



wwPDB X-ray Structure Validation Summary Report i

Oct 9, 2014 – 11:14 PM BST

PDB ID : 4U3U
Title : Crystal structure of Cycloheximide bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-22
Resolution : 2.90 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>

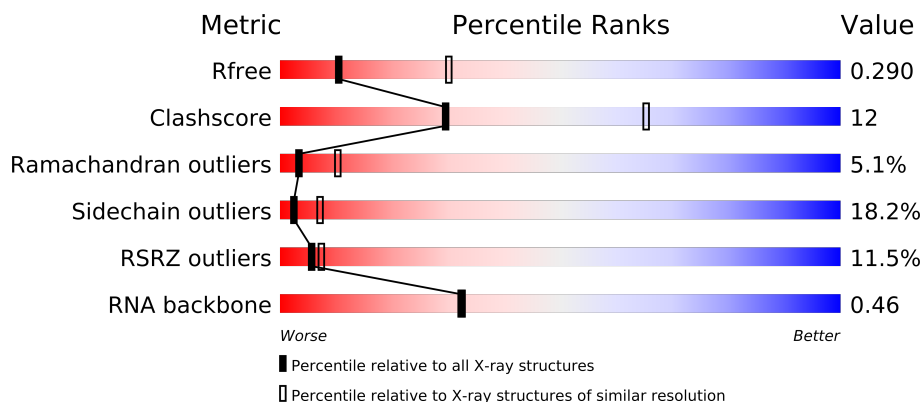
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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	
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	
49	m3	198	

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Mol	Chain	Length	Quality of chain
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	
70	o4	119	

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Mol	Chain	Length	Quality of chain
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	e1	76	
82	m2	160	
83	p0	311	
84	p1	47	
85	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
86	MG	1	3401	-	X
86	MG	1	3402	-	X
86	MG	1	3404	-	X
86	MG	1	3405	-	X
86	MG	1	3408	-	X
86	MG	1	3409	-	X
86	MG	1	3410	-	X
86	MG	1	3412	-	X
86	MG	1	3413	-	X
86	MG	1	3414	-	X
86	MG	1	3417	-	X
86	MG	1	3418	-	X
86	MG	1	3419	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3420	-	X
86	MG	1	3421	-	X
86	MG	1	3423	-	X
86	MG	1	3426	-	X
86	MG	1	3429	-	X
86	MG	1	3430	-	X
86	MG	1	3431	-	X
86	MG	1	3432	-	X
86	MG	1	3435	-	X
86	MG	1	3436	-	X
86	MG	1	3437	-	X
86	MG	1	3438	-	X
86	MG	1	3439	-	X
86	MG	1	3442	-	X
86	MG	1	3443	-	X
86	MG	1	3444	-	X
86	MG	1	3446	-	X
86	MG	1	3447	-	X
86	MG	1	3449	-	X
86	MG	1	3450	-	X
86	MG	1	3451	-	X
86	MG	1	3452	-	X
86	MG	1	3453	-	X
86	MG	1	3455	-	X
86	MG	1	3456	-	X
86	MG	1	3457	-	X
86	MG	1	3458	-	X
86	MG	1	3459	-	X
86	MG	1	3460	-	X
86	MG	1	3461	-	X
86	MG	1	3462	-	X
86	MG	1	3463	-	X
86	MG	1	3464	-	X
86	MG	1	3465	-	X
86	MG	1	3466	-	X
86	MG	1	3468	-	X
86	MG	1	3473	-	X
86	MG	1	3474	-	X
86	MG	1	3477	-	X
86	MG	1	3478	-	X
86	MG	1	3479	-	X
86	MG	1	3480	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3481	-	X
86	MG	1	3483	-	X
86	MG	1	3484	-	X
86	MG	1	3485	-	X
86	MG	1	3486	-	X
86	MG	1	3487	-	X
86	MG	1	3491	-	X
86	MG	1	3492	-	X
86	MG	1	3493	-	X
86	MG	1	3496	-	X
86	MG	1	3497	-	X
86	MG	1	3498	-	X
86	MG	1	3499	-	X
86	MG	1	3501	-	X
86	MG	1	3502	-	X
86	MG	1	3503	-	X
86	MG	1	3504	-	X
86	MG	1	3505	-	X
86	MG	1	3506	-	X
86	MG	1	3507	-	X
86	MG	1	3508	-	X
86	MG	1	3509	-	X
86	MG	1	3510	-	X
86	MG	1	3511	-	X
86	MG	1	3512	-	X
86	MG	1	3513	-	X
86	MG	1	3514	-	X
86	MG	1	3515	-	X
86	MG	1	3516	-	X
86	MG	1	3517	-	X
86	MG	1	3518	-	X
86	MG	1	3519	-	X
86	MG	1	3520	-	X
86	MG	1	3521	-	X
86	MG	1	3522	-	X
86	MG	1	3524	-	X
86	MG	1	3526	-	X
86	MG	1	3527	-	X
86	MG	1	3528	-	X
86	MG	1	3529	-	X
86	MG	1	3530	-	X
86	MG	1	3531	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3532	-	X
86	MG	1	3533	-	X
86	MG	1	3535	-	X
86	MG	1	3536	-	X
86	MG	1	3537	-	X
86	MG	1	3538	-	X
86	MG	1	3539	-	X
86	MG	1	3540	-	X
86	MG	1	3541	-	X
86	MG	1	3542	-	X
86	MG	1	3543	-	X
86	MG	1	3544	-	X
86	MG	1	3545	-	X
86	MG	1	3547	-	X
86	MG	1	3549	-	X
86	MG	1	3550	-	X
86	MG	1	3551	-	X
86	MG	1	3552	-	X
86	MG	1	3553	-	X
86	MG	1	3554	-	X
86	MG	1	3555	-	X
86	MG	1	3556	-	X
86	MG	1	3557	-	X
86	MG	1	3559	-	X
86	MG	1	3560	-	X
86	MG	1	3561	-	X
86	MG	1	3562	-	X
86	MG	1	3563	-	X
86	MG	1	3564	-	X
86	MG	1	3565	-	X
86	MG	1	3566	-	X
86	MG	1	3567	-	X
86	MG	1	3568	-	X
86	MG	1	3569	-	X
86	MG	1	3570	-	X
86	MG	1	3571	-	X
86	MG	1	3572	-	X
86	MG	1	3573	-	X
86	MG	1	3574	-	X
86	MG	1	3575	-	X
86	MG	1	3576	-	X
86	MG	1	3577	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3579	-	X
86	MG	1	3580	-	X
86	MG	1	3581	-	X
86	MG	1	3584	-	X
86	MG	1	3585	-	X
86	MG	1	3586	-	X
86	MG	1	3587	-	X
86	MG	1	3588	-	X
86	MG	1	3589	-	X
86	MG	1	3590	-	X
86	MG	1	3591	-	X
86	MG	1	3592	-	X
86	MG	1	3593	-	X
86	MG	1	3594	-	X
86	MG	1	3595	-	X
86	MG	1	3596	-	X
86	MG	1	3597	-	X
86	MG	1	3598	-	X
86	MG	1	3599	-	X
86	MG	1	3600	-	X
86	MG	1	3601	-	X
86	MG	1	3603	-	X
86	MG	1	3605	-	X
86	MG	1	3606	-	X
86	MG	1	3608	-	X
86	MG	1	3609	-	X
86	MG	1	3611	-	X
86	MG	1	3613	-	X
86	MG	1	3614	-	X
86	MG	1	3615	-	X
86	MG	1	3616	-	X
86	MG	1	3618	-	X
86	MG	1	3619	-	X
86	MG	1	3620	-	X
86	MG	1	3621	-	X
86	MG	1	3623	-	X
86	MG	1	3624	-	X
86	MG	1	3625	-	X
86	MG	1	3626	-	X
86	MG	1	3630	-	X
86	MG	1	3632	-	X
86	MG	1	3633	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3635	-	X
86	MG	1	3638	-	X
86	MG	1	3642	-	X
86	MG	1	3645	-	X
86	MG	1	3647	-	X
86	MG	1	3648	-	X
86	MG	1	3649	-	X
86	MG	1	3650	-	X
86	MG	1	3651	-	X
86	MG	1	3652	-	X
86	MG	1	3656	-	X
86	MG	1	3657	-	X
86	MG	1	3658	-	X
86	MG	1	3660	-	X
86	MG	1	3664	-	X
86	MG	1	3667	-	X
86	MG	1	3669	-	X
86	MG	1	3673	-	X
86	MG	1	3674	-	X
86	MG	1	3675	-	X
86	MG	1	3677	-	X
86	MG	1	3679	-	X
86	MG	1	3682	-	X
86	MG	1	3684	-	X
86	MG	1	3685	-	X
86	MG	1	3686	-	X
86	MG	1	3687	-	X
86	MG	1	3690	-	X
86	MG	1	3693	-	X
86	MG	1	3694	-	X
86	MG	1	3696	-	X
86	MG	1	3697	-	X
86	MG	1	3699	-	X
86	MG	1	3700	-	X
86	MG	1	3701	-	X
86	MG	1	3702	-	X
86	MG	1	3703	-	X
86	MG	1	3704	-	X
86	MG	1	3705	-	X
86	MG	1	3709	-	X
86	MG	1	3711	-	X
86	MG	1	3712	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3713	-	X
86	MG	1	3718	-	X
86	MG	1	3720	-	X
86	MG	1	3721	-	X
86	MG	1	3725	-	X
86	MG	1	3729	-	X
86	MG	1	3730	-	X
86	MG	1	3732	-	X
86	MG	1	3733	-	X
86	MG	1	3734	-	X
86	MG	1	3737	-	X
86	MG	1	3739	-	X
86	MG	1	3740	-	X
86	MG	1	3741	-	X
86	MG	1	3745	-	X
86	MG	1	3746	-	X
86	MG	1	3747	-	X
86	MG	1	3750	-	X
86	MG	1	3752	-	X
86	MG	1	3754	-	X
86	MG	1	3759	-	X
86	MG	1	3761	-	X
86	MG	1	3762	-	X
86	MG	1	3763	-	X
86	MG	1	3764	-	X
86	MG	1	3765	-	X
86	MG	1	3769	-	X
86	MG	1	3775	-	X
86	MG	1	3778	-	X
86	MG	1	3783	-	X
86	MG	1	3785	-	X
86	MG	1	3787	-	X
86	MG	1	3792	-	X
86	MG	1	3793	-	X
86	MG	1	3795	-	X
86	MG	1	3797	-	X
86	MG	1	3803	-	X
86	MG	1	3804	-	X
86	MG	1	3805	-	X
86	MG	1	3807	-	X
86	MG	1	3808	-	X
86	MG	1	3812	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	1	3813	-	X
86	MG	1	3814	-	X
86	MG	1	3815	-	X
86	MG	1	3816	-	X
86	MG	1	3817	-	X
86	MG	1	3821	-	X
86	MG	1	3826	-	X
86	MG	1	3829	-	X
86	MG	1	3830	-	X
86	MG	1	3832	-	X
86	MG	1	3834	-	X
86	MG	1	3835	-	X
86	MG	1	3836	-	X
86	MG	1	3838	-	X
86	MG	1	3840	-	X
86	MG	1	3843	-	X
86	MG	1	3844	-	X
86	MG	1	3845	-	X
86	MG	1	3846	-	X
86	MG	1	3849	-	X
86	MG	1	3850	-	X
86	MG	1	3851	-	X
86	MG	1	3853	-	X
86	MG	1	3854	-	X
86	MG	1	3855	-	X
86	MG	1	3856	-	X
86	MG	1	3859	-	X
86	MG	1	3860	-	X
86	MG	1	3861	-	X
86	MG	1	4218	-	X
86	MG	1	4222	-	X
86	MG	1	4223	-	X
86	MG	2	1902	-	X
86	MG	2	1903	-	X
86	MG	2	1904	-	X
86	MG	2	1905	-	X
86	MG	2	1906	-	X
86	MG	2	1907	-	X
86	MG	2	1908	-	X
86	MG	2	1909	-	X
86	MG	2	1910	-	X
86	MG	2	1912	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	2	1913	-	X
86	MG	2	1914	-	X
86	MG	2	1915	-	X
86	MG	2	1917	-	X
86	MG	2	1918	-	X
86	MG	2	1919	-	X
86	MG	2	1921	-	X
86	MG	2	1922	-	X
86	MG	2	1923	-	X
86	MG	2	1924	-	X
86	MG	2	1925	-	X
86	MG	2	1926	-	X
86	MG	2	1927	-	X
86	MG	2	1928	-	X
86	MG	2	1929	-	X
86	MG	2	1930	-	X
86	MG	2	1931	-	X
86	MG	2	1932	-	X
86	MG	2	1933	-	X
86	MG	2	1934	-	X
86	MG	2	1935	-	X
86	MG	2	1936	-	X
86	MG	2	1937	-	X
86	MG	2	1938	-	X
86	MG	2	1940	-	X
86	MG	2	1941	-	X
86	MG	2	1942	-	X
86	MG	2	1945	-	X
86	MG	2	1947	-	X
86	MG	2	1949	-	X
86	MG	2	1951	-	X
86	MG	2	1953	-	X
86	MG	2	1954	-	X
86	MG	2	1955	-	X
86	MG	2	1956	-	X
86	MG	2	1957	-	X
86	MG	2	1958	-	X
86	MG	2	1959	-	X
86	MG	2	1960	-	X
86	MG	2	1961	-	X
86	MG	2	1962	-	X
86	MG	2	1963	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	2	1964	-	X
86	MG	2	1967	-	X
86	MG	2	1971	-	X
86	MG	2	1972	-	X
86	MG	2	1973	-	X
86	MG	2	1974	-	X
86	MG	2	1975	-	X
86	MG	2	1976	-	X
86	MG	2	1977	-	X
86	MG	2	1978	-	X
86	MG	2	1980	-	X
86	MG	2	1981	-	X
86	MG	2	1985	-	X
86	MG	2	1987	-	X
86	MG	2	1988	-	X
86	MG	2	1991	-	X
86	MG	2	1993	-	X
86	MG	2	1995	-	X
86	MG	2	1999	-	X
86	MG	2	2000	-	X
86	MG	2	2001	-	X
86	MG	2	2002	-	X
86	MG	2	2005	-	X
86	MG	2	2006	-	X
86	MG	2	2007	-	X
86	MG	2	2008	-	X
86	MG	2	2009	-	X
86	MG	2	2010	-	X
86	MG	2	2011	-	X
86	MG	2	2012	-	X
86	MG	2	2013	-	X
86	MG	2	2015	-	X
86	MG	2	2016	-	X
86	MG	2	2017	-	X
86	MG	2	2018	-	X
86	MG	3	201	-	X
86	MG	3	202	-	X
86	MG	3	204	-	X
86	MG	3	205	-	X
86	MG	3	206	-	X
86	MG	3	207	-	X
86	MG	3	209	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	3	212	-	X
86	MG	3	213	-	X
86	MG	3	214	-	X
86	MG	4	203	-	X
86	MG	4	204	-	X
86	MG	4	206	-	X
86	MG	4	207	-	X
86	MG	4	211	-	X
86	MG	4	215	-	X
86	MG	4	221	-	X
86	MG	4	222	-	X
86	MG	5	3401	-	X
86	MG	5	3402	-	X
86	MG	5	3403	-	X
86	MG	5	3405	-	X
86	MG	5	3406	-	X
86	MG	5	3409	-	X
86	MG	5	3410	-	X
86	MG	5	3411	-	X
86	MG	5	3413	-	X
86	MG	5	3414	-	X
86	MG	5	3416	-	X
86	MG	5	3417	-	X
86	MG	5	3418	-	X
86	MG	5	3420	-	X
86	MG	5	3421	-	X
86	MG	5	3422	-	X
86	MG	5	3424	-	X
86	MG	5	3425	-	X
86	MG	5	3426	-	X
86	MG	5	3428	-	X
86	MG	5	3429	-	X
86	MG	5	3431	-	X
86	MG	5	3433	-	X
86	MG	5	3434	-	X
86	MG	5	3435	-	X
86	MG	5	3438	-	X
86	MG	5	3439	-	X
86	MG	5	3440	-	X
86	MG	5	3441	-	X
86	MG	5	3443	-	X
86	MG	5	3444	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3445	-	X
86	MG	5	3447	-	X
86	MG	5	3448	-	X
86	MG	5	3450	-	X
86	MG	5	3451	-	X
86	MG	5	3452	-	X
86	MG	5	3455	-	X
86	MG	5	3456	-	X
86	MG	5	3458	-	X
86	MG	5	3459	-	X
86	MG	5	3462	-	X
86	MG	5	3464	-	X
86	MG	5	3465	-	X
86	MG	5	3467	-	X
86	MG	5	3468	-	X
86	MG	5	3469	-	X
86	MG	5	3471	-	X
86	MG	5	3472	-	X
86	MG	5	3473	-	X
86	MG	5	3475	-	X
86	MG	5	3477	-	X
86	MG	5	3478	-	X
86	MG	5	3479	-	X
86	MG	5	3480	-	X
86	MG	5	3481	-	X
86	MG	5	3482	-	X
86	MG	5	3484	-	X
86	MG	5	3485	-	X
86	MG	5	3487	-	X
86	MG	5	3489	-	X
86	MG	5	3491	-	X
86	MG	5	3493	-	X
86	MG	5	3494	-	X
86	MG	5	3496	-	X
86	MG	5	3498	-	X
86	MG	5	3499	-	X
86	MG	5	3500	-	X
86	MG	5	3501	-	X
86	MG	5	3502	-	X
86	MG	5	3504	-	X
86	MG	5	3505	-	X
86	MG	5	3506	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3507	-	X
86	MG	5	3508	-	X
86	MG	5	3509	-	X
86	MG	5	3510	-	X
86	MG	5	3511	-	X
86	MG	5	3512	-	X
86	MG	5	3514	-	X
86	MG	5	3515	-	X
86	MG	5	3516	-	X
86	MG	5	3517	-	X
86	MG	5	3518	-	X
86	MG	5	3519	-	X
86	MG	5	3520	-	X
86	MG	5	3521	-	X
86	MG	5	3522	-	X
86	MG	5	3523	-	X
86	MG	5	3524	-	X
86	MG	5	3525	-	X
86	MG	5	3526	-	X
86	MG	5	3527	-	X
86	MG	5	3528	-	X
86	MG	5	3530	-	X
86	MG	5	3531	-	X
86	MG	5	3532	-	X
86	MG	5	3533	-	X
86	MG	5	3534	-	X
86	MG	5	3536	-	X
86	MG	5	3537	-	X
86	MG	5	3538	-	X
86	MG	5	3539	-	X
86	MG	5	3540	-	X
86	MG	5	3541	-	X
86	MG	5	3542	-	X
86	MG	5	3543	-	X
86	MG	5	3544	-	X
86	MG	5	3545	-	X
86	MG	5	3546	-	X
86	MG	5	3547	-	X
86	MG	5	3549	-	X
86	MG	5	3550	-	X
86	MG	5	3551	-	X
86	MG	5	3552	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3553	-	X
86	MG	5	3554	-	X
86	MG	5	3555	-	X
86	MG	5	3556	-	X
86	MG	5	3557	-	X
86	MG	5	3558	-	X
86	MG	5	3560	-	X
86	MG	5	3561	-	X
86	MG	5	3562	-	X
86	MG	5	3563	-	X
86	MG	5	3564	-	X
86	MG	5	3565	-	X
86	MG	5	3566	-	X
86	MG	5	3567	-	X
86	MG	5	3568	-	X
86	MG	5	3569	-	X
86	MG	5	3570	-	X
86	MG	5	3571	-	X
86	MG	5	3572	-	X
86	MG	5	3573	-	X
86	MG	5	3574	-	X
86	MG	5	3575	-	X
86	MG	5	3576	-	X
86	MG	5	3577	-	X
86	MG	5	3578	-	X
86	MG	5	3579	-	X
86	MG	5	3580	-	X
86	MG	5	3581	-	X
86	MG	5	3582	-	X
86	MG	5	3583	-	X
86	MG	5	3584	-	X
86	MG	5	3585	-	X
86	MG	5	3586	-	X
86	MG	5	3587	-	X
86	MG	5	3588	-	X
86	MG	5	3589	-	X
86	MG	5	3590	-	X
86	MG	5	3591	-	X
86	MG	5	3592	-	X
86	MG	5	3593	-	X
86	MG	5	3594	-	X
86	MG	5	3595	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3596	-	X
86	MG	5	3597	-	X
86	MG	5	3598	-	X
86	MG	5	3599	-	X
86	MG	5	3601	-	X
86	MG	5	3609	-	X
86	MG	5	3610	-	X
86	MG	5	3611	-	X
86	MG	5	3612	-	X
86	MG	5	3614	-	X
86	MG	5	3616	-	X
86	MG	5	3617	-	X
86	MG	5	3620	-	X
86	MG	5	3622	-	X
86	MG	5	3623	-	X
86	MG	5	3624	-	X
86	MG	5	3626	-	X
86	MG	5	3627	-	X
86	MG	5	3628	-	X
86	MG	5	3629	-	X
86	MG	5	3630	-	X
86	MG	5	3631	-	X
86	MG	5	3632	-	X
86	MG	5	3634	-	X
86	MG	5	3636	-	X
86	MG	5	3637	-	X
86	MG	5	3638	-	X
86	MG	5	3639	-	X
86	MG	5	3641	-	X
86	MG	5	3644	-	X
86	MG	5	3647	-	X
86	MG	5	3648	-	X
86	MG	5	3649	-	X
86	MG	5	3650	-	X
86	MG	5	3651	-	X
86	MG	5	3652	-	X
86	MG	5	3653	-	X
86	MG	5	3655	-	X
86	MG	5	3657	-	X
86	MG	5	3658	-	X
86	MG	5	3659	-	X
86	MG	5	3660	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3662	-	X
86	MG	5	3664	-	X
86	MG	5	3665	-	X
86	MG	5	3667	-	X
86	MG	5	3668	-	X
86	MG	5	3670	-	X
86	MG	5	3673	-	X
86	MG	5	3675	-	X
86	MG	5	3676	-	X
86	MG	5	3680	-	X
86	MG	5	3681	-	X
86	MG	5	3683	-	X
86	MG	5	3687	-	X
86	MG	5	3689	-	X
86	MG	5	3692	-	X
86	MG	5	3694	-	X
86	MG	5	3697	-	X
86	MG	5	3699	-	X
86	MG	5	3701	-	X
86	MG	5	3704	-	X
86	MG	5	3705	-	X
86	MG	5	3709	-	X
86	MG	5	3710	-	X
86	MG	5	3711	-	X
86	MG	5	3717	-	X
86	MG	5	3719	-	X
86	MG	5	3720	-	X
86	MG	5	3721	-	X
86	MG	5	3725	-	X
86	MG	5	3726	-	X
86	MG	5	3729	-	X
86	MG	5	3730	-	X
86	MG	5	3731	-	X
86	MG	5	3732	-	X
86	MG	5	3734	-	X
86	MG	5	3736	-	X
86	MG	5	3737	-	X
86	MG	5	3738	-	X
86	MG	5	3739	-	X
86	MG	5	3740	-	X
86	MG	5	3742	-	X
86	MG	5	3744	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3747	-	X
86	MG	5	3749	-	X
86	MG	5	3753	-	X
86	MG	5	3754	-	X
86	MG	5	3757	-	X
86	MG	5	3759	-	X
86	MG	5	3760	-	X
86	MG	5	3763	-	X
86	MG	5	3764	-	X
86	MG	5	3765	-	X
86	MG	5	3766	-	X
86	MG	5	3770	-	X
86	MG	5	3772	-	X
86	MG	5	3774	-	X
86	MG	5	3775	-	X
86	MG	5	3778	-	X
86	MG	5	3780	-	X
86	MG	5	3781	-	X
86	MG	5	3782	-	X
86	MG	5	3783	-	X
86	MG	5	3785	-	X
86	MG	5	3786	-	X
86	MG	5	3787	-	X
86	MG	5	3792	-	X
86	MG	5	3793	-	X
86	MG	5	3802	-	X
86	MG	5	3804	-	X
86	MG	5	3805	-	X
86	MG	5	3807	-	X
86	MG	5	3809	-	X
86	MG	5	3812	-	X
86	MG	5	3814	-	X
86	MG	5	3822	-	X
86	MG	5	3823	-	X
86	MG	5	3825	-	X
86	MG	5	3826	-	X
86	MG	5	3828	-	X
86	MG	5	3829	-	X
86	MG	5	3830	-	X
86	MG	5	3834	-	X
86	MG	5	3835	-	X
86	MG	5	3836	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	5	3837	-	X
86	MG	5	3844	-	X
86	MG	5	3846	-	X
86	MG	5	3848	-	X
86	MG	5	3849	-	X
86	MG	5	3850	-	X
86	MG	5	3851	-	X
86	MG	5	3852	-	X
86	MG	5	3854	-	X
86	MG	5	3857	-	X
86	MG	5	3858	-	X
86	MG	5	3861	-	X
86	MG	5	3862	-	X
86	MG	5	3864	-	X
86	MG	5	3865	-	X
86	MG	5	3866	-	X
86	MG	5	3867	-	X
86	MG	5	3868	-	X
86	MG	5	3872	-	X
86	MG	5	3874	-	X
86	MG	5	3875	-	X
86	MG	5	3877	-	X
86	MG	5	3878	-	X
86	MG	5	3880	-	X
86	MG	5	3881	-	X
86	MG	5	3882	-	X
86	MG	5	3883	-	X
86	MG	5	3884	-	X
86	MG	5	3885	-	X
86	MG	5	3889	-	X
86	MG	5	3890	-	X
86	MG	5	3894	-	X
86	MG	5	3895	-	X
86	MG	5	3896	-	X
86	MG	5	3897	-	X
86	MG	5	3899	-	X
86	MG	5	4253	-	X
86	MG	5	4254	-	X
86	MG	5	4255	-	X
86	MG	5	4256	-	X
86	MG	5	4257	-	X
86	MG	5	4258	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	6	1901	-	X
86	MG	6	1902	-	X
86	MG	6	1903	-	X
86	MG	6	1904	-	X
86	MG	6	1906	-	X
86	MG	6	1907	-	X
86	MG	6	1908	-	X
86	MG	6	1909	-	X
86	MG	6	1911	-	X
86	MG	6	1912	-	X
86	MG	6	1914	-	X
86	MG	6	1916	-	X
86	MG	6	1917	-	X
86	MG	6	1918	-	X
86	MG	6	1919	-	X
86	MG	6	1920	-	X
86	MG	6	1921	-	X
86	MG	6	1922	-	X
86	MG	6	1923	-	X
86	MG	6	1925	-	X
86	MG	6	1926	-	X
86	MG	6	1927	-	X
86	MG	6	1928	-	X
86	MG	6	1929	-	X
86	MG	6	1930	-	X
86	MG	6	1931	-	X
86	MG	6	1932	-	X
86	MG	6	1933	-	X
86	MG	6	1934	-	X
86	MG	6	1935	-	X
86	MG	6	1936	-	X
86	MG	6	1937	-	X
86	MG	6	1938	-	X
86	MG	6	1939	-	X
86	MG	6	1940	-	X
86	MG	6	1941	-	X
86	MG	6	1942	-	X
86	MG	6	1943	-	X
86	MG	6	1944	-	X
86	MG	6	1945	-	X
86	MG	6	1946	-	X
86	MG	6	1947	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	6	1948	-	X
86	MG	6	1949	-	X
86	MG	6	1950	-	X
86	MG	6	1951	-	X
86	MG	6	1952	-	X
86	MG	6	1953	-	X
86	MG	6	1954	-	X
86	MG	6	1955	-	X
86	MG	6	1956	-	X
86	MG	6	1958	-	X
86	MG	6	1959	-	X
86	MG	6	1960	-	X
86	MG	6	1961	-	X
86	MG	6	1963	-	X
86	MG	6	1964	-	X
86	MG	6	1966	-	X
86	MG	6	1967	-	X
86	MG	6	1968	-	X
86	MG	6	1972	-	X
86	MG	6	1974	-	X
86	MG	6	1975	-	X
86	MG	6	1977	-	X
86	MG	6	1979	-	X
86	MG	6	1980	-	X
86	MG	6	1981	-	X
86	MG	6	1982	-	X
86	MG	6	1983	-	X
86	MG	6	1985	-	X
86	MG	6	1986	-	X
86	MG	6	1989	-	X
86	MG	6	1992	-	X
86	MG	6	1993	-	X
86	MG	6	2001	-	X
86	MG	6	2008	-	X
86	MG	6	2011	-	X
86	MG	6	2012	-	X
86	MG	6	2013	-	X
86	MG	6	2014	-	X
86	MG	6	2016	-	X
86	MG	6	2017	-	X
86	MG	6	2019	-	X
86	MG	6	2020	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	6	2023	-	X
86	MG	6	2027	-	X
86	MG	6	2028	-	X
86	MG	6	2029	-	X
86	MG	6	2031	-	X
86	MG	6	2034	-	X
86	MG	6	2035	-	X
86	MG	6	2037	-	X
86	MG	6	2038	-	X
86	MG	6	2039	-	X
86	MG	6	2040	-	X
86	MG	6	2042	-	X
86	MG	6	2043	-	X
86	MG	6	2046	-	X
86	MG	7	201	-	X
86	MG	7	202	-	X
86	MG	7	203	-	X
86	MG	7	204	-	X
86	MG	7	205	-	X
86	MG	7	206	-	X
86	MG	7	207	-	X
86	MG	7	209	-	X
86	MG	7	212	-	X
86	MG	7	213	-	X
86	MG	7	214	-	X
86	MG	8	201	-	X
86	MG	8	203	-	X
86	MG	8	206	-	X
86	MG	8	208	-	X
86	MG	8	212	-	X
86	MG	D0	201	-	X
86	MG	L3	401	-	X
86	MG	L5	301	-	X
86	MG	M0	301	-	X
86	MG	M1	201	-	X
86	MG	M3	203	-	X
86	MG	M7	202	-	X
86	MG	M7	203	-	X
86	MG	N3	201	-	X
86	MG	N3	202	-	X
86	MG	N3	203	-	X
86	MG	N8	202	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	MG	N8	204	-	X
86	MG	O1	201	-	X
86	MG	O3	201	-	X
86	MG	c7	202	-	X
86	MG	c8	201	-	X
86	MG	d3	201	-	X
86	MG	d4	201	-	X
86	MG	l2	301	-	X
86	MG	l3	401	-	X
86	MG	l5	302	-	X
86	MG	l7	301	-	X
86	MG	l8	301	-	X
86	MG	m1	201	-	X
86	MG	m7	201	-	X
86	MG	m7	202	-	X
86	MG	m7	203	-	X
86	MG	n0	201	-	X
86	MG	n3	201	-	X
86	MG	n8	202	-	X
86	MG	o1	202	-	X
86	MG	o3	201	-	X
86	MG	q0	202	-	X
86	MG	s6	301	-	X
87	OHX	1	3864	-	X
87	OHX	1	3865	-	X
87	OHX	1	3870	-	X
87	OHX	1	3872	-	X
87	OHX	1	3877	-	X
87	OHX	1	3881	-	X
87	OHX	1	3888	-	X
87	OHX	1	3903	-	X
87	OHX	1	3908	-	X
87	OHX	1	3977	-	X
87	OHX	1	4013	-	X
87	OHX	1	4033	-	X
87	OHX	1	4042	-	X
87	OHX	1	4045	-	X
87	OHX	1	4057	-	X
87	OHX	1	4061	-	X
87	OHX	1	4062	-	X
87	OHX	1	4063	-	X
87	OHX	1	4066	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	1	4067	-	X
87	OHX	1	4069	-	X
87	OHX	1	4072	-	X
87	OHX	1	4081	-	X
87	OHX	1	4094	-	X
87	OHX	1	4095	-	X
87	OHX	1	4097	-	X
87	OHX	1	4098	-	X
87	OHX	1	4100	-	X
87	OHX	1	4104	-	X
87	OHX	1	4107	-	X
87	OHX	1	4109	-	X
87	OHX	1	4110	-	X
87	OHX	1	4111	-	X
87	OHX	1	4112	-	X
87	OHX	1	4114	-	X
87	OHX	1	4115	-	X
87	OHX	1	4118	-	X
87	OHX	1	4119	-	X
87	OHX	1	4120	-	X
87	OHX	1	4121	-	X
87	OHX	1	4122	-	X
87	OHX	1	4125	-	X
87	OHX	1	4127	-	X
87	OHX	1	4128	-	X
87	OHX	1	4129	-	X
87	OHX	1	4132	-	X
87	OHX	1	4133	-	X
87	OHX	1	4135	-	X
87	OHX	1	4137	-	X
87	OHX	1	4138	-	X
87	OHX	1	4139	-	X
87	OHX	1	4141	-	X
87	OHX	1	4142	-	X
87	OHX	1	4143	-	X
87	OHX	1	4146	-	X
87	OHX	1	4147	-	X
87	OHX	1	4148	-	X
87	OHX	1	4149	-	X
87	OHX	1	4152	-	X
87	OHX	1	4153	-	X
87	OHX	1	4154	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	1	4157	-	X
87	OHX	1	4158	-	X
87	OHX	1	4159	-	X
87	OHX	1	4160	-	X
87	OHX	1	4162	-	X
87	OHX	1	4163	-	X
87	OHX	1	4164	-	X
87	OHX	1	4166	-	X
87	OHX	1	4167	-	X
87	OHX	1	4168	-	X
87	OHX	1	4169	-	X
87	OHX	1	4170	-	X
87	OHX	1	4171	-	X
87	OHX	1	4173	-	X
87	OHX	1	4174	-	X
87	OHX	1	4175	-	X
87	OHX	1	4176	-	X
87	OHX	1	4177	-	X
87	OHX	1	4179	-	X
87	OHX	1	4180	-	X
87	OHX	1	4181	-	X
87	OHX	1	4182	-	X
87	OHX	1	4184	-	X
87	OHX	1	4185	-	X
87	OHX	1	4186	-	X
87	OHX	1	4188	-	X
87	OHX	1	4189	-	X
87	OHX	1	4190	-	X
87	OHX	1	4191	-	X
87	OHX	1	4192	-	X
87	OHX	1	4195	-	X
87	OHX	1	4197	-	X
87	OHX	1	4200	-	X
87	OHX	1	4201	-	X
87	OHX	1	4202	-	X
87	OHX	1	4203	-	X
87	OHX	1	4204	-	X
87	OHX	1	4205	-	X
87	OHX	1	4207	-	X
87	OHX	1	4208	-	X
87	OHX	1	4209	-	X
87	OHX	1	4210	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	1	4211	-	X
87	OHX	1	4213	-	X
87	OHX	1	4214	-	X
87	OHX	2	2022	-	X
87	OHX	2	2024	-	X
87	OHX	2	2039	-	X
87	OHX	2	2063	-	X
87	OHX	2	2073	-	X
87	OHX	2	2074	-	X
87	OHX	2	2078	-	X
87	OHX	2	2083	-	X
87	OHX	2	2090	-	X
87	OHX	2	2098	-	X
87	OHX	2	2107	-	X
87	OHX	2	2111	-	X
87	OHX	2	2112	-	X
87	OHX	2	2115	-	X
87	OHX	2	2116	-	X
87	OHX	2	2118	-	X
87	OHX	2	2121	-	X
87	OHX	2	2122	-	X
87	OHX	2	2124	-	X
87	OHX	2	2127	-	X
87	OHX	2	2134	-	X
87	OHX	2	2135	-	X
87	OHX	2	2136	-	X
87	OHX	2	2142	-	X
87	OHX	2	2144	-	X
87	OHX	2	2145	-	X
87	OHX	2	2147	-	X
87	OHX	2	2151	-	X
87	OHX	2	2152	-	X
87	OHX	2	2153	-	X
87	OHX	2	2156	-	X
87	OHX	2	2158	-	X
87	OHX	2	2159	-	X
87	OHX	2	2161	-	X
87	OHX	2	2162	-	X
87	OHX	2	2163	-	X
87	OHX	2	2164	-	X
87	OHX	2	2168	-	X
87	OHX	2	2170	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	2	2171	-	X
87	OHX	2	2172	-	X
87	OHX	2	2174	-	X
87	OHX	2	2175	-	X
87	OHX	2	2177	-	X
87	OHX	2	2178	-	X
87	OHX	3	223	-	X
87	OHX	3	224	-	X
87	OHX	3	225	-	X
87	OHX	4	229	-	X
87	OHX	4	233	-	X
87	OHX	4	234	-	X
87	OHX	4	235	-	X
87	OHX	4	236	-	X
87	OHX	5	3901	-	X
87	OHX	5	3902	-	X
87	OHX	5	3905	-	X
87	OHX	5	3910	-	X
87	OHX	5	3913	-	X
87	OHX	5	3952	-	X
87	OHX	5	4040	-	X
87	OHX	5	4045	-	X
87	OHX	5	4054	-	X
87	OHX	5	4063	-	X
87	OHX	5	4073	-	X
87	OHX	5	4077	-	X
87	OHX	5	4083	-	X
87	OHX	5	4087	-	X
87	OHX	5	4092	-	X
87	OHX	5	4093	-	X
87	OHX	5	4100	-	X
87	OHX	5	4105	-	X
87	OHX	5	4111	-	X
87	OHX	5	4113	-	X
87	OHX	5	4115	-	X
87	OHX	5	4124	-	X
87	OHX	5	4126	-	X
87	OHX	5	4128	-	X
87	OHX	5	4133	-	X
87	OHX	5	4135	-	X
87	OHX	5	4138	-	X
87	OHX	5	4139	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	5	4141	-	X
87	OHX	5	4142	-	X
87	OHX	5	4144	-	X
87	OHX	5	4146	-	X
87	OHX	5	4147	-	X
87	OHX	5	4148	-	X
87	OHX	5	4149	-	X
87	OHX	5	4150	-	X
87	OHX	5	4151	-	X
87	OHX	5	4152	-	X
87	OHX	5	4153	-	X
87	OHX	5	4154	-	X
87	OHX	5	4156	-	X
87	OHX	5	4158	-	X
87	OHX	5	4159	-	X
87	OHX	5	4160	-	X
87	OHX	5	4161	-	X
87	OHX	5	4162	-	X
87	OHX	5	4166	-	X
87	OHX	5	4172	-	X
87	OHX	5	4173	-	X
87	OHX	5	4174	-	X
87	OHX	5	4175	-	X
87	OHX	5	4176	-	X
87	OHX	5	4177	-	X
87	OHX	5	4178	-	X
87	OHX	5	4179	-	X
87	OHX	5	4181	-	X
87	OHX	5	4183	-	X
87	OHX	5	4184	-	X
87	OHX	5	4185	-	X
87	OHX	5	4186	-	X
87	OHX	5	4187	-	X
87	OHX	5	4188	-	X
87	OHX	5	4190	-	X
87	OHX	5	4191	-	X
87	OHX	5	4192	-	X
87	OHX	5	4193	-	X
87	OHX	5	4195	-	X
87	OHX	5	4196	-	X
87	OHX	5	4197	-	X
87	OHX	5	4201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	5	4202	-	X
87	OHX	5	4203	-	X
87	OHX	5	4204	-	X
87	OHX	5	4205	-	X
87	OHX	5	4207	-	X
87	OHX	5	4209	-	X
87	OHX	5	4212	-	X
87	OHX	5	4213	-	X
87	OHX	5	4215	-	X
87	OHX	5	4217	-	X
87	OHX	5	4218	-	X
87	OHX	5	4219	-	X
87	OHX	5	4220	-	X
87	OHX	5	4221	-	X
87	OHX	5	4222	-	X
87	OHX	5	4223	-	X
87	OHX	5	4226	-	X
87	OHX	5	4228	-	X
87	OHX	5	4229	-	X
87	OHX	5	4230	-	X
87	OHX	5	4231	-	X
87	OHX	5	4233	-	X
87	OHX	5	4234	-	X
87	OHX	5	4235	-	X
87	OHX	5	4236	-	X
87	OHX	5	4237	-	X
87	OHX	5	4239	-	X
87	OHX	5	4240	-	X
87	OHX	5	4244	-	X
87	OHX	5	4245	-	X
87	OHX	5	4246	-	X
87	OHX	5	4247	-	X
87	OHX	5	4248	-	X
87	OHX	5	4249	-	X
87	OHX	5	4250	-	X
87	OHX	6	2048	-	X
87	OHX	6	2051	-	X
87	OHX	6	2053	-	X
87	OHX	6	2092	-	X
87	OHX	6	2113	-	X
87	OHX	6	2116	-	X
87	OHX	6	2118	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	6	2122	-	X
87	OHX	6	2127	-	X
87	OHX	6	2134	-	X
87	OHX	6	2135	-	X
87	OHX	6	2137	-	X
87	OHX	6	2141	-	X
87	OHX	6	2145	-	X
87	OHX	6	2148	-	X
87	OHX	6	2158	-	X
87	OHX	6	2159	-	X
87	OHX	6	2161	-	X
87	OHX	6	2162	-	X
87	OHX	6	2164	-	X
87	OHX	6	2166	-	X
87	OHX	6	2169	-	X
87	OHX	6	2170	-	X
87	OHX	6	2171	-	X
87	OHX	6	2172	-	X
87	OHX	6	2175	-	X
87	OHX	6	2177	-	X
87	OHX	6	2178	-	X
87	OHX	6	2179	-	X
87	OHX	6	2181	-	X
87	OHX	6	2182	-	X
87	OHX	6	2184	-	X
87	OHX	6	2185	-	X
87	OHX	6	2187	-	X
87	OHX	6	2188	-	X
87	OHX	6	2189	-	X
87	OHX	6	2190	-	X
87	OHX	6	2191	-	X
87	OHX	6	2192	-	X
87	OHX	6	2195	-	X
87	OHX	6	2196	-	X
87	OHX	6	2198	-	X
87	OHX	6	2199	-	X
87	OHX	6	2200	-	X
87	OHX	6	2204	-	X
87	OHX	6	2205	-	X
87	OHX	7	223	-	X
87	OHX	7	226	-	X
87	OHX	7	227	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	OHX	8	220	-	X
87	OHX	8	224	-	X
87	OHX	8	225	-	X
87	OHX	8	227	-	X
87	OHX	8	228	-	X
87	OHX	L3	404	-	X
87	OHX	M7	207	-	X
87	OHX	O9	101	-	X
87	OHX	l4	404	-	X
87	OHX	l5	305	-	X
87	OHX	m4	201	-	X
87	OHX	m7	205	-	X
87	OHX	m8	201	-	X
87	OHX	s4	301	-	X
87	OHX	s9	201	-	X
89	3HE	5	4252	-	X

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411205 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 RNA (1750-MER).

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
			892	562	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	104	ALA	GLY	conflict	UNP P48589
C2	110	ALA	GLY	conflict	UNP P48589
c2	104	ALA	GLY	conflict	UNP P48589
c2	110	ALA	GLY	conflict	UNP P48589

- 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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	c6	142	Total	C	N	O	0	0	0
			1111	711	204	196			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 Uncultured eukaryote clone NS4T.275 18S ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence.

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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	l8	231	Total	C	N	O	S	0	0	0
			1764	1131	316	314	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
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	0	0	0
			1053	675	199	177			
50	m4	137	Total	C	N	O	0	0	0
			1059	678	200	179			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein 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 Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

- Molecule 82 is a protein called UNKNOWN PROTEIN m2.

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

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

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

- Molecule 84 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	L7	3	Total	Mg	0	0
			3	3		
86	m7	4	Total	Mg	0	0
			4	4		
86	n8	3	Total	Mg	0	0
			3	3		
86	o1	2	Total	Mg	0	0
			2	2		
86	N5	1	Total	Mg	0	0
			1	1		
86	6	147	Total	Mg	0	0
			147	147		
86	sM	2	Total	Mg	0	0
			2	2		
86	O4	2	Total	Mg	0	0
			2	2		
86	m5	2	Total	Mg	0	0
			2	2		
86	l3	1	Total	Mg	0	0
			1	1		
86	M1	1	Total	Mg	0	0
			1	1		
86	n0	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	d6	1	Total 1	Mg 1	0	0
86	2	122	Total 122	Mg 122	0	0
86	O3	1	Total 1	Mg 1	0	0
86	L4	1	Total 1	Mg 1	0	0
86	l7	1	Total 1	Mg 1	0	0
86	M5	2	Total 2	Mg 2	0	0
86	l4	2	Total 2	Mg 2	0	0
86	S2	1	Total 1	Mg 1	0	0
86	L8	1	Total 1	Mg 1	0	0
86	D3	1	Total 1	Mg 1	0	0
86	o4	2	Total 2	Mg 2	0	0
86	M9	1	Total 1	Mg 1	0	0
86	q0	1	Total 1	Mg 1	0	0
86	SM	1	Total 1	Mg 1	0	0
86	c8	2	Total 2	Mg 2	0	0
86	M0	2	Total 2	Mg 2	0	0
86	c1	1	Total 1	Mg 1	0	0
86	5	505	Total 505	Mg 505	0	0
86	L5	1	Total 1	Mg 1	0	0
86	O7	1	Total 1	Mg 1	0	0
86	s6	1	Total 1	Mg 1	0	0

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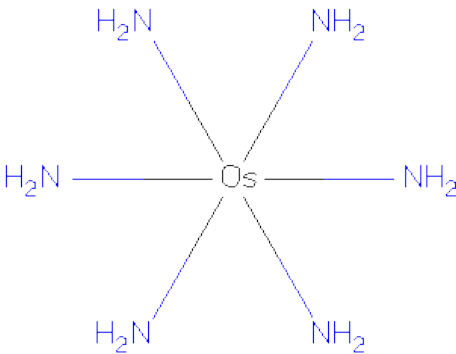
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	Q2	1	Total 1	Mg 1	0	0
86	1	471	Total 471	Mg 471	0	0
86	c4	1	Total 1	Mg 1	0	0
86	D0	1	Total 1	Mg 1	0	0
86	S8	1	Total 1	Mg 1	0	0
86	m1	2	Total 2	Mg 2	0	0
86	d3	1	Total 1	Mg 1	0	0
86	q3	2	Total 2	Mg 2	0	0
86	o3	1	Total 1	Mg 1	0	0
86	M3	4	Total 4	Mg 4	0	0
86	N3	3	Total 3	Mg 3	0	0
86	4	22	Total 22	Mg 22	0	0
86	n6	2	Total 2	Mg 2	0	0
86	S4	1	Total 1	Mg 1	0	0
86	L2	1	Total 1	Mg 1	0	0
86	o7	1	Total 1	Mg 1	0	0
86	l5	2	Total 2	Mg 2	0	0
86	C3	1	Total 1	Mg 1	0	0
86	M7	6	Total 6	Mg 6	0	0
86	N8	4	Total 4	Mg 4	0	0
86	s1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
86	m6	1	Total 1	Mg 1	0	0
86	O1	1	Total 1	Mg 1	0	0
86	s8	1	Total 1	Mg 1	0	0
86	l8	1	Total 1	Mg 1	0	0
86	c7	2	Total 2	Mg 2	0	0
86	7	15	Total 15	Mg 15	0	0
86	n3	2	Total 2	Mg 2	0	0
86	L3	3	Total 3	Mg 3	0	0
86	d4	1	Total 1	Mg 1	0	0
86	l2	2	Total 2	Mg 2	0	0
86	8	13	Total 13	Mg 13	0	0
86	M6	1	Total 1	Mg 1	0	0
86	N0	1	Total 1	Mg 1	0	0
86	3	14	Total 14	Mg 14	0	0

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
87	2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	C3	1	Total	N	Os	0	0
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87	C5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	1	1	Total	N	Os	0	0
			7	6	1		
87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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87	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
87	3	1	Total	N	Os	0	0
			7	6	1		
87	3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	3	1	Total	N	Os	0	0
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87	3	1	Total	N	Os	0	0
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87	4	1	Total	N	Os	0	0
			7	6	1		
87	4	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	4	1	Total 7	N 6	Os 1	0	0
87	4	1	Total 7	N 6	Os 1	0	0
87	L3	1	Total 7	N 6	Os 1	0	0
87	L3	1	Total 7	N 6	Os 1	0	0
87	L3	1	Total 7	N 6	Os 1	0	0
87	L4	1	Total 7	N 6	Os 1	0	0
87	M0	1	Total 7	N 6	Os 1	0	0
87	M5	1	Total 7	N 6	Os 1	0	0
87	M7	1	Total 7	N 6	Os 1	0	0
87	M7	1	Total 7	N 6	Os 1	0	0
87	M9	1	Total 7	N 6	Os 1	0	0
87	N1	1	Total 7	N 6	Os 1	0	0
87	N9	1	Total 7	N 6	Os 1	0	0
87	O2	1	Total 7	N 6	Os 1	0	0
87	O3	1	Total 7	N 6	Os 1	0	0
87	O7	1	Total 7	N 6	Os 1	0	0
87	O7	1	Total 7	N 6	Os 1	0	0
87	O9	1	Total 7	N 6	Os 1	0	0
87	Q2	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0
87	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
			7	6	1		
87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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87	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	5	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	7	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		
87	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	8	1	Total 7	N 6	Os 1	0	0
87	l3	1	Total 7	N 6	Os 1	0	0
87	l3	1	Total 7	N 6	Os 1	0	0
87	l3	1	Total 7	N 6	Os 1	0	0
87	l4	1	Total 7	N 6	Os 1	0	0
87	l4	1	Total 7	N 6	Os 1	0	0
87	l5	1	Total 7	N 6	Os 1	0	0
87	l5	1	Total 7	N 6	Os 1	0	0
87	l5	1	Total 7	N 6	Os 1	0	0
87	l9	1	Total 7	N 6	Os 1	0	0
87	m0	1	Total 7	N 6	Os 1	0	0
87	m0	1	Total 7	N 6	Os 1	0	0
87	m1	1	Total 7	N 6	Os 1	0	0
87	m4	1	Total 7	N 6	Os 1	0	0
87	m5	1	Total 7	N 6	Os 1	0	0
87	m6	1	Total 7	N 6	Os 1	0	0
87	m7	1	Total 7	N 6	Os 1	0	0
87	m8	1	Total 7	N 6	Os 1	0	0
87	n3	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	n9	1	Total	N	Os	0	0
			7	6	1		
87	o2	1	Total	N	Os	0	0
			7	6	1		
87	o3	1	Total	N	Os	0	0
			7	6	1		
87	o7	1	Total	N	Os	0	0
			7	6	1		
87	o9	1	Total	N	Os	0	0
			7	6	1		
87	q2	1	Total	N	Os	0	0
			7	6	1		

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

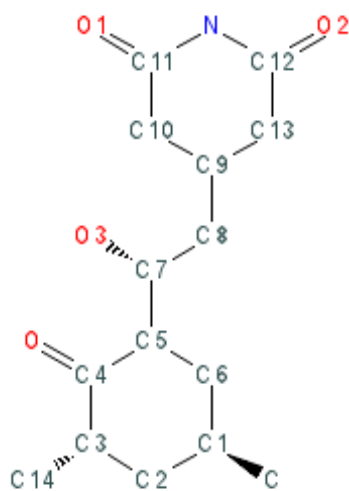
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	q0	1	Total	Zn	0	0
			1	1		
88	D6	1	Total	Zn	0	0
			1	1		
88	Q2	1	Total	Zn	0	0
			1	1		
88	e1	1	Total	Zn	0	0
			1	1		
88	Q3	1	Total	Zn	0	0
			1	1		
88	D9	1	Total	Zn	0	0
			1	1		
88	E1	1	Total	Zn	0	0
			1	1		
88	Q0	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0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

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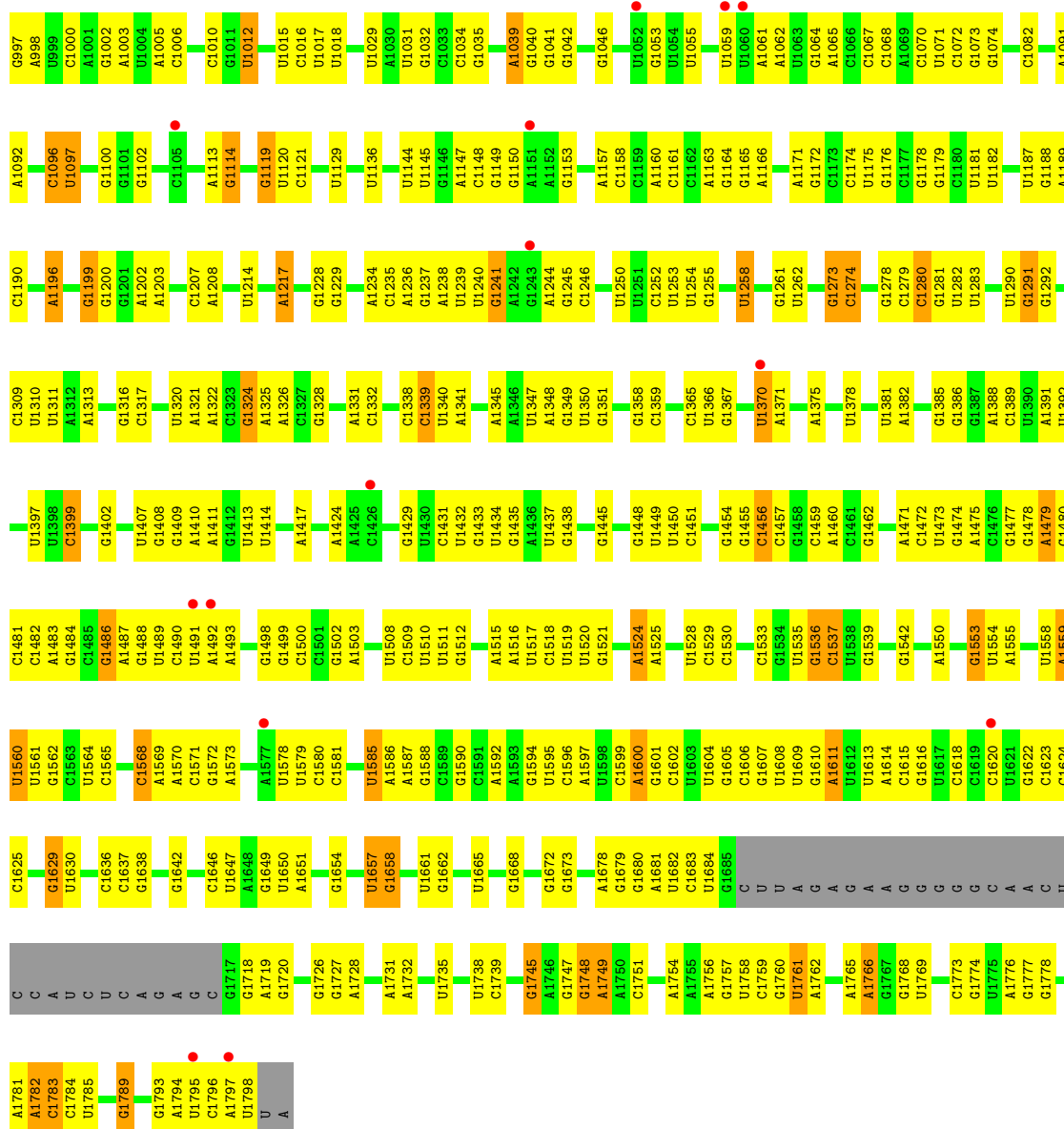
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	o7	1	Total	Zn	0	0
			1	1		
88	O7	1	Total	Zn	0	0
			1	1		
88	q2	1	Total	Zn	0	0
			1	1		

- Molecule 89 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: C₁₅H₂₃NO₄).

