



wwPDB X-ray Structure Validation Summary Report i

Oct 9, 2014 – 10:21 PM BST

PDB ID : 4U3N
Title : Crystal structure of CCA trinucleotide bound to the yeast 80S ribosome
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on : 2014-07-22
Resolution : 3.20 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>

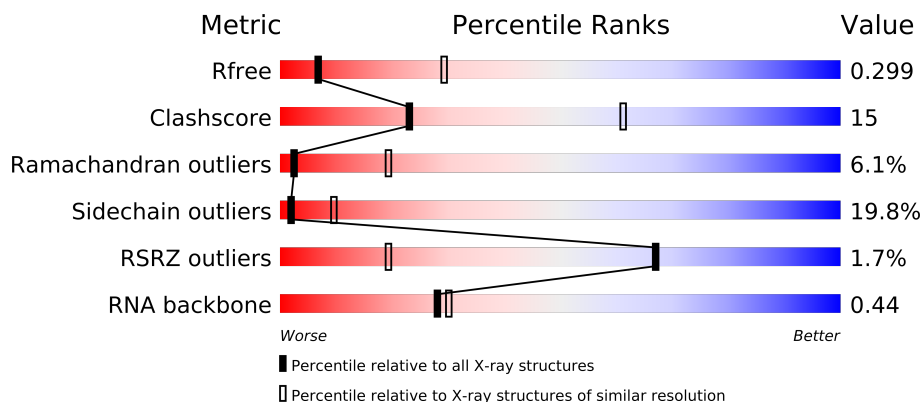
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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	
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	
28	D6	97	

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Mol	Chain	Length	Quality of chain
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	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	
50	M4	137	

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Mol	Chain	Length	Quality of chain
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	
71	O5	119	

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Mol	Chain	Length	Quality of chain
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	c0	105	
81	e0	62	
82	e1	76	
83	m2	160	
84	p0	311	
85	p1	47	
86	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
87	MG	1	3402	-	X
87	MG	1	3403	-	X
87	MG	1	3404	-	X
87	MG	1	3405	-	X
87	MG	1	3407	-	X
87	MG	1	3409	-	X
87	MG	1	3410	-	X
87	MG	1	3411	-	X
87	MG	1	3412	-	X
87	MG	1	3413	-	X
87	MG	1	3414	-	X
87	MG	1	3415	-	X
87	MG	1	3417	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	1	3418	-	X
87	MG	1	3419	-	X
87	MG	1	3420	-	X
87	MG	1	3422	-	X
87	MG	1	3424	-	X
87	MG	1	3425	-	X
87	MG	1	3428	-	X
87	MG	1	3430	-	X
87	MG	1	3431	-	X
87	MG	1	3432	-	X
87	MG	1	3433	-	X
87	MG	1	3434	-	X
87	MG	1	3437	-	X
87	MG	1	3438	-	X
87	MG	1	3439	-	X
87	MG	1	3440	-	X
87	MG	1	3441	-	X
87	MG	1	3443	-	X
87	MG	1	3445	-	X
87	MG	1	3446	-	X
87	MG	1	3448	-	X
87	MG	1	3449	-	X
87	MG	1	3451	-	X
87	MG	1	3452	-	X
87	MG	1	3454	-	X
87	MG	1	3455	-	X
87	MG	1	3456	-	X
87	MG	1	3457	-	X
87	MG	1	3458	-	X
87	MG	1	3459	-	X
87	MG	1	3460	-	X
87	MG	1	3461	-	X
87	MG	1	3462	-	X
87	MG	1	3463	-	X
87	MG	1	3464	-	X
87	MG	1	3465	-	X
87	MG	1	3466	-	X
87	MG	1	3469	-	X
87	MG	1	3470	-	X
87	MG	1	3471	-	X
87	MG	1	3472	-	X
87	MG	1	3473	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	1	3475	-	X
87	MG	1	3476	-	X
87	MG	1	3477	-	X
87	MG	1	3478	-	X
87	MG	1	3479	-	X
87	MG	1	3480	-	X
87	MG	1	3482	-	X
87	MG	1	3483	-	X
87	MG	1	3487	-	X
87	MG	1	3488	-	X
87	MG	1	3489	-	X
87	MG	1	3493	-	X
87	MG	1	3494	-	X
87	MG	1	3495	-	X
87	MG	1	3498	-	X
87	MG	1	3499	-	X
87	MG	1	3500	-	X
87	MG	1	3501	-	X
87	MG	1	3503	-	X
87	MG	1	3504	-	X
87	MG	1	3505	-	X
87	MG	1	3506	-	X
87	MG	1	3507	-	X
87	MG	1	3508	-	X
87	MG	1	3509	-	X
87	MG	1	3510	-	X
87	MG	1	3511	-	X
87	MG	1	3512	-	X
87	MG	1	3513	-	X
87	MG	1	3514	-	X
87	MG	1	3515	-	X
87	MG	1	3516	-	X
87	MG	1	3517	-	X
87	MG	1	3518	-	X
87	MG	1	3519	-	X
87	MG	1	3520	-	X
87	MG	1	3521	-	X
87	MG	1	3524	-	X
87	MG	1	3526	-	X
87	MG	1	3528	-	X
87	MG	1	3529	-	X
87	MG	1	3530	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	1	3531	-	X
87	MG	1	3532	-	X
87	MG	1	3533	-	X
87	MG	1	3534	-	X
87	MG	1	3535	-	X
87	MG	1	3536	-	X
87	MG	1	3537	-	X
87	MG	1	3538	-	X
87	MG	1	3540	-	X
87	MG	1	3541	-	X
87	MG	1	3542	-	X
87	MG	1	3544	-	X
87	MG	1	3545	-	X
87	MG	1	3546	-	X
87	MG	1	3548	-	X
87	MG	1	3550	-	X
87	MG	1	3551	-	X
87	MG	1	3552	-	X
87	MG	1	3553	-	X
87	MG	1	3554	-	X
87	MG	1	3555	-	X
87	MG	1	3556	-	X
87	MG	1	3557	-	X
87	MG	1	3558	-	X
87	MG	1	3559	-	X
87	MG	1	3561	-	X
87	MG	1	3562	-	X
87	MG	1	3563	-	X
87	MG	1	3564	-	X
87	MG	1	3565	-	X
87	MG	1	3566	-	X
87	MG	1	3568	-	X
87	MG	1	3569	-	X
87	MG	1	3570	-	X
87	MG	1	3571	-	X
87	MG	1	3572	-	X
87	MG	1	3574	-	X
87	MG	1	3575	-	X
87	MG	1	3576	-	X
87	MG	1	3577	-	X
87	MG	1	3578	-	X
87	MG	1	3579	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	1	3581	-	X
87	MG	1	3582	-	X
87	MG	1	3583	-	X
87	MG	1	3586	-	X
87	MG	1	3587	-	X
87	MG	1	3588	-	X
87	MG	1	3589	-	X
87	MG	1	3590	-	X
87	MG	1	3591	-	X
87	MG	1	3592	-	X
87	MG	1	3593	-	X
87	MG	1	3594	-	X
87	MG	1	3595	-	X
87	MG	1	3597	-	X
87	MG	1	3599	-	X
87	MG	1	3600	-	X
87	MG	1	3601	-	X
87	MG	1	3602	-	X
87	MG	1	3603	-	X
87	MG	1	3604	-	X
87	MG	1	3605	-	X
87	MG	1	3606	-	X
87	MG	1	3608	-	X
87	MG	1	3609	-	X
87	MG	1	3611	-	X
87	MG	1	3612	-	X
87	MG	1	3613	-	X
87	MG	1	3615	-	X
87	MG	1	3618	-	X
87	MG	1	3619	-	X
87	MG	1	3620	-	X
87	MG	1	3621	-	X
87	MG	1	3623	-	X
87	MG	1	3624	-	X
87	MG	1	3625	-	X
87	MG	1	3627	-	X
87	MG	1	3628	-	X
87	MG	1	3631	-	X
87	MG	1	3632	-	X
87	MG	1	3634	-	X
87	MG	1	3636	-	X
87	MG	1	3637	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	1	3638	-	X
87	MG	1	3639	-	X
87	MG	1	3641	-	X
87	MG	1	3643	-	X
87	MG	1	3645	-	X
87	MG	1	3646	-	X
87	MG	1	3647	-	X
87	MG	1	3648	-	X
87	MG	1	3649	-	X
87	MG	1	3650	-	X
87	MG	1	3651	-	X
87	MG	1	3652	-	X
87	MG	1	3653	-	X
87	MG	1	3656	-	X
87	MG	1	3657	-	X
87	MG	1	3658	-	X
87	MG	1	3659	-	X
87	MG	1	3660	-	X
87	MG	1	3661	-	X
87	MG	1	3662	-	X
87	MG	1	3663	-	X
87	MG	1	3668	-	X
87	MG	1	3669	-	X
87	MG	1	3670	-	X
87	MG	1	3671	-	X
87	MG	1	3672	-	X
87	MG	1	3673	-	X
87	MG	1	3674	-	X
87	MG	1	3675	-	X
87	MG	1	3676	-	X
87	MG	1	3677	-	X
87	MG	1	3680	-	X
87	MG	1	3681	-	X
87	MG	1	3682	-	X
87	MG	1	3685	-	X
87	MG	1	3686	-	X
87	MG	1	3687	-	X
87	MG	1	3688	-	X
87	MG	1	3689	-	X
87	MG	1	3691	-	X
87	MG	1	3692	-	X
87	MG	1	3693	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	1	3694	-	X
87	MG	1	3695	-	X
87	MG	1	3696	-	X
87	MG	1	3698	-	X
87	MG	1	3699	-	X
87	MG	1	3701	-	X
87	MG	1	3702	-	X
87	MG	1	3704	-	X
87	MG	1	3705	-	X
87	MG	1	3706	-	X
87	MG	1	3707	-	X
87	MG	1	3708	-	X
87	MG	1	3710	-	X
87	MG	1	3711	-	X
87	MG	1	3712	-	X
87	MG	1	3713	-	X
87	MG	1	3714	-	X
87	MG	1	3717	-	X
87	MG	1	3719	-	X
87	MG	1	3722	-	X
87	MG	1	3723	-	X
87	MG	1	3724	-	X
87	MG	1	3725	-	X
87	MG	1	3728	-	X
87	MG	1	3729	-	X
87	MG	1	3730	-	X
87	MG	1	3732	-	X
87	MG	1	3733	-	X
87	MG	1	3734	-	X
87	MG	1	3735	-	X
87	MG	1	3736	-	X
87	MG	1	3737	-	X
87	MG	1	3739	-	X
87	MG	1	3742	-	X
87	MG	1	3743	-	X
87	MG	1	3744	-	X
87	MG	1	3748	-	X
87	MG	1	3749	-	X
87	MG	1	3751	-	X
87	MG	1	3752	-	X
87	MG	1	3753	-	X
87	MG	1	3755	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	1	3756	-	X
87	MG	1	3759	-	X
87	MG	1	3760	-	X
87	MG	1	3761	-	X
87	MG	1	3763	-	X
87	MG	1	3764	-	X
87	MG	1	3765	-	X
87	MG	1	3766	-	X
87	MG	1	3767	-	X
87	MG	1	3771	-	X
87	MG	1	3772	-	X
87	MG	1	3777	-	X
87	MG	1	3778	-	X
87	MG	1	3779	-	X
87	MG	1	3780	-	X
87	MG	1	3781	-	X
87	MG	1	3782	-	X
87	MG	1	3785	-	X
87	MG	1	3786	-	X
87	MG	1	3787	-	X
87	MG	1	3788	-	X
87	MG	1	3790	-	X
87	MG	1	3791	-	X
87	MG	1	3792	-	X
87	MG	1	3793	-	X
87	MG	1	3794	-	X
87	MG	1	3795	-	X
87	MG	1	3797	-	X
87	MG	1	3798	-	X
87	MG	1	3799	-	X
87	MG	1	3801	-	X
87	MG	1	3802	-	X
87	MG	1	3803	-	X
87	MG	1	3804	-	X
87	MG	1	3806	-	X
87	MG	1	3811	-	X
87	MG	1	3812	-	X
87	MG	1	3816	-	X
87	MG	1	3819	-	X
87	MG	1	3820	-	X
87	MG	1	3821	-	X
87	MG	1	3822	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	1	3823	-	X
87	MG	1	3826	-	X
87	MG	1	3827	-	X
87	MG	1	3829	-	X
87	MG	1	3830	-	X
87	MG	1	3831	-	X
87	MG	1	3832	-	X
87	MG	1	3833	-	X
87	MG	1	3836	-	X
87	MG	1	3838	-	X
87	MG	1	3839	-	X
87	MG	1	3840	-	X
87	MG	1	3841	-	X
87	MG	1	3842	-	X
87	MG	1	3843	-	X
87	MG	1	3845	-	X
87	MG	1	3848	-	X
87	MG	1	3849	-	X
87	MG	1	3851	-	X
87	MG	1	3853	-	X
87	MG	1	3854	-	X
87	MG	1	3855	-	X
87	MG	1	3856	-	X
87	MG	1	3858	-	X
87	MG	1	3859	-	X
87	MG	1	3860	-	X
87	MG	1	3862	-	X
87	MG	1	3863	-	X
87	MG	1	3864	-	X
87	MG	1	3865	-	X
87	MG	1	3867	-	X
87	MG	1	3868	-	X
87	MG	1	3870	-	X
87	MG	1	3871	-	X
87	MG	1	3872	-	X
87	MG	1	4229	-	X
87	MG	1	4231	-	X
87	MG	1	4232	-	X
87	MG	2	1901	-	X
87	MG	2	1902	-	X
87	MG	2	1903	-	X
87	MG	2	1905	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	2	1906	-	X
87	MG	2	1907	-	X
87	MG	2	1908	-	X
87	MG	2	1909	-	X
87	MG	2	1910	-	X
87	MG	2	1911	-	X
87	MG	2	1912	-	X
87	MG	2	1913	-	X
87	MG	2	1914	-	X
87	MG	2	1915	-	X
87	MG	2	1916	-	X
87	MG	2	1917	-	X
87	MG	2	1918	-	X
87	MG	2	1919	-	X
87	MG	2	1921	-	X
87	MG	2	1922	-	X
87	MG	2	1923	-	X
87	MG	2	1924	-	X
87	MG	2	1925	-	X
87	MG	2	1926	-	X
87	MG	2	1928	-	X
87	MG	2	1929	-	X
87	MG	2	1930	-	X
87	MG	2	1931	-	X
87	MG	2	1932	-	X
87	MG	2	1933	-	X
87	MG	2	1934	-	X
87	MG	2	1935	-	X
87	MG	2	1936	-	X
87	MG	2	1937	-	X
87	MG	2	1938	-	X
87	MG	2	1939	-	X
87	MG	2	1941	-	X
87	MG	2	1942	-	X
87	MG	2	1945	-	X
87	MG	2	1946	-	X
87	MG	2	1948	-	X
87	MG	2	1949	-	X
87	MG	2	1951	-	X
87	MG	2	1952	-	X
87	MG	2	1955	-	X
87	MG	2	1957	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	2	1958	-	X
87	MG	2	1959	-	X
87	MG	2	1960	-	X
87	MG	2	1962	-	X
87	MG	2	1963	-	X
87	MG	2	1965	-	X
87	MG	2	1966	-	X
87	MG	2	1968	-	X
87	MG	2	1970	-	X
87	MG	2	1972	-	X
87	MG	2	1973	-	X
87	MG	2	1974	-	X
87	MG	2	1975	-	X
87	MG	2	1976	-	X
87	MG	2	1978	-	X
87	MG	2	1980	-	X
87	MG	2	1981	-	X
87	MG	2	1982	-	X
87	MG	2	1983	-	X
87	MG	2	1984	-	X
87	MG	2	1985	-	X
87	MG	2	1986	-	X
87	MG	2	1990	-	X
87	MG	2	1991	-	X
87	MG	2	1993	-	X
87	MG	2	2002	-	X
87	MG	2	2004	-	X
87	MG	2	2005	-	X
87	MG	2	2006	-	X
87	MG	2	2007	-	X
87	MG	2	2008	-	X
87	MG	2	2009	-	X
87	MG	2	2010	-	X
87	MG	2	2011	-	X
87	MG	2	2012	-	X
87	MG	2	2013	-	X
87	MG	2	2015	-	X
87	MG	2	2017	-	X
87	MG	2	2018	-	X
87	MG	2	2019	-	X
87	MG	2	2020	-	X
87	MG	2	2021	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	3	201	-	X
87	MG	3	202	-	X
87	MG	3	204	-	X
87	MG	3	205	-	X
87	MG	3	206	-	X
87	MG	3	208	-	X
87	MG	3	209	-	X
87	MG	3	210	-	X
87	MG	3	212	-	X
87	MG	3	213	-	X
87	MG	3	214	-	X
87	MG	4	201	-	X
87	MG	4	202	-	X
87	MG	4	204	-	X
87	MG	4	205	-	X
87	MG	4	206	-	X
87	MG	4	207	-	X
87	MG	4	209	-	X
87	MG	4	210	-	X
87	MG	4	211	-	X
87	MG	4	213	-	X
87	MG	4	217	-	X
87	MG	4	219	-	X
87	MG	5	3402	-	X
87	MG	5	3403	-	X
87	MG	5	3404	-	X
87	MG	5	3406	-	X
87	MG	5	3407	-	X
87	MG	5	3410	-	X
87	MG	5	3411	-	X
87	MG	5	3412	-	X
87	MG	5	3413	-	X
87	MG	5	3414	-	X
87	MG	5	3415	-	X
87	MG	5	3417	-	X
87	MG	5	3419	-	X
87	MG	5	3422	-	X
87	MG	5	3424	-	X
87	MG	5	3425	-	X
87	MG	5	3427	-	X
87	MG	5	3428	-	X
87	MG	5	3429	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3431	-	X
87	MG	5	3432	-	X
87	MG	5	3434	-	X
87	MG	5	3437	-	X
87	MG	5	3438	-	X
87	MG	5	3439	-	X
87	MG	5	3440	-	X
87	MG	5	3441	-	X
87	MG	5	3442	-	X
87	MG	5	3443	-	X
87	MG	5	3445	-	X
87	MG	5	3446	-	X
87	MG	5	3447	-	X
87	MG	5	3449	-	X
87	MG	5	3451	-	X
87	MG	5	3452	-	X
87	MG	5	3453	-	X
87	MG	5	3454	-	X
87	MG	5	3455	-	X
87	MG	5	3456	-	X
87	MG	5	3458	-	X
87	MG	5	3459	-	X
87	MG	5	3460	-	X
87	MG	5	3461	-	X
87	MG	5	3462	-	X
87	MG	5	3463	-	X
87	MG	5	3464	-	X
87	MG	5	3465	-	X
87	MG	5	3466	-	X
87	MG	5	3467	-	X
87	MG	5	3468	-	X
87	MG	5	3469	-	X
87	MG	5	3470	-	X
87	MG	5	3472	-	X
87	MG	5	3473	-	X
87	MG	5	3474	-	X
87	MG	5	3475	-	X
87	MG	5	3476	-	X
87	MG	5	3477	-	X
87	MG	5	3479	-	X
87	MG	5	3480	-	X
87	MG	5	3481	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3482	-	X
87	MG	5	3483	-	X
87	MG	5	3484	-	X
87	MG	5	3485	-	X
87	MG	5	3486	-	X
87	MG	5	3489	-	X
87	MG	5	3490	-	X
87	MG	5	3491	-	X
87	MG	5	3493	-	X
87	MG	5	3494	-	X
87	MG	5	3495	-	X
87	MG	5	3496	-	X
87	MG	5	3497	-	X
87	MG	5	3498	-	X
87	MG	5	3499	-	X
87	MG	5	3500	-	X
87	MG	5	3501	-	X
87	MG	5	3502	-	X
87	MG	5	3503	-	X
87	MG	5	3504	-	X
87	MG	5	3505	-	X
87	MG	5	3506	-	X
87	MG	5	3507	-	X
87	MG	5	3508	-	X
87	MG	5	3509	-	X
87	MG	5	3510	-	X
87	MG	5	3511	-	X
87	MG	5	3512	-	X
87	MG	5	3513	-	X
87	MG	5	3514	-	X
87	MG	5	3516	-	X
87	MG	5	3517	-	X
87	MG	5	3518	-	X
87	MG	5	3519	-	X
87	MG	5	3520	-	X
87	MG	5	3521	-	X
87	MG	5	3522	-	X
87	MG	5	3523	-	X
87	MG	5	3524	-	X
87	MG	5	3525	-	X
87	MG	5	3526	-	X
87	MG	5	3527	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3528	-	X
87	MG	5	3529	-	X
87	MG	5	3530	-	X
87	MG	5	3532	-	X
87	MG	5	3533	-	X
87	MG	5	3534	-	X
87	MG	5	3535	-	X
87	MG	5	3536	-	X
87	MG	5	3537	-	X
87	MG	5	3538	-	X
87	MG	5	3539	-	X
87	MG	5	3540	-	X
87	MG	5	3541	-	X
87	MG	5	3542	-	X
87	MG	5	3543	-	X
87	MG	5	3544	-	X
87	MG	5	3545	-	X
87	MG	5	3547	-	X
87	MG	5	3548	-	X
87	MG	5	3549	-	X
87	MG	5	3550	-	X
87	MG	5	3551	-	X
87	MG	5	3552	-	X
87	MG	5	3553	-	X
87	MG	5	3554	-	X
87	MG	5	3555	-	X
87	MG	5	3556	-	X
87	MG	5	3557	-	X
87	MG	5	3558	-	X
87	MG	5	3559	-	X
87	MG	5	3560	-	X
87	MG	5	3562	-	X
87	MG	5	3563	-	X
87	MG	5	3564	-	X
87	MG	5	3565	-	X
87	MG	5	3566	-	X
87	MG	5	3567	-	X
87	MG	5	3568	-	X
87	MG	5	3569	-	X
87	MG	5	3570	-	X
87	MG	5	3571	-	X
87	MG	5	3572	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3574	-	X
87	MG	5	3575	-	X
87	MG	5	3576	-	X
87	MG	5	3577	-	X
87	MG	5	3578	-	X
87	MG	5	3579	-	X
87	MG	5	3580	-	X
87	MG	5	3581	-	X
87	MG	5	3582	-	X
87	MG	5	3583	-	X
87	MG	5	3584	-	X
87	MG	5	3585	-	X
87	MG	5	3586	-	X
87	MG	5	3587	-	X
87	MG	5	3588	-	X
87	MG	5	3589	-	X
87	MG	5	3590	-	X
87	MG	5	3591	-	X
87	MG	5	3592	-	X
87	MG	5	3593	-	X
87	MG	5	3594	-	X
87	MG	5	3595	-	X
87	MG	5	3596	-	X
87	MG	5	3597	-	X
87	MG	5	3598	-	X
87	MG	5	3599	-	X
87	MG	5	3600	-	X
87	MG	5	3601	-	X
87	MG	5	3606	-	X
87	MG	5	3607	-	X
87	MG	5	3609	-	X
87	MG	5	3610	-	X
87	MG	5	3611	-	X
87	MG	5	3612	-	X
87	MG	5	3613	-	X
87	MG	5	3614	-	X
87	MG	5	3615	-	X
87	MG	5	3617	-	X
87	MG	5	3619	-	X
87	MG	5	3621	-	X
87	MG	5	3622	-	X
87	MG	5	3624	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3625	-	X
87	MG	5	3626	-	X
87	MG	5	3627	-	X
87	MG	5	3632	-	X
87	MG	5	3633	-	X
87	MG	5	3634	-	X
87	MG	5	3635	-	X
87	MG	5	3636	-	X
87	MG	5	3639	-	X
87	MG	5	3640	-	X
87	MG	5	3641	-	X
87	MG	5	3642	-	X
87	MG	5	3643	-	X
87	MG	5	3644	-	X
87	MG	5	3646	-	X
87	MG	5	3647	-	X
87	MG	5	3649	-	X
87	MG	5	3650	-	X
87	MG	5	3651	-	X
87	MG	5	3654	-	X
87	MG	5	3656	-	X
87	MG	5	3657	-	X
87	MG	5	3658	-	X
87	MG	5	3660	-	X
87	MG	5	3661	-	X
87	MG	5	3662	-	X
87	MG	5	3663	-	X
87	MG	5	3664	-	X
87	MG	5	3665	-	X
87	MG	5	3666	-	X
87	MG	5	3667	-	X
87	MG	5	3668	-	X
87	MG	5	3669	-	X
87	MG	5	3672	-	X
87	MG	5	3674	-	X
87	MG	5	3677	-	X
87	MG	5	3678	-	X
87	MG	5	3682	-	X
87	MG	5	3683	-	X
87	MG	5	3684	-	X
87	MG	5	3685	-	X
87	MG	5	3686	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3688	-	X
87	MG	5	3689	-	X
87	MG	5	3691	-	X
87	MG	5	3692	-	X
87	MG	5	3693	-	X
87	MG	5	3694	-	X
87	MG	5	3695	-	X
87	MG	5	3696	-	X
87	MG	5	3697	-	X
87	MG	5	3698	-	X
87	MG	5	3700	-	X
87	MG	5	3701	-	X
87	MG	5	3707	-	X
87	MG	5	3709	-	X
87	MG	5	3712	-	X
87	MG	5	3713	-	X
87	MG	5	3715	-	X
87	MG	5	3717	-	X
87	MG	5	3718	-	X
87	MG	5	3719	-	X
87	MG	5	3722	-	X
87	MG	5	3723	-	X
87	MG	5	3724	-	X
87	MG	5	3726	-	X
87	MG	5	3728	-	X
87	MG	5	3730	-	X
87	MG	5	3732	-	X
87	MG	5	3733	-	X
87	MG	5	3734	-	X
87	MG	5	3735	-	X
87	MG	5	3736	-	X
87	MG	5	3737	-	X
87	MG	5	3738	-	X
87	MG	5	3739	-	X
87	MG	5	3740	-	X
87	MG	5	3741	-	X
87	MG	5	3742	-	X
87	MG	5	3743	-	X
87	MG	5	3745	-	X
87	MG	5	3748	-	X
87	MG	5	3749	-	X
87	MG	5	3750	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3752	-	X
87	MG	5	3755	-	X
87	MG	5	3756	-	X
87	MG	5	3757	-	X
87	MG	5	3761	-	X
87	MG	5	3762	-	X
87	MG	5	3763	-	X
87	MG	5	3765	-	X
87	MG	5	3767	-	X
87	MG	5	3768	-	X
87	MG	5	3769	-	X
87	MG	5	3771	-	X
87	MG	5	3777	-	X
87	MG	5	3779	-	X
87	MG	5	3780	-	X
87	MG	5	3781	-	X
87	MG	5	3782	-	X
87	MG	5	3783	-	X
87	MG	5	3788	-	X
87	MG	5	3789	-	X
87	MG	5	3794	-	X
87	MG	5	3795	-	X
87	MG	5	3796	-	X
87	MG	5	3798	-	X
87	MG	5	3799	-	X
87	MG	5	3800	-	X
87	MG	5	3801	-	X
87	MG	5	3802	-	X
87	MG	5	3803	-	X
87	MG	5	3806	-	X
87	MG	5	3808	-	X
87	MG	5	3813	-	X
87	MG	5	3816	-	X
87	MG	5	3819	-	X
87	MG	5	3820	-	X
87	MG	5	3821	-	X
87	MG	5	3825	-	X
87	MG	5	3828	-	X
87	MG	5	3830	-	X
87	MG	5	3831	-	X
87	MG	5	3832	-	X
87	MG	5	3836	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3837	-	X
87	MG	5	3838	-	X
87	MG	5	3839	-	X
87	MG	5	3841	-	X
87	MG	5	3843	-	X
87	MG	5	3845	-	X
87	MG	5	3847	-	X
87	MG	5	3848	-	X
87	MG	5	3849	-	X
87	MG	5	3851	-	X
87	MG	5	3853	-	X
87	MG	5	3855	-	X
87	MG	5	3856	-	X
87	MG	5	3857	-	X
87	MG	5	3859	-	X
87	MG	5	3862	-	X
87	MG	5	3865	-	X
87	MG	5	3866	-	X
87	MG	5	3867	-	X
87	MG	5	3868	-	X
87	MG	5	3869	-	X
87	MG	5	3873	-	X
87	MG	5	3874	-	X
87	MG	5	3875	-	X
87	MG	5	3876	-	X
87	MG	5	3877	-	X
87	MG	5	3878	-	X
87	MG	5	3879	-	X
87	MG	5	3881	-	X
87	MG	5	3882	-	X
87	MG	5	3883	-	X
87	MG	5	3884	-	X
87	MG	5	3885	-	X
87	MG	5	3886	-	X
87	MG	5	3889	-	X
87	MG	5	3890	-	X
87	MG	5	3891	-	X
87	MG	5	3892	-	X
87	MG	5	3893	-	X
87	MG	5	3894	-	X
87	MG	5	3895	-	X
87	MG	5	3896	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	5	3897	-	X
87	MG	5	3898	-	X
87	MG	5	3899	-	X
87	MG	5	3900	-	X
87	MG	5	4260	-	X
87	MG	5	4261	-	X
87	MG	6	1901	-	X
87	MG	6	1902	-	X
87	MG	6	1903	-	X
87	MG	6	1904	-	X
87	MG	6	1905	-	X
87	MG	6	1906	-	X
87	MG	6	1907	-	X
87	MG	6	1908	-	X
87	MG	6	1909	-	X
87	MG	6	1910	-	X
87	MG	6	1911	-	X
87	MG	6	1912	-	X
87	MG	6	1913	-	X
87	MG	6	1914	-	X
87	MG	6	1915	-	X
87	MG	6	1916	-	X
87	MG	6	1917	-	X
87	MG	6	1918	-	X
87	MG	6	1919	-	X
87	MG	6	1920	-	X
87	MG	6	1921	-	X
87	MG	6	1922	-	X
87	MG	6	1925	-	X
87	MG	6	1926	-	X
87	MG	6	1927	-	X
87	MG	6	1928	-	X
87	MG	6	1929	-	X
87	MG	6	1930	-	X
87	MG	6	1931	-	X
87	MG	6	1932	-	X
87	MG	6	1933	-	X
87	MG	6	1934	-	X
87	MG	6	1935	-	X
87	MG	6	1936	-	X
87	MG	6	1937	-	X
87	MG	6	1938	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	6	1939	-	X
87	MG	6	1942	-	X
87	MG	6	1943	-	X
87	MG	6	1944	-	X
87	MG	6	1945	-	X
87	MG	6	1946	-	X
87	MG	6	1947	-	X
87	MG	6	1948	-	X
87	MG	6	1949	-	X
87	MG	6	1950	-	X
87	MG	6	1951	-	X
87	MG	6	1952	-	X
87	MG	6	1953	-	X
87	MG	6	1954	-	X
87	MG	6	1955	-	X
87	MG	6	1956	-	X
87	MG	6	1957	-	X
87	MG	6	1958	-	X
87	MG	6	1959	-	X
87	MG	6	1960	-	X
87	MG	6	1961	-	X
87	MG	6	1962	-	X
87	MG	6	1963	-	X
87	MG	6	1964	-	X
87	MG	6	1965	-	X
87	MG	6	1968	-	X
87	MG	6	1970	-	X
87	MG	6	1972	-	X
87	MG	6	1973	-	X
87	MG	6	1974	-	X
87	MG	6	1975	-	X
87	MG	6	1978	-	X
87	MG	6	1980	-	X
87	MG	6	1982	-	X
87	MG	6	1984	-	X
87	MG	6	1985	-	X
87	MG	6	1986	-	X
87	MG	6	1987	-	X
87	MG	6	1989	-	X
87	MG	6	1990	-	X
87	MG	6	1992	-	X
87	MG	6	1993	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	6	1994	-	X
87	MG	6	1999	-	X
87	MG	6	2003	-	X
87	MG	6	2004	-	X
87	MG	6	2006	-	X
87	MG	6	2007	-	X
87	MG	6	2008	-	X
87	MG	6	2009	-	X
87	MG	6	2012	-	X
87	MG	6	2015	-	X
87	MG	6	2016	-	X
87	MG	6	2018	-	X
87	MG	6	2020	-	X
87	MG	6	2025	-	X
87	MG	6	2026	-	X
87	MG	6	2028	-	X
87	MG	6	2029	-	X
87	MG	6	2031	-	X
87	MG	6	2032	-	X
87	MG	6	2033	-	X
87	MG	6	2034	-	X
87	MG	6	2035	-	X
87	MG	6	2037	-	X
87	MG	6	2038	-	X
87	MG	6	2039	-	X
87	MG	6	2040	-	X
87	MG	6	2042	-	X
87	MG	6	2043	-	X
87	MG	6	2203	-	X
87	MG	7	201	-	X
87	MG	7	202	-	X
87	MG	7	203	-	X
87	MG	7	205	-	X
87	MG	7	206	-	X
87	MG	7	208	-	X
87	MG	7	209	-	X
87	MG	7	210	-	X
87	MG	7	214	-	X
87	MG	7	227	-	X
87	MG	8	201	-	X
87	MG	8	202	-	X
87	MG	8	203	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	8	204	-	X
87	MG	8	205	-	X
87	MG	8	208	-	X
87	MG	8	209	-	X
87	MG	8	211	-	X
87	MG	8	213	-	X
87	MG	8	215	-	X
87	MG	L2	301	-	X
87	MG	L3	401	-	X
87	MG	L3	403	-	X
87	MG	L4	401	-	X
87	MG	L7	301	-	X
87	MG	L7	302	-	X
87	MG	L7	303	-	X
87	MG	L7	304	-	X
87	MG	M0	301	-	X
87	MG	M5	301	-	X
87	MG	M5	302	-	X
87	MG	M6	201	-	X
87	MG	M7	202	-	X
87	MG	N0	201	-	X
87	MG	N3	201	-	X
87	MG	N3	202	-	X
87	MG	N8	201	-	X
87	MG	N8	202	-	X
87	MG	N8	203	-	X
87	MG	N8	205	-	X
87	MG	O2	201	-	X
87	MG	O5	201	-	X
87	MG	O7	102	-	X
87	MG	S4	302	-	X
87	MG	S8	301	-	X
87	MG	c1	201	-	X
87	MG	c7	201	-	X
87	MG	c8	201	-	X
87	MG	d3	201	-	X
87	MG	l2	301	-	X
87	MG	l3	401	-	X
87	MG	l3	402	-	X
87	MG	l3	403	-	X
87	MG	l4	401	-	X
87	MG	l4	402	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
87	MG	l7	301	-	X
87	MG	m1	202	-	X
87	MG	m5	302	-	X
87	MG	m5	303	-	X
87	MG	m5	305	-	X
87	MG	m6	202	-	X
87	MG	m7	201	-	X
87	MG	m7	204	-	X
87	MG	n0	202	-	X
87	MG	n0	203	-	X
87	MG	n3	201	-	X
87	MG	n3	202	-	X
87	MG	n6	202	-	X
87	MG	n8	202	-	X
87	MG	o1	201	-	X
87	MG	o3	201	-	X
87	MG	o4	201	-	X
87	MG	q1	101	-	X
87	MG	q3	502	-	X
87	MG	s6	301	-	X
87	MG	s8	303	-	X
88	OHX	1	3919	-	X
88	OHX	1	3943	-	X
88	OHX	1	3963	-	X
88	OHX	1	3973	-	X
88	OHX	1	3989	-	X
88	OHX	1	3991	-	X
88	OHX	1	4015	-	X
88	OHX	1	4057	-	X
88	OHX	1	4058	-	X
88	OHX	1	4059	-	X
88	OHX	1	4074	-	X
88	OHX	1	4080	-	X
88	OHX	1	4082	-	X
88	OHX	1	4085	-	X
88	OHX	1	4090	-	X
88	OHX	1	4099	-	X
88	OHX	1	4123	-	X
88	OHX	1	4124	-	X
88	OHX	1	4125	-	X
88	OHX	1	4127	-	X
88	OHX	1	4132	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
88	OHX	1	4133	-	X
88	OHX	1	4138	-	X
88	OHX	1	4139	-	X
88	OHX	1	4140	-	X
88	OHX	1	4142	-	X
88	OHX	1	4146	-	X
88	OHX	1	4148	-	X
88	OHX	1	4149	-	X
88	OHX	1	4152	-	X
88	OHX	1	4153	-	X
88	OHX	1	4154	-	X
88	OHX	1	4155	-	X
88	OHX	1	4156	-	X
88	OHX	1	4159	-	X
88	OHX	1	4160	-	X
88	OHX	1	4166	-	X
88	OHX	1	4173	-	X
88	OHX	1	4176	-	X
88	OHX	1	4177	-	X
88	OHX	1	4180	-	X
88	OHX	1	4183	-	X
88	OHX	1	4184	-	X
88	OHX	1	4185	-	X
88	OHX	1	4186	-	X
88	OHX	1	4188	-	X
88	OHX	1	4189	-	X
88	OHX	1	4190	-	X
88	OHX	1	4191	-	X
88	OHX	1	4193	-	X
88	OHX	1	4196	-	X
88	OHX	1	4198	-	X
88	OHX	1	4200	-	X
88	OHX	1	4202	-	X
88	OHX	1	4203	-	X
88	OHX	1	4204	-	X
88	OHX	1	4206	-	X
88	OHX	1	4209	-	X
88	OHX	1	4210	-	X
88	OHX	1	4211	-	X
88	OHX	1	4212	-	X
88	OHX	1	4213	-	X
88	OHX	1	4215	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
88	OHX	1	4216	-	X
88	OHX	1	4217	-	X
88	OHX	1	4218	-	X
88	OHX	1	4219	-	X
88	OHX	1	4220	-	X
88	OHX	1	4221	-	X
88	OHX	1	4223	-	X
88	OHX	1	4225	-	X
88	OHX	2	2119	-	X
88	OHX	2	2120	-	X
88	OHX	2	2127	-	X
88	OHX	2	2128	-	X
88	OHX	2	2131	-	X
88	OHX	2	2136	-	X
88	OHX	2	2143	-	X
88	OHX	2	2146	-	X
88	OHX	2	2153	-	X
88	OHX	2	2157	-	X
88	OHX	2	2159	-	X
88	OHX	2	2160	-	X
88	OHX	2	2162	-	X
88	OHX	2	2163	-	X
88	OHX	2	2164	-	X
88	OHX	2	2169	-	X
88	OHX	2	2171	-	X
88	OHX	2	2172	-	X
88	OHX	2	2173	-	X
88	OHX	2	2176	-	X
88	OHX	2	2179	-	X
88	OHX	3	224	-	X
88	OHX	4	229	-	X
88	OHX	4	230	-	X
88	OHX	4	231	-	X
88	OHX	5	3917	-	X
88	OHX	5	3958	-	X
88	OHX	5	4006	-	X
88	OHX	5	4029	-	X
88	OHX	5	4046	-	X
88	OHX	5	4047	-	X
88	OHX	5	4054	-	X
88	OHX	5	4056	-	X
88	OHX	5	4065	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
88	OHX	5	4074	-	X
88	OHX	5	4075	-	X
88	OHX	5	4076	-	X
88	OHX	5	4079	-	X
88	OHX	5	4085	-	X
88	OHX	5	4086	-	X
88	OHX	5	4094	-	X
88	OHX	5	4096	-	X
88	OHX	5	4104	-	X
88	OHX	5	4130	-	X
88	OHX	5	4132	-	X
88	OHX	5	4141	-	X
88	OHX	5	4142	-	X
88	OHX	5	4143	-	X
88	OHX	5	4145	-	X
88	OHX	5	4146	-	X
88	OHX	5	4150	-	X
88	OHX	5	4152	-	X
88	OHX	5	4155	-	X
88	OHX	5	4157	-	X
88	OHX	5	4158	-	X
88	OHX	5	4160	-	X
88	OHX	5	4162	-	X
88	OHX	5	4163	-	X
88	OHX	5	4164	-	X
88	OHX	5	4165	-	X
88	OHX	5	4166	-	X
88	OHX	5	4169	-	X
88	OHX	5	4170	-	X
88	OHX	5	4174	-	X
88	OHX	5	4177	-	X
88	OHX	5	4180	-	X
88	OHX	5	4183	-	X
88	OHX	5	4184	-	X
88	OHX	5	4186	-	X
88	OHX	5	4188	-	X
88	OHX	5	4189	-	X
88	OHX	5	4190	-	X
88	OHX	5	4191	-	X
88	OHX	5	4192	-	X
88	OHX	5	4197	-	X
88	OHX	5	4200	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
88	OHX	5	4201	-	X
88	OHX	5	4204	-	X
88	OHX	5	4206	-	X
88	OHX	5	4207	-	X
88	OHX	5	4208	-	X
88	OHX	5	4209	-	X
88	OHX	5	4211	-	X
88	OHX	5	4212	-	X
88	OHX	5	4215	-	X
88	OHX	5	4216	-	X
88	OHX	5	4218	-	X
88	OHX	5	4219	-	X
88	OHX	5	4221	-	X
88	OHX	5	4223	-	X
88	OHX	5	4224	-	X
88	OHX	5	4226	-	X
88	OHX	5	4227	-	X
88	OHX	5	4229	-	X
88	OHX	5	4232	-	X
88	OHX	5	4234	-	X
88	OHX	5	4236	-	X
88	OHX	5	4237	-	X
88	OHX	5	4239	-	X
88	OHX	5	4240	-	X
88	OHX	5	4242	-	X
88	OHX	5	4244	-	X
88	OHX	5	4245	-	X
88	OHX	5	4252	-	X
88	OHX	5	4253	-	X
88	OHX	5	4254	-	X
88	OHX	5	4255	-	X
88	OHX	6	2045	-	X
88	OHX	6	2074	-	X
88	OHX	6	2107	-	X
88	OHX	6	2117	-	X
88	OHX	6	2122	-	X
88	OHX	6	2123	-	X
88	OHX	6	2143	-	X
88	OHX	6	2144	-	X
88	OHX	6	2156	-	X
88	OHX	6	2161	-	X
88	OHX	6	2168	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
88	OHX	6	2171	-	X
88	OHX	6	2174	-	X
88	OHX	6	2176	-	X
88	OHX	6	2181	-	X
88	OHX	6	2182	-	X
88	OHX	6	2184	-	X
88	OHX	6	2187	-	X
88	OHX	6	2188	-	X
88	OHX	6	2189	-	X
88	OHX	6	2196	-	X
88	OHX	6	2201	-	X
88	OHX	6	2202	-	X
88	OHX	7	224	-	X
88	OHX	7	225	-	X
88	OHX	7	226	-	X
88	OHX	8	227	-	X
88	OHX	8	229	-	X
88	OHX	M7	205	-	X
88	OHX	M7	206	-	X
88	OHX	14	404	-	X
88	OHX	15	306	-	X

