86	OHX	1	4088	7/7	0.14	-1.77	104,104,104,104	0
85	MG	5	3628	1/1	0.16	-1.78	32,32,32,32	0
86	OHX	6	2115	7/7	0.18	-1.78	95,95,95,95	0
85	MG	4	212	1/1	0.15	-1.78	29,29,29,29	0
85	MG	6	1915	1/1	0.13	-1.78	57,57,57,57	0
85	MG	5	3447	1/1	0.14	-1.79	29,29,29,29	0
85	MG	1	3833	1/1	0.09	-1.80	40,40,40,40	0
85	MG	5	3888	1/1	0.14	-1.80	32,32,32,32	0
85	MG	5	3878	1/1	0.18	-1.80	27,27,27,27	0
86	OHX	1	3952	7/7	0.10	-1.81	90,90,90,90	0
86	OHX	1	3927	7/7	0.13	-1.81	56,56,56,56	0
86	OHX	5	4030	7/7	0.14	-1.81	94,94,94,94	0
86	OHX	M5	304	7/7	0.13	-1.82	91,91,91,91	0
85	MG	1	3422	1/1	0.15	-1.82	23,23,23,23	0
86	OHX	5	3923	7/7	0.15	-1.83	57,57,57,57	0
86	OHX	4	223	7/7	0.12	-1.83	77,77,77,77	0
85	MG	4	213	1/1	0.18	-1.83	50,50,50,50	0
85	MG	5	3513	1/1	0.16	-1.84	27,27,27,27	0
85	MG	N3	203	1/1	0.10	-1.84	40,40,40,40	0
85	MG	1	3750	1/1	0.10	-1.85	38,38,38,38	0
86	OHX	1	4012	7/7	0.15	-1.85	101,101,101,101	0
86	OHX	2	2040	7/7	0.10	-1.85	79,79,79,79	0
86	OHX	1	4024	7/7	0.16	-1.85	94,94,94,94	0
86	OHX	6	2056	7/7	0.14	-1.86	57,57,57,57	0
85	MG	5	3699	1/1	0.15	-1.86	30,30,30,30	0
86	OHX	M0	303	7/7	0.13	-1.86	86,86,86,86	0
85	MG	1	3753	1/1	0.12	-1.87	44,44,44,44	0
86	OHX	1	3997	7/7	0.12	-1.87	111,111,111,111	0
85	MG	5	3417	1/1	0.14	-1.87	21,21,21,21	0
86	OHX	5	4101	7/7	0.12	-1.87	121,121,121,121	0
85	MG	1	3664	1/1	0.14	-1.88	39,39,39,39	0
87	ZN	d6	101	1/1	0.12	-1.90	48,48,48,48	0
86	OHX	1	3994	7/7	0.16	-1.90	92,92,92,92	0
86	OHX	6	2096	7/7	0.11	-1.91	105,105,105,105	0
86	OHX	1	3907	7/7	0.14	-1.91	61,61,61,61	0
86	OHX	5	4133	7/7	0.15	-1.91	102,102,102,102	0
86	OHX	2	2104	7/7	0.11	-1.92	169,169,169,169	0
85	MG	1	3712	1/1	0.12	-1.93	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3651	1/1	0.14	-1.93	31,31,31,31	0
86	OHX	1	3968	7/7	0.16	-1.93	65,65,65,65	0
85	MG	5	3694	1/1	0.13	-1.93	35,35,35,35	0
85	MG	8	208	1/1	0.15	-1.93	34,34,34,34	0
85	MG	5	3632	1/1	0.14	-1.94	30,30,30,30	0
86	OHX	2	2027	7/7	0.13	-1.94	69,69,69,69	0
86	OHX	5	4036	7/7	0.10	-1.94	105,105,105,105	0
86	OHX	2	2050	7/7	0.11	-1.95	95,95,95,95	0
85	MG	1	3602	1/1	0.15	-1.95	21,21,21,21	0
86	OHX	5	4131	7/7	0.13	-1.96	147,147,147,147	0
86	OHX	2	2054	7/7	0.12	-1.96	107,107,107,107	0
86	OHX	5	3962	7/7	0.10	-1.96	73,73,73,73	0
86	OHX	m5	302	7/7	0.11	-1.97	98,98,98,98	0
85	MG	1	3636	1/1	0.14	-1.97	43,43,43,43	0
85	MG	1	3690	1/1	0.16	-1.97	49,49,49,49	0
85	MG	2	2182	1/1	0.14	-1.98	54,54,54,54	0
86	OHX	n3	203	7/7	0.10	-1.98	69,69,69,69	0
86	OHX	6	2150	7/7	0.15	-1.98	115,115,115,115	0
85	MG	5	3761	1/1	0.16	-1.99	64,64,64,64	0
85	MG	c1	201	1/1	0.14	-1.99	41,41,41,41	0
86	OHX	5	4098	7/7	0.13	-1.99	114,114,114,114	0
85	MG	5	3692	1/1	0.14	-2.00	39,39,39,39	0
86	OHX	6	2077	7/7	0.14	-2.01	92,92,92,92	0
86	OHX	5	4088	7/7	0.15	-2.01	91,91,91,91	0
85	MG	5	3800	1/1	0.13	-2.01	35,35,35,35	0
86	OHX	6	2110	7/7	0.15	-2.01	93,93,93,93	0
85	MG	1	3424	1/1	0.12	-2.02	37,37,37,37	0
85	MG	1	3723	1/1	0.12	-2.03	43,43,43,43	0
86	OHX	1	4057	7/7	0.15	-2.03	114,114,114,114	0
86	OHX	SR	401	7/7	0.07	-2.03	136,136,136,136	0
85	MG	L2	301	1/1	0.11	-2.03	26,26,26,26	0
86	OHX	1	3902	7/7	0.14	-2.03	59,59,59,59	0
85	MG	5	3767	1/1	0.14	-2.04	29,29,29,29	0
85	MG	2	1985	1/1	0.15	-2.04	45,45,45,45	0
85	MG	5	3708	1/1	0.16	-2.04	36,36,36,36	0
86	OHX	7	222	7/7	0.06	-2.05	89,89,89,89	0
86	OHX	1	3879	7/7	0.17	-2.05	50,50,50,50	0
85	MG	8	202	1/1	0.14	-2.05	47,47,47,47	0
86	OHX	1	3949	7/7	0.09	-2.06	78,78,78,78	0
85	MG	M0	302	1/1	0.10	-2.06	37,37,37,37	0
86	OHX	2	2130	7/7	0.13	-2.06	150,150,150,150	0
86	OHX	1	3940	7/7	0.10	-2.07	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4002	7/7	0.08	-2.07	115,115,115,115	0
85	MG	5	3603	1/1	0.16	-2.08	19,19,19,19	0
86	OHX	6	2128	7/7	0.12	-2.09	109,109,109,109	0
85	MG	1	3601	1/1	0.16	-2.09	18,18,18,18	0
86	OHX	1	3913	7/7	0.14	-2.09	72,72,72,72	0
86	OHX	5	3943	7/7	0.16	-2.09	64,64,64,64	0
86	OHX	3	221	7/7	0.08	-2.10	102,102,102,102	0