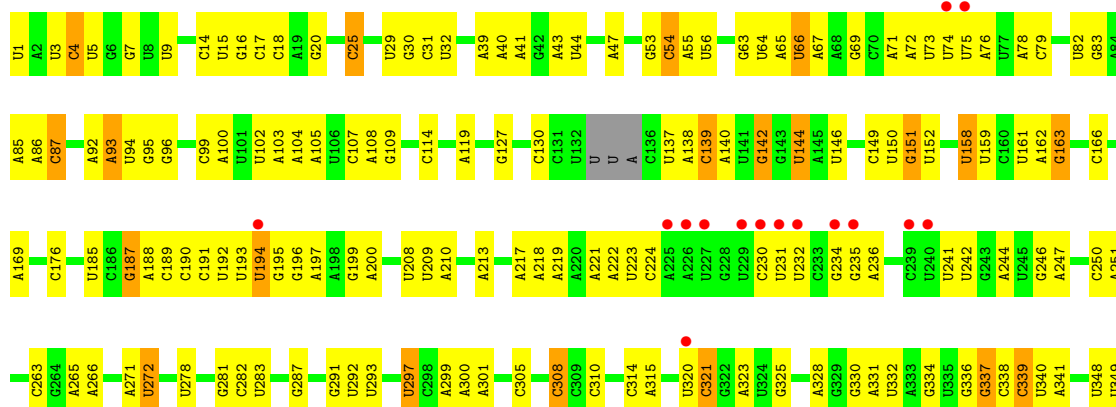


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			20	15	1	4		
89	5	1	Total	C	N	O	0	0
			20	15	1	4		

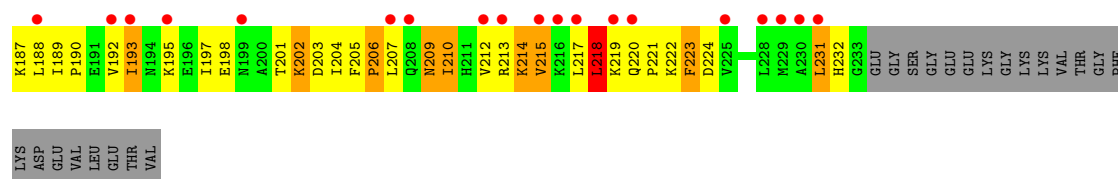


• Molecule 1: RNA (1750-MER)

Chain 6:







• Molecule 3: 40S ribosomal protein S1-A

Chain s1:

• Molecule 4: 40S ribosomal protein S2

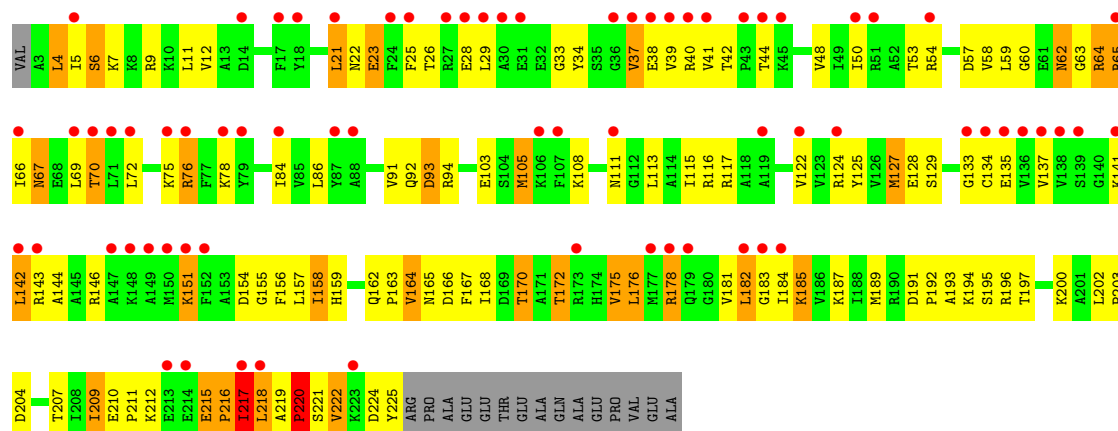
Chain S2:

• Molecule 4: 40S ribosomal protein S2

Chain s2:

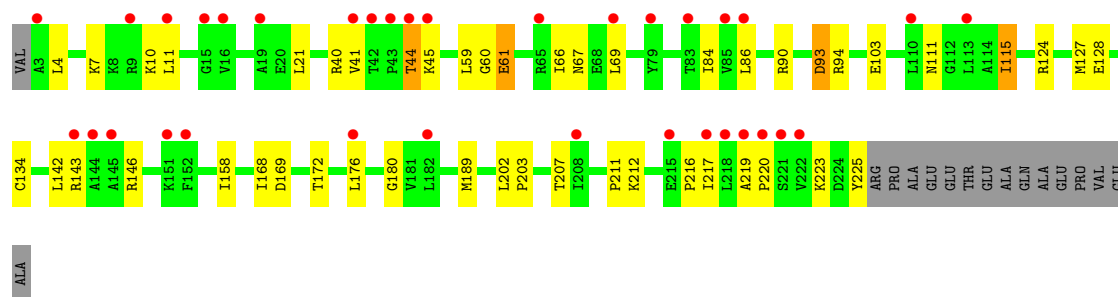
• Molecule 5: 40S ribosomal protein S3

Chain S3:



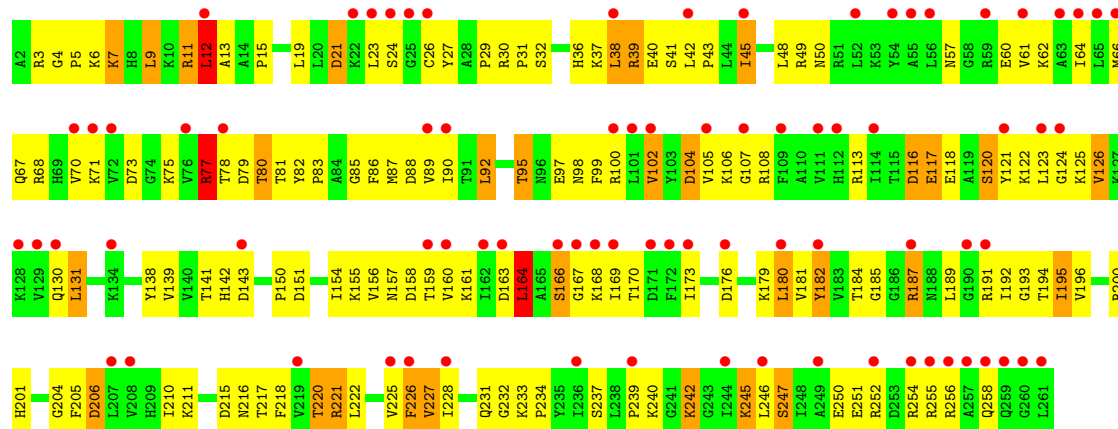
- Molecule 5: 40S ribosomal protein S3

Chain s3: 



- Molecule 6: 40S ribosomal protein S4-A

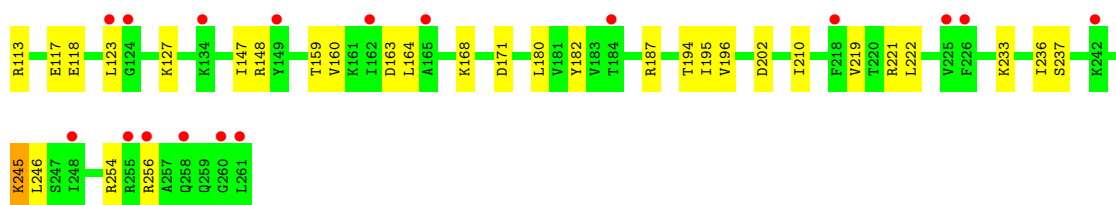
Chain S4:



- Molecule 6: 40S ribosomal protein S4-A

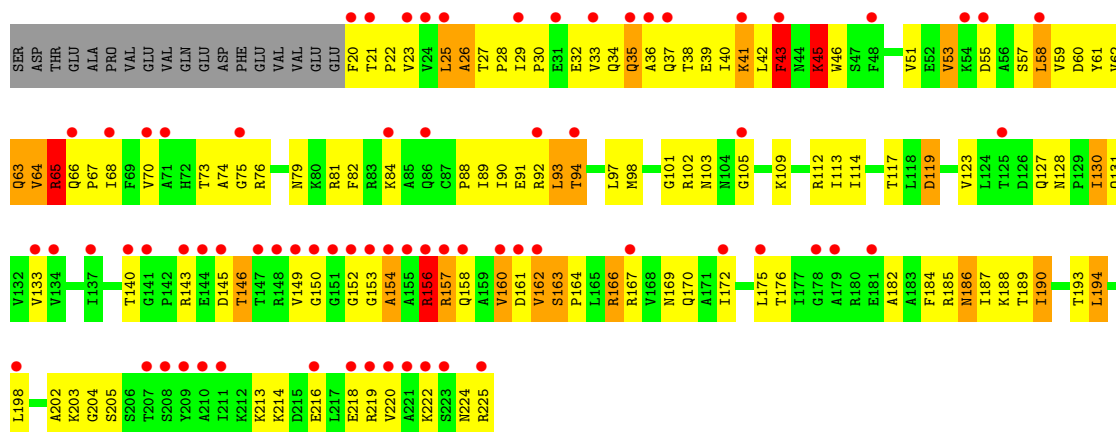
Chain s4:





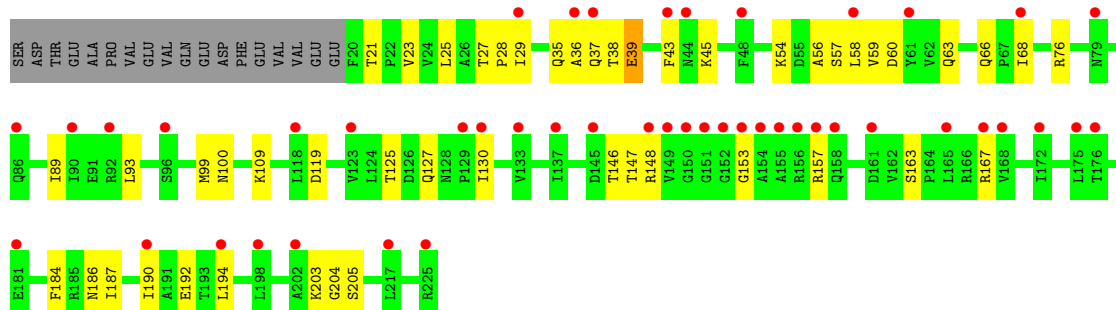
• Molecule 7: 40S ribosomal protein S5

Chain S5:



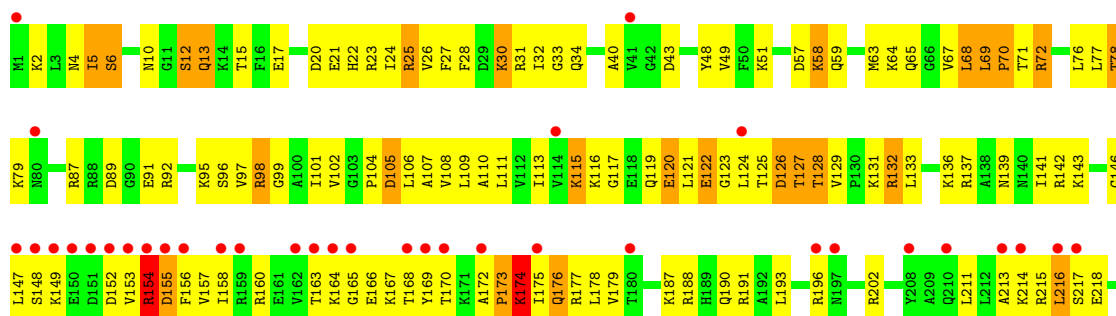
• Molecule 7: 40S ribosomal protein S5

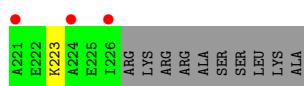
Chain s5:



• Molecule 8: 40S ribosomal protein S6-A

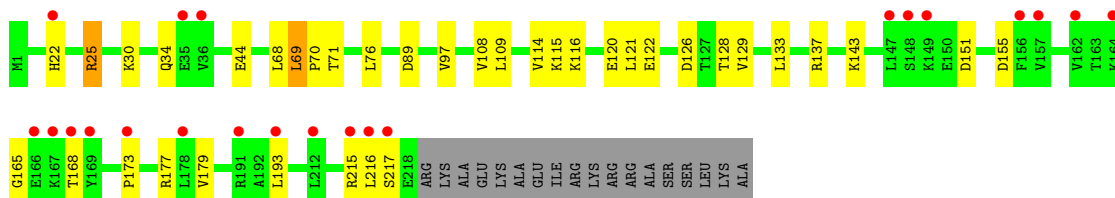
Chain S6:





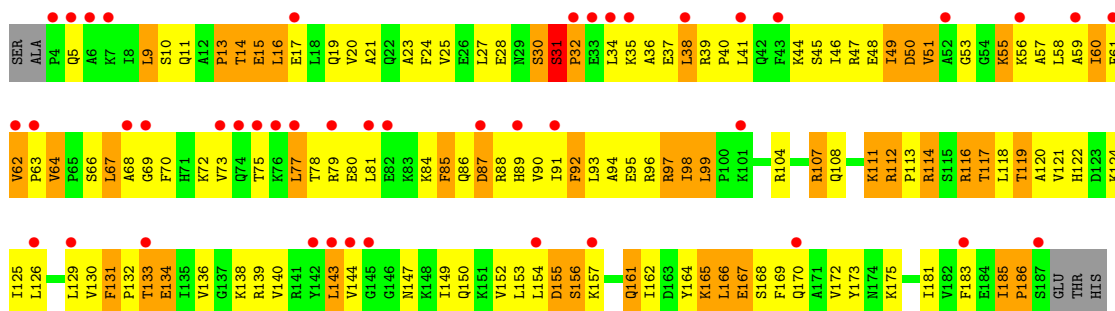
- Molecule 8: 40S ribosomal protein S6-A

Chain s6:



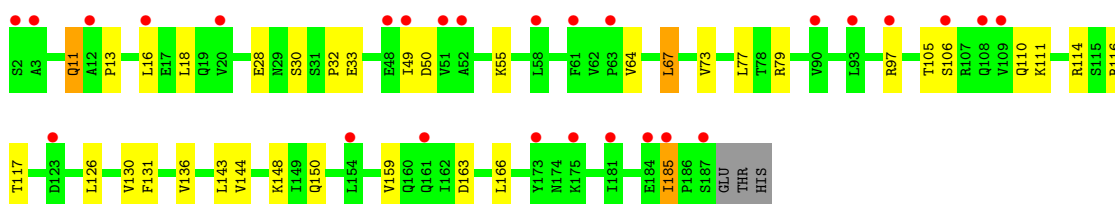
- Molecule 9: 40S ribosomal protein S7-A

Chain S7:



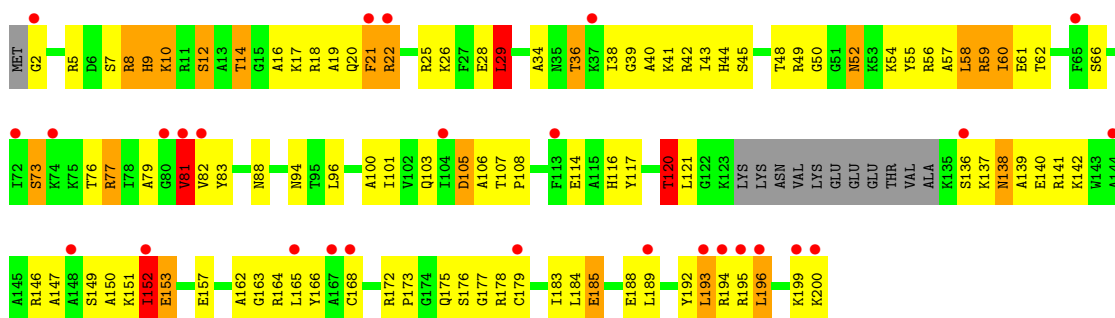
- Molecule 9: 40S ribosomal protein S7-A

Chain s7:



- Molecule 10: 40S ribosomal protein S8-A

Chain S8:



- Molecule 10: 40S ribosomal protein S8-A

[illegible]

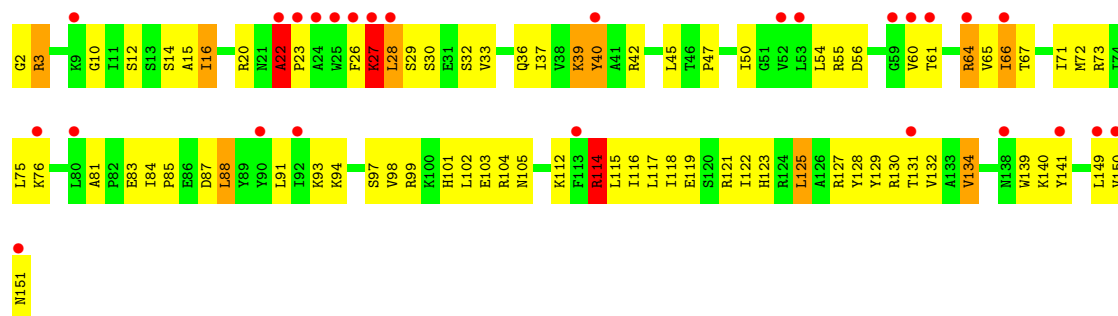
Category ID	Category Name	Frequency (approx.)
K139	Q138	10
K140	Q139	10
V141	Q140	10
I142	Q141	10
N143	Q142	10
P144	Q143	10
S145	Q144	10
F146	Q145	10
M147	Q146	10
R148	Q147	10
L149	Q148	10
D150	Q149	10
S152	Q150	10
E153	Q151	10
K154	Q152	10
H155	Q153	10
I156	Q154	10
D157	Q155	10
F158	Q156	10
A159	Q157	10
P160	Q158	10
T161	Q159	10
S162	Q160	10
P163	Q161	10
F164	Q162	10
G165	Q163	10
G166	Q164	10
A167	Q165	10
R168	Q166	10
P169	Q167	10
G170	Q168	10
R171	Q169	10
V172	Q170	10
A173	Q171	10
R174	Q172	10
R175	Q173	10
N176	Q174	10
A177	Q175	10
A178	Q176	10
R179	Q177	10
K180	Q178	10
E181	Q179	10
A182	Q180	10
G185	Q181	10
E186	Q182	10
A1A	Q183	10
ALA	Q184	10
ASP	Q185	10
GLU	Q186	10
ALA	Q187	10
ASP	Q188	10
GLU	Q189	10
ALA	Q190	10
ASP	Q191	10
GLU	Q192	10
ALA	Q193	10
ASP	Q194	10
GLU	Q195	10
ALA	Q196	10
ASP	Q197	10
GLU	Q198	10
ALA	Q199	10

Category	Number of Genes
G17	10
S121	20
R126	30
T130	40
H133	50
I134	60
I140	70
F146	80
M147	90
V148	100
R149	10
S162	20
A167	30
R188	40
V172	50
K180	60
E181	70
E182	80
A183	90
S184	100
G185	10
E186	20
ALA	30
ALA	40
ASP	50
ASP	60
GLU	70
GLU	80
ASP	90
ASP	100
GLU	10
GLU	20
GLU	30

● ●

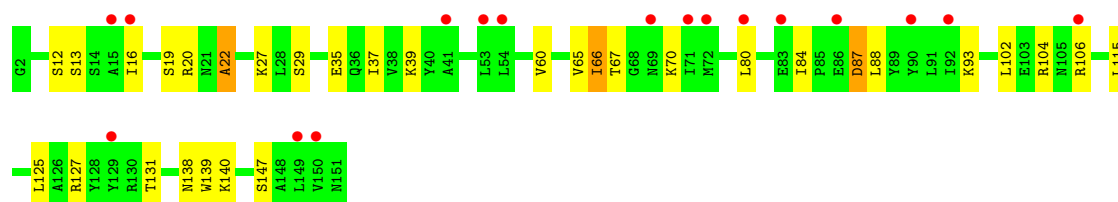
P97	T98	GLN	ARG	PRO	GLN	ARG	ARG	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain C3: 



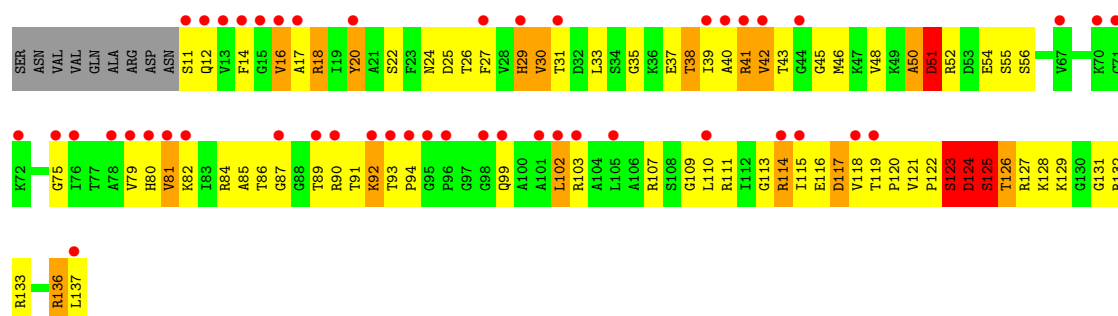
- Molecule 15: 40S ribosomal protein S13

Chain c3: 



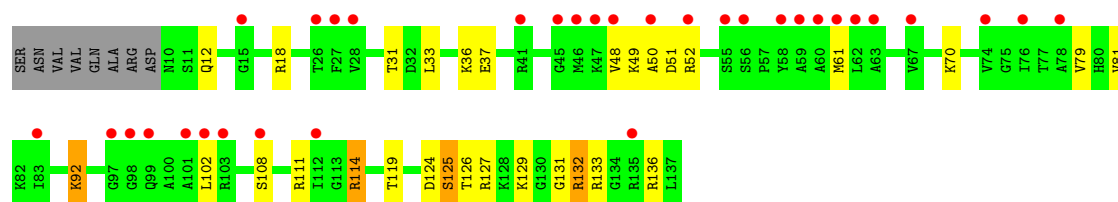
- Molecule 16: 40S ribosomal protein S14-A

Chain C4: 



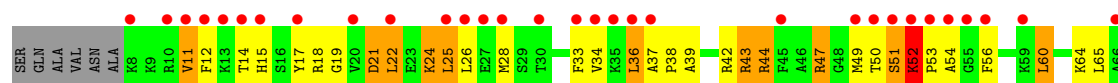
- Molecule 16: 40S ribosomal protein S14-A

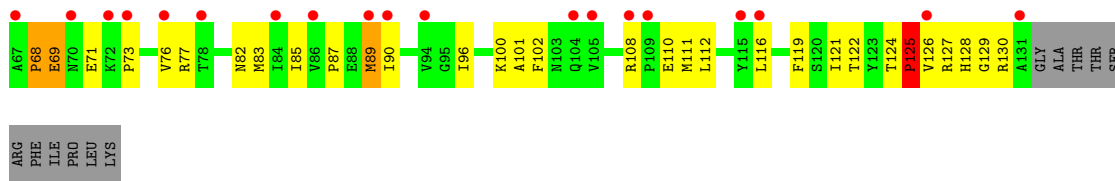
Chain c4: 



- Molecule 17: 40S ribosomal protein S15

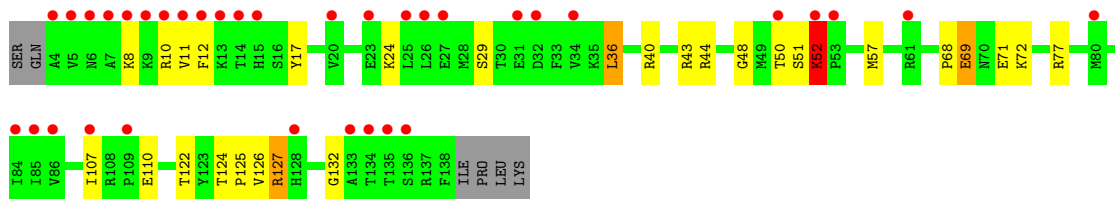
Chain C5: 





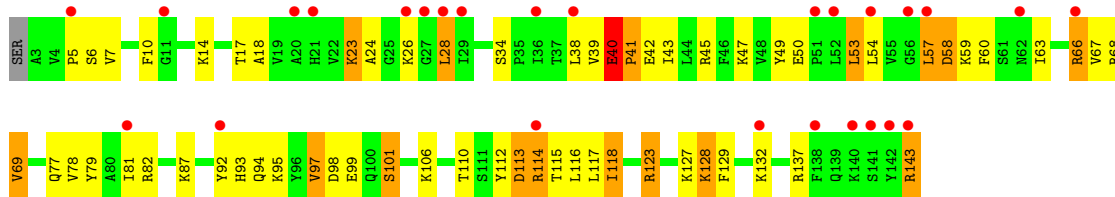
- Molecule 17: 40S ribosomal protein S15

Chain c5:



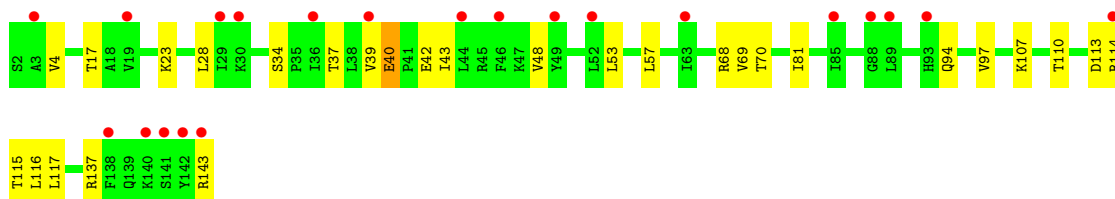
- Molecule 18: 40S ribosomal protein S16-A

Chain C6:



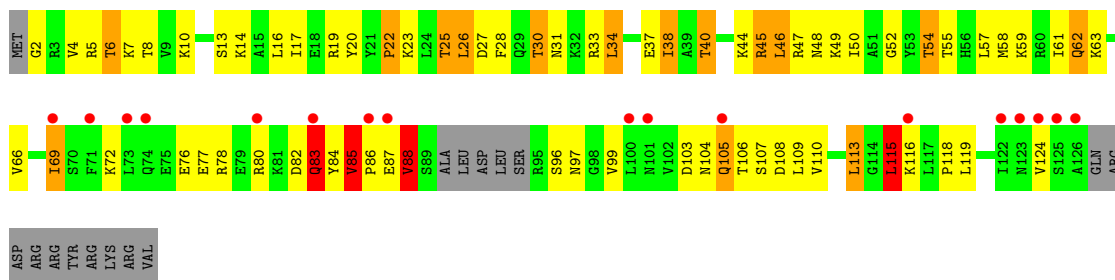
- Molecule 18: 40S ribosomal protein S16-A

Chain c6:



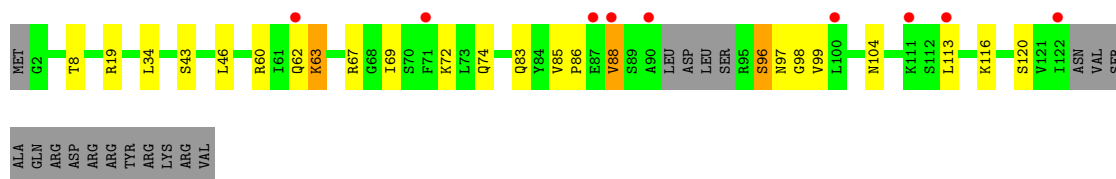
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:



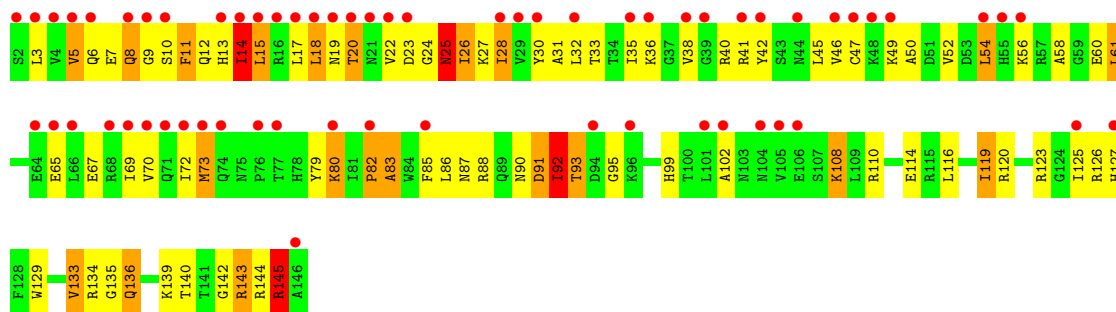
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:



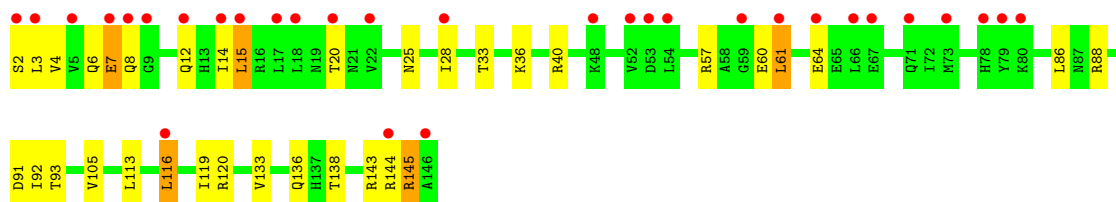
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:



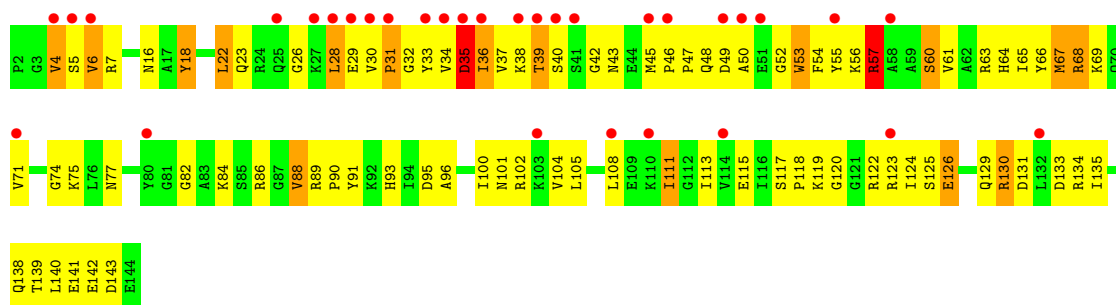
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



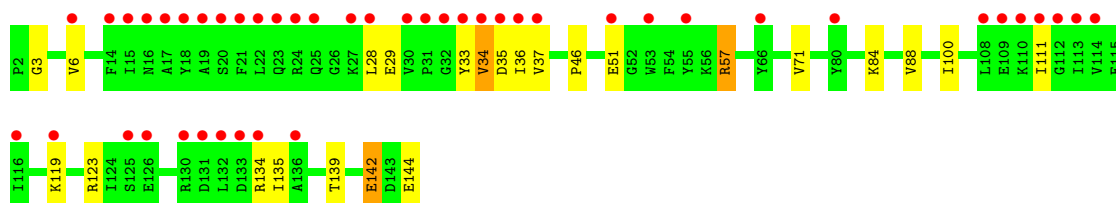
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:

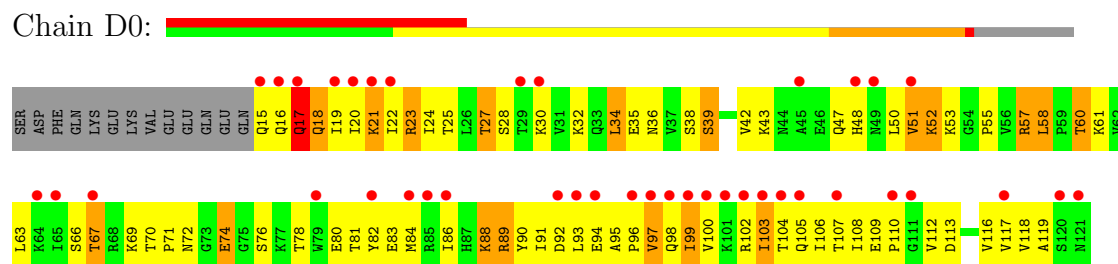


- Molecule 21: 40S ribosomal protein S19-A

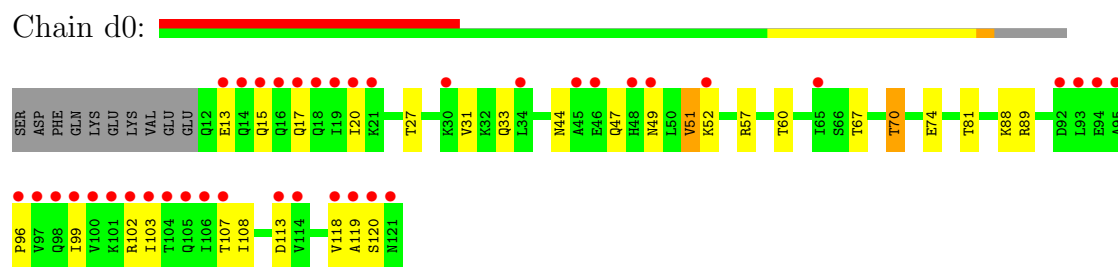
Chain c9:



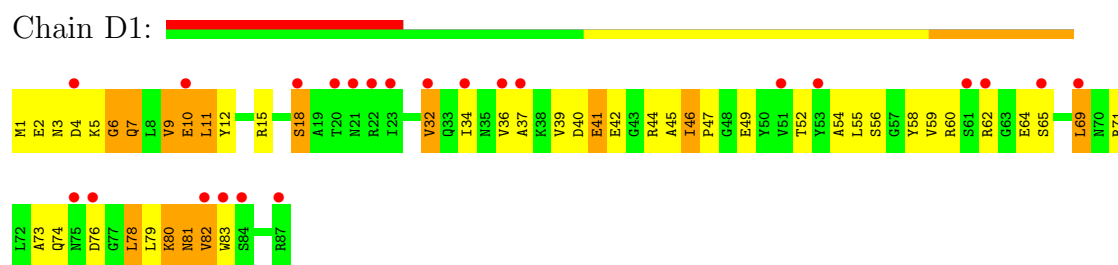
- Molecule 22: 40S ribosomal protein S20



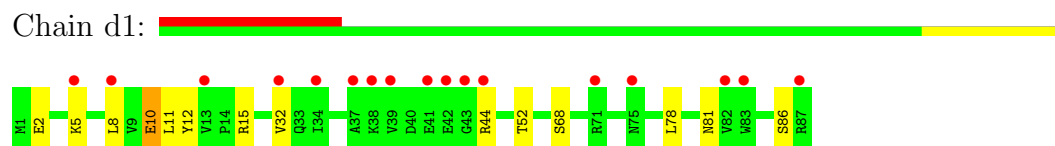
- Molecule 22: 40S ribosomal protein S20



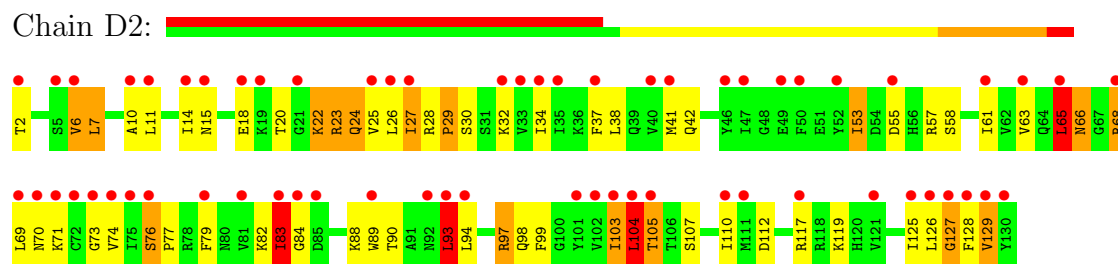
- Molecule 23: 40S ribosomal protein S21-A



- Molecule 23: 40S ribosomal protein S21-A

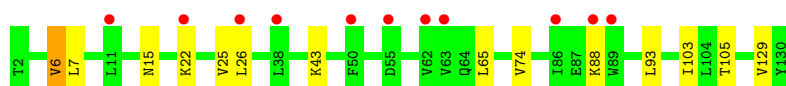


- Molecule 24: 40S ribosomal protein S22-A



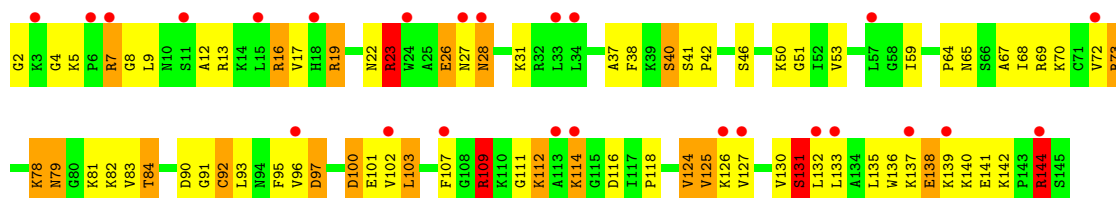
- Molecule 24: 40S ribosomal protein S22-A





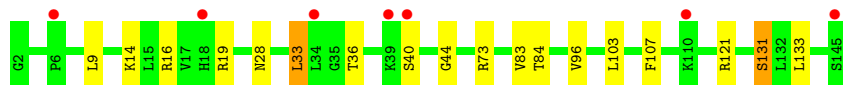
- Molecule 25: 40S ribosomal protein S23-A

Chain D3:



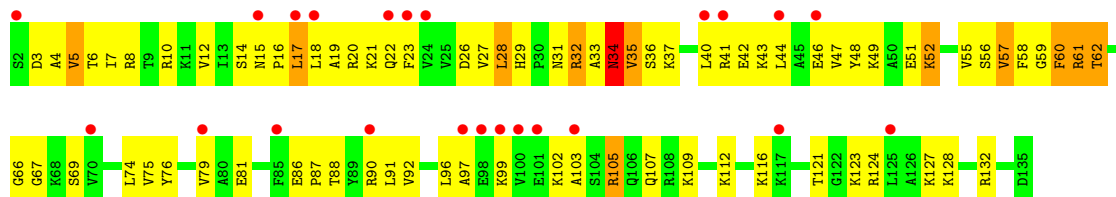
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



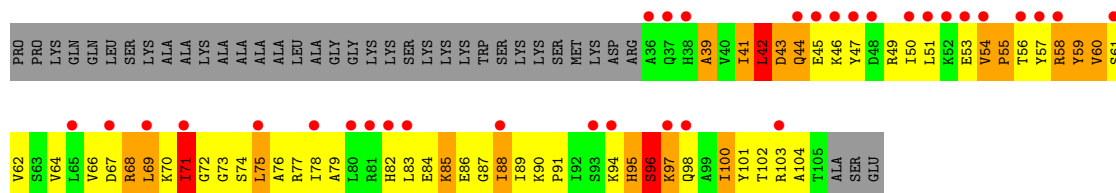
- Molecule 26: 40S ribosomal protein S24-A

Chain d4:



- Molecule 27: 40S ribosomal protein S25-A

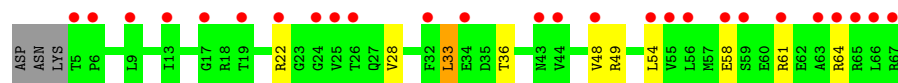
Chain D5:



- Molecule 27: 40S ribosomal protein S25-A

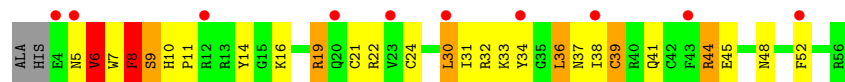
Chain d5:

Chain d8:



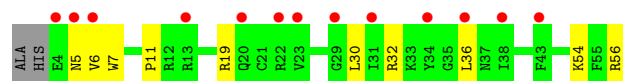
- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



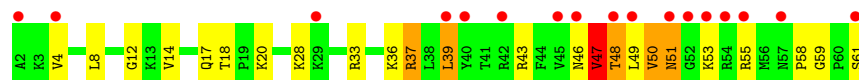
- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



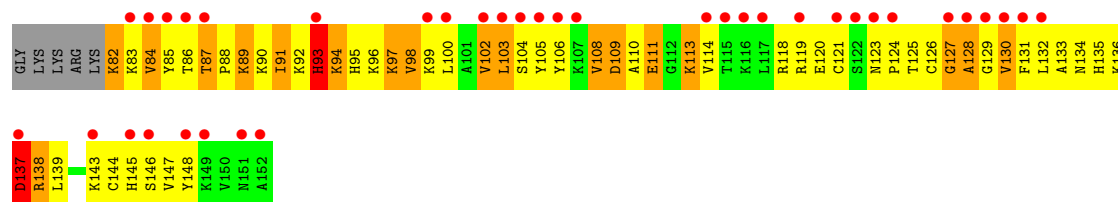
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



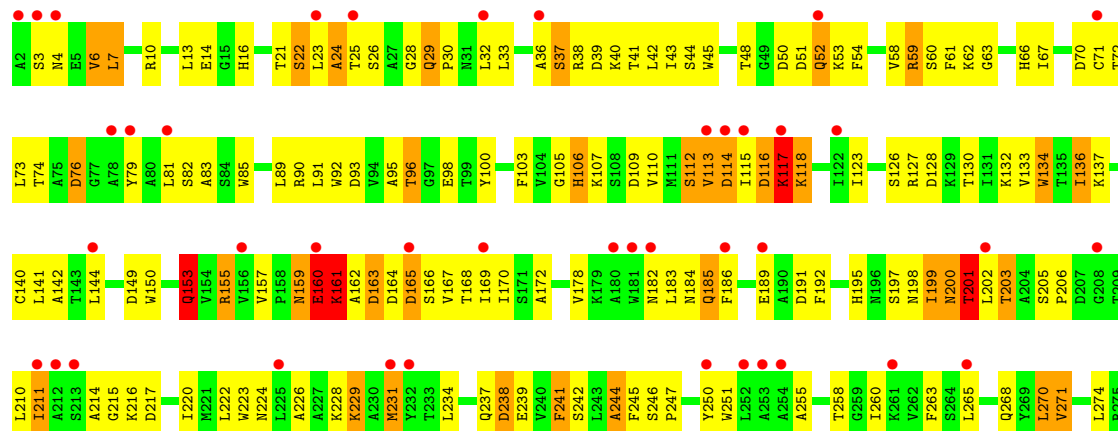
- Molecule 33: Ubiquitin-40S ribosomal protein S31

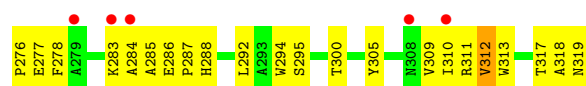
Chain E1:



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

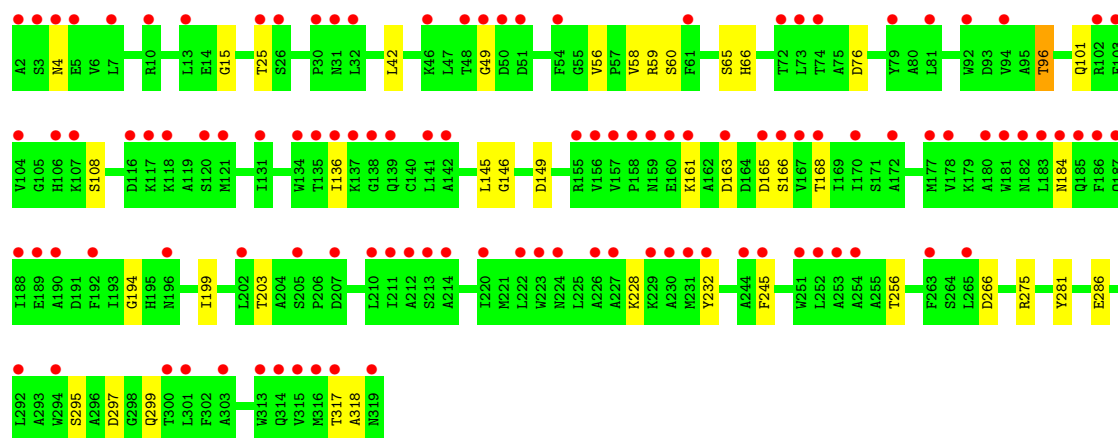
Chain SR:





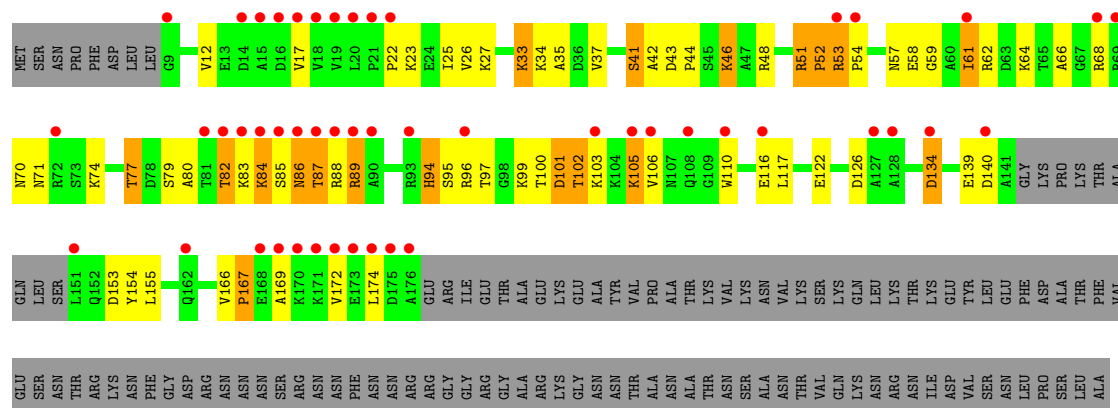
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



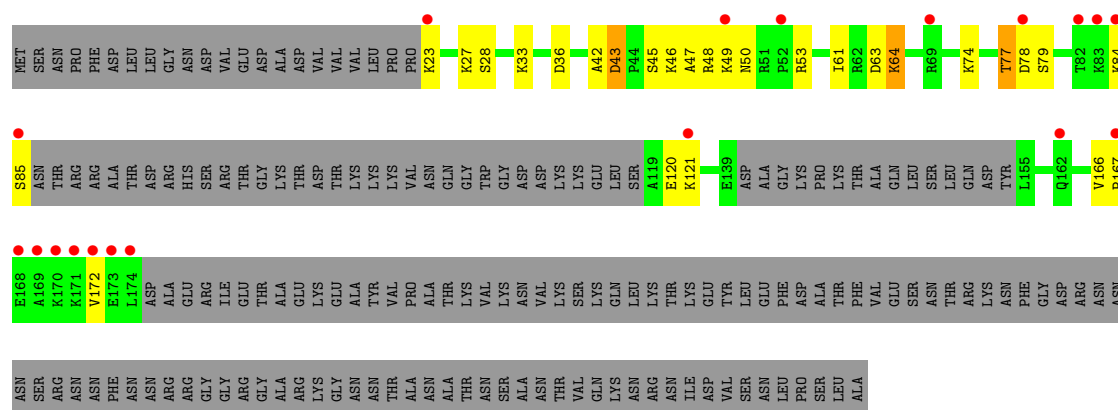
- Molecule 35: Suppressor protein STM1

Chain SM:



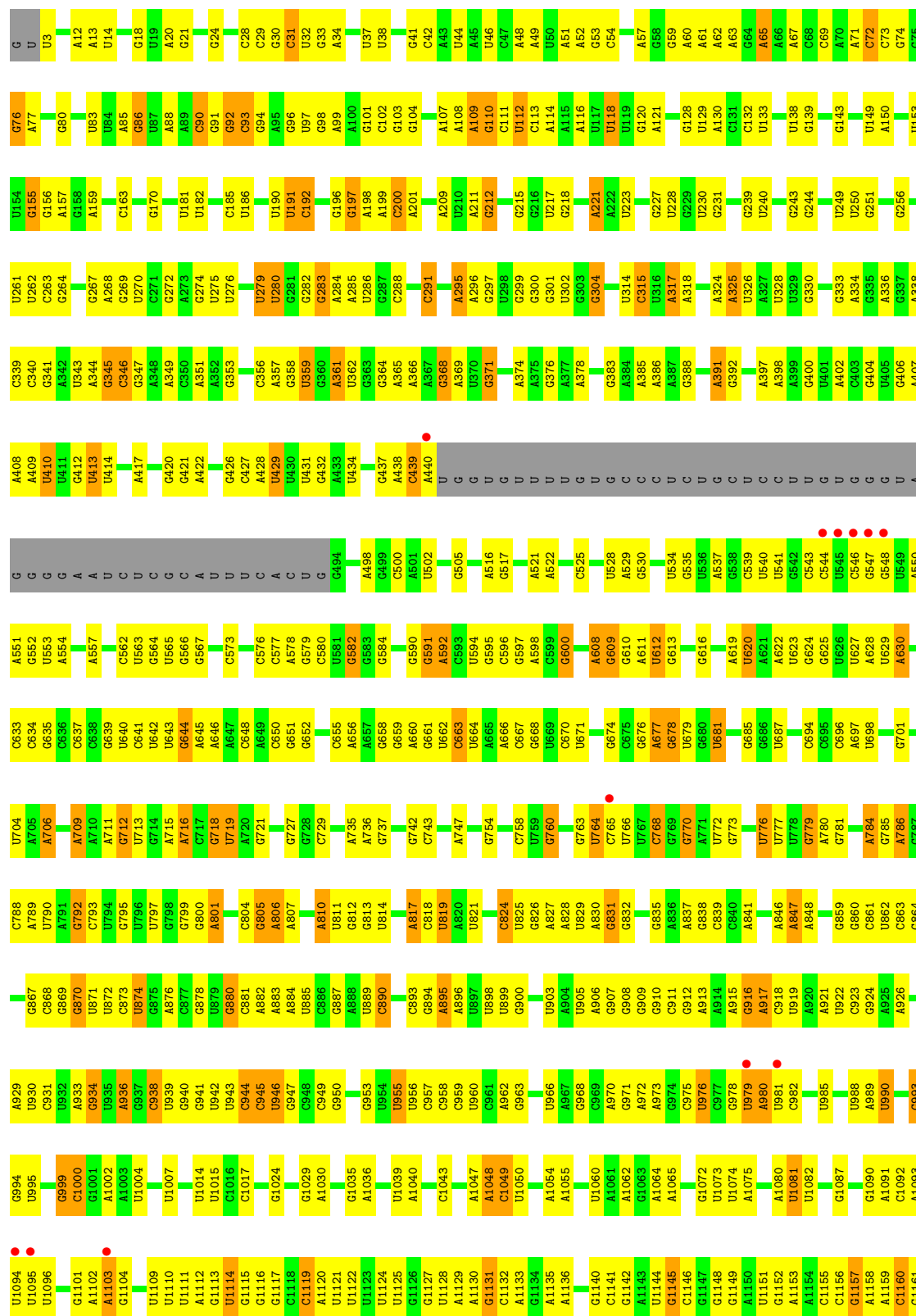
- Molecule 35: Suppressor protein STM1

Chain sM:



● Molecule 36: *Saccharomyces cerevisiae* chromosome XII cosmid 9634

Chain 1: 