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 411288 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence.

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 TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called Saccharomyces cerevisiae genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
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 S10-A.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 81 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S31.

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

- Molecule 83 is a protein called UNKNOWN PROTEIN m2.

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

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

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

- Molecule 85 is a protein called UNKNOWN PROTEIN p1.

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

- Molecule 86 is a protein called UNKNOWN PROTEIN p2.

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

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	L7	4	Total	Mg	0	0
			4	4		
87	n8	3	Total	Mg	0	0
			3	3		
87	o1	1	Total	Mg	0	0
			1	1		
87	N5	1	Total	Mg	0	0
			1	1		
87	6	144	Total	Mg	0	0
			144	144		
87	sM	1	Total	Mg	0	0
			1	1		
87	O4	1	Total	Mg	0	0
			1	1		
87	m5	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	l3	3	Total 3	Mg 3	0	0
87	M1	1	Total 1	Mg 1	0	0
87	d6	1	Total 1	Mg 1	0	0
87	2	124	Total 124	Mg 124	0	0
87	n0	3	Total 3	Mg 3	0	0
87	L4	1	Total 1	Mg 1	0	0
87	l7	1	Total 1	Mg 1	0	0
87	M5	2	Total 2	Mg 2	0	0
87	c9	1	Total 1	Mg 1	0	0
87	L8	1	Total 1	Mg 1	0	0
87	D3	1	Total 1	Mg 1	0	0
87	o4	1	Total 1	Mg 1	0	0
87	M9	1	Total 1	Mg 1	0	0
87	q0	1	Total 1	Mg 1	0	0
87	SM	1	Total 1	Mg 1	0	0
87	c8	1	Total 1	Mg 1	0	0
87	M0	2	Total 2	Mg 2	0	0
87	c1	1	Total 1	Mg 1	0	0
87	5	502	Total 502	Mg 502	0	0
87	L5	1	Total 1	Mg 1	0	0
87	O7	1	Total 1	Mg 1	0	0

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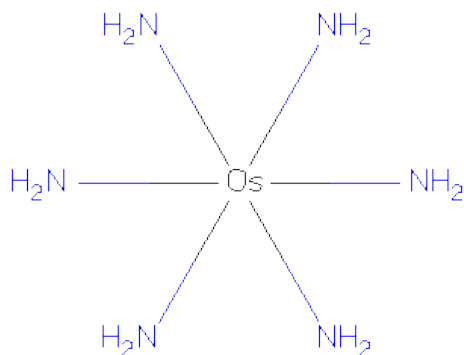
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	s6	1	Total 1	Mg 1	0	0
87	l4	2	Total 2	Mg 2	0	0
87	d4	1	Total 1	Mg 1	0	0
87	1	477	Total 477	Mg 477	0	0
87	d3	1	Total 1	Mg 1	0	0
87	S8	1	Total 1	Mg 1	0	0
87	m1	2	Total 2	Mg 2	0	0
87	O2	1	Total 1	Mg 1	0	0
87	q3	2	Total 2	Mg 2	0	0
87	o3	1	Total 1	Mg 1	0	0
87	M3	2	Total 2	Mg 2	0	0
87	N3	3	Total 3	Mg 3	0	0
87	4	19	Total 19	Mg 19	0	0
87	n6	2	Total 2	Mg 2	0	0
87	S4	2	Total 2	Mg 2	0	0
87	L2	1	Total 1	Mg 1	0	0
87	l5	2	Total 2	Mg 2	0	0
87	m7	5	Total 5	Mg 5	0	0
87	M7	4	Total 4	Mg 4	0	0
87	N8	5	Total 5	Mg 5	0	0
87	s1	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	m6	2	Total 2	Mg 2	0	0
87	s8	3	Total 3	Mg 3	0	0
87	c7	2	Total 2	Mg 2	0	0
87	7	15	Total 15	Mg 15	0	0
87	n3	2	Total 2	Mg 2	0	0
87	q1	1	Total 1	Mg 1	0	0
87	L3	3	Total 3	Mg 3	0	0
87	O5	1	Total 1	Mg 1	0	0
87	l2	1	Total 1	Mg 1	0	0
87	8	16	Total 16	Mg 16	0	0
87	M6	1	Total 1	Mg 1	0	0
87	N0	1	Total 1	Mg 1	0	0
87	3	14	Total 14	Mg 14	0	0

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
88	2	1	Total	N	Os	0	0
			7	6	1		
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	2	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	C3	1	Total	N	Os	0	0
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88	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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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	4	1	Total 7	N 6	Os 1	0	0
88	L3	1	Total 7	N 6	Os 1	0	0
88	L3	1	Total 7	N 6	Os 1	0	0
88	L3	1	Total 7	N 6	Os 1	0	0
88	L4	1	Total 7	N 6	Os 1	0	0
88	M0	1	Total 7	N 6	Os 1	0	0
88	M5	1	Total 7	N 6	Os 1	0	0
88	M7	1	Total 7	N 6	Os 1	0	0
88	M7	1	Total 7	N 6	Os 1	0	0
88	M8	1	Total 7	N 6	Os 1	0	0
88	M9	1	Total 7	N 6	Os 1	0	0
88	N9	1	Total 7	N 6	Os 1	0	0
88	O3	1	Total 7	N 6	Os 1	0	0
88	O7	1	Total 7	N 6	Os 1	0	0
88	O7	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	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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88	6	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	6	1	Total 7	N 6	Os 1	0	0
88	s1	1	Total 7	N 6	Os 1	0	0
88	s1	1	Total 7	N 6	Os 1	0	0
88	s8	1	Total 7	N 6	Os 1	0	0
88	c1	1	Total 7	N 6	Os 1	0	0
88	c3	1	Total 7	N 6	Os 1	0	0
88	c5	1	Total 7	N 6	Os 1	0	0
88	c8	1	Total 7	N 6	Os 1	0	0
88	d4	1	Total 7	N 6	Os 1	0	0
88	d9	1	Total 7	N 6	Os 1	0	0
88	sR	1	Total 7	N 6	Os 1	0	0
88	5	1	Total 7	N 6	Os 1	0	0

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	8	1	Total 7	N 6	Os 1	0	0
88	8	1	Total 7	N 6	Os 1	0	0
88	8	1	Total 7	N 6	Os 1	0	0
88	8	1	Total 7	N 6	Os 1	0	0
88	8	1	Total 7	N 6	Os 1	0	0
88	l3	1	Total 7	N 6	Os 1	0	0
88	l3	1	Total 7	N 6	Os 1	0	0
88	l3	1	Total 7	N 6	Os 1	0	0
88	l4	1	Total 7	N 6	Os 1	0	0
88	l4	1	Total 7	N 6	Os 1	0	0
88	l5	1	Total 7	N 6	Os 1	0	0
88	l5	1	Total 7	N 6	Os 1	0	0
88	l5	1	Total 7	N 6	Os 1	0	0
88	l5	1	Total 7	N 6	Os 1	0	0
88	l9	1	Total 7	N 6	Os 1	0	0
88	m0	1	Total 7	N 6	Os 1	0	0
88	m0	1	Total 7	N 6	Os 1	0	0
88	m1	1	Total 7	N 6	Os 1	0	0
88	m4	1	Total 7	N 6	Os 1	0	0
88	m5	1	Total 7	N 6	Os 1	0	0
88	m6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
88	n3	1	Total	N	Os	0	0
			7	6	1		
88	n3	1	Total	N	Os	0	0
			7	6	1		
88	n9	1	Total	N	Os	0	0
			7	6	1		
88	o3	1	Total	N	Os	0	0
			7	6	1		
88	o7	1	Total	N	Os	0	0
			7	6	1		
88	q2	1	Total	N	Os	0	0
			7	6	1		

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

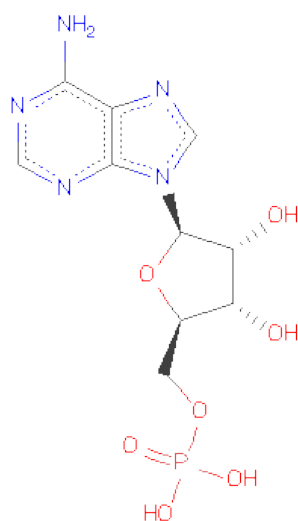
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	q0	1	Total	Zn	0	0
			1	1		
89	D6	1	Total	Zn	0	0
			1	1		
89	Q2	1	Total	Zn	0	0
			1	1		
89	e1	1	Total	Zn	0	0
			1	1		
89	Q3	1	Total	Zn	0	0
			1	1		
89	D9	1	Total	Zn	0	0
			1	1		
89	E1	1	Total	Zn	0	0
			1	1		
89	Q0	1	Total	Zn	0	0
			1	1		
89	d7	1	Total	Zn	0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

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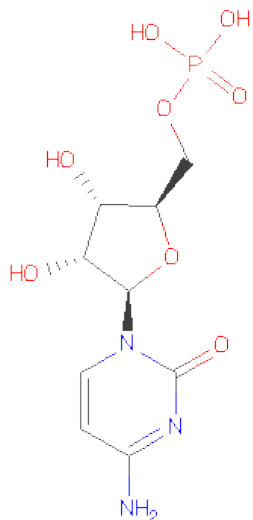
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
89	o7	1	Total	Zn	0	0
			1	1		
89	O7	1	Total	Zn	0	0
			1	1		
89	q2	1	Total	Zn	0	0
			1	1		

- Molecule 90 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
90	1	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
90	5	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 91 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).

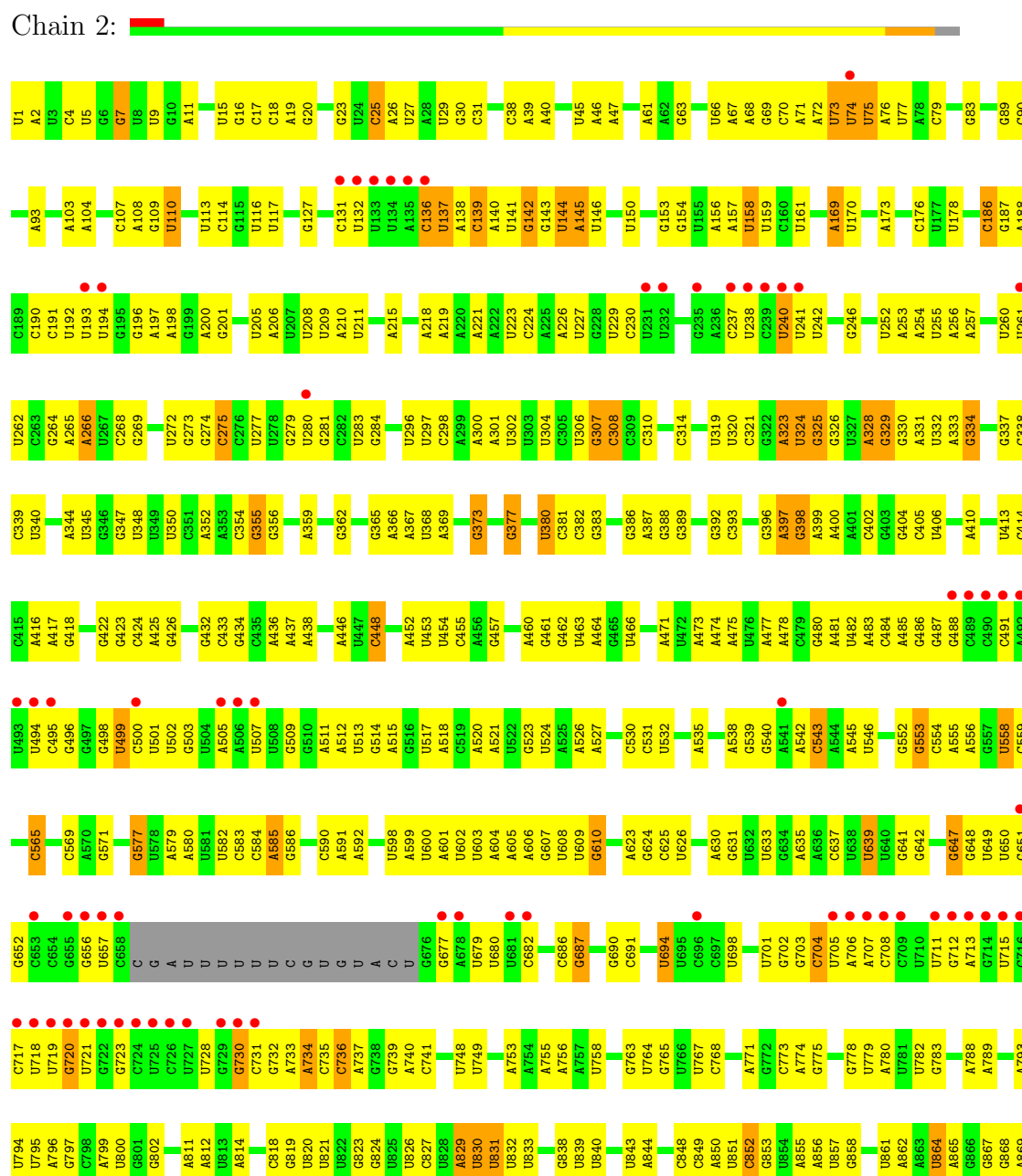


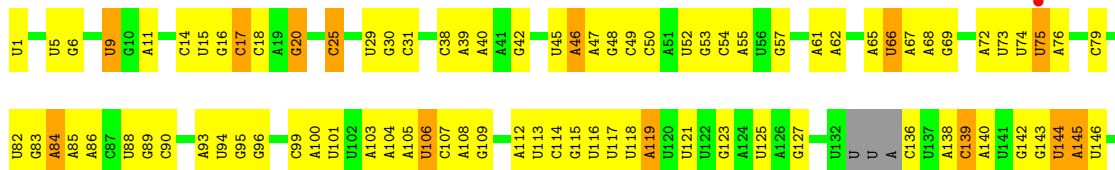
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	Q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		
91	q2	1	Total	C	N	O	P	0	0
			20	9	3	7	1		

3 Residue-property plots

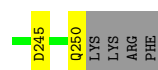
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 18S rRNA



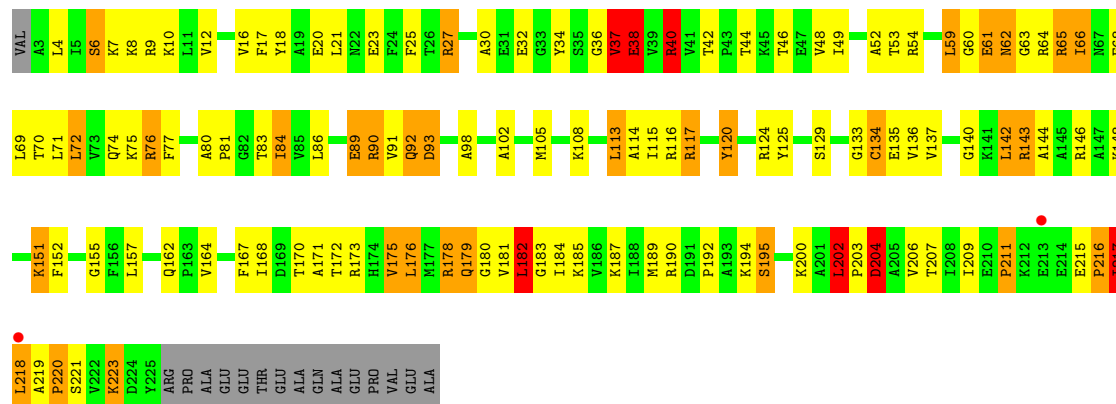


G1385	G1308	A1224	C1121	A1036	C956	G875	U805	G712	C637	A550	A483	U395	U320	C224	U150
U1389	C1309	U1225	G1126	C1037	G957	G876	A806	A713	G647	G557	C484	G396	U321	A225	G151
A1391	U1390	A1227	G1127	U1038	U958	G879	A807	G714	G648	G558	C485	A397	C321	A226	U152
U1392	A1312	G1228	G1130	G1041	U961	G880	A809	C716	U649	U558	G486	A399	G325	U227	G153
C1393	U1314	A1230	G1131	G1042	C962	A881	U813	C717	U650	U563	G487	A400	G329	G228	U155
G1394	U1315	U1231	A1133	C1045	A963	A884	A814	U718	G651	G564	C488		G330	U229	A156
U1396	G1316	U1232	C1134	G1050	A967	G885	G815	U719	G652	G565	C489		A331	C230	U157
U1397	U1135	G1233	U1136	G1060	A970	U886	G819	G721	C654	C566	C490		U332	U232	U158
U1398	A1137	G1063	A1137	U1059	A971	U887	U820	G722	G655	G568	C491		A333		C160
A1400	U1239	U1054	U1145	G1053	A974	A891	U821	U727	G656	C569	C407		G336	G235	U161
G1401	U1240	U1055	G1146	U1056	A974	A892	U822	U728	U657	A570	C408		G337	C237	A162
C1402	G1241	U1056	A1147	U1056	C975	A893	G823	U729	C658	G571	A416		C338	U238	G163
C1403	A1242	U1057	G1148	U1057	G976	U894	U825	G730	C659		G496		C339	C239	A164
	G1243	U1058	G1149	U1058	G976	U894	U826	A737	G660	G574	G497		U340	C239	G165
	U1059	U1059	G1150	U1059	U882	G895	U827	A738	G661	G574	G498		U341	U241	A168
	C1066	C1066	C1159	C1066	G985	G901	U828	G738	U662	G577	C500		C342		A169
	C1067	C1067	A1160	C1067	G986	G902	U829	A753	U663	U578	U501		C343	G246	U170
	C1068	C1068	C1161	C1068	G987	A905	U830	A754	U664	A579	U502		G346	A247	A171
	U1071	U1071	A1162	U1071	C990	A906	U831	A755	U665	U582	G503			U248	C176
	C1072	C1072	A1163	U1072	U911	U911	U832	A760	U666	C583	U507		U350	C250	U177
	G1073	G1073	G1164	C1073	U912	G912	U833	U764	U670	C584	U508		U351	A251	U178
	C1075	C1075	G1165	C1075	G913	G913	G837	G765	U670	C587	U508		U355	C258	A180
	C1076	C1076	G1166	C1076	G914	G914	G838	G766	U671	U588	G509		G356	U262	A181
	C1077	C1077	G1167	C1077	A915	A915	U839	U767	A673	A591	A511		G357	C263	C184
	C1078	C1078	A1171	C1078	U916	U916	U840	C768	C674	A592	U513		U358	G264	U185
	C1079	C1079	G1172	C1079	U917	U917	U841	C769	U675	C596	U514		A359	A285	G186
	U1080	U1080	C1173	U1080	A1002	A1002	U842	C770	U676				C361	A286	G187
	A1081	A1081	C1174	U1081	U1004	U1004	U843	A771	G677	U600	U517		G362	C276	C188
	C1082	C1082	A1176	C1082	C1006	C1006	U844	A772	A678	U600	U518		C363	U277	C190
	A1087	A1087	C1177	C1087	C1007	C1007	G845	A773	U679	A604	A521		A366		C191
	A1088	A1088	G1178	C1088	A923	A923	U847	G775	C682	U609	U522		A367	U280	U192
	A1091	A1091	C1180	C1091	A924	A924	C948	G776	C683	G610	G523		G371	G281	U193
	A1092	A1092	U1185	C1092	G925	G925	C949	G777	A684	U611	U524		G372	C282	U194
	U1095	U1095	U1185	C1095	A926	A926	G853	G778	A685	U612	A525		G373	U283	G195
	C1096	C1096	A1193	C1096	C927	C927	U854	A780	C686	G613	A526		G376	G291	G196
	U1097	U1097	A1198	C1097	U832	U832	G858	U781	U694	C614	A527		G377	U292	A197
	U1098	U1098	G1199	C1098	A933	A933	U859	G787	U695	A615	U528		C376	U293	U198
	U1099	U1099	G1200	C1099	C934	C934	U861	A788	C696	U616	A529		U380	C294	G199
	G1100	G1100	G1201	C1100	C937	C937	A862	A789	C697	U618	A534		A381	A206	A206
	C1101	C1101	A1202	C1101	A939	A939	U863	U792	C700	A619	A535		C382	A300	U209
	G1107	G1107	U1203	C1107	U840	U840	U864	A793	U701	A620	A538		G383	A301	A210
	U1108	U1108	G1212	C1108	A941	A941	A865	A794	G702	A621	A538		C384	C308	A213
	G1109	G1109	G1213	C1109	A942	A942	U866	U795	G703	A622	G539		A385	C309	G214
	G1111	G1111	U1214	C1111	A944	A944	G867	U796	C704	A623	G540		A386	C310	A215
	U1117	U1117	C1215	C1117	C950	C950	U868	A797	U705	G625	A541		A387	U311	U216
	G1118	G1118	G1216	C1118	A951	A951	C870	G797	U706	U626	A542		G390	A312	A217
	C1119	C1119	U1219	C1119	A952	A952	U871	U800	C708	A544	A544		C393	U313	A218
	U1120	U1120	G1220	C1120	A955	A955	U872	G801	C709	U629	A545		C394	C314	A219
							C874	A804	U711	G634	U547			C317	A221



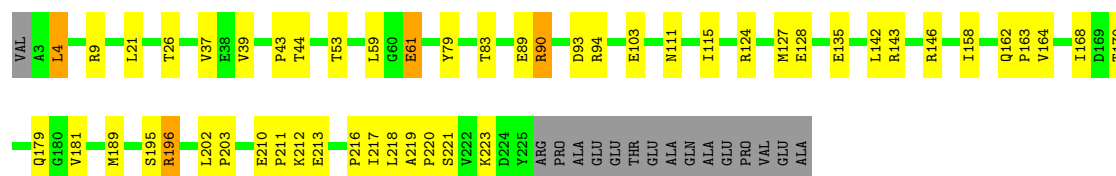
• Molecule 5: 40S ribosomal protein S3

Chain S3:



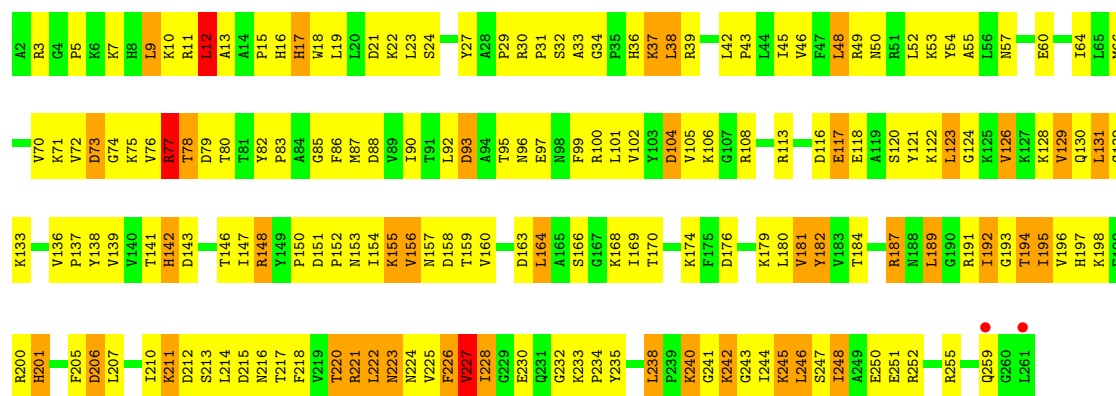
• Molecule 5: 40S ribosomal protein S3

Chain s3:



• Molecule 6: 40S ribosomal protein S4-A

Chain S4:



• Molecule 6: 40S ribosomal protein S4-A

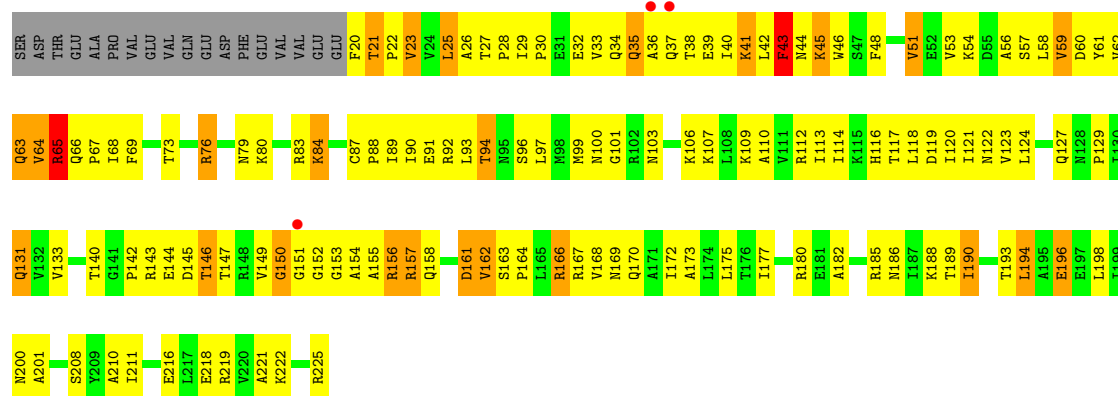
Chain s4:





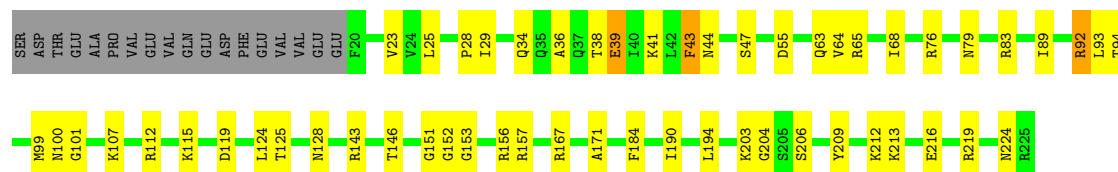
• Molecule 7: 40S ribosomal protein S5

Chain S5:



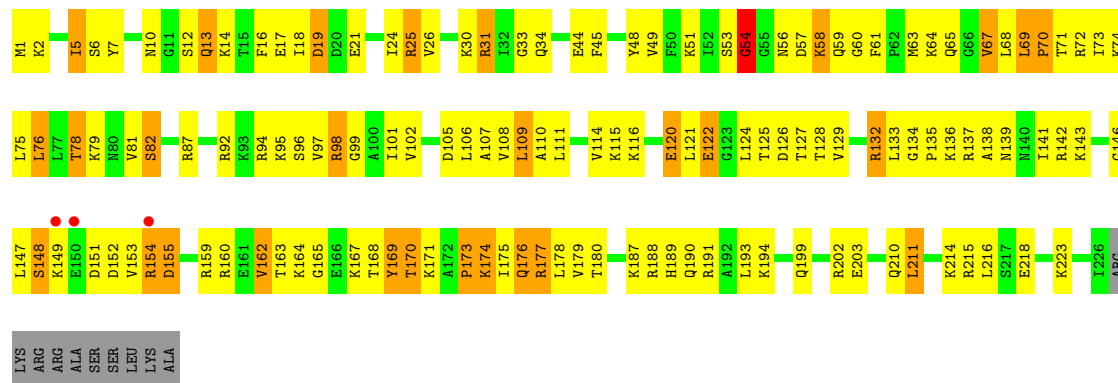
• Molecule 7: 40S ribosomal protein S5

Chain s5:



• Molecule 8: 40S ribosomal protein S6-A

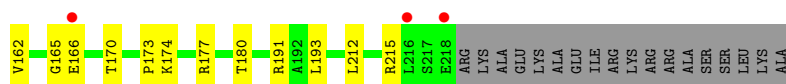
Chain S6:



• Molecule 8: 40S ribosomal protein S6-A

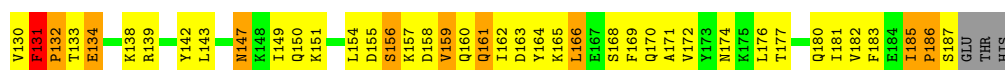
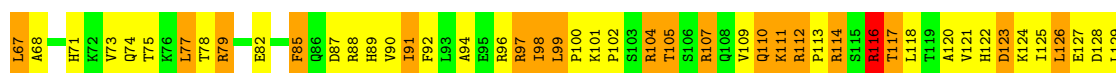
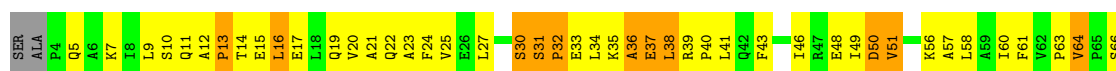
Chain s6:





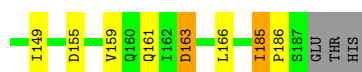
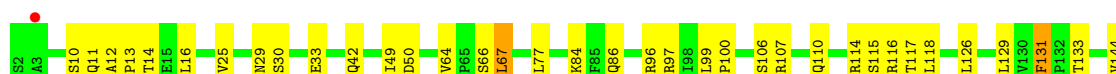
- Molecule 9: 40S ribosomal protein S7-A

Chain S7:



- Molecule 9: 40S ribosomal protein S7-A

Chain s7:



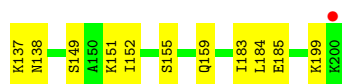
- Molecule 10: 40S ribosomal protein S8-A

Chain S8:



- Molecule 10: 40S ribosomal protein S8-A

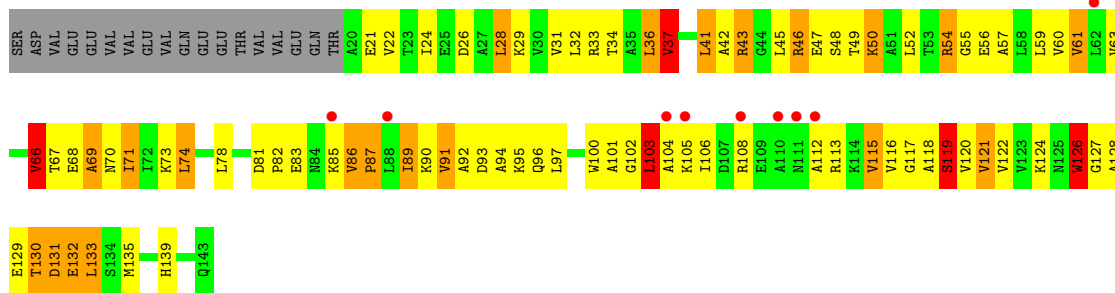
Chain s8:



- Molecule 11: 40S ribosomal protein S9-A

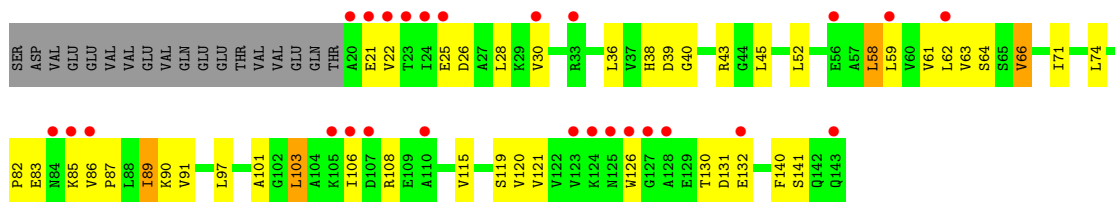
Chain S9:

Chain C2:



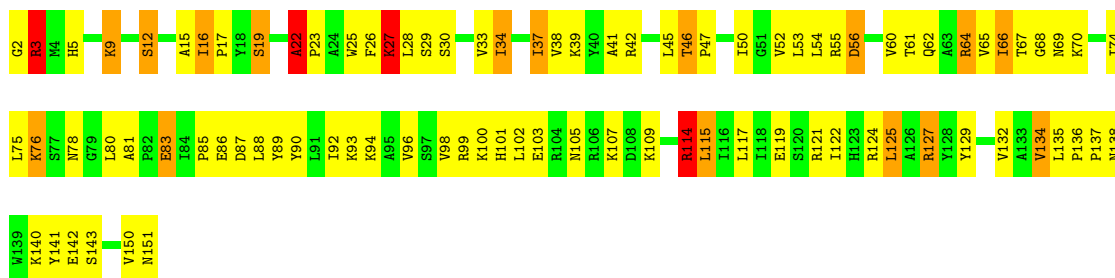
- Molecule 14: 40S ribosomal protein S12

Chain c2:



- Molecule 15: 40S ribosomal protein S13

Chain C3:



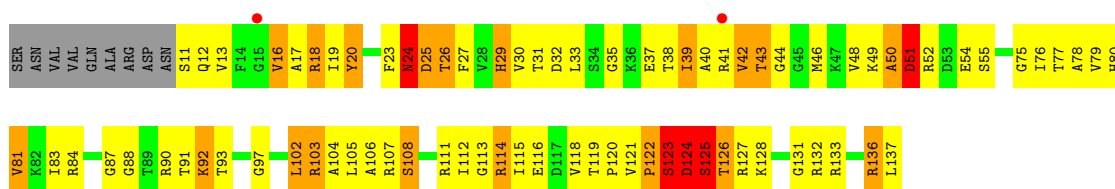
- Molecule 15: 40S ribosomal protein S13

Chain c3: 



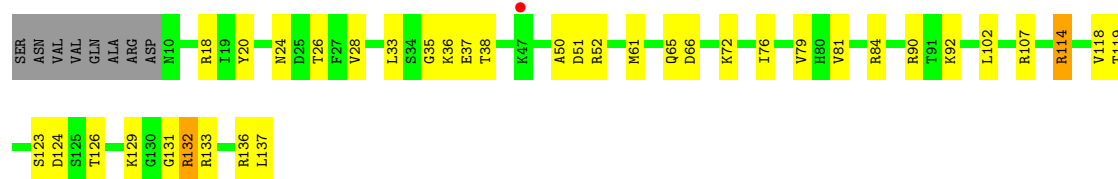
- Molecule 16: 40S ribosomal protein S14-A

Chain C4:



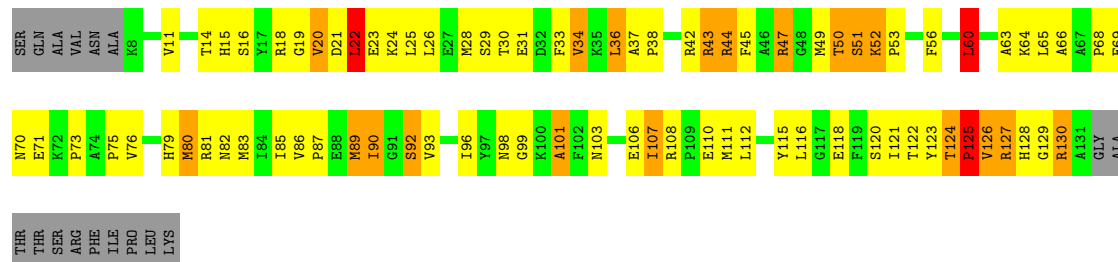
- Molecule 16: 40S ribosomal protein S14-A

Chain c4: 



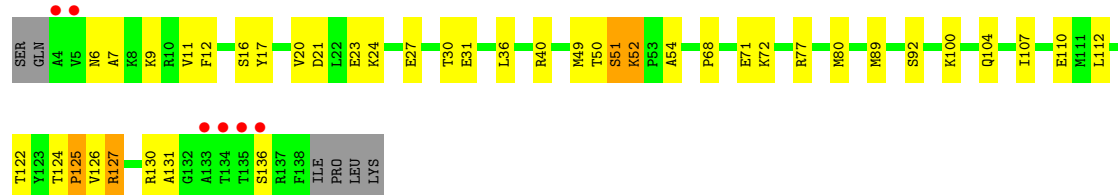
- Molecule 17: 40S ribosomal protein S15

Chain C5: 



- Molecule 17: 40S ribosomal protein S15

Chain c5: 



- Molecule 18: 40S ribosomal protein S16-A

Chain C6: 



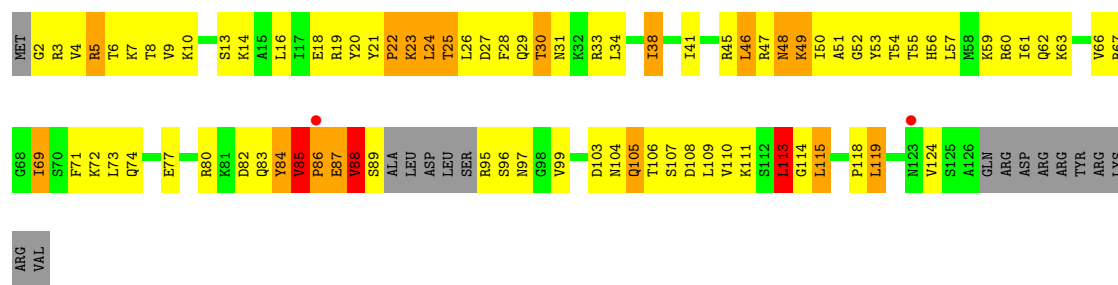
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 



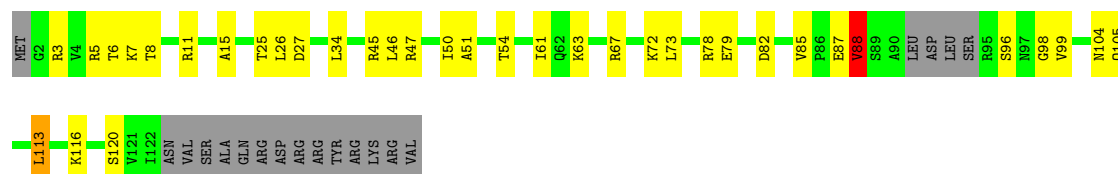
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 



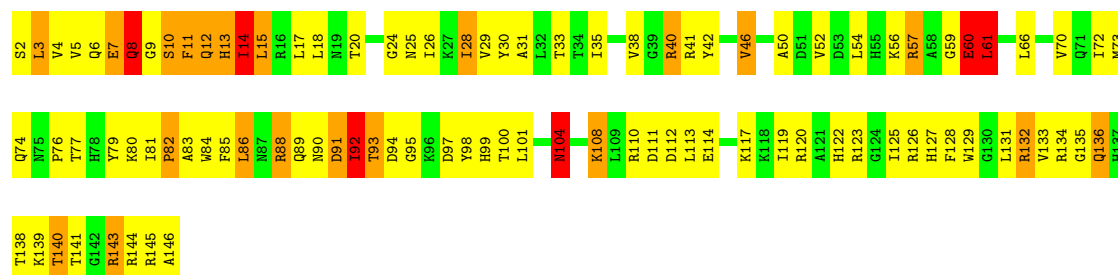
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:



- Molecule 20: 40S ribosomal protein S18-A

Chain C8:



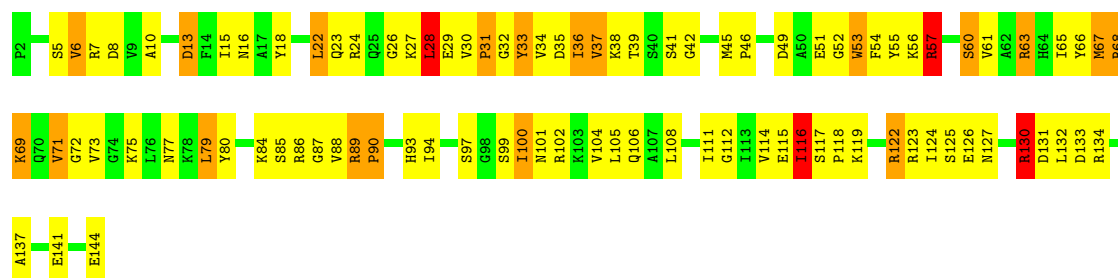
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



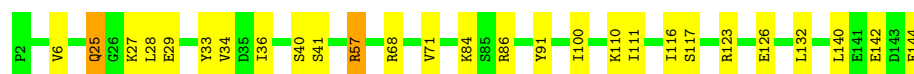
- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



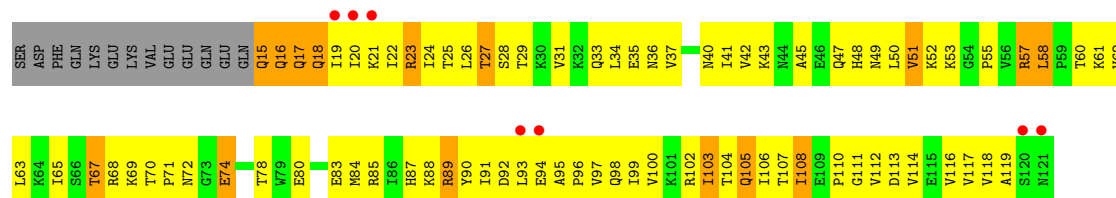
- Molecule 21: 40S ribosomal protein S19-A

Chain c9: 



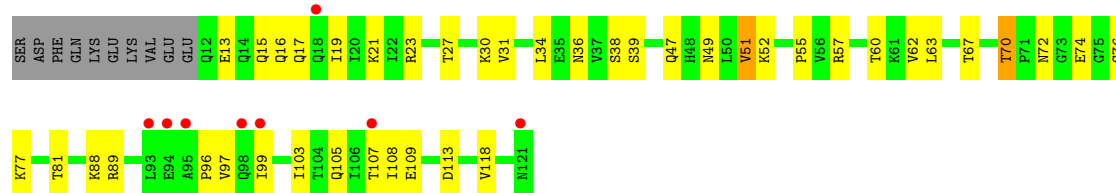
- Molecule 22: 40S ribosomal protein S20

Chain D0: 



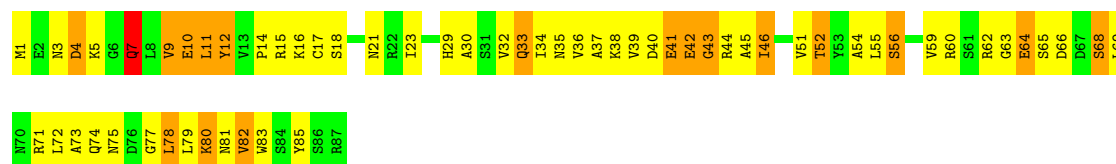
- Molecule 22: 40S ribosomal protein S20

Chain d0: 



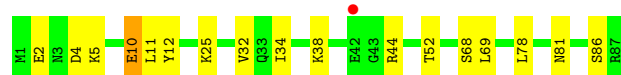
- Molecule 23: 40S ribosomal protein S21-A

Chain D1: 



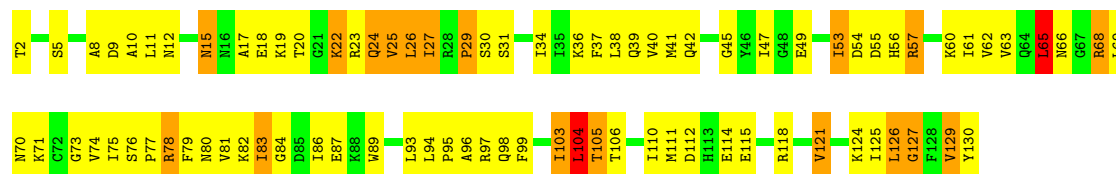
- Molecule 23: 40S ribosomal protein S21-A

Chain d1: 



- Molecule 24: 40S ribosomal protein S22-A

Chain D2: 



- Molecule 24: 40S ribosomal protein S22-A

- Molecule 25: 40S ribosomal protein S23-A

- Molecule 25: 40S ribosomal protein S23-A

- Molecule 26: 40S ribosomal protein S24-A

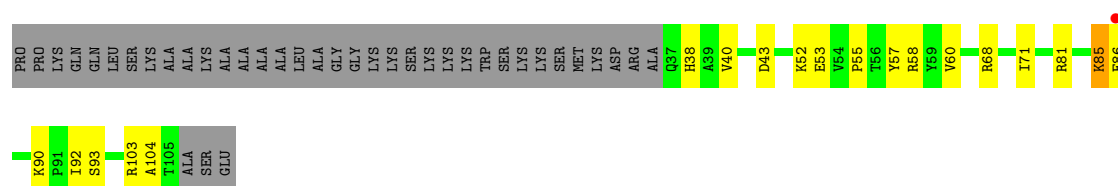
- Molecule 26: 40S ribosomal protein S24-A

- Molecule 27: 40S ribosomal protein S25-A



- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



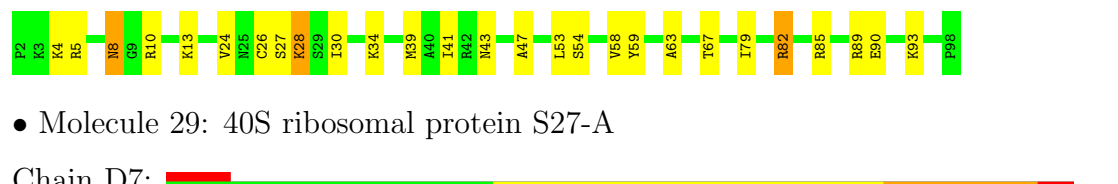
- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



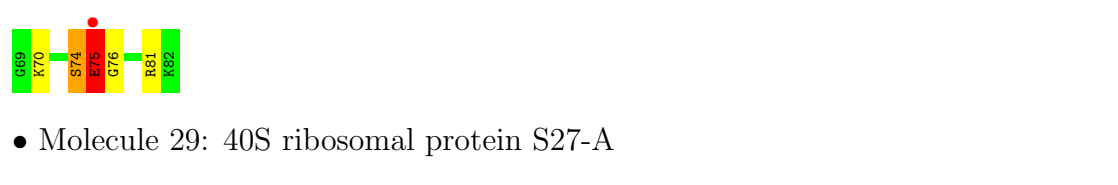
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



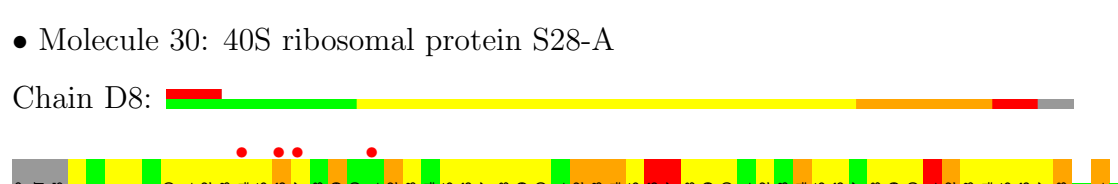
- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



- Molecule 29: 40S ribosomal protein S27-A

Chain d7:



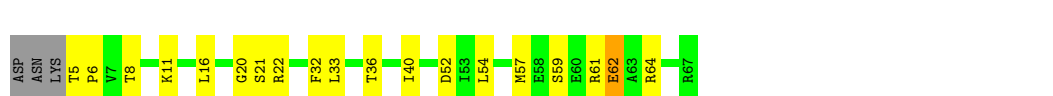
- Molecule 30: 40S ribosomal protein S28-A

Chain D8:



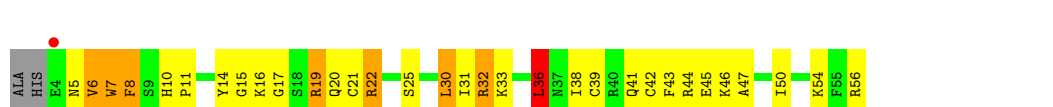
- Molecule 30: 40S ribosomal protein S28-A

Chain d8:



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



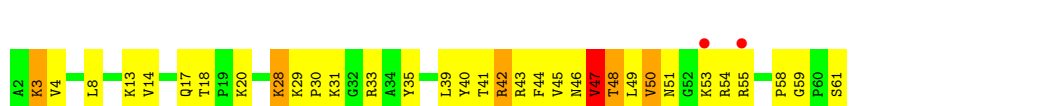
- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



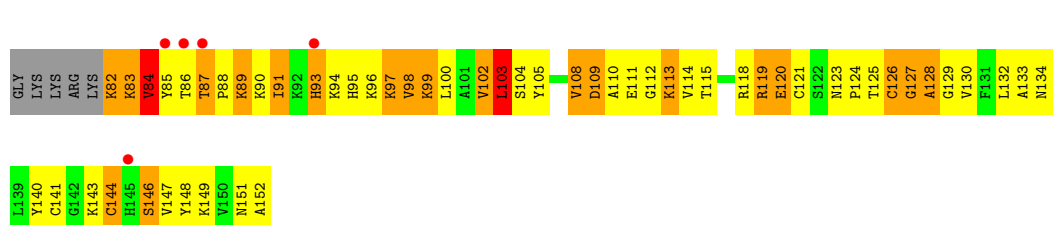
- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



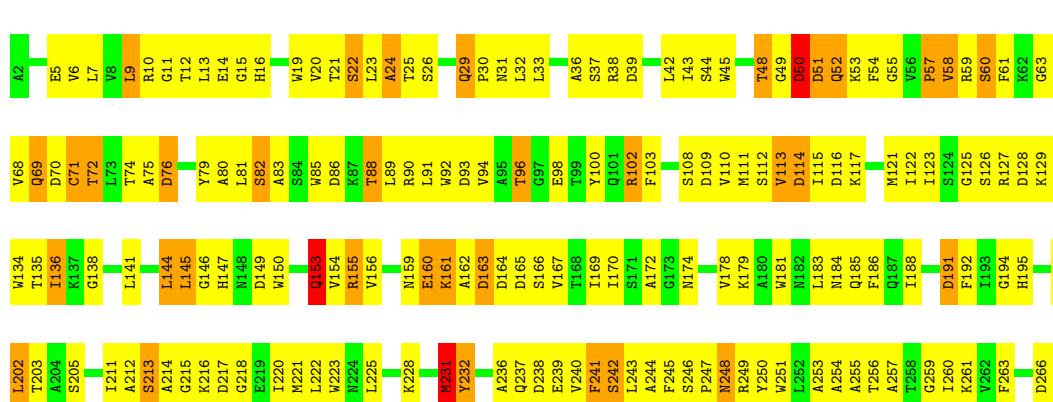
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



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

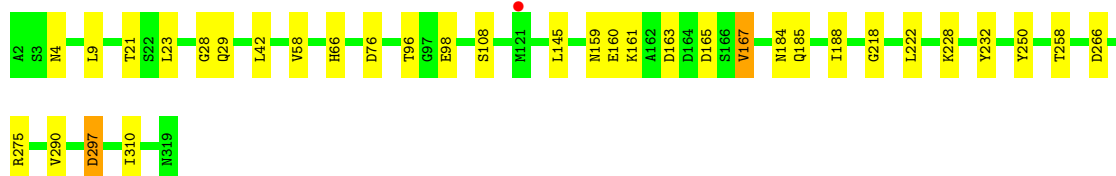
Chain SR:





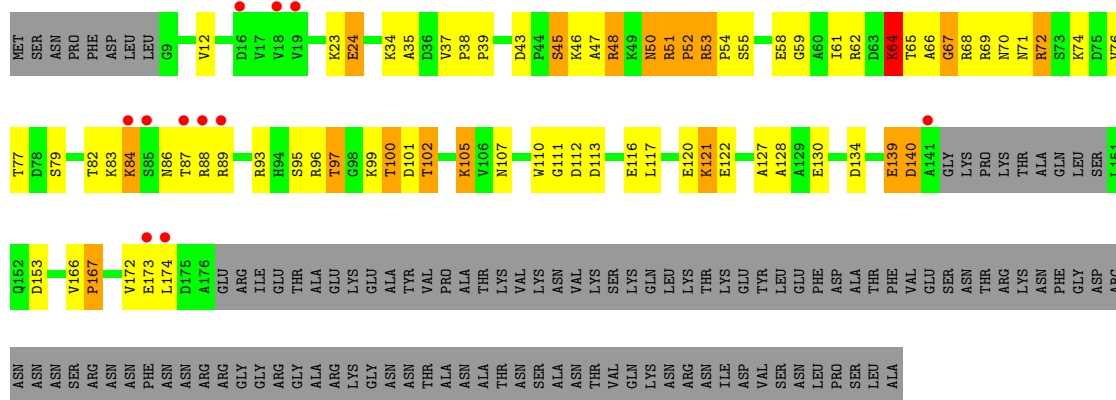
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



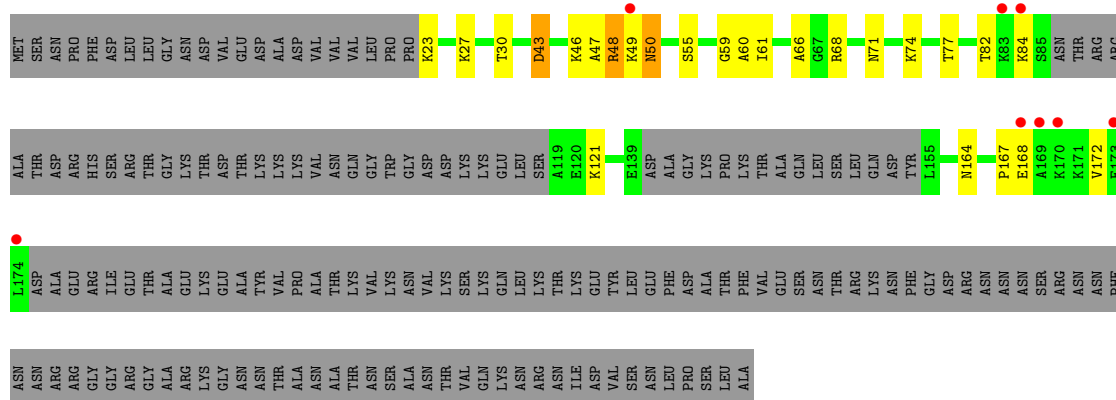
- Molecule 35: Suppressor protein STM1

Chain SM:



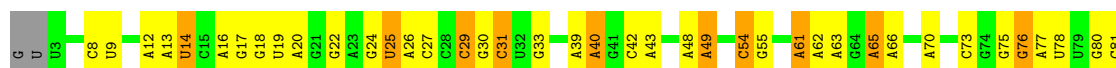
- Molecule 35: Suppressor protein STM1

Chain sM:



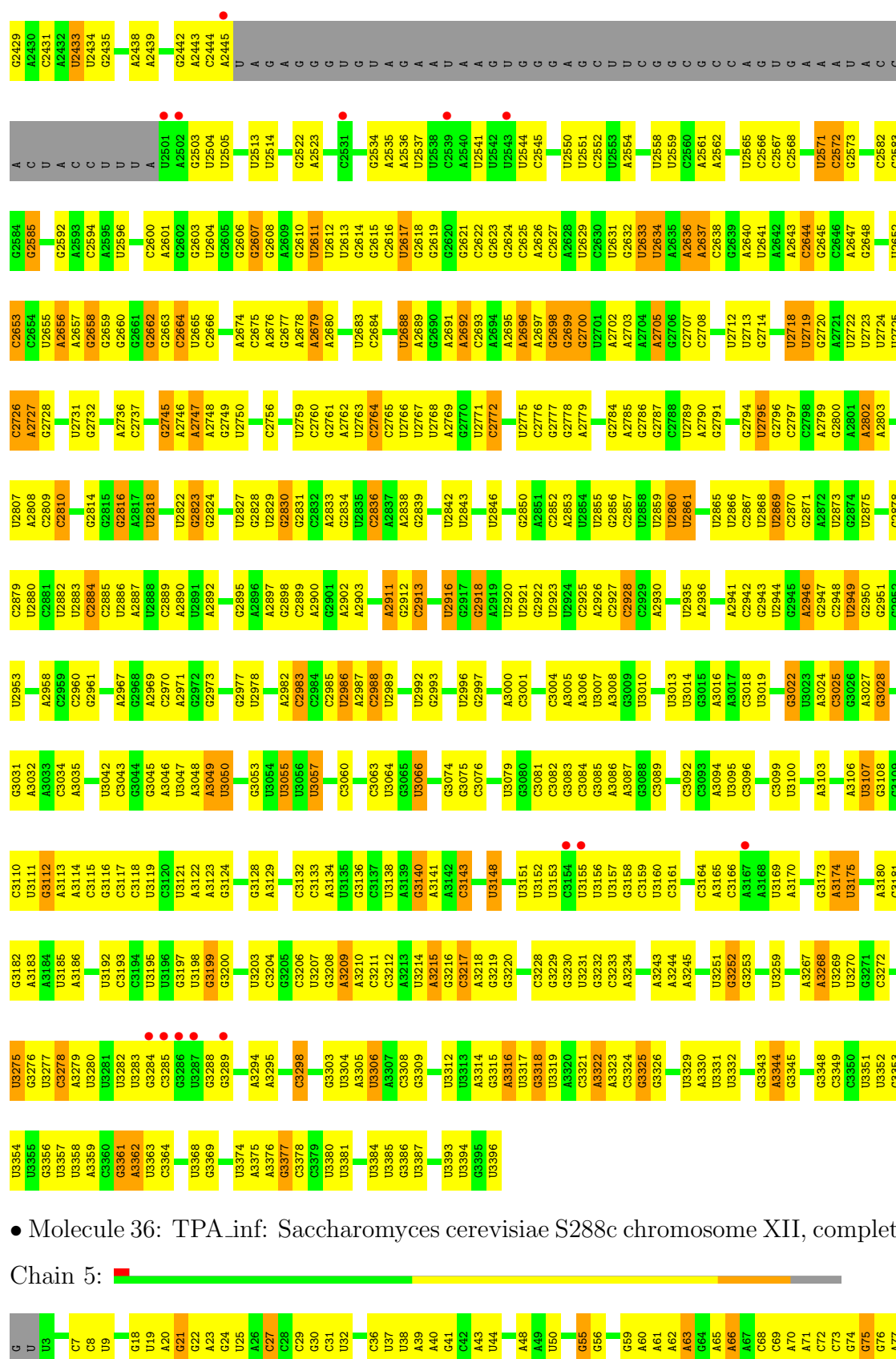
- Molecule 36: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 1:



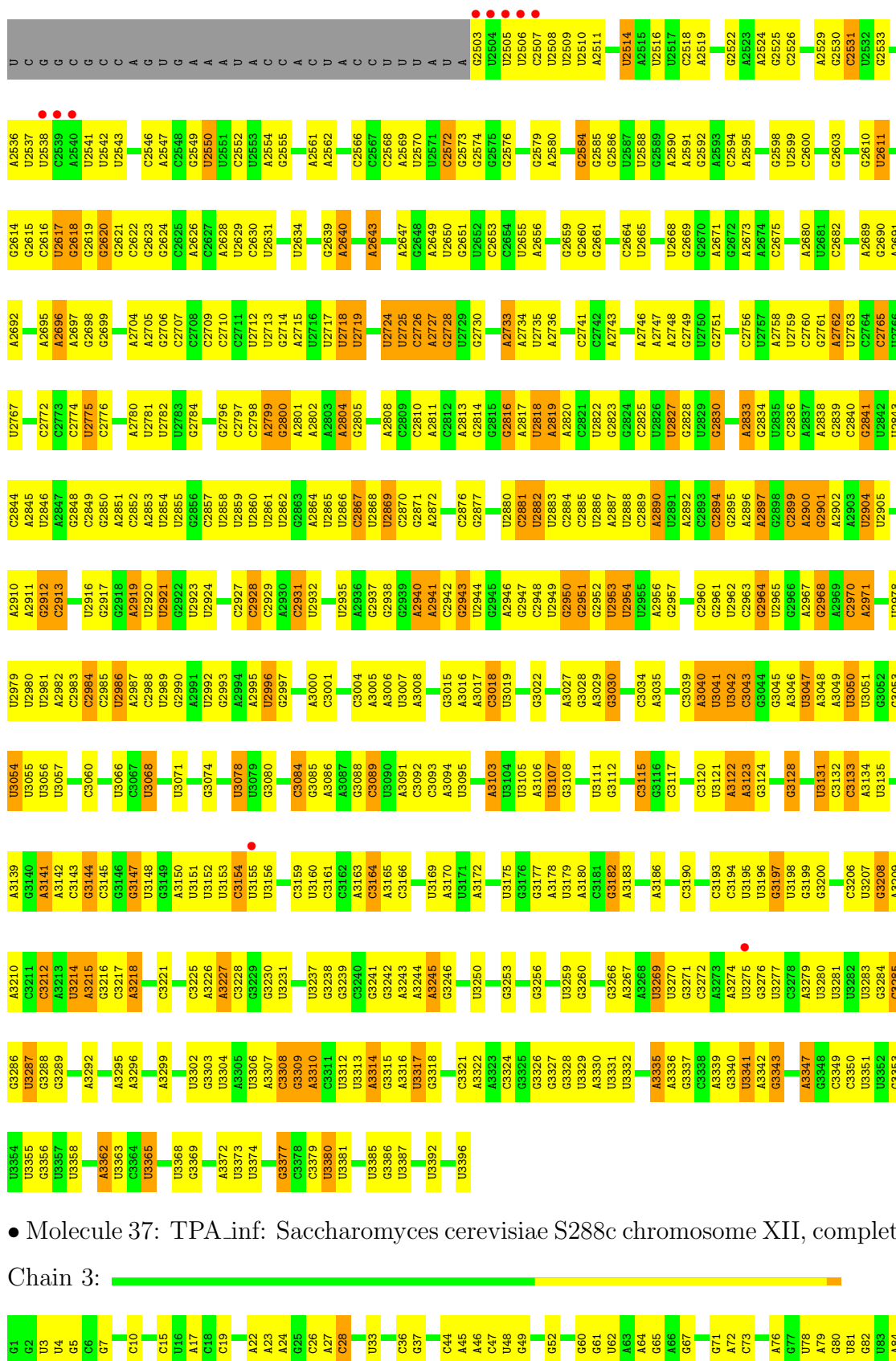
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G1177	G1178	A1179	A1180	U1181	A1182	C1183	A1184	C1185	G1186	C1187	U1188	U1189	C1190	A1191	C1192	A1193	G1194	A1195	A1196	A1197	C1198	C1199	A1200	A1201	A1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	C1216	U1220	U1221	G1222	A1223	C1224	A1225	G1226	C1227	C1228	G1229	C1230	A1231	C1232	C1233	G1234	U1235	G1236	C1237	C1238	C1239	C1240	U1241	G1242	A1244																																																																																																																																																																																																																																																																																																																																																																											
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G415	A416	A417	A418	G419	A420	G421	A422	G423	A424	G425	G426	C427	A428	U429	G432	A433	U434	C435	A436	G437	A438	C439	A440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803																																								
G333	A334	A338	C339	G340	G341	A342	U343	A344	G345	G346	G347	A350	A351	A352	G353	C356	A361	A365	A366	A367	A368	A369	U370	C371	C372	A373	A374	A375	A385	A386	A387	G388	A391	C392	U393	G394	A395	A396	A397	A398	U401	A402	C403	G406	A407	A408	A409	U410	U411	G412	G415	A416	A417	A418	G419	A420	G421	A422	G423	A424	G425	G426	C427	A428	U429	G432	A433	U434	C435	A436	G437	A438	C439	A440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792