86	OHX	5	3954	7/7	0.13	-2.10	74,74,74,74	0
85	MG	2	1964	1/1	0.12	-2.11	117,117,117,117	0
86	OHX	5	4011	7/7	0.12	-2.11	82,82,82,82	0
86	OHX	1	4089	7/7	0.09	-2.11	159,159,159,159	0
85	MG	5	3740	1/1	0.14	-2.11	34,34,34,34	0
85	MG	6	2034	1/1	0.13	-2.11	50,50,50,50	0
86	OHX	2	2039	7/7	0.12	-2.12	83,83,83,83	0
86	OHX	1	4101	7/7	0.12	-2.12	122,122,122,122	0
86	OHX	1	3936	7/7	0.13	-2.13	76,76,76,76	0
85	MG	5	3459	1/1	0.14	-2.13	23,23,23,23	0
86	OHX	5	3996	7/7	0.14	-2.13	78,78,78,78	0
86	OHX	2	2028	7/7	0.13	-2.13	62,62,62,62	0
85	MG	5	3484	1/1	0.15	-2.14	42,42,42,42	0
86	OHX	C3	202	7/7	0.12	-2.16	131,131,131,131	0
85	MG	5	3839	1/1	0.15	-2.16	30,30,30,30	0
85	MG	1	3828	1/1	0.12	-2.17	35,35,35,35	0
85	MG	5	3599	1/1	0.14	-2.17	31,31,31,31	0
85	MG	7	211	1/1	0.14	-2.17	46,46,46,46	0
86	OHX	5	4073	7/7	0.14	-2.18	93,93,93,93	0
86	OHX	6	2089	7/7	0.10	-2.19	108,108,108,108	0
86	OHX	2	2056	7/7	0.11	-2.19	93,93,93,93	0
86	OHX	1	4015	7/7	0.12	-2.20	98,98,98,98	0
86	OHX	5	4083	7/7	0.16	-2.20	94,94,94,94	0
86	OHX	6	2129	7/7	0.10	-2.22	113,113,113,113	0
86	OHX	5	3961	7/7	0.07	-2.22	72,72,72,72	0
85	MG	1	3406	1/1	0.14	-2.22	26,26,26,26	0
86	OHX	1	4095	7/7	0.15	-2.22	95,95,95,95	0
86	OHX	1	4078	7/7	0.12	-2.22	101,101,101,101	0
85	MG	6	2025	1/1	0.12	-2.23	52,52,52,52	0
86	OHX	2	2047	7/7	0.07	-2.23	94,94,94,94	0
86	OHX	6	2122	7/7	0.08	-2.23	115,115,115,115	0
87	ZN	D6	500	1/1	0.08	-2.24	67,67,67,67	0
85	MG	5	4256	1/1	0.15	-2.25	23,23,23,23	0
85	MG	M5	301	1/1	0.13	-2.25	43,43,43,43	0
85	MG	1	3478	1/1	0.14	-2.25	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2052	7/7	0.15	-2.26	56,56,56,56	0
86	OHX	1	3912	7/7	0.15	-2.27	66,66,66,66	0
86	OHX	2	2114	7/7	0.15	-2.27	124,124,124,124	0
86	OHX	6	2071	7/7	0.10	-2.27	96,96,96,96	0
85	MG	1	3584	1/1	0.14	-2.27	31,31,31,31	0
85	MG	5	3759	1/1	0.14	-2.28	32,32,32,32	0
86	OHX	1	3989	7/7	0.14	-2.29	72,72,72,72	0
86	OHX	5	3970	7/7	0.11	-2.29	77,77,77,77	0
85	MG	n8	202	1/1	0.15	-2.29	19,19,19,19	0
85	MG	6	1974	1/1	0.15	-2.29	45,45,45,45	0
86	OHX	2	2157	7/7	0.13	-2.30	195,195,195,195	0
85	MG	1	3645	1/1	0.07	-2.30	54,54,54,54	0
86	OHX	O7	104	7/7	0.12	-2.30	75,75,75,75	0
86	OHX	c8	203	7/7	0.07	-2.31	113,113,113,113	0
85	MG	1	3866	1/1	0.15	-2.31	49,49,49,49	0
85	MG	1	3794	1/1	0.09	-2.32	45,45,45,45	0
86	OHX	6	2116	7/7	0.12	-2.33	100,100,100,100	0
85	MG	1	3846	1/1	0.16	-2.33	24,24,24,24	0
86	OHX	5	4008	7/7	0.09	-2.34	64,64,64,64	0
86	OHX	3	222	7/7	0.10	-2.35	119,119,119,119	0
86	OHX	5	3968	7/7	0.14	-2.36	74,74,74,74	0
85	MG	5	3407	1/1	0.12	-2.36	32,32,32,32	0
85	MG	5	3715	1/1	0.13	-2.39	58,58,58,58	0
85	MG	5	3527	1/1	0.16	-2.39	26,26,26,26	0
85	MG	O7	102	1/1	0.15	-2.40	32,32,32,32	0
85	MG	1	3611	1/1	0.11	-2.41	36,36,36,36	0
86	OHX	1	4018	7/7	0.14	-2.41	93,93,93,93	0
86	OHX	2	2095	7/7	0.06	-2.41	132,132,132,132	0
85	MG	1	3783	1/1	0.13	-2.42	36,36,36,36	0
86	OHX	6	2070	7/7	0.11	-2.44	67,67,67,67	0
86	OHX	6	2097	7/7	0.08	-2.44	119,119,119,119	0
86	OHX	1	4139	7/7	0.14	-2.45	87,87,87,87	0
86	OHX	6	2123	7/7	0.11	-2.45	114,114,114,114	0
86	OHX	7	221	7/7	0.11	-2.45	82,82,82,82	0
86	OHX	1	3918	7/7	0.14	-2.46	72,72,72,72	0
85	MG	6	1994	1/1	0.05	-2.47	51,51,51,51	0
86	OHX	5	3995	7/7	0.12	-2.47	86,86,86,86	0
86	OHX	2	2057	7/7	0.10	-2.47	105,105,105,105	0
86	OHX	6	2164	7/7	0.09	-2.48	153,153,153,153	0
85	MG	1	4220	1/1	0.10	-2.48	23,23,23,23	0
85	MG	1	3662	1/1	0.10	-2.49	22,22,22,22	0
85	MG	5	3840	1/1	0.06	-2.51	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	5	3703	1/1	0.09	-2.51	32,32,32,32	0
86	OHX	1	3963	7/7	0.08	-2.51	88,88,88,88	0
86	OHX	5	4045	7/7	0.14	-2.51	95,95,95,95	0
86	OHX	4	225	7/7	0.10	-2.52	97,97,97,97	0
85	MG	5	3854	1/1	0.13	-2.52	54,54,54,54	0
85	MG	m7	205	1/1	0.13	-2.53	26,26,26,26	0
87	ZN	Q2	501	1/1	0.05	-2.54	63,63,63,63	0
85	MG	5	3461	1/1	0.17	-2.54	29,29,29,29	0
86	OHX	6	2062	7/7	0.12	-2.55	71,71,71,71	0
85	MG	m7	201	1/1	0.14	-2.55	24,24,24,24	0