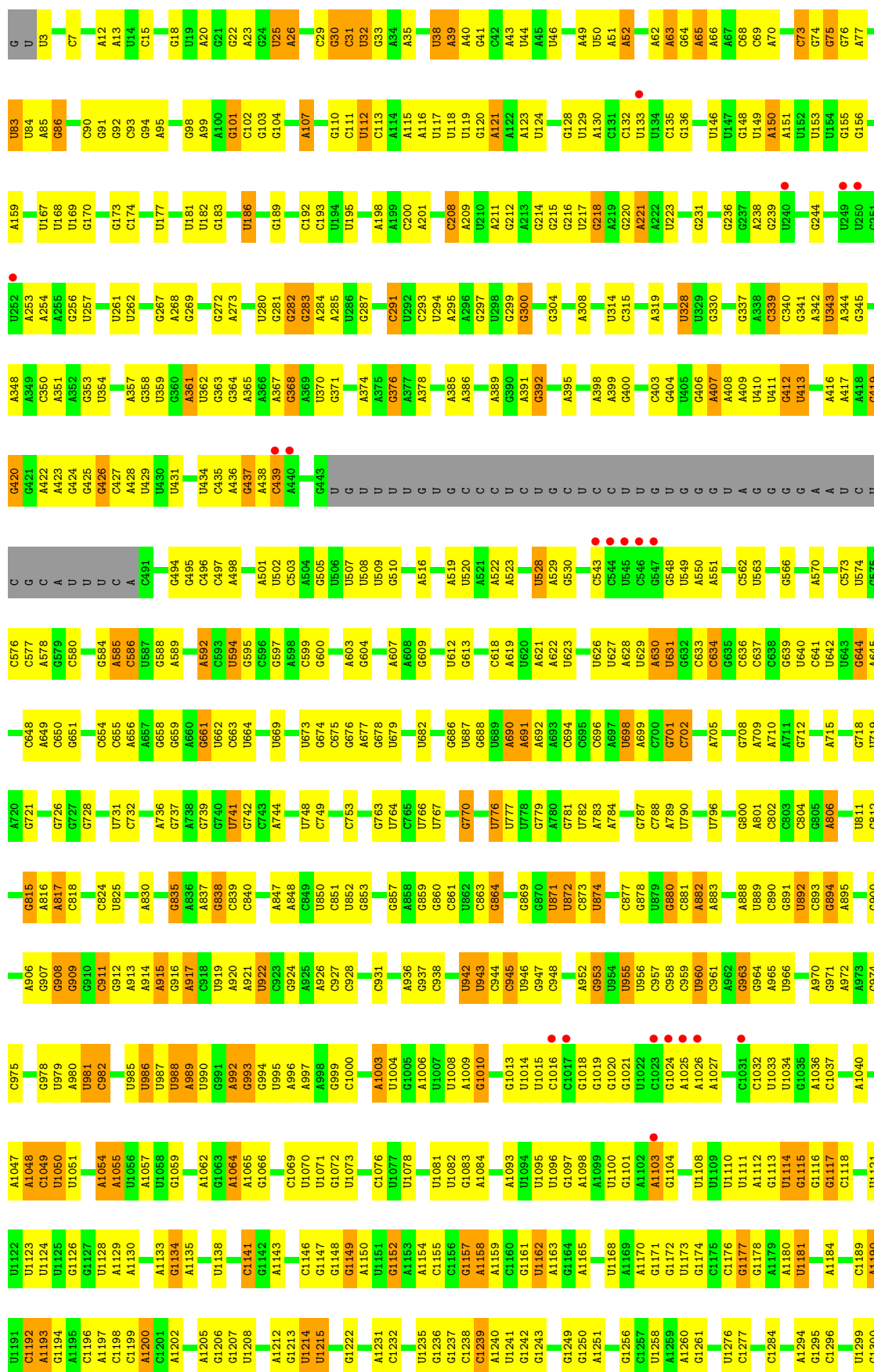


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A2262	A2183	C2108	U1840	U1742	U1629	G1547	A1467	C1403	A1330	A1245	A1163
C2263	U2184	U2112	A1841	G1748	U1630	G1547	A1468	G1404	U1331	G1246	G1164
U2264	A2113	A2113	A1842	A1749	C1631	U1553	U1405	U1405	A1332	U1247	G1165
G2273	U2186	C2114	G1845	A1752	A1632	U1554	A1477	A1406	U1334	G1167	U1167
G2278	G2187	G2115	C1846	A1752	C1633	U1555	C1478	A1407	G1335	U1168	U1168
C2278	A2188	C2118	A1847	G1758	G1634	U1556	U1479	G1408	U1336	A1170	A1170
A2279	U2189	C2118	A1848	G1758	G1635	C1559	G1480	G1409	A1337	A1260	G1171
A2280	U2190	A2119	A1849	C1761	U1636	A1559	A1481	U1410	U1338	G1261	G1172
A2281	U2191	A2120	A1850	U1762	C1639	G1560	A1482	C1411	C1339	G1262	U1173
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G2288	U2200	G2124	U1854	G1766	G1646	U1565	G1486	U1415	G1343	A1270	G1177
G2288	G2201	A2125	U1855	G1767	G1650	G1566	A1487	C1416	G1344	A1271	G1177
U2289	C2202	G2126	C1856	C1767	U1651	U1567	G1488	G1345	G1345	A1180	A1180
U2289	U2203	G2130	C1857	A1770	U1651	U1567	A1489	A1419	G1346	U1181	U1181
C2293	C2204	A2131	A1858	G1770	G1658	U1568	G1493	C1420	G1349	A1182	A1182
G2296	U2205	C2132	A1859	C1771	U1659	U1569	U1493	G1421	A1350	C1183	C1183
A2297	G2206	U2133	G1860	G1778	U1660	U1570	U1494	G1422	G1351	A1184	A1184
A2297	A2207	G2134	G1861	U1778	C1660	A1571	U1495	C1423	U1351	C1279	C1279
A2298	A2208	U2135	G1862	G1780	U1664	U1572	C1496	C1424	A1352	C1280	C1189
C2300	A2213	C2136	A1866	G1780	C1665	G1573	C1497	U1425	U1353	G1285	C1192
A2302	A2214	A2138	G1867	G1780	C1665	C1574	C1498	C1426	G1354	A1286	C1196
G2305	A2215	A2139	G1868	G1784	G1674	A1575	C1499	U1427	A1355	A1287	C1196
C2306	U2217	G2142	A1874	U1785	G1675	G1577	A1504	G1428	U1356	G1292	A1200
C2307	U2218	A2143	G1878	G1786	A1676	G1577	C1505	A1429	U1357	U1293	A1204
C2308	A2219	A2144	G1879	G1787	U1686	C1579	A1506	G1430	G1362	A1294	U1211
A2309	A2222	A2147	U1880	G1790	U1687	C1580	G1507	G1432	A1363	C1296	U1212
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G2315	A2228	G2150	U1888	G1796	U1695	C1585	G1510	A1336	G1366	U1299	U1215
G2316	A2229	C2151	G1889	A1797	C1701	A1589	U1511	U1436	U1369	G1300	C1216
A2317	A2233	A2152	U1890	A1798	U1702	G1590	U1512	C1437	A1363	U1305	U1220
U2318	G2236	U2153	U1891	A1799	U1706	G1592	U1513	U1438	A1294	G1306	A1221
U2319	G2237	U2154	G1892	A1799	U1706	G1592	U1514	U1439	G1376	G1307	G1222
A2320	C2237	C2156	U1893	G1807	A1707	A1593	U1518	G1444	G1377	U1309	C1228
C2322	G2237	G2157	U1894	G1807	U1707	U1594	G1519	U1445	U1309	G1310	G1229
G2323	U2241	A2158	A1895	A1814	A1715	C1596	G1520	U1446	G1380	G1230	G1230
A2242	A2242	U2159	G1898	U1815	U1716	C1597	G1521	A1447	A1381	G1232	G1233
A2243	A2243	G2160	G1899	U1815	U1717	G1598	U1522	G1447	G1382	G1233	G1233
U2334	A2244	G2161	A1900	U1818	G1718	G1599	A1524	G1450	U1315	G1234	G1234
C2245	C2245	A2164	A1901	U1819	U1719	A1594	U1524	G1451	G1383	G1235	G1235
G2247	G2247	G2165	G1902	U1820	U1720	U1596	G1525	A1452	G1387	G1236	G1236
C2248	A2167	A2166	U1903	U1821	U1721	A1603	G1530	A1453	A1317	G1237	G1237
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A2341	A2341	G2169	G1905	U1825	U1723	G1610	A1534	U1455	A1319	C1239	C1239
U2342	U2254	G2169	C1907	U1831	C1725	G1611	A1534	U1455	C1391	U1322	A1240
C2343	A2255	U2175	A1908	G1832	U1730	A1612	A1537	U1458	A1394	G1323	A1241
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C2350	C2257	G2177	A1910	U1834	G1733	C1614	G1541	A1460	C1396	A1326	G1243
A2351	U2258	A2178	A1911	A1835	G1734	C1615	U1616	A1461	U1399		
	U2260	C2179	A1915	G1838	U1740	G1617	G1543	A1463	A1399		

A3330	A3243	C3161	G3088	G3003	A2930	U2860	G2786	C2707	A2637	G2563	A	A2419	G2355
U3334	A3244	A3165	C3089	C3004	C2931	U2861	G2787	C2708	G2638	G2564	A	C2420	A2356
A3335	A3245	C3166	C3092	A3006	U2932	U2862	C2788	C2710	U2669	U2565	U	U2421	A2357
A3336	A3247	A3167	C3093	U3007	U2935	G2863	A2789	C2714	A2640	C2566	A	U2422	A2358
	C3248	A3168	A3094	A3008	A2936	U2864	A2790	G2715	U2641	C2567	C	A2424	C2359
		U3169	U3095	G3009	G2937	U2865	G2791	A2715	A2642	C2568	C	G2426	C2362
	U3251	A3170	C3096	U3010	G2938	U2866	A2792	G2716		A2569	C	U2427	A2363
G3252	G3252	U3171	C3097	U3020	G2939	C2867	G2793	U2717	A2647	U2570	C	U2428	A2364
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		U3175	U3101	U3024	C2943	C2871	C2799		U2651	C2574	C	U2435	A2368
		G3176	G3102	A3024	U2944	A2872	A2799		U2652	G2575	U	U2436	C2369
	A3268	A3177	A3103	A3029	G2945	U2873	G2800	C2726	C2653	G2576	U	G2437	G2370
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		A3179	A3105	A3033	G2947	U2875	A2802	G2728	U2655	U2578	A	A2439	A2372
	C3272	C3181	U3107	A3034	C2948	C2876	A2804	U2731	A2656	C2582			A2373
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A3274	A3274	A3183	G3109	C3034	G2950	U2880	A2733	A2733	C2658	G2584			C2375
	U3275	A3187	C3110	A3035	G2951	C2879	C2809	A2734	G2659	G2585			G2376
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	C3278		G3112	A3040	U2954	C2884	A2811	A2736	G2663				C2378
A3279	A3279	G3190	U3115	U3041	U2955	C2885	A2812	C2737	C2664				U2379
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U3281	U3281	C3193	C3118	U3043	U2958	U2887	G2816		U2668	A2593			A2384
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	G3286			A3049	G2964	U2897	U2822	A2748	A2601	G2520			A2390
				U3050		C2898	G2823		A2674				C2391
				G3053	A2969	G2899	G2824	G2751	G2605	C2526			C2392
A3294	A3294	C3206	C3133	U3054	C2970	C2898	U2826	U2752	G2606	G2527			G2393
A3295	A3295	U3207	A3134	U3055	A2971	G2899	G2827	G2753		G2528			G2394
		G3208	U3135	U3056	G2972	A2902		G2754	A2609				C2395
U3302	U3302	A3209	G3136	U3057	G2973	U2903		C2755	U2610				C2396
G3303	G3303		G3137	U3058	U2974	U2904	G2830	C2756	G2611				A2397
U3304	U3304	U3214	U3138	U3059	G2975	U2905	G2831	U2757	U2612				A2398
A3305	A3305	A3215	A3139	G3060	A2976	C2906	G2834	U2758	U2613				A2399
U3306	U3306	G3216	G3140	C3061	G2977	U2909	U2835	C2760	U2637				G2400
A3307	A3307	G3217	A3141	G3065	U2978	U2910	C2836	G2761	G2614				A2401
	G3308	A3218	A3142	U3066	U2980	A2911	A2837	A2762	G2615				A2402
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					A2982	C2913		C2764	U2617				A2404
U3312	U3312	U3222	U3148	G3074	C2983	U2916	U2842	C2765	G2618				C2405
A3314	A3314	G3224	A3150	G3075	C2984	C2985	U2843	U2766	G2619				C2406
G3315	G3315		U3151	U3078	U2986	U2987	C2844	U2767	C2620				C2407
A3316	A3316	A3227	U3152	U3079	U2987	U2988	A2845	U2768	G2621				U2408
G3317	G3317	C3228	U3153	G3080	C2988	U2991	U2846		C2622				G2409
G3318	G3318	G3229	C3081	C3082	U2989	U2992	A2847	C2772	G2623				U2410
U3319	U3319	G3230	U3154	U3083	U2990	U2993	G2848	C2775	U2551				G2411
A3320	A3320		U3155	G3084	U2991	U2994	C2849	G2776	C2625				G2412
			U3156	C3085	C2995	C2996	G2850	G2700	U2552				A2413
C3321	C3321	C3233	U3157	C3086	A2996	A2926	A2851	C2777	U2631				C2414
A3322	A3322	A3234	G3158	A3087	C2997	C2927	C2852	A2704	G2632				C2415
			U3160	A3087	U2998	C2928	A2853	G2778	U2633				U2416
							U2854	A2779	G2634				G2418

• Molecule 36: *Saccharomyces cerevisiae* chromosome XII cosmid 9634

Chain 5:



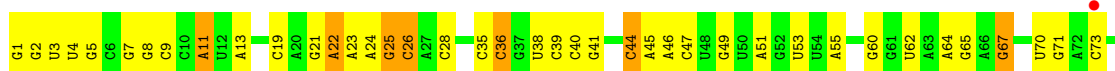






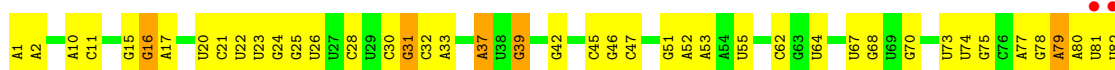
• Molecule 37: Yeast 5S rRNA gene

Chain 7:



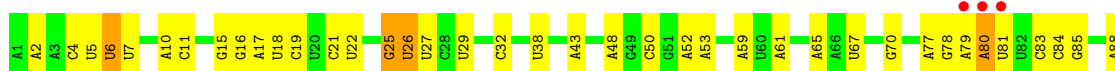
• Molecule 38: Uncultured eukaryote clone NS4T_275 18S ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence

Chain 4:



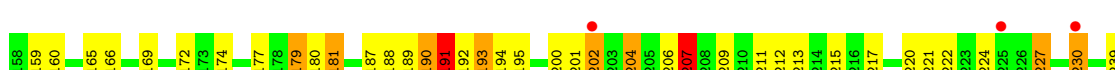
• Molecule 38: Uncultured eukaryote clone NS4T_275 18S ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence

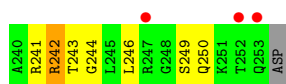
Chain 8:



• Molecule 39: 60S ribosomal protein L2-A

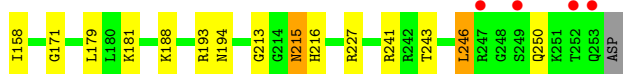
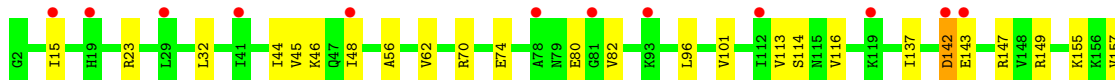
Chain L2:





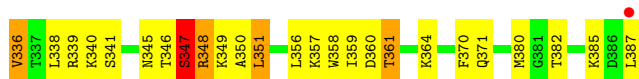
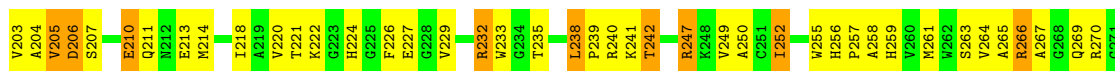
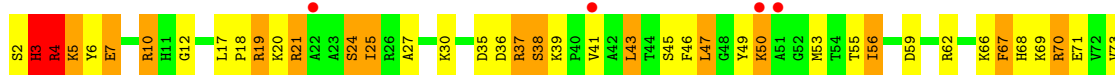
• Molecule 39: 60S ribosomal protein L2-A

Chain 12:



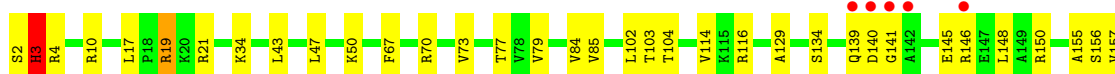
• Molecule 40: 60S ribosomal protein L3

Chain L3:



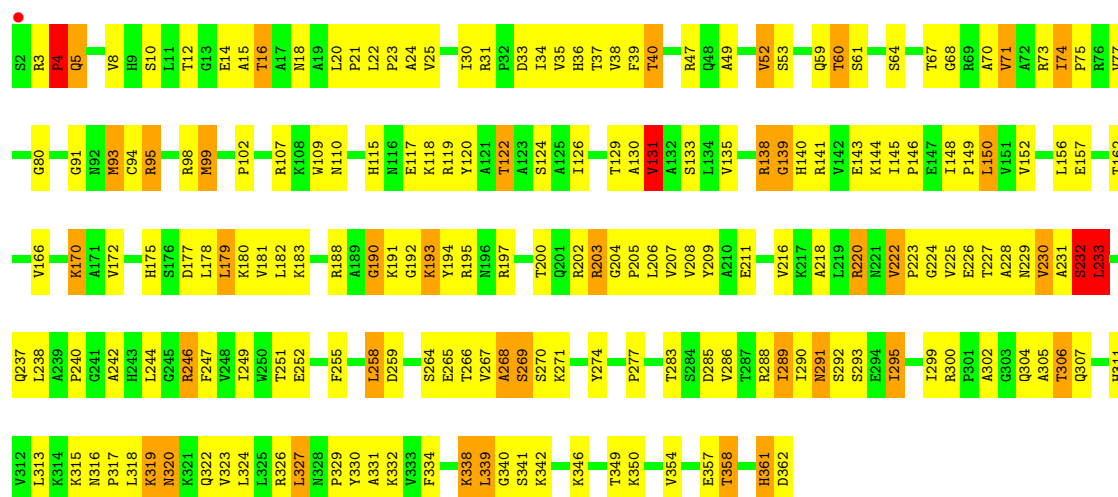
• Molecule 40: 60S ribosomal protein L3

Chain l3:



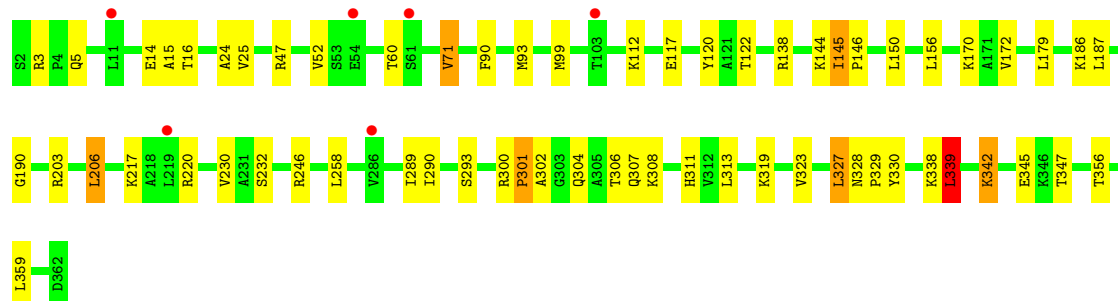
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



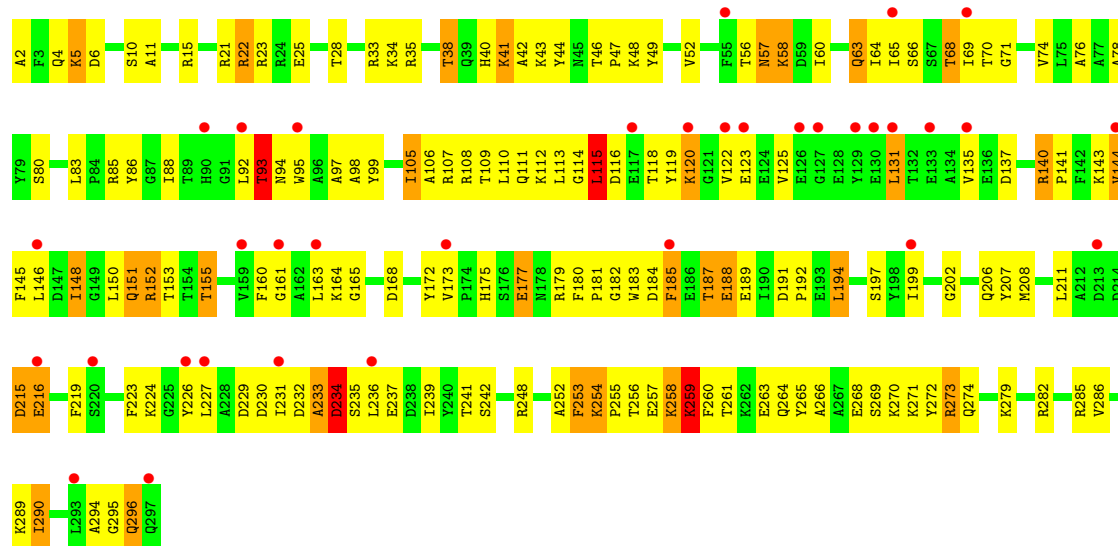
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:

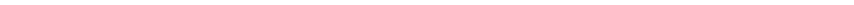


• Molecule 42: 60S ribosomal protein L5

Chain L5:



• Molecule 42: 60S ribosomal protein L5

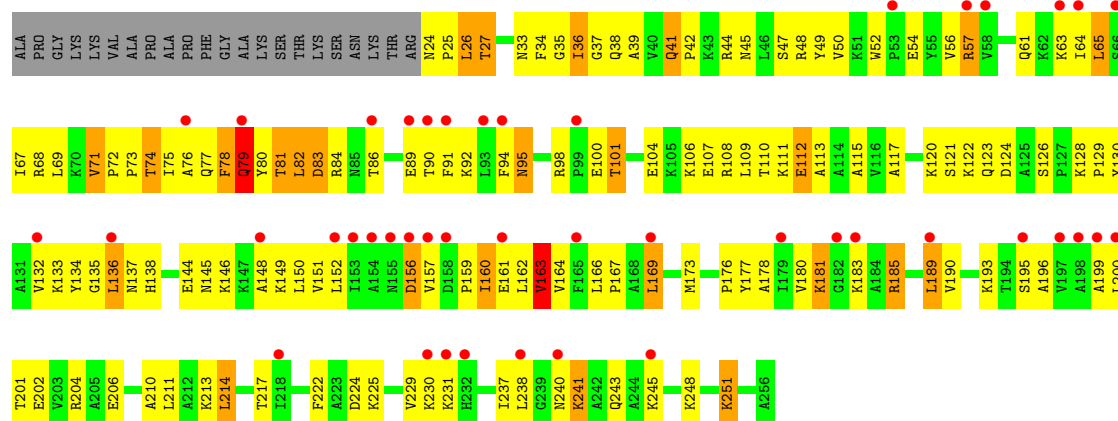
Chain 17: 

ALA	T22	A23	E24	Q25	V26	A27	A28	R41	E56	E59	R60	V77	L83	R88	K98	P99	R100	L103	R110	L124	I130	I156	K157	K158	Q159	L173
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------



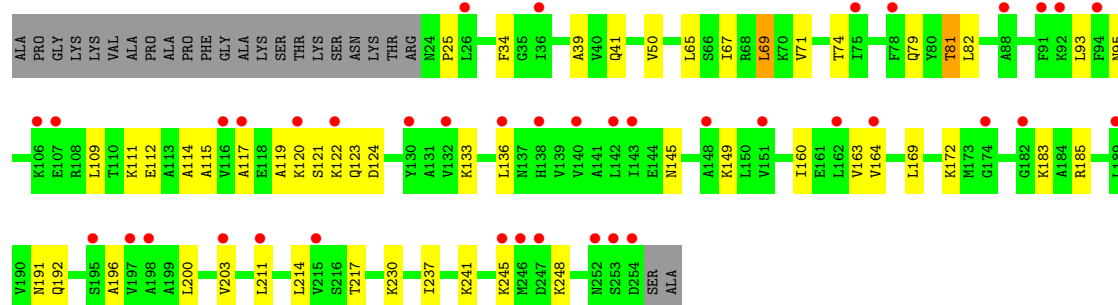
• Molecule 45: 60S ribosomal protein L8-A

Chain L8:



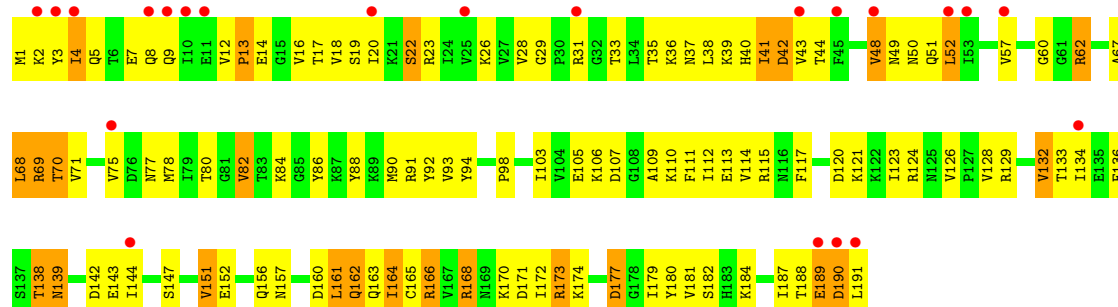
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



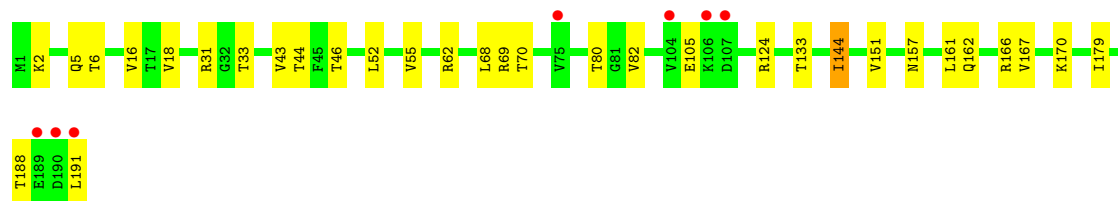
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



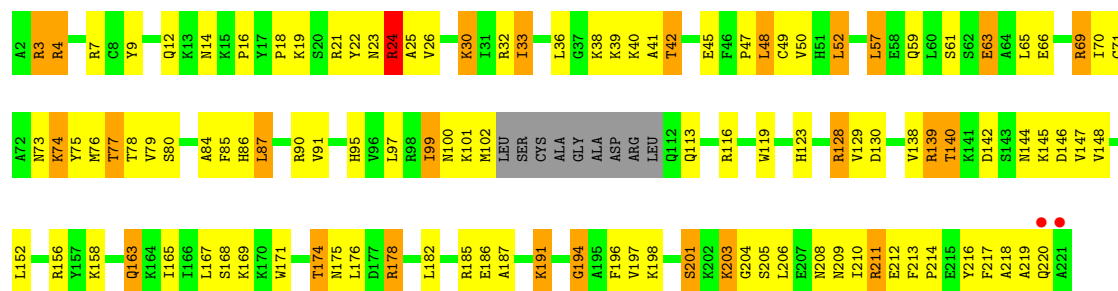
• Molecule 46: 60S ribosomal protein L9-A

Chain l9:



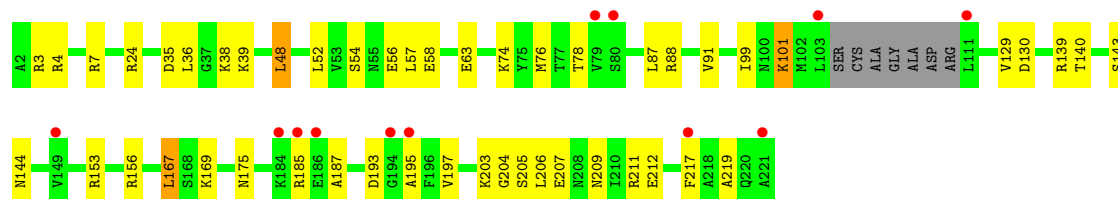
- Molecule 47: 60S ribosomal protein L10

Chain M0:



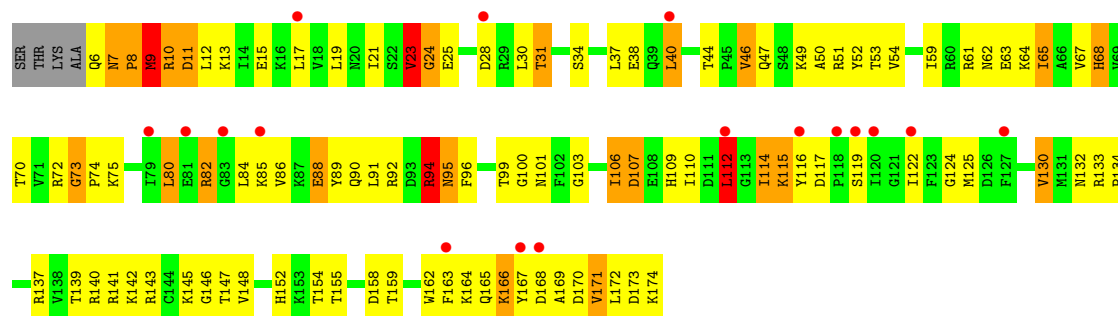
- Molecule 47: 60S ribosomal protein L10

Chain m0:



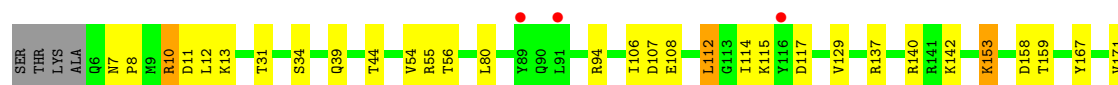
- Molecule 48: 60S ribosomal protein L11-B

Chain M1:



- Molecule 48: 60S ribosomal protein L11-B

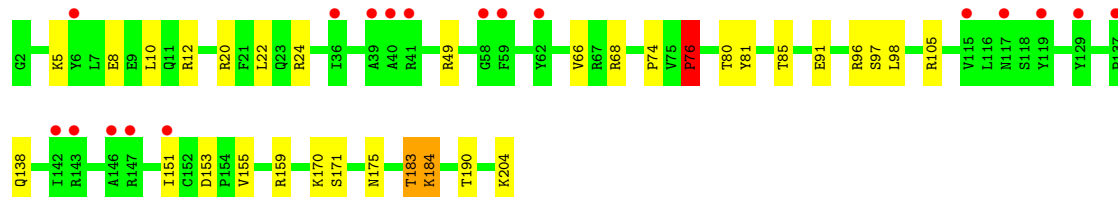
Chain m1:





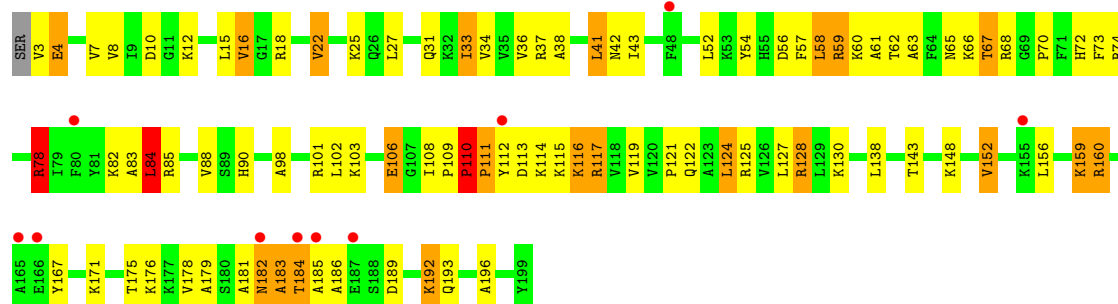
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



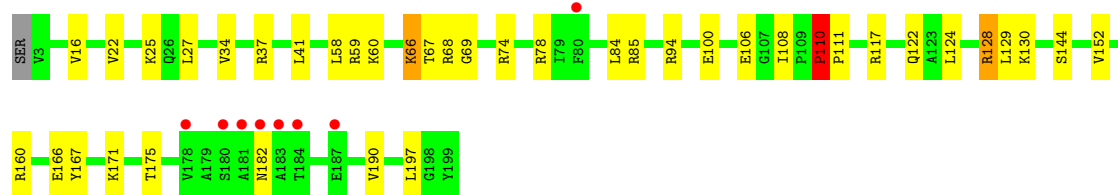
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



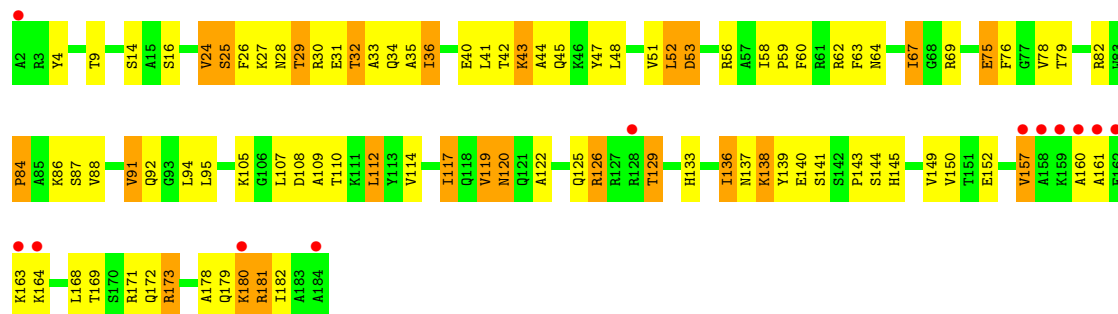
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



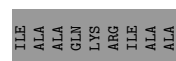
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



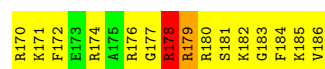
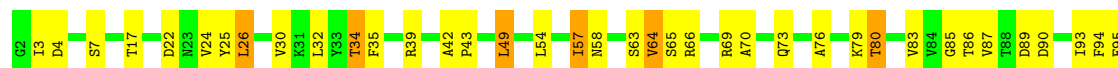
• Molecule 53: 60S ribosomal protein L17-A

Chain m7: 



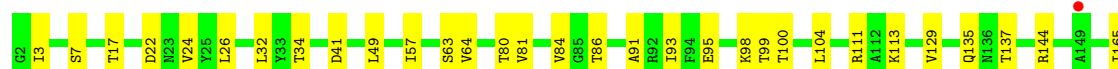
- Molecule 54: 60S ribosomal protein L18-A

Chain M8: 



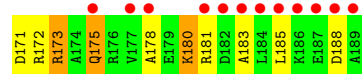
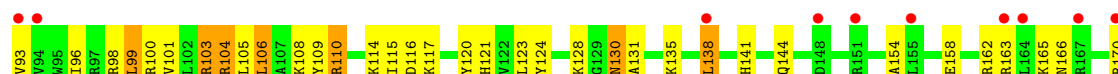
- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 



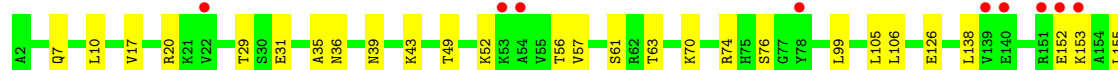
- Molecule 55: 60S ribosomal protein L19-A

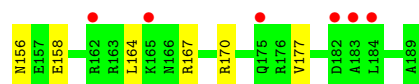
Chain M9: 



- Molecule 55: 60S ribosomal protein L19-A

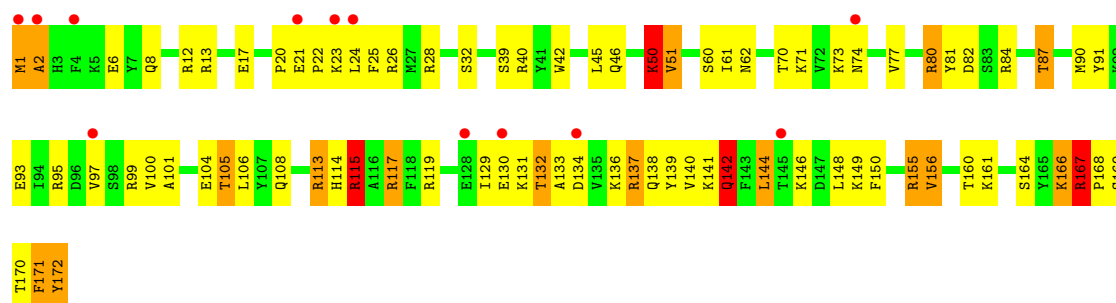
Chain m9: 





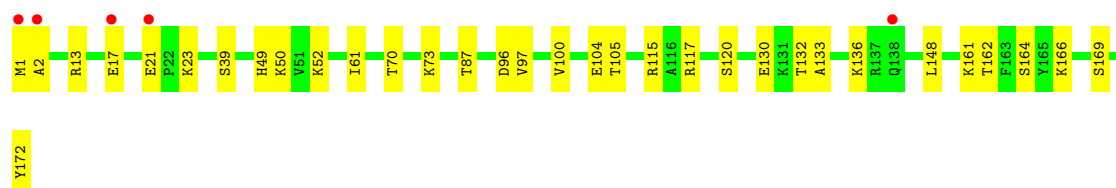
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



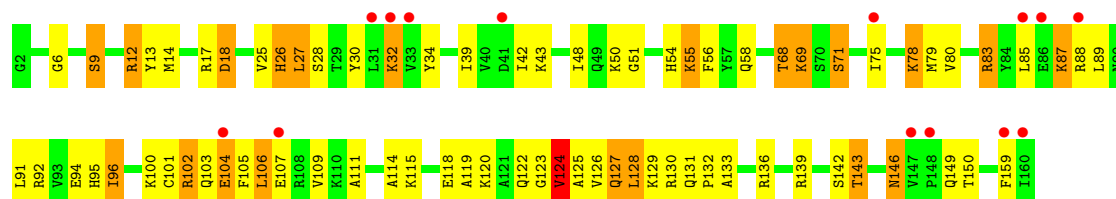
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



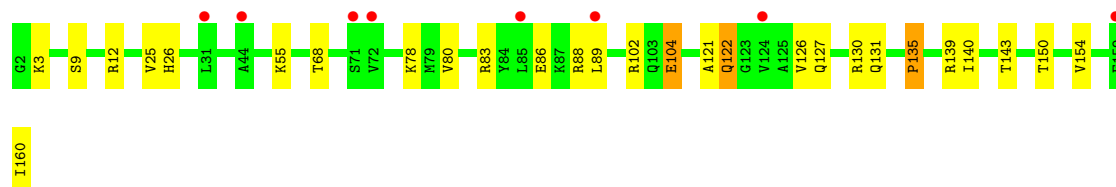
- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



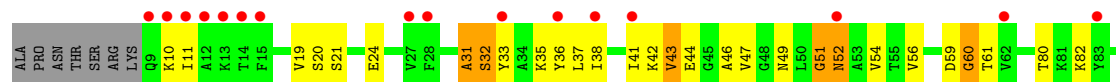
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



- Molecule 58: 60S ribosomal protein L22-A

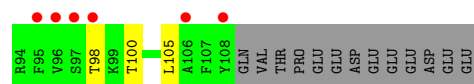
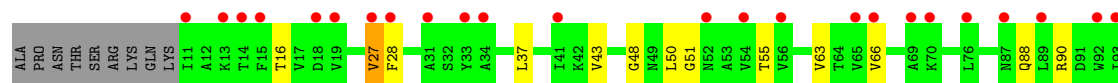
Chain N2:





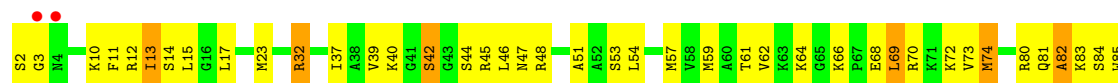
- Molecule 58: 60S ribosomal protein L22-A

Chain n2:



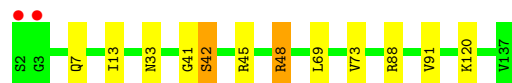
- Molecule 59: 60S ribosomal protein L23-A

Chain N3:



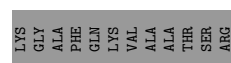
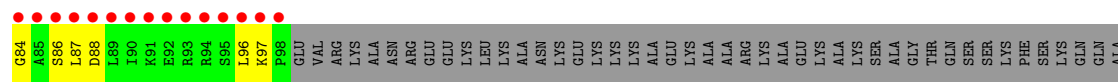
- Molecule 59: 60S ribosomal protein L23-A

Chain n3:



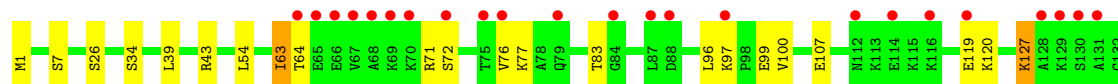
- Molecule 60: 60S ribosomal protein L24-A

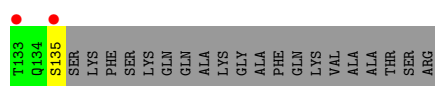
Chain N4:



- Molecule 60: 60S ribosomal protein L24-A

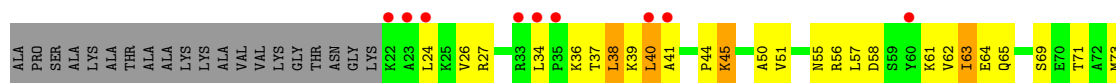
Chain n4:





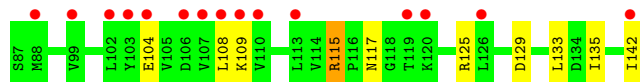
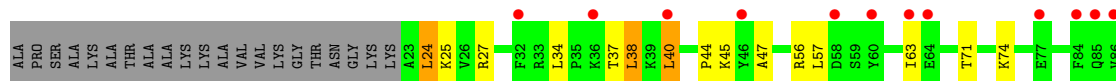
- Molecule 61: 60S ribosomal protein L25

Chain N5:



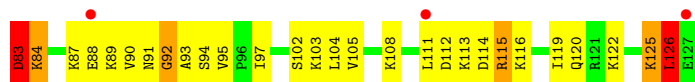
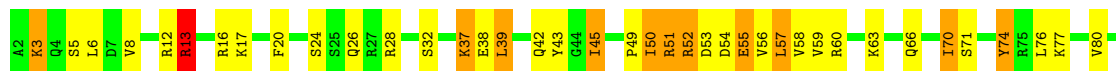
- Molecule 61: 60S ribosomal protein L25

Chain n5:



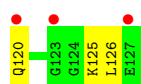
- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



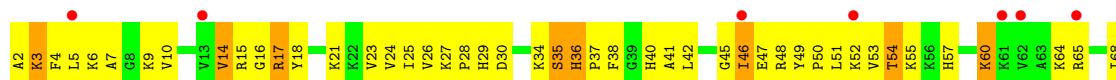
- Molecule 62: 60S ribosomal protein L26-A

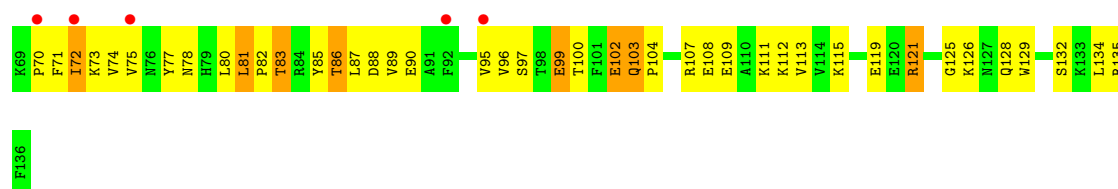
Chain n6:



- Molecule 63: 60S ribosomal protein L27-A

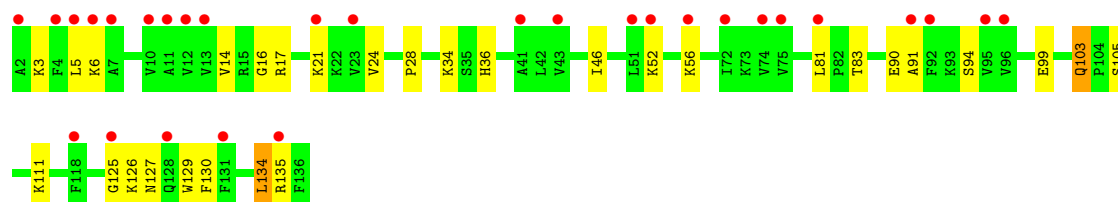
Chain N7:





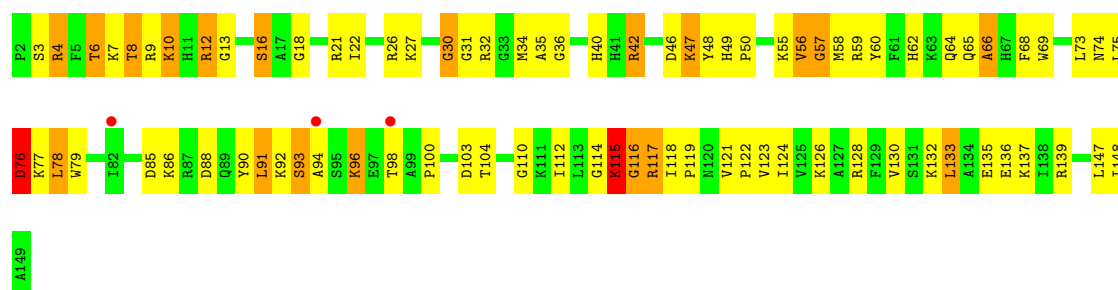
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



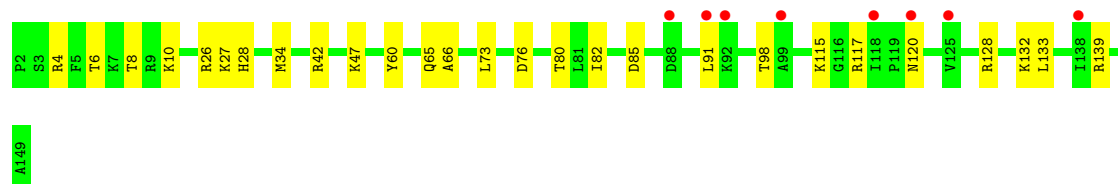
- Molecule 64: 60S ribosomal protein L28

Chain N8:



- Molecule 64: 60S ribosomal protein L28

Chain n8:



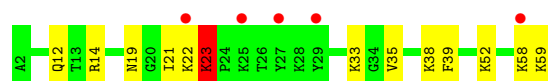
- Molecule 65: 60S ribosomal protein L29

Chain N9:



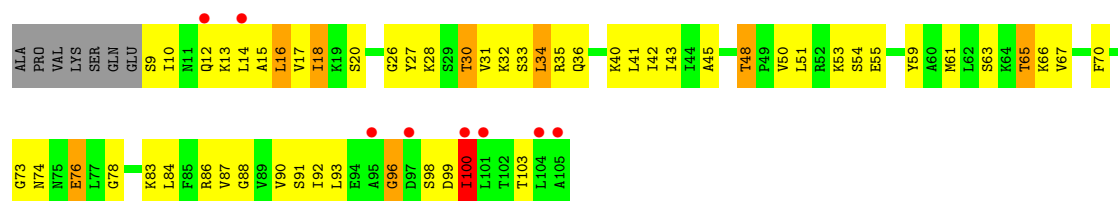
- Molecule 65: 60S ribosomal protein L29

Chain n9:



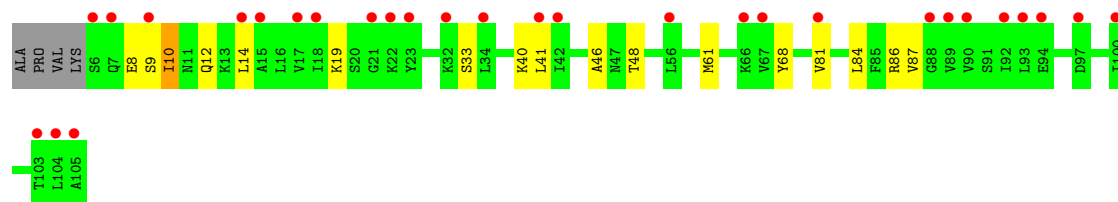
- Molecule 66: 60S ribosomal protein L30

Chain O0:



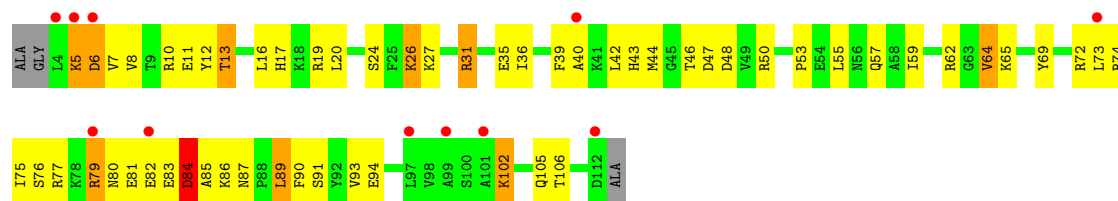
- Molecule 66: 60S ribosomal protein L30

Chain o0:



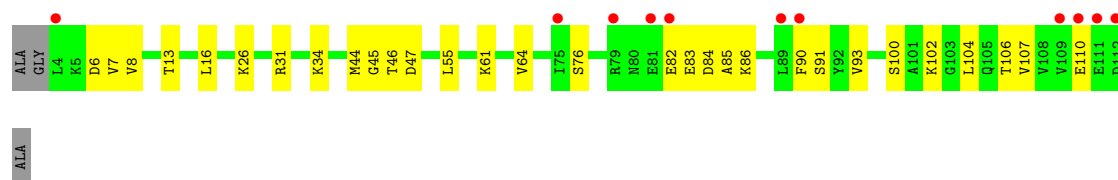
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



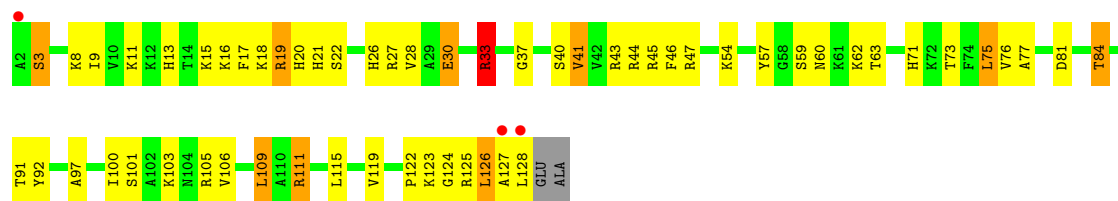
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



- Molecule 68: 60S ribosomal protein L32

Chain O2:



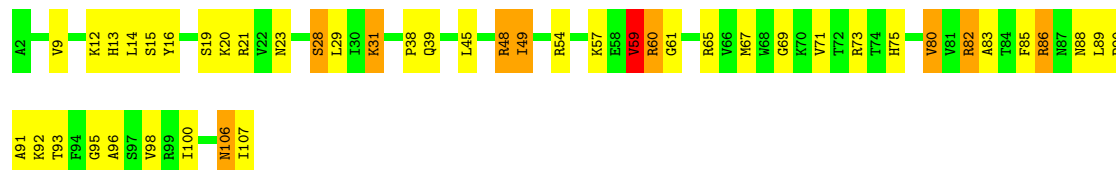
- Molecule 68: 60S ribosomal protein L32

Chain o2: 



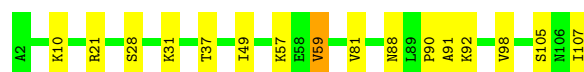
- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 



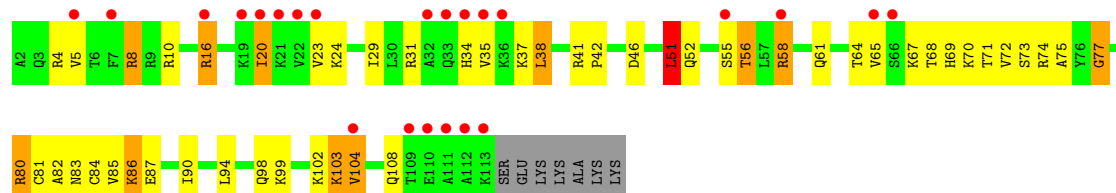
- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 



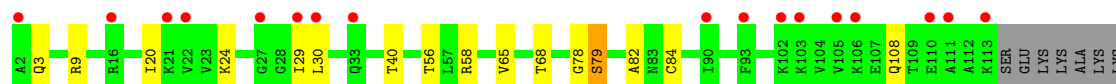
- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 



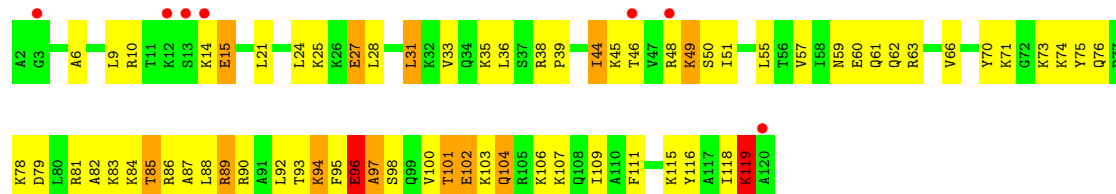
- Molecule 70: 60S ribosomal protein L34-A

Chain o4: 



- Molecule 71: 60S ribosomal protein L35-A

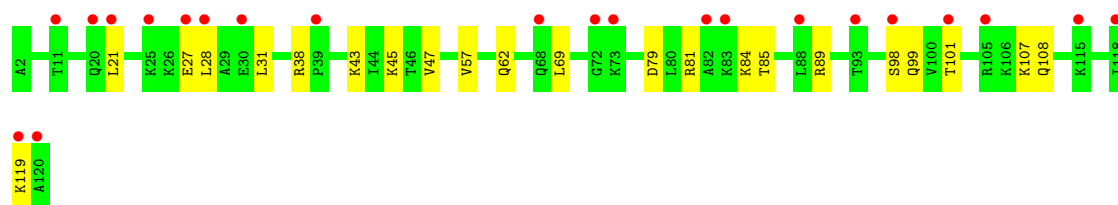
Chain O5: 



- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 





- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



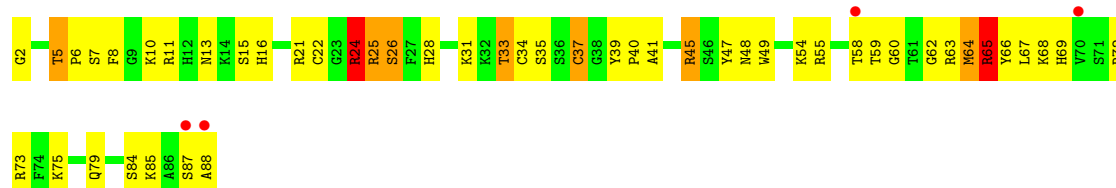
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