A2367	A2368	C2283	A2208	G2122	U1937	G1863	A1787	G1700	A1502	A1535	A1454	U1378	G1310
C2284	C2285	C2286	U2209	G2123	U1938	G1864	C1788	C1701	A1603	G1536	A1455	G1379	G1313
U2286	U2287	U2288	G2210	U2212	G1939	A1865	G1789	U1702	G1604	A1537	A1456	A1381	C1314
A2289	U2289	A2290	C2211	G2130	C1940	C1866	C1791	C1706	C1608	U1540	U1457	G1382	C1315
C2291	C2292	C2293	A2213	U2133	C1942	A1867	C1792	C1708	C1609	G1541	U1458	C1385	G1316
C2294	C2295	C2296	A2214	U2134	C1943	G1868	U1795	U1712	G1610	G1542	C1459	A1317	A1318
C2297	C2298	C2299	U2215	U2135	U1944	U1877	G1796	G1715	A1612	G1543	A1460	G1389	G1319
C2300	C2301	C2302	U2216	U2136	U1945	G1878	A1797	A1716	A1613	U1544	A1461	A1390	C1320
C2303	C2304	C2305	C2227	U2141	G1946	A1879	A1798	U1717	C1614	G1547	U1462	G1321	G1321
C2306	C2307	C2308	A2232	U2142	G1947	U1880	A1799	G1718	C1615	U1548	A1463	U1322	G1323
C2309	C2310	C2311	U2233	U2143	G1948	A1881	G1882	U1719	U1616	G1550	A1465	U1323	G1323
C2312	C2313	C2314	C2234	U2144	U1950	G1882	A1804	G1720	G1617	U1551	G1466	C1327	C1327
C2315	C2316	C2317	C2235	U2145	C1951	A1883	C1805	U1721	A1618	U1552	U1470	U1330	U1331
C2318	C2319	C2320	C2236	U2146	C1952	U1884	A1806	U1722	U1620	U1553	U1471	U1332	U1333
C2321	C2322	C2323	C2237	U2147	G1953	U1885	G1807	U1723	U1621	U1554	U1472	U1334	U1335
C2324	C2325	C2326	C2238	U2148	U1954	A1886	G1808	G1724	U1622	C1556	U1473	U1336	U1337
C2327	C2328	C2329	C2239	U2149	U1955	A1887	A1813	U1725	A1632	U1559	G1476	G1403	G1403
C2330	C2331	C2332	C2240	U2150	A	U1888	A1814	C1726	A1633	G1560	A1477	C1404	U1342
C2333	C2334	C2335	U2241	U2151	G	G1889	U1815	G1727	G1634	G1561	G1480	U1405	U1343
C2336	C2337	C2338	U2242	U2152	C	U1890	A1816	U1731	G1635	C1562	A1481	U1406	U1344
C2339	C2340	C2341	U2243	U2153	A	A1891	G1817	G1734	U1636	U1564	A1482	G1407	U1345
C2342	C2343	C2344	U2244	U2154	G	U1895	U1818	G1735	A1637	U1565	G1483	G1408	U1346
C2345	C2346	C2347	U2245	U2155	C	G1898	U1819	U1740	G1638	G1566	U1484	G1409	U1347
C2348	C2349	C2350	U2246	U2156	C	U1899	U1820	U1741	A1639	U1567	G1485	U1410	U1348
C2351	C2352	C2353	U2247	U2157	C	U1900	U1821	U1742	G1640	U1568	A1489	G1411	U1349
C2354	C2355	C2356	U2248	U2158	C	A1901	C1822	U1743	C1644	U1569	G1488	G1412	U1350
C2357	C2358	C2359	U2249	U2159	C	G1902	U1823	U1744	U1645	U1570	A1489	G1413	U1351
C2360	C2361	C2362	U2250	U2160	C	U1903	U1824	U1745	G1646	U1571	A1490	G1414	U1352
C2363	C2364	C2365	U2251	U2161	C	G1904	C1826	U1746	G1662	U1572	A1491	U1415	U1353
C2366	C2367	C2368	U2252	U2162	C	U1905	C1827	U1747	G1663	C1573	G1492	U1416	U1354
C2369	C2370	C2371	U2253	U2163	C	G1906	U1830	U1748	G1664	C1574	G1493	G1417	U1355
C2372	C2373	C2374	U2254	U2164	C	A1909	U1831	U1749	G1665	C1575	U1494	C1420	U1356
C2375	C2376	C2377	U2255	U2165	C	U1910	G1832	U1750	U1659	G1576	U1495	U1421	U1357
C2378	C2379	C2380	U2256	U2166	C	A1911	U1833	U1751	G1660	C1577	C1496	G1421	U1358
C2381	C2382	C2383	U2257	U2167	C	U1912	U1834	U1752	G1661	C1578	C1497	U1425	U1359
C2384	C2385	C2386	U2258	U2168	C	A1913	U1835	U1753	G1662	C1579	A1498	G1426	U1360
C2387	C2388	C2389	U2259	U2169	C	G1914	U1836	U1754	G1663	C1580	G1500	U1427	U1361
C2390	C2391	C2392	U2260	U2170	C	U1915	U1837	U1755	C1664	C1581	G1501	A1428	U1362
C2393	C2394	C2395	U2261	U2171	C	U1916	U1838	U1756	G1665	C1582	C1502	U1429	G1363
C2396	C2397	C2398	U2262	U2172	C	G1917	U1839	U1757	G1666	C1583	A1503	U1430	A1362
C2399	C2400	C2401	U2263	U2173	C	U1918	U1840	U1758	G1667	C1584	A1504	G1431	A1363
C2402	C2403	C2404	U2264	U2174	C	U1919	U1841	U1759	G1668	C1585	A1505	A1432	C1364
C2405	C2406	C2407	U2265	U2175	C	A1920	U1842	U1760	G1669	C1586	A1506	A1433	G1365
C2408	C2409	C2410	U2266	U2176	C	U1921	U1843	U1761	U1687	C1587	G1507	A1434	G1366
C2411	C2412	C2413	U2267	U2177	C	A1922	U1844	U1762	U1688	C1588	C1508	A1435	G1367
C2414	C2415	C2416	U2268	U2178	C	U1923	U1845	U1763	U1689	C1589	A1509	A1436	U1368
C2417	C2418	C2419	U2269	U2179	C	U1924	U1846	U1764	U1690	C1590	G1510	U1437	G1369
C2420	C2421	C2422	U2270	U2180	C	U1925	U1847	U1765	U1691	C1591	C1516	G1441	G1370
C2423	C2424	C2425	U2271	U2181	C	U1926	U1848	U1766	U1692	C1592	G1517	U1442	G1371
C2426	C2427	C2428	U2272	U2182	C	U1927	U1849	U1767	U1693	C1593	G1518	G1443	C1372
C2429	C2430	C2431	U2273	U2183	C	U1928	U1850	U1768	U1694	C1594	C1519	G1444	A1373
C2432	C2433	C2434	U2274	U2184	C	U1929	U1851	U1769	U1695	C1595	G1520	U1445	G1374
C2435	C2436	C2437	U2275	U2185	C	U1930	U1852	U1770	U1696	C1596	G1521	U1446	U1375
C2438	C2439	C2440	U2276	U2186	C	U1931	U1853	U1771	U1697	C1597	G1522	A1447	G1376
C2441	C2442	C2443	U2277	U2187	C	U1932	U1854	U1772	U1698	C1598	G1523	U1448	U1377
C2444	C2445	C2446	U2278	U2188	C	U1933	U1855	U1773	U1699	C1599	G1524	U1449	U1378
C2447	C2448	C2449	U2279	U2189	C	U1934	U1856	U1774	U1700	C1600	G1525	U1450	U1379
C2450	C2451	C2452	U2280	U2190	C	U1935	U1857	U1775	U1701	C1601	G1526	U1451	U1380
C2453	C2454	C2455	U2281	U2191	C	U1936	U1858	U1776	U1702	C1602	G1527	U1452	U1381
C2456	C2457	C2458	U2282	U2192	C	U1937	U1859	U1777	U1703	C1603	G1528	U1453	U1382
C2459	C2460	C2461	U2283	U2193	C	U1938	U1860	U1778	U1704	C1604	G1529	U1454	U1383
C2462	C2463	C2464	U2284	U2194	C	U1939	U1861	U1779	U1705	C1605	G1530	U1455	U1384
C2465	C2466	C2467	U2285	U2195	C	U1940	U1862	U1780	U1706	C1606	G1531	U1456	U1385
C2468	C2469	C2470	U2286	U2196	C	U1941	U1863	U1781	U1707	C1607	G1532	U1457	U1386
C2471	C2472	C2473	U2287	U2197	C	U1942	U1864	U1782	U1708	C1608	G1533	U1458	U1387
C2474	C2475	C2476	U2288	U2198	C	U1943	U1865	U1783	U1709	C1609	G1534	U1459	U1388
C2477	C2478	C2479	U2289	U2199	C	U1944	U1866	U1784	U1710	C1610	G1535	U1460	U1389
C2480	C2481	C2482	U2290	U2200	C	U1945	U1867	U1785	U1711	G1611	G1536	A1461	A1390
C2483	C2484	C2485	U2291	U2201	C	U1946	U1868	U1786	U1712	G1612	G1537	A1462	A1391
C2486	C2487	C2488	U2292	U2202	C	U1947	U1869	U1787	U1713	G1613	G1538	A1463	A1392
C2489	C2490	C2491	U2293	U2203	C	U1948	U1870	U1788	U1714	G1614	G1539	A1464	A1393
C2492	C2493	C2494	U2294	U2204	C	U1949	U1871	U1789	U1715	G1615	G1540	A1465	A1394
C2495	C2496	C2497	U2295	U2205	C	U1950	U1872	U1790	U1716	G1616	G1541	A1466	A1395
C2498	C2499	C2500	U2296	U2206	C	U1951	U1873	U1791	U1717	G1617	G1542	A1467	A1396
C2501	C2502	C2503	U2297	U2207	C	U1952	U1874	U1792	U1718	G1618	G1543	A1468	A1397
C2504	C2505	C2506	U2298	U2208	C	U1953	U1875	U1793	U1719	U1619	G1544	A1469	A1398
C2507	C2508	C2509	U2299	U2209	C	U1954	U1876	U1794	U1720	U1620	G1545	A1470	A1399
C2510	C2511	C2512	U2300	U2210	C	U1955	U1877	U1795	U1721	U1621	G1546	U1471	U1400
C2513	C2514	C2515	U2301	U2211	C	U1956	U1878	U1796	U1722	U1622	G1547	U1472	U1401
C2516	C2517	C2518	U2302	U2212	C	U1957	U1879	U1797	U1723	U1623	G1548	U1473	U1402
C2519	C2520	C2521	U2303	U2213	C	U1958	U1880	U1798	U1724	U1624	G1549	U1474	U1403
C2522	C2523	C2524	U2304	U2214	C	U1959	U1881	U1799	U1725	U1625	G1550	U1475	U1404
C2525	C2526	C2527	U2305	U2215	C	U1960	U1882	U1800	U1726	U1626	G1551	U1476	U1405
C2528	C2529	C2530	U2306	U2216	C	U1961	U1883	U1801	U1727	U1627	G1552	U1477	U1406
C2531	C2532	C2533	U2307	U2217	C	U1962	U1884	U1802	U1728	U1628	G1553	U1478	U1407
C2534	C2535	C2536	U2308	U2218	C	U1963	U1885	U1803	U1729	U1629	G1554	U1479	U1408
C2537	C2538	C2539	U2309	U2219	C	U1964	U1886	U1804	U1730	U1630	G1555	U1480	U1409
C2540	C2541	C2542	U2310	U2220	C	U1965	U1887	U1805	U1731	U1631	G1556	U1481	U1410
C2543	C2544	C2545	U2311	U2221	C	U1966	U1888	U1806	U1732	U1632	G1557	U1482	U1411
C2546	C2547	C2548	U2312	U2222	C	U1967	U1889	U1807	U1733	U1633	G1558	U1483	U1412
C2549	C2550	C2551	U2313	U2223	C	U1968	U1890	U1808	U1734	U1634	G1559	U1484	U1413
C2552	C2553	C2554	U2314	U2224	C	U1969	U1891	U1809	U1735	U1635	G1560	U1485	U1414



A1263	A1180	U1109	A1036	C959	C804	G718	G632	G548	A409	G335	U250	G158	U78
G1264	U1181	U1110	A1037	U960	G805	U719	C633	U549	U410	A336	G251	C166	U79
U1276	C1182	A1111	C1038	A961	A806	A720	C634	A550	U411	G337	U252	U167	U83
C1280	C1187	G1113	U1039	G963	G809	G726	C637	G552	U413	A342	A254	U168	C90
G1281	U1183	U1114	A1040	U966	A810	G727	G638	U555	U414	U343	G264	U169	G91
G1282	C1189	G1116	U1041	A967	U811	G727	G639	U556	U419	G344	A265	G170	G92
C1283	A1190	G1117	A1048	G968	G812	U731	C641	C561	G420	G345	U276	G173	C93
U1191	U1191	C1118	U1049	C969	G815	G732	U642	C562	G421	G346	A268	C174	G94
A1294	C1192	U1119	U1050	G970	A816	G733	U643	C567	G422	G347	G269	C175	A95
G1295	A1193	U1120	U1051	G971	A817	G734	U644	C566	A423	A348	U270	G176	G96
C1298	U1196	U1121	A1054	A972	C818	A735	A645	G567	G424	A349	C271	U177	G101
A1301	A1197	U1122	A1055	A973	U821	A736	A646	G568	G425	A352	G272	C180	C102
A1302	C1198	U1123	U1056	G974	U822	G737	A647	A569	G426	C356	U276	U180	G103
A1303	U1199	U1124	A1057	C975	C824	A738	C648	U570	C427	A357	G277	G104	G105
A1304	A1200	U1125	U1058	U976	U825	G739	G651	A572	U429	C358	U278	U188	C106
U1305	C1201	G1126	A1060	U979	U831	G742	G652	C573	U430	A361	U280	U190	A108
C1306	A1202	U1128	A1061	U980	G834	G743	C655	U574	A433	G364	G281	U191	A109
G1307	U1203	A1129	U1062	U981	U835	A744	A656	G575	U434	C365	U282	C192	A110
A1308	A1204	G1130	G1063	C982	G836	C745	A657	C580	U435	A366	G283	C193	G111
U1309	U1205	U1131	A1064	U983	A837	A746	G658	U581	A436	A367	A284	C197	C112
G1310	G1206	U1132	A1065	G984	G838	U748	U662	A589	G437	G368	A285	G197	U112
C1313	U1207	A1135	U1066	G994	C839	C749	C663	G590	A501	A369	U286	A201	C113
G1314	U1208	A1136	U1067	U995	U847	C757	G668	G591	U502	U370	G287	C205	A114
C1315	C1213	U1137	C1068	A996	A848	C757	U669	U594	C503	G371	A289	G206	A115
U1214	U1214	U1138	U1070	A997	A849	C757	C670	G595	A504	A372	G290	U207	U116
C1316	U1215	G1141	U1071	A998	C849	U766	U671	A598	U507	A373	C291	C208	U118
A1317	U1215	A1142	G1072	A999	U921	U766	U671	C599	U508	A374	U207	C208	U119
A1318	A1221	A1143	U1073	G999	C850	U767	A677	G600	U509	G376	U208	A209	G120
G1321	G1222	U1144	U1074	C1000	C923	U767	G678	U601	G510	A377	U210	A122	A121
U1322	A1231	G1145	A1075	G1001	G924	G770	U678	G514	U519	C378	G212	G215	G127
C1323	C1232	G1146	C1076	A1002	U855	G770	U678	A602	G	C379	G300	G216	G128
G1233	U1329	G1147	U1077	A1003	G857	G773	U683	A603	U	G383	G304	U217	U129
U1330	A1330	G1148	A1080	A1006	A858	U776	G684	G604	U	A384	U305	A218	A130
U1331	U1235	A1150	U1081	G1010	G859	U776	G685	A608	G	A385	A306	G219	G136
C1333	G1236	U1151	U1082	U930	G860	G779	U687	G609	C	A386	A307	A221	G137
U1334	C1237	G1152	U1083	G934	C861	A780	G688	G610	C	A387	G220	A222	G139
C1335	U1238	C1155	A1084	U935	U862	G781	U689	A611	U	A391	A313	C242	C142
U1336	C1239	A1156	A1085	U936	C863	U782	A690	G612	C	G392	U314	U223	G143
A1337	U1240	G1157	C1086	C938	U864	A783	A699	U613	U	U393	C315	C224	C144
C1338	U1241	A1158	U1087	U939	U865	A784	A699	G614	C	G394	A316	G234	G145
C1339	G1242	C1159	A1091	G940	A866	G788	C700	G618	U	A395	A317	G239	U146
G1340	U1243	A1160	C1092	U942	G870	C788	G701	A621	U	A396	A318	C243	G148
U1341	A1244	C1161	U1093	U943	U871	A789	G702	G624	U	A397	U326	U245	U149
G1342	G1245	G1161	U1094	C944	U872	U790	U704	A619	C	A398	A319	U246	A150
A1343	U1247	U1167	U1095	U1022	U873	U797	A706	G625	U	A399	A323	U328	G145
G1344	G1248	U1168	U1096	C1023	U874	C793	A706	A622	U	C403	U327	C247	U147
G1345	U1249	A1169	G1097	U946	U875	U797	U712	G626	U	G404	A326	U248	G148
G1346	G1250	A1170	A1098	G947	G875	U798	G713	U626	U	U405	U327	U249	A157
U1347	U1251	G1171	A1099	C948	U876	G798	G714	U626	U	U406	U328	U249	G155
C1348	U1258	U1171	G1101	U954	C877	U798	G715	U626	U	U407	U329	U249	G156
A1349	A1259	C1176	A1102	U955	G878	A801	A716	A630	U	A408	U330	U249	G157
U1350	U1260	G1177	A1103	U956	U879	C902	A716	A630	U				
U1351	G1261	U1178	A1104	C957	G880	C903	A716	A630	U				
A1352	G1262	A1179	C958	C958	C881	C903	C717	U631	U				

WORLDWIDE
PDB
PROTEIN DATA BANK



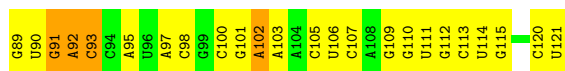
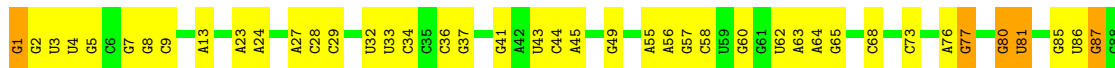
- Molecule 37: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 3:



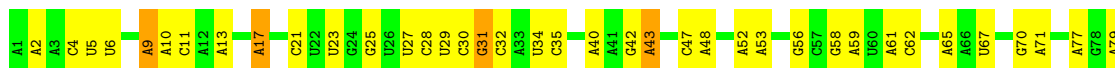
- Molecule 37: TPA_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 7:



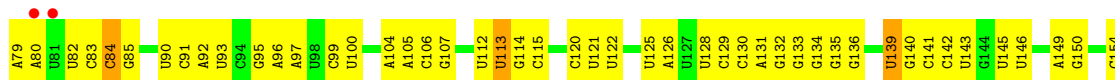
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



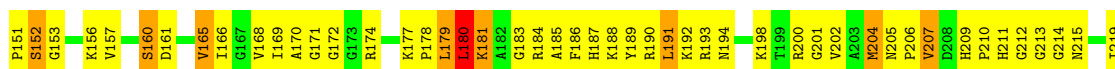
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 8:



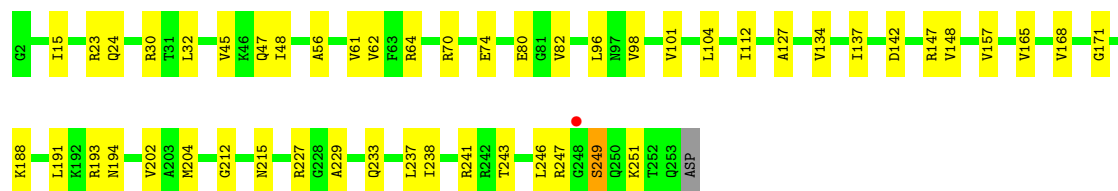
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



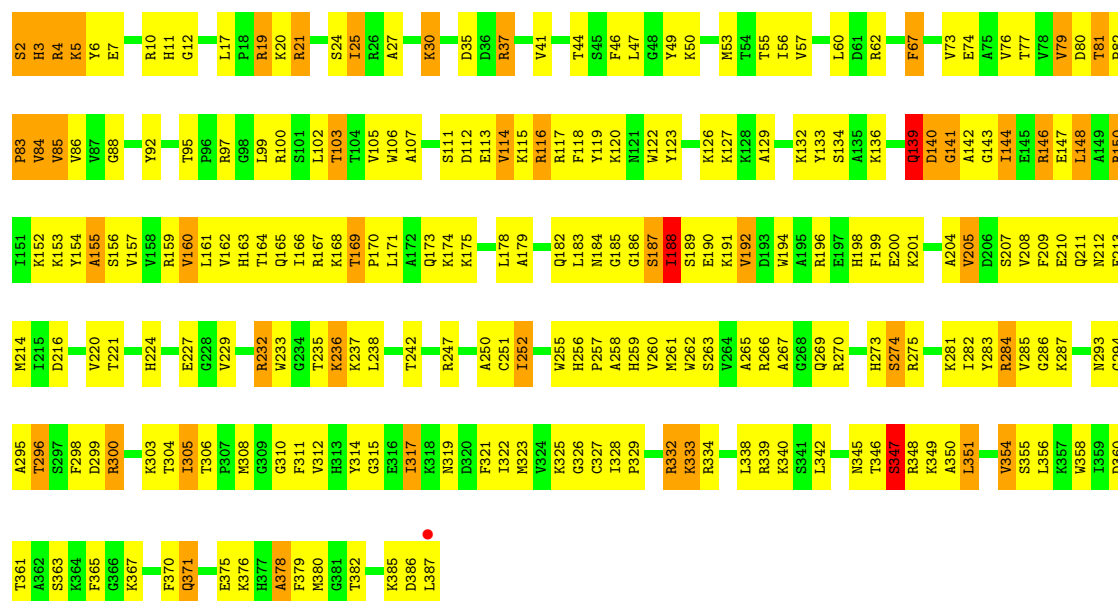
- Molecule 39: 60S ribosomal protein L2-A

Chain 12:



- Molecule 40: 60S ribosomal protein L3

Chain L3:



- Molecule 40: 60S ribosomal protein L3

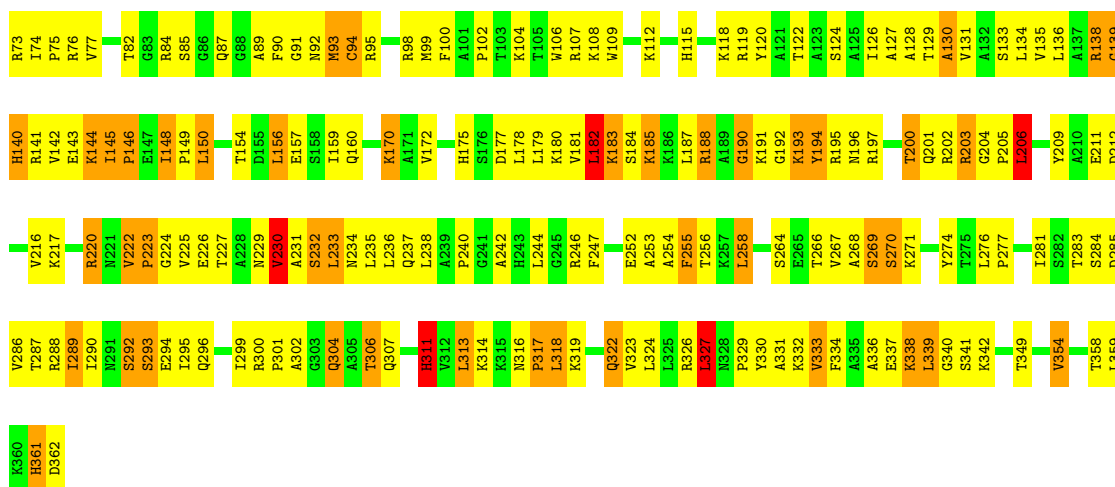
Chain 13:



- Molecule 41: 60S ribosomal protein L4-A

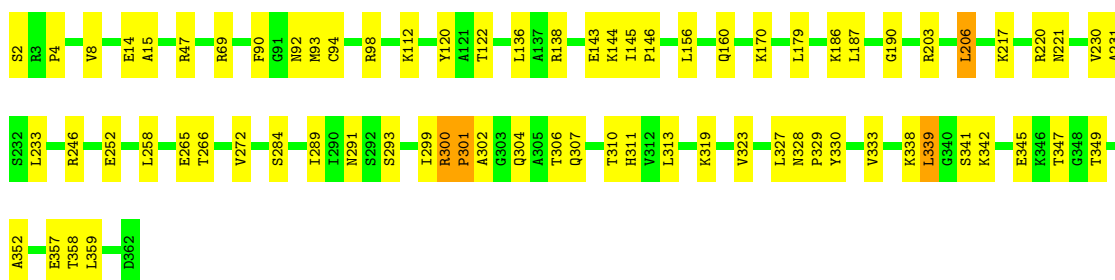
Chain L4:





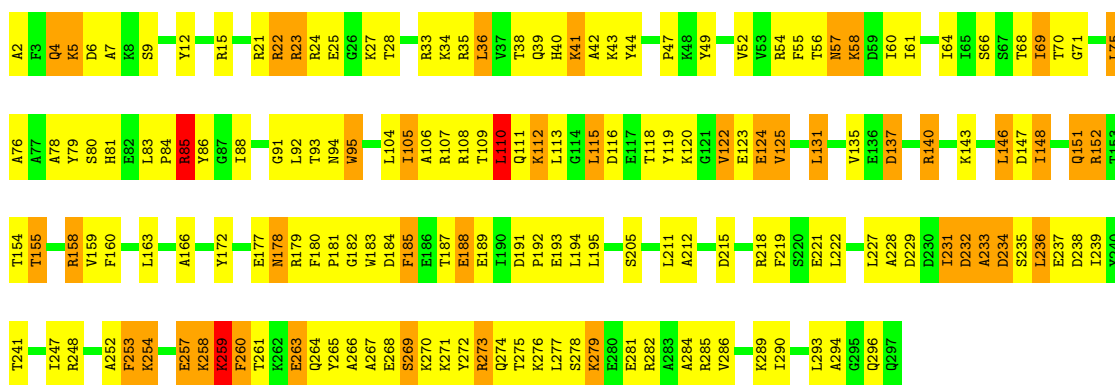
• Molecule 41: 60S ribosomal protein L4-A

Chain 14:



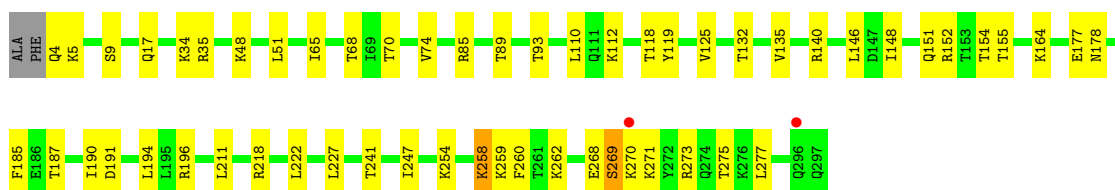
• Molecule 42: 60S ribosomal protein L5

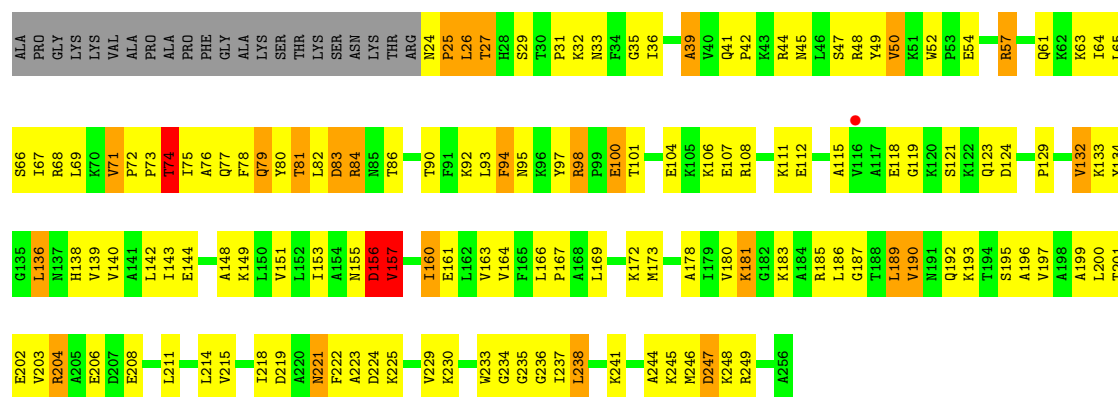
Chain L5:



• Molecule 42: 60S ribosomal protein L5

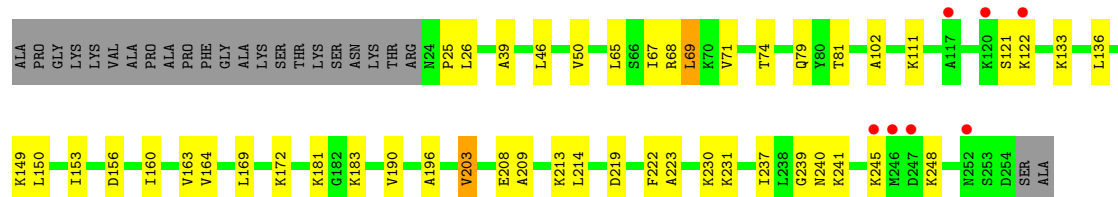
Chain l5:





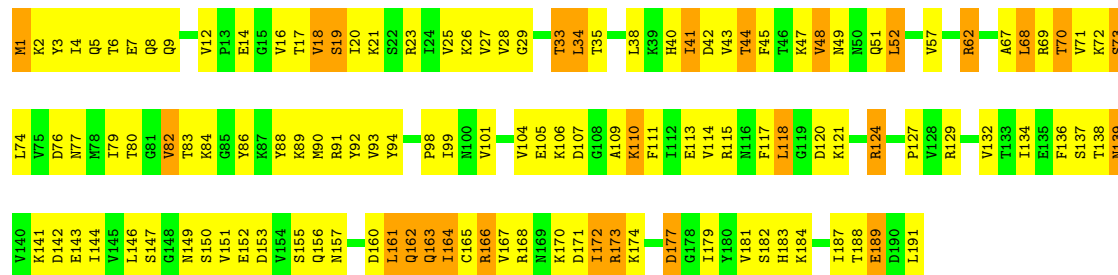
• Molecule 45: 60S ribosomal protein L8-A

Chain 18:



• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



• Molecule 46: 60S ribosomal protein L9-A

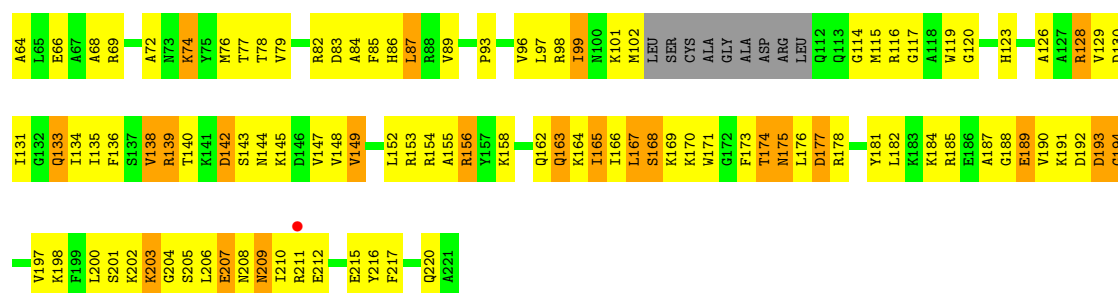
Chain 19:



• Molecule 47: 60S ribosomal protein L10

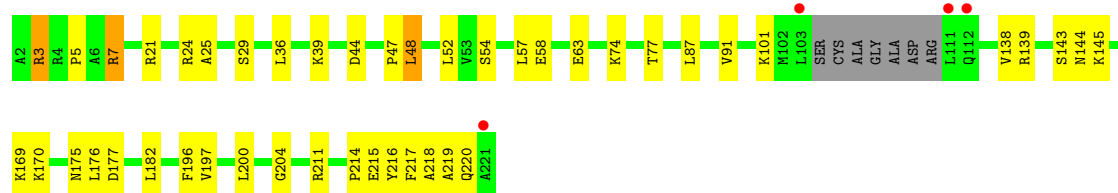
Chain M0:





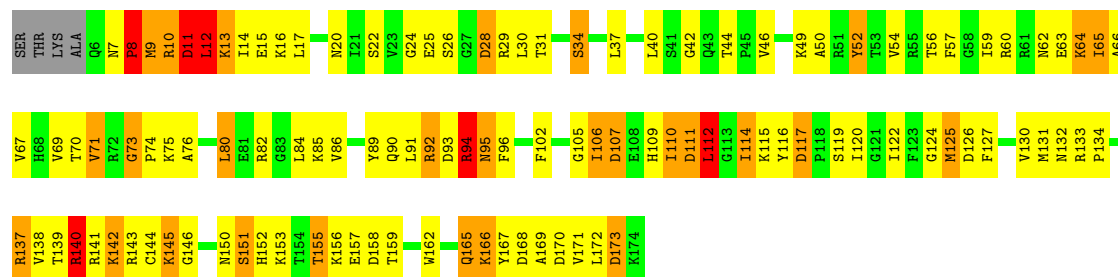
- Molecule 47: 60S ribosomal protein L10

Chain m0:



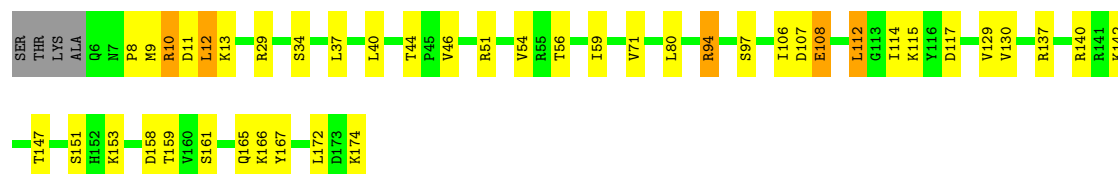
- Molecule 48: 60S ribosomal protein L11-B

Chain M1:



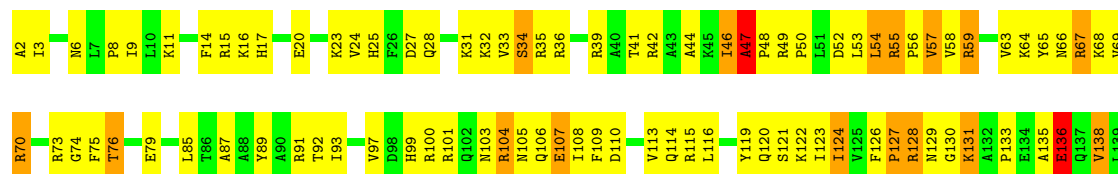
- Molecule 48: 60S ribosomal protein L11-B

Chain m1:



- Molecule 49: 60S ribosomal protein L13-A

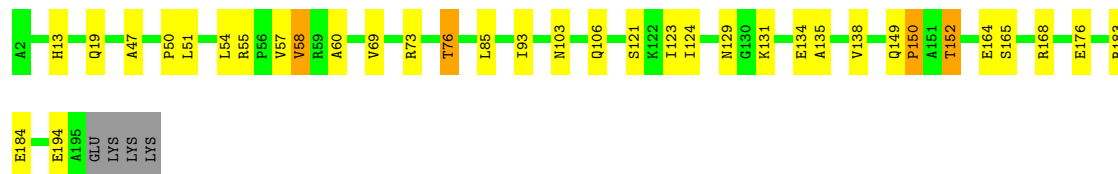
Chain M3:





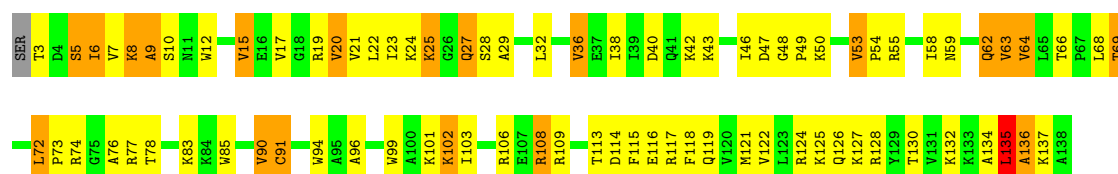
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



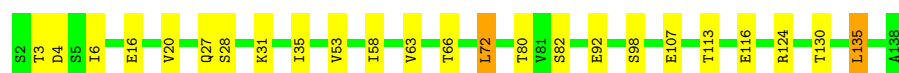
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



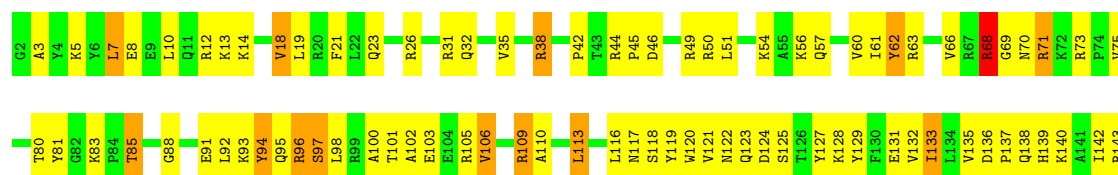
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