85	MG	5	3787	1/1	0.13	-2.55	33,33,33,33	0
85	MG	5	3444	1/1	0.14	-2.55	21,21,21,21	0
85	MG	5	3600	1/1	0.11	-2.55	50,50,50,50	0
86	OHX	6	2058	7/7	0.13	-2.56	61,61,61,61	0
86	OHX	5	4063	7/7	0.14	-2.57	106,106,106,106	0
86	OHX	1	3950	7/7	0.10	-2.57	89,89,89,89	0
86	OHX	1	3975	7/7	0.10	-2.57	88,88,88,88	0
86	OHX	1	4112	7/7	0.12	-2.57	102,102,102,102	0
86	OHX	6	2106	7/7	0.10	-2.57	92,92,92,92	0
86	OHX	5	3911	7/7	0.16	-2.57	44,44,44,44	0
86	OHX	5	4028	7/7	0.15	-2.58	73,73,73,73	0
86	OHX	1	4003	7/7	0.14	-2.58	90,90,90,90	0
86	OHX	1	3911	7/7	0.14	-2.58	70,70,70,70	0
86	OHX	2	2091	7/7	0.12	-2.60	100,100,100,100	0
86	OHX	6	2099	7/7	0.10	-2.60	124,124,124,124	0
85	MG	1	4223	1/1	0.15	-2.60	20,20,20,20	0
85	MG	5	3795	1/1	0.11	-2.61	42,42,42,42	0
86	OHX	5	4064	7/7	0.08	-2.61	125,125,125,125	0
85	MG	6	2016	1/1	0.12	-2.62	38,38,38,38	0
86	OHX	2	2055	7/7	0.10	-2.62	100,100,100,100	0
86	OHX	1	4154	7/7	0.15	-2.62	109,109,109,109	0
85	MG	1	3793	1/1	0.11	-2.63	73,73,73,73	0
85	MG	5	3674	1/1	0.13	-2.63	33,33,33,33	0
85	MG	5	3510	1/1	0.11	-2.64	20,20,20,20	0
86	OHX	2	2065	7/7	0.13	-2.65	87,87,87,87	0
86	OHX	5	3969	7/7	0.10	-2.66	76,76,76,76	0
85	MG	5	3831	1/1	0.07	-2.66	59,59,59,59	0
86	OHX	5	4071	7/7	0.17	-2.66	106,106,106,106	0
86	OHX	2	2074	7/7	0.06	-2.66	111,111,111,111	0
85	MG	12	302	1/1	0.11	-2.66	28,28,28,28	0
86	OHX	5	3991	7/7	0.10	-2.68	69,69,69,69	0
86	OHX	1	3906	7/7	0.12	-2.68	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	2	2082	7/7	0.12	-2.69	110,110,110,110	0
86	OHX	5	4007	7/7	0.11	-2.69	101,101,101,101	0
86	OHX	5	4002	7/7	0.13	-2.70	58,58,58,58	0
86	OHX	5	3980	7/7	0.10	-2.70	81,81,81,81	0
86	OHX	q2	502	7/7	0.12	-2.71	67,67,67,67	0
85	MG	1	3724	1/1	0.11	-2.71	43,43,43,43	0
85	MG	1	3642	1/1	0.12	-2.72	36,36,36,36	0
85	MG	1	3640	1/1	0.14	-2.72	28,28,28,28	0
85	MG	5	3654	1/1	0.10	-2.73	35,35,35,35	0
85	MG	1	3779	1/1	0.16	-2.73	24,24,24,24	0
86	OHX	1	3920	7/7	0.11	-2.74	70,70,70,70	0
85	MG	5	3843	1/1	0.16	-2.75	25,25,25,25	0
86	OHX	3	224	7/7	0.14	-2.75	132,132,132,132	0
85	MG	5	3437	1/1	0.11	-2.76	45,45,45,45	0
86	OHX	o7	502	7/7	0.12	-2.77	80,80,80,80	0
86	OHX	M5	303	7/7	0.11	-2.77	68,68,68,68	0
86	OHX	5	3936	7/7	0.12	-2.77	54,54,54,54	0
86	OHX	5	4025	7/7	0.09	-2.78	88,88,88,88	0
86	OHX	1	4036	7/7	0.11	-2.78	87,87,87,87	0
86	OHX	5	3957	7/7	0.09	-2.78	65,65,65,65	0
86	OHX	2	2133	7/7	0.11	-2.79	119,119,119,119	0
85	MG	5	3440	1/1	0.10	-2.79	31,31,31,31	0
85	MG	N3	202	1/1	0.08	-2.79	51,51,51,51	0
86	OHX	1	3947	7/7	0.14	-2.79	70,70,70,70	0
85	MG	5	3750	1/1	0.14	-2.80	34,34,34,34	0
86	OHX	2	2094	7/7	0.11	-2.80	119,119,119,119	0
86	OHX	5	4032	7/7	0.14	-2.80	88,88,88,88	0
86	OHX	1	3956	7/7	0.13	-2.82	86,86,86,86	0
86	OHX	1	4059	7/7	0.10	-2.82	117,117,117,117	0
85	MG	1	3477	1/1	0.10	-2.83	30,30,30,30	0
86	OHX	6	2086	7/7	0.12	-2.83	88,88,88,88	0
86	OHX	5	3930	7/7	0.12	-2.84	48,48,48,48	0
86	OHX	1	3899	7/7	0.13	-2.84	48,48,48,48	0
86	OHX	5	4022	7/7	0.09	-2.86	87,87,87,87	0
86	OHX	6	2153	7/7	0.14	-2.86	118,118,118,118	0
85	MG	5	3830	1/1	0.09	-2.87	46,46,46,46	0
85	MG	6	1984	1/1	0.14	-2.87	70,70,70,70	0
85	MG	1	3823	1/1	0.11	-2.87	30,30,30,30	0
86	OHX	1	4010	7/7	0.13	-2.87	82,82,82,82	0
85	MG	1	3681	1/1	0.09	-2.88	56,56,56,56	0
86	OHX	5	3986	7/7	0.11	-2.88	72,72,72,72	0
85	MG	1	3692	1/1	0.13	-2.89	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	1	4077	7/7	0.10	-2.89	97,97,97,97	0
86	OHX	2	2098	7/7	0.07	-2.90	126,126,126,126	0
86	OHX	5	3934	7/7	0.13	-2.91	62,62,62,62	0
86	OHX	1	4014	7/7	0.13	-2.92	104,104,104,104	0
85	MG	12	301	1/1	0.18	-2.92	43,43,43,43	0
86	OHX	5	3953	7/7	0.10	-2.93	55,55,55,55	0
86	OHX	5	3981	7/7	0.11	-2.93	71,71,71,71	0
85	MG	M7	205	1/1	0.14	-2.96	34,34,34,34	0
85	MG	5	3733	1/1	0.13	-2.97	32,32,32,32	0
86	OHX	5	3941	7/7	0.10	-2.97	67,67,67,67	0
86	OHX	5	3963	7/7	0.14	-2.98	77,77,77,77	0
86	OHX	4	228	7/7	0.13	-2.98	96,96,96,96	0