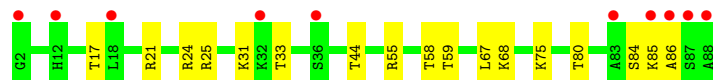
- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



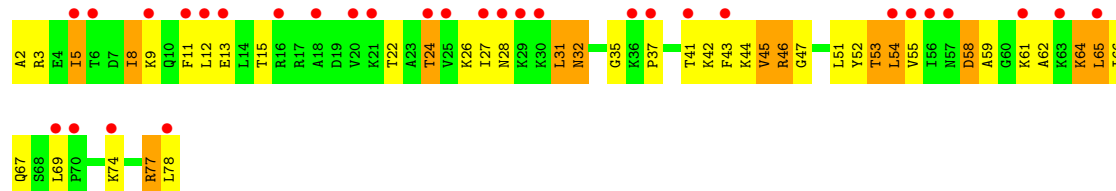
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

- Chain 09:



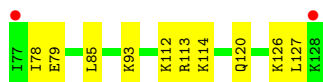
- Chain o9: 



- Chain Q0: 



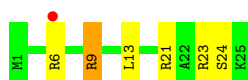
- Chain q0:



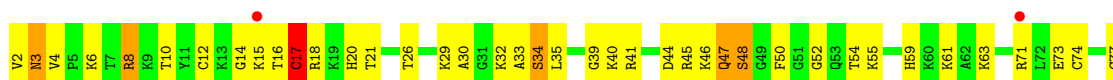
- Chain Q1:

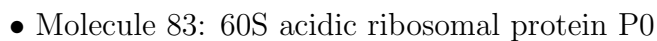


- Chain q1:



- Chain Q2:





ALA	ASP	ILE	ASP	P92	GLY
ALA	VAL	SER	VAL	L93	G3
SER	LYS	LEU	LYS	L96	I4
GLY	VAL	ALA	VAL	K97	R5
ASP	VAL	ILE	VAL	H98	L16
ALA	ASP	GLY	ASP	H99	
ALA	ALA	TYR	ALA	V99	
PRO	ALA	PRO	GLY	I100	
PRO	GLY	THR	ALA		
GLU	ASN	LEU	ASN	N103	Y22
GLU	LYS	PRO	LYS	R104	K23
ALA	VAL	SER	VAL		S24
ALA	GLY	ILE	GLY	A107	L25
ALA	GLN	VAL	GLN		F26
ALA	GLY	SER	GLY		V27
ALA	GLY	GLY	GLY		V28
GLU	GLU	HIS	GLU	ALA	G29
GLU	THR	THR	ALA	ARG	V30
GLU	LEU	LEU	SER	ALA	
GLU	ILE	LEU	LEU	GLY	V33
GLU	ASN	LEU	LEU	ALA	
SER	ASN	ASN	ASN	VAL	H39
ASP	TYR	LEU	LEU	ALA	
ASP	LYS	LEU	LEU	PRO	K43
ASP	ASN	ASP	ASN	GLU	
MET	ILE	LEU	ILE	ASP	G47
GLY	LEU	LEU	SER	ILE	R48
PHE	ALA	ALA	PRO	TRP	A49
GLY	VAL	VAL	PHE	VAL	V50
LEU	VAL	THR	THR	ARG	V51
PHE	ILE	PHE	PHE	ALA	
ASP	ALA	G184	ALA	VAL	T57
	ALA	L185	ASN	VAL	M58
	SER	T186	THR	THR	V59
	TYR	V187	GLY	MET	R60
	HIS	V188	GLY	GLU	
	TYR	Q189	PRO	PRO	I63
	PRO	V190	GLY	GLY	R64
	GLU	V191	LYS	THR	G65
	ILE	D192	THR	THR	F66
	GLU	N193	THR	SER	L67
	ASP	G194	SER	PHE	S68
	LEU	Q195	PHE	GLN	D69
	VAL	V196	PHE	VAL	L70
	ASP	P197	GLN	ALA	F71
	ARG	P198	ALA	LEU	D72
	ILE	T205	THR	VAL	E74
	GLU	D206	PRO	PRO	K75
	ASN		THR	THR	L76
	PRO		ALA	ALA	
	GLU	L209	LYS	ILE	F79
	TYR	V210	SER	ILE	V80
	ALA	S211	ALA	ARG	K81
	ALA	H212	ARG	GLY	
	ALA	F213	THR	THR	V84
	ALA		ILE	ILE	G85
	ALA	S218	ILE	ILE	F86
	PRO	T219	GLU	ILE	V87
	ALA	T220	ILE	ILE	F88
	ALA		VAL	VAL	
	THR	A221	SER	SER	F91

- Chain p1:
- 

- Molecule 85: 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	436.43Å 288.22Å 305.08Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	267.37 – 2.90 267.37 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (267.37-2.90) 99.9 (267.37-2.90)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.204 , 0.245 0.252 , 0.290	Depositor DCC
R_{free} test set	25170 reflections (1.54%)	DCC
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 1639575 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	411205	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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, OHX, MG, 3HE

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	0.69	3/41698 (0.0%)	1.25	259/64972 (0.4%)
1	6	0.83	9/42765 (0.0%)	1.36	416/66634 (0.6%)
2	S0	0.45	0/1617	0.63	0/2215
2	s0	0.50	0/1623	0.70	0/2222
3	S1	0.35	0/1735	0.63	2/2335 (0.1%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.49	0/1665	0.66	1/2263 (0.0%)
4	s2	0.60	0/1665	0.76	2/2263 (0.1%)
5	S3	0.49	0/1759	0.62	0/2368
5	s3	0.47	0/1759	0.60	0/2368
6	S4	0.48	0/2109	0.71	1/2839 (0.0%)
6	s4	0.57	0/2109	0.77	1/2839 (0.0%)
7	S5	0.39	0/1629	0.58	0/2202
7	s5	0.45	0/1629	0.63	0/2202
8	S6	0.45	0/1823	0.64	0/2439
8	s6	0.55	0/1779	0.69	0/2379
9	S7	0.43	0/1506	0.63	0/2028
9	s7	0.49	0/1516	0.68	0/2043
10	S8	0.53	0/1514	0.74	1/2021 (0.0%)
10	s8	0.62	0/1514	0.76	1/2021 (0.0%)
11	S9	0.46	0/1519	0.64	0/2035
11	s9	0.56	0/1519	0.72	1/2035 (0.0%)
12	C0	0.42	0/790	0.67	1/1069 (0.1%)
12	c0	0.39	0/777	0.63	3/1049 (0.3%)
13	C1	0.61	0/1240	0.80	1/1675 (0.1%)
13	c1	0.63	0/1194	0.78	0/1610
14	C2	0.36	0/900	0.63	0/1224
14	c2	0.30	0/900	0.56	0/1224
15	C3	0.46	0/1215	0.66	3/1638 (0.2%)
15	c3	0.56	0/1215	0.73	1/1638 (0.1%)
16	C4	0.36	0/901	0.63	0/1217
16	c4	0.51	0/960	0.72	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.46	0/998	0.65	0/1341
17	c5	0.51	0/1060	0.66	1/1426 (0.1%)
18	C6	0.45	0/1125	0.66	2/1510 (0.1%)
18	c6	0.49	0/1131	0.71	0/1518
19	C7	0.43	0/935	0.63	0/1254
19	c7	0.51	0/914	0.73	0/1224
20	C8	0.46	0/1211	0.64	0/1628
20	c8	0.49	0/1211	0.71	2/1628 (0.1%)
21	C9	0.46	0/1130	0.67	1/1517 (0.1%)
21	c9	0.51	0/1130	0.74	2/1517 (0.1%)
22	D0	0.46	0/865	0.65	0/1169
22	d0	0.51	0/892	0.68	0/1205
23	D1	0.43	0/693	0.60	0/935
23	d1	0.54	0/693	0.71	0/935
24	D2	0.53	0/1038	0.73	3/1395 (0.2%)
24	d2	0.62	0/1038	0.74	0/1395
25	D3	0.60	0/1139	0.81	3/1518 (0.2%)
25	d3	0.70	0/1139	0.79	1/1518 (0.1%)
26	D4	0.45	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.68	0/1449
27	D5	0.40	0/571	0.71	1/768 (0.1%)
27	d5	0.44	0/566	0.63	0/761
28	D6	0.44	0/782	0.67	0/1047
28	d6	0.54	0/782	0.72	0/1047
29	D7	0.43	0/620	0.67	1/838 (0.1%)
29	d7	0.49	0/620	0.68	0/838
30	D8	0.34	0/499	0.55	0/670
30	d8	0.42	0/499	0.66	0/670
31	D9	0.52	0/452	0.73	1/600 (0.2%)
31	d9	0.54	0/452	0.67	0/600
32	E0	0.46	0/483	0.61	0/643
33	E1	0.45	0/577	0.73	0/770
34	SR	0.89	2/2494 (0.1%)	1.42	4/3393 (0.1%)
34	sR	0.41	0/2495	0.58	0/3395
35	SM	0.52	0/1113	0.68	2/1502 (0.1%)
35	sM	0.50	0/683	0.66	1/923 (0.1%)
36	1	1.08	69/75394 (0.1%)	1.60	1618/117545 (1.4%)
36	5	1.10	113/75414 (0.1%)	1.60	1498/117575 (1.3%)
37	3	0.87	1/2883 (0.0%)	1.39	30/4491 (0.7%)
37	7	1.10	5/2883 (0.2%)	1.61	64/4491 (1.4%)
38	4	1.01	0/3746	1.51	61/5832 (1.0%)
38	8	0.87	0/3746	1.37	23/5832 (0.4%)
39	L2	0.72	0/1948	0.87	4/2617 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	l2	0.72	1/1946 (0.1%)	0.86	2/2614 (0.1%)
40	L3	0.73	0/3146	0.83	3/4228 (0.1%)
40	l3	0.82	2/3146 (0.1%)	0.89	7/4228 (0.2%)
41	L4	0.79	0/2800	0.94	6/3790 (0.2%)
41	l4	0.73	0/2800	0.88	3/3790 (0.1%)
42	L5	0.58	0/2425	0.70	0/3271
42	l5	0.71	0/2408	0.76	0/3248
43	L6	0.77	0/1260	0.84	1/1694 (0.1%)
43	l6	0.72	0/1269	0.82	1/1705 (0.1%)
44	L7	0.79	0/1821	0.85	1/2451 (0.0%)
44	l7	0.82	0/1828	0.86	3/2461 (0.1%)
45	L8	0.55	0/1836	0.67	1/2481 (0.0%)
45	l8	0.52	0/1796	0.69	1/2431 (0.0%)
46	L9	0.64	0/1539	0.76	1/2073 (0.0%)
46	l9	0.78	0/1539	0.82	0/2073
47	M0	0.72	0/1741	0.83	3/2335 (0.1%)
47	m0	0.77	1/1758 (0.1%)	0.85	3/2358 (0.1%)
48	M1	0.52	0/1374	0.71	1/1842 (0.1%)
48	m1	0.64	0/1374	0.79	1/1842 (0.1%)
49	M3	0.73	0/1568	0.84	3/2106 (0.1%)
49	m3	0.66	0/1573	0.82	3/2113 (0.1%)
50	M4	0.70	0/1068	0.80	1/1438 (0.1%)
50	m4	0.77	0/1074	0.81	1/1446 (0.1%)
51	M5	0.76	0/1757	0.82	0/2354
51	m5	0.65	0/1757	0.78	1/2354 (0.0%)
52	M6	0.83	1/1585 (0.1%)	0.92	3/2128 (0.1%)
52	m6	0.98	1/1585 (0.1%)	0.98	8/2128 (0.4%)
53	M7	0.78	1/1443 (0.1%)	0.83	0/1944
53	m7	0.84	0/1250	0.81	0/1683
54	M8	0.76	0/1465	0.91	4/1965 (0.2%)
54	m8	0.71	0/1465	0.87	1/1965 (0.1%)
55	M9	0.54	0/1538	0.66	0/2050
55	m9	0.59	0/1538	0.66	0/2050
56	N0	0.76	0/1481	0.83	1/1990 (0.1%)
56	n0	0.86	0/1481	0.83	0/1990
57	N1	0.78	1/1300 (0.1%)	0.81	0/1743
57	n1	0.82	1/1300 (0.1%)	0.81	0/1743
58	N2	0.44	0/812	0.61	0/1099
58	n2	0.51	0/794	0.67	0/1076
59	N3	0.72	0/1018	0.80	0/1369
59	n3	0.83	0/1018	0.94	3/1369 (0.2%)
60	N4	0.60	0/712	0.66	0/958
60	n4	0.66	0/1052	0.75	0/1398

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	N5	0.61	0/979	0.77	1/1321 (0.1%)
61	n5	0.62	0/974	0.75	1/1314 (0.1%)
62	N6	0.70	0/1004	0.88	3/1341 (0.2%)
62	n6	0.63	0/1004	0.80	1/1341 (0.1%)
63	N7	0.50	0/1118	0.65	0/1497
63	n7	0.45	0/1118	0.61	0/1497
64	N8	0.82	0/1204	0.92	2/1612 (0.1%)
64	n8	0.76	0/1204	0.95	3/1612 (0.2%)
65	N9	0.73	0/473	0.80	1/629 (0.2%)
65	n9	0.81	0/473	1.00	1/629 (0.2%)
66	O0	0.45	0/751	0.63	0/1008
66	o0	0.49	0/775	0.66	0/1040
67	O1	0.61	0/890	0.72	0/1196
67	o1	0.77	0/897	0.82	0/1205
68	O2	0.83	0/1041	0.92	2/1394 (0.1%)
68	o2	0.82	0/1041	0.92	3/1394 (0.2%)
69	O3	0.89	0/868	0.88	1/1168 (0.1%)
69	o3	0.89	0/868	0.84	0/1168
70	O4	0.59	0/890	0.75	1/1189 (0.1%)
70	o4	0.61	1/890 (0.1%)	0.73	0/1189
71	O5	0.67	0/978	0.78	0/1301
71	o5	0.58	0/974	0.66	0/1297
72	O6	0.63	0/778	0.82	1/1034 (0.1%)
72	o6	0.52	0/777	0.68	0/1033
73	O7	0.81	1/696 (0.1%)	0.95	2/923 (0.2%)
73	o7	0.70	0/696	0.79	0/923
74	O8	0.51	0/618	0.63	0/826
74	o8	0.44	0/614	0.61	0/822
75	O9	0.77	0/443	0.89	0/588
75	o9	0.69	0/443	0.76	1/588 (0.2%)
76	Q0	0.67	0/423	0.76	0/562
76	q0	0.81	0/423	0.90	0/562
77	Q1	0.68	0/234	1.04	0/300
77	q1	0.83	0/234	0.94	1/300 (0.3%)
78	Q2	0.93	1/860 (0.1%)	0.87	2/1136 (0.2%)
78	q2	0.86	1/860 (0.1%)	0.81	0/1136
79	Q3	0.77	0/701	0.82	0/934
79	q3	0.70	0/701	0.85	2/934 (0.2%)
80	e0	0.52	0/499	0.72	0/665
81	e1	0.39	0/619	0.73	1/822 (0.1%)
83	p0	0.43	0/1092	0.60	0/1474
All	All	0.85	215/430075 (0.0%)	1.27	4114/631366 (0.7%)

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
3	s1	0	1
6	s4	0	1
7	s5	0	1
9	S7	0	1
9	s7	0	1
10	S8	0	1
13	C1	0	1
16	C4	0	2
17	c5	0	1
19	C7	0	2
19	c7	0	1
20	c8	0	1
22	d0	0	1
25	d3	0	1
27	D5	0	3
28	D6	0	3
34	SR	0	2
39	L2	0	1
39	l2	0	2
42	l5	0	1
43	L6	0	1
44	L7	0	1
44	l7	0	2
52	M6	0	1
52	m6	0	1
53	M7	0	1
53	m7	0	1
56	n0	0	1
59	n3	0	1
62	n6	0	1
64	N8	0	2
64	n8	0	1
65	N9	0	1
65	n9	0	1
67	O1	0	1
67	o1	0	1
75	o9	0	1
78	Q2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
81	e1	0	1
All	All	0	50

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	SR	160	GLU	C-N	-30.25	0.64	1.34
34	SR	161	LYS	C-N	-24.97	0.76	1.34
78	Q2	17	CYS	CB-SG	16.00	2.09	1.82
36	5	1152	G	N9-C4	-13.57	1.27	1.38
78	q2	17	CYS	CB-SG	12.94	2.04	1.82

The worst 5 of 4114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	SR	161	LYS	O-C-N	-44.54	51.44	122.70
34	SR	160	GLU	C-N-CA	-39.83	22.12	121.70
34	SR	160	GLU	CA-C-N	-34.85	40.53	117.20
36	5	1152	G	N3-C4-C5	27.52	142.36	128.60
36	5	1152	G	N3-C4-N9	-27.23	109.66	126.00

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	88	ARG	Peptide
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
9	S7	31	SER	Peptide
10	S8	79	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	754	1
1	6	38238	0	19241	711	0
2	S0	1577	0	1567	124	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	143	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	108	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	138	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	134	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	123	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	116	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	102	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	124	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	48	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	64	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	56	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	70	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	84	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	66	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	70	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	64	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	84	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	90	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	79	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	55	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	68	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	56	0
27	d5	558	0	598	0	0
28	D6	769	0	814	77	0
28	d6	769	0	814	0	0
29	D7	610	0	631	34	0
29	d7	610	0	631	0	0
30	D8	497	0	535	45	0
30	d8	497	0	535	0	0
31	D9	442	0	428	29	0
31	d9	442	0	428	0	0
32	E0	475	0	525	22	0
33	E1	566	0	602	64	0
34	SR	2441	0	2395	134	1
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	58	0
35	sM	680	0	607	0	0
36	1	67355	0	33847	1105	0
36	5	67376	0	33858	1049	1
37	3	2579	0	1304	38	0
37	7	2579	0	1304	37	0
38	4	3353	0	1695	56	1
38	8	3353	0	1695	56	0
39	L2	1914	0	1981	124	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	239	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	170	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	153	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	61	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	l7	1791	0	1869	0	0
45	L8	1804	0	1875	126	0
45	l8	1764	0	1821	0	0
46	L9	1518	0	1587	107	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1736	112	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	87	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	111	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	58	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	104	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	97	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	87	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	88	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	73	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	82	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	68	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	35	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	58	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	20	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	48	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	59	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	79	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	103	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	n9	462	0	491	0	0
66	O0	743	0	797	48	0
66	o0	767	0	816	0	0
67	O1	876	0	912	47	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	51	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	41	0
69	o3	850	0	880	0	0
70	O4	880	0	945	45	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	64	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	50	0
72	o6	770	0	846	0	0
73	O7	681	0	683	50	0
73	o7	681	0	683	0	0
74	O8	612	0	682	32	0
74	o8	608	0	671	0	0
75	O9	436	0	475	36	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	20	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	22	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	45	0
78	q2	847	0	916	0	0
79	Q3	694	0	734	49	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	e1	608	0	654	0	0
82	m2	750	0	176	0	0
83	p0	1077	0	1041	0	0
84	p1	235	0	51	0	0
85	p2	230	0	52	0	0
86	1	471	0	0	0	0
86	2	122	0	0	0	0
86	3	14	0	0	0	0
86	4	22	0	0	0	0
86	5	505	0	0	0	0
86	6	147	0	0	0	0
86	7	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	8	13	0	0	0	0
86	C3	1	0	0	0	0
86	D0	1	0	0	0	0
86	D3	1	0	0	0	0
86	L2	1	0	0	0	0
86	L3	3	0	0	0	0
86	L4	1	0	0	0	0
86	L5	1	0	0	0	0
86	L7	3	0	0	0	0
86	L8	1	0	0	0	0
86	M0	2	0	0	0	0
86	M1	1	0	0	0	0
86	M3	4	0	0	0	0
86	M5	2	0	0	0	0
86	M6	1	0	0	0	0
86	M7	6	0	0	0	0
86	M9	1	0	0	0	0
86	N0	1	0	0	0	0
86	N3	3	0	0	0	0
86	N5	1	0	0	0	0
86	N8	4	0	0	0	0
86	O1	1	0	0	0	0
86	O3	1	0	0	0	0
86	O4	2	0	0	0	0
86	O7	1	0	0	0	0
86	Q2	1	0	0	0	0
86	S2	1	0	0	0	0
86	S4	1	0	0	0	0
86	S8	1	0	0	0	0
86	SM	1	0	0	0	0
86	c1	1	0	0	0	0
86	c4	1	0	0	0	0
86	c7	2	0	0	0	0
86	c8	2	0	0	0	0
86	d3	1	0	0	0	0
86	d4	1	0	0	0	0
86	d6	1	0	0	0	0
86	l2	2	0	0	0	0
86	l3	1	0	0	0	0
86	l4	2	0	0	0	0
86	l5	2	0	0	0	0
86	l7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	l8	1	0	0	0	0
86	m1	2	0	0	0	0
86	m5	2	0	0	0	0
86	m6	1	0	0	0	0
86	m7	4	0	0	0	0
86	n0	2	0	0	0	0
86	n3	2	0	0	0	0
86	n6	2	0	0	0	0
86	n8	3	0	0	0	0
86	o1	2	0	0	0	0
86	o3	1	0	0	0	0
86	o4	2	0	0	0	0
86	o7	1	0	0	0	0
86	q0	1	0	0	0	0
86	q3	2	0	0	0	0
86	s1	1	0	0	0	0
86	s6	1	0	0	0	0
86	s8	1	0	0	0	0
86	sM	2	0	0	0	0
87	1	2457	0	0	251	0
87	2	1106	0	0	121	0
87	3	77	0	0	6	0
87	4	98	0	0	8	0
87	5	2464	0	0	245	0
87	6	1113	0	0	103	0
87	7	91	0	0	11	0
87	8	112	0	0	19	0
87	C3	7	0	0	0	0
87	C5	7	0	0	6	0
87	C8	7	0	0	1	0
87	D3	7	0	0	0	0
87	D9	7	0	0	4	0
87	L3	21	0	0	1	0
87	L4	7	0	0	2	0
87	M0	7	0	0	0	0
87	M5	7	0	0	0	0
87	M7	14	0	0	2	0
87	M9	7	0	0	1	0
87	N1	7	0	0	0	0
87	N9	7	0	0	0	0
87	O2	7	0	0	0	0
87	O3	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	O7	14	0	0	6	0
87	O9	7	0	0	4	0
87	Q2	7	0	0	2	0
87	S8	7	0	0	1	0
87	SR	7	0	0	0	0
87	c1	7	0	0	0	0
87	c3	7	0	0	0	0
87	c5	7	0	0	0	0
87	c8	7	0	0	0	0
87	d4	7	0	0	0	0
87	d9	7	0	0	0	0
87	l3	21	0	0	0	0
87	l4	14	0	0	0	0
87	l5	21	0	0	0	0
87	l9	7	0	0	0	0
87	m0	14	0	0	0	0
87	m1	7	0	0	0	0
87	m4	7	0	0	0	0
87	m5	7	0	0	0	0
87	m6	7	0	0	0	0
87	m7	7	0	0	0	0
87	m8	7	0	0	0	0
87	n3	7	0	0	0	0
87	n9	7	0	0	0	0
87	o2	7	0	0	0	0
87	o3	7	0	0	0	0
87	o7	7	0	0	0	0
87	o9	7	0	0	0	0
87	q2	7	0	0	0	0
87	s1	7	0	0	0	0
87	s4	7	0	0	0	0
87	s8	7	0	0	0	0
87	s9	7	0	0	0	0
87	sR	7	0	0	0	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	0	0
88	Q3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
89	1	20	0	0	0	0
89	5	20	0	0	0	0
All	All	411205	0	297289	8429	2

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 8429 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	1.49	1.52
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.09	1.45
36:1:1481:A:O2'	36:1:1858:A:N3	1.85	1.07
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.52	1.03
40:L3:296:THR:HG22	40:L3:298:PHE:H	1.44	0.99

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:236:A:O2'	38:4:158:U:O2'[2_556]	2.06	0.14
34:SR:137:LYS:NZ	36:5:3293:U:O4[2_546]	2.10	0.10

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%)	151 (74%)	36 (18%)	17 (8%)	1	3
2	s0	204/251 (81%)	157 (77%)	30 (15%)	17 (8%)	1	3
3	S1	212/254 (84%)	145 (68%)	35 (16%)	32 (15%)	0	1
3	s1	214/254 (84%)	179 (84%)	21 (10%)	14 (6%)	2	5
4	S2	215/253 (85%)	190 (88%)	17 (8%)	8 (4%)	5	20
4	s2	215/253 (85%)	184 (86%)	20 (9%)	11 (5%)	3	10
5	S3	221/239 (92%)	194 (88%)	19 (9%)	8 (4%)	5	22
5	s3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	2	5
6	S4	258/260 (99%)	213 (83%)	34 (13%)	11 (4%)	4	15
6	s4	258/260 (99%)	224 (87%)	19 (7%)	15 (6%)	3	7
7	S5	204/224 (91%)	166 (81%)	20 (10%)	18 (9%)	1	3
7	s5	204/224 (91%)	167 (82%)	18 (9%)	19 (9%)	1	2
8	S6	224/236 (95%)	194 (87%)	19 (8%)	11 (5%)	3	12
8	s6	216/236 (92%)	189 (88%)	20 (9%)	7 (3%)	6	25
9	S7	182/189 (96%)	137 (75%)	26 (14%)	19 (10%)	1	2
9	s7	184/189 (97%)	154 (84%)	21 (11%)	9 (5%)	3	12
10	S8	184/200 (92%)	156 (85%)	13 (7%)	15 (8%)	1	3
10	s8	184/200 (92%)	163 (89%)	15 (8%)	6 (3%)	6	24
11	S9	183/196 (93%)	153 (84%)	21 (12%)	9 (5%)	3	12
11	s9	183/196 (93%)	154 (84%)	19 (10%)	10 (6%)	3	8
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	2	4
12	c0	92/105 (88%)	65 (71%)	15 (16%)	12 (13%)	0	1
13	C1	153/155 (99%)	125 (82%)	14 (9%)	14 (9%)	1	2
13	c1	144/155 (93%)	123 (85%)	14 (10%)	7 (5%)	3	12
14	C2	122/142 (86%)	76 (62%)	24 (20%)	22 (18%)	0	0
14	c2	122/142 (86%)	74 (61%)	30 (25%)	18 (15%)	0	1
15	C3	148/150 (99%)	129 (87%)	13 (9%)	6 (4%)	4	17
15	c3	148/150 (99%)	124 (84%)	14 (10%)	10 (7%)	2	5
16	C4	125/136 (92%)	98 (78%)	16 (13%)	11 (9%)	1	3
16	c4	126/136 (93%)	102 (81%)	12 (10%)	12 (10%)	1	2
17	C5	122/141 (86%)	91 (75%)	21 (17%)	10 (8%)	1	3
17	c5	133/141 (94%)	97 (73%)	22 (16%)	14 (10%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	C6	139/142 (98%)	122 (88%)	11 (8%)	6 (4%)	4	15
18	c6	140/142 (99%)	124 (89%)	10 (7%)	6 (4%)	4	15
19	C7	116/136 (85%)	87 (75%)	20 (17%)	9 (8%)	1	3
19	c7	113/136 (83%)	92 (81%)	10 (9%)	11 (10%)	1	2
20	C8	143/145 (99%)	117 (82%)	14 (10%)	12 (8%)	1	3
20	c8	143/145 (99%)	120 (84%)	16 (11%)	7 (5%)	3	12
21	C9	141/143 (99%)	121 (86%)	14 (10%)	6 (4%)	4	15
21	c9	141/143 (99%)	117 (83%)	17 (12%)	7 (5%)	3	11
22	D0	105/120 (88%)	87 (83%)	14 (13%)	4 (4%)	5	19
22	d0	108/120 (90%)	86 (80%)	13 (12%)	9 (8%)	1	3
23	D1	85/87 (98%)	67 (79%)	11 (13%)	7 (8%)	1	3
23	d1	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	19	57
24	D2	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	9	35
24	d2	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	27	68
25	D3	142/144 (99%)	109 (77%)	17 (12%)	16 (11%)	1	1
25	d3	142/144 (99%)	124 (87%)	17 (12%)	1 (1%)	30	72
26	D4	132/134 (98%)	111 (84%)	14 (11%)	7 (5%)	3	9
26	d4	132/134 (98%)	109 (83%)	18 (14%)	5 (4%)	5	19
27	D5	68/107 (64%)	48 (71%)	10 (15%)	10 (15%)	0	1
27	d5	67/107 (63%)	52 (78%)	10 (15%)	5 (8%)	2	4
28	D6	95/97 (98%)	66 (70%)	10 (10%)	19 (20%)	0	0
28	d6	95/97 (98%)	74 (78%)	13 (14%)	8 (8%)	1	3
29	D7	79/81 (98%)	61 (77%)	15 (19%)	3 (4%)	5	19
29	d7	79/81 (98%)	62 (78%)	12 (15%)	5 (6%)	2	6
30	D8	61/66 (92%)	51 (84%)	6 (10%)	4 (7%)	2	5
30	d8	61/66 (92%)	46 (75%)	13 (21%)	2 (3%)	6	24
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	5	18
31	d9	51/55 (93%)	43 (84%)	4 (8%)	4 (8%)	1	3
32	E0	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	3	10
33	E1	69/76 (91%)	35 (51%)	19 (28%)	15 (22%)	0	0
34	SR	316/318 (99%)	252 (80%)	36 (11%)	28 (9%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	sR	316/318 (99%)	274 (87%)	30 (10%)	12 (4%)	5	19
35	SM	155/273 (57%)	112 (72%)	22 (14%)	21 (14%)	0	1
35	sM	98/273 (36%)	65 (66%)	18 (18%)	15 (15%)	0	1
39	L2	250/253 (99%)	222 (89%)	25 (10%)	3 (1%)	19	57
39	l2	250/253 (99%)	219 (88%)	25 (10%)	6 (2%)	9	35
40	L3	384/386 (100%)	339 (88%)	31 (8%)	14 (4%)	5	22
40	l3	384/386 (100%)	343 (89%)	31 (8%)	10 (3%)	8	32
41	L4	359/361 (99%)	303 (84%)	37 (10%)	19 (5%)	3	9
41	l4	359/361 (99%)	309 (86%)	31 (9%)	19 (5%)	3	9
42	L5	294/296 (99%)	249 (85%)	27 (9%)	18 (6%)	2	7
42	l5	292/296 (99%)	256 (88%)	32 (11%)	4 (1%)	16	52
43	L6	152/175 (87%)	140 (92%)	10 (7%)	2 (1%)	18	54
43	l6	153/175 (87%)	130 (85%)	19 (12%)	4 (3%)	8	32
44	L7	220/243 (90%)	202 (92%)	11 (5%)	7 (3%)	6	25
44	l7	221/243 (91%)	204 (92%)	14 (6%)	3 (1%)	16	52
45	L8	231/255 (91%)	189 (82%)	30 (13%)	12 (5%)	3	10
45	l8	229/255 (90%)	185 (81%)	23 (10%)	21 (9%)	1	2
46	L9	189/191 (99%)	170 (90%)	15 (8%)	4 (2%)	11	39
46	l9	189/191 (99%)	173 (92%)	13 (7%)	3 (2%)	14	47
47	M0	207/220 (94%)	182 (88%)	18 (9%)	7 (3%)	6	23
47	m0	209/220 (95%)	175 (84%)	25 (12%)	9 (4%)	4	15
48	M1	167/173 (96%)	127 (76%)	26 (16%)	14 (8%)	1	3
48	m1	167/173 (96%)	143 (86%)	15 (9%)	9 (5%)	3	9
49	M3	191/198 (96%)	170 (89%)	17 (9%)	4 (2%)	11	39
49	m3	192/198 (97%)	162 (84%)	18 (9%)	12 (6%)	2	6
50	M4	134/137 (98%)	116 (87%)	11 (8%)	7 (5%)	3	10
50	m4	135/137 (98%)	126 (93%)	7 (5%)	2 (2%)	15	50
51	M5	201/203 (99%)	186 (92%)	8 (4%)	7 (4%)	6	23
51	m5	201/203 (99%)	179 (89%)	16 (8%)	6 (3%)	7	27
52	M6	195/198 (98%)	183 (94%)	7 (4%)	5 (3%)	8	32
52	m6	195/198 (98%)	184 (94%)	8 (4%)	3 (2%)	15	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	M7	181/183 (99%)	156 (86%)	17 (9%)	8 (4%)	4	15
53	m7	153/183 (84%)	136 (89%)	16 (10%)	1 (1%)	30	72
54	M8	183/185 (99%)	166 (91%)	12 (7%)	5 (3%)	8	30
54	m8	183/185 (99%)	161 (88%)	15 (8%)	7 (4%)	5	19
55	M9	186/188 (99%)	177 (95%)	7 (4%)	2 (1%)	21	60
55	m9	186/188 (99%)	169 (91%)	14 (8%)	3 (2%)	14	47
56	N0	170/172 (99%)	156 (92%)	10 (6%)	4 (2%)	9	35
56	n0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	33	76
57	N1	157/159 (99%)	137 (87%)	14 (9%)	6 (4%)	5	19
57	n1	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	12	42
58	N2	98/120 (82%)	73 (74%)	19 (19%)	6 (6%)	2	7
58	n2	96/120 (80%)	79 (82%)	13 (14%)	4 (4%)	4	16
59	N3	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	30	72
59	n3	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	15	50
60	N4	96/155 (62%)	72 (75%)	15 (16%)	9 (9%)	1	2
60	n4	133/155 (86%)	113 (85%)	11 (8%)	9 (7%)	2	5
61	N5	119/141 (84%)	108 (91%)	9 (8%)	2 (2%)	14	45
61	n5	118/141 (84%)	97 (82%)	15 (13%)	6 (5%)	3	10
62	N6	124/126 (98%)	111 (90%)	7 (6%)	6 (5%)	4	12
62	n6	124/126 (98%)	109 (88%)	10 (8%)	5 (4%)	5	17
63	N7	133/135 (98%)	115 (86%)	11 (8%)	7 (5%)	3	9
63	n7	133/135 (98%)	109 (82%)	11 (8%)	13 (10%)	1	2
64	N8	146/148 (99%)	120 (82%)	18 (12%)	8 (6%)	3	8
64	n8	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	30	72
65	N9	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	5	22
65	n9	56/58 (97%)	44 (79%)	9 (16%)	3 (5%)	3	9
66	O0	95/104 (91%)	89 (94%)	4 (4%)	2 (2%)	11	39
66	o0	98/104 (94%)	88 (90%)	8 (8%)	2 (2%)	11	40
67	O1	107/112 (96%)	96 (90%)	7 (6%)	4 (4%)	5	20
67	o1	107/112 (96%)	89 (83%)	10 (9%)	8 (8%)	2	4
68	O2	125/129 (97%)	113 (90%)	11 (9%)	1 (1%)	27	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	o2	125/129 (97%)	108 (86%)	14 (11%)	3 (2%)	9	35
69	O3	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	22	63
69	o3	104/106 (98%)	95 (91%)	6 (6%)	3 (3%)	7	28
70	O4	110/119 (92%)	102 (93%)	7 (6%)	1 (1%)	25	66
70	o4	110/119 (92%)	102 (93%)	5 (4%)	3 (3%)	8	30
71	O5	117/119 (98%)	104 (89%)	9 (8%)	4 (3%)	6	23
71	o5	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	14	45
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	2	6
72	o6	97/99 (98%)	84 (87%)	5 (5%)	8 (8%)	1	3
73	O7	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
73	o7	85/87 (98%)	74 (87%)	9 (11%)	2 (2%)	9	35
74	O8	75/77 (97%)	65 (87%)	8 (11%)	2 (3%)	8	30
74	o8	75/77 (97%)	67 (89%)	5 (7%)	3 (4%)	5	17
75	O9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o9	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	11	39
76	Q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	5	17
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	11	40
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	89 (86%)	9 (9%)	5 (5%)	3	12
78	q2	103/105 (98%)	94 (91%)	7 (7%)	2 (2%)	12	42
79	Q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	10	37
79	q3	89/91 (98%)	81 (91%)	6 (7%)	2 (2%)	10	37
80	e0	60/62 (97%)	51 (85%)	5 (8%)	4 (7%)	2	5
81	e1	74/76 (97%)	37 (50%)	18 (24%)	19 (26%)	0	0
83	p0	139/311 (45%)	114 (82%)	21 (15%)	4 (3%)	7	28
All	All	22333/24141 (92%)	18964 (85%)	2226 (10%)	1143 (5%)	3	10

5 of 1143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN

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Mol	Chain	Res	Type
2	S0	39	ASN
2	S0	95	ALA
2	S0	158	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	130 (79%)	34 (21%)	2	5
2	s0	165/209 (79%)	138 (84%)	27 (16%)	3	10
3	S1	191/223 (86%)	159 (83%)	32 (17%)	3	9
3	s1	192/223 (86%)	162 (84%)	30 (16%)	4	11
4	S2	176/204 (86%)	140 (80%)	36 (20%)	2	5
4	s2	176/204 (86%)	137 (78%)	39 (22%)	1	4
5	S3	182/194 (94%)	142 (78%)	40 (22%)	1	4
5	s3	182/194 (94%)	145 (80%)	37 (20%)	2	5
6	S4	221/221 (100%)	178 (80%)	43 (20%)	2	6
6	s4	221/221 (100%)	179 (81%)	42 (19%)	2	6
7	S5	173/190 (91%)	148 (86%)	25 (14%)	5	13
7	s5	173/190 (91%)	144 (83%)	29 (17%)	3	9
8	S6	188/201 (94%)	150 (80%)	38 (20%)	2	5
8	s6	187/201 (93%)	155 (83%)	32 (17%)	3	8
9	S7	165/169 (98%)	127 (77%)	38 (23%)	1	3
9	s7	165/169 (98%)	136 (82%)	29 (18%)	3	8
10	S8	150/161 (93%)	128 (85%)	22 (15%)	4	13
10	s8	150/161 (93%)	126 (84%)	24 (16%)	3	10
11	S9	158/165 (96%)	122 (77%)	36 (23%)	1	3
11	s9	158/165 (96%)	123 (78%)	35 (22%)	1	4
12	C0	77/98 (79%)	62 (80%)	15 (20%)	2	6
12	c0	73/98 (74%)	63 (86%)	10 (14%)	5	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	C1	129/136 (95%)	108 (84%)	21 (16%)	3	10
13	c1	129/136 (95%)	105 (81%)	24 (19%)	2	7
14	C2	88/118 (75%)	67 (76%)	21 (24%)	1	3
14	c2	88/118 (75%)	70 (80%)	18 (20%)	2	5
15	C3	127/127 (100%)	106 (84%)	21 (16%)	3	9
15	c3	127/127 (100%)	103 (81%)	24 (19%)	2	7
16	C4	81/104 (78%)	58 (72%)	23 (28%)	0	2
16	c4	97/104 (93%)	75 (77%)	22 (23%)	1	4
17	C5	101/117 (86%)	86 (85%)	15 (15%)	4	12
17	c5	103/117 (88%)	85 (82%)	18 (18%)	3	8
18	C6	117/118 (99%)	97 (83%)	20 (17%)	3	8
18	c6	118/118 (100%)	95 (80%)	23 (20%)	2	6
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1	4
19	c7	92/124 (74%)	77 (84%)	15 (16%)	3	10
20	C8	128/128 (100%)	102 (80%)	26 (20%)	2	5
20	c8	128/128 (100%)	98 (77%)	30 (23%)	1	3
21	C9	115/115 (100%)	95 (83%)	20 (17%)	3	8
21	c9	115/115 (100%)	96 (84%)	19 (16%)	3	9
22	D0	100/113 (88%)	76 (76%)	24 (24%)	1	3
22	d0	103/113 (91%)	81 (79%)	22 (21%)	1	4
23	D1	74/74 (100%)	61 (82%)	13 (18%)	3	8
23	d1	74/74 (100%)	60 (81%)	14 (19%)	2	7
24	D2	110/110 (100%)	88 (80%)	22 (20%)	2	6
24	d2	110/110 (100%)	96 (87%)	14 (13%)	6	18
25	D3	119/119 (100%)	96 (81%)	23 (19%)	2	6
25	d3	119/119 (100%)	102 (86%)	17 (14%)	5	13
26	D4	112/112 (100%)	95 (85%)	17 (15%)	4	12
26	d4	112/112 (100%)	98 (88%)	14 (12%)	7	19
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1	3
27	d5	61/88 (69%)	52 (85%)	9 (15%)	4	13
28	D6	83/83 (100%)	68 (82%)	15 (18%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	d6	83/83 (100%)	72 (87%)	11 (13%)	6	16
29	D7	70/70 (100%)	59 (84%)	11 (16%)	4	11
29	d7	70/70 (100%)	63 (90%)	7 (10%)	11	32
30	D8	56/59 (95%)	42 (75%)	14 (25%)	1	3
30	d8	56/59 (95%)	47 (84%)	9 (16%)	3	10
31	D9	47/48 (98%)	39 (83%)	8 (17%)	3	9
31	d9	47/48 (98%)	41 (87%)	6 (13%)	6	18
32	E0	51/51 (100%)	44 (86%)	7 (14%)	5	15
33	E1	62/66 (94%)	51 (82%)	11 (18%)	3	8
34	SR	260/261 (100%)	223 (86%)	37 (14%)	5	13
34	sR	260/261 (100%)	230 (88%)	30 (12%)	8	23
35	SM	97/228 (42%)	79 (81%)	18 (19%)	2	7
35	sM	54/228 (24%)	39 (72%)	15 (28%)	0	2
39	L2	193/195 (99%)	156 (81%)	37 (19%)	2	6
39	l2	192/195 (98%)	160 (83%)	32 (17%)	3	9
40	L3	321/322 (100%)	250 (78%)	71 (22%)	1	4
40	l3	319/322 (99%)	250 (78%)	69 (22%)	1	4
41	L4	288/288 (100%)	241 (84%)	47 (16%)	3	10
41	l4	288/288 (100%)	239 (83%)	49 (17%)	3	9
42	L5	244/244 (100%)	206 (84%)	38 (16%)	4	11
42	l5	243/244 (100%)	198 (82%)	45 (18%)	2	7
43	L6	134/152 (88%)	115 (86%)	19 (14%)	5	13
43	l6	135/152 (89%)	111 (82%)	24 (18%)	2	7
44	L7	186/204 (91%)	169 (91%)	17 (9%)	14	38
44	l7	187/204 (92%)	160 (86%)	27 (14%)	5	13
45	L8	187/207 (90%)	152 (81%)	35 (19%)	2	7
45	l8	177/207 (86%)	146 (82%)	31 (18%)	3	8
46	L9	171/171 (100%)	140 (82%)	31 (18%)	2	7
46	l9	171/171 (100%)	141 (82%)	30 (18%)	3	8
47	M0	177/186 (95%)	139 (78%)	38 (22%)	1	4
47	m0	179/186 (96%)	140 (78%)	39 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	M1	147/150 (98%)	117 (80%)	30 (20%)	2	5
48	m1	147/150 (98%)	123 (84%)	24 (16%)	3	10
49	M3	154/158 (98%)	124 (80%)	30 (20%)	2	6
49	m3	154/158 (98%)	132 (86%)	22 (14%)	5	13
50	M4	107/108 (99%)	89 (83%)	18 (17%)	3	9
50	m4	108/108 (100%)	88 (82%)	20 (18%)	2	7
51	M5	175/175 (100%)	145 (83%)	30 (17%)	3	8
51	m5	175/175 (100%)	146 (83%)	29 (17%)	3	9
52	M6	160/161 (99%)	138 (86%)	22 (14%)	5	14
52	m6	160/161 (99%)	127 (79%)	33 (21%)	2	5
53	M7	140/145 (97%)	112 (80%)	28 (20%)	2	6
53	m7	125/145 (86%)	106 (85%)	19 (15%)	4	12
54	M8	150/150 (100%)	126 (84%)	24 (16%)	3	10
54	m8	150/150 (100%)	120 (80%)	30 (20%)	2	6
55	M9	153/153 (100%)	128 (84%)	25 (16%)	3	10
55	m9	153/153 (100%)	123 (80%)	30 (20%)	2	6
56	N0	156/156 (100%)	125 (80%)	31 (20%)	2	6
56	n0	156/156 (100%)	125 (80%)	31 (20%)	2	6
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	3
57	n1	136/136 (100%)	109 (80%)	27 (20%)	2	6
58	N2	87/106 (82%)	79 (91%)	8 (9%)	13	38
58	n2	85/106 (80%)	72 (85%)	13 (15%)	4	12
59	N3	104/104 (100%)	91 (88%)	13 (12%)	7	19
59	n3	104/104 (100%)	96 (92%)	8 (8%)	18	47
60	N4	57/129 (44%)	52 (91%)	5 (9%)	14	40
60	n4	100/129 (78%)	84 (84%)	16 (16%)	3	10
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1	4
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1	5
62	N6	109/109 (100%)	86 (79%)	23 (21%)	1	5
62	n6	109/109 (100%)	82 (75%)	27 (25%)	1	3
63	N7	115/115 (100%)	93 (81%)	22 (19%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	n7	115/115 (100%)	96 (84%)	19 (16%)	3	9
64	N8	118/118 (100%)	101 (86%)	17 (14%)	5	13
64	n8	118/118 (100%)	96 (81%)	22 (19%)	2	7
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	4
65	n9	46/46 (100%)	36 (78%)	10 (22%)	1	4
66	O0	81/87 (93%)	70 (86%)	11 (14%)	5	15
66	o0	84/87 (97%)	68 (81%)	16 (19%)	2	6
67	O1	92/96 (96%)	75 (82%)	17 (18%)	2	7
67	o1	94/96 (98%)	73 (78%)	21 (22%)	1	4
68	O2	109/110 (99%)	91 (84%)	18 (16%)	3	9
68	o2	109/110 (99%)	88 (81%)	21 (19%)	2	6
69	O3	90/90 (100%)	78 (87%)	12 (13%)	6	16
69	o3	90/90 (100%)	76 (84%)	14 (16%)	4	11
70	O4	95/101 (94%)	75 (79%)	20 (21%)	1	5
70	o4	95/101 (94%)	82 (86%)	13 (14%)	5	15
71	O5	104/104 (100%)	82 (79%)	22 (21%)	1	5
71	o5	103/104 (99%)	83 (81%)	20 (19%)	2	6
72	O6	81/81 (100%)	63 (78%)	18 (22%)	1	4
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	58 (83%)	12 (17%)	3	8
73	o7	70/70 (100%)	55 (79%)	15 (21%)	1	4
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	4
74	o8	67/68 (98%)	56 (84%)	11 (16%)	3	10
75	O9	45/45 (100%)	39 (87%)	6 (13%)	6	16
75	o9	45/45 (100%)	40 (89%)	5 (11%)	9	26
76	Q0	47/47 (100%)	42 (89%)	5 (11%)	10	28
76	q0	47/47 (100%)	38 (81%)	9 (19%)	2	6
77	Q1	23/23 (100%)	15 (65%)	8 (35%)	0	1
77	q1	23/23 (100%)	17 (74%)	6 (26%)	1	2
78	Q2	90/90 (100%)	74 (82%)	16 (18%)	2	7
78	q2	90/90 (100%)	72 (80%)	18 (20%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	Q3	71/71 (100%)	57 (80%)	14 (20%)	2	6
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	5
80	e0	53/53 (100%)	42 (79%)	11 (21%)	2	5
81	e1	66/66 (100%)	48 (73%)	18 (27%)	0	2
83	p0	105/253 (42%)	83 (79%)	22 (21%)	1	5
All	All	18728/20239 (92%)	15327 (82%)	3401 (18%)	2	7

5 of 3401 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
68	O2	41	VAL
8	s6	22	HIS
64	n8	26	ARG
71	O5	15	GLU
3	s1	25	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	s1	209	ASN
8	s6	197	ASN
51	m5	194	GLN
3	s1	211	HIS
6	s4	231	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	$\# Z > 2$
87	OHX	1	3864	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3880	-	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
87	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3923	-	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
87	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3966	-	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
87	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4009	-	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
87	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4052	-	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
87	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4095	-	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
87	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4138	-	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
87	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4181	-	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
87	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
89	3HE	1	4215	-	21,21,21	0.50	0	30,30,30	0.68	0
87	OHX	2	2022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2030	-	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
87	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2073	-	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
87	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2116	-	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
87	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2159	-	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
87	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	234	-	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
87	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3940	-	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
87	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3983	-	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
87	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4026	-	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
87	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4069	-	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
87	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4112	-	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
87	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4155	-	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
87	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4198	-	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
87	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4241	-	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
87	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
89	3HE	5	4252	-	21,21,21	0.81	1 (4%)	30,30,30	1.09	2 (6%)
87	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2078	-	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
87	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2121	-	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
87	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2164	-	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
87	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	6	2205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	L4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M7	208	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	N9	101	-	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
87	OHX	O2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	O9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	c8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m6	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	o9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
87	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
87	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
87	OHX	1	3864	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3865	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3866	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3867	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	1	3902	-	-	0/0/0/0	0/0/0/0

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4112	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4154	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4196	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
87	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
89	3HE	1	4215	-	-	0/8/36/36	0/2/2/2
87	OHX	2	2022	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2044	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2086	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2128	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2170	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	3	215	-	-	0/0/0/0	0/0/0/0
87	OHX	3	216	-	-	0/0/0/0	0/0/0/0
87	OHX	3	217	-	-	0/0/0/0	0/0/0/0
87	OHX	3	218	-	-	0/0/0/0	0/0/0/0
87	OHX	3	219	-	-	0/0/0/0	0/0/0/0
87	OHX	3	220	-	-	0/0/0/0	0/0/0/0
87	OHX	3	221	-	-	0/0/0/0	0/0/0/0
87	OHX	3	222	-	-	0/0/0/0	0/0/0/0
87	OHX	3	223	-	-	0/0/0/0	0/0/0/0
87	OHX	3	224	-	-	0/0/0/0	0/0/0/0
87	OHX	3	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	223	-	-	0/0/0/0	0/0/0/0
87	OHX	4	224	-	-	0/0/0/0	0/0/0/0
87	OHX	4	225	-	-	0/0/0/0	0/0/0/0
87	OHX	4	226	-	-	0/0/0/0	0/0/0/0
87	OHX	4	227	-	-	0/0/0/0	0/0/0/0
87	OHX	4	228	-	-	0/0/0/0	0/0/0/0
87	OHX	4	229	-	-	0/0/0/0	0/0/0/0
87	OHX	4	230	-	-	0/0/0/0	0/0/0/0
87	OHX	4	231	-	-	0/0/0/0	0/0/0/0
87	OHX	4	232	-	-	0/0/0/0	0/0/0/0
87	OHX	4	233	-	-	0/0/0/0	0/0/0/0
87	OHX	4	234	-	-	0/0/0/0	0/0/0/0
87	OHX	4	235	-	-	0/0/0/0	0/0/0/0
87	OHX	4	236	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3907	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3949	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3991	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
87	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4033	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4075	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4117	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4159	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4201	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4243	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
87	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
89	3HE	5	4252	-	-	0/8/36/36	0/2/2/2
87	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2079	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2121	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2163	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
87	OHX	6	2205	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	7	215	-	-	0/0/0/0	0/0/0/0
87	OHX	7	216	-	-	0/0/0/0	0/0/0/0
87	OHX	7	217	-	-	0/0/0/0	0/0/0/0
87	OHX	7	218	-	-	0/0/0/0	0/0/0/0
87	OHX	7	219	-	-	0/0/0/0	0/0/0/0
87	OHX	7	220	-	-	0/0/0/0	0/0/0/0
87	OHX	7	221	-	-	0/0/0/0	0/0/0/0
87	OHX	7	222	-	-	0/0/0/0	0/0/0/0
87	OHX	7	223	-	-	0/0/0/0	0/0/0/0
87	OHX	7	224	-	-	0/0/0/0	0/0/0/0
87	OHX	7	225	-	-	0/0/0/0	0/0/0/0
87	OHX	7	226	-	-	0/0/0/0	0/0/0/0
87	OHX	7	227	-	-	0/0/0/0	0/0/0/0
87	OHX	8	214	-	-	0/0/0/0	0/0/0/0
87	OHX	8	215	-	-	0/0/0/0	0/0/0/0
87	OHX	8	216	-	-	0/0/0/0	0/0/0/0
87	OHX	8	217	-	-	0/0/0/0	0/0/0/0
87	OHX	8	218	-	-	0/0/0/0	0/0/0/0
87	OHX	8	219	-	-	0/0/0/0	0/0/0/0
87	OHX	8	220	-	-	0/0/0/0	0/0/0/0
87	OHX	8	221	-	-	0/0/0/0	0/0/0/0
87	OHX	8	222	-	-	0/0/0/0	0/0/0/0
87	OHX	8	223	-	-	0/0/0/0	0/0/0/0
87	OHX	8	224	-	-	0/0/0/0	0/0/0/0
87	OHX	8	225	-	-	0/0/0/0	0/0/0/0
87	OHX	8	226	-	-	0/0/0/0	0/0/0/0
87	OHX	8	227	-	-	0/0/0/0	0/0/0/0
87	OHX	8	228	-	-	0/0/0/0	0/0/0/0
87	OHX	8	229	-	-	0/0/0/0	0/0/0/0
87	OHX	C3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
87	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
87	OHX	L4	402	-	-	0/0/0/0	0/0/0/0
87	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
87	OHX	M7	208	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
87	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
87	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	O2	201	-	-	0/0/0/0	0/0/0/0
87	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
87	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
87	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
87	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
87	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
87	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
87	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
87	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
87	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
87	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	402	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
87	OHX	l4	404	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
87	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
87	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
87	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
87	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
87	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
87	OHX	m5	303	-	-	0/0/0/0	0/0/0/0
87	OHX	m6	202	-	-	0/0/0/0	0/0/0/0
87	OHX	m7	205	-	-	0/0/0/0	0/0/0/0
87	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
87	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
87	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
87	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
87	OHX	o7	103	-	-	0/0/0/0	0/0/0/0
87	OHX	o9	101	-	-	0/0/0/0	0/0/0/0
87	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
87	OHX	s1	302	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
87	OHX	s8	302	-	-	0/0/0/0	0/0/0/0
87	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
87	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	5	4252	3HE	C5-C7	3.07	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	5	4252	3HE	C7-C5-C4	3.85	119.68	111.65
89	5	4252	3HE	C6-C5-C7	-2.30	105.01	110.95