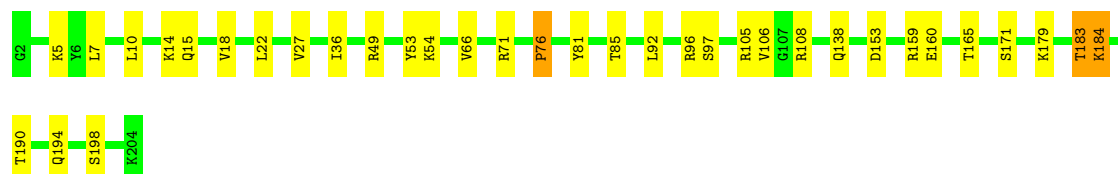
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



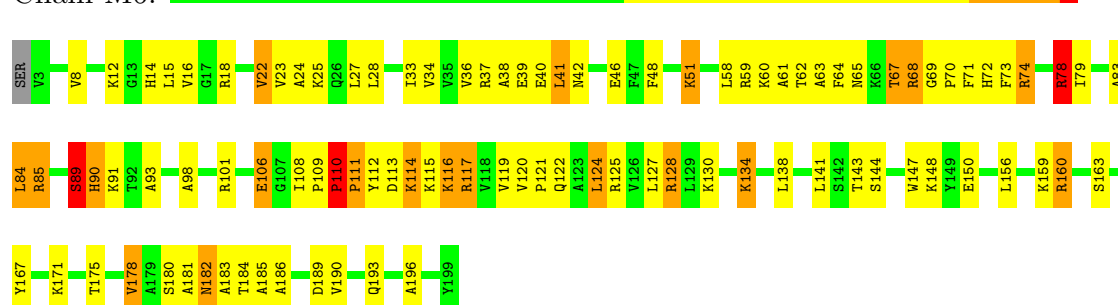
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



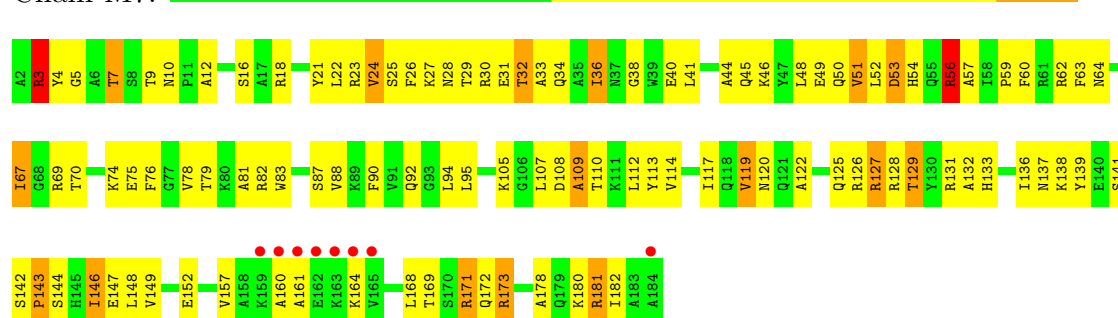
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



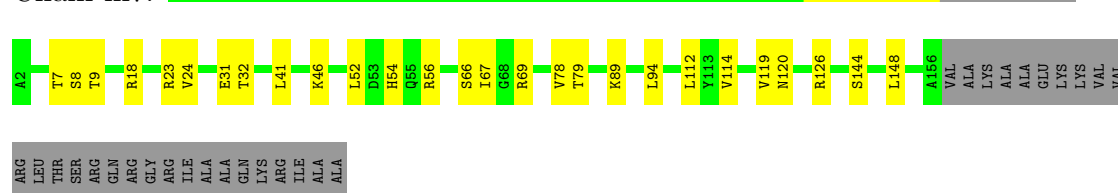
- Molecule 53: 60S ribosomal protein L17-A

Chain M7:



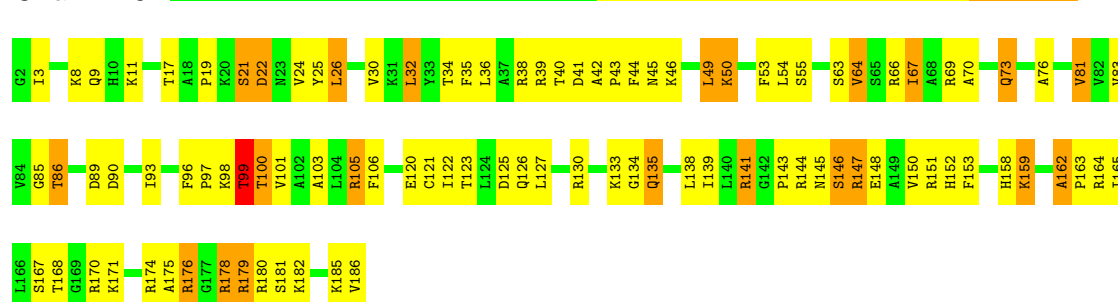
- Molecule 53: 60S ribosomal protein L17-A

Chain m7:



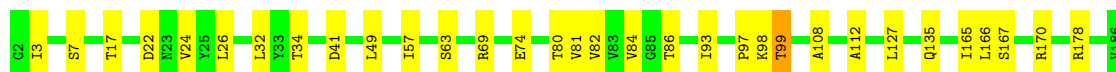
- Molecule 54: 60S ribosomal protein L18-A

Chain M8:



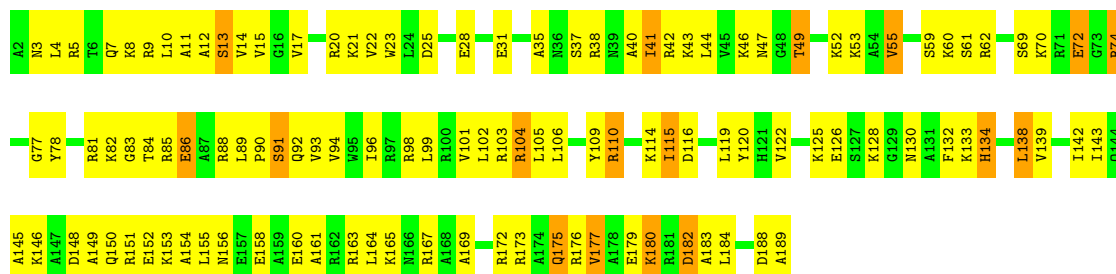
- Molecule 54: 60S ribosomal protein L18-A

Chain m8:



- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



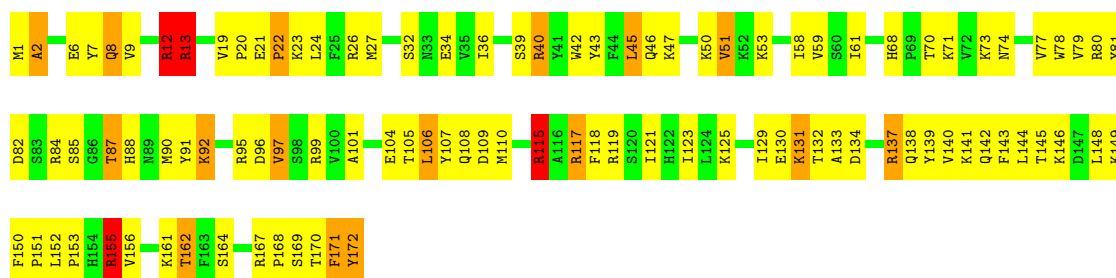
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:



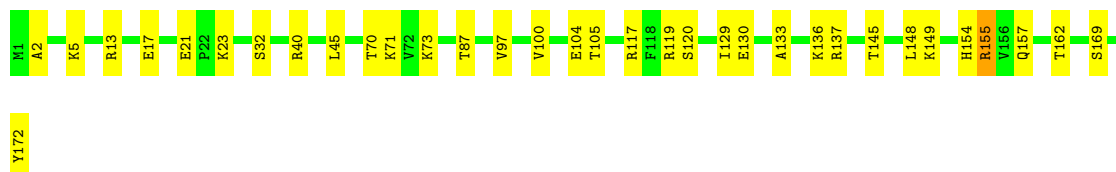
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



- Molecule 56: 60S ribosomal protein L20-A

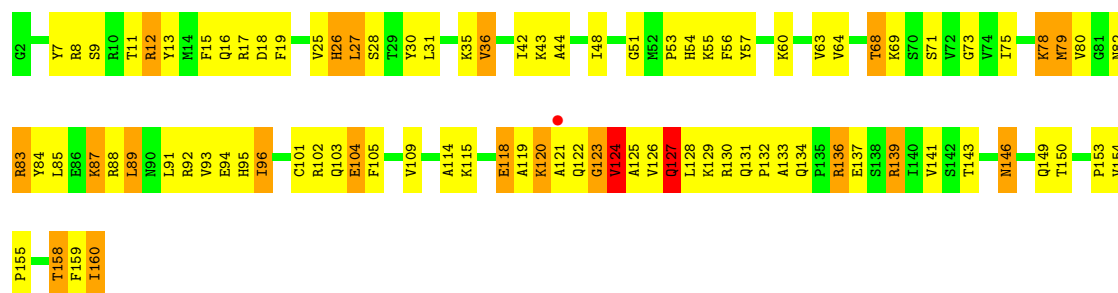
Chain n0:



- Molecule 57: 60S ribosomal protein L21-A

Chain N1:





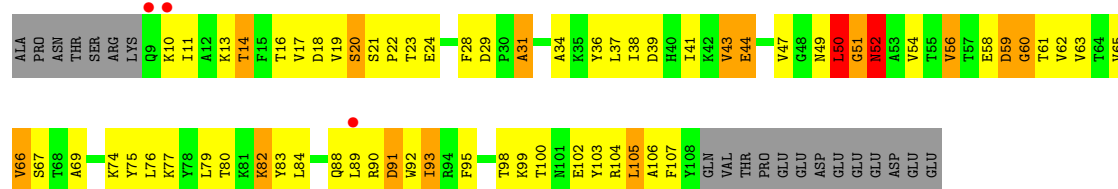
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



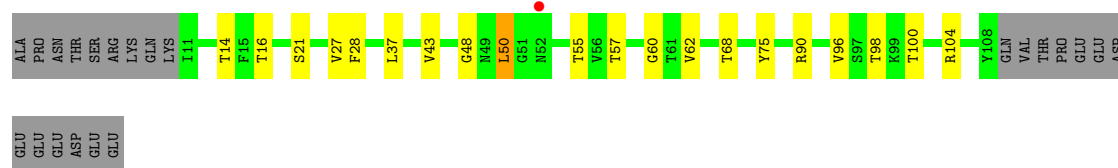
- Molecule 58: 60S ribosomal protein L22-A

Chain N2:



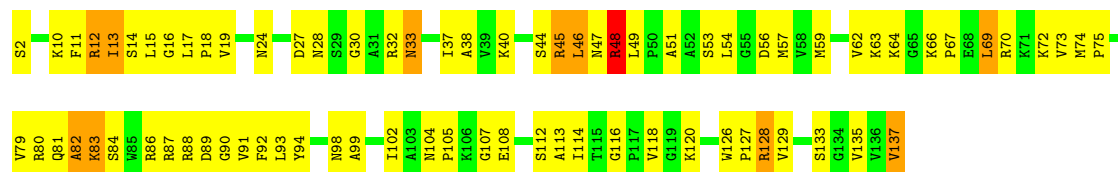
- Molecule 58: 60S ribosomal protein L22-A

Chain n2:



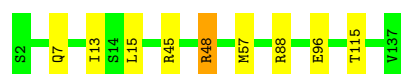
- Molecule 59: 60S ribosomal protein L23-A

Chain N3:



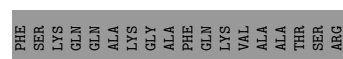
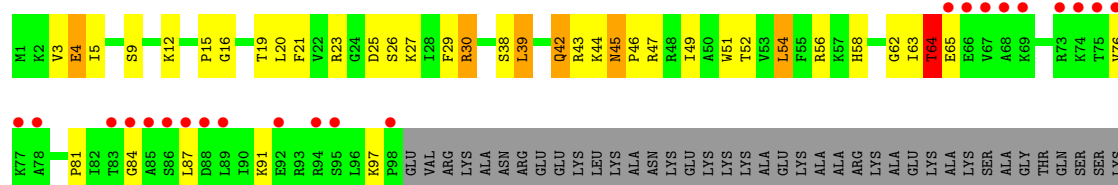
- Molecule 59: 60S ribosomal protein L23-A

Chain n3:



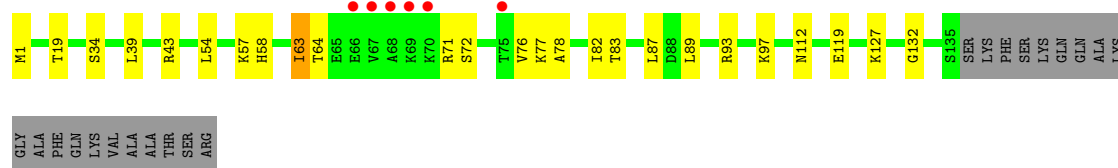
- Molecule 60: 60S ribosomal protein L24-A

Chain N4:



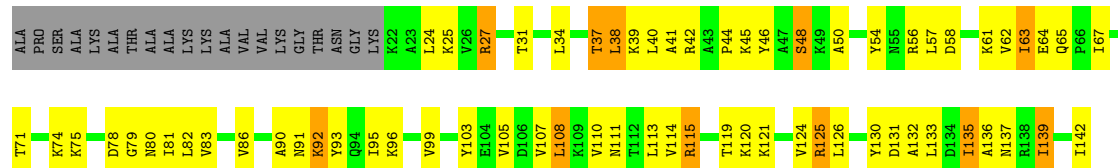
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:



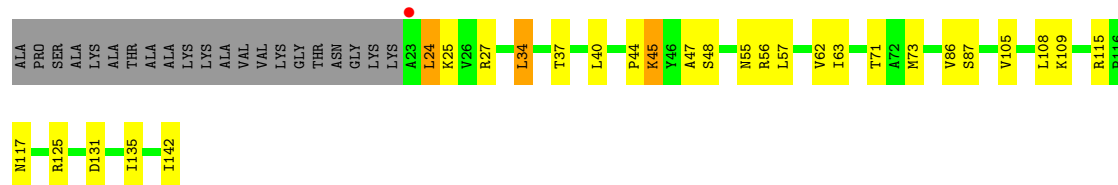
- Molecule 61: 60S ribosomal protein L25

Chain N5:



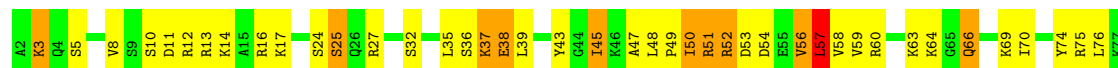
- Molecule 61: 60S ribosomal protein L25

Chain n5:



- Molecule 62: 60S ribosomal protein L26-A

Chain N6:





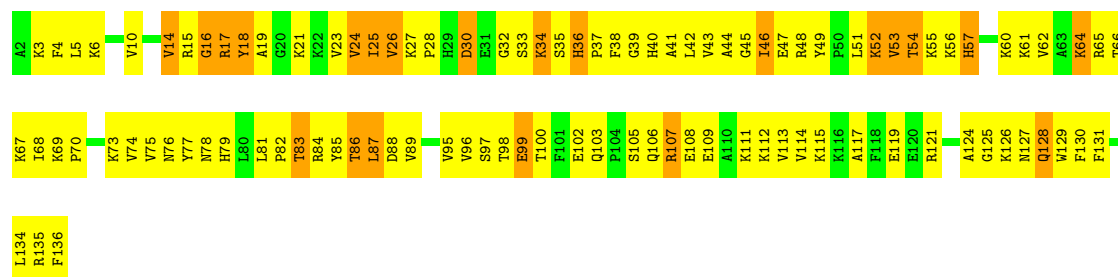
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



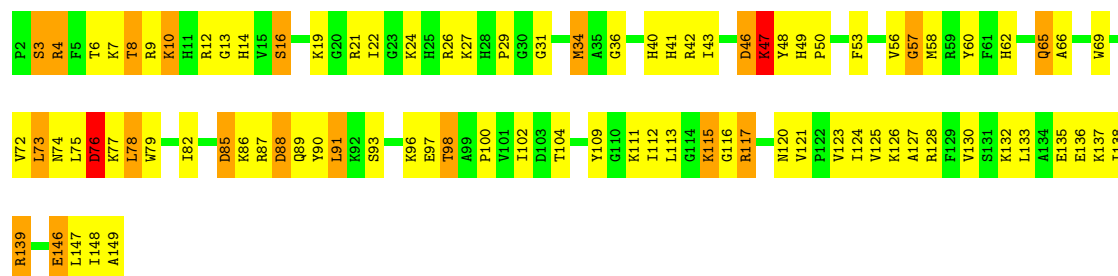
- Molecule 63: 60S ribosomal protein L27-A

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:



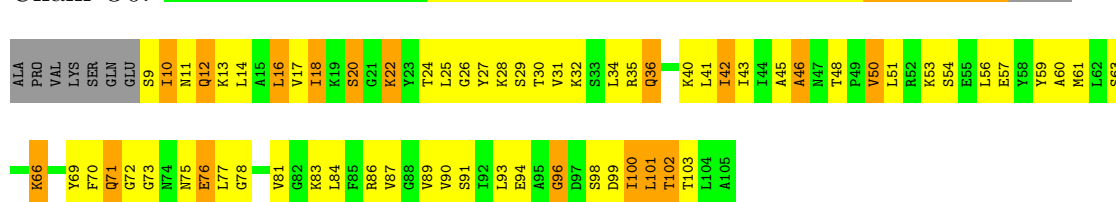
- Molecule 65: 60S ribosomal protein L29

Chain n9:



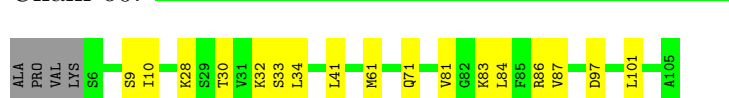
- Molecule 66: 60S ribosomal protein L30

Chain O0:



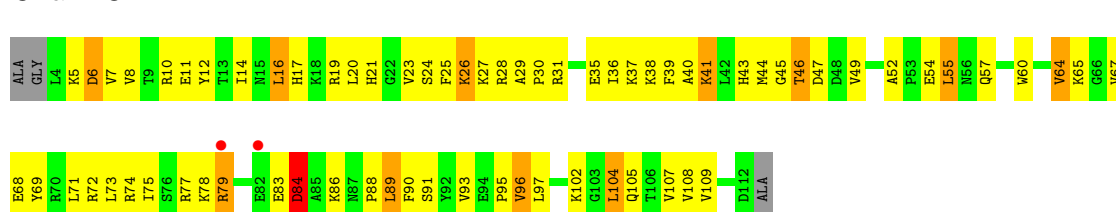
- Molecule 66: 60S ribosomal protein L30

Chain o0:



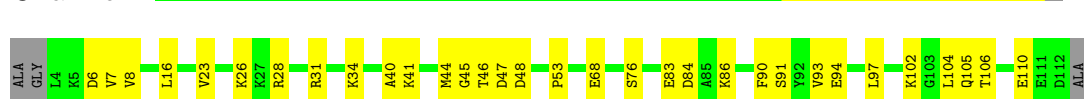
- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



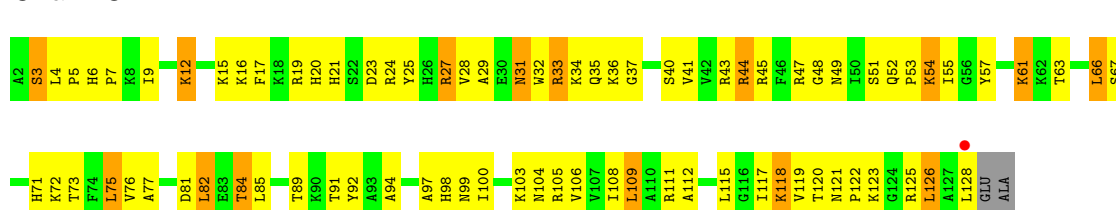
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



- Molecule 68: 60S ribosomal protein L32

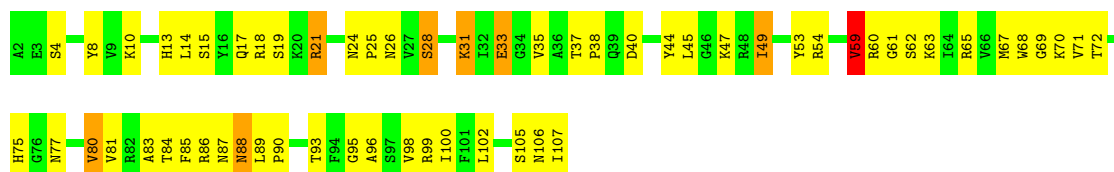
Chain O2:



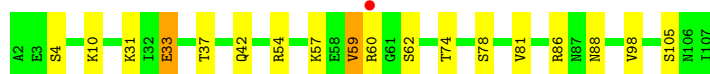
- Molecule 68: 60S ribosomal protein L32

Chain o2: 

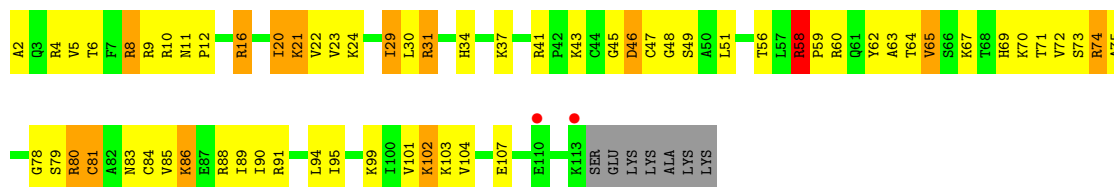
- Molecule 69: 60S ribosomal protein L33-A

Chain O3: 

- Molecule 69: 60S ribosomal protein L33-A

Chain o3: 

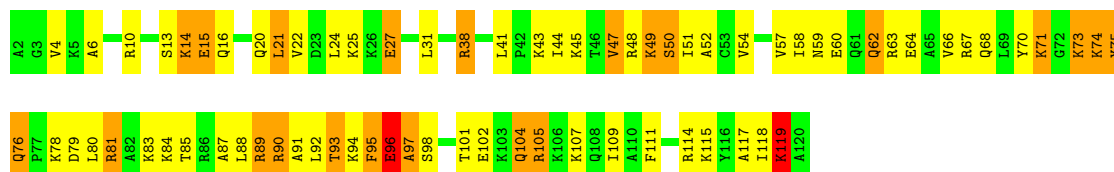
- Molecule 70: 60S ribosomal protein L34-A

Chain O4: 

- Molecule 70: 60S ribosomal protein L34-A

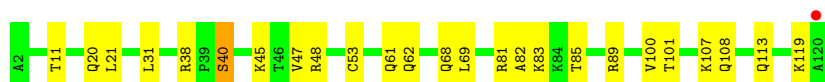
Chain o4: 

- Molecule 71: 60S ribosomal protein L35-A

Chain O5: 

- Molecule 71: 60S ribosomal protein L35-A

Chain o5: 



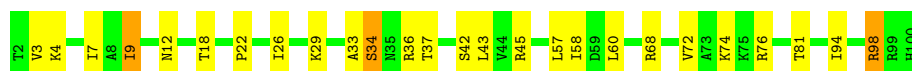
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



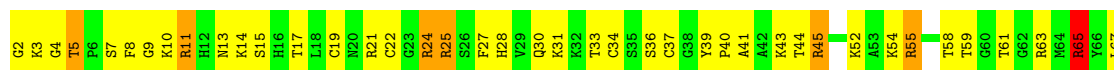
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



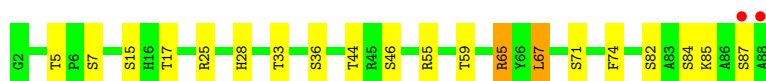
- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



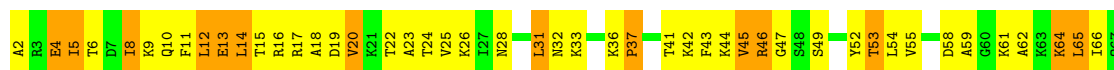
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

Chain o8:



- Molecule 75: 60S ribosomal protein L39

Chain O9:



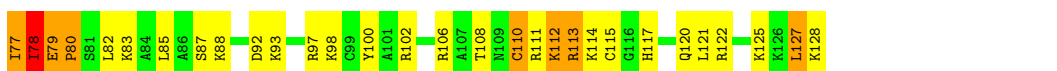
- Molecule 75: 60S ribosomal protein L39

Chain o9:



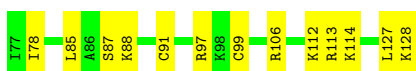
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



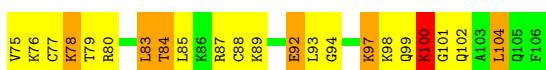
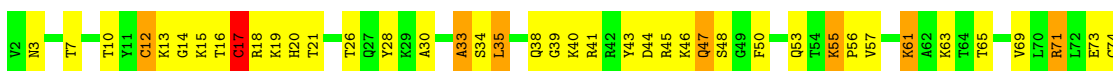
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



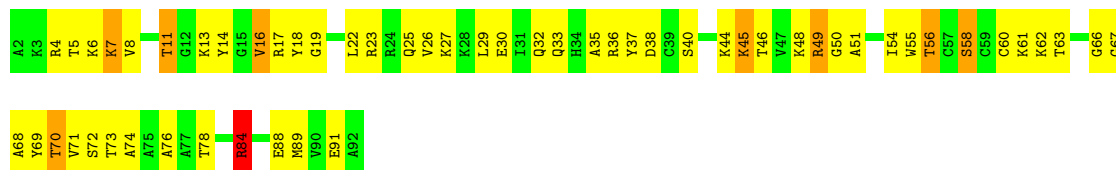
- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



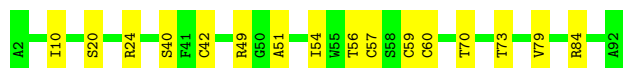
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:



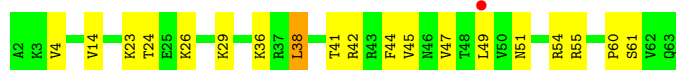
- Molecule 80: 40S ribosomal protein S10-A

Chain c0:



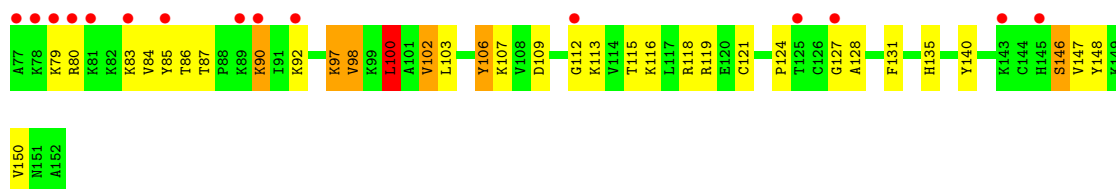
- Molecule 81: 40S ribosomal protein S30-A

Chain e0:



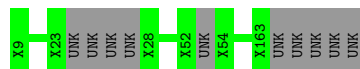
- Molecule 82: Ubiquitin-40S ribosomal protein S31

Chain e1:



- Molecule 83: UNKNOWN PROTEIN m2

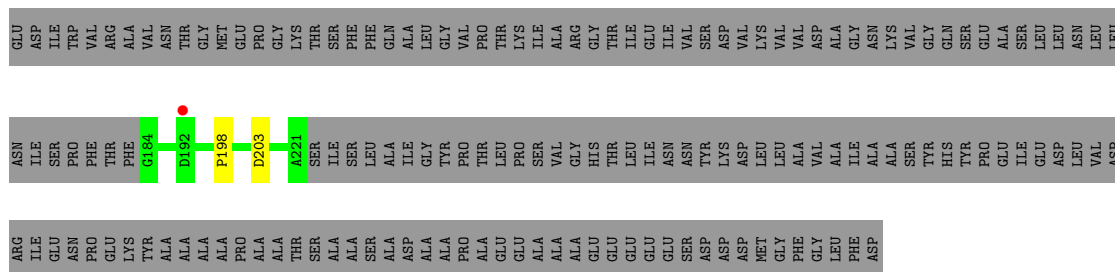
Chain m2:



- Molecule 84: 60S acidic ribosomal protein P0

Chain p0:





- Molecule 85: UNKNOWN PROTEIN p1

Chain p1: 

There are no outlier residues recorded for this chain.

- Molecule 86: 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	436.02Å 287.59Å 304.52Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	49.82 – 3.20 49.82 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.82-3.20) 99.9 (49.82-3.20)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.181 , 0.237 0.259 , 0.299	Depositor DCC
R_{free} test set	24045 reflections (1.98%)	DCC
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	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	1 of 1214488 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	411288	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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

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	0.68	1/41698 (0.0%)	1.28	292/64972 (0.4%)
1	6	0.81	13/42765 (0.0%)	1.38	456/66634 (0.7%)
2	S0	0.43	0/1617	0.67	0/2215
2	s0	0.49	0/1623	0.72	0/2222
3	S1	0.37	0/1735	0.69	2/2335 (0.1%)
3	s1	0.51	0/1748	0.70	1/2352 (0.0%)
4	S2	0.45	0/1665	0.65	0/2263
4	s2	0.54	0/1665	0.72	1/2263 (0.0%)
5	S3	0.45	0/1759	0.68	2/2368 (0.1%)
5	s3	0.45	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.71	0/2839
6	s4	0.52	0/2109	0.75	2/2839 (0.1%)
7	S5	0.38	0/1629	0.60	0/2202
7	s5	0.46	0/1629	0.71	1/2202 (0.0%)
8	S6	0.45	0/1823	0.63	1/2439 (0.0%)
8	s6	0.51	0/1779	0.68	0/2379
9	S7	0.42	0/1506	0.63	0/2028
9	s7	0.44	0/1516	0.70	1/2043 (0.0%)
10	S8	0.51	0/1514	0.76	1/2021 (0.0%)
10	s8	0.59	0/1514	0.77	1/2021 (0.0%)
11	S9	0.43	0/1519	0.65	0/2035
11	s9	0.53	0/1519	0.75	1/2035 (0.0%)
12	C0	0.43	0/790	0.66	1/1069 (0.1%)
13	C1	0.55	0/1240	0.69	0/1675
13	c1	0.60	0/1194	0.80	2/1610 (0.1%)
14	C2	0.35	0/900	0.65	1/1224 (0.1%)
14	c2	0.32	0/900	0.60	1/1224 (0.1%)
15	C3	0.47	0/1215	0.69	3/1638 (0.2%)
15	c3	0.54	0/1215	0.75	1/1638 (0.1%)
16	C4	0.37	0/901	0.64	0/1217
16	c4	0.52	0/960	0.73	0/1290
17	C5	0.44	0/998	0.66	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	c5	0.47	0/1060	0.66	0/1426
18	C6	0.43	0/1125	0.69	2/1510 (0.1%)
18	c6	0.48	0/1131	0.71	1/1518 (0.1%)
19	C7	0.40	0/935	0.66	0/1254
19	c7	0.48	0/914	0.72	0/1224
20	C8	0.43	0/1211	0.66	1/1628 (0.1%)
20	c8	0.50	0/1211	0.70	2/1628 (0.1%)
21	C9	0.44	0/1130	0.67	1/1517 (0.1%)
21	c9	0.49	0/1130	0.72	2/1517 (0.1%)
22	D0	0.45	0/865	0.66	0/1169
22	d0	0.49	0/892	0.70	0/1205
23	D1	0.39	0/693	0.59	0/935
23	d1	0.49	0/693	0.70	0/935
24	D2	0.46	0/1038	0.75	2/1395 (0.1%)
24	d2	0.64	0/1038	0.78	1/1395 (0.1%)
25	D3	0.58	0/1139	0.74	0/1518
25	d3	0.64	0/1139	0.82	2/1518 (0.1%)
26	D4	0.41	0/1087	0.59	0/1449
26	d4	0.51	0/1087	0.69	0/1449
27	D5	0.39	0/571	0.77	2/768 (0.3%)
27	d5	0.42	0/566	0.69	0/761
28	D6	0.40	0/782	0.60	0/1047
28	d6	0.53	0/782	0.69	0/1047
29	D7	0.42	0/620	0.68	0/838
29	d7	0.44	0/620	0.68	0/838
30	D8	0.34	0/499	0.62	0/670
30	d8	0.38	0/499	0.64	0/670
31	D9	0.50	0/452	0.74	1/600 (0.2%)
31	d9	0.56	0/452	0.71	0/600
32	E0	0.40	0/483	0.64	0/643
33	E1	0.41	0/577	0.78	0/770
34	SR	0.39	0/2494	0.63	0/3393
34	sR	0.39	0/2495	0.60	0/3395
35	SM	0.45	0/1113	0.68	2/1502 (0.1%)
35	sM	0.41	0/683	0.63	1/923 (0.1%)
36	1	1.01	59/75394 (0.1%)	1.57	1453/117545 (1.2%)
36	5	1.05	74/75414 (0.1%)	1.58	1442/117575 (1.2%)
37	3	0.87	0/2883	1.32	14/4491 (0.3%)
37	7	1.02	1/2883 (0.0%)	1.60	54/4491 (1.2%)
38	4	0.95	1/3746 (0.0%)	1.51	47/5832 (0.8%)
38	8	0.89	0/3746	1.43	43/5832 (0.7%)
39	L2	0.65	0/1948	0.81	2/2617 (0.1%)
39	l2	0.64	0/1946	0.83	0/2614