86	OHX	1	3898	7/7	0.11	-3.00	55,55,55,55	0
85	MG	5	3769	1/1	0.21	-3.00	86,86,86,86	0
85	MG	1	3780	1/1	0.15	-3.00	53,53,53,53	0
86	OHX	1	4175	7/7	0.13	-3.01	86,86,86,86	0
86	OHX	1	4062	7/7	0.06	-3.01	133,133,133,133	0
86	OHX	1	3964	7/7	0.09	-3.02	90,90,90,90	0
86	OHX	2	2032	7/7	0.12	-3.02	89,89,89,89	0
85	MG	5	3666	1/1	0.13	-3.03	21,21,21,21	0
86	OHX	5	4043	7/7	0.15	-3.05	96,96,96,96	0
86	OHX	5	4111	7/7	0.14	-3.06	104,104,104,104	0
86	OHX	1	3923	7/7	0.10	-3.06	69,69,69,69	0
86	OHX	5	4003	7/7	0.13	-3.07	95,95,95,95	0
85	MG	5	3719	1/1	0.16	-3.08	31,31,31,31	0
86	OHX	2	2061	7/7	0.12	-3.10	84,84,84,84	0
85	MG	5	3860	1/1	0.13	-3.10	51,51,51,51	0
86	OHX	5	4197	7/7	0.14	-3.10	92,92,92,92	0
86	OHX	2	2088	7/7	0.09	-3.10	101,101,101,101	0
85	MG	1	3857	1/1	0.13	-3.11	59,59,59,59	0
86	OHX	2	2081	7/7	0.09	-3.11	127,127,127,127	0
86	OHX	6	2135	7/7	0.09	-3.12	116,116,116,116	0
85	MG	5	3711	1/1	0.10	-3.12	51,51,51,51	0
86	OHX	2	2096	7/7	0.11	-3.12	121,121,121,121	0
86	OHX	1	4119	7/7	0.15	-3.12	103,103,103,103	0
86	OHX	1	4051	7/7	0.10	-3.14	99,99,99,99	0
86	OHX	5	4096	7/7	0.13	-3.15	115,115,115,115	0
86	OHX	6	2078	7/7	0.11	-3.15	76,76,76,76	0
86	OHX	1	4109	7/7	0.09	-3.16	120,120,120,120	0
86	OHX	5	3920	7/7	0.14	-3.17	51,51,51,51	0
85	MG	1	3772	1/1	0.14	-3.18	47,47,47,47	0
86	OHX	1	4022	7/7	0.14	-3.18	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3603	1/1	0.14	-3.21	24,24,24,24	0
85	MG	5	3408	1/1	0.11	-3.21	17,17,17,17	0
85	MG	1	3830	1/1	0.14	-3.21	16,16,16,16	0
86	OHX	1	3938	7/7	0.13	-3.23	58,58,58,58	0
85	MG	1	3605	1/1	0.14	-3.23	29,29,29,29	0
86	OHX	5	4038	7/7	0.08	-3.23	105,105,105,105	0
86	OHX	o3	203	7/7	0.08	-3.24	88,88,88,88	0
85	MG	5	3820	1/1	0.11	-3.25	52,52,52,52	0
86	OHX	5	3922	7/7	0.15	-3.26	53,53,53,53	0
86	OHX	6	2082	7/7	0.06	-3.27	83,83,83,83	0
85	MG	1	3446	1/1	0.08	-3.27	31,31,31,31	0
85	MG	6	1978	1/1	0.13	-3.27	67,67,67,67	0
85	MG	1	3427	1/1	0.13	-3.28	27,27,27,27	0
86	OHX	2	2052	7/7	0.14	-3.29	83,83,83,83	0
86	OHX	6	2063	7/7	0.11	-3.30	71,71,71,71	0
86	OHX	2	2083	7/7	0.08	-3.31	114,114,114,114	0
85	MG	6	2017	1/1	0.11	-3.32	58,58,58,58	0
86	OHX	6	2085	7/7	0.10	-3.32	109,109,109,109	0
86	OHX	1	4056	7/7	0.09	-3.34	112,112,112,112	0
86	OHX	1	3998	7/7	0.09	-3.35	96,96,96,96	0
86	OHX	6	2069	7/7	0.10	-3.36	79,79,79,79	0
86	OHX	5	3977	7/7	0.11	-3.36	81,81,81,81	0
86	OHX	8	222	7/7	0.07	-3.37	114,114,114,114	0
86	OHX	2	2076	7/7	0.13	-3.37	115,115,115,115	0
86	OHX	6	2083	7/7	0.11	-3.37	98,98,98,98	0
86	OHX	2	2059	7/7	0.08	-3.38	91,91,91,91	0
85	MG	1	3831	1/1	0.11	-3.38	39,39,39,39	0
85	MG	5	3682	1/1	0.16	-3.39	22,22,22,22	0
85	MG	1	3812	1/1	0.14	-3.39	27,27,27,27	0
86	OHX	5	3989	7/7	0.14	-3.40	62,62,62,62	0
86	OHX	1	4080	7/7	0.10	-3.41	106,106,106,106	0
86	OHX	7	223	7/7	0.08	-3.42	106,106,106,106	0
85	MG	5	3837	1/1	0.14	-3.43	40,40,40,40	0
86	OHX	5	4006	7/7	0.11	-3.46	87,87,87,87	0
85	MG	1	3476	1/1	0.15	-3.46	21,21,21,21	0
86	OHX	1	3884	7/7	0.12	-3.46	50,50,50,50	0
86	OHX	5	4085	7/7	0.10	-3.47	95,95,95,95	0
85	MG	5	3664	1/1	0.12	-3.47	37,37,37,37	0
86	OHX	5	4068	7/7	0.13	-3.48	81,81,81,81	0
86	OHX	1	3974	7/7	0.10	-3.48	86,86,86,86	0
86	OHX	2	2131	7/7	0.12	-3.49	93,93,93,93	0
86	OHX	1	3916	7/7	0.13	-3.50	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	1	3744	1/1	0.12	-3.50	29,29,29,29	0
85	MG	1	3497	1/1	0.11	-3.51	33,33,33,33	0
86	OHX	5	4084	7/7	0.10	-3.52	112,112,112,112	0
86	OHX	1	4181	7/7	0.09	-3.53	192,192,192,192	0
85	MG	2	2002	1/1	0.10	-3.54	87,87,87,87	0
86	OHX	2	2097	7/7	0.08	-3.55	131,131,131,131	0
86	OHX	1	4006	7/7	0.10	-3.55	102,102,102,102	0
86	OHX	5	3916	7/7	0.13	-3.56	51,51,51,51	0
85	MG	2	1942	1/1	0.10	-3.57	63,63,63,63	0
86	OHX	6	2068	7/7	0.09	-3.57	71,71,71,71	0
85	MG	5	3857	1/1	0.12	-3.58	37,37,37,37	0
86	OHX	2	2067	7/7	0.10	-3.58	114,114,114,114	0
85	MG	O3	201	1/1	0.10	-3.60	28,28,28,28	0
86	OHX	1	3976	7/7	0.10	-3.61	80,80,80,80	0
85	MG	1	3565	1/1	0.15	-3.61	27,27,27,27	0