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	0.76
1	SR	160:GLU	C	161:LYS	N	0.64

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%)	0.32	70 (4%) 36 43	44, 77, 148, 252	0
1	6	1795/1800 (99%)	0.40	77 (4%) 34 40	32, 62, 155, 269	0
2	S0	206/251 (82%)	1.39	63 (30%) 1 1	80, 96, 108, 136	0
2	s0	206/251 (82%)	0.99	38 (18%) 2 3	59, 77, 93, 103	0
3	S1	214/254 (84%)	2.23	98 (45%) 1 0	84, 119, 149, 159	0
3	s1	216/254 (85%)	1.29	46 (21%) 1 2	57, 71, 93, 103	0
4	S2	217/253 (85%)	1.00	45 (20%) 1 2	59, 74, 90, 106	0
4	s2	217/253 (85%)	0.78	21 (9%) 8 10	46, 61, 77, 88	0
5	S3	223/239 (93%)	1.56	71 (31%) 1 1	66, 79, 102, 119	0
5	s3	223/239 (93%)	0.80	34 (15%) 3 4	58, 83, 105, 114	0
6	S4	260/260 (100%)	1.41	80 (30%) 1 1	54, 76, 90, 118	0
6	s4	260/260 (100%)	0.87	30 (11%) 5 7	40, 62, 76, 107	0
7	S5	206/224 (91%)	1.76	71 (34%) 1 1	80, 100, 117, 133	0
7	s5	206/224 (91%)	1.23	46 (22%) 1 2	58, 78, 106, 120	0
8	S6	226/236 (95%)	0.76	38 (16%) 2 3	55, 91, 109, 139	0
8	s6	218/236 (92%)	0.71	22 (10%) 7 10	42, 71, 93, 116	0
9	S7	184/189 (97%)	1.17	44 (23%) 1 2	72, 104, 135, 144	0
9	s7	186/189 (98%)	0.87	27 (14%) 3 5	55, 87, 121, 134	0
10	S8	188/200 (94%)	0.76	27 (14%) 3 5	46, 61, 99, 114	0
10	s8	188/200 (94%)	0.95	31 (16%) 2 3	37, 58, 100, 113	0
11	S9	185/196 (94%)	1.64	59 (31%) 1 1	71, 86, 123, 155	0
11	s9	185/196 (94%)	0.86	23 (12%) 5 6	53, 67, 103, 136	0
12	C0	96/105 (91%)	1.42	28 (29%) 1 1	70, 92, 122, 137	0
12	c0	96/105 (91%)	1.38	24 (25%) 1 2	75, 105, 133, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	2.22	56 (36%)	1	1	47, 59, 115, 127	0
13	c1	146/155 (94%)	1.77	41 (28%)	1	1	38, 53, 82, 101	0
14	C2	124/142 (87%)	3.00	74 (59%)	0	0	114, 127, 149, 164	0
14	c2	124/142 (87%)	3.92	86 (69%)	0	0	145, 165, 186, 197	0
15	C3	150/150 (100%)	1.05	27 (18%)	2	3	57, 75, 89, 95	0
15	c3	150/150 (100%)	0.70	17 (11%)	6	7	45, 60, 75, 93	0
16	C4	127/136 (93%)	1.71	47 (37%)	1	0	58, 120, 136, 138	0
16	c4	128/136 (94%)	1.33	33 (25%)	1	1	42, 74, 84, 91	0
17	C5	124/141 (87%)	1.86	50 (40%)	1	0	64, 80, 120, 139	0
17	c5	135/141 (95%)	1.52	35 (25%)	1	1	60, 79, 110, 132	0
18	C6	141/142 (99%)	0.89	26 (18%)	2	3	68, 90, 96, 99	0
18	c6	142/142 (100%)	0.82	21 (14%)	3	4	54, 72, 86, 107	0
19	C7	120/136 (88%)	0.44	17 (14%)	3	5	73, 92, 119, 122	0
19	c7	117/136 (86%)	0.33	9 (7%)	13	16	62, 77, 105, 109	0
20	C8	145/145 (100%)	2.16	62 (42%)	1	0	64, 87, 113, 122	0
20	c8	145/145 (100%)	1.09	31 (21%)	1	2	57, 67, 93, 106	0
21	C9	143/143 (100%)	1.08	32 (22%)	1	2	72, 88, 105, 116	0
21	c9	143/143 (100%)	1.48	45 (31%)	1	1	54, 65, 84, 104	0
22	D0	107/120 (89%)	1.79	40 (37%)	1	0	64, 93, 128, 134	0
22	d0	110/120 (91%)	2.43	39 (35%)	1	1	53, 86, 129, 150	0
23	D1	87/87 (100%)	1.44	23 (26%)	1	1	77, 83, 105, 115	0
23	d1	87/87 (100%)	1.21	17 (19%)	2	2	57, 64, 86, 98	0
24	D2	129/129 (100%)	2.01	62 (48%)	1	0	58, 68, 75, 85	0
24	d2	129/129 (100%)	0.68	11 (8%)	11	13	41, 51, 57, 66	0
25	D3	144/144 (100%)	0.94	25 (17%)	2	3	49, 56, 67, 82	0
25	d3	144/144 (100%)	0.39	7 (4%)	28	34	36, 42, 57, 69	0
26	D4	134/134 (100%)	0.91	23 (17%)	2	3	67, 91, 109, 114	0
26	d4	134/134 (100%)	0.63	13 (9%)	8	10	50, 72, 86, 107	0
27	D5	70/107 (65%)	2.00	33 (47%)	1	0	95, 111, 123, 128	0
27	d5	69/107 (64%)	1.67	28 (40%)	1	0	68, 90, 104, 109	0
28	D6	97/97 (100%)	3.29	65 (67%)	0	0	65, 81, 138, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
28	d6	97/97 (100%)	1.26	21 (21%)	1	2	46, 59, 89, 98	0
29	D7	81/81 (100%)	2.14	31 (38%)	1	0	71, 89, 128, 138	0
29	d7	81/81 (100%)	1.32	18 (22%)	1	2	55, 71, 117, 119	0
30	D8	63/66 (95%)	3.43	39 (61%)	0	0	94, 112, 127, 147	0
30	d8	63/66 (95%)	1.92	26 (41%)	1	0	76, 92, 108, 120	0
31	D9	53/55 (96%)	0.99	10 (18%)	2	2	63, 67, 91, 102	0
31	d9	53/55 (96%)	1.16	13 (24%)	1	2	57, 62, 101, 118	0
32	E0	60/60 (100%)	1.87	17 (28%)	1	1	56, 86, 127, 132	0
33	E1	71/76 (93%)	2.52	37 (52%)	0	0	91, 110, 126, 129	0
34	SR	318/318 (100%)	0.67	46 (14%)	3	5	60, 95, 117, 143	0
34	sR	318/318 (100%)	1.68	111 (34%)	1	1	75, 95, 114, 135	0
35	SM	159/273 (58%)	1.93	49 (30%)	1	1	55, 80, 128, 136	0
35	sM	104/273 (38%)	0.78	19 (18%)	2	3	45, 81, 162, 167	0
36	1	3149/3396 (92%)	0.32	75 (2%)	56	65	20, 43, 119, 234	0
36	5	3150/3396 (92%)	0.29	63 (2%)	62	71	20, 42, 111, 229	0
37	3	121/121 (100%)	0.12	1 (0%)	83	89	33, 59, 76, 81	0
37	7	121/121 (100%)	0.24	1 (0%)	83	89	27, 43, 56, 64	0
38	4	158/158 (100%)	0.36	3 (1%)	64	72	26, 45, 83, 114	0
38	8	158/158 (100%)	0.32	4 (2%)	54	64	33, 53, 91, 112	0
39	L2	252/253 (99%)	0.55	17 (6%)	17	21	25, 40, 58, 66	0
39	l2	252/253 (99%)	0.45	16 (6%)	19	23	26, 44, 61, 74	0
40	L3	386/386 (100%)	0.30	18 (4%)	30	37	27, 47, 60, 97	0
40	l3	386/386 (100%)	0.15	6 (1%)	68	78	20, 34, 47, 83	0
41	L4	361/361 (100%)	-0.08	1 (0%)	91	95	21, 37, 54, 65	0
41	l4	361/361 (100%)	0.07	6 (1%)	67	76	26, 44, 62, 70	0
42	L5	296/296 (100%)	0.58	34 (11%)	5	7	41, 65, 83, 105	0
42	l5	294/296 (99%)	0.33	13 (4%)	33	40	34, 48, 71, 110	0
43	L6	156/175 (89%)	0.30	4 (2%)	53	63	33, 40, 60, 80	0
43	l6	157/175 (89%)	0.12	0	100	100	35, 43, 63, 75	0
44	L7	222/243 (91%)	0.18	1 (0%)	88	93	26, 33, 62, 110	0
44	l7	223/243 (91%)	0.07	1 (0%)	90	94	24, 33, 69, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	L8	233/255 (91%)	0.91	44 (18%) 2 2	48, 62, 96, 114	0
45	l8	231/255 (90%)	1.03	40 (17%) 2 3	58, 70, 98, 105	0
46	L9	191/191 (100%)	0.67	22 (11%) 5 7	43, 55, 66, 86	0
46	l9	191/191 (100%)	0.43	7 (3%) 39 47	31, 38, 58, 78	0
47	M0	211/220 (95%)	0.03	2 (0%) 81 88	28, 44, 78, 113	0
47	m0	213/220 (96%)	0.43	12 (5%) 24 28	26, 45, 71, 90	0
48	M1	169/173 (97%)	0.56	17 (10%) 7 10	49, 68, 80, 92	0
48	m1	169/173 (97%)	0.13	4 (2%) 56 65	36, 52, 64, 76	0
49	M3	193/198 (97%)	0.16	7 (3%) 41 48	24, 46, 83, 111	0
49	m3	194/198 (97%)	0.41	5 (2%) 53 63	31, 55, 90, 114	0
50	M4	136/137 (99%)	0.56	7 (5%) 27 33	35, 43, 57, 65	0
50	m4	137/137 (100%)	0.27	4 (2%) 49 58	31, 36, 55, 65	0
51	M5	203/203 (100%)	0.34	5 (2%) 54 64	23, 39, 49, 55	0
51	m5	203/203 (100%)	0.65	18 (8%) 10 12	29, 48, 58, 61	0
52	M6	197/198 (99%)	0.50	10 (5%) 27 33	27, 35, 55, 60	0
52	m6	197/198 (99%)	0.18	8 (4%) 35 43	21, 26, 51, 57	0
53	M7	183/183 (100%)	0.58	12 (6%) 18 21	29, 36, 88, 118	0
53	m7	155/183 (84%)	-0.07	0 100 100	24, 34, 48, 81	0
54	M8	185/185 (100%)	0.08	0 100 100	26, 36, 48, 60	0
54	m8	185/185 (100%)	0.18	1 (0%) 88 93	30, 42, 52, 59	0
55	M9	188/188 (100%)	0.68	24 (12%) 4 6	43, 57, 135, 146	0
55	m9	188/188 (100%)	0.46	15 (7%) 12 15	40, 52, 115, 132	0
56	N0	172/172 (100%)	0.68	12 (6%) 16 19	35, 41, 55, 62	0
56	n0	172/172 (100%)	0.34	5 (2%) 49 58	27, 34, 44, 54	0
57	N1	159/159 (100%)	0.57	14 (8%) 10 13	30, 40, 77, 83	0
57	n1	159/159 (100%)	0.50	8 (5%) 28 33	27, 35, 70, 76	0
58	N2	100/120 (83%)	1.27	21 (21%) 1 2	72, 89, 104, 120	0
58	n2	98/120 (81%)	1.35	30 (30%) 1 1	64, 77, 86, 89	0
59	N3	136/136 (100%)	-0.13	3 (2%) 59 67	31, 42, 58, 66	0
59	n3	136/136 (100%)	0.09	2 (1%) 70 79	22, 33, 47, 51	0
60	N4	98/155 (63%)	2.27	30 (30%) 1 1	43, 54, 140, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	n4	135/155 (87%)	1.02	25 (18%) 2 3	32, 80, 117, 135	0
61	N5	121/141 (85%)	0.93	17 (14%) 3 5	38, 52, 70, 94	0
61	n5	120/141 (85%)	1.16	27 (22%) 1 2	43, 57, 75, 83	0
62	N6	126/126 (100%)	0.24	3 (2%) 56 65	30, 47, 59, 71	0
62	n6	126/126 (100%)	0.68	11 (8%) 10 13	37, 53, 69, 75	0
63	N7	135/135 (100%)	0.59	12 (8%) 10 12	59, 74, 88, 96	0
63	n7	135/135 (100%)	0.91	29 (21%) 1 2	65, 81, 105, 113	0
64	N8	148/148 (100%)	0.39	3 (2%) 62 71	21, 37, 61, 71	0
64	n8	148/148 (100%)	0.50	8 (5%) 25 30	23, 45, 64, 68	0
65	N9	58/58 (100%)	0.58	8 (13%) 4 5	25, 45, 91, 106	0
65	n9	58/58 (100%)	0.45	5 (8%) 11 13	24, 46, 67, 78	0
66	O0	97/104 (93%)	0.55	8 (8%) 12 15	59, 69, 95, 100	0
66	o0	100/104 (96%)	1.53	29 (29%) 1 1	62, 72, 104, 120	0
67	O1	109/112 (97%)	0.76	11 (10%) 7 10	41, 53, 89, 104	0
67	o1	109/112 (97%)	0.54	11 (10%) 7 10	33, 44, 84, 103	0
68	O2	127/129 (98%)	0.09	3 (2%) 56 65	21, 34, 44, 63	0
68	o2	127/129 (98%)	0.17	3 (2%) 56 65	22, 40, 53, 69	0
69	O3	106/106 (100%)	-0.06	0 100 100	26, 32, 52, 60	0
69	o3	106/106 (100%)	-0.09	0 100 100	24, 32, 56, 67	0
70	O4	112/119 (94%)	1.10	23 (20%) 1 2	39, 57, 97, 111	0
70	o4	112/119 (94%)	0.72	17 (15%) 3 4	40, 59, 95, 105	0
71	O5	119/119 (100%)	0.52	7 (5%) 22 25	36, 56, 63, 64	0
71	o5	119/119 (100%)	1.04	22 (18%) 2 3	45, 61, 70, 74	0
72	O6	99/99 (100%)	0.54	12 (12%) 5 7	41, 52, 79, 92	0
72	o6	99/99 (100%)	0.40	10 (10%) 7 10	50, 61, 81, 103	0
73	O7	87/87 (100%)	0.55	4 (4%) 31 38	27, 34, 59, 83	0
73	o7	87/87 (100%)	0.95	10 (11%) 5 7	28, 36, 65, 101	0
74	O8	77/77 (100%)	1.86	31 (40%) 1 0	63, 77, 97, 106	0
74	o8	77/77 (100%)	0.81	11 (14%) 3 5	65, 78, 97, 104	0
75	O9	50/50 (100%)	0.76	6 (12%) 5 7	36, 40, 50, 53	0
75	o9	50/50 (100%)	1.25	11 (22%) 1 2	40, 44, 56, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
76	Q0	52/52 (100%)	0.43	3 (5%) 22 26	40, 45, 63, 72	0
76	q0	52/52 (100%)	0.11	2 (3%) 38 45	28, 31, 42, 51	0
77	Q1	25/25 (100%)	0.67	3 (12%) 5 7	45, 48, 51, 56	0
77	q1	25/25 (100%)	0.04	1 (4%) 36 43	34, 39, 50, 58	0
78	Q2	105/105 (100%)	0.43	6 (5%) 23 28	25, 43, 64, 96	0
78	q2	105/105 (100%)	0.35	2 (1%) 64 72	29, 43, 64, 81	0
79	Q3	91/91 (100%)	0.43	4 (4%) 33 40	33, 43, 63, 79	0
79	q3	91/91 (100%)	0.41	3 (3%) 44 53	31, 45, 61, 67	0
80	e0	62/62 (100%)	0.77	10 (16%) 2 3	51, 67, 108, 114	0
81	e1	76/76 (100%)	3.42	48 (63%) 0 0	122, 134, 156, 162	0
82	m2	0/160	-	-	-	-
83	p0	143/311 (45%)	1.86	54 (37%) 1 0	78, 99, 163, 171	0
84	p1	0/47	-	-	-	-
85	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	0.69	3811 (11%) 5 7	20, 58, 118, 269	0

The worst 5 of 3811 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	76	VAL	38.6
7	S5	152	GLY	20.1
53	M7	161	ALA	19.2
81	e1	112	GLY	18.7
16	C4	15	GLY	18.6