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	L3	0.62	0/3146	0.77	0/4228
40	l3	0.76	0/3146	0.84	3/4228 (0.1%)
41	L4	0.70	1/2800 (0.0%)	0.88	3/3790 (0.1%)
41	l4	0.68	1/2800 (0.0%)	0.85	3/3790 (0.1%)
42	L5	0.51	0/2425	0.67	0/3271
42	l5	0.65	0/2408	0.76	0/3248
43	L6	0.65	0/1260	0.79	0/1694
43	l6	0.66	0/1269	0.76	1/1705 (0.1%)
44	L7	0.68	0/1821	0.85	2/2451 (0.1%)
44	l7	0.74	0/1828	0.80	2/2461 (0.1%)
45	L8	0.51	0/1836	0.69	0/2481
45	l8	0.52	0/1795	0.67	0/2429
46	L9	0.60	0/1539	0.71	0/2073
46	l9	0.70	0/1539	0.80	0/2073
47	M0	0.64	0/1741	0.76	2/2335 (0.1%)
47	m0	0.67	0/1758	0.80	3/2358 (0.1%)
48	M1	0.49	0/1374	0.71	1/1842 (0.1%)
48	m1	0.59	0/1374	0.81	2/1842 (0.1%)
49	M3	0.68	0/1568	0.80	1/2106 (0.0%)
49	m3	0.61	0/1573	0.78	0/2113
50	M4	0.61	0/1068	0.74	0/1438
50	m4	0.68	0/1074	0.80	1/1446 (0.1%)
51	M5	0.65	0/1757	0.79	1/2354 (0.0%)
51	m5	0.64	0/1757	0.77	0/2354
52	M6	0.70	0/1585	0.86	3/2128 (0.1%)
52	m6	0.84	0/1585	0.92	3/2128 (0.1%)
53	M7	0.67	0/1443	0.80	1/1944 (0.1%)
53	m7	0.78	0/1250	0.81	0/1683
54	M8	0.67	0/1465	0.85	2/1965 (0.1%)
54	m8	0.66	0/1465	0.86	2/1965 (0.1%)
55	M9	0.51	0/1538	0.66	0/2050
55	m9	0.57	0/1538	0.65	0/2050
56	N0	0.64	0/1481	0.82	3/1990 (0.2%)
56	n0	0.73	0/1481	0.83	2/1990 (0.1%)
57	N1	0.68	0/1300	0.79	0/1743
57	n1	0.74	0/1300	0.79	0/1743
58	N2	0.44	0/812	0.63	0/1099
58	n2	0.46	0/794	0.62	0/1076
59	N3	0.62	0/1018	0.78	1/1369 (0.1%)
59	n3	0.69	0/1018	0.83	1/1369 (0.1%)
60	N4	0.50	0/712	0.64	0/958
60	n4	0.61	0/1052	0.70	0/1398
61	N5	0.53	0/979	0.74	1/1321 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
61	n5	0.58	0/974	0.74	1/1314 (0.1%)
62	N6	0.63	0/1004	0.82	1/1341 (0.1%)
62	n6	0.57	0/1004	0.78	1/1341 (0.1%)
63	N7	0.49	0/1118	0.66	0/1497
63	n7	0.47	0/1118	0.67	0/1497
64	N8	0.72	0/1204	0.86	1/1612 (0.1%)
64	n8	0.69	0/1204	0.82	0/1612
65	N9	0.60	0/473	0.78	0/629
65	n9	0.63	0/473	0.89	1/629 (0.2%)
66	O0	0.47	0/751	0.64	0/1008
66	o0	0.49	0/775	0.69	0/1040
67	O1	0.60	0/890	0.74	0/1196
67	o1	0.66	0/897	0.81	0/1205
68	O2	0.79	0/1041	0.87	0/1394
68	o2	0.74	0/1041	0.87	2/1394 (0.1%)
69	O3	0.79	0/868	0.85	0/1168
69	o3	0.79	0/868	0.83	0/1168
70	O4	0.59	0/890	0.79	2/1189 (0.2%)
70	o4	0.57	0/890	0.81	0/1189
71	O5	0.62	0/978	0.77	0/1301
71	o5	0.53	0/974	0.67	0/1297
72	O6	0.57	0/778	0.74	0/1034
72	o6	0.55	0/777	0.70	0/1033
73	O7	0.67	0/696	0.94	4/923 (0.4%)
73	o7	0.64	0/696	0.81	1/923 (0.1%)
74	O8	0.48	0/618	0.64	1/826 (0.1%)
74	o8	0.45	0/614	0.64	0/822
75	O9	0.64	0/443	0.83	0/588
75	o9	0.63	0/443	0.76	0/588
76	Q0	0.64	0/423	0.73	0/562
76	q0	0.81	1/423 (0.2%)	0.85	0/562
77	Q1	0.66	0/234	0.84	0/300
77	q1	0.65	0/234	0.98	2/300 (0.7%)
78	Q2	0.74	1/860 (0.1%)	0.83	0/1136
78	q2	0.69	0/860	0.79	1/1136 (0.1%)
79	Q3	0.67	0/701	0.77	0/934
79	q3	0.65	0/701	0.80	0/934
80	c0	0.40	0/777	0.66	3/1049 (0.3%)
81	e0	0.49	0/499	0.72	0/665
82	e1	0.38	0/619	0.74	1/822 (0.1%)
84	p0	0.44	0/1092	0.63	1/1474 (0.1%)
All	All	0.80	153/430074 (0.0%)	1.26	3913/631364 (0.6%)

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
3	s1	0	1
7	s5	0	2
9	S7	0	1
9	s7	0	1
10	s8	0	1
13	C1	0	1
15	c3	0	1
16	C4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	2
19	c7	0	3
22	d0	0	1
25	D3	0	1
26	d4	0	2
27	D5	0	3
27	d5	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	2
42	l5	0	2
43	l6	0	1
44	l7	0	2
45	L8	0	2
48	M1	0	2
51	m5	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	2
56	n0	0	1
57	N1	0	1
60	n4	0	1
63	n7	0	1
64	n8	0	2
65	N9	0	1
65	n9	0	1
82	e1	0	1
All	All	0	52

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.64	1.28	1.38
36	5	3008	A	N9-C4	-8.98	1.32	1.37
36	5	2358	A	N9-C4	-8.04	1.33	1.37
36	1	1114	U	C2-N3	-7.72	1.32	1.37
36	1	2714	G	N9-C4	-7.69	1.31	1.38

The worst 5 of 3913 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-21.84	112.90	126.00
36	5	1152	G	N3-C4-C5	21.63	139.41	128.60
36	5	1152	G	C2-N3-C4	-18.18	102.81	111.90
36	1	2714	G	N3-C4-C5	17.75	137.47	128.60
36	1	1308	A	O5'-P-OP2	-16.96	90.35	110.70

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	C1	127	GLN	Peptide
16	C4	124	ASP	Peptide
18	C6	40	GLU	Peptide
19	C7	22	PRO	Peptide
9	S7	131	PHE	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	18758	895	0
1	6	38238	0	19240	845	0
2	S0	1577	0	1567	166	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	187	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	119	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	110	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	184	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	153	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	138	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	126	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	131	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	148	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	74	0
13	C1	1214	0	1259	101	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	65	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	95	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	94	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	89	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	117	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	94	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	109	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	96	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	88	0
22	d0	882	0	939	0	0
23	D1	684	0	672	78	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	88	0
24	d2	1021	0	1060	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D3	1121	0	1196	86	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	94	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	70	0
27	d5	558	0	598	0	0
28	D6	769	0	814	99	0
28	d6	769	0	815	0	0
29	D7	610	0	630	51	0
29	d7	610	0	631	0	0
30	D8	497	0	535	47	0
30	d8	497	0	535	0	0
31	D9	442	0	428	32	0
31	d9	442	0	428	0	0
32	E0	475	0	525	37	0
33	E1	566	0	602	58	0
34	SR	2441	0	2397	183	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	74	0
35	sM	680	0	607	0	0
36	1	67355	0	33846	1234	0
36	5	67376	0	33861	1200	0
37	3	2579	0	1304	46	0
37	7	2579	0	1304	51	0
38	4	3353	0	1695	60	0
38	8	3353	0	1695	72	0
39	L2	1914	0	1981	157	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	260	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	204	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	182	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	86	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	131	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	126	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	131	0
46	l9	1518	0	1587	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	M0	1705	0	1736	158	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	103	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	134	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	89	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	125	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	103	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	100	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	102	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1616	110	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	107	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	105	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	51	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	70	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	25	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	60	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	80	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	103	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1215	94	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	31	0
65	n9	462	0	491	0	0
66	O0	743	0	797	61	0
66	o0	767	0	816	0	0
67	O1	876	0	912	57	0
67	o1	883	0	918	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	O2	1020	0	1090	88	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	47	0
69	o3	850	0	880	0	0
70	O4	880	0	945	69	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	81	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	66	0
72	o6	770	0	846	0	0
73	O7	681	0	683	47	0
73	o7	681	0	683	0	0
74	O8	612	0	682	49	0
74	o8	608	0	671	0	0
75	O9	436	0	475	32	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	22	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	26	0
77	q1	233	0	284	0	0
78	Q2	847	0	915	56	0
78	q2	847	0	915	0	0
79	Q3	694	0	734	57	0
79	q3	694	0	734	0	0
80	c0	762	0	699	0	0
81	e0	491	0	542	0	0
82	e1	608	0	654	0	0
83	m2	750	0	178	0	0
84	p0	1077	0	1041	0	0
85	p1	235	0	50	0	0
86	p2	230	0	52	0	0
87	1	477	0	0	0	0
87	2	124	0	0	0	0
87	3	14	0	0	0	0
87	4	19	0	0	0	0
87	5	502	0	0	0	0
87	6	144	0	0	0	0
87	7	15	0	0	0	0
87	8	16	0	0	0	0
87	D3	1	0	0	0	0
87	L2	1	0	0	0	0
87	L3	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	L4	1	0	0	0	0
87	L5	1	0	0	0	0
87	L7	4	0	0	0	0
87	L8	1	0	0	0	0
87	M0	2	0	0	0	0
87	M1	1	0	0	0	0
87	M3	2	0	0	0	0
87	M5	2	0	0	0	0
87	M6	1	0	0	0	0
87	M7	4	0	0	0	0
87	M9	1	0	0	0	0
87	N0	1	0	0	0	0
87	N3	3	0	0	0	0
87	N5	1	0	0	0	0
87	N8	5	0	0	0	0
87	O2	1	0	0	0	0
87	O4	1	0	0	0	0
87	O5	1	0	0	0	0
87	O7	1	0	0	0	0
87	S4	2	0	0	0	0
87	S8	1	0	0	0	0
87	SM	1	0	0	0	0
87	c1	1	0	0	0	0
87	c7	2	0	0	0	0
87	c8	1	0	0	0	0
87	c9	1	0	0	0	0
87	d3	1	0	0	0	0
87	d4	1	0	0	0	0
87	d6	1	0	0	0	0
87	l2	1	0	0	0	0
87	l3	3	0	0	0	0
87	l4	2	0	0	0	0
87	l5	2	0	0	0	0
87	l7	1	0	0	0	0
87	m1	2	0	0	0	0
87	m5	5	0	0	0	0
87	m6	2	0	0	0	0
87	m7	5	0	0	0	0
87	n0	3	0	0	0	0
87	n3	2	0	0	0	0
87	n6	2	0	0	0	0
87	n8	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	o1	1	0	0	0	0
87	o3	1	0	0	0	0
87	o4	1	0	0	0	0
87	q0	1	0	0	0	0
87	q1	1	0	0	0	0
87	q3	2	0	0	0	0
87	s1	1	0	0	0	0
87	s6	1	0	0	0	0
87	s8	3	0	0	0	0
87	sM	1	0	0	0	0
88	1	2478	0	0	145	0
88	2	1106	0	0	73	0
88	3	77	0	0	1	0
88	4	98	0	0	6	0
88	5	2506	0	0	157	0
88	6	1113	0	0	73	0
88	7	84	0	0	5	0
88	8	98	0	0	11	0
88	C3	7	0	0	1	0
88	C5	7	0	0	5	0
88	C8	7	0	0	0	0
88	D3	7	0	0	0	0
88	D9	7	0	0	0	0
88	L3	21	0	0	2	0
88	L4	7	0	0	3	0
88	M0	7	0	0	0	0
88	M5	7	0	0	1	0
88	M7	14	0	0	1	0
88	M8	7	0	0	0	0
88	M9	7	0	0	0	0
88	N9	7	0	0	0	0
88	O3	7	0	0	0	0
88	O7	14	0	0	2	0
88	S8	7	0	0	1	0
88	SR	7	0	0	0	0
88	c1	7	0	0	0	0
88	c3	7	0	0	0	0
88	c5	7	0	0	0	0
88	c8	7	0	0	0	0
88	d4	7	0	0	0	0
88	d9	7	0	0	0	0
88	l3	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	l4	14	0	0	0	0
88	l5	28	0	0	0	0
88	l9	7	0	0	0	0
88	m0	14	0	0	0	0
88	m1	7	0	0	0	0
88	m4	7	0	0	0	0
88	m5	7	0	0	0	0
88	m6	7	0	0	0	0
88	n3	14	0	0	0	0
88	n9	7	0	0	0	0
88	o3	7	0	0	0	0
88	o7	7	0	0	0	0
88	q2	7	0	0	0	0
88	s1	14	0	0	0	0
88	s8	7	0	0	0	0
88	sR	7	0	0	0	0
89	D6	1	0	0	0	0
89	D7	1	0	0	0	0
89	D9	1	0	0	0	0
89	E1	1	0	0	0	0
89	O7	1	0	0	0	0
89	Q0	1	0	0	0	0
89	Q2	1	0	0	0	0
89	Q3	1	0	0	0	0
89	d6	1	0	0	0	0
89	d7	1	0	0	0	0
89	d9	1	0	0	0	0
89	e1	1	0	0	0	0
89	o7	1	0	0	0	0
89	q0	1	0	0	0	0
89	q2	1	0	0	0	0
89	q3	1	0	0	0	0
90	1	22	0	12	0	0
90	5	22	0	12	0	0
91	Q2	40	0	22	3	0
91	q2	40	0	22	0	0
All	All	411288	0	297360	10031	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 10031 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.56	1.11
40:L3:296:THR:HG22	40:L3:298:PHE:H	2.66	1.06
1:6:1636:C:H4'	1:6:1637:C:H5'	1.34	1.05
28:D6:26:CYS:SG	28:D6:77:CYS:SG	3.43	1.01
36:5:3274:A:H3'	36:5:3275:U:H5''	1.42	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	143 (70%)	34 (17%)	27 (13%)	0	2
2	s0	204/251 (81%)	152 (74%)	33 (16%)	19 (9%)	1	8
3	S1	212/254 (84%)	141 (66%)	38 (18%)	33 (16%)	0	1
3	s1	214/254 (84%)	171 (80%)	30 (14%)	13 (6%)	2	19
4	S2	215/253 (85%)	173 (80%)	27 (13%)	15 (7%)	2	13
4	s2	215/253 (85%)	184 (86%)	21 (10%)	10 (5%)	4	27
5	S3	221/239 (92%)	182 (82%)	24 (11%)	15 (7%)	2	15
5	s3	221/239 (92%)	174 (79%)	31 (14%)	16 (7%)	2	13
6	S4	258/260 (99%)	206 (80%)	34 (13%)	18 (7%)	2	13
6	s4	258/260 (99%)	210 (81%)	28 (11%)	20 (8%)	1	11
7	S5	204/224 (91%)	154 (76%)	34 (17%)	16 (8%)	1	11
7	s5	204/224 (91%)	154 (76%)	35 (17%)	15 (7%)	2	12
8	S6	224/236 (95%)	197 (88%)	15 (7%)	12 (5%)	3	24
8	s6	216/236 (92%)	184 (85%)	22 (10%)	10 (5%)	4	28
9	S7	182/189 (96%)	136 (75%)	25 (14%)	21 (12%)	1	4
9	s7	184/189 (97%)	141 (77%)	28 (15%)	15 (8%)	1	10
10	S8	184/200 (92%)	148 (80%)	23 (12%)	13 (7%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	s8	184/200 (92%)	155 (84%)	16 (9%)	13 (7%)	2	13
11	S9	183/196 (93%)	147 (80%)	26 (14%)	10 (6%)	3	23
11	s9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	5	34
12	C0	94/105 (90%)	68 (72%)	17 (18%)	9 (10%)	1	7
13	C1	153/155 (99%)	114 (74%)	24 (16%)	15 (10%)	1	7
13	c1	144/155 (93%)	122 (85%)	16 (11%)	6 (4%)	4	31
14	C2	122/142 (86%)	67 (55%)	34 (28%)	21 (17%)	0	1
14	c2	122/142 (86%)	67 (55%)	32 (26%)	23 (19%)	0	0
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	4	32
15	c3	148/150 (99%)	120 (81%)	18 (12%)	10 (7%)	2	15
16	C4	125/136 (92%)	90 (72%)	19 (15%)	16 (13%)	0	3
16	c4	126/136 (93%)	96 (76%)	19 (15%)	11 (9%)	1	8
17	C5	122/141 (86%)	88 (72%)	22 (18%)	12 (10%)	1	7
17	c5	133/141 (94%)	94 (71%)	20 (15%)	19 (14%)	0	2
18	C6	139/142 (98%)	117 (84%)	11 (8%)	11 (8%)	1	11
18	c6	140/142 (99%)	120 (86%)	12 (9%)	8 (6%)	3	22
19	C7	116/136 (85%)	87 (75%)	21 (18%)	8 (7%)	2	14
19	c7	113/136 (83%)	84 (74%)	19 (17%)	10 (9%)	1	8
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	9
20	c8	143/145 (99%)	115 (80%)	18 (13%)	10 (7%)	2	13
21	C9	141/143 (99%)	120 (85%)	14 (10%)	7 (5%)	3	26
21	c9	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	4	30
22	D0	105/120 (88%)	82 (78%)	19 (18%)	4 (4%)	5	34
22	d0	108/120 (90%)	87 (81%)	10 (9%)	11 (10%)	1	6
23	D1	85/87 (98%)	64 (75%)	12 (14%)	9 (11%)	1	5
23	d1	85/87 (98%)	72 (85%)	10 (12%)	3 (4%)	6	37
24	D2	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	9	51
24	d2	127/129 (98%)	112 (88%)	14 (11%)	1 (1%)	27	77
25	D3	142/144 (99%)	109 (77%)	19 (13%)	14 (10%)	1	7
25	d3	142/144 (99%)	119 (84%)	18 (13%)	5 (4%)	6	37
26	D4	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	d4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	2	12
27	D5	68/107 (64%)	44 (65%)	11 (16%)	13 (19%)	0	0
27	d5	67/107 (63%)	49 (73%)	11 (16%)	7 (10%)	1	5
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0	2
28	d6	95/97 (98%)	67 (70%)	18 (19%)	10 (10%)	1	5
29	D7	79/81 (98%)	63 (80%)	9 (11%)	7 (9%)	1	8
29	d7	79/81 (98%)	60 (76%)	12 (15%)	7 (9%)	1	8
30	D8	61/66 (92%)	49 (80%)	6 (10%)	6 (10%)	1	7
30	d8	61/66 (92%)	43 (70%)	13 (21%)	5 (8%)	1	10
31	D9	51/55 (93%)	41 (80%)	8 (16%)	2 (4%)	5	33
31	d9	51/55 (93%)	36 (71%)	9 (18%)	6 (12%)	1	4
32	E0	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	14	62
33	E1	69/76 (91%)	38 (55%)	12 (17%)	19 (28%)	0	0
34	SR	316/318 (99%)	244 (77%)	45 (14%)	27 (8%)	1	9
34	sR	316/318 (99%)	261 (83%)	42 (13%)	13 (4%)	4	32
35	SM	155/273 (57%)	111 (72%)	27 (17%)	17 (11%)	1	5
35	sM	98/273 (36%)	57 (58%)	28 (29%)	13 (13%)	0	2
39	L2	250/253 (99%)	224 (90%)	17 (7%)	9 (4%)	5	36
39	l2	250/253 (99%)	214 (86%)	23 (9%)	13 (5%)	3	25
40	L3	384/386 (100%)	322 (84%)	45 (12%)	17 (4%)	4	29
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	6	38
41	L4	359/361 (99%)	297 (83%)	34 (10%)	28 (8%)	1	11
41	l4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	2	19
42	L5	294/296 (99%)	237 (81%)	35 (12%)	22 (8%)	2	12
42	l5	292/296 (99%)	253 (87%)	32 (11%)	7 (2%)	9	51
43	L6	152/175 (87%)	134 (88%)	12 (8%)	6 (4%)	5	33
43	l6	153/175 (87%)	130 (85%)	17 (11%)	6 (4%)	5	33
44	L7	220/243 (90%)	184 (84%)	26 (12%)	10 (4%)	4	29
44	l7	221/243 (91%)	189 (86%)	27 (12%)	5 (2%)	10	52
45	L8	231/255 (91%)	189 (82%)	31 (13%)	11 (5%)	4	27
45	l8	229/255 (90%)	188 (82%)	23 (10%)	18 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	L9	189/191 (99%)	166 (88%)	21 (11%)	2 (1%)	21	72
46	l9	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	6	39
47	M0	207/220 (94%)	171 (83%)	28 (14%)	8 (4%)	5	33
47	m0	209/220 (95%)	172 (82%)	23 (11%)	14 (7%)	2	16
48	M1	167/173 (96%)	122 (73%)	29 (17%)	16 (10%)	1	7
48	m1	167/173 (96%)	141 (84%)	15 (9%)	11 (7%)	2	16
49	M3	191/198 (96%)	154 (81%)	26 (14%)	11 (6%)	3	21
49	m3	192/198 (97%)	150 (78%)	28 (15%)	14 (7%)	2	12
50	M4	134/137 (98%)	113 (84%)	12 (9%)	9 (7%)	2	16
50	m4	135/137 (98%)	118 (87%)	16 (12%)	1 (1%)	30	80
51	M5	201/203 (99%)	183 (91%)	14 (7%)	4 (2%)	11	56
51	m5	201/203 (99%)	181 (90%)	16 (8%)	4 (2%)	11	56
52	M6	195/198 (98%)	176 (90%)	12 (6%)	7 (4%)	5	36
52	m6	195/198 (98%)	179 (92%)	10 (5%)	6 (3%)	7	41
53	M7	181/183 (99%)	144 (80%)	27 (15%)	10 (6%)	3	23
53	m7	153/183 (84%)	132 (86%)	18 (12%)	3 (2%)	11	56
54	M8	183/185 (99%)	154 (84%)	24 (13%)	5 (3%)	8	46
54	m8	183/185 (99%)	151 (82%)	26 (14%)	6 (3%)	6	38
55	M9	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	38	85
55	m9	186/188 (99%)	167 (90%)	14 (8%)	5 (3%)	8	46
56	N0	170/172 (99%)	154 (91%)	13 (8%)	3 (2%)	13	60
56	n0	170/172 (99%)	160 (94%)	7 (4%)	3 (2%)	13	60
57	N1	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	4	29
57	n1	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	6	39
58	N2	98/120 (82%)	72 (74%)	15 (15%)	11 (11%)	1	4
58	n2	96/120 (80%)	78 (81%)	15 (16%)	3 (3%)	7	41
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	15	64
59	n3	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
60	N4	96/155 (62%)	78 (81%)	13 (14%)	5 (5%)	3	25
60	n4	133/155 (86%)	109 (82%)	15 (11%)	9 (7%)	2	15
61	N5	119/141 (84%)	106 (89%)	11 (9%)	2 (2%)	14	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	n5	118/141 (84%)	98 (83%)	11 (9%)	9 (8%)	2	12
62	N6	124/126 (98%)	104 (84%)	14 (11%)	6 (5%)	4	27
62	n6	124/126 (98%)	112 (90%)	8 (6%)	4 (3%)	6	39
63	N7	133/135 (98%)	111 (84%)	11 (8%)	11 (8%)	1	9
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	1	9
64	N8	146/148 (99%)	121 (83%)	18 (12%)	7 (5%)	4	27
64	n8	146/148 (99%)	119 (82%)	22 (15%)	5 (3%)	6	38
65	N9	56/58 (97%)	47 (84%)	6 (11%)	3 (5%)	3	24
65	n9	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	8
66	O0	95/104 (91%)	76 (80%)	15 (16%)	4 (4%)	4	31
66	o0	98/104 (94%)	85 (87%)	13 (13%)	0	100	100
67	O1	107/112 (96%)	91 (85%)	8 (8%)	8 (8%)	2	12
67	o1	107/112 (96%)	85 (79%)	13 (12%)	9 (8%)	1	9
68	O2	125/129 (97%)	108 (86%)	17 (14%)	0	100	100
68	o2	125/129 (97%)	109 (87%)	9 (7%)	7 (6%)	3	23
69	O3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	7	43
69	o3	104/106 (98%)	96 (92%)	4 (4%)	4 (4%)	5	34
70	O4	110/119 (92%)	94 (86%)	14 (13%)	2 (2%)	13	60
70	o4	110/119 (92%)	100 (91%)	9 (8%)	1 (1%)	25	76
71	O5	117/119 (98%)	99 (85%)	10 (8%)	8 (7%)	2	15
71	o5	117/119 (98%)	95 (81%)	17 (14%)	5 (4%)	4	30
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	2	19
72	o6	97/99 (98%)	76 (78%)	15 (16%)	6 (6%)	2	19
73	O7	85/87 (98%)	74 (87%)	8 (9%)	3 (4%)	6	37
73	o7	85/87 (98%)	70 (82%)	11 (13%)	4 (5%)	4	27
74	O8	75/77 (97%)	65 (87%)	7 (9%)	3 (4%)	5	32
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	5	32
75	O9	48/50 (96%)	40 (83%)	6 (12%)	2 (4%)	4	31
75	o9	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
76	Q0	50/52 (96%)	39 (78%)	9 (18%)	2 (4%)	5	32
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	11	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	4	30
78	Q2	103/105 (98%)	84 (82%)	13 (13%)	6 (6%)	3	21
78	q2	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	12	59
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	6	38
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	21	72
80	c0	92/105 (88%)	59 (64%)	16 (17%)	17 (18%)	0	1
81	e0	60/62 (97%)	43 (72%)	10 (17%)	7 (12%)	1	4
82	e1	74/76 (97%)	34 (46%)	21 (28%)	19 (26%)	0	0
84	p0	139/311 (45%)	116 (84%)	16 (12%)	7 (5%)	3	26
All	All	22333/24141 (92%)	18253 (82%)	2722 (12%)	1358 (6%)	2	19

5 of 1358 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	30	GLN
2	S0	39	ASN
2	S0	66	ALA
2	S0	111	ILE

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%)	136 (83%)	28 (17%)	3	14
2	s0	165/209 (79%)	127 (77%)	38 (23%)	1	5
3	S1	191/223 (86%)	151 (79%)	40 (21%)	1	8
3	s1	192/223 (86%)	153 (80%)	39 (20%)	2	9
4	S2	176/204 (86%)	130 (74%)	46 (26%)	1	2
4	s2	176/204 (86%)	129 (73%)	47 (27%)	1	2
5	S3	182/194 (94%)	143 (79%)	39 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	s3	182/194 (94%)	143 (79%)	39 (21%)	1	7
6	S4	221/221 (100%)	178 (80%)	43 (20%)	2	10
6	s4	221/221 (100%)	184 (83%)	37 (17%)	3	14
7	S5	173/190 (91%)	145 (84%)	28 (16%)	3	15
7	s5	173/190 (91%)	133 (77%)	40 (23%)	1	5
8	S6	188/201 (94%)	151 (80%)	37 (20%)	2	10
8	s6	187/201 (93%)	150 (80%)	37 (20%)	2	9
9	S7	165/169 (98%)	136 (82%)	29 (18%)	3	13
9	s7	165/169 (98%)	134 (81%)	31 (19%)	2	11
10	S8	150/161 (93%)	122 (81%)	28 (19%)	2	11
10	s8	150/161 (93%)	124 (83%)	26 (17%)	3	13
11	S9	158/165 (96%)	124 (78%)	34 (22%)	1	7
11	s9	158/165 (96%)	126 (80%)	32 (20%)	2	9
12	C0	77/98 (79%)	64 (83%)	13 (17%)	3	14
13	C1	129/136 (95%)	107 (83%)	22 (17%)	3	14
13	c1	129/136 (95%)	109 (84%)	20 (16%)	4	17
14	C2	88/118 (75%)	66 (75%)	22 (25%)	1	3
14	c2	88/118 (75%)	63 (72%)	25 (28%)	0	2
15	C3	127/127 (100%)	100 (79%)	27 (21%)	1	7
15	c3	127/127 (100%)	103 (81%)	24 (19%)	2	11
16	C4	81/104 (78%)	60 (74%)	21 (26%)	1	2
16	c4	97/104 (93%)	69 (71%)	28 (29%)	0	1
17	C5	101/117 (86%)	80 (79%)	21 (21%)	2	8
17	c5	103/117 (88%)	78 (76%)	25 (24%)	1	3
18	C6	117/118 (99%)	89 (76%)	28 (24%)	1	4
18	c6	118/118 (100%)	95 (80%)	23 (20%)	2	10
19	C7	94/124 (76%)	75 (80%)	19 (20%)	2	9
19	c7	92/124 (74%)	66 (72%)	26 (28%)	0	2
20	C8	128/128 (100%)	96 (75%)	32 (25%)	1	3
20	c8	128/128 (100%)	101 (79%)	27 (21%)	1	8
21	C9	115/115 (100%)	83 (72%)	32 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	c9	115/115 (100%)	93 (81%)	22 (19%)	2	11
22	D0	100/113 (88%)	83 (83%)	17 (17%)	3	14
22	d0	103/113 (91%)	71 (69%)	32 (31%)	0	1
23	D1	74/74 (100%)	59 (80%)	15 (20%)	2	9
23	d1	74/74 (100%)	59 (80%)	15 (20%)	2	9
24	D2	110/110 (100%)	88 (80%)	22 (20%)	2	9
24	d2	110/110 (100%)	93 (84%)	17 (16%)	4	17
25	D3	119/119 (100%)	98 (82%)	21 (18%)	3	13
25	d3	119/119 (100%)	92 (77%)	27 (23%)	1	6
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2	12
26	d4	112/112 (100%)	91 (81%)	21 (19%)	2	11
27	D5	61/88 (69%)	50 (82%)	11 (18%)	2	12
27	d5	61/88 (69%)	49 (80%)	12 (20%)	2	10
28	D6	83/83 (100%)	66 (80%)	17 (20%)	2	8
28	d6	83/83 (100%)	63 (76%)	20 (24%)	1	4
29	D7	70/70 (100%)	55 (79%)	15 (21%)	1	7
29	d7	70/70 (100%)	59 (84%)	11 (16%)	4	17
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0	1
30	d8	56/59 (95%)	41 (73%)	15 (27%)	1	2
31	D9	47/48 (98%)	41 (87%)	6 (13%)	6	28
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	7
32	E0	51/51 (100%)	42 (82%)	9 (18%)	3	13
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	2
34	SR	260/261 (100%)	214 (82%)	46 (18%)	3	13
34	sR	260/261 (100%)	237 (91%)	23 (9%)	14	50
35	SM	97/228 (42%)	79 (81%)	18 (19%)	2	11
35	sM	54/228 (24%)	40 (74%)	14 (26%)	1	2
39	L2	193/195 (99%)	153 (79%)	40 (21%)	2	8
39	l2	192/195 (98%)	156 (81%)	36 (19%)	2	11
40	L3	320/322 (99%)	260 (81%)	60 (19%)	2	11
40	l3	319/322 (99%)	259 (81%)	60 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	L4	288/288 (100%)	241 (84%)	47 (16%)	3	15
41	l4	288/288 (100%)	236 (82%)	52 (18%)	2	12
42	L5	244/244 (100%)	199 (82%)	45 (18%)	2	11
42	l5	243/244 (100%)	194 (80%)	49 (20%)	2	9
43	L6	134/152 (88%)	113 (84%)	21 (16%)	4	17
43	l6	135/152 (89%)	113 (84%)	22 (16%)	3	15
44	L7	186/204 (91%)	162 (87%)	24 (13%)	6	28
44	l7	187/204 (92%)	163 (87%)	24 (13%)	6	28
45	L8	187/207 (90%)	151 (81%)	36 (19%)	2	10
45	l8	177/207 (86%)	145 (82%)	32 (18%)	2	12
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	8
46	l9	171/171 (100%)	132 (77%)	39 (23%)	1	6
47	M0	177/186 (95%)	136 (77%)	41 (23%)	1	5
47	m0	179/186 (96%)	148 (83%)	31 (17%)	3	13
48	M1	147/150 (98%)	115 (78%)	32 (22%)	1	7
48	m1	147/150 (98%)	112 (76%)	35 (24%)	1	4
49	M3	154/158 (98%)	124 (80%)	30 (20%)	2	10
49	m3	154/158 (98%)	129 (84%)	25 (16%)	3	15
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	13
50	m4	108/108 (100%)	84 (78%)	24 (22%)	1	6
51	M5	175/175 (100%)	148 (85%)	27 (15%)	4	18
51	m5	175/175 (100%)	142 (81%)	33 (19%)	2	11
52	M6	160/161 (99%)	134 (84%)	26 (16%)	3	15
52	m6	160/161 (99%)	136 (85%)	24 (15%)	4	19
53	M7	140/145 (97%)	114 (81%)	26 (19%)	2	11
53	m7	125/145 (86%)	101 (81%)	24 (19%)	2	10
54	M8	150/150 (100%)	123 (82%)	27 (18%)	2	12
54	m8	150/150 (100%)	125 (83%)	25 (17%)	3	14
55	M9	153/153 (100%)	130 (85%)	23 (15%)	4	19
55	m9	153/153 (100%)	121 (79%)	32 (21%)	1	8
56	N0	156/156 (100%)	125 (80%)	31 (20%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	n0	156/156 (100%)	127 (81%)	29 (19%)	2	11
57	N1	136/136 (100%)	104 (76%)	32 (24%)	1	5
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	7
58	N2	87/106 (82%)	72 (83%)	15 (17%)	3	14
58	n2	85/106 (80%)	67 (79%)	18 (21%)	1	8
59	N3	104/104 (100%)	85 (82%)	19 (18%)	2	12
59	n3	104/104 (100%)	95 (91%)	9 (9%)	15	51
60	N4	57/129 (44%)	47 (82%)	10 (18%)	3	13
60	n4	100/129 (78%)	84 (84%)	16 (16%)	3	16
61	N5	104/117 (89%)	88 (85%)	16 (15%)	4	18
61	n5	104/117 (89%)	83 (80%)	21 (20%)	2	9
62	N6	109/109 (100%)	87 (80%)	22 (20%)	2	9
62	n6	109/109 (100%)	75 (69%)	34 (31%)	0	1
63	N7	115/115 (100%)	96 (84%)	19 (16%)	3	14
63	n7	115/115 (100%)	89 (77%)	26 (23%)	1	6
64	N8	118/118 (100%)	90 (76%)	28 (24%)	1	4
64	n8	118/118 (100%)	96 (81%)	22 (19%)	2	11
65	N9	46/46 (100%)	37 (80%)	9 (20%)	2	10
65	n9	46/46 (100%)	38 (83%)	8 (17%)	3	13
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1	5
66	o0	84/87 (97%)	67 (80%)	17 (20%)	2	9
67	O1	92/96 (96%)	75 (82%)	17 (18%)	2	11
67	o1	94/96 (98%)	71 (76%)	23 (24%)	1	3
68	O2	109/110 (99%)	82 (75%)	27 (25%)	1	3
68	o2	109/110 (99%)	89 (82%)	20 (18%)	2	12
69	O3	90/90 (100%)	75 (83%)	15 (17%)	3	14
69	o3	90/90 (100%)	74 (82%)	16 (18%)	2	13
70	O4	95/101 (94%)	76 (80%)	19 (20%)	2	9
70	o4	95/101 (94%)	78 (82%)	17 (18%)	2	12
71	O5	104/104 (100%)	79 (76%)	25 (24%)	1	4
71	o5	103/104 (99%)	82 (80%)	21 (20%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	O6	81/81 (100%)	60 (74%)	21 (26%)	1	2
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0	1
73	O7	70/70 (100%)	57 (81%)	13 (19%)	2	11
73	o7	70/70 (100%)	53 (76%)	17 (24%)	1	3
74	O8	68/68 (100%)	50 (74%)	18 (26%)	1	2
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	12
75	O9	45/45 (100%)	34 (76%)	11 (24%)	1	3
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2	13
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	1	3
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	5
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	3	13
77	q1	23/23 (100%)	18 (78%)	5 (22%)	1	7
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	1	3
78	q2	90/90 (100%)	65 (72%)	25 (28%)	0	2
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	3	14
79	q3	71/71 (100%)	56 (79%)	15 (21%)	1	8
80	c0	73/98 (74%)	65 (89%)	8 (11%)	9	36
81	e0	53/53 (100%)	40 (76%)	13 (24%)	1	3
82	e1	66/66 (100%)	45 (68%)	21 (32%)	0	1
84	p0	105/253 (42%)	84 (80%)	21 (20%)	2	9
All	All	18727/20239 (92%)	15017 (80%)	3710 (20%)	2	9

5 of 3710 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	O4	8	ARG
8	s6	12	SER
63	n7	135	ARG
72	O6	45	ARG
3	s1	77	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
47	M0	162	GLN
3	s1	149	GLN
53	m7	34	GLN
54	M8	152	HIS
59	N3	33	ASN