85	MG	1	3738	1/1	0.13	-3.61	24,24,24,24	0
85	MG	m5	301	1/1	0.10	-3.63	45,45,45,45	0
86	OHX	6	2095	7/7	0.11	-3.64	100,100,100,100	0
86	OHX	5	4000	7/7	0.10	-3.64	94,94,94,94	0
86	OHX	1	3890	7/7	0.14	-3.65	53,53,53,53	0
86	OHX	1	4028	7/7	0.12	-3.65	92,92,92,92	0
86	OHX	1	3910	7/7	0.09	-3.65	66,66,66,66	0
85	MG	1	3433	1/1	0.11	-3.65	29,29,29,29	0
86	OHX	1	4069	7/7	0.07	-3.65	119,119,119,119	0
85	MG	5	3450	1/1	0.14	-3.66	20,20,20,20	0
86	OHX	1	3962	7/7	0.09	-3.66	59,59,59,59	0
86	OHX	6	2079	7/7	0.08	-3.68	88,88,88,88	0
86	OHX	6	2061	7/7	0.12	-3.70	65,65,65,65	0
86	OHX	1	3958	7/7	0.11	-3.71	75,75,75,75	0
85	MG	5	3806	1/1	0.11	-3.71	30,30,30,30	0
85	MG	1	3558	1/1	0.16	-3.73	40,40,40,40	0
85	MG	5	3724	1/1	0.16	-3.74	28,28,28,28	0
85	MG	1	3729	1/1	0.14	-3.74	61,61,61,61	0
86	OHX	5	3952	7/7	0.11	-3.75	83,83,83,83	0
85	MG	1	3764	1/1	0.11	-3.76	42,42,42,42	0
85	MG	5	3774	1/1	0.13	-3.77	27,27,27,27	0
86	OHX	5	4014	7/7	0.09	-3.82	77,77,77,77	0
86	OHX	1	4021	7/7	0.13	-3.83	99,99,99,99	0
86	OHX	1	3896	7/7	0.11	-3.84	52,52,52,52	0
85	MG	1	3710	1/1	0.13	-3.85	25,25,25,25	0
85	MG	5	3678	1/1	0.13	-3.85	37,37,37,37	0
85	MG	1	3672	1/1	0.13	-3.85	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
85	MG	2	1999	1/1	0.12	-3.86	83,83,83,83	0
86	OHX	2	2029	7/7	0.13	-3.86	75,75,75,75	0
86	OHX	1	3895	7/7	0.14	-3.86	54,54,54,54	0
86	OHX	6	2166	7/7	0.11	-3.87	115,115,115,115	0
86	OHX	1	3993	7/7	0.11	-3.89	84,84,84,84	0
86	OHX	1	3908	7/7	0.11	-3.90	54,54,54,54	0
86	OHX	1	3987	7/7	0.10	-3.93	80,80,80,80	0
86	OHX	13	402	7/7	0.07	-3.93	79,79,79,79	0
86	OHX	7	220	7/7	0.13	-3.93	76,76,76,76	0
86	OHX	1	4011	7/7	0.10	-3.97	89,89,89,89	0
86	OHX	5	4128	7/7	0.12	-3.98	112,112,112,112	0
85	MG	6	2008	1/1	0.13	-3.99	41,41,41,41	0
86	OHX	1	3946	7/7	0.12	-4.03	71,71,71,71	0
85	MG	1	3438	1/1	0.14	-4.03	36,36,36,36	0
85	MG	5	3704	1/1	0.14	-4.03	41,41,41,41	0
86	OHX	1	4026	7/7	0.07	-4.03	116,116,116,116	0
86	OHX	1	4032	7/7	0.12	-4.06	108,108,108,108	0
85	MG	6	1970	1/1	0.13	-4.06	49,49,49,49	0
86	OHX	5	4103	7/7	0.10	-4.08	123,123,123,123	0
86	OHX	1	4052	7/7	0.07	-4.10	108,108,108,108	0
86	OHX	5	4060	7/7	0.09	-4.10	113,113,113,113	0
86	OHX	5	4065	7/7	0.12	-4.12	91,91,91,91	0
85	MG	1	3775	1/1	0.14	-4.14	29,29,29,29	0
85	MG	5	3597	1/1	0.12	-4.14	28,28,28,28	0
85	MG	1	3760	1/1	0.14	-4.14	30,30,30,30	0
86	OHX	1	3881	7/7	0.13	-4.15	46,46,46,46	0
85	MG	5	3430	1/1	0.13	-4.15	27,27,27,27	0
86	OHX	2	2072	7/7	0.06	-4.15	100,100,100,100	0
85	MG	5	3485	1/1	0.11	-4.16	41,41,41,41	0
86	OHX	1	3933	7/7	0.12	-4.18	86,86,86,86	0
85	MG	1	3468	1/1	0.10	-4.18	37,37,37,37	0
86	OHX	5	4016	7/7	0.14	-4.19	87,87,87,87	0
86	OHX	2	2060	7/7	0.08	-4.19	99,99,99,99	0
86	OHX	6	2108	7/7	0.12	-4.19	88,88,88,88	0
85	MG	5	3779	1/1	0.15	-4.19	38,38,38,38	0
86	OHX	1	3985	7/7	0.11	-4.20	69,69,69,69	0
86	OHX	1	3961	7/7	0.11	-4.22	72,72,72,72	0
85	MG	1	3745	1/1	0.12	-4.23	39,39,39,39	0
85	MG	6	1930	1/1	0.14	-4.25	46,46,46,46	0
85	MG	1	3695	1/1	0.10	-4.26	36,36,36,36	0
86	OHX	1	3965	7/7	0.12	-4.27	85,85,85,85	0
86	OHX	7	217	7/7	0.12	-4.29	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	4048	7/7	0.10	-4.30	94,94,94,94	0
86	OHX	2	2045	7/7	0.09	-4.30	82,82,82,82	0
86	OHX	2	2073	7/7	0.07	-4.32	95,95,95,95	0
86	OHX	8	220	7/7	0.07	-4.33	101,101,101,101	0
85	MG	5	3817	1/1	0.12	-4.33	33,33,33,33	0
86	OHX	1	3984	7/7	0.11	-4.33	94,94,94,94	0
86	OHX	1	3925	7/7	0.11	-4.34	66,66,66,66	0
86	OHX	5	4055	7/7	0.11	-4.37	86,86,86,86	0
86	OHX	2	2063	7/7	0.10	-4.38	95,95,95,95	0
86	OHX	5	3925	7/7	0.12	-4.39	46,46,46,46	0
86	OHX	1	3960	7/7	0.10	-4.40	78,78,78,78	0
86	OHX	4	224	7/7	0.09	-4.40	93,93,93,93	0
86	OHX	1	3892	7/7	0.11	-4.41	56,56,56,56	0
85	MG	5	3698	1/1	0.10	-4.41	44,44,44,44	0
85	MG	1	3732	1/1	0.09	-4.42	37,37,37,37	0
85	MG	1	3705	1/1	0.12	-4.42	47,47,47,47	0
85	MG	1	3480	1/1	0.15	-4.43	57,57,57,57	0
86	OHX	5	4168	7/7	0.07	-4.44	154,154,154,154	0