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
86	MG	5	3753	1/1	0.42	515.00	52,52,52,52	0
86	MG	6	1933	1/1	0.40	455.00	59,59,59,59	0
86	MG	1	3419	1/1	0.31	331.00	80,80,80,80	0
86	MG	4	222	1/1	0.41	245.00	48,48,48,48	0
86	MG	4	221	1/1	0.53	245.00	94,94,94,94	0
86	MG	6	1945	1/1	0.48	232.33	49,49,49,49	0
86	MG	1	3836	1/1	0.29	231.00	41,41,41,41	0
86	MG	2	1958	1/1	0.42	212.33	74,74,74,74	0
86	MG	6	2019	1/1	0.41	183.34	48,48,48,48	0
87	OHX	1	4067	7/7	0.29	176.78	112,112,112,112	0
86	MG	2	2001	1/1	0.59	156.67	98,98,98,98	0
86	MG	6	2040	1/1	0.48	147.80	92,92,92,92	0
86	MG	2	2018	1/1	0.40	142.18	67,67,67,67	0
86	MG	5	3680	1/1	0.24	141.00	39,39,39,39	0
86	MG	1	3635	1/1	0.40	127.00	71,71,71,71	0
86	MG	6	2039	1/1	0.42	117.80	72,72,72,72	0
86	MG	1	3647	1/1	0.26	110.00	37,37,37,37	0
86	MG	1	3861	1/1	0.39	95.40	62,62,62,62	0
86	MG	5	3568	1/1	0.44	91.43	28,28,28,28	0
86	MG	6	2016	1/1	0.20	85.00	67,67,67,67	0
86	MG	5	3884	1/1	0.35	82.60	83,83,83,83	0
86	MG	2	2013	1/1	0.31	79.00	58,58,58,58	0
87	OHX	1	4186	7/7	0.42	78.67	156,156,156,156	0
86	MG	2	1904	1/1	0.42	75.57	70,70,70,70	0
86	MG	5	3410	1/1	0.32	74.60	41,41,41,41	0
86	MG	5	3676	1/1	0.34	74.20	39,39,39,39	0
86	MG	4	204	1/1	0.36	72.67	47,47,47,47	0
86	MG	5	3431	1/1	0.32	72.60	67,67,67,67	0
86	MG	2	1987	1/1	0.18	69.00	79,79,79,79	0
86	MG	1	3514	1/1	0.34	66.98	31,31,31,31	0
86	MG	6	1944	1/1	0.50	66.82	51,51,51,51	0
86	MG	1	3737	1/1	0.35	59.33	60,60,60,60	0
86	MG	5	3673	1/1	0.37	56.75	50,50,50,50	0
86	MG	5	3592	1/1	0.35	54.82	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3868	1/1	0.19	54.00	44,44,44,44	0
86	MG	1	3567	1/1	0.50	53.73	34,34,34,34	0
86	MG	2	1935	1/1	0.44	52.00	47,47,47,47	0
86	MG	1	3468	1/1	0.40	51.05	59,59,59,59	0
86	MG	1	3575	1/1	0.35	48.74	34,34,34,34	0
86	MG	2	2011	1/1	0.31	47.86	48,48,48,48	0
86	MG	5	3782	1/1	0.37	47.77	82,82,82,82	0
86	MG	6	1981	1/1	0.35	47.00	52,52,52,52	0
86	MG	5	3468	1/1	0.51	46.79	89,89,89,89	0
86	MG	1	3594	1/1	0.38	44.33	66,66,66,66	0
87	OHX	2	2158	7/7	0.48	44.19	128,128,128,128	0
86	MG	1	3775	1/1	0.25	43.51	57,57,57,57	0
86	MG	1	3537	1/1	0.41	43.50	51,51,51,51	0
86	MG	5	3491	1/1	0.28	43.31	43,43,43,43	0
86	MG	5	3622	1/1	0.30	40.43	39,39,39,39	0
86	MG	6	2011	1/1	0.35	40.35	56,56,56,56	0
86	MG	2	1945	1/1	0.38	39.76	75,75,75,75	0
86	MG	5	3877	1/1	0.50	39.75	40,40,40,40	0
86	MG	5	3732	1/1	0.20	39.55	47,47,47,47	0
86	MG	13	401	1/1	0.42	39.19	22,22,22,22	0
86	MG	1	3493	1/1	0.25	39.00	74,74,74,74	0
86	MG	1	3538	1/1	0.45	38.71	31,31,31,31	0
86	MG	5	3895	1/1	0.44	38.33	104,104,104,104	0
86	MG	5	3519	1/1	0.42	38.25	23,23,23,23	0
86	MG	1	3450	1/1	0.29	37.55	36,36,36,36	0
86	MG	1	3684	1/1	0.24	37.50	40,40,40,40	0
86	MG	5	3881	1/1	0.31	36.08	29,29,29,29	0
87	OHX	8	227	7/7	0.26	36.02	116,116,116,116	0
86	MG	5	3547	1/1	0.41	35.47	45,45,45,45	0
86	MG	5	3573	1/1	0.32	35.44	34,34,34,34	0
87	OHX	1	4163	7/7	0.35	35.33	144,144,144,144	0
86	MG	5	3576	1/1	0.33	35.19	33,33,33,33	0
86	MG	1	3545	1/1	0.24	35.17	37,37,37,37	0
86	MG	5	3435	1/1	0.30	34.71	76,76,76,76	0
86	MG	1	3851	1/1	0.40	34.31	68,68,68,68	0
86	MG	2	1953	1/1	0.47	33.95	111,111,111,111	0
86	MG	5	3563	1/1	0.38	33.77	24,24,24,24	0
86	MG	2	1977	1/1	0.36	33.15	91,91,91,91	0
86	MG	5	3664	1/1	0.48	33.08	54,54,54,54	0
86	MG	6	1948	1/1	0.33	32.46	41,41,41,41	0
86	MG	2	1914	1/1	0.40	32.40	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3711	1/1	0.30	32.27	90,90,90,90	0
86	MG	1	3856	1/1	0.27	32.25	52,52,52,52	0
86	MG	2	2008	1/1	0.30	32.25	68,68,68,68	0
86	MG	1	3409	1/1	0.34	32.19	34,34,34,34	0
86	MG	1	3449	1/1	0.31	32.12	38,38,38,38	0
86	MG	2	1921	1/1	0.41	32.06	48,48,48,48	0
86	MG	6	1931	1/1	0.44	32.01	53,53,53,53	0
86	MG	5	3526	1/1	0.40	31.96	26,26,26,26	0
86	MG	5	3687	1/1	0.43	31.82	63,63,63,63	0
86	MG	5	3623	1/1	0.26	31.50	41,41,41,41	0
86	MG	5	3541	1/1	0.32	31.49	19,19,19,19	0
86	MG	1	3559	1/1	0.27	31.29	49,49,49,49	0
86	MG	1	3547	1/1	0.45	31.25	58,58,58,58	0
86	MG	2	1988	1/1	0.31	31.09	54,54,54,54	0
86	MG	2	1932	1/1	0.35	30.69	54,54,54,54	0
86	MG	2	2016	1/1	0.40	30.22	79,79,79,79	0
86	MG	1	3844	1/1	0.27	29.86	52,52,52,52	0
86	MG	1	3544	1/1	0.38	29.74	32,32,32,32	0
86	MG	1	3574	1/1	0.44	29.61	32,32,32,32	0
86	MG	1	3667	1/1	0.38	29.59	65,65,65,65	0
86	MG	6	1921	1/1	0.35	29.52	40,40,40,40	0
86	MG	6	2038	1/1	0.47	29.35	45,45,45,45	0
86	MG	2	1924	1/1	0.39	29.28	70,70,70,70	0
86	MG	5	3469	1/1	0.29	29.25	37,37,37,37	0
86	MG	5	3484	1/1	0.38	29.18	52,52,52,52	0
86	MG	2	2012	1/1	0.39	29.12	71,71,71,71	0
86	MG	5	3730	1/1	0.35	28.82	90,90,90,90	0
86	MG	1	3805	1/1	0.74	28.75	157,157,157,157	0
86	MG	5	3447	1/1	0.28	28.60	38,38,38,38	0
86	MG	1	3855	1/1	0.57	28.50	76,76,76,76	0
86	MG	2	2000	1/1	0.54	28.38	78,78,78,78	0
86	MG	2	1913	1/1	0.41	28.21	68,68,68,68	0
86	MG	5	3532	1/1	0.33	28.18	23,23,23,23	0
86	MG	3	204	1/1	0.54	28.07	48,48,48,48	0
86	MG	1	3480	1/1	0.34	28.07	36,36,36,36	0
86	MG	1	3562	1/1	0.35	27.94	31,31,31,31	0
86	MG	5	3572	1/1	0.42	27.68	20,20,20,20	0
86	MG	1	3614	1/1	0.29	27.55	50,50,50,50	0
86	MG	2	1980	1/1	0.37	27.50	56,56,56,56	0
86	MG	1	3769	1/1	0.21	27.46	79,79,79,79	0
86	MG	1	3599	1/1	0.37	27.45	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	1916	1/1	0.29	27.21	55,55,55,55	0
87	OHX	4	236	7/7	0.31	27.16	118,118,118,118	0
86	MG	2	2007	1/1	0.34	27.15	45,45,45,45	0
86	MG	5	3414	1/1	0.30	27.15	31,31,31,31	0
86	MG	6	2029	1/1	0.48	26.91	77,77,77,77	0
86	MG	1	3829	1/1	0.34	26.58	28,28,28,28	0
86	MG	1	3529	1/1	0.40	26.58	41,41,41,41	0
86	MG	5	3614	1/1	0.34	26.33	44,44,44,44	0
87	OHX	1	4192	7/7	0.32	26.29	126,126,126,126	0
86	MG	6	1943	1/1	0.39	26.25	38,38,38,38	0
86	MG	1	3556	1/1	0.42	26.05	26,26,26,26	0
86	MG	6	1909	1/1	0.44	26.00	82,82,82,82	0
86	MG	1	3530	1/1	0.42	25.78	34,34,34,34	0
86	MG	1	3830	1/1	0.38	25.70	17,17,17,17	0
86	MG	1	3677	1/1	0.33	25.65	56,56,56,56	0
86	MG	1	3444	1/1	0.46	25.60	57,57,57,57	0
86	MG	5	3620	1/1	0.27	25.52	39,39,39,39	0
86	MG	2	1956	1/1	0.41	25.50	56,56,56,56	0
86	MG	5	3509	1/1	0.34	25.50	27,27,27,27	0
86	MG	1	3591	1/1	0.43	25.49	36,36,36,36	0
86	MG	7	214	1/1	0.34	25.46	47,47,47,47	0
86	MG	1	3579	1/1	0.32	25.20	23,23,23,23	0
86	MG	1	3580	1/1	0.41	25.17	34,34,34,34	0
86	MG	1	3516	1/1	0.40	25.16	32,32,32,32	0
86	MG	5	3599	1/1	0.42	25.02	27,27,27,27	0
86	MG	3	213	1/1	0.39	24.71	51,51,51,51	0
86	MG	2	1973	1/1	0.29	24.51	63,63,63,63	0
86	MG	1	3557	1/1	0.37	24.50	36,36,36,36	0
86	MG	1	3549	1/1	0.32	24.47	52,52,52,52	0
86	MG	5	3649	1/1	0.32	24.33	43,43,43,43	0
86	MG	6	1903	1/1	0.34	24.31	43,43,43,43	0
86	MG	5	3658	1/1	0.36	24.25	51,51,51,51	0
86	MG	1	3835	1/1	0.34	24.16	32,32,32,32	0
86	MG	5	3652	1/1	0.45	24.06	66,66,66,66	0
86	MG	5	3554	1/1	0.34	24.00	41,41,41,41	0
86	MG	2	1957	1/1	0.31	24.00	74,74,74,74	0
86	MG	5	3636	1/1	0.48	23.90	72,72,72,72	0
86	MG	1	3512	1/1	0.37	23.81	24,24,24,24	0
86	MG	6	1959	1/1	0.34	23.74	51,51,51,51	0
86	MG	5	3588	1/1	0.33	23.72	23,23,23,23	0
86	MG	5	3505	1/1	0.43	23.71	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3780	1/1	0.20	23.67	61,61,61,61	0
86	MG	2	2006	1/1	0.42	23.60	45,45,45,45	0
86	MG	5	3597	1/1	0.46	23.58	27,27,27,27	0
86	MG	1	3709	1/1	0.29	23.56	30,30,30,30	0
86	MG	5	3438	1/1	0.31	23.50	45,45,45,45	0
86	MG	5	3634	1/1	0.48	23.50	87,87,87,87	0
86	MG	5	3889	1/1	0.47	23.42	52,52,52,52	0
86	MG	1	3713	1/1	0.43	23.32	74,74,74,74	0
86	MG	1	3854	1/1	0.32	23.25	43,43,43,43	0
86	MG	6	1953	1/1	0.45	23.24	57,57,57,57	0
87	OHX	1	4176	7/7	0.35	23.16	109,109,109,109	0
87	OHX	1	4207	7/7	0.41	23.16	110,110,110,110	0
86	MG	5	3511	1/1	0.41	23.15	26,26,26,26	0
86	MG	5	3611	1/1	0.28	23.14	24,24,24,24	0
86	MG	5	3518	1/1	0.33	23.02	34,34,34,34	0
86	MG	6	1908	1/1	0.25	22.67	44,44,44,44	0
86	MG	5	3591	1/1	0.41	22.54	33,33,33,33	0
86	MG	1	3593	1/1	0.46	22.48	47,47,47,47	0
87	OHX	5	4187	7/7	0.36	22.34	105,105,105,105	0
86	MG	5	3754	1/1	0.27	22.33	39,39,39,39	0
87	OHX	5	4204	7/7	0.32	22.31	127,127,127,127	0
86	MG	1	3581	1/1	0.36	22.17	34,34,34,34	0
87	OHX	5	4237	7/7	0.29	22.13	134,134,134,134	0
86	MG	5	3598	1/1	0.32	21.97	27,27,27,27	0
86	MG	2	1974	1/1	0.44	21.92	76,76,76,76	0
86	MG	5	3508	1/1	0.35	21.86	34,34,34,34	0
86	MG	5	3418	1/1	0.36	21.80	21,21,21,21	0
86	MG	1	3625	1/1	0.54	21.78	77,77,77,77	0
86	MG	2	1928	1/1	0.38	21.77	74,74,74,74	0
87	OHX	2	2163	7/7	0.40	21.73	142,142,142,142	0
86	MG	1	3595	1/1	0.35	21.71	25,25,25,25	0
86	MG	5	3862	1/1	0.19	21.67	51,51,51,51	0
86	MG	1	3484	1/1	0.45	21.66	42,42,42,42	0
86	MG	1	3531	1/1	0.28	21.65	56,56,56,56	0
86	MG	1	3565	1/1	0.37	21.65	47,47,47,47	0
86	MG	1	3750	1/1	0.37	21.62	58,58,58,58	0
86	MG	1	3785	1/1	0.55	21.52	36,36,36,36	0
86	MG	2	2017	1/1	0.42	21.50	68,68,68,68	0
86	MG	1	3417	1/1	0.29	21.44	37,37,37,37	0
86	MG	1	3528	1/1	0.41	21.42	30,30,30,30	0
86	MG	1	3563	1/1	0.41	21.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3536	1/1	0.33	21.14	33,33,33,33	0
86	MG	3	207	1/1	0.39	21.09	58,58,58,58	0
86	MG	8	203	1/1	0.40	21.04	47,47,47,47	0
86	MG	1	3504	1/1	0.45	21.04	36,36,36,36	0
86	MG	5	3894	1/1	0.21	21.00	53,53,53,53	0
86	MG	5	3872	1/1	0.33	20.99	31,31,31,31	0
86	MG	2	1941	1/1	0.35	20.82	73,73,73,73	0
86	MG	5	3551	1/1	0.48	20.70	50,50,50,50	0
86	MG	n3	201	1/1	0.38	20.66	22,22,22,22	0
86	MG	5	3450	1/1	0.28	20.64	52,52,52,52	0
86	MG	1	3729	1/1	0.39	20.61	28,28,28,28	0
86	MG	5	3729	1/1	0.26	20.61	38,38,38,38	0
86	MG	1	3408	1/1	0.34	20.54	32,32,32,32	0
86	MG	1	3404	1/1	0.42	20.52	50,50,50,50	0
86	MG	7	205	1/1	0.36	20.24	26,26,26,26	0
86	MG	1	3812	1/1	0.33	20.20	52,52,52,52	0
87	OHX	1	4204	7/7	0.32	20.15	119,119,119,119	0
87	OHX	5	4195	7/7	0.30	20.09	118,118,118,118	0
86	MG	6	1918	1/1	0.40	20.09	64,64,64,64	0
86	MG	6	1961	1/1	0.34	20.07	62,62,62,62	0
86	MG	1	3499	1/1	0.37	19.87	66,66,66,66	0
87	OHX	1	4171	7/7	0.33	19.86	123,123,123,123	0
86	MG	6	1960	1/1	0.40	19.74	41,41,41,41	0
86	MG	1	3553	1/1	0.45	19.69	35,35,35,35	0
86	MG	5	3506	1/1	0.23	19.58	45,45,45,45	0
86	MG	2	1910	1/1	0.28	19.49	51,51,51,51	0
86	MG	1	3592	1/1	0.30	19.39	35,35,35,35	0
86	MG	5	3550	1/1	0.43	19.16	37,37,37,37	0
86	MG	1	3843	1/1	0.39	18.99	54,54,54,54	0
86	MG	5	3736	1/1	0.32	18.90	65,65,65,65	0
86	MG	5	3586	1/1	0.41	18.87	31,31,31,31	0
86	MG	5	3655	1/1	0.39	18.87	65,65,65,65	0
86	MG	1	3462	1/1	0.30	18.80	25,25,25,25	0
86	MG	5	3557	1/1	0.26	18.79	37,37,37,37	0
86	MG	1	3576	1/1	0.35	18.74	23,23,23,23	0
86	MG	5	3472	1/1	0.29	18.67	29,29,29,29	0
86	MG	1	3694	1/1	0.25	18.65	34,34,34,34	0
86	MG	3	214	1/1	0.32	18.60	60,60,60,60	0
86	MG	5	3525	1/1	0.27	18.59	36,36,36,36	0
86	MG	7	202	1/1	0.29	18.54	26,26,26,26	0
86	MG	1	3849	1/1	0.25	18.49	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2142	7/7	0.37	18.47	115,115,115,115	0
86	MG	7	209	1/1	0.39	18.46	38,38,38,38	0
86	MG	2	1959	1/1	0.49	18.40	94,94,94,94	0
86	MG	5	3585	1/1	0.47	18.40	34,34,34,34	0
86	MG	1	3535	1/1	0.34	18.34	31,31,31,31	0
86	MG	5	3475	1/1	0.28	18.33	51,51,51,51	0
86	MG	6	1925	1/1	0.43	18.24	36,36,36,36	0
87	OHX	1	4141	7/7	0.33	18.23	124,124,124,124	0
86	MG	6	1955	1/1	0.44	18.16	34,34,34,34	0
87	OHX	6	2148	7/7	0.26	17.91	96,96,96,96	0
86	MG	5	3540	1/1	0.27	17.87	36,36,36,36	0
86	MG	3	206	1/1	0.38	17.85	31,31,31,31	0
86	MG	1	3795	1/1	0.30	17.82	24,24,24,24	0
87	OHX	5	4209	7/7	0.27	17.79	119,119,119,119	0
86	MG	1	3518	1/1	0.34	17.74	23,23,23,23	0
87	OHX	5	4228	7/7	0.32	17.72	108,108,108,108	0
86	MG	1	3739	1/1	0.24	17.70	50,50,50,50	0
86	MG	5	3583	1/1	0.27	17.68	37,37,37,37	0
86	MG	8	201	1/1	0.34	17.65	35,35,35,35	0
86	MG	5	3524	1/1	0.42	17.58	41,41,41,41	0
86	MG	1	3543	1/1	0.38	17.55	32,32,32,32	0
86	MG	1	3817	1/1	0.34	17.52	52,52,52,52	0
86	MG	5	3890	1/1	0.39	17.43	46,46,46,46	0
86	MG	1	3754	1/1	0.25	17.41	21,21,21,21	0
86	MG	5	3899	1/1	0.41	17.40	52,52,52,52	0
86	MG	4	215	1/1	0.34	17.36	50,50,50,50	0
86	MG	5	3534	1/1	0.28	17.36	35,35,35,35	0
87	OHX	5	4213	7/7	0.32	17.34	112,112,112,112	0
86	MG	N3	201	1/1	0.39	17.31	30,30,30,30	0
86	MG	1	3432	1/1	0.31	17.24	38,38,38,38	0
86	MG	5	3502	1/1	0.36	17.21	24,24,24,24	0
86	MG	5	3574	1/1	0.35	17.11	28,28,28,28	0
86	MG	5	3575	1/1	0.38	17.10	36,36,36,36	0
87	OHX	5	4222	7/7	0.29	17.09	124,124,124,124	0
86	MG	1	3513	1/1	0.37	16.97	21,21,21,21	0
86	MG	6	2046	1/1	0.37	16.93	60,60,60,60	0
87	OHX	2	2171	7/7	0.40	16.92	127,127,127,127	0
86	MG	5	3458	1/1	0.31	16.92	23,23,23,23	0
86	MG	5	4256	1/1	0.55	16.92	29,29,29,29	0
86	MG	5	3485	1/1	0.39	16.90	31,31,31,31	0
86	MG	6	1937	1/1	0.29	16.87	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3637	1/1	0.30	16.81	37,37,37,37	0
86	MG	5	3577	1/1	0.40	16.76	44,44,44,44	0
86	MG	5	3850	1/1	0.32	16.76	49,49,49,49	0
86	MG	6	1963	1/1	0.38	16.70	68,68,68,68	0
86	MG	5	3558	1/1	0.34	16.60	23,23,23,23	0
86	MG	2	1929	1/1	0.40	16.58	57,57,57,57	0
86	MG	1	3506	1/1	0.35	16.56	38,38,38,38	0
87	OHX	1	4189	7/7	0.44	16.54	116,116,116,116	0
86	MG	5	3581	1/1	0.39	16.53	36,36,36,36	0
86	MG	5	3533	1/1	0.42	16.48	40,40,40,40	0
86	MG	5	3697	1/1	0.22	16.47	67,67,67,67	0
86	MG	1	3511	1/1	0.34	16.41	27,27,27,27	0
86	MG	1	3696	1/1	0.20	16.40	38,38,38,38	0
86	MG	1	3522	1/1	0.39	16.39	33,33,33,33	0
86	MG	5	3543	1/1	0.38	16.39	31,31,31,31	0
86	MG	3	205	1/1	0.34	16.37	34,34,34,34	0
86	MG	5	3837	1/1	0.26	16.33	56,56,56,56	0
86	MG	1	3465	1/1	0.24	16.28	58,58,58,58	0
86	MG	6	1914	1/1	0.34	16.26	35,35,35,35	0
86	MG	1	3597	1/1	0.34	16.15	19,19,19,19	0
86	MG	5	3434	1/1	0.35	16.11	51,51,51,51	0
86	MG	1	3461	1/1	0.27	16.11	28,28,28,28	0
86	MG	5	3627	1/1	0.27	16.08	36,36,36,36	0
86	MG	5	3501	1/1	0.35	16.06	34,34,34,34	0
86	MG	5	3549	1/1	0.37	16.04	48,48,48,48	0
86	MG	5	3451	1/1	0.33	16.00	55,55,55,55	0
86	MG	6	1919	1/1	0.34	15.99	38,38,38,38	0
86	MG	1	3853	1/1	0.33	15.95	78,78,78,78	0
86	MG	3	201	1/1	0.36	15.95	66,66,66,66	0
86	MG	5	3523	1/1	0.30	15.88	26,26,26,26	0
86	MG	5	3564	1/1	0.47	15.81	33,33,33,33	0
87	OHX	1	4137	7/7	0.32	15.65	113,113,113,113	0
86	MG	5	3766	1/1	0.37	15.59	36,36,36,36	0
86	MG	6	1920	1/1	0.36	15.46	52,52,52,52	0
86	MG	5	3639	1/1	0.20	15.39	49,49,49,49	0
86	MG	5	3772	1/1	0.35	15.38	69,69,69,69	0
86	MG	5	3561	1/1	0.37	15.35	29,29,29,29	0
86	MG	6	1917	1/1	0.33	15.35	48,48,48,48	0
87	OHX	1	4177	7/7	0.31	15.32	128,128,128,128	0
86	MG	5	3874	1/1	0.48	15.25	48,48,48,48	0
86	MG	1	3552	1/1	0.35	15.24	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	5	4215	7/7	0.33	15.19	121,121,121,121	0
86	MG	5	3428	1/1	0.33	15.04	39,39,39,39	0
86	MG	6	1922	1/1	0.33	15.03	47,47,47,47	0
86	MG	1	3859	1/1	0.37	15.02	120,120,120,120	0
86	MG	5	3444	1/1	0.26	15.00	31,31,31,31	0
86	MG	1	3649	1/1	0.36	14.96	43,43,43,43	0
86	MG	6	2014	1/1	0.53	14.77	124,124,124,124	0
86	MG	6	1929	1/1	0.35	14.76	48,48,48,48	0
86	MG	1	3509	1/1	0.33	14.73	42,42,42,42	0
86	MG	5	3774	1/1	0.35	14.72	28,28,28,28	0
87	OHX	6	2182	7/7	0.34	14.63	124,124,124,124	0
86	MG	5	3778	1/1	0.26	14.61	65,65,65,65	0
86	MG	1	3605	1/1	0.29	14.60	30,30,30,30	0
86	MG	5	3740	1/1	0.32	14.59	69,69,69,69	0
86	MG	5	3482	1/1	0.39	14.54	62,62,62,62	0
86	MG	1	3459	1/1	0.35	14.48	29,29,29,29	0
86	MG	1	3711	1/1	0.31	14.48	56,56,56,56	0
87	OHX	2	2161	7/7	0.31	14.48	146,146,146,146	0
86	MG	1	3740	1/1	0.30	14.46	57,57,57,57	0
86	MG	1	3761	1/1	0.24	14.44	27,27,27,27	0
86	MG	5	3403	1/1	0.42	14.43	58,58,58,58	0
86	MG	1	3412	1/1	0.35	14.42	37,37,37,37	0
86	MG	6	1951	1/1	0.39	14.41	60,60,60,60	0
86	MG	5	3578	1/1	0.34	14.41	29,29,29,29	0
87	OHX	5	4218	7/7	0.34	14.40	117,117,117,117	0
86	MG	1	3584	1/1	0.32	14.39	34,34,34,34	0
86	MG	5	3566	1/1	0.27	14.36	20,20,20,20	0
86	MG	5	3565	1/1	0.38	14.35	27,27,27,27	0
86	MG	5	3641	1/1	0.40	14.30	34,34,34,34	0
86	MG	4	207	1/1	0.35	14.25	34,34,34,34	0
86	MG	2	1971	1/1	0.32	14.17	69,69,69,69	0
86	MG	6	2008	1/1	0.17	14.14	47,47,47,47	0
86	MG	1	3572	1/1	0.37	14.13	38,38,38,38	0
86	MG	2	1908	1/1	0.25	14.12	65,65,65,65	0
86	MG	1	3615	1/1	0.30	14.06	33,33,33,33	0
86	MG	6	1958	1/1	0.33	14.06	47,47,47,47	0
86	MG	1	3600	1/1	0.42	14.04	19,19,19,19	0
86	MG	1	3515	1/1	0.41	14.03	31,31,31,31	0
86	MG	5	3650	1/1	0.30	14.00	45,45,45,45	0
86	MG	7	201	1/1	0.46	13.99	39,39,39,39	0
86	MG	2	1918	1/1	0.37	13.99	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3573	1/1	0.33	13.95	27,27,27,27	0
86	MG	6	1942	1/1	0.26	13.94	30,30,30,30	0
86	MG	1	3745	1/1	0.25	13.94	26,26,26,26	0
86	MG	1	3720	1/1	0.37	13.93	51,51,51,51	0
86	MG	2	2015	1/1	0.41	13.82	67,67,67,67	0
86	MG	6	1946	1/1	0.41	13.77	55,55,55,55	0
87	OHX	6	2166	7/7	0.23	13.68	132,132,132,132	0
86	MG	5	3596	1/1	0.41	13.65	35,35,35,35	0
86	MG	5	3883	1/1	0.28	13.59	47,47,47,47	0
86	MG	5	3822	1/1	0.37	13.57	37,37,37,37	0
86	MG	5	3835	1/1	0.34	13.51	37,37,37,37	0
86	MG	6	1977	1/1	0.29	13.47	56,56,56,56	0
86	MG	5	3538	1/1	0.40	13.45	36,36,36,36	0
86	MG	1	3815	1/1	0.55	13.43	110,110,110,110	0
87	OHX	6	2184	7/7	0.36	13.38	127,127,127,127	0
86	MG	5	3739	1/1	0.32	13.37	43,43,43,43	0
87	OHX	1	4184	7/7	0.38	13.32	120,120,120,120	0
86	MG	6	1906	1/1	0.37	13.27	44,44,44,44	0
86	MG	1	3527	1/1	0.32	13.25	24,24,24,24	0
87	OHX	5	4178	7/7	0.37	13.18	97,97,97,97	0
86	MG	4	211	1/1	0.23	13.14	51,51,51,51	0
86	MG	5	3480	1/1	0.27	13.11	63,63,63,63	0
86	MG	1	3431	1/1	0.30	13.08	42,42,42,42	0
86	MG	5	3875	1/1	0.35	13.06	41,41,41,41	0
86	MG	1	3402	1/1	0.35	13.06	46,46,46,46	0
86	MG	6	2042	1/1	0.38	13.05	71,71,71,71	0
86	MG	1	3455	1/1	0.34	13.04	54,54,54,54	0
87	OHX	2	2168	7/7	0.36	12.97	139,139,139,139	0
87	OHX	1	4146	7/7	0.22	12.88	118,118,118,118	0
86	MG	5	3880	1/1	0.33	12.84	21,21,21,21	0
86	MG	5	3521	1/1	0.41	12.81	33,33,33,33	0
86	MG	6	2001	1/1	0.43	12.80	46,46,46,46	0
86	MG	5	3562	1/1	0.30	12.79	24,24,24,24	0
86	MG	5	3587	1/1	0.41	12.72	21,21,21,21	0
87	OHX	5	4186	7/7	0.29	12.71	109,109,109,109	0
86	MG	1	3588	1/1	0.31	12.70	30,30,30,30	0
87	OHX	2	2170	7/7	0.30	12.68	127,127,127,127	0
86	MG	5	3866	1/1	0.22	12.67	52,52,52,52	0
86	MG	5	3443	1/1	0.35	12.63	27,27,27,27	0
87	OHX	1	4188	7/7	0.28	12.61	114,114,114,114	0
86	MG	6	1928	1/1	0.36	12.61	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	4	206	1/1	0.32	12.59	46,46,46,46	0
86	MG	1	3458	1/1	0.28	12.58	55,55,55,55	0
86	MG	1	3418	1/1	0.34	12.58	48,48,48,48	0
86	MG	5	3744	1/1	0.34	12.56	26,26,26,26	0
87	OHX	5	4159	7/7	0.26	12.54	96,96,96,96	0
87	OHX	2	2152	7/7	0.21	12.53	146,146,146,146	0
86	MG	1	3682	1/1	0.25	12.42	52,52,52,52	0
86	MG	1	3697	1/1	0.21	12.40	52,52,52,52	0
86	MG	5	3662	1/1	0.31	12.33	27,27,27,27	0
86	MG	1	3536	1/1	0.32	12.32	42,42,42,42	0
86	MG	5	3424	1/1	0.28	12.30	54,54,54,54	0
86	MG	5	3749	1/1	0.41	12.30	33,33,33,33	0
86	MG	5	3504	1/1	0.21	12.25	36,36,36,36	0
87	OHX	5	4239	7/7	0.30	12.24	124,124,124,124	0
87	OHX	5	4154	7/7	0.28	12.23	102,102,102,102	0
87	OHX	1	4209	7/7	0.30	12.18	111,111,111,111	0
86	MG	1	3561	1/1	0.34	12.14	35,35,35,35	0
87	OHX	8	224	7/7	0.33	12.13	123,123,123,123	0
86	MG	5	3499	1/1	0.27	12.11	46,46,46,46	0
87	OHX	2	2124	7/7	0.28	12.06	110,110,110,110	0
86	MG	1	3613	1/1	0.21	11.95	42,42,42,42	0
87	OHX	6	2179	7/7	0.30	11.94	123,123,123,123	0
86	MG	1	3502	1/1	0.34	11.89	36,36,36,36	0
86	MG	5	3448	1/1	0.28	11.86	37,37,37,37	0
86	MG	5	3531	1/1	0.34	11.81	26,26,26,26	0
86	MG	2	1919	1/1	0.46	11.77	66,66,66,66	0
86	MG	5	3456	1/1	0.23	11.76	43,43,43,43	0
86	MG	1	3485	1/1	0.28	11.72	34,34,34,34	0
86	MG	5	3580	1/1	0.33	11.71	30,30,30,30	0
86	MG	1	3813	1/1	0.34	11.71	53,53,53,53	0
87	OHX	1	4167	7/7	0.21	11.68	109,109,109,109	0
86	MG	1	3526	1/1	0.28	11.65	24,24,24,24	0
86	MG	1	3793	1/1	0.26	11.64	20,20,20,20	0
87	OHX	2	2135	7/7	0.25	11.61	116,116,116,116	0
86	MG	1	3533	1/1	0.26	11.61	31,31,31,31	0
86	MG	6	1940	1/1	0.45	11.60	76,76,76,76	0
87	OHX	1	4112	7/7	0.24	11.56	102,102,102,102	0
86	MG	2	1925	1/1	0.38	11.56	63,63,63,63	0
86	MG	1	3452	1/1	0.28	11.56	41,41,41,41	0
86	MG	2	1962	1/1	0.43	11.55	68,68,68,68	0
86	MG	5	3530	1/1	0.28	11.53	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3867	1/1	0.25	11.50	61,61,61,61	0
86	MG	1	3481	1/1	0.29	11.48	26,26,26,26	0
86	MG	5	3747	1/1	0.27	11.44	49,49,49,49	0
86	MG	6	1947	1/1	0.41	11.41	48,48,48,48	0
86	MG	5	3433	1/1	0.36	11.37	45,45,45,45	0
86	MG	1	3478	1/1	0.30	11.36	71,71,71,71	0
86	MG	1	3542	1/1	0.27	11.23	20,20,20,20	0
86	MG	5	3689	1/1	0.25	11.20	39,39,39,39	0
86	MG	5	3610	1/1	0.30	11.19	23,23,23,23	0
86	MG	5	3657	1/1	0.22	11.15	41,41,41,41	0
86	MG	5	3681	1/1	0.19	11.14	44,44,44,44	0
87	OHX	5	4151	7/7	0.23	11.06	108,108,108,108	0
87	OHX	5	4179	7/7	0.27	11.03	118,118,118,118	0
87	OHX	2	2177	7/7	0.27	11.02	156,156,156,156	0
86	MG	6	1907	1/1	0.38	10.98	55,55,55,55	0
86	MG	5	3409	1/1	0.35	10.92	40,40,40,40	0
86	MG	5	3786	1/1	0.26	10.90	25,25,25,25	0
87	OHX	1	4201	7/7	0.32	10.88	122,122,122,122	0
86	MG	6	1950	1/1	0.28	10.86	35,35,35,35	0
86	MG	1	3587	1/1	0.41	10.78	39,39,39,39	0
86	MG	6	2035	1/1	0.31	10.77	72,72,72,72	0
86	MG	1	3510	1/1	0.34	10.75	25,25,25,25	0
87	OHX	6	2205	7/7	0.33	10.75	129,129,129,129	0
86	MG	5	3612	1/1	0.30	10.71	32,32,32,32	0
86	MG	6	1956	1/1	0.43	10.68	42,42,42,42	0
87	OHX	6	2187	7/7	0.43	10.66	127,127,127,127	0
87	OHX	5	4230	7/7	0.29	10.65	136,136,136,136	0
86	MG	5	3834	1/1	0.30	10.62	41,41,41,41	0
86	MG	5	3493	1/1	0.27	10.56	56,56,56,56	0
86	MG	2	1917	1/1	0.35	10.56	53,53,53,53	0
86	MG	2	1964	1/1	0.33	10.54	85,85,85,85	0
86	MG	1	3797	1/1	0.22	10.51	43,43,43,43	0
86	MG	6	1972	1/1	0.28	10.50	58,58,58,58	0
86	MG	2	1915	1/1	0.38	10.49	61,61,61,61	0
86	MG	6	1939	1/1	0.33	10.47	54,54,54,54	0
87	OHX	1	4139	7/7	0.34	10.46	97,97,97,97	0
86	MG	5	3836	1/1	0.23	10.44	40,40,40,40	0
86	MG	6	2028	1/1	0.28	10.41	56,56,56,56	0
86	MG	5	3459	1/1	0.22	10.39	36,36,36,36	0
86	MG	5	3630	1/1	0.19	10.38	47,47,47,47	0
86	MG	1	3609	1/1	0.36	10.38	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	5	4149	7/7	0.30	10.35	114,114,114,114	0
86	MG	6	1982	1/1	0.32	10.35	64,64,64,64	0
86	MG	5	3507	1/1	0.31	10.35	28,28,28,28	0
86	MG	1	3626	1/1	0.32	10.34	31,31,31,31	0
87	OHX	5	4231	7/7	0.40	10.33	110,110,110,110	0
86	MG	1	3590	1/1	0.27	10.32	27,27,27,27	0
86	MG	1	3554	1/1	0.27	10.30	50,50,50,50	0
86	MG	5	3552	1/1	0.32	10.27	26,26,26,26	0
86	MG	1	3792	1/1	0.54	10.23	37,37,37,37	0
86	MG	1	3540	1/1	0.33	10.22	22,22,22,22	0
86	MG	1	3608	1/1	0.31	10.22	48,48,48,48	0
86	MG	5	3528	1/1	0.33	10.18	29,29,29,29	0
87	OHX	5	4139	7/7	0.33	10.14	110,110,110,110	0
87	OHX	6	2191	7/7	0.33	10.14	123,123,123,123	0
86	MG	5	3726	1/1	0.25	10.13	42,42,42,42	0
86	MG	5	3515	1/1	0.38	10.11	26,26,26,26	0
86	MG	1	3429	1/1	0.32	10.11	41,41,41,41	0
86	MG	5	3411	1/1	0.27	10.11	33,33,33,33	0
86	MG	5	3500	1/1	0.26	10.10	26,26,26,26	0
86	MG	1	3721	1/1	0.31	10.08	50,50,50,50	0
86	MG	1	3436	1/1	0.34	10.06	38,38,38,38	0
87	OHX	1	4061	7/7	0.28	10.05	126,126,126,126	0
87	OHX	5	4092	7/7	0.24	10.04	104,104,104,104	0
87	OHX	6	2175	7/7	0.41	10.03	114,114,114,114	0
86	MG	1	3814	1/1	0.16	10.00	45,45,45,45	0
86	MG	1	3505	1/1	0.28	10.00	29,29,29,29	0
86	MG	N3	202	1/1	0.29	9.96	57,57,57,57	0
87	OHX	1	4213	7/7	0.30	9.95	118,118,118,118	0
87	OHX	5	4181	7/7	0.27	9.95	121,121,121,121	0
86	MG	2	1993	1/1	0.33	9.91	88,88,88,88	0
87	OHX	1	4170	7/7	0.32	9.89	147,147,147,147	0
86	MG	5	3631	1/1	0.32	9.86	57,57,57,57	0
87	OHX	1	4169	7/7	0.32	9.85	137,137,137,137	0
86	MG	5	3496	1/1	0.35	9.83	23,23,23,23	0
87	OHX	1	4173	7/7	0.24	9.80	148,148,148,148	0
86	MG	1	3586	1/1	0.33	9.80	41,41,41,41	0
86	MG	6	1964	1/1	0.23	9.80	46,46,46,46	0
86	MG	5	3514	1/1	0.34	9.79	48,48,48,48	0
86	MG	1	3410	1/1	0.32	9.78	41,41,41,41	0
86	MG	o1	202	1/1	0.53	9.76	68,68,68,68	0
86	MG	5	3804	1/1	0.25	9.75	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4175	7/7	0.28	9.74	137,137,137,137	0
86	MG	1	3675	1/1	0.28	9.73	21,21,21,21	0
86	MG	1	3446	1/1	0.36	9.71	44,44,44,44	0
86	MG	1	3453	1/1	0.30	9.69	35,35,35,35	0
86	MG	1	3764	1/1	0.31	9.57	42,42,42,42	0
86	MG	5	3569	1/1	0.32	9.56	25,25,25,25	0
86	MG	5	3594	1/1	0.31	9.56	30,30,30,30	0
87	OHX	1	4168	7/7	0.31	9.54	98,98,98,98	0
86	MG	2	1934	1/1	0.42	9.54	64,64,64,64	0
86	MG	5	3829	1/1	0.26	9.53	23,23,23,23	0
86	MG	1	3606	1/1	0.21	9.52	35,35,35,35	0
86	MG	2	1940	1/1	0.29	9.48	58,58,58,58	0
86	MG	1	3496	1/1	0.29	9.48	28,28,28,28	0
87	OHX	8	228	7/7	0.33	9.47	112,112,112,112	0
86	MG	5	3647	1/1	0.31	9.46	31,31,31,31	0
87	OHX	1	4153	7/7	0.22	9.40	115,115,115,115	0
86	MG	6	1968	1/1	0.31	9.40	62,62,62,62	0
87	OHX	1	4152	7/7	0.28	9.39	123,123,123,123	0
86	MG	6	1993	1/1	0.29	9.39	60,60,60,60	0
86	MG	1	3497	1/1	0.25	9.38	39,39,39,39	0
86	MG	2	1985	1/1	0.36	9.38	99,99,99,99	0
87	OHX	1	4062	7/7	0.31	9.37	120,120,120,120	0
86	MG	1	3414	1/1	0.34	9.33	30,30,30,30	0
86	MG	6	2034	1/1	0.31	9.32	63,63,63,63	0
86	MG	1	3550	1/1	0.27	9.29	27,27,27,27	0
86	MG	1	3702	1/1	0.25	9.28	44,44,44,44	0
86	MG	5	3717	1/1	0.24	9.28	46,46,46,46	0
86	MG	2	1942	1/1	0.28	9.24	62,62,62,62	0
87	OHX	6	2113	7/7	0.27	9.20	110,110,110,110	0
87	OHX	2	2162	7/7	0.26	9.19	156,156,156,156	0
87	OHX	6	2172	7/7	0.29	9.19	101,101,101,101	0
86	MG	1	3598	1/1	0.34	9.18	26,26,26,26	0
87	OHX	1	4115	7/7	0.22	9.17	112,112,112,112	0
87	OHX	8	225	7/7	0.27	9.12	118,118,118,118	0
86	MG	5	3421	1/1	0.18	9.10	90,90,90,90	0
86	MG	1	3638	1/1	0.32	9.09	49,49,49,49	0
87	OHX	M7	207	7/7	0.37	9.04	93,93,93,93	0
87	OHX	1	4045	7/7	0.24	9.01	101,101,101,101	0
87	OHX	5	4142	7/7	0.30	9.00	117,117,117,117	0
86	MG	1	3517	1/1	0.33	9.00	28,28,28,28	0
86	MG	5	3445	1/1	0.30	8.89	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	MG	1	3693	1/1	0.25	8.88	44,44,44,44	0
86	MG	6	1966	1/1	0.41	8.86	76,76,76,76	0
86	MG	5	3683	1/1	0.39	8.83	79,79,79,79	0
86	MG	5	3527	1/1	0.27	8.82	45,45,45,45	0
87	OHX	1	4114	7/7	0.28	8.82	108,108,108,108	0
86	MG	1	3460	1/1	0.22	8.79	21,21,21,21	0
86	MG	5	3520	1/1	0.28	8.76	20,20,20,20	0
87	OHX	5	4192	7/7	0.27	8.74	109,109,109,109	0
86	MG	1	3443	1/1	0.34	8.73	73,73,73,73	0
87	OHX	5	4202	7/7	0.25	8.70	124,124,124,124	0
86	MG	6	1935	1/1	0.27	8.67	51,51,51,51	0
86	MG	5	3489	1/1	0.38	8.67	29,29,29,29	0
86	MG	2	1909	1/1	0.21	8.65	63,63,63,63	0
86	MG	1	3560	1/1	0.27	8.65	22,22,22,22	0
87	OHX	5	4160	7/7	0.25	8.63	113,113,113,113	0
86	MG	5	3556	1/1	0.34	8.62	43,43,43,43	0
86	MG	2	1976	1/1	0.33	8.62	86,86,86,86	0
86	MG	2	1933	1/1	0.39	8.61	64,64,64,64	0
87	OHX	5	4161	7/7	0.29	8.60	113,113,113,113	0
86	MG	5	3593	1/1	0.34	8.58	27,27,27,27	0
87	OHX	1	4057	7/7	0.32	8.57	105,105,105,105	0
86	MG	5	3440	1/1	0.32	8.56	62,62,62,62	0
86	MG	1	3601	1/1	0.24	8.56	30,30,30,30	0
86	MG	1	3840	1/1	0.20	8.56	44,44,44,44	0
86	MG	1	3732	1/1	0.26	8.55	73,73,73,73	0
87	OHX	5	4229	7/7	0.26	8.53	156,156,156,156	0
87	OHX	1	4095	7/7	0.20	8.52	126,126,126,126	0
86	MG	1	3439	1/1	0.34	8.50	46,46,46,46	0
87	OHX	6	2127	7/7	0.31	8.50	91,91,91,91	0
86	MG	1	3451	1/1	0.30	8.48	29,29,29,29	0
87	OHX	5	4245	7/7	0.23	8.46	133,133,133,133	0
86	MG	1	3679	1/1	0.18	8.46	42,42,42,42	0
86	MG	2	2005	1/1	0.56	8.42	62,62,62,62	0
87	OHX	2	2116	7/7	0.23	8.41	123,123,123,123	0
86	MG	1	3401	1/1	0.31	8.39	36,36,36,36	0
86	MG	1	3705	1/1	0.20	8.38	57,57,57,57	0
86	MG	8	208	1/1	0.35	8.38	76,76,76,76	0
87	OHX	1	4142	7/7	0.26	8.37	125,125,125,125	0
86	MG	5	3477	1/1	0.26	8.37	68,68,68,68	0
87	OHX	1	4182	7/7	0.27	8.36	125,125,125,125	0
86	MG	1	3704	1/1	0.26	8.33	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3685	1/1	0.26	8.32	51,51,51,51	0
86	MG	2	1922	1/1	0.36	8.32	60,60,60,60	0
87	OHX	1	4072	7/7	0.29	8.25	90,90,90,90	0
86	MG	5	3560	1/1	0.30	8.24	22,22,22,22	0
86	MG	5	3429	1/1	0.27	8.16	23,23,23,23	0
87	OHX	5	4185	7/7	0.30	8.13	111,111,111,111	0
86	MG	1	3718	1/1	0.55	8.12	39,39,39,39	0
87	OHX	5	4162	7/7	0.27	8.12	104,104,104,104	0
86	MG	6	1983	1/1	0.38	8.11	47,47,47,47	0
87	OHX	2	2178	7/7	0.31	8.10	125,125,125,125	0
86	MG	2	1972	1/1	0.21	8.05	63,63,63,63	0
86	MG	5	3579	1/1	0.41	8.03	41,41,41,41	0
86	MG	2	1931	1/1	0.35	8.01	52,52,52,52	0
86	MG	1	3674	1/1	0.26	8.00	52,52,52,52	0
87	OHX	6	2188	7/7	0.22	8.00	160,160,160,160	0
87	OHX	5	4248	7/7	0.26	7.97	113,113,113,113	0
87	OHX	5	4138	7/7	0.26	7.96	115,115,115,115	0
86	MG	1	3616	1/1	0.26	7.96	34,34,34,34	0
87	OHX	2	2134	7/7	0.25	7.96	120,120,120,120	0
86	MG	5	3455	1/1	0.34	7.95	35,35,35,35	0
86	MG	5	3537	1/1	0.38	7.95	26,26,26,26	0
86	MG	3	202	1/1	0.24	7.93	40,40,40,40	0
86	MG	5	3545	1/1	0.32	7.93	62,62,62,62	0
86	MG	5	3882	1/1	0.28	7.90	33,33,33,33	0
86	MG	2	1927	1/1	0.40	7.89	49,49,49,49	0
86	MG	5	3807	1/1	0.42	7.88	94,94,94,94	0
86	MG	2	1906	1/1	0.24	7.83	45,45,45,45	0
86	MG	1	3498	1/1	0.27	7.83	22,22,22,22	0
87	OHX	1	4127	7/7	0.25	7.79	129,129,129,129	0
87	OHX	1	4125	7/7	0.27	7.78	107,107,107,107	0
86	MG	1	3569	1/1	0.26	7.76	23,23,23,23	0
87	OHX	6	2181	7/7	0.32	7.75	117,117,117,117	0
86	MG	1	3551	1/1	0.29	7.74	37,37,37,37	0
87	OHX	1	4190	7/7	0.25	7.71	123,123,123,123	0
86	MG	1	3521	1/1	0.35	7.69	61,61,61,61	0
87	OHX	1	4159	7/7	0.25	7.67	134,134,134,134	0
86	MG	1	3532	1/1	0.30	7.65	21,21,21,21	0
86	MG	6	1934	1/1	0.34	7.64	65,65,65,65	0
86	MG	5	3582	1/1	0.35	7.60	31,31,31,31	0
86	MG	6	1980	1/1	0.19	7.60	70,70,70,70	0
86	MG	D0	201	1/1	0.36	7.57	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	1926	1/1	0.24	7.57	45,45,45,45	0
86	MG	5	3406	1/1	0.22	7.57	30,30,30,30	0
86	MG	5	3539	1/1	0.28	7.56	34,34,34,34	0
86	MG	6	1904	1/1	0.32	7.55	57,57,57,57	0
86	MG	1	3589	1/1	0.27	7.53	27,27,27,27	0
87	OHX	6	2161	7/7	0.46	7.53	115,115,115,115	0
87	OHX	5	4176	7/7	0.24	7.52	121,121,121,121	0
86	MG	5	3487	1/1	0.29	7.48	34,34,34,34	0
87	OHX	1	4185	7/7	0.27	7.44	131,131,131,131	0
86	MG	5	3848	1/1	0.30	7.44	39,39,39,39	0
86	MG	5	3709	1/1	0.24	7.39	43,43,43,43	0
87	OHX	6	2190	7/7	0.33	7.38	123,123,123,123	0
87	OHX	5	4173	7/7	0.26	7.37	83,83,83,83	0
86	MG	6	1985	1/1	0.32	7.36	40,40,40,40	0
86	MG	m1	201	1/1	0.36	7.34	54,54,54,54	0
87	OHX	6	2204	7/7	0.28	7.34	125,125,125,125	0
87	OHX	2	2147	7/7	0.27	7.27	110,110,110,110	0
86	MG	7	203	1/1	0.26	7.27	45,45,45,45	0
86	MG	1	3519	1/1	0.36	7.27	35,35,35,35	0
87	OHX	1	4174	7/7	0.24	7.26	122,122,122,122	0
86	MG	6	1911	1/1	0.23	7.21	41,41,41,41	0
86	MG	5	3420	1/1	0.27	7.21	62,62,62,62	0
86	MG	1	3699	1/1	0.24	7.21	35,35,35,35	0
87	OHX	5	4115	7/7	0.24	7.19	108,108,108,108	0
86	MG	5	3701	1/1	0.28	7.18	35,35,35,35	0
87	OHX	5	4128	7/7	0.24	7.16	113,113,113,113	0
87	OHX	1	4200	7/7	0.30	7.13	122,122,122,122	0
86	MG	1	3701	1/1	0.26	7.09	34,34,34,34	0
86	MG	5	3516	1/1	0.23	7.09	29,29,29,29	0
86	MG	5	3609	1/1	0.24	7.08	50,50,50,50	0
86	MG	5	3584	1/1	0.29	7.07	41,41,41,41	0
86	MG	5	3595	1/1	0.30	7.07	36,36,36,36	0
86	MG	2	1907	1/1	0.33	7.05	51,51,51,51	0
87	OHX	1	4135	7/7	0.24	7.05	104,104,104,104	0
86	MG	1	3473	1/1	0.27	7.03	22,22,22,22	0
87	OHX	1	4197	7/7	0.27	7.03	116,116,116,116	0
87	OHX	4	233	7/7	0.27	6.98	108,108,108,108	0
87	OHX	5	4226	7/7	0.25	6.97	119,119,119,119	0
86	MG	1	3457	1/1	0.25	6.97	35,35,35,35	0
86	MG	2	1949	1/1	0.23	6.97	53,53,53,53	0
86	MG	5	3553	1/1	0.29	6.96	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	1926	1/1	0.34	6.96	84,84,84,84	0
86	MG	6	1979	1/1	0.27	6.93	42,42,42,42	0
86	MG	1	3657	1/1	0.22	6.93	29,29,29,29	0
86	MG	2	1938	1/1	0.36	6.93	58,58,58,58	0
86	MG	5	3498	1/1	0.25	6.92	32,32,32,32	0
86	MG	5	3764	1/1	0.26	6.90	37,37,37,37	0
86	MG	5	3464	1/1	0.32	6.89	26,26,26,26	0
86	MG	5	3830	1/1	0.23	6.86	42,42,42,42	0
86	MG	1	3479	1/1	0.22	6.86	64,64,64,64	0
86	MG	5	3757	1/1	0.19	6.86	53,53,53,53	0
87	OHX	6	2164	7/7	0.31	6.84	120,120,120,120	0
86	MG	5	3413	1/1	0.33	6.84	37,37,37,37	0
87	OHX	3	224	7/7	0.29	6.83	112,112,112,112	0
86	MG	5	3720	1/1	0.22	6.82	44,44,44,44	0
86	MG	5	3417	1/1	0.26	6.80	20,20,20,20	0
86	MG	3	212	1/1	0.29	6.80	68,68,68,68	0
86	MG	1	3570	1/1	0.30	6.80	24,24,24,24	0
86	MG	12	301	1/1	0.32	6.80	45,45,45,45	0
87	OHX	5	4126	7/7	0.18	6.78	126,126,126,126	0
87	OHX	6	2158	7/7	0.26	6.77	122,122,122,122	0
87	OHX	1	4203	7/7	0.35	6.75	120,120,120,120	0
87	OHX	5	4175	7/7	0.27	6.75	120,120,120,120	0
87	OHX	5	4184	7/7	0.30	6.74	106,106,106,106	0
86	MG	5	3857	1/1	0.21	6.71	59,59,59,59	0
86	MG	1	3405	1/1	0.52	6.68	82,82,82,82	0
87	OHX	2	2156	7/7	0.39	6.68	104,104,104,104	0
86	MG	1	3501	1/1	0.31	6.66	23,23,23,23	0
86	MG	1	3466	1/1	0.27	6.66	44,44,44,44	0
86	MG	1	4218	1/1	0.40	6.64	28,28,28,28	0
86	MG	1	3763	1/1	0.21	6.62	46,46,46,46	0
86	MG	1	3734	1/1	0.25	6.56	37,37,37,37	0
86	MG	6	1901	1/1	0.24	6.53	41,41,41,41	0
86	MG	1	3838	1/1	0.26	6.51	26,26,26,26	0
87	OHX	1	4013	7/7	0.21	6.48	108,108,108,108	0
87	OHX	1	4202	7/7	0.44	6.48	123,123,123,123	0
86	MG	5	3628	1/1	0.21	6.48	24,24,24,24	0
86	MG	5	3422	1/1	0.27	6.47	34,34,34,34	0
86	MG	1	3423	1/1	0.24	6.46	34,34,34,34	0
86	MG	1	3803	1/1	0.25	6.46	30,30,30,30	0
87	OHX	5	4219	7/7	0.18	6.46	158,158,158,158	0
86	MG	2	1937	1/1	0.36	6.45	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4100	7/7	0.22	6.41	128,128,128,128	0
87	OHX	2	2145	7/7	0.35	6.41	122,122,122,122	0
86	MG	N8	204	1/1	0.49	6.41	30,30,30,30	0
86	MG	1	3564	1/1	0.25	6.41	42,42,42,42	0
86	MG	5	3570	1/1	0.33	6.39	29,29,29,29	0
86	MG	5	3885	1/1	0.27	6.39	23,23,23,23	0
86	MG	6	1932	1/1	0.21	6.37	38,38,38,38	0
87	OHX	5	4188	7/7	0.27	6.36	132,132,132,132	0
87	OHX	5	4150	7/7	0.25	6.36	129,129,129,129	0
86	MG	5	3785	1/1	0.18	6.35	56,56,56,56	0
86	MG	5	3644	1/1	0.30	6.34	54,54,54,54	0
87	OHX	5	4220	7/7	0.26	6.33	127,127,127,127	0
86	MG	1	3524	1/1	0.28	6.32	25,25,25,25	0
86	MG	5	3617	1/1	0.25	6.31	40,40,40,40	0
86	MG	2	1955	1/1	0.26	6.28	57,57,57,57	0
86	MG	1	3821	1/1	0.25	6.28	64,64,64,64	0
86	MG	1	3503	1/1	0.28	6.27	21,21,21,21	0
86	MG	6	1938	1/1	0.29	6.27	35,35,35,35	0
87	OHX	5	4223	7/7	0.33	6.25	116,116,116,116	0
86	MG	1	3651	1/1	0.30	6.24	61,61,61,61	0
86	MG	3	209	1/1	0.38	6.24	52,52,52,52	0
87	OHX	4	234	7/7	0.24	6.21	136,136,136,136	0
86	MG	5	3590	1/1	0.26	6.20	26,26,26,26	0
86	MG	5	3624	1/1	0.23	6.19	34,34,34,34	0
87	OHX	5	4183	7/7	0.25	6.17	119,119,119,119	0
86	MG	17	301	1/1	0.28	6.17	36,36,36,36	0
87	OHX	5	4146	7/7	0.25	6.15	108,108,108,108	0
86	MG	1	3611	1/1	0.23	6.13	42,42,42,42	0
87	OHX	5	4207	7/7	0.26	6.13	127,127,127,127	0
86	MG	6	1975	1/1	0.22	6.04	50,50,50,50	0
87	OHX	1	4063	7/7	0.29	6.04	111,111,111,111	0
86	MG	6	1930	1/1	0.24	6.03	50,50,50,50	0
86	MG	5	3734	1/1	0.22	6.03	63,63,63,63	0
86	MG	5	3787	1/1	0.23	6.03	33,33,33,33	0
86	MG	1	3435	1/1	0.17	6.02	35,35,35,35	0
86	MG	1	3491	1/1	0.24	6.01	24,24,24,24	0
86	MG	1	3624	1/1	0.21	6.00	44,44,44,44	0
86	MG	1	3816	1/1	0.26	5.99	34,34,34,34	0
87	OHX	1	4107	7/7	0.25	5.99	123,123,123,123	0
86	MG	2	1975	1/1	0.26	5.97	50,50,50,50	0
87	OHX	6	2048	7/7	0.21	5.95	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3660	1/1	0.22	5.95	31,31,31,31	0
86	MG	5	3705	1/1	0.26	5.94	61,61,61,61	0
86	MG	5	3626	1/1	0.26	5.93	36,36,36,36	0
86	MG	1	3778	1/1	0.18	5.93	64,64,64,64	0
86	MG	1	3832	1/1	0.26	5.92	29,29,29,29	0
86	MG	6	2043	1/1	0.24	5.92	41,41,41,41	0
86	MG	1	3741	1/1	0.26	5.89	42,42,42,42	0
86	MG	1	3539	1/1	0.23	5.89	38,38,38,38	0
86	MG	5	3544	1/1	0.23	5.86	25,25,25,25	0
86	MG	6	1927	1/1	0.27	5.85	43,43,43,43	0
86	MG	5	3738	1/1	0.24	5.85	50,50,50,50	0
86	MG	6	1912	1/1	0.32	5.84	62,62,62,62	0
86	MG	5	3721	1/1	0.24	5.82	57,57,57,57	0
86	MG	1	3508	1/1	0.36	5.82	22,22,22,22	0
86	MG	d3	201	1/1	0.71	5.82	44,44,44,44	0
86	MG	7	212	1/1	0.34	5.82	41,41,41,41	0
86	MG	1	3541	1/1	0.22	5.81	49,49,49,49	0
86	MG	8	206	1/1	0.37	5.81	46,46,46,46	0
87	OHX	5	4105	7/7	0.25	5.80	94,94,94,94	0
86	MG	1	3577	1/1	0.30	5.79	22,22,22,22	0
86	MG	5	3571	1/1	0.39	5.79	29,29,29,29	0
87	OHX	6	2122	7/7	0.23	5.78	100,100,100,100	0
87	OHX	5	4190	7/7	0.23	5.77	125,125,125,125	0
86	MG	1	3648	1/1	0.26	5.70	30,30,30,30	0
87	OHX	5	4135	7/7	0.24	5.70	111,111,111,111	0
86	MG	1	3486	1/1	0.27	5.69	39,39,39,39	0
86	MG	5	3737	1/1	0.20	5.69	33,33,33,33	0
86	MG	5	3402	1/1	0.24	5.67	22,22,22,22	0
87	OHX	5	4236	7/7	0.25	5.67	117,117,117,117	0
86	MG	5	3844	1/1	0.21	5.65	42,42,42,42	0
86	MG	d4	201	1/1	0.24	5.62	46,46,46,46	0
87	OHX	7	227	7/7	0.27	5.61	140,140,140,140	0
86	MG	5	3849	1/1	0.29	5.60	61,61,61,61	0
86	MG	1	3725	1/1	0.20	5.60	40,40,40,40	0
87	OHX	1	4195	7/7	0.21	5.59	132,132,132,132	0
86	MG	5	3555	1/1	0.32	5.58	28,28,28,28	0
86	MG	6	1923	1/1	0.33	5.57	61,61,61,61	0
87	OHX	5	4234	7/7	0.38	5.54	138,138,138,138	0
87	OHX	O9	101	7/7	0.43	5.53	100,100,100,100	0
86	MG	6	1949	1/1	0.28	5.53	46,46,46,46	0
86	MG	o3	201	1/1	0.32	5.52	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	5	4201	7/7	0.28	5.51	108,108,108,108	0
86	MG	5	3793	1/1	0.24	5.48	85,85,85,85	0
87	OHX	5	4217	7/7	0.25	5.47	127,127,127,127	0
86	MG	5	3667	1/1	0.22	5.47	40,40,40,40	0
86	MG	5	3828	1/1	0.32	5.44	34,34,34,34	0
87	OHX	5	4152	7/7	0.26	5.44	131,131,131,131	0
86	MG	1	3633	1/1	0.27	5.44	57,57,57,57	0
86	MG	5	3826	1/1	0.29	5.43	33,33,33,33	0
86	MG	2	1960	1/1	0.24	5.39	57,57,57,57	0
87	OHX	7	226	7/7	0.28	5.39	109,109,109,109	0
86	MG	1	3430	1/1	0.24	5.38	47,47,47,47	0
87	OHX	1	4138	7/7	0.31	5.38	120,120,120,120	0
86	MG	1	4223	1/1	0.32	5.37	25,25,25,25	0
86	MG	1	3487	1/1	0.25	5.35	30,30,30,30	0
86	MG	1	3658	1/1	0.23	5.33	44,44,44,44	0
86	MG	5	3512	1/1	0.34	5.33	23,23,23,23	0
86	MG	5	4253	1/1	0.23	5.32	33,33,33,33	0
87	OHX	5	4197	7/7	0.23	5.32	103,103,103,103	0
86	MG	1	3845	1/1	0.26	5.31	38,38,38,38	0
87	OHX	5	4111	7/7	0.28	5.31	118,118,118,118	0
87	OHX	5	3910	7/7	0.22	5.23	64,64,64,64	0
86	MG	1	3566	1/1	0.23	5.19	32,32,32,32	0
87	OHX	5	4249	7/7	0.25	5.17	141,141,141,141	0
87	OHX	14	404	7/7	0.45	5.15	128,128,128,128	0
87	OHX	6	2177	7/7	0.23	5.14	95,95,95,95	0
86	MG	5	3809	1/1	0.26	5.12	33,33,33,33	0
87	OHX	m4	201	7/7	0.25	5.12	189,189,189,189	0
87	OHX	1	4205	7/7	0.22	5.11	121,121,121,121	0
86	MG	1	3477	1/1	0.20	5.11	32,32,32,32	0
86	MG	6	1936	1/1	0.26	5.09	62,62,62,62	0
86	MG	5	3699	1/1	0.20	5.07	54,54,54,54	0
87	OHX	5	4203	7/7	0.43	5.07	117,117,117,117	0
86	MG	5	3517	1/1	0.26	5.06	23,23,23,23	0
87	OHX	1	4128	7/7	0.22	5.03	110,110,110,110	0
86	MG	1	3656	1/1	0.27	5.03	43,43,43,43	0
86	MG	5	3648	1/1	0.23	5.03	48,48,48,48	0
86	MG	5	3522	1/1	0.18	5.00	36,36,36,36	0
86	MG	1	3621	1/1	0.20	5.00	59,59,59,59	0
86	MG	5	3854	1/1	0.28	4.98	52,52,52,52	0
86	MG	6	2027	1/1	0.25	4.96	65,65,65,65	0
87	OHX	2	2078	7/7	0.26	4.90	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	1	3888	7/7	0.18	4.89	73,73,73,73	0
86	MG	5	3478	1/1	0.24	4.88	30,30,30,30	0
86	MG	2	1963	1/1	0.19	4.88	126,126,126,126	0
86	MG	6	1989	1/1	0.21	4.87	57,57,57,57	0
87	OHX	1	4210	7/7	0.29	4.85	119,119,119,119	0
86	MG	1	3730	1/1	0.29	4.84	32,32,32,32	0
86	MG	6	2037	1/1	0.19	4.84	55,55,55,55	0
86	MG	1	3787	1/1	0.39	4.84	25,25,25,25	0
86	MG	5	3861	1/1	0.22	4.82	82,82,82,82	0
86	MG	1	3673	1/1	0.45	4.82	61,61,61,61	0