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 2563 ligands modelled in this entry, 1424 are monoatomic - leaving 1139 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	$\# Z > 2$
90	A	1	3401	-	22,24,25	0.89	1 (4%)	32,35,38	1.33	4 (12%)
88	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	1	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	1	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
90	A	5	3401	-	22,24,25	0.66	0	32,35,38	0.94	1 (3%)
88	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4248	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4249	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4250	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4251	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4252	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4253	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4254	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4255	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4256	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4257	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	5	4258	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2046	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	6	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2049	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2089	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	6	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2092	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2105	1	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2132	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	6	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2135	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	215	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	216	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	D3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L3	406	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	L4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M7	205	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	O7	104	-	0,6,6	0.00	-	0,15,15	0.00	-
91	C	Q2	502	-	19,21,22	1.18	1 (5%)	24,30,33	1.00	1 (4%)
91	C	Q2	503	-	19,21,22	0.99	1 (5%)	24,30,33	1.54	4 (16%)
88	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c1	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	c8	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	405	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l3	406	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l4	404	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	l9	600	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m1	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	m6	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	n9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
91	C	q2	502	-	19,21,22	1.19	3 (15%)	24,30,33	1.00	1 (4%)
91	C	q2	503	-	19,21,22	1.31	3 (15%)	24,30,33	0.85	1 (4%)
88	OHX	q2	504	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	s8	304	-	0,6,6	0.00	-	0,15,15	0.00	-
88	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	A	1	3401	-	-	0/8/25/26	0/3/3/3
88	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3875	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3881	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3917	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3923	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3959	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3965	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
88	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4001	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4007	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4043	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4049	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4085	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4091	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4127	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4133	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4169	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4175	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4211	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4213	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4214	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4215	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4216	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4217	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	1	4218	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4219	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4220	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4221	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4222	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4223	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4224	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4225	-	-	0/0/0/0	0/0/0/0
88	OHX	1	4226	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2055	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2063	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2097	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2105	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2139	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
88	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
88	OHX	3	215	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	3	216	-	-	0/0/0/0	0/0/0/0
88	OHX	3	217	-	-	0/0/0/0	0/0/0/0
88	OHX	3	218	-	-	0/0/0/0	0/0/0/0
88	OHX	3	219	-	-	0/0/0/0	0/0/0/0
88	OHX	3	220	-	-	0/0/0/0	0/0/0/0
88	OHX	3	221	-	-	0/0/0/0	0/0/0/0
88	OHX	3	222	-	-	0/0/0/0	0/0/0/0
88	OHX	3	223	-	-	0/0/0/0	0/0/0/0
88	OHX	3	224	-	-	0/0/0/0	0/0/0/0
88	OHX	3	225	-	-	0/0/0/0	0/0/0/0
88	OHX	4	220	-	-	0/0/0/0	0/0/0/0
88	OHX	4	221	-	-	0/0/0/0	0/0/0/0
88	OHX	4	222	-	-	0/0/0/0	0/0/0/0
88	OHX	4	223	-	-	0/0/0/0	0/0/0/0
88	OHX	4	224	-	-	0/0/0/0	0/0/0/0
88	OHX	4	225	-	-	0/0/0/0	0/0/0/0
88	OHX	4	226	-	-	0/0/0/0	0/0/0/0
88	OHX	4	227	-	-	0/0/0/0	0/0/0/0
88	OHX	4	228	-	-	0/0/0/0	0/0/0/0
88	OHX	4	229	-	-	0/0/0/0	0/0/0/0
88	OHX	4	230	-	-	0/0/0/0	0/0/0/0
88	OHX	4	231	-	-	0/0/0/0	0/0/0/0
88	OHX	4	232	-	-	0/0/0/0	0/0/0/0
88	OHX	4	233	-	-	0/0/0/0	0/0/0/0
90	A	5	3401	-	-	0/8/25/26	0/3/3/3
88	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3917	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3958	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3959	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
88	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4000	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4001	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4042	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4043	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4084	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4085	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4126	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4127	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4168	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4169	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4211	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4248	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4249	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4250	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4251	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4252	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4253	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	5	4254	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4255	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4256	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4257	-	-	0/0/0/0	0/0/0/0
88	OHX	5	4258	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2080	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2088	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2105	1	-	0/0/0/0	0/0/0/0
88	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2122	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2130	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2164	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2172	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
88	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
88	OHX	7	215	-	-	0/0/0/0	0/0/0/0
88	OHX	7	216	-	-	0/0/0/0	0/0/0/0
88	OHX	7	217	-	-	0/0/0/0	0/0/0/0
88	OHX	7	218	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	OHX	7	219	-	-	0/0/0/0	0/0/0/0
88	OHX	7	220	-	-	0/0/0/0	0/0/0/0
88	OHX	7	221	-	-	0/0/0/0	0/0/0/0
88	OHX	7	222	-	-	0/0/0/0	0/0/0/0
88	OHX	7	223	-	-	0/0/0/0	0/0/0/0
88	OHX	7	224	-	-	0/0/0/0	0/0/0/0
88	OHX	7	225	-	-	0/0/0/0	0/0/0/0
88	OHX	7	226	-	-	0/0/0/0	0/0/0/0
88	OHX	8	217	-	-	0/0/0/0	0/0/0/0
88	OHX	8	218	-	-	0/0/0/0	0/0/0/0
88	OHX	8	219	-	-	0/0/0/0	0/0/0/0
88	OHX	8	220	-	-	0/0/0/0	0/0/0/0
88	OHX	8	221	-	-	0/0/0/0	0/0/0/0
88	OHX	8	222	-	-	0/0/0/0	0/0/0/0
88	OHX	8	223	-	-	0/0/0/0	0/0/0/0
88	OHX	8	224	-	-	0/0/0/0	0/0/0/0
88	OHX	8	225	-	-	0/0/0/0	0/0/0/0
88	OHX	8	226	-	-	0/0/0/0	0/0/0/0
88	OHX	8	227	-	-	0/0/0/0	0/0/0/0
88	OHX	8	228	-	-	0/0/0/0	0/0/0/0
88	OHX	8	229	-	-	0/0/0/0	0/0/0/0
88	OHX	8	230	-	-	0/0/0/0	0/0/0/0
88	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
88	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
88	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
88	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
88	OHX	L3	406	-	-	0/0/0/0	0/0/0/0
88	OHX	L4	402	-	-	0/0/0/0	0/0/0/0
88	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
88	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
88	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
88	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
88	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
88	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
88	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
88	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
88	OHX	O7	104	-	-	0/0/0/0	0/0/0/0
91	C	Q2	502	-	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	C	Q2	503	-	-	0/6/25/26	0/2/2/2
88	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
88	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
88	OHX	c1	202	-	-	0/0/0/0	0/0/0/0
88	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
88	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
88	OHX	c8	202	-	-	0/0/0/0	0/0/0/0
88	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
88	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	405	-	-	0/0/0/0	0/0/0/0
88	OHX	l3	406	-	-	0/0/0/0	0/0/0/0
88	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
88	OHX	l4	404	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
88	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
88	OHX	l9	600	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
88	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
88	OHX	m1	203	-	-	0/0/0/0	0/0/0/0
88	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
88	OHX	m5	306	-	-	0/0/0/0	0/0/0/0
88	OHX	m6	203	-	-	0/0/0/0	0/0/0/0
88	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
88	OHX	n3	204	-	-	0/0/0/0	0/0/0/0
88	OHX	n9	101	-	-	0/0/0/0	0/0/0/0
88	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
88	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
91	C	q2	502	-	-	0/6/25/26	0/2/2/2
91	C	q2	503	-	-	0/6/25/26	0/2/2/2
88	OHX	q2	504	-	-	0/0/0/0	0/0/0/0
88	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
88	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
88	OHX	s8	304	-	-	0/0/0/0	0/0/0/0
88	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	q2	502	C	C2-N1	3.23	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	q2	503	C	C2-N1	3.22	1.41	1.38
91	Q2	502	C	C2-N1	3.01	1.41	1.38
91	q2	503	C	O2-C2	2.72	1.25	1.21
91	Q2	503	C	O2-C2	2.55	1.25	1.21

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	1	3401	A	C8-N9-C4	-5.21	102.72	106.96
91	Q2	503	C	C6-C5-C4	4.50	119.66	117.51
91	q2	502	C	C2-N3-C4	3.28	120.38	115.65
91	Q2	502	C	C2-N3-C4	3.12	120.15	115.65
91	Q2	503	C	C6-N1-C1'	2.92	126.58	119.33

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

There are no chain breaks in this entry.

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%)	-0.07	78 (4%) 32 6	41, 78, 197, 349	0
1	6	1795/1800 (99%)	-0.07	82 (4%) 31 6	32, 61, 204, 344	0
2	S0	206/251 (82%)	-0.06	2 (0%) 79 29	76, 100, 158, 210	0
2	s0	206/251 (82%)	-0.29	0 100 100	61, 79, 124, 217	0
3	S1	214/254 (84%)	0.40	11 (5%) 27 5	67, 120, 182, 222	0
3	s1	216/254 (85%)	-0.10	1 (0%) 88 46	46, 68, 110, 185	0
4	S2	217/253 (85%)	-0.22	0 100 100	54, 83, 116, 182	0
4	s2	217/253 (85%)	-0.13	5 (2%) 57 13	41, 64, 119, 179	0
5	S3	223/239 (93%)	-0.00	2 (0%) 81 32	60, 84, 140, 236	0
5	s3	223/239 (93%)	-0.08	0 100 100	45, 85, 143, 177	0
6	S4	260/260 (100%)	0.02	2 (0%) 83 35	60, 79, 120, 181	0
6	s4	260/260 (100%)	-0.21	1 (0%) 90 51	44, 62, 100, 176	0
7	S5	206/224 (91%)	-0.02	3 (1%) 70 21	65, 104, 159, 238	0
7	s5	206/224 (91%)	-0.16	0 100 100	46, 78, 134, 205	0
8	S6	226/236 (95%)	0.17	3 (1%) 74 24	50, 89, 148, 187	0
8	s6	218/236 (92%)	-0.03	3 (1%) 72 22	41, 70, 119, 221	0
9	S7	184/189 (97%)	0.09	0 100 100	69, 106, 164, 214	0
9	s7	186/189 (98%)	-0.04	1 (0%) 88 46	55, 91, 155, 206	0
10	S8	188/200 (94%)	0.01	1 (0%) 88 46	41, 62, 120, 183	0
10	s8	188/200 (94%)	-0.05	1 (0%) 88 46	31, 57, 109, 136	0
11	S9	185/196 (94%)	0.19	5 (2%) 52 11	66, 92, 140, 223	0
11	s9	185/196 (94%)	-0.12	0 100 100	49, 69, 132, 176	0
12	C0	96/105 (91%)	-0.04	0 100 100	64, 97, 146, 220	0
13	C1	155/155 (100%)	0.08	7 (4%) 32 6	41, 63, 169, 234	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	c1	146/155 (94%)	-0.13	1 (0%) 84 38	33, 51, 124, 195	0
14	C2	124/142 (87%)	0.72	9 (7%) 15 3	92, 132, 206, 244	0
14	c2	124/142 (87%)	1.46	26 (20%) 1 1	137, 181, 244, 299	0
15	C3	150/150 (100%)	-0.09	0 100 100	48, 78, 119, 191	0
15	c3	150/150 (100%)	-0.29	0 100 100	37, 60, 94, 127	0
16	C4	127/136 (93%)	0.12	2 (1%) 68 20	57, 121, 166, 204	0
16	c4	128/136 (94%)	-0.12	1 (0%) 83 35	45, 71, 97, 130	0
17	C5	124/141 (87%)	0.03	0 100 100	61, 84, 159, 203	0
17	c5	135/141 (95%)	0.18	6 (4%) 33 7	51, 85, 161, 201	0
18	C6	141/142 (99%)	-0.03	0 100 100	74, 90, 121, 198	0
18	c6	142/142 (100%)	-0.05	2 (1%) 72 22	51, 71, 116, 160	0
19	C7	120/136 (88%)	0.12	2 (1%) 67 19	68, 95, 174, 194	0
19	c7	117/136 (86%)	-0.05	0 100 100	55, 78, 134, 204	0
20	C8	145/145 (100%)	0.10	0 100 100	59, 93, 139, 156	0
20	c8	145/145 (100%)	-0.07	1 (0%) 84 38	54, 73, 119, 147	0
21	C9	143/143 (100%)	0.07	0 100 100	76, 94, 136, 178	0
21	c9	143/143 (100%)	-0.20	0 100 100	44, 66, 109, 166	0
22	D0	107/120 (89%)	0.55	7 (6%) 18 4	66, 92, 178, 217	0
22	d0	110/120 (91%)	0.50	8 (7%) 15 3	49, 86, 182, 238	0
23	D1	87/87 (100%)	-0.18	0 100 100	83, 95, 132, 169	0
23	d1	87/87 (100%)	-0.30	1 (1%) 77 27	56, 69, 102, 179	0
24	D2	129/129 (100%)	-0.13	0 100 100	58, 74, 98, 108	0
24	d2	129/129 (100%)	-0.32	0 100 100	36, 50, 70, 90	0
25	D3	144/144 (100%)	-0.14	0 100 100	37, 57, 90, 136	0
25	d3	144/144 (100%)	-0.30	0 100 100	30, 40, 69, 138	0
26	D4	134/134 (100%)	0.23	1 (0%) 84 38	56, 96, 146, 223	0
26	d4	134/134 (100%)	-0.09	0 100 100	43, 71, 118, 198	0
27	D5	70/107 (65%)	0.36	1 (1%) 72 22	89, 121, 178, 209	0
27	d5	69/107 (64%)	0.16	1 (1%) 72 22	67, 95, 152, 160	0
28	D6	97/97 (100%)	0.37	2 (2%) 60 15	58, 94, 181, 235	0
28	d6	97/97 (100%)	-0.07	0 100 100	41, 65, 113, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	D7	81/81 (100%)	0.41	6 (7%) 14 3	71, 95, 164, 222	0
29	d7	81/81 (100%)	0.01	1 (1%) 75 26	50, 71, 154, 206	0
30	D8	63/66 (95%)	0.77	4 (6%) 19 4	77, 118, 179, 231	0
30	d8	63/66 (95%)	0.52	0 100 100	69, 100, 144, 166	0
31	D9	53/55 (96%)	-0.17	1 (1%) 64 18	64, 71, 100, 146	0
31	d9	53/55 (96%)	-0.01	1 (1%) 64 18	51, 64, 97, 161	0
32	E0	60/60 (100%)	0.37	2 (3%) 44 9	53, 93, 160, 200	0
33	E1	71/76 (93%)	0.61	5 (7%) 16 4	89, 119, 186, 212	0
34	SR	318/318 (100%)	0.08	2 (0%) 86 41	81, 106, 156, 226	0
34	sR	318/318 (100%)	0.08	1 (0%) 91 58	70, 99, 155, 211	0
35	SM	159/273 (58%)	0.31	11 (6%) 17 4	50, 93, 168, 196	0
35	sM	104/273 (38%)	0.40	8 (7%) 13 3	60, 105, 190, 220	0
36	1	3149/3396 (92%)	-0.27	79 (2%) 54 12	26, 44, 162, 334	0
36	5	3150/3396 (92%)	-0.29	58 (1%) 65 18	24, 42, 142, 343	0
37	3	121/121 (100%)	-0.51	0 100 100	32, 60, 82, 126	0
37	7	121/121 (100%)	-0.49	0 100 100	25, 47, 61, 125	0
38	4	158/158 (100%)	-0.41	3 (1%) 64 18	29, 47, 96, 203	0
38	8	158/158 (100%)	-0.34	3 (1%) 64 18	33, 53, 121, 197	0
39	L2	252/253 (99%)	-0.31	0 100 100	29, 42, 71, 140	0
39	l2	252/253 (99%)	-0.29	1 (0%) 90 51	24, 42, 74, 143	0
40	L3	386/386 (100%)	-0.31	1 (0%) 91 58	27, 49, 80, 169	0
40	l3	386/386 (100%)	-0.33	1 (0%) 91 58	21, 34, 60, 126	0
41	L4	361/361 (100%)	-0.32	0 100 100	24, 41, 72, 119	0
41	l4	361/361 (100%)	-0.29	0 100 100	28, 44, 75, 122	0
42	L5	296/296 (100%)	-0.14	0 100 100	42, 68, 118, 173	0
42	l5	294/296 (99%)	-0.24	2 (0%) 84 38	30, 49, 96, 193	0
43	L6	156/175 (89%)	-0.30	0 100 100	31, 43, 80, 134	0
43	l6	157/175 (89%)	-0.33	1 (0%) 86 41	31, 44, 93, 154	0
44	L7	222/243 (91%)	-0.37	0 100 100	21, 34, 79, 196	0
44	l7	223/243 (91%)	-0.39	0 100 100	22, 33, 80, 178	0
45	L8	233/255 (91%)	-0.12	1 (0%) 90 51	42, 63, 133, 225	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	l8	231/255 (90%)	0.11	7 (3%) 48 10	51, 72, 118, 185	0
46	L9	191/191 (100%)	-0.11	0 100 100	42, 58, 87, 163	0
46	l9	191/191 (100%)	-0.36	1 (0%) 88 46	26, 37, 76, 194	0
47	M0	211/220 (95%)	-0.12	1 (0%) 88 46	33, 50, 118, 262	0
47	m0	213/220 (96%)	-0.13	4 (1%) 64 18	34, 52, 102, 205	0
48	M1	169/173 (97%)	-0.08	0 100 100	49, 73, 110, 143	0
48	m1	169/173 (97%)	-0.27	0 100 100	37, 51, 84, 139	0
49	M3	193/198 (97%)	-0.20	0 100 100	26, 48, 115, 223	0
49	m3	194/198 (97%)	-0.12	0 100 100	34, 56, 114, 166	0
50	M4	136/137 (99%)	-0.24	0 100 100	35, 45, 81, 125	0
50	m4	137/137 (100%)	-0.37	0 100 100	26, 38, 75, 153	0
51	M5	203/203 (100%)	-0.38	0 100 100	27, 39, 55, 81	0
51	m5	203/203 (100%)	-0.31	0 100 100	30, 48, 63, 88	0
52	M6	197/198 (99%)	-0.34	0 100 100	26, 37, 67, 132	0
52	m6	197/198 (99%)	-0.40	0 100 100	19, 26, 65, 146	0
53	M7	183/183 (100%)	0.04	8 (4%) 33 7	27, 39, 151, 209	0
53	m7	155/183 (84%)	-0.17	0 100 100	21, 34, 61, 156	0
54	M8	185/185 (100%)	-0.34	0 100 100	27, 38, 52, 79	0
54	m8	185/185 (100%)	-0.30	0 100 100	31, 42, 60, 112	0
55	M9	188/188 (100%)	0.06	0 100 100	43, 60, 162, 210	0
55	m9	188/188 (100%)	0.01	3 (1%) 68 20	36, 51, 137, 218	0
56	N0	172/172 (100%)	-0.37	0 100 100	33, 43, 75, 150	0
56	n0	172/172 (100%)	-0.40	0 100 100	23, 33, 61, 127	0
57	N1	159/159 (100%)	-0.21	1 (0%) 86 41	29, 42, 93, 164	0
57	n1	159/159 (100%)	-0.22	0 100 100	28, 37, 91, 153	0
58	N2	100/120 (83%)	0.28	3 (3%) 48 10	62, 91, 143, 184	0
58	n2	98/120 (81%)	0.27	1 (1%) 79 29	56, 80, 117, 161	0
59	N3	136/136 (100%)	-0.24	0 100 100	29, 46, 84, 164	0
59	n3	136/136 (100%)	-0.24	0 100 100	22, 33, 68, 140	0
60	N4	98/155 (63%)	0.87	22 (22%) 1 1	39, 63, 228, 293	0
60	n4	135/155 (87%)	0.17	6 (4%) 33 7	30, 80, 169, 219	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
61	N5	121/141 (85%)	-0.14	0 100 100	39, 56, 88, 144	0
61	n5	120/141 (85%)	-0.07	1 (0%) 83 35	40, 55, 99, 123	0
62	N6	126/126 (100%)	-0.07	1 (0%) 83 35	33, 51, 82, 112	0
62	n6	126/126 (100%)	-0.09	0 100 100	41, 53, 87, 149	0
63	N7	135/135 (100%)	-0.13	0 100 100	55, 74, 112, 152	0
63	n7	135/135 (100%)	-0.12	0 100 100	61, 85, 131, 164	0
64	N8	148/148 (100%)	-0.31	0 100 100	25, 37, 72, 164	0
64	n8	148/148 (100%)	-0.27	0 100 100	25, 44, 77, 118	0
65	N9	58/58 (100%)	-0.16	0 100 100	27, 46, 114, 158	0
65	n9	58/58 (100%)	-0.17	0 100 100	29, 50, 103, 131	0
66	O0	97/104 (93%)	-0.04	0 100 100	58, 75, 124, 140	0
66	o0	100/104 (96%)	-0.09	0 100 100	52, 72, 129, 173	0
67	O1	109/112 (97%)	-0.02	2 (1%) 65 18	31, 56, 132, 172	0
67	o1	109/112 (97%)	-0.02	0 100 100	29, 45, 118, 181	0
68	O2	127/129 (98%)	-0.19	1 (0%) 83 35	20, 34, 64, 138	0
68	o2	127/129 (98%)	-0.21	2 (1%) 68 20	19, 38, 68, 128	0
69	O3	106/106 (100%)	-0.35	0 100 100	26, 34, 62, 144	0
69	o3	106/106 (100%)	-0.24	1 (0%) 81 32	23, 31, 60, 141	0
70	O4	112/119 (94%)	-0.03	2 (1%) 65 18	41, 56, 119, 212	0
70	o4	112/119 (94%)	-0.11	0 100 100	34, 55, 108, 175	0
71	O5	119/119 (100%)	-0.17	0 100 100	36, 57, 88, 130	0
71	o5	119/119 (100%)	-0.09	1 (0%) 83 35	44, 62, 94, 134	0
72	O6	99/99 (100%)	-0.11	0 100 100	44, 57, 102, 178	0
72	o6	99/99 (100%)	-0.11	0 100 100	50, 62, 108, 159	0
73	O7	87/87 (100%)	-0.25	0 100 100	27, 38, 64, 197	0
73	o7	87/87 (100%)	-0.15	2 (2%) 57 13	29, 38, 76, 175	0
74	O8	77/77 (100%)	0.19	0 100 100	59, 82, 116, 161	0
74	o8	77/77 (100%)	0.34	0 100 100	59, 80, 129, 144	0
75	O9	50/50 (100%)	-0.26	0 100 100	40, 46, 66, 89	0
75	o9	50/50 (100%)	-0.21	0 100 100	41, 46, 71, 103	0
76	Q0	52/52 (100%)	-0.19	0 100 100	42, 51, 75, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
76	q0	52/52 (100%)	-0.28	0	100	100	26, 32, 63, 145	0
77	Q1	25/25 (100%)	0.03	0	100	100	45, 49, 68, 83	0
77	q1	25/25 (100%)	-0.28	0	100	100	34, 42, 60, 73	0
78	Q2	105/105 (100%)	0.02	0	100	100	28, 45, 83, 170	0
78	q2	105/105 (100%)	-0.09	0	100	100	30, 46, 83, 174	0
79	Q3	91/91 (100%)	-0.13	0	100	100	31, 49, 85, 117	0
79	q3	91/91 (100%)	-0.36	0	100	100	24, 47, 79, 97	0
80	c0	96/105 (91%)	0.35	3 (3%)	47	10	68, 108, 166, 240	0
81	e0	62/62 (100%)	0.24	1 (1%)	68	20	53, 69, 167, 247	0
82	e1	76/76 (100%)	1.30	15 (19%)	2	1	112, 154, 206, 247	0
83	m2	0/160	-	-	-	-	-	-
84	p0	143/311 (45%)	0.26	2 (1%)	72	22	62, 102, 177, 269	0
85	p1	0/47	-	-	-	-	-	-
86	p2	0/46	-	-	-	-	-	-
All	All	33063/35344 (93%)	-0.12	562 (1%)	67	19	19, 60, 147, 349	0

The worst 5 of 562 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
60	N4	76	VAL	13.5
1	2	238	U	9.6
1	6	662	U	9.2
1	6	663	U	9.1
1	2	656	G	8.5