86	OHX	1	4040	7/7	0.10	-4.45	114,114,114,114	0
85	MG	5	3749	1/1	0.09	-4.46	38,38,38,38	0
86	OHX	2	2077	7/7	0.11	-4.46	98,98,98,98	0
85	MG	1	3811	1/1	0.12	-4.46	40,40,40,40	0
85	MG	1	3665	1/1	0.10	-4.47	37,37,37,37	0
86	OHX	1	3980	7/7	0.14	-4.50	87,87,87,87	0
85	MG	5	3492	1/1	0.12	-4.50	22,22,22,22	0
86	OHX	1	3967	7/7	0.15	-4.53	82,82,82,82	0
86	OHX	1	3999	7/7	0.07	-4.53	105,105,105,105	0
86	OHX	5	4196	7/7	0.12	-4.54	65,65,65,65	0
86	OHX	5	3924	7/7	0.12	-4.55	52,52,52,52	0
86	OHX	5	3946	7/7	0.12	-4.59	62,62,62,62	0
86	OHX	5	4051	7/7	0.15	-4.61	88,88,88,88	0
86	OHX	1	3887	7/7	0.13	-4.63	49,49,49,49	0
86	OHX	5	4097	7/7	0.13	-4.63	93,93,93,93	0
85	MG	1	3606	1/1	0.11	-4.63	42,42,42,42	0
86	OHX	2	2066	7/7	0.12	-4.65	89,89,89,89	0
85	MG	1	3746	1/1	0.14	-4.65	50,50,50,50	0
85	MG	1	3706	1/1	0.07	-4.65	30,30,30,30	0
86	OHX	5	4080	7/7	0.09	-4.68	95,95,95,95	0
86	OHX	5	4050	7/7	0.07	-4.68	111,111,111,111	0
85	MG	6	1973	1/1	0.14	-4.70	43,43,43,43	0
86	OHX	2	2051	7/7	0.09	-4.71	91,91,91,91	0
85	MG	1	3434	1/1	0.13	-4.72	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	OHX	1	4009	7/7	0.10	-4.72	93,93,93,93	0
86	OHX	2	2042	7/7	0.11	-4.72	79,79,79,79	0
86	OHX	5	3982	7/7	0.08	-4.74	63,63,63,63	0
86	OHX	6	2138	7/7	0.11	-4.78	100,100,100,100	0
85	MG	1	3442	1/1	0.15	-4.79	19,19,19,19	0
86	OHX	2	2111	7/7	0.09	-4.80	93,93,93,93	0
86	OHX	1	3929	7/7	0.10	-4.83	63,63,63,63	0
86	OHX	6	2102	7/7	0.07	-4.84	96,96,96,96	0
86	OHX	1	4064	7/7	0.07	-4.87	123,123,123,123	0
86	OHX	1	3990	7/7	0.11	-4.89	97,97,97,97	0
86	OHX	1	4019	7/7	0.12	-4.90	89,89,89,89	0
85	MG	1	3715	1/1	0.12	-4.91	31,31,31,31	0
86	OHX	8	218	7/7	0.12	-4.94	97,97,97,97	0
86	OHX	3	218	7/7	0.11	-4.95	81,81,81,81	0
86	OHX	5	4023	7/7	0.08	-4.97	89,89,89,89	0
86	OHX	1	4013	7/7	0.08	-4.97	105,105,105,105	0
85	MG	1	3453	1/1	0.17	-5.00	37,37,37,37	0
85	MG	7	214	1/1	0.15	-5.00	54,54,54,54	0
86	OHX	6	2149	7/7	0.14	-5.00	87,87,87,87	0
86	OHX	1	3969	7/7	0.10	-5.02	80,80,80,80	0
86	OHX	5	3998	7/7	0.08	-5.04	91,91,91,91	0
85	MG	1	3628	1/1	0.11	-5.07	52,52,52,52	0
85	MG	5	3637	1/1	0.11	-5.08	35,35,35,35	0
86	OHX	5	4086	7/7	0.14	-5.11	98,98,98,98	0
85	MG	1	3864	1/1	0.16	-5.13	33,33,33,33	0
86	OHX	5	4035	7/7	0.14	-5.14	102,102,102,102	0
86	OHX	5	3972	7/7	0.10	-5.17	66,66,66,66	0
86	OHX	5	4123	7/7	0.16	-5.17	116,116,116,116	0
85	MG	5	3739	1/1	0.10	-5.18	31,31,31,31	0
86	OHX	5	3960	7/7	0.12	-5.21	61,61,61,61	0
86	OHX	5	3993	7/7	0.13	-5.22	66,66,66,66	0
86	OHX	1	3991	7/7	0.12	-5.28	92,92,92,92	0
86	OHX	1	4030	7/7	0.08	-5.28	103,103,103,103	0
86	OHX	6	2092	7/7	0.09	-5.32	94,94,94,94	0
85	MG	5	3616	1/1	0.14	-5.33	36,36,36,36	0
86	OHX	5	4129	7/7	0.07	-5.33	114,114,114,114	0
85	MG	1	3691	1/1	0.14	-5.33	28,28,28,28	0
86	OHX	5	3950	7/7	0.13	-5.33	67,67,67,67	0
86	OHX	3	216	7/7	0.14	-5.36	87,87,87,87	0
86	OHX	5	3937	7/7	0.12	-5.36	62,62,62,62	0
85	MG	6	1989	1/1	0.13	-5.37	60,60,60,60	0
86	OHX	5	3992	7/7	0.10	-5.37	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2131	7/7	0.09	-5.38	119,119,119,119	0
86	OHX	5	4215	7/7	0.11	-5.38	85,85,85,85	0
86	OHX	5	3984	7/7	0.12	-5.38	71,71,71,71	0
86	OHX	1	3934	7/7	0.10	-5.40	68,68,68,68	0
86	OHX	6	2119	7/7	0.07	-5.40	107,107,107,107	0
85	MG	5	3725	1/1	0.07	-5.41	41,41,41,41	0
86	OHX	M6	202	7/7	0.09	-5.42	80,80,80,80	0
85	MG	1	3852	1/1	0.16	-5.47	43,43,43,43	0
86	OHX	5	4057	7/7	0.07	-5.48	105,105,105,105	0
86	OHX	5	4153	7/7	0.10	-5.51	95,95,95,95	0
86	OHX	6	2060	7/7	0.11	-5.52	69,69,69,69	0
86	OHX	5	4015	7/7	0.10	-5.55	83,83,83,83	0
86	OHX	1	3983	7/7	0.08	-5.59	89,89,89,89	0
85	MG	5	3804	1/1	0.08	-5.61	27,27,27,27	0
85	MG	5	3688	1/1	0.13	-5.62	33,33,33,33	0
86	OHX	2	2071	7/7	0.08	-5.66	108,108,108,108	0
85	MG	5	3747	1/1	0.11	-5.75	47,47,47,47	0
86	OHX	5	3967	7/7	0.10	-5.79	70,70,70,70	0
86	OHX	5	4021	7/7	0.09	-5.79	90,90,90,90	0
86	OHX	1	3951	7/7	0.11	-5.79	72,72,72,72	0