87	OHX	6	2178	7/7	0.23	4.81	108,108,108,108	0
86	MG	m7	201	1/1	0.35	4.78	30,30,30,30	0
86	MG	5	3510	1/1	0.28	4.77	36,36,36,36	0
86	MG	5	3405	1/1	0.21	4.76	22,22,22,22	0
87	OHX	1	4118	7/7	0.33	4.76	116,116,116,116	0
86	MG	5	4257	1/1	0.36	4.73	25,25,25,25	0
87	OHX	1	4069	7/7	0.22	4.72	104,104,104,104	0
86	MG	1	3807	1/1	0.19	4.69	30,30,30,30	0
86	MG	1	3687	1/1	0.21	4.69	80,80,80,80	0
87	OHX	1	4208	7/7	0.28	4.69	115,115,115,115	0
87	OHX	1	4158	7/7	0.24	4.67	116,116,116,116	0
87	OHX	5	4148	7/7	0.26	4.66	112,112,112,112	0
86	MG	N3	203	1/1	0.21	4.65	51,51,51,51	0
86	MG	5	3439	1/1	0.30	4.64	47,47,47,47	0
87	OHX	1	4166	7/7	0.23	4.63	101,101,101,101	0
86	MG	1	3596	1/1	0.33	4.62	28,28,28,28	0
87	OHX	1	4119	7/7	0.22	4.62	103,103,103,103	0
87	OHX	1	4143	7/7	0.24	4.61	104,104,104,104	0
86	MG	5	4255	1/1	0.32	4.60	22,22,22,22	0
87	OHX	1	4110	7/7	0.28	4.60	101,101,101,101	0
87	OHX	2	2164	7/7	0.22	4.60	160,160,160,160	0
87	OHX	5	4153	7/7	0.23	4.58	103,103,103,103	0
86	MG	5	3812	1/1	0.24	4.58	37,37,37,37	0
86	MG	2	1967	1/1	0.59	4.58	105,105,105,105	0
87	OHX	1	4094	7/7	0.27	4.57	119,119,119,119	0
87	OHX	5	4177	7/7	0.22	4.57	118,118,118,118	0
86	MG	2	1912	1/1	0.26	4.55	56,56,56,56	0
86	MG	1	3456	1/1	0.25	4.55	20,20,20,20	0
87	OHX	5	4235	7/7	0.61	4.54	128,128,128,128	0
86	MG	5	3775	1/1	0.24	4.54	97,97,97,97	0
87	OHX	5	4073	7/7	0.21	4.54	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2023	1/1	0.23	4.54	43,43,43,43	0
86	MG	1	3826	1/1	0.23	4.52	44,44,44,44	0
86	MG	5	4254	1/1	0.29	4.51	35,35,35,35	0
86	MG	5	3494	1/1	0.25	4.47	44,44,44,44	0
86	MG	1	3571	1/1	0.28	4.45	16,16,16,16	0
86	MG	1	3664	1/1	0.28	4.45	45,45,45,45	0
87	OHX	5	4246	7/7	0.21	4.45	129,129,129,129	0
87	OHX	6	2192	7/7	0.27	4.45	141,141,141,141	0
87	OHX	5	4144	7/7	0.27	4.44	103,103,103,103	0
86	MG	1	3438	1/1	0.21	4.42	41,41,41,41	0
86	MG	5	3616	1/1	0.22	4.40	29,29,29,29	0
87	OHX	6	2170	7/7	0.21	4.40	132,132,132,132	0
87	OHX	6	2135	7/7	0.21	4.36	111,111,111,111	0
87	OHX	6	2200	7/7	0.26	4.36	126,126,126,126	0
87	OHX	2	2112	7/7	0.31	4.35	120,120,120,120	0
87	OHX	5	4156	7/7	0.24	4.34	116,116,116,116	0
87	OHX	2	2153	7/7	0.24	4.32	129,129,129,129	0
86	MG	1	3712	1/1	0.31	4.31	46,46,46,46	0
86	MG	2	1930	1/1	0.22	4.31	54,54,54,54	0
86	MG	5	3852	1/1	0.22	4.29	65,65,65,65	0
86	MG	1	3660	1/1	0.23	4.29	38,38,38,38	0
86	MG	M3	203	1/1	0.45	4.28	94,94,94,94	0
86	MG	6	1941	1/1	0.24	4.28	45,45,45,45	0
87	OHX	1	3870	7/7	0.21	4.28	55,55,55,55	0
86	MG	O3	201	1/1	0.22	4.27	33,33,33,33	0
87	OHX	5	4191	7/7	0.19	4.23	111,111,111,111	0
86	MG	5	3897	1/1	0.19	4.23	53,53,53,53	0
86	MG	2	1999	1/1	0.17	4.23	66,66,66,66	0
86	MG	5	3846	1/1	0.22	4.21	28,28,28,28	0
87	OHX	5	4240	7/7	0.29	4.19	174,174,174,174	0
87	OHX	1	4214	7/7	0.26	4.18	132,132,132,132	0
86	MG	2	2009	1/1	0.24	4.15	68,68,68,68	0
87	OHX	5	3952	7/7	0.21	4.14	101,101,101,101	0
86	MG	1	3759	1/1	0.16	4.14	36,36,36,36	0
86	MG	5	3865	1/1	0.19	4.13	35,35,35,35	0
87	OHX	5	4158	7/7	0.25	4.10	117,117,117,117	0
86	MG	5	3670	1/1	0.20	4.10	33,33,33,33	0
87	OHX	6	2196	7/7	0.26	4.09	151,151,151,151	0
86	MG	5	3781	1/1	0.20	4.04	44,44,44,44	0
86	MG	1	3474	1/1	0.19	4.02	70,70,70,70	0
86	MG	5	3878	1/1	0.23	4.02	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	2	2074	7/7	0.22	4.01	126,126,126,126	0
86	MG	5	3770	1/1	0.32	4.01	43,43,43,43	0
86	MG	6	1902	1/1	0.23	4.00	50,50,50,50	0
86	MG	1	3630	1/1	0.23	3.99	34,34,34,34	0
87	OHX	2	2115	7/7	0.32	3.98	121,121,121,121	0
86	MG	L3	401	1/1	0.23	3.98	31,31,31,31	0
86	MG	5	3896	1/1	0.24	3.97	50,50,50,50	0
87	OHX	6	2195	7/7	0.22	3.97	161,161,161,161	0
86	MG	5	3710	1/1	0.25	3.96	47,47,47,47	0
86	MG	1	3846	1/1	0.26	3.96	45,45,45,45	0
87	OHX	5	4174	7/7	0.26	3.96	116,116,116,116	0
87	OHX	6	2162	7/7	0.25	3.95	110,110,110,110	0
87	OHX	1	4133	7/7	0.31	3.95	114,114,114,114	0
86	MG	M1	201	1/1	0.28	3.94	68,68,68,68	0
86	MG	5	3765	1/1	0.21	3.94	31,31,31,31	0
86	MG	2	1981	1/1	0.19	3.93	74,74,74,74	0
87	OHX	6	2185	7/7	0.22	3.93	122,122,122,122	0
87	OHX	3	225	7/7	0.19	3.92	127,127,127,127	0
86	MG	2	1961	1/1	0.25	3.90	50,50,50,50	0
87	OHX	2	2151	7/7	0.24	3.89	131,131,131,131	0
87	OHX	8	220	7/7	0.21	3.89	105,105,105,105	0
87	OHX	1	4111	7/7	0.23	3.89	117,117,117,117	0
87	OHX	5	4247	7/7	0.29	3.88	125,125,125,125	0
87	OHX	2	2144	7/7	0.28	3.88	127,127,127,127	0
86	MG	5	3659	1/1	0.22	3.88	42,42,42,42	0
87	OHX	4	229	7/7	0.23	3.86	94,94,94,94	0
86	MG	6	2020	1/1	0.20	3.86	107,107,107,107	0
86	MG	1	3442	1/1	0.23	3.84	22,22,22,22	0
86	MG	5	3567	1/1	0.38	3.83	42,42,42,42	0
87	OHX	5	4233	7/7	0.26	3.83	106,106,106,106	0
87	OHX	2	2172	7/7	0.27	3.82	129,129,129,129	0
86	MG	1	3804	1/1	0.20	3.80	33,33,33,33	0
87	OHX	1	4164	7/7	0.20	3.80	112,112,112,112	0
86	MG	s6	301	1/1	0.33	3.79	65,65,65,65	0
86	MG	1	3618	1/1	0.21	3.77	54,54,54,54	0
86	MG	5	3783	1/1	0.22	3.76	69,69,69,69	0
86	MG	1	3783	1/1	0.20	3.75	45,45,45,45	0
86	MG	1	3652	1/1	0.39	3.74	87,87,87,87	0
86	MG	2	1902	1/1	0.22	3.73	41,41,41,41	0
87	OHX	5	4045	7/7	0.20	3.72	87,87,87,87	0
87	OHX	5	4166	7/7	0.21	3.70	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	5	3905	7/7	0.20	3.70	50,50,50,50	0
86	MG	5	3675	1/1	0.22	3.68	63,63,63,63	0
87	OHX	2	2090	7/7	0.18	3.68	115,115,115,115	0
86	MG	6	1992	1/1	0.19	3.68	62,62,62,62	0
86	MG	6	2013	1/1	0.18	3.67	57,57,57,57	0
87	OHX	1	4154	7/7	0.32	3.65	114,114,114,114	0
86	MG	5	3731	1/1	0.24	3.65	24,24,24,24	0
87	OHX	1	4104	7/7	0.20	3.64	108,108,108,108	0
87	OHX	3	223	7/7	0.17	3.62	154,154,154,154	0
86	MG	5	3759	1/1	0.38	3.62	68,68,68,68	0
87	OHX	6	2199	7/7	0.28	3.60	129,129,129,129	0
86	MG	4	203	1/1	0.36	3.60	45,45,45,45	0
86	MG	5	3805	1/1	0.20	3.59	145,145,145,145	0
86	MG	5	3858	1/1	0.25	3.59	43,43,43,43	0
86	MG	O1	201	1/1	0.24	3.59	59,59,59,59	0
86	MG	5	3665	1/1	0.21	3.57	57,57,57,57	0
87	OHX	6	2137	7/7	0.23	3.57	117,117,117,117	0
86	MG	1	3555	1/1	0.30	3.56	28,28,28,28	0
86	MG	6	2031	1/1	0.23	3.56	64,64,64,64	0
86	MG	L5	301	1/1	0.35	3.55	57,57,57,57	0
86	MG	n8	202	1/1	0.23	3.55	40,40,40,40	0
86	MG	5	3802	1/1	0.19	3.55	29,29,29,29	0
87	OHX	5	4083	7/7	0.24	3.55	98,98,98,98	0
87	OHX	2	2063	7/7	0.19	3.54	97,97,97,97	0
86	MG	n0	201	1/1	0.35	3.53	38,38,38,38	0
86	MG	5	3471	1/1	0.20	3.53	106,106,106,106	0
86	MG	1	3413	1/1	0.23	3.48	58,58,58,58	0
86	MG	7	206	1/1	0.19	3.47	40,40,40,40	0
86	MG	5	3542	1/1	0.35	3.47	27,27,27,27	0
86	MG	5	3546	1/1	0.21	3.45	28,28,28,28	0
87	OHX	6	2198	7/7	0.27	3.43	124,124,124,124	0
87	OHX	2	2118	7/7	0.21	3.42	120,120,120,120	0
86	MG	1	3603	1/1	0.23	3.39	25,25,25,25	0
86	MG	2	1978	1/1	0.30	3.38	51,51,51,51	0
86	MG	2	1995	1/1	0.29	3.36	87,87,87,87	0
86	MG	6	1986	1/1	0.22	3.36	74,74,74,74	0
87	OHX	1	4121	7/7	0.24	3.35	128,128,128,128	0
86	MG	5	3629	1/1	0.23	3.35	53,53,53,53	0
87	OHX	2	2073	7/7	0.29	3.34	107,107,107,107	0
86	MG	2	1991	1/1	0.34	3.34	51,51,51,51	0
86	MG	5	3425	1/1	0.21	3.32	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2024	7/7	0.20	3.30	75,75,75,75	0
87	OHX	2	2175	7/7	0.18	3.29	127,127,127,127	0
86	MG	5	3668	1/1	0.22	3.29	25,25,25,25	0
86	MG	m7	202	1/1	0.29	3.28	29,29,29,29	0
87	OHX	5	3901	7/7	0.20	3.27	39,39,39,39	0
86	MG	6	1954	1/1	0.28	3.27	39,39,39,39	0
86	MG	2	1936	1/1	0.28	3.26	50,50,50,50	0
87	OHX	2	2159	7/7	0.43	3.25	121,121,121,121	0
86	MG	5	3601	1/1	0.23	3.24	38,38,38,38	0
87	OHX	5	4087	7/7	0.18	3.23	115,115,115,115	0
86	MG	1	3669	1/1	0.19	3.23	40,40,40,40	0
86	MG	1	3733	1/1	0.19	3.22	60,60,60,60	0
87	OHX	6	2053	7/7	0.17	3.22	68,68,68,68	0
87	OHX	6	2171	7/7	0.20	3.21	131,131,131,131	0
86	MG	2	2002	1/1	0.23	3.21	74,74,74,74	0
86	MG	1	3765	1/1	0.20	3.21	32,32,32,32	0
87	OHX	1	4066	7/7	0.23	3.19	102,102,102,102	0
87	OHX	5	4250	7/7	0.28	3.16	120,120,120,120	0
87	OHX	1	4162	7/7	0.24	3.16	136,136,136,136	0
87	OHX	m8	201	7/7	0.29	3.16	121,121,121,121	0
86	MG	2	1905	1/1	0.27	3.14	55,55,55,55	0
87	OHX	5	4244	7/7	0.27	3.13	124,124,124,124	0
86	MG	5	3465	1/1	0.23	3.13	48,48,48,48	0
86	MG	1	3426	1/1	0.20	3.12	53,53,53,53	0
87	OHX	1	4157	7/7	0.22	3.12	126,126,126,126	0
87	OHX	6	2169	7/7	0.25	3.11	108,108,108,108	0
87	OHX	1	4122	7/7	0.20	3.10	97,97,97,97	0
87	OHX	1	4211	7/7	0.21	3.09	113,113,113,113	0
86	MG	1	3585	1/1	0.22	3.09	35,35,35,35	0
86	MG	1	3437	1/1	0.22	3.08	26,26,26,26	0
86	MG	5	3462	1/1	0.21	3.05	28,28,28,28	0
87	OHX	2	2127	7/7	0.23	3.04	133,133,133,133	0
86	MG	1	3650	1/1	0.20	3.03	39,39,39,39	0
87	OHX	1	4120	7/7	0.21	3.03	119,119,119,119	0
86	MG	1	3860	1/1	0.23	3.02	37,37,37,37	0
86	MG	1	3700	1/1	0.20	3.02	37,37,37,37	0
87	OHX	5	4205	7/7	0.32	3.02	120,120,120,120	0
86	MG	1	3483	1/1	0.19	3.02	36,36,36,36	0
86	MG	5	3452	1/1	0.26	3.02	25,25,25,25	0
86	MG	5	3441	1/1	0.20	3.01	26,26,26,26	0
87	OHX	5	4093	7/7	0.25	3.01	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4180	7/7	0.32	3.00	123,123,123,123	0
86	MG	2	1903	1/1	0.27	2.99	40,40,40,40	0
86	MG	5	4258	1/1	0.21	2.98	33,33,33,33	0
87	OHX	1	3903	7/7	0.17	2.98	75,75,75,75	0
86	MG	1	4222	1/1	0.23	2.97	25,25,25,25	0
86	MG	5	3760	1/1	0.23	2.97	58,58,58,58	0
87	OHX	2	2022	7/7	0.17	2.97	68,68,68,68	0
87	OHX	1	3872	7/7	0.20	2.97	56,56,56,56	0
86	MG	1	3447	1/1	0.23	2.95	31,31,31,31	0
86	MG	1	3568	1/1	0.31	2.94	22,22,22,22	0
86	MG	5	3864	1/1	0.15	2.94	35,35,35,35	0
87	OHX	1	3977	7/7	0.21	2.93	78,78,78,78	0
87	OHX	5	4172	7/7	0.25	2.92	88,88,88,88	0
87	OHX	1	4160	7/7	0.19	2.92	137,137,137,137	0
86	MG	1	3762	1/1	0.19	2.92	43,43,43,43	0
87	OHX	1	4081	7/7	0.17	2.89	124,124,124,124	0
86	MG	5	3823	1/1	0.35	2.89	86,86,86,86	0
86	MG	5	3416	1/1	0.21	2.88	29,29,29,29	0
86	MG	1	3507	1/1	0.25	2.87	28,28,28,28	0
86	MG	1	3421	1/1	0.32	2.87	36,36,36,36	0
86	MG	1	3690	1/1	0.21	2.87	53,53,53,53	0
86	MG	N8	202	1/1	0.22	2.86	20,20,20,20	0
86	MG	5	3479	1/1	0.22	2.85	22,22,22,22	0
86	MG	1	3492	1/1	0.25	2.83	58,58,58,58	0
87	OHX	6	2159	7/7	0.20	2.82	120,120,120,120	0
86	MG	M7	202	1/1	0.27	2.81	30,30,30,30	0
86	MG	5	3481	1/1	0.32	2.80	57,57,57,57	0
87	OHX	5	4113	7/7	0.23	2.79	92,92,92,92	0
86	MG	5	3825	1/1	0.19	2.78	37,37,37,37	0
87	OHX	6	2189	7/7	0.25	2.76	127,127,127,127	0
86	MG	5	3692	1/1	0.22	2.75	35,35,35,35	0
86	MG	1	3645	1/1	0.24	2.75	59,59,59,59	0
87	OHX	5	4040	7/7	0.25	2.74	78,78,78,78	0
87	OHX	l5	305	7/7	0.30	2.72	125,125,125,125	0
87	OHX	2	2107	7/7	0.19	2.72	125,125,125,125	0
86	MG	c8	201	1/1	0.31	2.71	59,59,59,59	0
87	OHX	2	2111	7/7	0.20	2.71	142,142,142,142	0
86	MG	1	3463	1/1	0.15	2.71	34,34,34,34	0
86	MG	5	3704	1/1	0.46	2.70	59,59,59,59	0
87	OHX	5	3913	7/7	0.17	2.70	57,57,57,57	0
86	MG	5	3426	1/1	0.20	2.69	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	MG	6	2017	1/1	0.29	2.69	39,39,39,39	0
87	OHX	2	2136	7/7	0.19	2.68	147,147,147,147	0
87	OHX	5	4196	7/7	0.21	2.67	132,132,132,132	0
87	OHX	2	2098	7/7	0.19	2.66	103,103,103,103	0
86	MG	1	3632	1/1	0.29	2.64	63,63,63,63	0
87	OHX	1	3864	7/7	0.19	2.64	38,38,38,38	0
87	OHX	5	4193	7/7	0.29	2.64	109,109,109,109	0
87	OHX	5	4100	7/7	0.17	2.63	112,112,112,112	0
86	MG	5	3725	1/1	0.29	2.63	51,51,51,51	0
87	OHX	2	2039	7/7	0.17	2.61	96,96,96,96	0
86	MG	1	3808	1/1	0.22	2.60	30,30,30,30	0
87	OHX	s9	201	7/7	0.35	2.59	110,110,110,110	0
86	MG	2	1954	1/1	0.18	2.58	89,89,89,89	0
86	MG	6	2012	1/1	0.21	2.57	45,45,45,45	0
87	OHX	2	2083	7/7	0.19	2.56	108,108,108,108	0
87	OHX	5	4147	7/7	0.19	2.55	103,103,103,103	0
86	MG	6	1974	1/1	0.19	2.55	54,54,54,54	0
86	MG	5	3763	1/1	0.20	2.55	71,71,71,71	0
86	MG	2	2010	1/1	0.19	2.54	64,64,64,64	0
87	OHX	2	2122	7/7	0.16	2.54	122,122,122,122	0
87	OHX	1	4191	7/7	0.23	2.53	126,126,126,126	0
87	OHX	1	4132	7/7	0.23	2.53	105,105,105,105	0
87	OHX	1	4042	7/7	0.21	2.53	87,87,87,87	0
87	OHX	2	2174	7/7	0.35	2.52	141,141,141,141	0
86	MG	5	3851	1/1	0.18	2.51	43,43,43,43	0
86	MG	1	3520	1/1	0.21	2.51	26,26,26,26	0
86	MG	1	3464	1/1	0.19	2.50	47,47,47,47	0
86	MG	7	204	1/1	0.21	2.47	67,67,67,67	0
86	MG	5	3651	1/1	0.19	2.47	81,81,81,81	0
86	MG	5	3467	1/1	0.16	2.46	56,56,56,56	0
87	OHX	4	235	7/7	0.26	2.46	128,128,128,128	0
86	MG	1	3619	1/1	0.25	2.45	55,55,55,55	0
86	MG	7	213	1/1	0.18	2.45	58,58,58,58	0
86	MG	5	3694	1/1	0.22	2.44	40,40,40,40	0
87	OHX	5	4063	7/7	0.20	2.44	111,111,111,111	0
86	MG	1	3686	1/1	0.24	2.44	44,44,44,44	0
87	OHX	7	223	7/7	0.19	2.43	109,109,109,109	0
86	MG	1	3623	1/1	0.21	2.43	43,43,43,43	0
86	MG	1	3747	1/1	0.23	2.42	49,49,49,49	0
86	MG	m7	203	1/1	0.29	2.40	44,44,44,44	0
86	MG	l8	301	1/1	0.33	2.39	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3473	1/1	0.20	2.39	42,42,42,42	0
86	MG	c7	202	1/1	0.28	2.39	70,70,70,70	0
87	OHX	5	4054	7/7	0.20	2.38	95,95,95,95	0
87	OHX	1	4148	7/7	0.20	2.37	127,127,127,127	0
87	OHX	5	4133	7/7	0.19	2.37	110,110,110,110	0
86	MG	5	3719	1/1	0.24	2.37	59,59,59,59	0
87	OHX	5	4212	7/7	0.19	2.37	131,131,131,131	0
87	OHX	1	4098	7/7	0.20	2.35	100,100,100,100	0
87	OHX	1	4179	7/7	0.41	2.35	119,119,119,119	0
86	MG	5	3589	1/1	0.22	2.34	62,62,62,62	0
87	OHX	6	2116	7/7	0.21	2.33	110,110,110,110	0
86	MG	1	3703	1/1	0.17	2.33	46,46,46,46	0
87	OHX	6	2118	7/7	0.18	2.32	115,115,115,115	0
86	MG	2	1951	1/1	0.35	2.32	80,80,80,80	0
87	OHX	5	4077	7/7	0.30	2.32	109,109,109,109	0
87	OHX	s4	301	7/7	0.23	2.30	130,130,130,130	0
87	OHX	1	4149	7/7	0.20	2.30	131,131,131,131	0
86	MG	1	3642	1/1	0.21	2.30	36,36,36,36	0
86	MG	1	3620	1/1	0.18	2.29	54,54,54,54	0
86	MG	1	3752	1/1	0.21	2.29	50,50,50,50	0
86	MG	M7	203	1/1	0.25	2.27	30,30,30,30	0
87	OHX	2	2121	7/7	0.23	2.26	129,129,129,129	0
86	MG	1	3850	1/1	0.20	2.25	45,45,45,45	0
86	MG	1	3420	1/1	0.42	2.25	56,56,56,56	0
87	OHX	1	4097	7/7	0.18	2.25	133,133,133,133	0
87	OHX	1	4109	7/7	0.21	2.25	120,120,120,120	0
86	MG	8	212	1/1	0.18	2.25	56,56,56,56	0
87	OHX	6	2134	7/7	0.20	2.24	136,136,136,136	0
86	MG	M0	301	1/1	0.25	2.24	33,33,33,33	0
87	OHX	6	2051	7/7	0.18	2.23	66,66,66,66	0
86	MG	6	1967	1/1	0.23	2.23	62,62,62,62	0
87	OHX	5	4124	7/7	0.20	2.22	127,127,127,127	0
87	OHX	1	4129	7/7	0.20	2.21	144,144,144,144	0
87	OHX	5	4221	7/7	0.31	2.20	141,141,141,141	0
86	MG	6	1952	1/1	0.32	2.19	53,53,53,53	0
87	OHX	6	2092	7/7	0.20	2.19	108,108,108,108	0
86	MG	2	1947	1/1	0.38	2.18	61,61,61,61	0
87	OHX	1	3881	7/7	0.18	2.17	62,62,62,62	0
87	OHX	m7	205	7/7	0.35	2.16	111,111,111,111	0
89	3HE	5	4252	20/20	0.23	2.16	32,32,32,32	0
86	MG	1	3834	1/1	0.33	2.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	5	3653	1/1	0.20	2.15	24,24,24,24	0
86	MG	2	1923	1/1	0.20	2.15	52,52,52,52	0
87	OHX	1	3908	7/7	0.20	2.14	80,80,80,80	0
86	MG	q0	202	1/1	0.21	2.13	38,38,38,38	0
86	MG	5	3814	1/1	0.30	2.12	52,52,52,52	0
87	OHX	6	2141	7/7	0.19	2.12	120,120,120,120	0
87	OHX	5	4141	7/7	0.25	2.11	117,117,117,117	0
86	MG	5	3742	1/1	0.19	2.10	52,52,52,52	0
86	MG	5	3401	1/1	0.21	2.09	41,41,41,41	0
87	OHX	6	2145	7/7	0.22	2.09	117,117,117,117	0
86	MG	5	3638	1/1	0.23	2.07	43,43,43,43	0
87	OHX	1	4033	7/7	0.19	2.06	100,100,100,100	0
86	MG	5	3632	1/1	0.23	2.06	34,34,34,34	0
87	OHX	1	4147	7/7	0.19	2.06	128,128,128,128	0
86	MG	5	3792	1/1	0.19	2.05	34,34,34,34	0
86	MG	l5	302	1/1	0.28	2.05	56,56,56,56	0
86	MG	7	207	1/1	0.19	2.05	47,47,47,47	0
87	OHX	L3	404	7/7	0.24	2.04	103,103,103,103	0
87	OHX	1	3865	7/7	0.18	2.04	45,45,45,45	0
87	OHX	1	4181	7/7	0.20	2.03	94,94,94,94	0
87	OHX	5	3902	7/7	0.19	2.03	39,39,39,39	0
87	OHX	1	3877	7/7	0.17	2.03	59,59,59,59	0
86	MG	1	3746	1/1	0.18	2.00	33,33,33,33	0
86	MG	5	3824	1/1	0.19	1.98	55,55,55,55	0
87	OHX	2	2138	7/7	0.20	1.96	137,137,137,137	0
86	MG	1	3494	1/1	0.17	1.95	35,35,35,35	0
87	OHX	5	4089	7/7	0.18	1.95	98,98,98,98	0
86	MG	1	3583	1/1	0.31	1.95	34,34,34,34	0
86	MG	5	3436	1/1	0.20	1.95	27,27,27,27	0
86	MG	1	3546	1/1	0.20	1.95	49,49,49,49	0
87	OHX	6	2149	7/7	0.18	1.94	123,123,123,123	0
87	OHX	5	4206	7/7	0.38	1.93	126,126,126,126	0
87	OHX	2	2165	7/7	0.28	1.93	144,144,144,144	0
87	OHX	5	4075	7/7	0.20	1.93	107,107,107,107	0
86	MG	6	1957	1/1	0.46	1.91	53,53,53,53	0
86	MG	5	3460	1/1	0.19	1.90	60,60,60,60	0
86	MG	M7	201	1/1	0.37	1.90	65,65,65,65	0
87	OHX	d4	202	7/7	0.22	1.90	131,131,131,131	0
86	MG	5	3454	1/1	0.16	1.89	38,38,38,38	0
87	OHX	1	4071	7/7	0.17	1.88	125,125,125,125	0
87	OHX	6	2194	7/7	0.33	1.87	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2010	1/1	0.20	1.87	46,46,46,46	0
86	MG	1	3722	1/1	0.18	1.87	44,44,44,44	0
87	OHX	M7	208	7/7	0.36	1.85	125,125,125,125	0
86	MG	1	3839	1/1	0.20	1.84	55,55,55,55	0
87	OHX	6	2197	7/7	0.20	1.84	153,153,153,153	0
86	MG	1	3774	1/1	0.20	1.84	38,38,38,38	0
87	OHX	5	3903	7/7	0.18	1.82	44,44,44,44	0
86	MG	1	3802	1/1	0.26	1.81	54,54,54,54	0
87	OHX	6	2153	7/7	0.19	1.80	135,135,135,135	0
86	MG	2	2180	1/1	0.18	1.80	81,81,81,81	0
86	MG	1	3773	1/1	0.17	1.79	48,48,48,48	0
87	OHX	4	224	7/7	0.18	1.77	57,57,57,57	0
87	OHX	1	3868	7/7	0.20	1.77	51,51,51,51	0
86	MG	1	4216	1/1	0.22	1.77	23,23,23,23	0
87	OHX	2	2146	7/7	0.19	1.75	155,155,155,155	0
87	OHX	5	4243	7/7	0.17	1.75	141,141,141,141	0
86	MG	1	3637	1/1	0.23	1.75	44,44,44,44	0
87	OHX	1	4046	7/7	0.20	1.74	102,102,102,102	0
87	OHX	8	226	7/7	0.19	1.74	129,129,129,129	0
87	OHX	7	224	7/7	0.19	1.74	102,102,102,102	0
86	MG	5	3679	1/1	0.18	1.74	83,83,83,83	0
86	MG	6	1973	1/1	0.20	1.73	45,45,45,45	0
87	OHX	1	4140	7/7	0.18	1.72	114,114,114,114	0
86	MG	6	1976	1/1	0.17	1.72	52,52,52,52	0
87	OHX	1	4005	7/7	0.18	1.72	101,101,101,101	0
86	MG	5	3503	1/1	0.17	1.70	35,35,35,35	0
86	MG	5	3606	1/1	0.19	1.70	34,34,34,34	0
87	OHX	1	4083	7/7	0.17	1.70	123,123,123,123	0
87	OHX	5	4189	7/7	0.23	1.68	108,108,108,108	0
86	MG	SM	301	1/1	0.18	1.68	44,44,44,44	0
86	MG	2	1901	1/1	0.40	1.68	72,72,72,72	0
87	OHX	1	3926	7/7	0.18	1.65	88,88,88,88	0
87	OHX	6	2128	7/7	0.19	1.64	110,110,110,110	0
87	OHX	5	3915	7/7	0.18	1.64	62,62,62,62	0
86	MG	o4	201	1/1	0.24	1.64	58,58,58,58	0
89	3HE	1	4215	20/20	0.23	1.64	27,27,27,27	0
87	OHX	5	3927	7/7	0.20	1.59	66,66,66,66	0
87	OHX	5	4227	7/7	0.30	1.57	144,144,144,144	0
87	OHX	5	4137	7/7	0.44	1.57	113,113,113,113	0
87	OHX	1	4187	7/7	0.22	1.56	123,123,123,123	0
87	OHX	1	3886	7/7	0.17	1.56	70,70,70,70	0
86	MG	1	3716	1/1	0.38	1.56	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3655	1/1	0.18	1.54	28,28,28,28	0
86	MG	1	3786	1/1	0.16	1.54	34,34,34,34	0
86	MG	5	3633	1/1	0.20	1.54	44,44,44,44	0
87	OHX	7	225	7/7	0.19	1.54	128,128,128,128	0
87	OHX	1	3878	7/7	0.18	1.53	58,58,58,58	0
86	MG	5	3548	1/1	0.23	1.50	46,46,46,46	0
87	OHX	1	4082	7/7	0.19	1.50	112,112,112,112	0
87	OHX	5	4171	7/7	0.22	1.49	146,146,146,146	0
86	MG	7	210	1/1	0.20	1.49	55,55,55,55	0
86	MG	5	3745	1/1	0.18	1.48	32,32,32,32	0
87	OHX	1	4088	7/7	0.24	1.48	89,89,89,89	0
86	MG	5	3840	1/1	0.15	1.48	55,55,55,55	0
86	MG	1	3683	1/1	0.15	1.47	38,38,38,38	0
87	OHX	2	2023	7/7	0.17	1.47	74,74,74,74	0
87	OHX	1	3873	7/7	0.18	1.46	57,57,57,57	0
87	OHX	5	3914	7/7	0.18	1.46	63,63,63,63	0
87	OHX	5	4082	7/7	0.21	1.45	97,97,97,97	0
86	MG	2	1944	1/1	0.17	1.45	58,58,58,58	0
87	OHX	5	4164	7/7	0.18	1.44	130,130,130,130	0
87	OHX	1	3866	7/7	0.18	1.44	42,42,42,42	0
86	MG	2	1966	1/1	0.18	1.44	77,77,77,77	0
86	MG	L8	301	1/1	0.37	1.44	57,57,57,57	0
87	OHX	2	2108	7/7	0.15	1.44	135,135,135,135	0
86	MG	1	3403	1/1	0.19	1.42	32,32,32,32	0
86	MG	5	3529	1/1	0.28	1.42	50,50,50,50	0
87	OHX	6	2186	7/7	0.15	1.42	154,154,154,154	0
87	OHX	6	2114	7/7	0.18	1.40	97,97,97,97	0
86	MG	5	3483	1/1	0.21	1.40	34,34,34,34	0
87	OHX	o9	101	7/7	0.38	1.40	99,99,99,99	0
87	OHX	1	4198	7/7	0.32	1.39	127,127,127,127	0
86	MG	1	3636	1/1	0.34	1.39	55,55,55,55	0
86	MG	5	3404	1/1	0.18	1.38	37,37,37,37	0
86	MG	1	3744	1/1	0.17	1.38	53,53,53,53	0
86	MG	2	1916	1/1	0.24	1.38	48,48,48,48	0
86	MG	1	3411	1/1	0.18	1.37	35,35,35,35	0
87	OHX	1	4035	7/7	0.18	1.37	110,110,110,110	0
86	MG	6	1913	1/1	0.36	1.36	48,48,48,48	0
87	OHX	1	4130	7/7	0.21	1.36	138,138,138,138	0
86	MG	4	205	1/1	0.33	1.36	69,69,69,69	0
86	MG	5	3535	1/1	0.17	1.35	44,44,44,44	0
87	OHX	2	2133	7/7	0.23	1.34	120,120,120,120	0
87	OHX	1	4151	7/7	0.20	1.34	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	n6	201	1/1	0.26	1.33	57,57,57,57	0
87	OHX	5	4232	7/7	0.16	1.33	157,157,157,157	0
87	OHX	2	2173	7/7	0.21	1.32	135,135,135,135	0
87	OHX	5	4200	7/7	0.24	1.31	109,109,109,109	0
87	OHX	6	2157	7/7	0.25	1.31	130,130,130,130	0
86	MG	6	2021	1/1	0.17	1.31	76,76,76,76	0
86	MG	1	3448	1/1	0.18	1.29	37,37,37,37	0
87	OHX	5	4251	7/7	0.20	1.28	142,142,142,142	0
87	OHX	5	4163	7/7	0.19	1.28	103,103,103,103	0
86	MG	1	3768	1/1	0.20	1.27	58,58,58,58	0
87	OHX	5	4143	7/7	0.18	1.26	116,116,116,116	0
87	OHX	5	3908	7/7	0.17	1.26	49,49,49,49	0
86	MG	1	3433	1/1	0.20	1.26	31,31,31,31	0
87	OHX	2	2114	7/7	0.23	1.25	111,111,111,111	0
86	MG	6	2025	1/1	0.16	1.25	59,59,59,59	0
87	OHX	1	4194	7/7	0.39	1.24	125,125,125,125	0
86	MG	5	3423	1/1	0.19	1.24	36,36,36,36	0
86	MG	1	3794	1/1	0.17	1.23	44,44,44,44	0
87	OHX	2	2126	7/7	0.34	1.23	118,118,118,118	0
87	OHX	5	4091	7/7	0.23	1.23	100,100,100,100	0
86	MG	5	3800	1/1	0.25	1.22	66,66,66,66	0
87	OHX	5	3940	7/7	0.18	1.22	80,80,80,80	0
86	MG	1	3469	1/1	0.18	1.21	43,43,43,43	0
86	MG	5	3791	1/1	0.20	1.20	48,48,48,48	0
87	OHX	5	4238	7/7	0.14	1.20	130,130,130,130	0
87	OHX	8	215	7/7	0.18	1.20	55,55,55,55	0
87	OHX	6	2151	7/7	0.19	1.20	125,125,125,125	0
87	OHX	2	2139	7/7	0.16	1.19	148,148,148,148	0
86	MG	5	3453	1/1	0.21	1.19	29,29,29,29	0
87	OHX	5	4165	7/7	0.18	1.18	159,159,159,159	0
86	MG	6	2005	1/1	0.18	1.18	81,81,81,81	0
87	OHX	6	2201	7/7	0.18	1.18	129,129,129,129	0
86	MG	1	3672	1/1	0.17	1.18	38,38,38,38	0
86	MG	L7	301	1/1	0.21	1.18	37,37,37,37	0
87	OHX	6	2055	7/7	0.17	1.17	75,75,75,75	0
86	MG	2	2004	1/1	0.24	1.17	55,55,55,55	0
87	OHX	6	2176	7/7	0.31	1.17	136,136,136,136	0
87	OHX	1	3918	7/7	0.16	1.16	107,107,107,107	0
87	OHX	5	4121	7/7	0.26	1.14	133,133,133,133	0
87	OHX	1	4183	7/7	0.17	1.12	131,131,131,131	0
87	OHX	2	2167	7/7	0.23	1.12	108,108,108,108	0
87	OHX	6	2174	7/7	0.26	1.12	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3825	1/1	0.17	1.12	19,19,19,19	0
87	OHX	1	4145	7/7	0.17	1.11	132,132,132,132	0
86	MG	5	3642	1/1	0.20	1.11	50,50,50,50	0
87	OHX	1	4030	7/7	0.19	1.11	98,98,98,98	0
87	OHX	1	4126	7/7	0.16	1.09	132,132,132,132	0
86	MG	5	3794	1/1	0.18	1.09	40,40,40,40	0
86	MG	6	1999	1/1	0.22	1.09	54,54,54,54	0
87	OHX	2	2091	7/7	0.22	1.07	103,103,103,103	0
87	OHX	5	3900	7/7	0.20	1.06	42,42,42,42	0
86	MG	1	3610	1/1	0.26	1.06	59,59,59,59	0
87	OHX	1	4134	7/7	0.19	1.05	105,105,105,105	0
86	MG	n8	203	1/1	0.20	1.03	42,42,42,42	0
87	OHX	5	3924	7/7	0.17	1.02	65,65,65,65	0
86	MG	5	3797	1/1	0.17	1.01	52,52,52,52	0
86	MG	2	1979	1/1	0.19	1.01	62,62,62,62	0
87	OHX	2	2085	7/7	0.17	1.00	104,104,104,104	0
87	OHX	8	229	7/7	0.25	1.00	121,121,121,121	0
87	OHX	1	4090	7/7	0.19	0.99	137,137,137,137	0
87	OHX	5	4211	7/7	0.21	0.99	122,122,122,122	0
87	OHX	5	4106	7/7	0.18	0.99	99,99,99,99	0
86	MG	c4	201	1/1	0.24	0.98	52,52,52,52	0
87	OHX	6	2078	7/7	0.17	0.98	99,99,99,99	0
86	MG	8	205	1/1	0.18	0.98	67,67,67,67	0
86	MG	2	2014	1/1	0.35	0.98	56,56,56,56	0
86	MG	5	3625	1/1	0.16	0.97	55,55,55,55	0
86	MG	5	3722	1/1	0.18	0.97	45,45,45,45	0
86	MG	5	3891	1/1	0.17	0.95	35,35,35,35	0
86	MG	6	1965	1/1	0.17	0.94	63,63,63,63	0
87	OHX	5	4169	7/7	0.19	0.93	122,122,122,122	0
87	OHX	2	2077	7/7	0.20	0.93	116,116,116,116	0
86	MG	5	3427	1/1	0.24	0.90	34,34,34,34	0
87	OHX	2	2128	7/7	0.14	0.89	171,171,171,171	0
86	MG	1	3822	1/1	0.16	0.88	38,38,38,38	0
87	OHX	6	2152	7/7	0.23	0.88	101,101,101,101	0
87	OHX	1	4019	7/7	0.19	0.88	103,103,103,103	0
87	OHX	1	4084	7/7	0.18	0.84	116,116,116,116	0
86	MG	8	209	1/1	0.17	0.83	62,62,62,62	0
87	OHX	5	4109	7/7	0.18	0.83	109,109,109,109	0
86	MG	2	1970	1/1	0.20	0.82	63,63,63,63	0
87	OHX	6	2050	7/7	0.18	0.82	64,64,64,64	0
86	MG	5	3873	1/1	0.20	0.81	38,38,38,38	0
86	MG	l5	301	1/1	0.24	0.81	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
86	MG	5	3746	1/1	0.18	0.81	36,36,36,36	0
87	OHX	8	214	7/7	0.18	0.80	53,53,53,53	0
86	MG	5	3686	1/1	0.17	0.80	46,46,46,46	0
87	OHX	1	4099	7/7	0.21	0.80	105,105,105,105	0
86	MG	5	3712	1/1	0.16	0.79	44,44,44,44	0
86	MG	5	3446	1/1	0.17	0.79	27,27,27,27	0
86	MG	2	1969	1/1	0.23	0.79	65,65,65,65	0
87	OHX	2	2033	7/7	0.16	0.79	93,93,93,93	0
86	MG	1	3695	1/1	0.18	0.78	40,40,40,40	0
86	MG	5	3442	1/1	0.21	0.78	36,36,36,36	0
87	OHX	1	4079	7/7	0.24	0.78	112,112,112,112	0
86	MG	1	3475	1/1	0.18	0.78	25,25,25,25	0
87	OHX	2	2119	7/7	0.19	0.78	121,121,121,121	0
87	OHX	5	3933	7/7	0.17	0.78	83,83,83,83	0
86	MG	1	3440	1/1	0.21	0.77	38,38,38,38	0
87	OHX	5	4076	7/7	0.18	0.76	104,104,104,104	0
88	ZN	q2	501	1/1	0.26	0.76	77,77,77,77	0
87	OHX	5	3945	7/7	0.15	0.75	80,80,80,80	0
87	OHX	6	2049	7/7	0.17	0.74	60,60,60,60	0
87	OHX	1	4206	7/7	0.24	0.74	123,123,123,123	0
87	OHX	5	4107	7/7	0.23	0.74	108,108,108,108	0
86	MG	5	3831	1/1	0.19	0.74	65,65,65,65	0
86	MG	5	3816	1/1	0.20	0.74	39,39,39,39	0
86	MG	1	3757	1/1	0.23	0.73	26,26,26,26	0
86	MG	6	1905	1/1	0.18	0.72	53,53,53,53	0
87	OHX	6	2146	7/7	0.26	0.72	119,119,119,119	0
86	MG	6	1987	1/1	0.17	0.71	69,69,69,69	0
87	OHX	2	2148	7/7	0.23	0.71	145,145,145,145	0
86	MG	1	3760	1/1	0.15	0.71	53,53,53,53	0
87	OHX	2	2029	7/7	0.16	0.70	86,86,86,86	0
86	MG	5	3750	1/1	0.20	0.69	51,51,51,51	0
86	MG	1	3612	1/1	0.18	0.69	39,39,39,39	0
87	OHX	6	2183	7/7	0.36	0.68	116,116,116,116	0
86	MG	2	1911	1/1	0.28	0.68	53,53,53,53	0
87	OHX	5	3948	7/7	0.15	0.68	83,83,83,83	0
86	MG	1	3756	1/1	0.17	0.67	42,42,42,42	0
86	MG	1	3644	1/1	0.19	0.66	43,43,43,43	0
86	MG	1	3482	1/1	0.23	0.64	48,48,48,48	0
86	MG	1	3766	1/1	0.18	0.64	58,58,58,58	0
87	OHX	5	4157	7/7	0.21	0.64	117,117,117,117	0
87	OHX	6	2163	7/7	0.24	0.64	108,108,108,108	0
86	MG	5	3449	1/1	0.18	0.63	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	L3	406	7/7	0.41	0.62	146,146,146,146	0
87	OHX	6	2126	7/7	0.21	0.62	118,118,118,118	0
86	MG	1	3659	1/1	0.22	0.62	43,43,43,43	0
87	OHX	6	2160	7/7	0.22	0.61	105,105,105,105	0
87	OHX	s1	302	7/7	0.27	0.60	136,136,136,136	0
86	MG	n8	201	1/1	0.21	0.60	32,32,32,32	0
86	MG	5	3700	1/1	0.19	0.60	39,39,39,39	0
87	OHX	5	4168	7/7	0.15	0.59	133,133,133,133	0
87	OHX	1	4080	7/7	0.20	0.59	104,104,104,104	0
86	MG	7	208	1/1	0.18	0.58	43,43,43,43	0
87	OHX	1	3913	7/7	0.13	0.58	88,88,88,88	0
87	OHX	5	3939	7/7	0.15	0.57	80,80,80,80	0
86	MG	5	3476	1/1	0.26	0.56	45,45,45,45	0
87	OHX	5	4224	7/7	0.31	0.55	132,132,132,132	0
86	MG	1	3582	1/1	0.22	0.54	31,31,31,31	0
86	MG	5	3461	1/1	0.17	0.54	24,24,24,24	0
86	MG	1	3488	1/1	0.23	0.54	46,46,46,46	0
86	MG	6	2018	1/1	0.25	0.53	52,52,52,52	0
86	MG	4	209	1/1	0.17	0.52	46,46,46,46	0
87	OHX	1	4196	7/7	0.20	0.52	145,145,145,145	0
87	OHX	5	4050	7/7	0.17	0.52	92,92,92,92	0
87	OHX	4	232	7/7	0.18	0.51	124,124,124,124	0
86	MG	1	3726	1/1	0.15	0.50	55,55,55,55	0
86	MG	5	3777	1/1	0.18	0.50	26,26,26,26	0
88	ZN	d7	101	1/1	0.46	0.50	132,132,132,132	0
87	OHX	5	4034	7/7	0.19	0.49	95,95,95,95	0
86	MG	1	3470	1/1	0.15	0.48	39,39,39,39	0
86	MG	1	3663	1/1	0.20	0.48	41,41,41,41	0
86	MG	5	3415	1/1	0.17	0.48	43,43,43,43	0
86	MG	1	3820	1/1	0.23	0.47	31,31,31,31	0
87	OHX	4	230	7/7	0.17	0.47	110,110,110,110	0
87	OHX	1	4150	7/7	0.17	0.47	105,105,105,105	0
87	OHX	1	4000	7/7	0.21	0.47	104,104,104,104	0
87	OHX	O3	202	7/7	0.19	0.46	103,103,103,103	0
86	MG	1	3724	1/1	0.18	0.45	52,52,52,52	0
87	OHX	5	3922	7/7	0.17	0.45	59,59,59,59	0
87	OHX	1	4016	7/7	0.14	0.44	137,137,137,137	0
86	MG	5	3645	1/1	0.17	0.44	30,30,30,30	0
87	OHX	5	3932	7/7	0.17	0.43	66,66,66,66	0
87	OHX	5	4110	7/7	0.21	0.43	92,92,92,92	0
87	OHX	D3	202	7/7	0.28	0.42	130,130,130,130	0
86	MG	7	228	1/1	0.18	0.41	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	6	2202	7/7	0.22	0.41	127,127,127,127	0
87	OHX	2	2105	7/7	0.19	0.40	119,119,119,119	0
86	MG	6	1996	1/1	0.16	0.39	35,35,35,35	0
87	OHX	6	2156	7/7	0.20	0.39	104,104,104,104	0
86	MG	5	3839	1/1	0.20	0.39	38,38,38,38	0
86	MG	2	1952	1/1	0.15	0.38	86,86,86,86	0
87	OHX	5	4097	7/7	0.17	0.38	106,106,106,106	0
87	OHX	1	4113	7/7	0.17	0.38	151,151,151,151	0
87	OHX	3	222	7/7	0.19	0.38	108,108,108,108	0
87	OHX	5	4030	7/7	0.19	0.37	84,84,84,84	0
87	OHX	1	4041	7/7	0.17	0.36	100,100,100,100	0
87	OHX	1	4172	7/7	0.17	0.36	98,98,98,98	0
86	MG	1	3717	1/1	0.18	0.35	62,62,62,62	0
86	MG	5	3672	1/1	0.17	0.35	31,31,31,31	0
86	MG	5	3437	1/1	0.17	0.34	37,37,37,37	0
86	MG	1	3454	1/1	0.22	0.34	50,50,50,50	0
86	MG	o1	201	1/1	0.17	0.33	46,46,46,46	0
87	OHX	1	3995	7/7	0.18	0.33	91,91,91,91	0
87	OHX	5	4053	7/7	0.17	0.33	92,92,92,92	0
87	OHX	2	2160	7/7	0.32	0.32	138,138,138,138	0
87	OHX	1	4131	7/7	0.20	0.32	136,136,136,136	0
86	MG	L7	302	1/1	0.17	0.32	37,37,37,37	0
86	MG	1	3828	1/1	0.20	0.32	36,36,36,36	0
86	MG	1	3472	1/1	0.17	0.31	23,23,23,23	0
87	OHX	1	4044	7/7	0.17	0.31	98,98,98,98	0
87	OHX	2	2169	7/7	0.15	0.31	121,121,121,121	0
87	OHX	d9	102	7/7	0.22	0.30	124,124,124,124	0
86	MG	4	210	1/1	0.20	0.30	43,43,43,43	0
87	OHX	2	2132	7/7	0.14	0.30	139,139,139,139	0
86	MG	5	3856	1/1	0.21	0.29	33,33,33,33	0
87	OHX	1	4101	7/7	0.25	0.29	119,119,119,119	0
87	OHX	5	4140	7/7	0.14	0.28	128,128,128,128	0
87	OHX	1	4212	7/7	0.23	0.28	144,144,144,144	0
87	OHX	5	4117	7/7	0.18	0.27	94,94,94,94	0
86	MG	6	1969	1/1	0.22	0.27	39,39,39,39	0
87	OHX	6	2140	7/7	0.15	0.27	119,119,119,119	0
87	OHX	19	600	7/7	0.19	0.26	113,113,113,113	0
86	MG	M7	206	1/1	0.19	0.26	51,51,51,51	0
87	OHX	1	3897	7/7	0.15	0.26	76,76,76,76	0
86	MG	12	302	1/1	0.20	0.26	30,30,30,30	0
87	OHX	2	2166	7/7	0.16	0.25	143,143,143,143	0
86	MG	5	3813	1/1	0.14	0.25	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	2	2109	7/7	0.15	0.25	126,126,126,126	0
86	MG	s8	301	1/1	0.18	0.24	44,44,44,44	0
87	OHX	5	4080	7/7	0.18	0.24	112,112,112,112	0
86	MG	1	3751	1/1	0.15	0.23	50,50,50,50	0
87	OHX	6	2047	7/7	0.17	0.22	52,52,52,52	0
86	MG	N8	203	1/1	0.24	0.22	44,44,44,44	0
87	OHX	1	4025	7/7	0.17	0.21	115,115,115,115	0
87	OHX	5	4180	7/7	0.16	0.21	141,141,141,141	0
87	OHX	6	2138	7/7	0.27	0.21	109,109,109,109	0
86	MG	N0	201	1/1	0.21	0.21	44,44,44,44	0
86	MG	1	3736	1/1	0.22	0.21	30,30,30,30	0
87	OHX	2	2176	7/7	0.27	0.21	149,149,149,149	0
87	OHX	6	2117	7/7	0.16	0.20	112,112,112,112	0
87	OHX	2	2179	7/7	0.28	0.20	147,147,147,147	0
87	OHX	6	2109	7/7	0.16	0.19	98,98,98,98	0
86	MG	5	3646	1/1	0.17	0.19	53,53,53,53	0
86	MG	1	3698	1/1	0.22	0.18	71,71,71,71	0
87	OHX	5	4028	7/7	0.16	0.18	98,98,98,98	0
88	ZN	D7	101	1/1	0.39	0.17	142,142,142,142	0
86	MG	1	3833	1/1	0.18	0.17	35,35,35,35	0
87	OHX	2	2137	7/7	0.17	0.17	127,127,127,127	0
87	OHX	1	4106	7/7	0.20	0.16	101,101,101,101	0
87	OHX	1	3949	7/7	0.12	0.15	105,105,105,105	0
86	MG	5	3688	1/1	0.16	0.15	68,68,68,68	0
86	MG	5	3761	1/1	0.16	0.15	38,38,38,38	0
86	MG	1	3731	1/1	0.19	0.14	46,46,46,46	0
87	OHX	6	2168	7/7	0.16	0.13	159,159,159,159	0
87	OHX	D9	102	7/7	0.20	0.13	120,120,120,120	0
87	OHX	6	2125	7/7	0.15	0.13	100,100,100,100	0
87	OHX	5	4120	7/7	0.16	0.13	107,107,107,107	0
86	MG	2	1943	1/1	0.15	0.12	61,61,61,61	0
87	OHX	5	3941	7/7	0.16	0.11	72,72,72,72	0
87	OHX	6	2101	7/7	0.13	0.11	143,143,143,143	0
87	OHX	5	4057	7/7	0.17	0.11	98,98,98,98	0
86	MG	5	3714	1/1	0.17	0.10	35,35,35,35	0
86	MG	3	210	1/1	0.18	0.09	59,59,59,59	0
86	MG	1	3678	1/1	0.17	0.09	43,43,43,43	0
87	OHX	6	2133	7/7	0.21	0.09	110,110,110,110	0
86	MG	1	3680	1/1	0.16	0.09	36,36,36,36	0
87	OHX	1	4015	7/7	0.16	0.08	102,102,102,102	0
87	OHX	1	4021	7/7	0.16	0.08	100,100,100,100	0
87	OHX	5	4199	7/7	0.17	0.07	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3427	1/1	0.17	0.07	32,32,32,32	0
87	OHX	l3	404	7/7	0.27	0.07	128,128,128,128	0
87	OHX	5	4129	7/7	0.24	0.05	125,125,125,125	0
86	MG	4	220	1/1	0.17	0.05	47,47,47,47	0
87	OHX	2	2099	7/7	0.17	0.05	125,125,125,125	0
87	OHX	1	3894	7/7	0.17	0.04	73,73,73,73	0
87	OHX	5	3949	7/7	0.17	0.04	93,93,93,93	0
86	MG	6	1962	1/1	0.18	0.04	38,38,38,38	0
86	MG	1	4219	1/1	0.21	0.03	41,41,41,41	0
87	OHX	6	2142	7/7	0.14	0.03	140,140,140,140	0
87	OHX	1	4089	7/7	0.15	0.03	119,119,119,119	0
86	MG	6	1991	1/1	0.15	0.02	64,64,64,64	0
87	OHX	5	4242	7/7	0.29	0.02	92,92,92,92	0
86	MG	1	3801	1/1	0.23	0.02	52,52,52,52	0
86	MG	2	1983	1/1	0.17	0.02	51,51,51,51	0
87	OHX	6	2173	7/7	0.19	0.02	122,122,122,122	0
86	MG	C3	201	1/1	0.24	0.01	64,64,64,64	0
86	MG	5	3605	1/1	0.20	0.01	29,29,29,29	0
87	OHX	5	3967	7/7	0.15	-0.02	94,94,94,94	0
86	MG	6	2036	1/1	0.24	-0.02	65,65,65,65	0
86	MG	M7	204	1/1	0.20	-0.02	32,32,32,32	0
86	MG	o4	202	1/1	0.24	-0.03	65,65,65,65	0
86	MG	O4	201	1/1	0.24	-0.04	46,46,46,46	0
87	OHX	1	3883	7/7	0.15	-0.04	63,63,63,63	0
87	OHX	2	2036	7/7	0.13	-0.04	103,103,103,103	0
86	MG	5	3666	1/1	0.19	-0.04	38,38,38,38	0
87	OHX	1	3931	7/7	0.15	-0.05	97,97,97,97	0
86	MG	5	3860	1/1	0.16	-0.05	47,47,47,47	0
87	OHX	5	4155	7/7	0.17	-0.05	105,105,105,105	0
87	OHX	5	3916	7/7	0.15	-0.05	63,63,63,63	0
87	OHX	5	3909	7/7	0.16	-0.05	47,47,47,47	0
86	MG	2	1965	1/1	0.21	-0.06	58,58,58,58	0
86	MG	M3	204	1/1	0.21	-0.06	34,34,34,34	0
86	MG	5	3832	1/1	0.15	-0.07	48,48,48,48	0
87	OHX	1	3906	7/7	0.15	-0.07	83,83,83,83	0
87	OHX	1	3915	7/7	0.15	-0.07	84,84,84,84	0
86	MG	1	3789	1/1	0.15	-0.07	73,73,73,73	0
87	OHX	1	3895	7/7	0.16	-0.07	74,74,74,74	0
86	MG	6	2206	1/1	0.21	-0.08	46,46,46,46	0
87	OHX	1	3867	7/7	0.19	-0.08	51,51,51,51	0
86	MG	d6	102	1/1	0.25	-0.08	48,48,48,48	0
86	MG	5	3713	1/1	0.16	-0.09	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	4094	7/7	0.20	-0.09	112,112,112,112	0
87	OHX	1	4096	7/7	0.12	-0.09	127,127,127,127	0
87	OHX	5	3904	7/7	0.20	-0.09	50,50,50,50	0
87	OHX	2	2130	7/7	0.15	-0.11	115,115,115,115	0
87	OHX	5	4225	7/7	0.19	-0.11	126,126,126,126	0
87	OHX	1	4092	7/7	0.15	-0.12	134,134,134,134	0
86	MG	S8	301	1/1	0.16	-0.12	50,50,50,50	0
88	ZN	q0	201	1/1	0.18	-0.12	28,28,28,28	0
87	OHX	5	4114	7/7	0.17	-0.13	105,105,105,105	0
86	MG	5	3693	1/1	0.17	-0.13	49,49,49,49	0
86	MG	5	3756	1/1	0.20	-0.14	48,48,48,48	0
87	OHX	6	2193	7/7	0.23	-0.14	141,141,141,141	0
86	MG	6	1997	1/1	0.19	-0.14	65,65,65,65	0
86	MG	5	3490	1/1	0.16	-0.14	27,27,27,27	0
86	MG	5	3419	1/1	0.17	-0.14	27,27,27,27	0
87	OHX	5	4145	7/7	0.16	-0.15	120,120,120,120	0
87	OHX	5	4108	7/7	0.17	-0.15	115,115,115,115	0
87	OHX	1	4056	7/7	0.17	-0.16	86,86,86,86	0
87	OHX	4	223	7/7	0.17	-0.17	51,51,51,51	0
86	MG	M6	201	1/1	0.24	-0.17	45,45,45,45	0
86	MG	5	3838	1/1	0.15	-0.17	23,23,23,23	0
87	OHX	m0	302	7/7	0.21	-0.18	110,110,110,110	0
86	MG	5	3708	1/1	0.17	-0.19	45,45,45,45	0
86	MG	1	3654	1/1	0.16	-0.19	41,41,41,41	0
87	OHX	1	4038	7/7	0.16	-0.19	104,104,104,104	0
86	MG	6	2024	1/1	0.20	-0.20	43,43,43,43	0
86	MG	5	3497	1/1	0.18	-0.20	29,29,29,29	0
86	MG	1	3415	1/1	0.20	-0.20	43,43,43,43	0
86	MG	5	3654	1/1	0.16	-0.21	35,35,35,35	0
87	OHX	2	2032	7/7	0.17	-0.21	97,97,97,97	0
87	OHX	1	4087	7/7	0.18	-0.22	110,110,110,110	0
87	OHX	1	3996	7/7	0.13	-0.23	147,147,147,147	0
86	MG	5	3841	1/1	0.15	-0.23	49,49,49,49	0
86	MG	6	2006	1/1	0.19	-0.23	57,57,57,57	0
87	OHX	2	2149	7/7	0.20	-0.24	151,151,151,151	0
87	OHX	2	2154	7/7	0.19	-0.25	125,125,125,125	0
87	OHX	S8	302	7/7	0.24	-0.25	141,141,141,141	0
87	OHX	1	4144	7/7	0.20	-0.25	131,131,131,131	0
86	MG	5	3743	1/1	0.16	-0.26	36,36,36,36	0
86	MG	6	1910	1/1	0.16	-0.26	57,57,57,57	0
87	OHX	6	2180	7/7	0.15	-0.27	135,135,135,135	0
86	MG	1	3445	1/1	0.15	-0.28	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	2	1998	1/1	0.23	-0.29	61,61,61,61	0
87	OHX	c1	202	7/7	0.21	-0.30	117,117,117,117	0
87	OHX	5	3906	7/7	0.17	-0.31	52,52,52,52	0
86	MG	5	3600	1/1	0.16	-0.31	35,35,35,35	0
87	OHX	1	3891	7/7	0.15	-0.31	66,66,66,66	0
87	OHX	m1	203	7/7	0.32	-0.31	135,135,135,135	0
86	MG	2	1986	1/1	0.17	-0.32	71,71,71,71	0
86	MG	5	3815	1/1	0.16	-0.32	55,55,55,55	0
87	OHX	6	2067	7/7	0.16	-0.33	101,101,101,101	0
87	OHX	6	2144	7/7	0.16	-0.33	124,124,124,124	0
86	MG	5	3842	1/1	0.14	-0.34	35,35,35,35	0
86	MG	8	204	1/1	0.18	-0.35	46,46,46,46	0
86	MG	1	3424	1/1	0.17	-0.35	41,41,41,41	0
87	OHX	1	3869	7/7	0.17	-0.35	48,48,48,48	0
86	MG	1	3634	1/1	0.16	-0.36	41,41,41,41	0
86	MG	1	3670	1/1	0.15	-0.36	75,75,75,75	0
87	OHX	5	4136	7/7	0.17	-0.36	120,120,120,120	0
87	OHX	2	2068	7/7	0.18	-0.36	101,101,101,101	0
87	OHX	1	4123	7/7	0.16	-0.37	123,123,123,123	0
87	OHX	6	2074	7/7	0.14	-0.37	108,108,108,108	0
86	MG	5	3769	1/1	0.15	-0.37	34,34,34,34	0
87	OHX	6	2054	7/7	0.17	-0.38	75,75,75,75	0
86	MG	2	1948	1/1	0.18	-0.38	75,75,75,75	0
87	OHX	n9	101	7/7	0.16	-0.38	62,62,62,62	0
86	MG	m7	204	1/1	0.19	-0.39	32,32,32,32	0
87	OHX	L4	402	7/7	0.17	-0.39	113,113,113,113	0
86	MG	5	3495	1/1	0.17	-0.39	32,32,32,32	0
87	OHX	l5	304	7/7	0.19	-0.40	121,121,121,121	0
87	OHX	2	2100	7/7	0.14	-0.40	126,126,126,126	0
86	MG	1	3495	1/1	0.17	-0.40	41,41,41,41	0
86	MG	2	2021	1/1	0.17	-0.40	104,104,104,104	0
87	OHX	1	3991	7/7	0.12	-0.41	125,125,125,125	0
87	OHX	6	2065	7/7	0.14	-0.41	88,88,88,88	0
87	OHX	1	3884	7/7	0.16	-0.42	64,64,64,64	0
86	MG	l4	401	1/1	0.24	-0.43	33,33,33,33	0
87	OHX	N9	101	7/7	0.17	-0.43	57,57,57,57	0
87	OHX	1	3999	7/7	0.16	-0.43	84,84,84,84	0
86	MG	M9	201	1/1	0.20	-0.43	61,61,61,61	0
87	OHX	6	2129	7/7	0.16	-0.43	117,117,117,117	0
87	OHX	1	3885	7/7	0.16	-0.44	61,61,61,61	0
86	MG	L3	403	1/1	0.14	-0.44	41,41,41,41	0
88	ZN	d9	101	1/1	0.16	-0.45	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3767	1/1	0.15	-0.45	54,54,54,54	0
87	OHX	5	4194	7/7	0.17	-0.45	151,151,151,151	0
87	OHX	6	2057	7/7	0.16	-0.46	74,74,74,74	0
86	MG	1	3422	1/1	0.17	-0.46	29,29,29,29	0
86	MG	5	3608	1/1	0.16	-0.47	34,34,34,34	0
86	MG	1	3676	1/1	0.15	-0.47	62,62,62,62	0
87	OHX	6	2108	7/7	0.18	-0.47	109,109,109,109	0
87	OHX	l3	403	7/7	0.16	-0.49	99,99,99,99	0
86	MG	n6	202	1/1	0.18	-0.49	43,43,43,43	0
86	MG	5	3663	1/1	0.15	-0.49	45,45,45,45	0
87	OHX	1	3932	7/7	0.16	-0.49	60,60,60,60	0
86	MG	1	3841	1/1	0.16	-0.49	51,51,51,51	0
87	OHX	2	2034	7/7	0.14	-0.49	94,94,94,94	0
87	OHX	1	4103	7/7	0.16	-0.49	114,114,114,114	0
87	OHX	6	2075	7/7	0.13	-0.50	108,108,108,108	0
86	MG	2	1946	1/1	0.19	-0.50	52,52,52,52	0
87	OHX	1	4156	7/7	0.14	-0.50	103,103,103,103	0
87	OHX	2	2125	7/7	0.16	-0.51	126,126,126,126	0
87	OHX	5	4042	7/7	0.13	-0.51	137,137,137,137	0
87	OHX	6	2110	7/7	0.14	-0.52	109,109,109,109	0
86	MG	5	3843	1/1	0.17	-0.52	49,49,49,49	0
87	OHX	5	3966	7/7	0.15	-0.53	90,90,90,90	0
87	OHX	5	3920	7/7	0.14	-0.53	62,62,62,62	0
86	MG	5	3752	1/1	0.15	-0.53	38,38,38,38	0
86	MG	2	2003	1/1	0.20	-0.54	59,59,59,59	0
87	OHX	1	4064	7/7	0.17	-0.54	89,89,89,89	0
87	OHX	5	3956	7/7	0.15	-0.54	88,88,88,88	0
87	OHX	1	4091	7/7	0.16	-0.55	110,110,110,110	0
87	OHX	5	4216	7/7	0.17	-0.55	96,96,96,96	0
86	MG	5	3470	1/1	0.17	-0.55	32,32,32,32	0
87	OHX	5	3975	7/7	0.13	-0.56	94,94,94,94	0
87	OHX	5	4060	7/7	0.15	-0.56	105,105,105,105	0
88	ZN	Q0	500	1/1	0.16	-0.57	42,42,42,42	0
86	MG	1	3407	1/1	0.16	-0.58	37,37,37,37	0
86	MG	5	3604	1/1	0.14	-0.58	37,37,37,37	0
87	OHX	1	4059	7/7	0.17	-0.59	116,116,116,116	0
87	OHX	1	3875	7/7	0.16	-0.59	52,52,52,52	0
86	MG	1	3467	1/1	0.15	-0.59	42,42,42,42	0
86	MG	1	3748	1/1	0.16	-0.59	43,43,43,43	0
86	MG	1	3622	1/1	0.15	-0.60	34,34,34,34	0
86	MG	5	3463	1/1	0.18	-0.60	36,36,36,36	0
86	MG	1	3749	1/1	0.15	-0.61	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	1	4077	7/7	0.16	-0.61	108,108,108,108	0
87	OHX	5	3974	7/7	0.10	-0.62	77,77,77,77	0
86	MG	5	3869	1/1	0.15	-0.62	32,32,32,32	0
86	MG	S2	301	1/1	0.22	-0.62	65,65,65,65	0
86	MG	5	3893	1/1	0.14	-0.62	64,64,64,64	0
87	OHX	2	2028	7/7	0.14	-0.63	89,89,89,89	0
87	OHX	5	4210	7/7	0.18	-0.63	100,100,100,100	0
87	OHX	1	3880	7/7	0.16	-0.63	60,60,60,60	0
87	OHX	c5	201	7/7	0.21	-0.63	140,140,140,140	0
86	MG	1	3558	1/1	0.16	-0.64	43,43,43,43	0
86	MG	5	3696	1/1	0.14	-0.64	40,40,40,40	0
87	OHX	1	4023	7/7	0.13	-0.65	122,122,122,122	0
87	OHX	5	3953	7/7	0.15	-0.66	90,90,90,90	0
86	MG	6	1978	1/1	0.16	-0.66	37,37,37,37	0
88	ZN	Q2	501	1/1	0.14	-0.66	75,75,75,75	0
86	MG	1	3799	1/1	0.19	-0.67	47,47,47,47	0
87	OHX	s8	302	7/7	0.27	-0.68	141,141,141,141	0
86	MG	1	3782	1/1	0.17	-0.69	32,32,32,32	0
86	MG	o7	101	1/1	0.19	-0.70	40,40,40,40	0
87	OHX	1	4124	7/7	0.15	-0.73	128,128,128,128	0
86	MG	4	217	1/1	0.12	-0.73	58,58,58,58	0
86	MG	8	207	1/1	0.14	-0.73	59,59,59,59	0
87	OHX	8	223	7/7	0.18	-0.73	113,113,113,113	0
86	MG	1	3602	1/1	0.16	-0.74	23,23,23,23	0
87	OHX	14	403	7/7	0.18	-0.74	114,114,114,114	0
87	OHX	1	3970	7/7	0.15	-0.75	97,97,97,97	0
87	OHX	1	4075	7/7	0.15	-0.75	110,110,110,110	0
87	OHX	2	2106	7/7	0.12	-0.76	106,106,106,106	0
87	OHX	2	2150	7/7	0.11	-0.76	157,157,157,157	0
86	MG	6	1971	1/1	0.14	-0.77	54,54,54,54	0
87	OHX	1	4037	7/7	0.16	-0.77	93,93,93,93	0
87	OHX	5	4038	7/7	0.16	-0.78	104,104,104,104	0
86	MG	1	3784	1/1	0.14	-0.79	47,47,47,47	0
87	OHX	6	2060	7/7	0.14	-0.79	87,87,87,87	0
86	MG	5	3871	1/1	0.15	-0.79	50,50,50,50	0
87	OHX	6	2147	7/7	0.11	-0.79	119,119,119,119	0
87	OHX	2	2095	7/7	0.15	-0.80	112,112,112,112	0
87	OHX	1	3937	7/7	0.13	-0.80	100,100,100,100	0
86	MG	5	3727	1/1	0.15	-0.80	36,36,36,36	0
87	OHX	5	4069	7/7	0.14	-0.81	89,89,89,89	0
86	MG	m5	302	1/1	0.16	-0.81	47,47,47,47	0
86	MG	4	208	1/1	0.14	-0.81	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3942	7/7	0.12	-0.82	98,98,98,98	0
87	OHX	1	3924	7/7	0.13	-0.82	101,101,101,101	0
88	ZN	O7	101	1/1	0.14	-0.82	32,32,32,32	0
87	OHX	1	4050	7/7	0.15	-0.82	105,105,105,105	0
87	OHX	2	2101	7/7	0.13	-0.83	121,121,121,121	0
87	OHX	2	2066	7/7	0.11	-0.84	127,127,127,127	0
87	OHX	1	4053	7/7	0.14	-0.84	119,119,119,119	0
87	OHX	2	2123	7/7	0.13	-0.84	128,128,128,128	0
87	OHX	1	4161	7/7	0.19	-0.84	122,122,122,122	0
87	OHX	1	3927	7/7	0.12	-0.84	92,92,92,92	0
86	MG	D3	201	1/1	0.15	-0.84	53,53,53,53	0
87	OHX	6	2056	7/7	0.14	-0.84	65,65,65,65	0
87	OHX	5	4125	7/7	0.12	-0.84	133,133,133,133	0
86	MG	6	2026	1/1	0.12	-0.86	73,73,73,73	0
86	MG	1	3743	1/1	0.14	-0.86	37,37,37,37	0
86	MG	1	3668	1/1	0.14	-0.87	48,48,48,48	0
87	OHX	5	4119	7/7	0.15	-0.88	106,106,106,106	0
87	OHX	5	3907	7/7	0.16	-0.88	57,57,57,57	0
86	MG	1	3689	1/1	0.17	-0.88	30,30,30,30	0
86	MG	5	3695	1/1	0.15	-0.89	43,43,43,43	0
87	OHX	5	4018	7/7	0.14	-0.90	139,139,139,139	0
87	OHX	1	4165	7/7	0.11	-0.90	170,170,170,170	0
86	MG	6	1970	1/1	0.15	-0.90	52,52,52,52	0
86	MG	c8	202	1/1	0.23	-0.91	61,61,61,61	0
86	MG	5	3803	1/1	0.14	-0.91	43,43,43,43	0
87	OHX	5	4079	7/7	0.15	-0.91	92,92,92,92	0
87	OHX	1	4004	7/7	0.14	-0.91	110,110,110,110	0
86	MG	5	3817	1/1	0.12	-0.91	41,41,41,41	0
88	ZN	D9	101	1/1	0.11	-0.91	66,66,66,66	0
86	MG	M5	301	1/1	0.15	-0.91	26,26,26,26	0
86	MG	s1	301	1/1	0.19	-0.91	72,72,72,72	0
86	MG	L3	402	1/1	0.16	-0.92	62,62,62,62	0
86	MG	q3	502	1/1	0.18	-0.92	56,56,56,56	0
87	OHX	6	2121	7/7	0.14	-0.92	105,105,105,105	0
86	MG	5	3677	1/1	0.14	-0.93	38,38,38,38	0
87	OHX	4	231	7/7	0.10	-0.93	133,133,133,133	0
86	MG	n0	202	1/1	0.15	-0.94	37,37,37,37	0
86	MG	5	3806	1/1	0.14	-0.94	30,30,30,30	0
86	MG	1	3809	1/1	0.14	-0.94	46,46,46,46	0
86	MG	1	3548	1/1	0.15	-0.95	36,36,36,36	0
87	OHX	1	4029	7/7	0.14	-0.96	118,118,118,118	0
86	MG	O4	202	1/1	0.15	-0.96	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	6	2022	1/1	0.17	-0.97	58,58,58,58	0
87	OHX	2	2084	7/7	0.10	-0.97	122,122,122,122	0
86	MG	5	3788	1/1	0.14	-0.97	41,41,41,41	0
87	OHX	5	4047	7/7	0.16	-0.97	91,91,91,91	0
87	OHX	2	2092	7/7	0.12	-0.98	128,128,128,128	0
87	OHX	1	4043	7/7	0.12	-0.98	93,93,93,93	0
86	MG	1	3842	1/1	0.17	-0.99	30,30,30,30	0
87	OHX	5	3970	7/7	0.11	-0.99	87,87,87,87	0
87	OHX	5	4182	7/7	0.14	-0.99	129,129,129,129	0
87	OHX	2	2140	7/7	0.10	-1.00	142,142,142,142	0
87	OHX	2	2030	7/7	0.13	-1.00	97,97,97,97	0
87	OHX	L3	405	7/7	0.15	-1.00	100,100,100,100	0
87	OHX	2	2104	7/7	0.15	-1.01	105,105,105,105	0
87	OHX	1	3898	7/7	0.13	-1.02	78,78,78,78	0
87	OHX	2	2120	7/7	0.12	-1.02	128,128,128,128	0
86	MG	Q2	502	1/1	0.12	-1.02	58,58,58,58	0
87	OHX	7	215	7/7	0.14	-1.02	80,80,80,80	0
87	OHX	2	2025	7/7	0.14	-1.02	78,78,78,78	0
87	OHX	5	3957	7/7	0.14	-1.03	82,82,82,82	0
87	OHX	1	4078	7/7	0.13	-1.03	105,105,105,105	0
87	OHX	5	4167	7/7	0.14	-1.04	114,114,114,114	0
87	OHX	1	4068	7/7	0.12	-1.04	112,112,112,112	0
86	MG	1	3666	1/1	0.14	-1.05	33,33,33,33	0
86	MG	5	3779	1/1	0.12	-1.05	53,53,53,53	0
86	MG	1	4221	1/1	0.13	-1.05	53,53,53,53	0
87	OHX	2	2143	7/7	0.14	-1.06	142,142,142,142	0
87	OHX	2	2086	7/7	0.13	-1.07	114,114,114,114	0
86	MG	2	2020	1/1	0.11	-1.08	85,85,85,85	0
87	OHX	1	3905	7/7	0.14	-1.09	75,75,75,75	0
87	OHX	1	4007	7/7	0.15	-1.09	100,100,100,100	0
86	MG	2	1939	1/1	0.13	-1.10	56,56,56,56	0
87	OHX	m0	301	7/7	0.08	-1.10	116,116,116,116	0
87	OHX	2	2046	7/7	0.05	-1.11	116,116,116,116	0
87	OHX	8	216	7/7	0.08	-1.11	100,100,100,100	0
87	OHX	2	2031	7/7	0.14	-1.11	84,84,84,84	0
87	OHX	6	2150	7/7	0.15	-1.12	96,96,96,96	0
86	MG	1	3425	1/1	0.14	-1.12	26,26,26,26	0
87	OHX	O7	103	7/7	0.09	-1.12	85,85,85,85	0
86	MG	2	1920	1/1	0.20	-1.13	52,52,52,52	0
87	OHX	6	2203	7/7	0.09	-1.14	171,171,171,171	0
86	MG	n3	202	1/1	0.14	-1.14	37,37,37,37	0
86	MG	8	211	1/1	0.16	-1.15	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2087	7/7	0.14	-1.15	114,114,114,114	0
87	OHX	1	4076	7/7	0.13	-1.15	117,117,117,117	0
87	OHX	1	3951	7/7	0.15	-1.16	95,95,95,95	0
86	MG	5	3724	1/1	0.15	-1.16	32,32,32,32	0
86	MG	m1	202	1/1	0.15	-1.16	52,52,52,52	0
86	MG	1	3416	1/1	0.14	-1.17	27,27,27,27	0
86	MG	5	3819	1/1	0.13	-1.17	57,57,57,57	0
86	MG	5	3784	1/1	0.12	-1.17	70,70,70,70	0
86	MG	1	3428	1/1	0.11	-1.18	48,48,48,48	0
87	OHX	5	4064	7/7	0.13	-1.18	115,115,115,115	0
87	OHX	1	3901	7/7	0.15	-1.19	71,71,71,71	0
87	OHX	2	2056	7/7	0.12	-1.21	116,116,116,116	0
87	OHX	5	4241	7/7	0.18	-1.21	211,211,211,211	0
87	OHX	1	3965	7/7	0.11	-1.22	104,104,104,104	0
87	OHX	5	4123	7/7	0.12	-1.22	121,121,121,121	0
86	MG	5	3811	1/1	0.10	-1.22	37,37,37,37	0
86	MG	6	1984	1/1	0.12	-1.24	38,38,38,38	0
87	OHX	8	217	7/7	0.12	-1.24	99,99,99,99	0
86	MG	1	3628	1/1	0.15	-1.25	37,37,37,37	0
87	OHX	6	2143	7/7	0.14	-1.25	113,113,113,113	0
87	OHX	2	2052	7/7	0.11	-1.26	119,119,119,119	0
86	MG	5	3755	1/1	0.12	-1.26	48,48,48,48	0
86	MG	1	4217	1/1	0.15	-1.28	22,22,22,22	0
86	MG	M3	201	1/1	0.14	-1.28	42,42,42,42	0
86	MG	5	3741	1/1	0.16	-1.29	34,34,34,34	0
87	OHX	1	4102	7/7	0.15	-1.30	124,124,124,124	0
86	MG	1	3627	1/1	0.14	-1.30	38,38,38,38	0
86	MG	1	3735	1/1	0.15	-1.30	59,59,59,59	0
87	OHX	6	2090	7/7	0.10	-1.31	116,116,116,116	0
86	MG	1	3578	1/1	0.15	-1.31	22,22,22,22	0
86	MG	5	3643	1/1	0.13	-1.31	43,43,43,43	0
87	OHX	5	3990	7/7	0.14	-1.31	63,63,63,63	0
86	MG	6	2007	1/1	0.14	-1.32	52,52,52,52	0
87	OHX	2	2117	7/7	0.14	-1.32	141,141,141,141	0
86	MG	1	3489	1/1	0.14	-1.35	27,27,27,27	0
87	OHX	6	2165	7/7	0.14	-1.36	168,168,168,168	0
86	MG	5	3768	1/1	0.13	-1.36	35,35,35,35	0
87	OHX	1	4199	7/7	0.14	-1.36	112,112,112,112	0
86	MG	6	2033	1/1	0.16	-1.37	45,45,45,45	0
87	OHX	1	3941	7/7	0.15	-1.38	80,80,80,80	0
87	OHX	1	3944	7/7	0.12	-1.38	93,93,93,93	0
87	OHX	1	3948	7/7	0.12	-1.38	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3961	7/7	0.12	-1.38	107,107,107,107	0
87	OHX	5	4032	7/7	0.11	-1.38	121,121,121,121	0
87	OHX	5	4074	7/7	0.14	-1.39	104,104,104,104	0
87	OHX	5	3934	7/7	0.13	-1.39	67,67,67,67	0
86	MG	1	3665	1/1	0.13	-1.40	43,43,43,43	0
87	OHX	1	3981	7/7	0.07	-1.40	106,106,106,106	0
86	MG	5	3432	1/1	0.16	-1.40	34,34,34,34	0
87	OHX	1	4027	7/7	0.15	-1.41	99,99,99,99	0
86	MG	5	3674	1/1	0.13	-1.41	23,23,23,23	0
87	OHX	2	2141	7/7	0.13	-1.42	124,124,124,124	0
86	MG	1	3771	1/1	0.14	-1.42	57,57,57,57	0
87	OHX	5	4003	7/7	0.13	-1.42	68,68,68,68	0
87	OHX	1	3933	7/7	0.12	-1.43	91,91,91,91	0
87	OHX	5	3993	7/7	0.13	-1.43	92,92,92,92	0
87	OHX	1	4108	7/7	0.13	-1.43	113,113,113,113	0
86	MG	5	3621	1/1	0.10	-1.43	36,36,36,36	0
88	ZN	Q3	501	1/1	0.09	-1.44	61,61,61,61	0
86	MG	1	3863	1/1	0.15	-1.44	25,25,25,25	0
86	MG	5	3863	1/1	0.15	-1.44	55,55,55,55	0
87	OHX	1	4026	7/7	0.12	-1.44	114,114,114,114	0
86	MG	1	3681	1/1	0.13	-1.45	56,56,56,56	0
86	MG	2	1992	1/1	0.16	-1.45	62,62,62,62	0
87	OHX	2	2131	7/7	0.13	-1.45	129,129,129,129	0
86	MG	1	3753	1/1	0.14	-1.45	31,31,31,31	0
87	OHX	5	3911	7/7	0.15	-1.45	53,53,53,53	0
87	OHX	1	3916	7/7	0.13	-1.46	82,82,82,82	0
87	OHX	6	2130	7/7	0.10	-1.46	124,124,124,124	0
87	OHX	5	3988	7/7	0.10	-1.46	92,92,92,92	0
86	MG	1	3708	1/1	0.14	-1.47	40,40,40,40	0
87	OHX	6	2102	7/7	0.10	-1.47	141,141,141,141	0
87	OHX	5	3963	7/7	0.11	-1.47	80,80,80,80	0
87	OHX	6	2068	7/7	0.11	-1.47	76,76,76,76	0
87	OHX	5	3912	7/7	0.14	-1.48	52,52,52,52	0
87	OHX	5	4014	7/7	0.10	-1.48	138,138,138,138	0
88	ZN	e1	501	1/1	0.05	-1.49	143,143,143,143	0
87	OHX	sR	401	7/7	0.10	-1.49	145,145,145,145	0
86	MG	sM	302	1/1	0.13	-1.49	35,35,35,35	0
87	OHX	l5	303	7/7	0.13	-1.49	127,127,127,127	0
87	OHX	c8	203	7/7	0.12	-1.50	123,123,123,123	0
87	OHX	2	2047	7/7	0.07	-1.50	103,103,103,103	0
87	OHX	5	4000	7/7	0.13	-1.51	102,102,102,102	0
87	OHX	2	2042	7/7	0.12	-1.51	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	q2	502	7/7	0.13	-1.52	77,77,77,77	0
87	OHX	2	2102	7/7	0.13	-1.52	124,124,124,124	0
87	OHX	5	4020	7/7	0.14	-1.52	99,99,99,99	0
86	MG	1	3806	1/1	0.14	-1.53	44,44,44,44	0
87	OHX	SR	401	7/7	0.06	-1.54	148,148,148,148	0
86	MG	2	1990	1/1	0.08	-1.54	85,85,85,85	0
88	ZN	E1	501	1/1	0.09	-1.54	105,105,105,105	0
87	OHX	1	3871	7/7	0.16	-1.55	50,50,50,50	0
87	OHX	1	4040	7/7	0.07	-1.56	118,118,118,118	0
87	OHX	C8	201	7/7	0.14	-1.58	99,99,99,99	0
87	OHX	6	2059	7/7	0.12	-1.58	68,68,68,68	0
87	OHX	5	3980	7/7	0.11	-1.58	84,84,84,84	0
88	ZN	o7	102	1/1	0.11	-1.59	37,37,37,37	0
86	MG	5	3488	1/1	0.15	-1.60	50,50,50,50	0
87	OHX	Q2	503	7/7	0.12	-1.60	76,76,76,76	0
86	MG	S4	301	1/1	0.10	-1.61	61,61,61,61	0
87	OHX	2	2026	7/7	0.13	-1.61	71,71,71,71	0
87	OHX	1	4054	7/7	0.14	-1.61	95,95,95,95	0
87	OHX	5	4127	7/7	0.16	-1.61	114,114,114,114	0
87	OHX	1	3922	7/7	0.11	-1.63	83,83,83,83	0
86	MG	5	3790	1/1	0.09	-1.66	35,35,35,35	0
86	MG	L4	401	1/1	0.13	-1.66	28,28,28,28	0
87	OHX	5	4118	7/7	0.14	-1.66	106,106,106,106	0
87	OHX	5	3976	7/7	0.11	-1.67	86,86,86,86	0
87	OHX	1	3896	7/7	0.14	-1.67	68,68,68,68	0
87	OHX	6	2119	7/7	0.11	-1.69	99,99,99,99	0
86	MG	5	3723	1/1	0.14	-1.69	41,41,41,41	0
87	OHX	5	4102	7/7	0.14	-1.69	92,92,92,92	0
87	OHX	5	4096	7/7	0.15	-1.71	127,127,127,127	0
87	OHX	5	4208	7/7	0.13	-1.71	135,135,135,135	0
87	OHX	1	4052	7/7	0.11	-1.73	127,127,127,127	0
87	OHX	2	2035	7/7	0.10	-1.73	78,78,78,78	0
86	MG	5	3613	1/1	0.14	-1.74	30,30,30,30	0
86	MG	6	1915	1/1	0.09	-1.75	59,59,59,59	0
87	OHX	1	3899	7/7	0.13	-1.75	62,62,62,62	0
87	OHX	5	3937	7/7	0.11	-1.76	67,67,67,67	0
87	OHX	N1	201	7/7	0.14	-1.76	60,60,60,60	0
86	MG	1	3714	1/1	0.15	-1.76	28,28,28,28	0
87	OHX	5	4081	7/7	0.12	-1.78	107,107,107,107	0
87	OHX	1	4116	7/7	0.14	-1.78	121,121,121,121	0
86	MG	5	3703	1/1	0.16	-1.79	35,35,35,35	0
87	OHX	1	4012	7/7	0.07	-1.79	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3471	1/1	0.15	-1.79	35,35,35,35	0
87	OHX	6	2106	7/7	0.13	-1.80	106,106,106,106	0
87	OHX	1	3953	7/7	0.12	-1.80	84,84,84,84	0
87	OHX	1	3976	7/7	0.11	-1.80	82,82,82,82	0
86	MG	14	402	1/1	0.09	-1.81	43,43,43,43	0
87	OHX	c3	201	7/7	0.26	-1.82	135,135,135,135	0
87	OHX	1	4070	7/7	0.12	-1.83	117,117,117,117	0
86	MG	5	3669	1/1	0.14	-1.83	23,23,23,23	0
87	OHX	5	4078	7/7	0.09	-1.84	147,147,147,147	0
87	OHX	2	2129	7/7	0.13	-1.85	107,107,107,107	0
88	ZN	D6	500	1/1	0.09	-1.85	72,72,72,72	0
86	MG	2	1996	1/1	0.13	-1.86	67,67,67,67	0
87	OHX	2	2048	7/7	0.11	-1.86	111,111,111,111	0
87	OHX	4	228	7/7	0.13	-1.87	112,112,112,112	0
86	MG	5	3682	1/1	0.14	-1.87	32,32,32,32	0
87	OHX	O2	201	7/7	0.11	-1.88	79,79,79,79	0
87	OHX	5	3950	7/7	0.12	-1.88	91,91,91,91	0
87	OHX	O7	104	7/7	0.11	-1.89	88,88,88,88	0
87	OHX	2	2110	7/7	0.12	-1.92	102,102,102,102	0
87	OHX	5	3962	7/7	0.08	-1.92	83,83,83,83	0
87	OHX	5	3918	7/7	0.15	-1.92	59,59,59,59	0
87	OHX	1	3973	7/7	0.07	-1.92	114,114,114,114	0
87	OHX	5	4214	7/7	0.11	-1.93	177,177,177,177	0
87	OHX	5	3989	7/7	0.10	-1.93	107,107,107,107	0
86	MG	1	3780	1/1	0.11	-1.94	55,55,55,55	0
87	OHX	2	2072	7/7	0.07	-1.94	130,130,130,130	0
87	OHX	1	3984	7/7	0.14	-1.95	84,84,84,84	0
86	MG	L2	301	1/1	0.12	-1.95	30,30,30,30	0
87	OHX	6	2072	7/7	0.11	-1.97	104,104,104,104	0
87	OHX	7	221	7/7	0.07	-1.97	99,99,99,99	0
87	OHX	5	3923	7/7	0.13	-1.97	62,62,62,62	0
87	OHX	2	2027	7/7	0.12	-1.98	81,81,81,81	0
87	OHX	5	4134	7/7	0.15	-1.98	114,114,114,114	0
86	MG	1	3790	1/1	0.10	-2.00	50,50,50,50	0
87	OHX	1	4055	7/7	0.11	-2.01	132,132,132,132	0
86	MG	5	3457	1/1	0.14	-2.01	82,82,82,82	0
87	OHX	1	3989	7/7	0.15	-2.02	106,106,106,106	0
86	MG	5	3685	1/1	0.13	-2.03	28,28,28,28	0
87	OHX	6	2066	7/7	0.11	-2.04	91,91,91,91	0
86	MG	5	3635	1/1	0.14	-2.04	37,37,37,37	0
86	MG	1	3727	1/1	0.14	-2.04	31,31,31,31	0
87	OHX	2	2038	7/7	0.10	-2.04	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	2	2155	7/7	0.11	-2.05	208,208,208,208	0
86	MG	M3	202	1/1	0.14	-2.05	36,36,36,36	0
87	OHX	1	3946	7/7	0.09	-2.05	97,97,97,97	0
87	OHX	m5	303	7/7	0.14	-2.05	111,111,111,111	0
87	OHX	5	4088	7/7	0.14	-2.06	99,99,99,99	0
88	ZN	d6	101	1/1	0.10	-2.07	54,54,54,54	0
87	OHX	M5	303	7/7	0.12	-2.08	104,104,104,104	0
86	MG	q3	503	1/1	0.15	-2.08	56,56,56,56	0
87	OHX	C5	201	7/7	0.17	-2.09	151,151,151,151	0
87	OHX	5	3971	7/7	0.11	-2.09	87,87,87,87	0
86	MG	1	3781	1/1	0.13	-2.09	43,43,43,43	0
86	MG	1	3604	1/1	0.14	-2.10	33,33,33,33	0
87	OHX	2	2089	7/7	0.12	-2.12	114,114,114,114	0
87	OHX	5	4067	7/7	0.11	-2.12	106,106,106,106	0
87	OHX	3	218	7/7	0.06	-2.12	108,108,108,108	0
87	OHX	o2	201	7/7	0.08	-2.12	85,85,85,85	0
86	MG	1	3641	1/1	0.12	-2.12	35,35,35,35	0
86	MG	5	3799	1/1	0.11	-2.13	41,41,41,41	0
87	OHX	5	3959	7/7	0.11	-2.14	78,78,78,78	0
87	OHX	5	3955	7/7	0.10	-2.15	83,83,83,83	0
87	OHX	M0	303	7/7	0.11	-2.16	101,101,101,101	0
87	OHX	5	4085	7/7	0.11	-2.16	124,124,124,124	0
87	OHX	1	3910	7/7	0.10	-2.17	75,75,75,75	0
87	OHX	1	4086	7/7	0.16	-2.20	113,113,113,113	0
87	OHX	1	4074	7/7	0.11	-2.20	111,111,111,111	0
86	MG	5	3821	1/1	0.12	-2.20	52,52,52,52	0
86	MG	5	3707	1/1	0.11	-2.21	36,36,36,36	0
87	OHX	4	225	7/7	0.11	-2.22	69,69,69,69	0
87	OHX	1	4105	7/7	0.11	-2.22	130,130,130,130	0
87	OHX	2	2070	7/7	0.09	-2.22	112,112,112,112	0
87	OHX	1	3876	7/7	0.14	-2.22	53,53,53,53	0
86	MG	5	3833	1/1	0.08	-2.23	64,64,64,64	0
87	OHX	1	4006	7/7	0.15	-2.23	90,90,90,90	0
86	MG	1	3719	1/1	0.13	-2.23	31,31,31,31	0
86	MG	1	3738	1/1	0.14	-2.24	52,52,52,52	0
87	OHX	1	4085	7/7	0.07	-2.24	166,166,166,166	0
87	OHX	1	4034	7/7	0.05	-2.25	134,134,134,134	0
86	MG	5	3847	1/1	0.10	-2.25	52,52,52,52	0
87	OHX	5	4072	7/7	0.14	-2.25	114,114,114,114	0
87	OHX	6	2052	7/7	0.14	-2.25	64,64,64,64	0
87	OHX	6	2098	7/7	0.07	-2.26	128,128,128,128	0
87	OHX	5	3947	7/7	0.14	-2.26	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	c1	201	1/1	0.11	-2.26	42,42,42,42	0
87	OHX	1	4014	7/7	0.14	-2.27	107,107,107,107	0
87	OHX	2	2093	7/7	0.06	-2.27	142,142,142,142	0
87	OHX	5	4084	7/7	0.15	-2.27	104,104,104,104	0
87	OHX	1	4047	7/7	0.12	-2.27	108,108,108,108	0
87	OHX	5	4101	7/7	0.10	-2.28	130,130,130,130	0
86	MG	5	3559	1/1	0.15	-2.29	45,45,45,45	0
87	OHX	1	3904	7/7	0.14	-2.29	78,78,78,78	0
86	MG	2	1997	1/1	0.13	-2.29	91,91,91,91	0
86	MG	1	3723	1/1	0.12	-2.31	48,48,48,48	0
86	MG	5	3771	1/1	0.15	-2.31	96,96,96,96	0
87	OHX	2	2041	7/7	0.10	-2.31	93,93,93,93	0
87	OHX	5	4015	7/7	0.10	-2.31	86,86,86,86	0
87	OHX	5	4043	7/7	0.13	-2.32	116,116,116,116	0
86	MG	5	3492	1/1	0.13	-2.35	46,46,46,46	0
86	MG	5	3748	1/1	0.12	-2.35	56,56,56,56	0
87	OHX	1	3980	7/7	0.13	-2.35	80,80,80,80	0
87	OHX	5	4132	7/7	0.13	-2.36	160,160,160,160	0
87	OHX	7	222	7/7	0.10	-2.36	114,114,114,114	0
86	MG	O7	102	1/1	0.16	-2.36	36,36,36,36	0
86	MG	5	3718	1/1	0.12	-2.37	51,51,51,51	0
87	OHX	1	4049	7/7	0.15	-2.37	102,102,102,102	0
87	OHX	1	4032	7/7	0.13	-2.38	98,98,98,98	0
86	MG	m6	201	1/1	0.10	-2.38	27,27,27,27	0
87	OHX	6	2124	7/7	0.10	-2.38	126,126,126,126	0
86	MG	5	3716	1/1	0.12	-2.39	41,41,41,41	0
87	OHX	3	221	7/7	0.10	-2.39	125,125,125,125	0
86	MG	1	3852	1/1	0.14	-2.40	23,23,23,23	0
86	MG	1	3824	1/1	0.13	-2.40	55,55,55,55	0
87	OHX	1	4065	7/7	0.08	-2.41	131,131,131,131	0
87	OHX	1	3935	7/7	0.13	-2.41	86,86,86,86	0
87	OHX	5	4116	7/7	0.13	-2.41	135,135,135,135	0
87	OHX	1	4036	7/7	0.10	-2.41	128,128,128,128	0
87	OHX	1	4003	7/7	0.15	-2.41	97,97,97,97	0
87	OHX	2	2096	7/7	0.07	-2.41	145,145,145,145	0
87	OHX	5	4104	7/7	0.10	-2.42	119,119,119,119	0
86	MG	5	3853	1/1	0.11	-2.42	53,53,53,53	0
87	OHX	6	2058	7/7	0.13	-2.43	73,73,73,73	0
86	MG	6	1988	1/1	0.13	-2.43	39,39,39,39	0
87	OHX	C3	202	7/7	0.13	-2.44	152,152,152,152	0
87	OHX	5	4036	7/7	0.12	-2.44	110,110,110,110	0
86	MG	1	3827	1/1	0.12	-2.45	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	1	3692	1/1	0.14	-2.45	34,34,34,34	0
86	MG	5	3735	1/1	0.14	-2.45	38,38,38,38	0
87	OHX	2	2057	7/7	0.10	-2.46	99,99,99,99	0
87	OHX	2	2079	7/7	0.09	-2.46	139,139,139,139	0
86	MG	6	1998	1/1	0.12	-2.46	47,47,47,47	0
87	OHX	2	2088	7/7	0.07	-2.47	101,101,101,101	0
87	OHX	1	3990	7/7	0.12	-2.48	93,93,93,93	0
86	MG	6	2003	1/1	0.11	-2.48	50,50,50,50	0
86	MG	M0	302	1/1	0.12	-2.48	40,40,40,40	0
87	OHX	1	4011	7/7	0.11	-2.48	116,116,116,116	0
87	OHX	6	2154	7/7	0.13	-2.50	129,129,129,129	0
87	OHX	6	2139	7/7	0.13	-2.51	109,109,109,109	0
86	MG	1	3525	1/1	0.13	-2.52	28,28,28,28	0
86	MG	1	4220	1/1	0.12	-2.52	41,41,41,41	0
87	OHX	1	3943	7/7	0.08	-2.52	84,84,84,84	0
87	OHX	1	3998	7/7	0.13	-2.53	104,104,104,104	0
87	OHX	5	4070	7/7	0.09	-2.55	119,119,119,119	0
86	MG	5	3412	1/1	0.15	-2.56	33,33,33,33	0
87	OHX	1	3921	7/7	0.14	-2.56	72,72,72,72	0
87	OHX	2	2065	7/7	0.08	-2.57	125,125,125,125	0
87	OHX	2	2037	7/7	0.12	-2.57	93,93,93,93	0
87	OHX	2	2053	7/7	0.08	-2.58	111,111,111,111	0
87	OHX	5	3958	7/7	0.08	-2.60	75,75,75,75	0
86	MG	1	3810	1/1	0.14	-2.60	33,33,33,33	0
86	MG	1	3779	1/1	0.14	-2.60	41,41,41,41	0
87	OHX	5	4090	7/7	0.13	-2.60	88,88,88,88	0
87	OHX	1	3938	7/7	0.15	-2.61	96,96,96,96	0
86	MG	6	2009	1/1	0.14	-2.63	45,45,45,45	0
87	OHX	5	4029	7/7	0.13	-2.63	86,86,86,86	0
86	MG	1	3406	1/1	0.14	-2.64	31,31,31,31	0
86	MG	5	3796	1/1	0.13	-2.65	63,63,63,63	0
87	OHX	6	2100	7/7	0.10	-2.69	135,135,135,135	0
87	OHX	5	4066	7/7	0.14	-2.69	102,102,102,102	0
86	MG	1	3662	1/1	0.10	-2.69	27,27,27,27	0
86	MG	c7	201	1/1	0.15	-2.69	64,64,64,64	0
87	OHX	2	2081	7/7	0.07	-2.69	127,127,127,127	0
87	OHX	1	3889	7/7	0.12	-2.70	67,67,67,67	0
87	OHX	1	3979	7/7	0.12	-2.71	101,101,101,101	0
87	OHX	5	4099	7/7	0.14	-2.71	106,106,106,106	0
87	OHX	1	4008	7/7	0.11	-2.72	112,112,112,112	0
87	OHX	1	4193	7/7	0.10	-2.72	161,161,161,161	0
87	OHX	6	2086	7/7	0.10	-2.72	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	5	3998	7/7	0.10	-2.73	107,107,107,107	0
87	OHX	2	2075	7/7	0.11	-2.74	111,111,111,111	0
87	OHX	5	4019	7/7	0.09	-2.75	114,114,114,114	0
87	OHX	5	4039	7/7	0.07	-2.75	117,117,117,117	0
87	OHX	5	4027	7/7	0.14	-2.76	91,91,91,91	0
86	MG	5	3698	1/1	0.10	-2.77	35,35,35,35	0
86	MG	5	3733	1/1	0.14	-2.78	46,46,46,46	0
87	OHX	5	3944	7/7	0.14	-2.78	73,73,73,73	0
87	OHX	1	3997	7/7	0.07	-2.78	127,127,127,127	0
86	MG	1	3818	1/1	0.09	-2.80	35,35,35,35	0
87	OHX	1	3994	7/7	0.07	-2.80	116,116,116,116	0
87	OHX	6	2120	7/7	0.09	-2.81	118,118,118,118	0
87	OHX	2	2080	7/7	0.10	-2.82	121,121,121,121	0
86	MG	6	1995	1/1	0.13	-2.83	44,44,44,44	0
86	MG	1	3643	1/1	0.12	-2.83	40,40,40,40	0
86	MG	sM	301	1/1	0.07	-2.83	37,37,37,37	0
87	OHX	7	218	7/7	0.12	-2.84	83,83,83,83	0
87	OHX	n3	203	7/7	0.07	-2.85	77,77,77,77	0
87	OHX	1	3982	7/7	0.09	-2.85	88,88,88,88	0
87	OHX	5	4025	7/7	0.08	-2.86	108,108,108,108	0
87	OHX	1	3890	7/7	0.11	-2.87	61,61,61,61	0
87	OHX	1	3887	7/7	0.12	-2.89	65,65,65,65	0
87	OHX	8	221	7/7	0.09	-2.89	115,115,115,115	0
86	MG	5	3474	1/1	0.14	-2.89	27,27,27,27	0
87	OHX	5	3992	7/7	0.10	-2.89	81,81,81,81	0
87	OHX	5	4006	7/7	0.09	-2.89	91,91,91,91	0
86	MG	1	3742	1/1	0.12	-2.89	34,34,34,34	0
87	OHX	o3	202	7/7	0.07	-2.90	98,98,98,98	0
87	OHX	2	2040	7/7	0.11	-2.90	88,88,88,88	0
87	OHX	1	3934	7/7	0.11	-2.90	90,90,90,90	0
87	OHX	5	4058	7/7	0.09	-2.91	115,115,115,115	0
87	OHX	1	4028	7/7	0.10	-2.92	117,117,117,117	0
87	OHX	6	2076	7/7	0.09	-2.92	78,78,78,78	0
86	MG	5	3513	1/1	0.10	-2.92	26,26,26,26	0
87	OHX	1	4002	7/7	0.08	-2.93	112,112,112,112	0
87	OHX	5	4049	7/7	0.15	-2.93	108,108,108,108	0
87	OHX	3	215	7/7	0.11	-2.97	89,89,89,89	0
86	MG	1	3758	1/1	0.10	-2.98	43,43,43,43	0
86	MG	1	3770	1/1	0.10	-2.98	35,35,35,35	0
87	OHX	1	4001	7/7	0.13	-2.99	87,87,87,87	0
87	OHX	1	3969	7/7	0.09	-3.00	94,94,94,94	0
87	OHX	8	222	7/7	0.07	-3.01	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	OHX	6	2111	7/7	0.13	-3.01	100,100,100,100	0
87	OHX	5	4052	7/7	0.11	-3.02	96,96,96,96	0
87	OHX	6	2112	7/7	0.09	-3.03	115,115,115,115	0
87	OHX	1	3962	7/7	0.12	-3.03	91,91,91,91	0
87	OHX	1	3914	7/7	0.10	-3.06	79,79,79,79	0
87	OHX	5	4046	7/7	0.11	-3.07	107,107,107,107	0
87	OHX	1	4060	7/7	0.08	-3.08	135,135,135,135	0
87	OHX	5	3978	7/7	0.09	-3.08	92,92,92,92	0
87	OHX	1	3966	7/7	0.08	-3.10	85,85,85,85	0
87	OHX	5	4013	7/7	0.14	-3.10	98,98,98,98	0
88	ZN	q3	501	1/1	0.06	-3.10	65,65,65,65	0
87	OHX	6	2061	7/7	0.11	-3.11	74,74,74,74	0
87	OHX	m6	202	7/7	0.10	-3.13	80,80,80,80	0
86	MG	5	3820	1/1	0.12	-3.14	52,52,52,52	0
86	MG	1	3534	1/1	0.15	-3.15	27,27,27,27	0
87	OHX	o7	103	7/7	0.10	-3.16	90,90,90,90	0
86	MG	5	3615	1/1	0.07	-3.16	27,27,27,27	0
87	OHX	1	3959	7/7	0.08	-3.17	101,101,101,101	0
87	OHX	2	2113	7/7	0.14	-3.18	137,137,137,137	0
87	OHX	2	2097	7/7	0.07	-3.19	138,138,138,138	0
87	OHX	5	3981	7/7	0.09	-3.19	93,93,93,93	0
87	OHX	1	3912	7/7	0.11	-3.20	78,78,78,78	0
86	MG	5	3430	1/1	0.13	-3.23	27,27,27,27	0
86	MG	1	3434	1/1	0.13	-3.23	39,39,39,39	0
86	MG	3	211	1/1	0.12	-3.25	69,69,69,69	0
87	OHX	7	217	7/7	0.12	-3.25	98,98,98,98	0
87	OHX	2	2067	7/7	0.10	-3.28	140,140,140,140	0
87	OHX	1	4155	7/7	0.12	-3.29	94,94,94,94	0
87	OHX	5	4022	7/7	0.09	-3.30	106,106,106,106	0
87	OHX	5	4010	7/7	0.12	-3.31	81,81,81,81	0
87	OHX	5	4033	7/7	0.13	-3.31	99,99,99,99	0
87	OHX	5	3925	7/7	0.11	-3.31	63,63,63,63	0
87	OHX	5	4065	7/7	0.07	-3.31	138,138,138,138	0
87	OHX	l3	402	7/7	0.06	-3.33	88,88,88,88	0
86	MG	1	3811	1/1	0.11	-3.33	45,45,45,45	0
87	OHX	6	2079	7/7	0.09	-3.36	87,87,87,87	0
87	OHX	2	2094	7/7	0.09	-3.37	132,132,132,132	0
86	MG	N5	201	1/1	0.14	-3.37	59,59,59,59	0
86	MG	1	3710	1/1	0.13	-3.38	30,30,30,30	0
87	OHX	5	4037	7/7	0.08	-3.38	116,116,116,116	0
87	OHX	5	4062	7/7	0.11	-3.39	95,95,95,95	0
87	OHX	1	4024	7/7	0.14	-3.39	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	3931	7/7	0.12	-3.40	59,59,59,59	0
87	OHX	1	4073	7/7	0.10	-3.41	113,113,113,113	0
87	OHX	5	4008	7/7	0.09	-3.41	113,113,113,113	0
86	MG	1	3441	1/1	0.12	-3.43	35,35,35,35	0
87	OHX	5	4055	7/7	0.13	-3.44	100,100,100,100	0
87	OHX	1	3967	7/7	0.10	-3.47	119,119,119,119	0
87	OHX	2	2045	7/7	0.08	-3.48	105,105,105,105	0
87	OHX	1	3958	7/7	0.09	-3.49	100,100,100,100	0
87	OHX	1	4018	7/7	0.12	-3.49	115,115,115,115	0
86	MG	1	3691	1/1	0.15	-3.51	29,29,29,29	0
87	OHX	2	2061	7/7	0.09	-3.52	107,107,107,107	0
87	OHX	1	3917	7/7	0.11	-3.52	77,77,77,77	0
86	MG	M5	302	1/1	0.11	-3.52	50,50,50,50	0
87	OHX	1	3874	7/7	0.17	-3.53	58,58,58,58	0
87	OHX	2	2071	7/7	0.07	-3.53	112,112,112,112	0
87	OHX	5	4061	7/7	0.08	-3.54	128,128,128,128	0
87	OHX	6	2107	7/7	0.10	-3.55	101,101,101,101	0
86	MG	5	3408	1/1	0.09	-3.55	22,22,22,22	0
87	OHX	2	2043	7/7	0.09	-3.57	89,89,89,89	0
87	OHX	5	4056	7/7	0.11	-3.58	97,97,97,97	0
86	MG	1	3646	1/1	0.07	-3.60	61,61,61,61	0
87	OHX	1	4048	7/7	0.08	-3.61	117,117,117,117	0
87	OHX	6	2104	7/7	0.10	-3.61	97,97,97,97	0
87	OHX	5	4002	7/7	0.10	-3.63	88,88,88,88	0
87	OHX	5	3936	7/7	0.12	-3.63	64,64,64,64	0
86	MG	8	210	1/1	0.09	-3.63	56,56,56,56	0
87	OHX	1	3978	7/7	0.08	-3.64	101,101,101,101	0
87	OHX	5	3984	7/7	0.09	-3.65	86,86,86,86	0
87	OHX	6	2123	7/7	0.09	-3.65	124,124,124,124	0
87	OHX	1	3930	7/7	0.10	-3.65	89,89,89,89	0
87	OHX	6	2155	7/7	0.11	-3.66	125,125,125,125	0
87	OHX	1	3909	7/7	0.14	-3.67	85,85,85,85	0
86	MG	4	201	1/1	0.15	-3.71	43,43,43,43	0
87	OHX	2	2050	7/7	0.10	-3.71	95,95,95,95	0
87	OHX	5	4051	7/7	0.07	-3.71	119,119,119,119	0
87	OHX	2	2076	7/7	0.10	-3.72	110,110,110,110	0
87	OHX	6	2097	7/7	0.08	-3.72	118,118,118,118	0
87	OHX	5	4103	7/7	0.09	-3.73	129,129,129,129	0
87	OHX	1	4051	7/7	0.11	-3.73	121,121,121,121	0
87	OHX	1	3925	7/7	0.09	-3.73	79,79,79,79	0
87	OHX	1	3975	7/7	0.11	-3.76	95,95,95,95	0
86	MG	1	3617	1/1	0.14	-3.76	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	4	227	7/7	0.07	-3.76	104,104,104,104	0
87	OHX	2	2044	7/7	0.07	-3.77	96,96,96,96	0
87	OHX	2	2058	7/7	0.09	-3.77	111,111,111,111	0
86	MG	6	2015	1/1	0.11	-3.79	41,41,41,41	0
87	OHX	1	3985	7/7	0.10	-3.79	109,109,109,109	0
87	OHX	5	4170	7/7	0.08	-3.82	164,164,164,164	0
87	OHX	5	4095	7/7	0.12	-3.83	113,113,113,113	0
87	OHX	5	4098	7/7	0.09	-3.84	123,123,123,123	0
87	OHX	1	3993	7/7	0.11	-3.85	90,90,90,90	0
87	OHX	1	4136	7/7	0.11	-3.85	97,97,97,97	0
86	MG	5	3602	1/1	0.14	-3.87	35,35,35,35	0
86	MG	4	214	1/1	0.11	-3.90	56,56,56,56	0
87	OHX	5	3926	7/7	0.12	-3.91	53,53,53,53	0
86	MG	5	3603	1/1	0.10	-3.92	53,53,53,53	0
87	OHX	5	4112	7/7	0.11	-3.93	112,112,112,112	0
86	MG	5	3661	1/1	0.12	-3.94	43,43,43,43	0
86	MG	5	3715	1/1	0.05	-3.94	65,65,65,65	0
87	OHX	5	3928	7/7	0.10	-3.95	68,68,68,68	0
86	MG	5	3640	1/1	0.08	-3.96	45,45,45,45	0
86	MG	1	3800	1/1	0.12	-3.98	52,52,52,52	0
87	OHX	5	4044	7/7	0.13	-3.98	109,109,109,109	0
86	MG	5	3798	1/1	0.15	-3.99	33,33,33,33	0
86	MG	M7	205	1/1	0.15	-4.00	35,35,35,35	0
87	OHX	6	2095	7/7	0.09	-4.00	114,114,114,114	0
86	MG	4	213	1/1	0.12	-4.03	37,37,37,37	0
86	MG	5	3773	1/1	0.07	-4.03	59,59,59,59	0
87	OHX	5	4059	7/7	0.07	-4.06	123,123,123,123	0
87	OHX	1	3988	7/7	0.09	-4.06	97,97,97,97	0
87	OHX	5	4041	7/7	0.09	-4.07	116,116,116,116	0
87	OHX	1	3892	7/7	0.11	-4.08	62,62,62,62	0
87	OHX	1	3907	7/7	0.11	-4.09	67,67,67,67	0
87	OHX	5	3961	7/7	0.12	-4.10	71,71,71,71	0
87	OHX	2	2103	7/7	0.08	-4.10	185,185,185,185	0
87	OHX	6	2087	7/7	0.11	-4.12	102,102,102,102	0
87	OHX	1	3963	7/7	0.10	-4.12	71,71,71,71	0
86	MG	5	3702	1/1	0.10	-4.13	52,52,52,52	0
86	MG	5	3691	1/1	0.12	-4.16	42,42,42,42	0
87	OHX	5	3960	7/7	0.11	-4.17	66,66,66,66	0
87	OHX	1	3882	7/7	0.12	-4.17	57,57,57,57	0
87	OHX	5	4122	7/7	0.09	-4.18	122,122,122,122	0
87	OHX	5	3917	7/7	0.12	-4.19	59,59,59,59	0
87	OHX	1	3971	7/7	0.10	-4.19	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	4010	7/7	0.11	-4.20	117,117,117,117	0
87	OHX	5	4004	7/7	0.11	-4.21	107,107,107,107	0
87	OHX	6	2070	7/7	0.09	-4.21	87,87,87,87	0
87	OHX	5	4024	7/7	0.11	-4.22	99,99,99,99	0
87	OHX	1	4093	7/7	0.09	-4.24	125,125,125,125	0
86	MG	5	3618	1/1	0.11	-4.25	32,32,32,32	0
87	OHX	6	2136	7/7	0.08	-4.26	127,127,127,127	0
87	OHX	6	2085	7/7	0.08	-4.27	105,105,105,105	0
86	MG	m5	301	1/1	0.10	-4.28	37,37,37,37	0
87	OHX	6	2115	7/7	0.11	-4.28	111,111,111,111	0
87	OHX	5	3987	7/7	0.08	-4.29	83,83,83,83	0
86	MG	5	3407	1/1	0.12	-4.30	34,34,34,34	0
87	OHX	5	4086	7/7	0.10	-4.30	106,106,106,106	0
87	OHX	1	3964	7/7	0.07	-4.31	93,93,93,93	0
87	OHX	5	4023	7/7	0.09	-4.32	98,98,98,98	0
87	OHX	5	3991	7/7	0.08	-4.33	96,96,96,96	0
87	OHX	1	3952	7/7	0.11	-4.34	92,92,92,92	0
87	OHX	5	4198	7/7	0.11	-4.35	76,76,76,76	0
87	OHX	2	2064	7/7	0.11	-4.35	95,95,95,95	0
86	MG	N8	201	1/1	0.08	-4.36	29,29,29,29	0
86	MG	5	3808	1/1	0.13	-4.38	36,36,36,36	0
87	OHX	5	4017	7/7	0.09	-4.40	101,101,101,101	0
87	OHX	5	3968	7/7	0.10	-4.42	83,83,83,83	0
87	OHX	2	2051	7/7	0.09	-4.44	108,108,108,108	0
87	OHX	7	219	7/7	0.12	-4.46	84,84,84,84	0
87	OHX	2	2060	7/7	0.07	-4.47	114,114,114,114	0
86	MG	1	3776	1/1	0.14	-4.47	46,46,46,46	0
87	OHX	5	4009	7/7	0.08	-4.47	70,70,70,70	0
87	OHX	1	4058	7/7	0.06	-4.50	143,143,143,143	0
86	MG	3	203	1/1	0.15	-4.51	84,84,84,84	0
87	OHX	6	2084	7/7	0.08	-4.52	108,108,108,108	0
87	OHX	6	2103	7/7	0.07	-4.53	106,106,106,106	0
87	OHX	5	3951	7/7	0.13	-4.55	76,76,76,76	0
87	OHX	6	2093	7/7	0.08	-4.56	105,105,105,105	0
87	OHX	5	3969	7/7	0.11	-4.57	84,84,84,84	0
87	OHX	1	4031	7/7	0.12	-4.58	112,112,112,112	0
86	MG	1	3688	1/1	0.16	-4.61	45,45,45,45	0
87	OHX	5	3977	7/7	0.09	-4.62	94,94,94,94	0
87	OHX	5	3943	7/7	0.11	-4.62	83,83,83,83	0
87	OHX	1	3968	7/7	0.09	-4.63	88,88,88,88	0
87	OHX	7	216	7/7	0.13	-4.64	79,79,79,79	0
87	OHX	1	4009	7/7	0.12	-4.68	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	3999	7/7	0.08	-4.71	96,96,96,96	0
86	MG	1	3523	1/1	0.09	-4.73	63,63,63,63	0
87	OHX	1	3992	7/7	0.07	-4.73	111,111,111,111	0
87	OHX	5	4007	7/7	0.09	-4.74	97,97,97,97	0
87	OHX	1	4022	7/7	0.06	-4.77	123,123,123,123	0
87	OHX	5	3938	7/7	0.12	-4.79	70,70,70,70	0
87	OHX	5	4012	7/7	0.10	-4.84	95,95,95,95	0
87	OHX	1	3957	7/7	0.09	-4.86	68,68,68,68	0
87	OHX	1	3923	7/7	0.10	-4.86	70,70,70,70	0
87	OHX	5	3930	7/7	0.13	-4.91	67,67,67,67	0
86	MG	5	3607	1/1	0.13	-4.93	22,22,22,22	0
87	OHX	6	2096	7/7	0.09	-4.94	111,111,111,111	0
86	MG	7	211	1/1	0.14	-4.94	67,67,67,67	0
86	MG	5	3845	1/1	0.16	-4.95	29,29,29,29	0
87	OHX	1	3902	7/7	0.09	-4.98	67,67,67,67	0
86	MG	1	3707	1/1	0.09	-4.98	54,54,54,54	0
87	OHX	5	3996	7/7	0.10	-5.00	99,99,99,99	0
87	OHX	1	3960	7/7	0.09	-5.00	89,89,89,89	0
86	MG	1	3772	1/1	0.12	-5.00	46,46,46,46	0
87	OHX	5	3997	7/7	0.11	-5.02	87,87,87,87	0
87	OHX	2	2055	7/7	0.07	-5.04	120,120,120,120	0
87	OHX	5	3982	7/7	0.10	-5.05	77,77,77,77	0
87	OHX	5	3972	7/7	0.07	-5.09	75,75,75,75	0
86	MG	8	202	1/1	0.11	-5.15	53,53,53,53	0
87	OHX	5	3942	7/7	0.10	-5.16	75,75,75,75	0
86	MG	1	3639	1/1	0.14	-5.16	55,55,55,55	0
87	OHX	6	2132	7/7	0.09	-5.17	129,129,129,129	0
86	MG	1	3476	1/1	0.11	-5.17	39,39,39,39	0
87	OHX	5	4026	7/7	0.09	-5.18	94,94,94,94	0
87	OHX	5	3973	7/7	0.09	-5.18	73,73,73,73	0
87	OHX	1	3956	7/7	0.08	-5.20	79,79,79,79	0
87	OHX	5	4131	7/7	0.08	-5.21	103,103,103,103	0
87	OHX	5	4130	7/7	0.07	-5.24	125,125,125,125	0
87	OHX	5	3929	7/7	0.12	-5.25	67,67,67,67	0
87	OHX	6	2099	7/7	0.09	-5.25	115,115,115,115	0
86	MG	5	3656	1/1	0.13	-5.28	53,53,53,53	0
87	OHX	1	3947	7/7	0.06	-5.28	92,92,92,92	0
87	OHX	3	220	7/7	0.08	-5.30	113,113,113,113	0
86	MG	5	3690	1/1	0.13	-5.30	35,35,35,35	0
87	OHX	1	3919	7/7	0.10	-5.30	73,73,73,73	0
87	OHX	6	2077	7/7	0.09	-5.32	96,96,96,96	0
86	MG	5	3870	1/1	0.09	-5.33	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	1	3900	7/7	0.12	-5.37	73,73,73,73	0
87	OHX	1	3879	7/7	0.12	-5.40	60,60,60,60	0
86	MG	1	3777	1/1	0.12	-5.46	31,31,31,31	0
86	MG	2	1984	1/1	0.10	-5.49	55,55,55,55	0
87	OHX	2	2069	7/7	0.08	-5.49	118,118,118,118	0
87	OHX	6	2064	7/7	0.09	-5.50	79,79,79,79	0
87	OHX	1	4017	7/7	0.07	-5.51	109,109,109,109	0
86	MG	6	1994	1/1	0.07	-5.52	46,46,46,46	0
87	OHX	1	3945	7/7	0.11	-5.58	82,82,82,82	0
87	OHX	1	4039	7/7	0.12	-5.59	99,99,99,99	0
87	OHX	2	2082	7/7	0.05	-5.59	123,123,123,123	0
87	OHX	3	219	7/7	0.07	-5.61	111,111,111,111	0
87	OHX	1	4178	7/7	0.11	-5.61	225,225,225,225	0
87	OHX	5	3979	7/7	0.10	-5.65	73,73,73,73	0
87	OHX	2	2059	7/7	0.11	-5.68	95,95,95,95	0
87	OHX	6	2131	7/7	0.10	-5.69	102,102,102,102	0
86	MG	4	216	1/1	0.08	-5.71	68,68,68,68	0
86	MG	5	3767	1/1	0.06	-5.75	51,51,51,51	0
87	OHX	1	3928	7/7	0.09	-5.76	78,78,78,78	0
86	MG	1	3819	1/1	0.12	-5.77	55,55,55,55	0
87	OHX	5	3964	7/7	0.09	-5.84	86,86,86,86	0
87	OHX	2	2054	7/7	0.08	-5.89	103,103,103,103	0
87	OHX	5	3919	7/7	0.13	-5.89	63,63,63,63	0
87	OHX	2	2049	7/7	0.10	-5.95	104,104,104,104	0
87	OHX	5	3935	7/7	0.12	-5.97	70,70,70,70	0
86	MG	1	3862	1/1	0.10	-6.00	60,60,60,60	0
86	MG	1	3629	1/1	0.07	-6.03	58,58,58,58	0
87	OHX	4	226	7/7	0.09	-6.10	85,85,85,85	0
87	OHX	5	4005	7/7	0.09	-6.11	84,84,84,84	0
86	MG	5	3827	1/1	0.13	-6.14	36,36,36,36	0
86	MG	1	3661	1/1	0.12	-6.15	26,26,26,26	0
87	OHX	1	3940	7/7	0.07	-6.17	82,82,82,82	0
87	OHX	6	2080	7/7	0.07	-6.18	97,97,97,97	0
87	OHX	6	2081	7/7	0.09	-6.31	91,91,91,91	0
87	OHX	5	3946	7/7	0.10	-6.34	71,71,71,71	0
86	MG	1	3607	1/1	0.07	-6.34	48,48,48,48	0
87	OHX	3	217	7/7	0.07	-6.42	98,98,98,98	0
87	OHX	3	216	7/7	0.09	-6.48	99,99,99,99	0
87	OHX	7	220	7/7	0.09	-6.48	94,94,94,94	0
87	OHX	6	2062	7/7	0.11	-6.50	73,73,73,73	0
86	MG	5	3751	1/1	0.09	-6.50	46,46,46,46	0
86	MG	5	3762	1/1	0.09	-6.51	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	4	212	1/1	0.17	-6.60	55,55,55,55	0
87	OHX	5	3994	7/7	0.12	-6.62	77,77,77,77	0
87	OHX	1	3893	7/7	0.12	-6.63	64,64,64,64	0
87	OHX	6	2091	7/7	0.07	-6.67	100,100,100,100	0
87	OHX	5	3954	7/7	0.07	-6.68	66,66,66,66	0
87	OHX	6	2069	7/7	0.10	-6.69	85,85,85,85	0
87	OHX	5	4031	7/7	0.10	-6.69	105,105,105,105	0
87	OHX	5	4016	7/7	0.10	-6.73	97,97,97,97	0
87	OHX	6	2088	7/7	0.07	-6.75	99,99,99,99	0
87	OHX	5	3965	7/7	0.09	-6.80	74,74,74,74	0
87	OHX	5	3921	7/7	0.13	-6.86	58,58,58,58	0
87	OHX	5	3983	7/7	0.08	-6.87	72,72,72,72	0
87	OHX	1	3911	7/7	0.12	-6.89	79,79,79,79	0
87	OHX	5	4071	7/7	0.10	-6.97	108,108,108,108	0
86	MG	5	3789	1/1	0.14	-7.03	45,45,45,45	0
86	MG	4	219	1/1	0.11	-7.07	36,36,36,36	0
87	OHX	6	2167	7/7	0.11	-7.14	133,133,133,133	0
87	OHX	1	4020	7/7	0.11	-7.14	107,107,107,107	0
86	MG	L7	303	1/1	0.13	-7.16	41,41,41,41	0
86	MG	5	3795	1/1	0.09	-7.16	39,39,39,39	0
87	OHX	5	3985	7/7	0.10	-7.21	83,83,83,83	0
86	MG	1	3706	1/1	0.10	-7.32	33,33,33,33	0
86	MG	2	1982	1/1	0.12	-7.35	70,70,70,70	0
86	MG	5	3728	1/1	0.06	-7.44	49,49,49,49	0
86	MG	5	3892	1/1	0.12	-7.48	25,25,25,25	0
87	OHX	1	4117	7/7	0.14	-7.55	112,112,112,112	0
87	OHX	5	4068	7/7	0.09	-7.57	114,114,114,114	0
87	OHX	1	3983	7/7	0.12	-7.67	83,83,83,83	0
86	MG	1	3858	1/1	0.11	-7.67	43,43,43,43	0
87	OHX	6	2073	7/7	0.09	-7.73	76,76,76,76	0
87	OHX	1	3972	7/7	0.09	-7.75	96,96,96,96	0
86	MG	5	3706	1/1	0.13	-7.86	47,47,47,47	0
87	OHX	2	2062	7/7	0.10	-7.86	116,116,116,116	0
87	OHX	6	2082	7/7	0.09	-7.89	91,91,91,91	0
87	OHX	5	4001	7/7	0.09	-7.91	101,101,101,101	0
86	MG	1	3728	1/1	0.08	-7.92	70,70,70,70	0
87	OHX	5	4021	7/7	0.11	-7.92	94,94,94,94	0
87	OHX	6	2063	7/7	0.10	-8.06	79,79,79,79	0
87	OHX	6	2083	7/7	0.07	-8.06	94,94,94,94	0
86	MG	6	2004	1/1	0.09	-8.18	67,67,67,67	0
87	OHX	6	2089	7/7	0.08	-8.27	107,107,107,107	0
87	OHX	5	4035	7/7	0.09	-8.27	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	OHX	5	3995	7/7	0.06	-8.32	107,107,107,107	0
87	OHX	1	3950	7/7	0.08	-8.56	87,87,87,87	0
86	MG	1	3848	1/1	0.09	-8.68	49,49,49,49	0
86	MG	1	3671	1/1	0.11	-8.86	44,44,44,44	0
86	MG	1	3715	1/1	0.10	-9.00	36,36,36,36	0
87	OHX	8	218	7/7	0.07	-9.06	118,118,118,118	0
86	MG	1	3823	1/1	0.13	-9.08	39,39,39,39	0
87	OHX	1	3954	7/7	0.08	-9.09	84,84,84,84	0
86	MG	5	3486	1/1	0.12	-9.12	41,41,41,41	0
86	MG	1	3796	1/1	0.10	-9.14	50,50,50,50	0
87	OHX	6	2105	7/7	0.07	-9.15	109,109,109,109	0
87	OHX	6	2094	7/7	0.09	-9.41	96,96,96,96	0
87	OHX	5	4048	7/7	0.12	-9.75	110,110,110,110	0
86	MG	5	3684	1/1	0.10	-9.80	33,33,33,33	0
87	OHX	1	3955	7/7	0.08	-9.81	92,92,92,92	0
86	MG	5	3810	1/1	0.09	-9.93	64,64,64,64	0
87	OHX	8	219	7/7	0.09	-10.33	114,114,114,114	0
87	OHX	1	3974	7/7	0.09	-10.85	99,99,99,99	0
87	OHX	5	4011	7/7	0.05	-10.96	105,105,105,105	0
86	MG	6	2032	1/1	0.09	-11.40	59,59,59,59	0
86	MG	5	3466	1/1	0.09	-11.43	34,34,34,34	0
86	MG	1	3640	1/1	0.07	-11.60	62,62,62,62	0
86	MG	5	3776	1/1	0.13	-12.02	31,31,31,31	0
86	MG	6	2002	1/1	0.09	-12.09	88,88,88,88	0
87	OHX	1	3987	7/7	0.07	-12.46	107,107,107,107	0
87	OHX	5	3986	7/7	0.06	-12.67	83,83,83,83	0
86	MG	6	2030	1/1	0.07	-12.73	96,96,96,96	0
86	MG	5	3678	1/1	0.06	-12.89	36,36,36,36	0
86	MG	6	1990	1/1	0.11	-13.12	37,37,37,37	0
87	OHX	1	3920	7/7	0.10	-13.48	80,80,80,80	0
87	OHX	1	3986	7/7	0.09	-14.17	103,103,103,103	0
86	MG	1	3631	1/1	0.10	-14.80	24,24,24,24	0
87	OHX	6	2071	7/7	0.09	-16.04	75,75,75,75	0
87	OHX	1	3939	7/7	0.08	-16.53	92,92,92,92	0
86	MG	1	3653	1/1	0.16	-17.00	69,69,69,69	0
87	OHX	1	3929	7/7	0.10	-19.44	75,75,75,75	0
86	MG	5	3671	1/1	0.08	-19.66	38,38,38,38	0
87	OHX	1	3936	7/7	0.07	-28.33	88,88,88,88	0
86	MG	5	3855	1/1	0.14	-33.00	59,59,59,59	0
86	MG	5	3818	1/1	0.11	-43.00	36,36,36,36	0
86	MG	1	3798	1/1	0.08	-67.00	88,88,88,88	0
86	MG	1	3755	1/1	0.28	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
86	MG	8	213	1/1	0.38	-	26,26,26,26	0
86	MG	5	3887	1/1	0.40	-	50,50,50,50	0
87	OHX	M9	202	7/7	0.25	-	149,149,149,149	0
86	MG	5	3758	1/1	0.15	-	36,36,36,36	0
86	MG	2	1989	1/1	0.23	-	107,107,107,107	0
86	MG	5	3898	1/1	0.29	-	117,117,117,117	0
86	MG	5	3886	1/1	0.15	-	56,56,56,56	0
86	MG	4	218	1/1	0.11	-	50,50,50,50	0
86	MG	5	3876	1/1	0.48	-	51,51,51,51	0
86	MG	6	2000	1/1	0.38	-	97,97,97,97	0
86	MG	1	3847	1/1	0.16	-	51,51,51,51	0
86	MG	2	1950	1/1	0.43	-	66,66,66,66	0
86	MG	1	3831	1/1	0.30	-	55,55,55,55	0
86	MG	6	1924	1/1	0.42	-	90,90,90,90	0
86	MG	2	1994	1/1	0.52	-	58,58,58,58	0
86	MG	6	2041	1/1	0.41	-	52,52,52,52	0
86	MG	5	3801	1/1	0.15	-	37,37,37,37	0
86	MG	1	3788	1/1	0.17	-	61,61,61,61	0
86	MG	6	2044	1/1	0.44	-	54,54,54,54	0
87	OHX	2	2157	7/7	0.13	-	291,291,291,291	0
86	MG	5	3879	1/1	0.35	-	42,42,42,42	0
86	MG	6	2045	1/1	0.34	-	67,67,67,67	0
86	MG	1	3791	1/1	0.21	-	49,49,49,49	0
86	MG	2	1968	1/1	0.29	-	83,83,83,83	0
86	MG	5	3888	1/1	0.55	-	84,84,84,84	0
86	MG	2	2019	1/1	0.46	-	64,64,64,64	0
86	MG	3	208	1/1	0.17	-	73,73,73,73	0
86	MG	1	3837	1/1	0.41	-	53,53,53,53	0
86	MG	1	3490	1/1	0.22	-	56,56,56,56	0
86	MG	5	3859	1/1	0.47	-	74,74,74,74	0
86	MG	5	3619	1/1	0.31	-	31,31,31,31	0
86	MG	4	202	1/1	0.36	-	50,50,50,50	0
86	MG	1	3857	1/1	0.49	-	104,104,104,104	0
86	MG	1	3500	1/1	0.37	-	61,61,61,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.