86	OHX	6	2084	7/7	0.10	-5.80	96,96,96,96	0
86	OHX	2	2053	7/7	0.07	-5.81	94,94,94,94	0
85	MG	5	3668	1/1	0.12	-5.83	29,29,29,29	0
85	MG	7	212	1/1	0.15	-5.93	64,64,64,64	0
86	OHX	6	2075	7/7	0.09	-5.94	69,69,69,69	0
86	OHX	5	4095	7/7	0.11	-5.96	104,104,104,104	0
85	MG	5	3452	1/1	0.14	-6.00	35,35,35,35	0
86	OHX	1	4158	7/7	0.15	-6.04	84,84,84,84	0
85	MG	5	3496	1/1	0.12	-6.08	39,39,39,39	0
85	MG	1	3441	1/1	0.09	-6.09	30,30,30,30	0
86	OHX	5	3994	7/7	0.07	-6.11	102,102,102,102	0
86	OHX	5	4047	7/7	0.09	-6.16	97,97,97,97	0
86	OHX	2	2084	7/7	0.07	-6.23	111,111,111,111	0
86	OHX	1	3959	7/7	0.09	-6.25	71,71,71,71	0
86	OHX	5	4130	7/7	0.09	-6.26	95,95,95,95	0
86	OHX	6	2111	7/7	0.10	-6.27	104,104,104,104	0
85	MG	5	3650	1/1	0.11	-6.29	22,22,22,22	0
86	OHX	1	3941	7/7	0.11	-6.33	76,76,76,76	0
85	MG	5	3838	1/1	0.13	-6.33	53,53,53,53	0
85	MG	1	3740	1/1	0.07	-6.34	49,49,49,49	0
86	OHX	5	3935	7/7	0.10	-6.35	56,56,56,56	0
85	MG	1	3678	1/1	0.16	-6.35	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	5	3959	7/7	0.12	-6.38	58,58,58,58	0
86	OHX	6	2091	7/7	0.12	-6.43	94,94,94,94	0
86	OHX	6	2098	7/7	0.09	-6.49	103,103,103,103	0
85	MG	1	3787	1/1	0.15	-6.50	46,46,46,46	0
85	MG	1	3632	1/1	0.12	-6.52	50,50,50,50	0
86	OHX	5	4058	7/7	0.08	-6.55	109,109,109,109	0
86	OHX	3	220	7/7	0.05	-6.57	101,101,101,101	0
86	OHX	1	3942	7/7	0.12	-6.58	78,78,78,78	0
85	MG	1	3616	1/1	0.14	-6.58	32,32,32,32	0
86	OHX	6	2103	7/7	0.10	-6.59	88,88,88,88	0
86	OHX	7	219	7/7	0.08	-6.63	76,76,76,76	0
86	OHX	2	2064	7/7	0.09	-6.65	104,104,104,104	0
85	MG	5	3483	1/1	0.11	-6.66	34,34,34,34	0
86	OHX	1	3979	7/7	0.07	-6.67	87,87,87,87	0
85	MG	5	3736	1/1	0.10	-6.69	36,36,36,36	0
86	OHX	1	3914	7/7	0.11	-6.71	58,58,58,58	0
86	OHX	m6	202	7/7	0.09	-6.75	73,73,73,73	0
85	MG	1	3464	1/1	0.14	-6.75	31,31,31,31	0
85	MG	1	3676	1/1	0.12	-6.76	59,59,59,59	0
86	OHX	1	3917	7/7	0.10	-6.79	70,70,70,70	0
85	MG	5	3636	1/1	0.10	-6.80	40,40,40,40	0
86	OHX	5	3942	7/7	0.08	-6.85	75,75,75,75	0
86	OHX	1	4035	7/7	0.10	-6.86	99,99,99,99	0
86	OHX	3	217	7/7	0.08	-6.90	86,86,86,86	0
85	MG	1	3524	1/1	0.14	-6.92	20,20,20,20	0
85	MG	1	3829	1/1	0.14	-6.95	47,47,47,47	0
86	OHX	5	4067	7/7	0.08	-6.97	105,105,105,105	0
86	OHX	5	3927	7/7	0.12	-6.98	59,59,59,59	0
85	MG	5	3891	1/1	0.15	-7.00	64,64,64,64	0
86	OHX	1	4099	7/7	0.13	-7.02	115,115,115,115	0
86	OHX	2	2102	7/7	0.07	-7.03	110,110,110,110	0
86	OHX	6	2087	7/7	0.07	-7.05	91,91,91,91	0
86	OHX	6	2072	7/7	0.10	-7.08	67,67,67,67	0
85	MG	1	3803	1/1	0.10	-7.09	41,41,41,41	0
86	OHX	1	3977	7/7	0.09	-7.09	85,85,85,85	0
86	OHX	5	3971	7/7	0.08	-7.09	65,65,65,65	0
86	OHX	6	2094	7/7	0.08	-7.09	105,105,105,105	0
86	OHX	2	2046	7/7	0.08	-7.13	86,86,86,86	0
86	OHX	5	3990	7/7	0.07	-7.17	84,84,84,84	0
86	OHX	1	4043	7/7	0.11	-7.18	88,88,88,88	0
86	OHX	1	3955	7/7	0.09	-7.29	80,80,80,80	0
85	MG	1	3741	1/1	0.13	-7.32	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	OHX	6	2090	7/7	0.06	-7.41	90,90,90,90	0
85	MG	6	2032	1/1	0.10	-7.43	56,56,56,56	0
86	OHX	5	3945	7/7	0.10	-7.56	61,61,61,61	0
86	OHX	6	2076	7/7	0.08	-7.63	86,86,86,86	0
85	MG	5	3836	1/1	0.12	-7.64	22,22,22,22	0
85	MG	1	3657	1/1	0.11	-7.66	23,23,23,23	0
86	OHX	6	2080	7/7	0.08	-7.68	79,79,79,79	0
86	OHX	5	3964	7/7	0.12	-7.69	66,66,66,66	0
85	MG	6	2007	1/1	0.12	-7.75	50,50,50,50	0
86	OHX	6	2093	7/7	0.06	-7.84	87,87,87,87	0
85	MG	6	2010	1/1	0.10	-7.85	36,36,36,36	0
85	MG	1	3435	1/1	0.10	-7.86	32,32,32,32	0
86	OHX	5	4087	7/7	0.09	-7.95	105,105,105,105	0
86	OHX	6	2104	7/7	0.08	-7.99	100,100,100,100	0
85	MG	5	3765	1/1	0.07	-8.00	46,46,46,46	0
86	OHX	5	4012	7/7	0.09	-8.02	82,82,82,82	0
86	OHX	1	3926	7/7	0.11	-8.12	72,72,72,72	0
86	OHX	8	217	7/7	0.08	-8.37	102,102,102,102	0
86	OHX	5	4069	7/7	0.11	-8.46	108,108,108,108	0
86	OHX	1	3972	7/7	0.12	-8.47	107,107,107,107	0
86	OHX	5	4010	7/7	0.05	-8.51	88,88,88,88	0
86	OHX	7	218	7/7	0.10	-8.57	84,84,84,84	0
86	OHX	5	4213	7/7	0.09	-8.60	166,166,166,166	0
86	OHX	5	4034	7/7	0.10	-8.63	86,86,86,86	0
85	MG	5	3826	1/1	0.09	-8.69	29,29,29,29	0
86	OHX	1	3945	7/7	0.10	-8.82	82,82,82,82	0
86	OHX	5	4070	7/7	0.10	-8.85	98,98,98,98	0
85	MG	5	3792	1/1	0.07	-8.97	32,32,32,32	0
86	OHX	6	2088	7/7	0.08	-9.25	95,95,95,95	0
86	OHX	5	3928	7/7	0.11	-9.26	55,55,55,55	0
85	MG	1	3725	1/1	0.10	-9.28	35,35,35,35	0
85	MG	1	3845	1/1	0.13	-9.29	43,43,43,43	0
86	OHX	1	3973	7/7	0.10	-9.49	82,82,82,82	0
85	MG	5	3702	1/1	0.12	-9.67	44,44,44,44	0
86	OHX	1	4048	7/7	0.13	-9.75	86,86,86,86	0
86	OHX	6	2081	7/7	0.09	-9.81	78,78,78,78	0
86	OHX	5	4020	7/7	0.10	-9.84	85,85,85,85	0
85	MG	5	3488	1/1	0.11	-10.00	41,41,41,41	0
86	OHX	1	4007	7/7	0.11	-10.02	90,90,90,90	0
85	MG	6	1986	1/1	0.10	-10.04	39,39,39,39	0
86	OHX	5	4066	7/7	0.07	-10.26	97,97,97,97	0
85	MG	5	3653	1/1	0.10	-10.51	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	4	210	1/1	0.09	-10.62	43,43,43,43	0
85	MG	1	3638	1/1	0.08	-10.66	49,49,49,49	0
85	MG	1	3770	1/1	0.14	-10.71	75,75,75,75	0
86	OHX	5	3978	7/7	0.10	-10.83	65,65,65,65	0
85	MG	5	3760	1/1	0.10	-10.87	35,35,35,35	0
86	OHX	5	3976	7/7	0.09	-10.95	85,85,85,85	0
85	MG	5	3788	1/1	0.09	-10.97	39,39,39,39	0
85	MG	5	3824	1/1	0.10	-11.57	37,37,37,37	0
86	OHX	5	3985	7/7	0.08	-12.02	71,71,71,71	0
85	MG	1	3440	1/1	0.14	-12.07	31,31,31,31	0
85	MG	5	3741	1/1	0.08	-12.09	46,46,46,46	0
86	OHX	1	3935	7/7	0.09	-12.12	68,68,68,68	0
86	OHX	6	2130	7/7	0.07	-12.94	96,96,96,96	0
85	MG	5	3794	1/1	0.14	-13.00	64,64,64,64	0
85	MG	5	3895	1/1	0.13	-13.00	51,51,51,51	0
85	MG	5	3687	1/1	0.07	-13.71	45,45,45,45	0
85	MG	8	210	1/1	0.05	-13.89	50,50,50,50	0
85	MG	5	3601	1/1	0.09	-13.98	35,35,35,35	0
85	MG	5	3862	1/1	0.10	-14.30	33,33,33,33	0
86	OHX	1	4055	7/7	0.08	-14.54	104,104,104,104	0
85	MG	1	3671	1/1	0.09	-14.77	40,40,40,40	0
85	MG	1	3639	1/1	0.09	-15.33	56,56,56,56	0
85	MG	5	3812	1/1	0.07	-15.39	74,74,74,74	0
86	OHX	5	4004	7/7	0.09	-15.45	69,69,69,69	0
85	MG	5	3686	1/1	0.10	-17.14	32,32,32,32	0
86	OHX	6	2114	7/7	0.11	-17.19	102,102,102,102	0
86	OHX	1	3992	7/7	0.08	-17.20	94,94,94,94	0
85	MG	5	3808	1/1	0.11	-17.86	59,59,59,59	0
85	MG	6	2001	1/1	0.10	-18.71	80,80,80,80	0
85	MG	5	3781	1/1	0.17	-19.00	64,64,64,64	0
85	MG	5	3471	1/1	0.14	-19.67	40,40,40,40	0
85	MG	4	215	1/1	0.12	-23.73	60,60,60,60	0
85	MG	5	3679	1/1	0.12	-29.03	28,28,28,28	0
86	OHX	2	2062	7/7	0.07	-36.09	105,105,105,105	0
85	MG	5	3464	1/1	0.13	-59.00	30,30,30,30	0
85	MG	5	3850	1/1	0.10	-161.00	56,56,56,56	0
85	MG	6	1979	1/1	0.25	-	51,51,51,51	0
85	MG	6	1999	1/1	0.32	-	87,87,87,87	0
85	MG	6	2045	1/1	0.36	-	63,63,63,63	0
85	MG	5	3773	1/1	0.28	-	83,83,83,83	0
85	MG	3	208	1/1	0.11	-	66,66,66,66	0
85	MG	1	3841	1/1	0.25	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
85	MG	5	3876	1/1	0.27	-	39,39,39,39	0
85	MG	1	3737	1/1	0.17	-	54,54,54,54	0
85	MG	1	3840	1/1	0.24	-	39,39,39,39	0
85	MG	1	3465	1/1	0.26	-	41,41,41,41	0
85	MG	1	3490	1/1	0.25	-	51,51,51,51	0
85	MG	5	3799	1/1	0.10	-	39,39,39,39	0
85	MG	1	3851	1/1	0.15	-	50,50,50,50	0
85	MG	2	2021	1/1	0.45	-	61,61,61,61	0
85	MG	6	2041	1/1	0.52	-	65,65,65,65	0
85	MG	5	3615	1/1	0.29	-	30,30,30,30	0
85	MG	1	3703	1/1	0.09	-	49,49,49,49	0
85	MG	6	2044	1/1	0.38	-	44,44,44,44	0
85	MG	1	3613	1/1	0.28	-	36,36,36,36	0
85	MG	2	1996	1/1	0.42	-	48,48,48,48	0
86	OHX	2	2159	7/7	0.11	-	260,260,260,260	0
85	MG	6	1924	1/1	0.61	-	87,87,87,87	0
85	MG	1	3500	1/1	0.26	-	51,51,51,51	0
85	MG	5	3883	1/1	0.13	-	48,48,48,48	0
85	MG	4	201	1/1	0.34	-	50,50,50,50	0
85	MG	1	3756	1/1	0.22	-	91,91,91,91	0
85	MG	1	3627	1/1	0.33	-	58,58,58,58	0
85	MG	5	3886	1/1	0.50	-	80,80,80,80	0
85	MG	5	3500	1/1	0.16	-	45,45,45,45	0
85	MG	8	212	1/1	0.22	-	47,47,47,47	0
85	MG	2	1954	1/1	0.57	-	87,87,87,87	0
85	MG	1	3792	1/1	0.18	-	58,58,58,58	0
85	MG	5	3873	1/1	0.39	-	47,47,47,47	0
85	MG	4	217	1/1	0.14	-	48,48,48,48	0
85	MG	1	3795	1/1	0.20	-	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.