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
87	MG	6	2018	1/1	0.64	537.05	88,88,88,88	0
88	OHX	1	4200	7/7	0.34	415.00	340,340,340,340	0
87	MG	1	3821	1/1	0.29	387.00	40,40,40,40	0
87	MG	3	202	1/1	0.48	359.21	58,58,58,58	0
87	MG	5	3446	1/1	0.31	321.00	31,31,31,31	0
87	MG	5	3493	1/1	0.40	248.00	34,34,34,34	0
87	MG	5	3877	1/1	0.60	225.50	35,35,35,35	0
87	MG	17	301	1/1	0.77	208.33	38,38,38,38	0
87	MG	6	2015	1/1	0.72	193.67	44,44,44,44	0
87	MG	1	3693	1/1	0.83	182.52	65,65,65,65	0
87	MG	1	3748	1/1	0.40	151.26	40,40,40,40	0
87	MG	1	3865	1/1	0.40	131.50	101,101,101,101	0
87	MG	5	3438	1/1	1.00	129.00	55,55,55,55	0
87	MG	5	3665	1/1	0.34	126.73	42,42,42,42	0
87	MG	5	3899	1/1	0.81	119.36	147,147,147,147	0
87	MG	1	3841	1/1	0.97	114.92	41,41,41,41	0
87	MG	5	3406	1/1	0.34	111.31	26,26,26,26	0
87	MG	1	3532	1/1	0.55	107.48	11,11,11,11	0
87	MG	5	3449	1/1	0.39	105.26	53,53,53,53	0
87	MG	8	215	1/1	0.55	104.20	43,43,43,43	0
87	MG	1	3765	1/1	0.55	103.45	62,62,62,62	0
87	MG	5	3736	1/1	0.39	99.69	49,49,49,49	0
87	MG	1	3551	1/1	0.53	94.50	34,34,34,34	0
87	MG	5	3559	1/1	0.78	93.54	39,39,39,39	0
87	MG	5	3566	1/1	0.60	92.31	19,19,19,19	0
87	MG	6	1928	1/1	0.69	90.50	51,51,51,51	0
87	MG	1	3819	1/1	0.38	89.80	56,56,56,56	0
87	MG	1	3743	1/1	0.36	86.60	43,43,43,43	0
87	MG	4	201	1/1	0.58	82.10	48,48,48,48	0
87	MG	5	3855	1/1	0.39	82.00	59,59,59,59	0
87	MG	1	3561	1/1	0.58	80.82	31,31,31,31	0
87	MG	4	219	1/1	0.46	76.37	201,201,201,201	0
87	MG	6	2006	1/1	0.58	76.25	41,41,41,41	0
87	MG	1	3864	1/1	0.50	75.77	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3724	1/1	0.61	74.78	41,41,41,41	0
87	MG	5	3696	1/1	0.86	73.62	54,54,54,54	0
87	MG	5	3624	1/1	0.68	73.36	41,41,41,41	0
87	MG	5	3800	1/1	0.36	73.13	79,79,79,79	0
87	MG	2	1951	1/1	0.41	73.00	50,50,50,50	0
87	MG	5	3432	1/1	0.45	72.36	49,49,49,49	0
87	MG	6	1975	1/1	0.51	69.49	47,47,47,47	0
87	MG	5	3524	1/1	0.51	68.80	30,30,30,30	0
88	OHX	1	4189	7/7	0.24	65.76	282,282,282,282	0
87	MG	6	1956	1/1	0.54	65.55	29,29,29,29	0
87	MG	1	3764	1/1	0.81	65.40	56,56,56,56	0
87	MG	5	3801	1/1	0.86	64.92	80,80,80,80	0
87	MG	5	3501	1/1	0.56	64.85	33,33,33,33	0
87	MG	5	3472	1/1	0.55	64.73	36,36,36,36	0
87	MG	1	3826	1/1	0.41	64.08	52,52,52,52	0
87	MG	1	3854	1/1	0.58	62.31	43,43,43,43	0
87	MG	2	2017	1/1	0.79	62.10	49,49,49,49	0
87	MG	5	3663	1/1	0.89	62.06	59,59,59,59	0
87	MG	5	3607	1/1	0.51	60.23	41,41,41,41	0
87	MG	5	3698	1/1	1.34	59.98	69,69,69,69	0
87	MG	5	3660	1/1	0.46	59.82	55,55,55,55	0
87	MG	5	3666	1/1	0.40	57.44	15,15,15,15	0
87	MG	2	2019	1/1	0.69	57.36	32,32,32,32	0
87	MG	6	1920	1/1	0.75	57.10	66,66,66,66	0
87	MG	5	3707	1/1	0.16	57.00	51,51,51,51	0
87	MG	5	3730	1/1	0.35	56.95	43,43,43,43	0
87	MG	1	3407	1/1	0.86	54.99	41,41,41,41	0
87	MG	1	3544	1/1	0.46	54.84	32,32,32,32	0
87	MG	2	1976	1/1	0.80	54.03	63,63,63,63	0
87	MG	5	3459	1/1	0.48	53.47	31,31,31,31	0
87	MG	1	3842	1/1	0.40	53.15	20,20,20,20	0
87	MG	5	3890	1/1	0.53	52.71	49,49,49,49	0
87	MG	5	3536	1/1	0.44	52.25	23,23,23,23	0
87	MG	1	3479	1/1	0.54	52.12	24,24,24,24	0
87	MG	8	213	1/1	0.47	51.78	30,30,30,30	0
87	MG	1	3405	1/1	0.48	51.67	39,39,39,39	0
87	MG	6	2034	1/1	0.60	51.51	47,47,47,47	0
87	MG	1	3680	1/1	0.33	50.83	30,30,30,30	0
87	MG	1	3600	1/1	0.60	49.79	11,11,11,11	0
87	MG	2	1966	1/1	0.52	49.33	44,44,44,44	0
87	MG	1	3650	1/1	0.50	48.60	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	4	204	1/1	0.53	48.55	30,30,30,30	0
87	MG	1	3454	1/1	0.33	48.50	47,47,47,47	0
87	MG	5	3891	1/1	0.75	48.48	56,56,56,56	0
87	MG	1	3582	1/1	0.50	48.25	11,11,11,11	0
87	MG	1	3699	1/1	0.36	48.00	40,40,40,40	0
87	MG	6	1903	1/1	0.70	47.28	33,33,33,33	0
87	MG	1	3695	1/1	0.43	47.02	27,27,27,27	0
87	MG	5	3453	1/1	0.54	47.00	28,28,28,28	0
87	MG	1	3540	1/1	0.78	46.87	19,19,19,19	0
87	MG	5	3586	1/1	0.51	46.53	24,24,24,24	0
87	MG	5	3743	1/1	0.58	46.13	31,31,31,31	0
87	MG	5	3542	1/1	0.40	45.30	27,27,27,27	0
87	MG	5	3625	1/1	0.58	45.23	24,24,24,24	0
87	MG	5	3447	1/1	0.78	44.89	44,44,44,44	0
87	MG	1	3851	1/1	0.66	44.56	42,42,42,42	0
87	MG	5	3521	1/1	0.49	44.49	7,7,7,7	0
87	MG	2	1982	1/1	0.59	44.11	40,40,40,40	0
87	MG	1	3674	1/1	1.27	42.99	80,80,80,80	0
87	MG	8	205	1/1	0.42	42.97	23,23,23,23	0
87	MG	1	3602	1/1	0.56	42.52	26,26,26,26	0
87	MG	n3	201	1/1	0.45	42.11	3,3,3,3	0
87	MG	2	1959	1/1	0.56	42.10	44,44,44,44	0
87	MG	5	3724	1/1	0.47	42.07	47,47,47,47	0
87	MG	5	3796	1/1	0.59	41.58	40,40,40,40	0
87	MG	5	3505	1/1	0.40	41.19	45,45,45,45	0
87	MG	6	1938	1/1	0.48	41.16	33,33,33,33	0
87	MG	1	3460	1/1	0.61	41.11	70,70,70,70	0
87	MG	5	3437	1/1	0.48	41.06	19,19,19,19	0
87	MG	1	3558	1/1	0.56	41.04	14,14,14,14	0
87	MG	1	3424	1/1	0.50	41.00	34,34,34,34	0
87	MG	1	3403	1/1	0.42	40.99	35,35,35,35	0
87	MG	1	3478	1/1	0.31	40.97	39,39,39,39	0
87	MG	6	2031	1/1	0.48	40.96	52,52,52,52	0
87	MG	1	3578	1/1	0.41	40.52	0,0,0,0	0
87	MG	L3	403	1/1	0.88	40.43	40,40,40,40	0
87	MG	5	3876	1/1	0.57	40.40	31,31,31,31	0
87	MG	1	3564	1/1	0.44	40.23	15,15,15,15	0
87	MG	1	3672	1/1	0.67	40.08	28,28,28,28	0
87	MG	5	3443	1/1	0.36	40.00	20,20,20,20	0
87	MG	5	3601	1/1	0.47	39.87	9,9,9,9	0
87	MG	1	3830	1/1	0.41	39.84	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	2009	1/1	0.34	39.26	33,33,33,33	0
87	MG	1	3867	1/1	0.59	39.26	98,98,98,98	0
87	MG	5	3816	1/1	0.33	39.12	51,51,51,51	0
87	MG	5	3672	1/1	0.42	39.06	30,30,30,30	0
87	MG	2	2011	1/1	0.58	38.85	40,40,40,40	0
87	MG	5	3737	1/1	0.32	38.09	24,24,24,24	0
87	MG	1	3772	1/1	0.33	38.00	43,43,43,43	0
87	MG	5	3581	1/1	0.67	37.96	19,19,19,19	0
87	MG	5	3574	1/1	0.45	37.93	8,8,8,8	0
87	MG	1	3504	1/1	0.74	37.77	28,28,28,28	0
87	MG	5	3485	1/1	0.36	37.62	42,42,42,42	0
87	MG	5	3534	1/1	0.49	37.40	1,1,1,1	0
87	MG	5	3481	1/1	0.33	37.36	48,48,48,48	0
87	MG	5	3825	1/1	0.45	37.14	32,32,32,32	0
87	MG	5	3626	1/1	0.49	36.81	64,64,64,64	0
87	MG	1	3730	1/1	0.76	36.35	42,42,42,42	0
87	MG	2	2002	1/1	0.80	36.35	177,177,177,177	0
87	MG	5	3741	1/1	0.29	36.32	24,24,24,24	0
87	MG	6	2038	1/1	0.52	35.80	39,39,39,39	0
87	MG	1	3707	1/1	0.59	35.24	35,35,35,35	0
87	MG	5	3869	1/1	0.29	35.22	38,38,38,38	0
87	MG	5	3545	1/1	0.42	35.18	6,6,6,6	0
87	MG	4	202	1/1	0.45	35.07	17,17,17,17	0
87	MG	5	3497	1/1	0.36	34.81	32,32,32,32	0
87	MG	5	3540	1/1	0.56	34.74	36,36,36,36	0
87	MG	4	217	1/1	0.49	34.64	35,35,35,35	0
87	MG	1	3736	1/1	0.26	34.63	65,65,65,65	0
87	MG	5	3578	1/1	0.45	34.28	6,6,6,6	0
87	MG	6	1922	1/1	0.54	34.25	28,28,28,28	0
87	MG	1	3420	1/1	0.39	34.00	35,35,35,35	0
87	MG	5	3740	1/1	0.36	34.00	55,55,55,55	0
87	MG	5	3853	1/1	0.53	33.78	47,47,47,47	0
87	MG	1	3639	1/1	0.30	33.73	26,26,26,26	0
87	MG	6	1945	1/1	0.45	33.67	16,16,16,16	0
87	MG	1	3632	1/1	0.41	33.63	76,76,76,76	0
87	MG	2	2018	1/1	0.75	33.25	46,46,46,46	0
87	MG	1	3590	1/1	0.63	33.25	28,28,28,28	0
87	MG	5	3454	1/1	0.43	33.21	17,17,17,17	0
87	MG	1	3859	1/1	0.30	33.07	31,31,31,31	0
87	MG	5	3867	1/1	0.52	32.92	29,29,29,29	0
87	MG	6	2040	1/1	0.31	32.78	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3469	1/1	0.48	32.70	33,33,33,33	0
87	MG	5	3564	1/1	0.44	32.41	10,10,10,10	0
87	MG	5	3483	1/1	0.46	32.35	37,37,37,37	0
87	MG	5	3718	1/1	0.44	32.16	73,73,73,73	0
87	MG	5	3749	1/1	0.38	31.81	47,47,47,47	0
87	MG	6	1986	1/1	0.40	31.81	45,45,45,45	0
87	MG	1	3537	1/1	0.44	31.74	8,8,8,8	0
87	MG	3	208	1/1	0.55	31.66	54,54,54,54	0
87	MG	1	3692	1/1	0.52	31.49	23,23,23,23	0
88	OHX	5	4132	7/7	0.27	31.31	195,195,195,195	0
87	MG	5	3848	1/1	0.42	31.09	59,59,59,59	0
87	MG	L7	304	1/1	0.61	30.93	44,44,44,44	0
87	MG	5	3587	1/1	0.40	30.92	10,10,10,10	0
87	MG	5	3526	1/1	0.45	30.81	27,27,27,27	0
87	MG	3	205	1/1	0.42	30.70	23,23,23,23	0
87	MG	5	3873	1/1	0.47	30.70	15,15,15,15	0
87	MG	5	3465	1/1	0.34	30.60	33,33,33,33	0
88	OHX	5	4192	7/7	0.35	30.48	301,301,301,301	0
87	MG	5	3588	1/1	0.53	30.43	18,18,18,18	0
87	MG	5	3695	1/1	0.47	30.41	56,56,56,56	0
87	MG	5	3552	1/1	0.43	30.10	11,11,11,11	0
87	MG	1	3663	1/1	0.34	30.04	39,39,39,39	0
87	MG	1	3714	1/1	0.66	29.74	52,52,52,52	0
87	MG	5	3565	1/1	0.58	29.69	9,9,9,9	0
87	MG	1	3833	1/1	0.25	29.67	47,47,47,47	0
87	MG	1	3599	1/1	0.50	29.63	3,3,3,3	0
87	MG	5	3794	1/1	0.28	29.44	45,45,45,45	0
87	MG	1	3691	1/1	0.59	29.35	42,42,42,42	0
87	MG	5	3709	1/1	0.62	29.30	45,45,45,45	0
87	MG	3	209	1/1	0.65	29.03	47,47,47,47	0
87	MG	5	3580	1/1	0.36	28.99	20,20,20,20	0
87	MG	2	2009	1/1	0.46	28.91	35,35,35,35	0
87	MG	6	1994	1/1	0.36	28.42	50,50,50,50	0
87	MG	1	3802	1/1	0.34	28.40	16,16,16,16	0
87	MG	5	3701	1/1	0.37	28.32	59,59,59,59	0
87	MG	1	3586	1/1	0.38	28.31	10,10,10,10	0
87	MG	5	3612	1/1	0.33	28.30	15,15,15,15	0
87	MG	6	1959	1/1	0.38	28.28	30,30,30,30	0
87	MG	5	3541	1/1	0.27	28.14	10,10,10,10	0
87	MG	5	3410	1/1	0.30	28.09	28,28,28,28	0
87	MG	5	3499	1/1	0.31	28.04	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	2	1905	1/1	0.70	27.96	60,60,60,60	0
87	MG	5	3886	1/1	0.41	27.95	25,25,25,25	0
87	MG	5	3456	1/1	0.37	27.95	21,21,21,21	0
87	MG	5	3589	1/1	0.53	27.77	6,6,6,6	0
87	MG	5	3715	1/1	0.49	27.73	65,65,65,65	0
87	MG	6	2029	1/1	0.66	27.67	49,49,49,49	0
87	MG	5	3820	1/1	0.56	27.58	39,39,39,39	0
87	MG	1	3611	1/1	0.48	27.57	26,26,26,26	0
87	MG	6	1946	1/1	0.45	27.53	44,44,44,44	0
87	MG	5	3572	1/1	0.46	27.47	19,19,19,19	0
87	MG	5	3735	1/1	0.36	27.34	40,40,40,40	0
87	MG	1	3591	1/1	0.48	27.04	15,15,15,15	0
87	MG	5	3489	1/1	0.67	27.00	49,49,49,49	0
87	MG	1	3471	1/1	0.41	26.93	33,33,33,33	0
87	MG	1	3482	1/1	0.39	26.90	64,64,64,64	0
87	MG	1	3771	1/1	0.49	26.73	68,68,68,68	0
87	MG	1	3526	1/1	0.33	26.66	12,12,12,12	0
87	MG	1	3645	1/1	0.25	26.48	35,35,35,35	0
87	MG	5	3832	1/1	0.34	26.33	35,35,35,35	0
88	OHX	5	4191	7/7	0.19	26.33	225,225,225,225	0
87	MG	7	208	1/1	0.72	26.21	47,47,47,47	0
87	MG	2	1957	1/1	0.47	26.20	35,35,35,35	0
87	MG	5	3780	1/1	0.40	26.14	21,21,21,21	0
87	MG	1	3465	1/1	0.19	26.00	38,38,38,38	0
87	MG	1	3793	1/1	0.28	25.96	44,44,44,44	0
87	MG	5	3466	1/1	0.45	25.95	33,33,33,33	0
87	MG	1	3698	1/1	0.47	25.94	29,29,29,29	0
87	MG	7	214	1/1	0.34	25.86	55,55,55,55	0
87	MG	1	3577	1/1	0.49	25.80	22,22,22,22	0
87	MG	2	1906	1/1	0.28	25.79	31,31,31,31	0
87	MG	1	3508	1/1	0.45	25.78	24,24,24,24	0
87	MG	5	3682	1/1	0.24	25.34	28,28,28,28	0
87	MG	8	201	1/1	0.36	25.32	54,54,54,54	0
87	MG	5	3495	1/1	0.50	25.28	29,29,29,29	0
87	MG	8	204	1/1	0.51	25.21	29,29,29,29	0
88	OHX	5	4184	7/7	0.38	25.12	295,295,295,295	0
87	MG	1	3803	1/1	0.30	25.02	54,54,54,54	0
87	MG	1	3530	1/1	0.55	24.91	25,25,25,25	0
87	MG	1	3778	1/1	0.40	24.90	47,47,47,47	0
87	MG	1	3516	1/1	0.38	24.89	22,22,22,22	0
87	MG	1	3777	1/1	0.29	24.71	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3415	1/1	0.34	24.68	11,11,11,11	0
87	MG	6	1958	1/1	0.51	24.60	31,31,31,31	0
87	MG	5	3728	1/1	0.30	24.54	9,9,9,9	0
87	MG	1	3711	1/1	0.27	24.53	47,47,47,47	0
87	MG	1	3722	1/1	0.28	24.36	38,38,38,38	0
87	MG	1	3501	1/1	0.49	24.27	54,54,54,54	0
87	MG	3	204	1/1	0.42	24.22	18,18,18,18	0
87	MG	1	3518	1/1	0.41	24.08	24,24,24,24	0
88	OHX	1	4212	7/7	0.26	24.07	364,364,364,364	0
87	MG	1	3621	1/1	0.47	24.06	35,35,35,35	0
87	MG	5	3440	1/1	0.39	24.03	21,21,21,21	0
87	MG	5	3632	1/1	0.51	24.00	60,60,60,60	0
87	MG	5	3883	1/1	0.34	23.92	21,21,21,21	0
87	MG	5	3693	1/1	0.47	23.88	35,35,35,35	0
87	MG	6	1907	1/1	0.31	23.75	35,35,35,35	0
87	MG	1	3559	1/1	0.31	23.57	7,7,7,7	0
87	MG	5	3550	1/1	0.48	23.50	39,39,39,39	0
87	MG	6	1916	1/1	0.95	23.47	38,38,38,38	0
87	MG	1	3470	1/1	0.37	23.16	36,36,36,36	0
87	MG	2	1928	1/1	0.46	23.11	53,53,53,53	0
87	MG	5	3713	1/1	0.48	23.09	62,62,62,62	0
87	MG	L2	301	1/1	0.55	23.01	41,41,41,41	0
87	MG	5	3558	1/1	0.63	23.00	32,32,32,32	0
87	MG	1	3609	1/1	0.42	23.00	30,30,30,30	0
87	MG	5	3412	1/1	0.47	22.88	20,20,20,20	0
87	MG	5	3530	1/1	0.48	22.83	17,17,17,17	0
87	MG	5	3757	1/1	0.49	22.82	37,37,37,37	0
87	MG	2	1985	1/1	0.24	22.50	53,53,53,53	0
87	MG	5	3549	1/1	0.50	22.48	27,27,27,27	0
87	MG	2	1923	1/1	0.29	22.40	31,31,31,31	0
87	MG	1	3739	1/1	0.42	22.39	40,40,40,40	0
87	MG	1	3457	1/1	0.57	22.34	28,28,28,28	0
87	MG	6	1925	1/1	0.53	22.33	20,20,20,20	0
87	MG	1	3462	1/1	0.30	22.27	3,3,3,3	0
87	MG	5	3856	1/1	0.39	22.24	30,30,30,30	0
87	MG	6	1949	1/1	0.58	22.23	35,35,35,35	0
87	MG	5	3407	1/1	0.39	22.14	12,12,12,12	0
87	MG	6	2025	1/1	0.47	22.09	43,43,43,43	0
87	MG	1	3514	1/1	0.44	22.07	9,9,9,9	0
87	MG	2	1991	1/1	0.40	21.99	42,42,42,42	0
87	MG	1	3790	1/1	0.47	21.91	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	1905	1/1	0.62	21.89	37,37,37,37	0
87	MG	1	3706	1/1	0.41	21.89	55,55,55,55	0
87	MG	5	3610	1/1	0.49	21.86	45,45,45,45	0
87	MG	5	3779	1/1	0.22	21.57	31,31,31,31	0
87	MG	5	3683	1/1	0.22	21.56	21,21,21,21	0
87	MG	5	3783	1/1	0.28	21.46	55,55,55,55	0
87	MG	1	3756	1/1	0.44	21.40	44,44,44,44	0
88	OHX	5	4234	7/7	0.27	21.39	318,318,318,318	0
87	MG	5	3769	1/1	0.40	21.35	64,64,64,64	0
87	MG	6	1944	1/1	0.64	21.35	29,29,29,29	0
87	MG	1	3520	1/1	0.46	21.22	8,8,8,8	0
87	MG	5	3642	1/1	0.26	21.16	17,17,17,17	0
87	MG	1	3801	1/1	0.71	21.09	29,29,29,29	0
87	MG	5	3677	1/1	0.41	21.07	33,33,33,33	0
87	MG	1	3798	1/1	0.27	21.00	54,54,54,54	0
87	MG	1	3710	1/1	0.36	20.99	47,47,47,47	0
87	MG	5	3510	1/1	0.37	20.89	6,6,6,6	0
87	MG	1	3432	1/1	0.46	20.88	35,35,35,35	0
87	MG	2	2020	1/1	0.62	20.79	53,53,53,53	0
87	MG	5	3475	1/1	0.34	20.77	38,38,38,38	0
87	MG	5	3413	1/1	0.36	20.73	20,20,20,20	0
87	MG	6	1970	1/1	0.33	20.65	67,67,67,67	0
87	MG	2	1911	1/1	0.50	20.56	29,29,29,29	0
87	MG	1	3535	1/1	0.43	20.53	23,23,23,23	0
87	MG	5	3722	1/1	0.57	20.42	50,50,50,50	0
87	MG	5	3646	1/1	0.55	20.36	40,40,40,40	0
87	MG	5	3445	1/1	0.20	20.18	24,24,24,24	0
87	MG	1	3734	1/1	0.43	20.17	44,44,44,44	0
87	MG	5	3579	1/1	0.58	20.13	29,29,29,29	0
87	MG	5	3621	1/1	0.29	20.09	44,44,44,44	0
87	MG	5	3513	1/1	0.51	20.03	10,10,10,10	0
87	MG	5	3507	1/1	0.52	20.01	22,22,22,22	0
87	MG	1	3552	1/1	0.48	19.98	19,19,19,19	0
87	MG	6	1948	1/1	0.40	19.98	30,30,30,30	0
87	MG	1	3820	1/1	0.26	19.90	39,39,39,39	0
87	MG	5	3470	1/1	0.36	19.90	28,28,28,28	0
87	MG	5	3577	1/1	0.47	19.90	12,12,12,12	0
87	MG	M5	302	1/1	0.31	19.86	40,40,40,40	0
87	MG	5	3882	1/1	0.57	19.84	28,28,28,28	0
87	MG	5	3600	1/1	0.39	19.84	14,14,14,14	0
87	MG	5	3402	1/1	0.24	19.84	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3570	1/1	0.40	19.82	10,10,10,10	0
87	MG	5	3425	1/1	0.34	19.72	42,42,42,42	0
87	MG	5	3599	1/1	0.39	19.72	0,0,0,0	0
87	MG	1	3628	1/1	0.30	19.58	44,44,44,44	0
87	MG	6	1951	1/1	0.43	19.56	36,36,36,36	0
87	MG	7	227	1/1	0.40	19.54	36,36,36,36	0
87	MG	6	1914	1/1	0.26	19.52	7,7,7,7	0
87	MG	5	3868	1/1	0.38	19.48	42,42,42,42	0
87	MG	1	3505	1/1	0.30	19.46	0,0,0,0	0
87	MG	7	201	1/1	0.43	19.41	9,9,9,9	0
87	MG	5	3668	1/1	0.39	19.40	45,45,45,45	0
87	MG	5	3647	1/1	0.41	19.33	43,43,43,43	0
87	MG	1	3840	1/1	0.31	19.20	1,1,1,1	0
87	MG	6	1972	1/1	0.37	19.11	57,57,57,57	0
87	MG	1	3594	1/1	0.70	19.08	37,37,37,37	0
87	MG	1	3713	1/1	0.43	19.07	34,34,34,34	0
87	MG	1	3414	1/1	0.34	19.05	39,39,39,39	0
87	MG	5	3838	1/1	0.34	19.01	33,33,33,33	0
87	MG	5	3494	1/1	0.24	19.00	41,41,41,41	0
87	MG	1	3503	1/1	0.46	18.95	11,11,11,11	0
87	MG	5	3452	1/1	0.44	18.86	38,38,38,38	0
87	MG	1	3554	1/1	0.47	18.85	13,13,13,13	0
87	MG	1	3831	1/1	0.34	18.85	54,54,54,54	0
87	MG	6	2020	1/1	0.28	18.83	46,46,46,46	0
87	MG	6	2026	1/1	0.44	18.78	45,45,45,45	0
87	MG	4	213	1/1	0.20	18.75	38,38,38,38	0
87	MG	5	3674	1/1	0.26	18.72	29,29,29,29	0
87	MG	6	1921	1/1	0.43	18.55	21,21,21,21	0
87	MG	5	3458	1/1	0.33	18.54	18,18,18,18	0
87	MG	1	3511	1/1	0.34	18.51	24,24,24,24	0
87	MG	5	3755	1/1	0.39	18.50	45,45,45,45	0
87	MG	1	3498	1/1	0.25	18.47	20,20,20,20	0
87	MG	2	1941	1/1	0.32	18.28	46,46,46,46	0
87	MG	5	3419	1/1	0.57	18.27	12,12,12,12	0
87	MG	1	3495	1/1	0.28	18.20	50,50,50,50	0
87	MG	1	3565	1/1	0.41	18.20	7,7,7,7	0
87	MG	5	3467	1/1	0.42	18.02	50,50,50,50	0
87	MG	1	3619	1/1	0.54	18.01	40,40,40,40	0
87	MG	1	3500	1/1	0.46	17.97	27,27,27,27	0
87	MG	6	1963	1/1	0.53	17.94	57,57,57,57	0
87	MG	1	3694	1/1	0.30	17.86	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3572	1/1	0.30	17.85	6,6,6,6	0
87	MG	5	3651	1/1	0.34	17.85	48,48,48,48	0
87	MG	5	3590	1/1	0.32	17.82	16,16,16,16	0
87	MG	1	3780	1/1	0.36	17.77	74,74,74,74	0
87	MG	1	3434	1/1	0.41	17.77	37,37,37,37	0
87	MG	1	3555	1/1	0.57	17.67	11,11,11,11	0
87	MG	5	3684	1/1	0.48	17.67	42,42,42,42	0
87	MG	5	3490	1/1	0.39	17.67	53,53,53,53	0
87	MG	8	202	1/1	0.47	17.65	40,40,40,40	0
87	MG	1	3475	1/1	0.44	17.65	8,8,8,8	0
87	MG	5	3480	1/1	0.36	17.61	19,19,19,19	0
88	OHX	1	4154	7/7	0.26	17.59	287,287,287,287	0
87	MG	6	1926	1/1	0.51	17.59	40,40,40,40	0
87	MG	5	3719	1/1	0.38	17.57	50,50,50,50	0
87	MG	1	3473	1/1	0.44	17.55	32,32,32,32	0
87	MG	6	2035	1/1	0.49	17.54	38,38,38,38	0
87	MG	1	3413	1/1	0.33	17.53	24,24,24,24	0
87	MG	1	3670	1/1	0.36	17.49	39,39,39,39	0
87	MG	1	3443	1/1	0.37	17.45	19,19,19,19	0
87	MG	1	3517	1/1	0.51	17.45	10,10,10,10	0
87	MG	1	3603	1/1	0.42	17.43	7,7,7,7	0
87	MG	5	3685	1/1	0.31	17.41	43,43,43,43	0
87	MG	5	3851	1/1	0.47	17.35	36,36,36,36	0
87	MG	5	3428	1/1	0.52	17.35	30,30,30,30	0
87	MG	1	3563	1/1	0.44	17.31	17,17,17,17	0
87	MG	5	3528	1/1	0.34	17.31	8,8,8,8	0
87	MG	5	3598	1/1	0.51	17.15	6,6,6,6	0
87	MG	1	3515	1/1	0.37	17.08	3,3,3,3	0
87	MG	1	3858	1/1	0.61	17.08	61,61,61,61	0
87	MG	3	212	1/1	0.37	17.04	87,87,87,87	0
87	MG	5	3560	1/1	0.39	16.88	19,19,19,19	0
87	MG	1	3593	1/1	0.53	16.86	21,21,21,21	0
87	MG	5	3543	1/1	0.28	16.83	0,0,0,0	0
87	MG	1	3627	1/1	0.39	16.77	30,30,30,30	0
87	MG	1	3589	1/1	0.67	16.76	28,28,28,28	0
87	MG	5	3841	1/1	0.46	16.74	26,26,26,26	0
87	MG	1	3494	1/1	0.39	16.73	44,44,44,44	0
87	MG	5	3644	1/1	0.31	16.65	51,51,51,51	0
87	MG	1	3870	1/1	0.35	16.65	43,43,43,43	0
87	MG	o3	201	1/1	0.55	16.64	61,61,61,61	0
87	MG	1	3761	1/1	0.35	16.64	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3687	1/1	0.30	16.60	28,28,28,28	0
87	MG	1	3717	1/1	0.26	16.56	42,42,42,42	0
87	MG	1	3646	1/1	0.39	16.53	44,44,44,44	0
87	MG	1	3871	1/1	0.31	16.50	62,62,62,62	0
87	MG	5	3808	1/1	0.38	16.48	40,40,40,40	0
87	MG	1	3812	1/1	0.39	16.43	43,43,43,43	0
87	MG	1	3657	1/1	0.39	16.36	44,44,44,44	0
87	MG	5	3544	1/1	0.35	16.31	14,14,14,14	0
87	MG	5	3422	1/1	0.34	16.31	10,10,10,10	0
88	OHX	5	4236	7/7	0.23	16.30	262,262,262,262	0
87	MG	6	1950	1/1	0.26	16.25	14,14,14,14	0
87	MG	5	3771	1/1	0.39	16.24	24,24,24,24	0
87	MG	1	3579	1/1	0.53	16.18	16,16,16,16	0
87	MG	8	203	1/1	0.42	16.12	50,50,50,50	0
87	MG	5	3862	1/1	0.24	16.08	33,33,33,33	0
87	MG	2	1946	1/1	0.34	16.07	31,31,31,31	0
87	MG	1	3458	1/1	0.31	16.05	3,3,3,3	0
87	MG	7	209	1/1	0.43	16.01	10,10,10,10	0
87	MG	6	1955	1/1	0.45	16.01	8,8,8,8	0
87	MG	1	3708	1/1	0.60	15.99	30,30,30,30	0
87	MG	5	3879	1/1	0.41	15.96	25,25,25,25	0
87	MG	1	3576	1/1	0.37	15.92	0,0,0,0	0
87	MG	5	3517	1/1	0.44	15.91	17,17,17,17	0
87	MG	2	1903	1/1	0.38	15.82	24,24,24,24	0
87	MG	6	1917	1/1	0.35	15.74	31,31,31,31	0
87	MG	1	3652	1/1	0.36	15.73	44,44,44,44	0
88	OHX	1	4203	7/7	0.43	15.67	364,364,364,364	0
87	MG	5	3845	1/1	0.49	15.67	53,53,53,53	0
87	MG	5	3584	1/1	0.34	15.64	17,17,17,17	0
87	MG	5	3639	1/1	0.37	15.59	40,40,40,40	0
87	MG	1	3451	1/1	0.37	15.53	14,14,14,14	0
87	MG	2	1938	1/1	0.50	15.52	31,31,31,31	0
87	MG	13	402	1/1	0.38	15.31	69,69,69,69	0
87	MG	1	3542	1/1	0.41	15.31	15,15,15,15	0
87	MG	1	3791	1/1	0.34	15.24	31,31,31,31	0
87	MG	5	3556	1/1	0.52	15.15	27,27,27,27	0
87	MG	1	3441	1/1	0.41	15.12	30,30,30,30	0
87	MG	1	3440	1/1	0.71	15.06	27,27,27,27	0
87	MG	2	2013	1/1	0.29	15.00	47,47,47,47	0
87	MG	7	205	1/1	0.38	14.97	11,11,11,11	0
88	OHX	4	230	7/7	0.30	14.95	283,283,283,283	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3410	1/1	0.29	14.94	10,10,10,10	0
87	MG	N3	201	1/1	0.35	14.90	10,10,10,10	0
87	MG	6	1974	1/1	0.29	14.90	54,54,54,54	0
87	MG	1	3499	1/1	0.39	14.87	18,18,18,18	0
88	OHX	1	4219	7/7	0.32	14.85	225,225,225,225	0
87	MG	1	3461	1/1	0.33	14.85	6,6,6,6	0
87	MG	8	209	1/1	0.34	14.82	63,63,63,63	0
87	MG	5	3563	1/1	0.48	14.79	28,28,28,28	0
87	MG	5	3742	1/1	0.42	14.76	40,40,40,40	0
87	MG	12	301	1/1	0.50	14.74	30,30,30,30	0
87	MG	1	3419	1/1	0.64	14.72	36,36,36,36	0
87	MG	1	3402	1/1	0.41	14.71	23,23,23,23	0
87	MG	5	3633	1/1	0.30	14.67	20,20,20,20	0
87	MG	5	3514	1/1	0.46	14.66	9,9,9,9	0
87	MG	5	3512	1/1	0.41	14.64	24,24,24,24	0
87	MG	2	1937	1/1	0.37	14.63	23,23,23,23	0
87	MG	1	3536	1/1	0.27	14.63	36,36,36,36	0
88	OHX	1	4202	7/7	0.34	14.60	269,269,269,269	0
87	MG	6	1901	1/1	0.32	14.50	18,18,18,18	0
87	MG	1	3546	1/1	0.36	14.49	15,15,15,15	0
87	MG	2	1913	1/1	0.61	14.48	29,29,29,29	0
87	MG	1	3701	1/1	0.20	14.48	42,42,42,42	0
87	MG	1	3548	1/1	0.36	14.45	43,43,43,43	0
87	MG	2	2010	1/1	0.53	14.40	46,46,46,46	0
87	MG	M5	301	1/1	0.52	14.38	39,39,39,39	0
87	MG	7	202	1/1	0.32	14.34	9,9,9,9	0
87	MG	6	1943	1/1	0.33	14.33	17,17,17,17	0
87	MG	5	3649	1/1	0.39	14.32	10,10,10,10	0
87	MG	2	2004	1/1	0.41	14.29	59,59,59,59	0
87	MG	5	3700	1/1	0.44	14.19	51,51,51,51	0
87	MG	N3	202	1/1	0.23	14.19	55,55,55,55	0
87	MG	5	3739	1/1	0.42	14.12	42,42,42,42	0
87	MG	1	3732	1/1	0.27	14.05	41,41,41,41	0
87	MG	1	3606	1/1	0.37	14.04	16,16,16,16	0
87	MG	5	3619	1/1	0.33	14.04	39,39,39,39	0
87	MG	1	3459	1/1	0.31	14.02	24,24,24,24	0
87	MG	1	3845	1/1	0.37	14.01	11,11,11,11	0
87	MG	5	3427	1/1	0.31	14.01	16,16,16,16	0
87	MG	6	1913	1/1	0.47	13.99	24,24,24,24	0
87	MG	5	3606	1/1	0.45	13.94	25,25,25,25	0
87	MG	5	3404	1/1	0.67	13.80	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3875	1/1	0.36	13.76	18,18,18,18	0
87	MG	2	1917	1/1	0.44	13.60	25,25,25,25	0
87	MG	4	206	1/1	0.38	13.59	19,19,19,19	0
87	MG	3	214	1/1	0.28	13.56	43,43,43,43	0
87	MG	5	3650	1/1	0.39	13.52	32,32,32,32	0
87	MG	5	3434	1/1	0.43	13.52	27,27,27,27	0
87	MG	3	213	1/1	0.47	13.44	25,25,25,25	0
87	MG	5	3763	1/1	0.34	13.42	31,31,31,31	0
87	MG	5	3557	1/1	0.33	13.41	10,10,10,10	0
87	MG	5	3782	1/1	0.72	13.38	45,45,45,45	0
87	MG	1	3872	1/1	0.37	13.37	28,28,28,28	0
87	MG	2	1939	1/1	0.40	13.33	29,29,29,29	0
87	MG	1	3660	1/1	0.48	13.32	29,29,29,29	0
87	MG	1	3647	1/1	0.29	13.29	35,35,35,35	0
87	MG	1	3689	1/1	0.44	13.29	47,47,47,47	0
88	OHX	5	4146	7/7	0.30	13.27	243,243,243,243	0
87	MG	5	3641	1/1	0.32	13.24	35,35,35,35	0
87	MG	1	3588	1/1	0.56	13.21	26,26,26,26	0
87	MG	1	3541	1/1	0.30	13.21	35,35,35,35	0
87	MG	6	2028	1/1	0.42	13.20	57,57,57,57	0
87	MG	6	1931	1/1	0.30	13.14	29,29,29,29	0
87	MG	5	3738	1/1	0.46	13.12	47,47,47,47	0
87	MG	1	3430	1/1	0.43	13.08	39,39,39,39	0
87	MG	1	3856	1/1	0.36	12.96	42,42,42,42	0
87	MG	4	211	1/1	0.40	12.94	34,34,34,34	0
87	MG	5	3712	1/1	0.24	12.86	43,43,43,43	0
87	MG	6	1947	1/1	0.32	12.85	28,28,28,28	0
87	MG	6	1911	1/1	0.41	12.81	26,26,26,26	0
87	MG	1	3806	1/1	0.30	12.81	59,59,59,59	0
87	MG	c7	201	1/1	0.64	12.79	64,64,64,64	0
87	MG	5	3865	1/1	0.34	12.75	54,54,54,54	0
87	MG	2	1909	1/1	0.42	12.75	43,43,43,43	0
87	MG	2	1975	1/1	0.41	12.74	66,66,66,66	0
87	MG	2	1924	1/1	0.36	12.73	50,50,50,50	0
87	MG	6	1906	1/1	0.37	12.70	27,27,27,27	0
87	MG	1	3587	1/1	0.45	12.68	28,28,28,28	0
87	MG	1	3848	1/1	0.37	12.67	10,10,10,10	0
88	OHX	1	4218	7/7	0.23	12.65	259,259,259,259	0
87	MG	5	3554	1/1	0.29	12.60	12,12,12,12	0
87	MG	2	1902	1/1	0.32	12.60	16,16,16,16	0
87	MG	1	3412	1/1	0.24	12.49	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3522	1/1	0.37	12.49	1,1,1,1	0
87	MG	1	3449	1/1	0.31	12.48	33,33,33,33	0
87	MG	1	3669	1/1	0.44	12.48	37,37,37,37	0
87	MG	5	3762	1/1	0.22	12.47	51,51,51,51	0
87	MG	5	3802	1/1	0.28	12.45	56,56,56,56	0
87	MG	1	4232	1/1	0.41	12.43	83,83,83,83	0
87	MG	5	3553	1/1	0.53	12.27	25,25,25,25	0
87	MG	5	3538	1/1	0.41	12.26	20,20,20,20	0
87	MG	1	3569	1/1	0.33	12.23	8,8,8,8	0
88	OHX	1	4217	7/7	0.28	12.23	287,287,287,287	0
87	MG	5	3523	1/1	0.20	12.22	6,6,6,6	0
87	MG	1	3506	1/1	0.36	12.21	23,23,23,23	0
87	MG	5	3511	1/1	0.34	12.19	2,2,2,2	0
87	MG	m5	305	1/1	0.41	12.14	39,39,39,39	0
87	MG	2	2008	1/1	0.69	12.13	33,33,33,33	0
87	MG	5	3884	1/1	0.25	12.11	34,34,34,34	0
87	MG	1	3597	1/1	0.37	12.04	1,1,1,1	0
87	MG	1	3755	1/1	0.33	12.02	40,40,40,40	0
87	MG	1	3839	1/1	0.31	12.00	22,22,22,22	0
87	MG	1	3464	1/1	0.29	11.95	10,10,10,10	0
87	MG	2	1918	1/1	0.48	11.95	26,26,26,26	0
87	MG	5	3881	1/1	0.25	11.91	7,7,7,7	0
87	MG	1	3513	1/1	0.35	11.91	19,19,19,19	0
88	OHX	1	4196	7/7	0.34	11.90	262,262,262,262	0
87	MG	1	3583	1/1	0.34	11.85	13,13,13,13	0
87	MG	1	3581	1/1	0.41	11.77	13,13,13,13	0
87	MG	5	3533	1/1	0.29	11.76	10,10,10,10	0
87	MG	5	3593	1/1	0.34	11.74	11,11,11,11	0
87	MG	2	1914	1/1	0.41	11.74	33,33,33,33	0
88	OHX	1	4074	7/7	0.32	11.73	255,255,255,255	0
87	MG	S4	302	1/1	0.65	11.70	53,53,53,53	0
87	MG	5	3732	1/1	0.35	11.68	15,15,15,15	0
87	MG	2	1919	1/1	0.34	11.65	25,25,25,25	0
87	MG	6	2007	1/1	0.29	11.64	32,32,32,32	0
87	MG	1	3524	1/1	0.39	11.61	5,5,5,5	0
87	MG	1	3463	1/1	0.30	11.58	12,12,12,12	0
87	MG	1	3528	1/1	0.28	11.57	15,15,15,15	0
87	MG	5	3469	1/1	0.20	11.57	12,12,12,12	0
87	MG	5	3575	1/1	0.38	11.56	21,21,21,21	0
87	MG	2	1960	1/1	0.38	11.56	54,54,54,54	0
87	MG	1	3612	1/1	0.56	11.50	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3521	1/1	0.44	11.46	30,30,30,30	0
87	MG	5	3476	1/1	0.24	11.42	26,26,26,26	0
87	MG	6	1929	1/1	0.22	11.39	27,27,27,27	0
88	OHX	5	4237	7/7	0.32	11.36	259,259,259,259	0
87	MG	1	3519	1/1	0.34	11.31	11,11,11,11	0
87	MG	5	3761	1/1	0.22	11.29	42,42,42,42	0
87	MG	5	3567	1/1	0.41	11.28	6,6,6,6	0
87	MG	1	3529	1/1	0.28	11.22	3,3,3,3	0
87	MG	1	3686	1/1	0.26	11.20	37,37,37,37	0
87	MG	5	3893	1/1	0.27	11.13	17,17,17,17	0
88	OHX	5	4180	7/7	0.31	11.10	273,273,273,273	0
87	MG	5	3717	1/1	0.23	11.10	38,38,38,38	0
87	MG	6	1985	1/1	0.31	11.07	47,47,47,47	0
88	OHX	1	4176	7/7	0.33	11.07	247,247,247,247	0
87	MG	5	3726	1/1	0.25	11.03	24,24,24,24	0
87	MG	1	3794	1/1	0.30	10.97	51,51,51,51	0
87	MG	1	3704	1/1	0.29	10.94	40,40,40,40	0
87	MG	5	3583	1/1	0.43	10.92	26,26,26,26	0
87	MG	6	2016	1/1	0.30	10.90	52,52,52,52	0
87	MG	5	3694	1/1	0.36	10.89	34,34,34,34	0
88	OHX	1	4215	7/7	0.26	10.83	272,272,272,272	0
87	MG	1	3624	1/1	0.31	10.79	34,34,34,34	0
87	MG	2	2021	1/1	0.37	10.78	127,127,127,127	0
88	OHX	5	4242	7/7	0.29	10.69	365,365,365,365	0
87	MG	5	3500	1/1	0.34	10.64	18,18,18,18	0
87	MG	N8	201	1/1	0.37	10.61	30,30,30,30	0
87	MG	1	3853	1/1	0.39	10.59	45,45,45,45	0
87	MG	2	1958	1/1	0.33	10.56	30,30,30,30	0
87	MG	3	206	1/1	0.33	10.48	11,11,11,11	0
87	MG	5	3678	1/1	0.23	10.47	33,33,33,33	0
87	MG	5	3551	1/1	0.35	10.39	23,23,23,23	0
87	MG	1	3804	1/1	0.28	10.39	59,59,59,59	0
88	OHX	5	4074	7/7	0.17	10.39	183,183,183,183	0
87	MG	2	1934	1/1	0.47	10.39	61,61,61,61	0
88	OHX	6	2168	7/7	0.48	10.36	346,346,346,346	0
87	MG	1	3788	1/1	0.34	10.35	25,25,25,25	0
87	MG	6	1960	1/1	0.43	10.34	11,11,11,11	0
87	MG	5	3688	1/1	0.46	10.34	48,48,48,48	0
88	OHX	5	4226	7/7	0.24	10.33	297,297,297,297	0
87	MG	5	3568	1/1	0.23	10.27	9,9,9,9	0
87	MG	2	1921	1/1	0.32	10.27	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	2	2146	7/7	0.57	10.27	358,358,358,358	0
87	MG	2	1926	1/1	0.33	10.21	46,46,46,46	0
87	MG	5	3461	1/1	0.26	10.20	15,15,15,15	0
87	MG	1	3428	1/1	0.36	10.16	18,18,18,18	0
87	MG	2	1962	1/1	0.26	10.16	21,21,21,21	0
87	MG	5	3803	1/1	0.50	10.15	43,43,43,43	0
87	MG	5	3765	1/1	0.34	10.15	49,49,49,49	0
87	MG	2	1972	1/1	0.23	10.13	36,36,36,36	0
87	MG	5	3491	1/1	0.43	10.12	1,1,1,1	0
87	MG	2	1968	1/1	0.49	10.12	27,27,27,27	0
87	MG	5	3474	1/1	0.30	10.10	43,43,43,43	0
87	MG	5	3576	1/1	0.33	10.09	12,12,12,12	0
87	MG	1	3422	1/1	0.36	10.09	25,25,25,25	0
87	MG	1	3719	1/1	0.31	10.03	66,66,66,66	0
87	MG	5	3597	1/1	0.49	10.02	23,23,23,23	0
87	MG	1	3466	1/1	0.35	10.00	21,21,21,21	0
88	OHX	6	2181	7/7	0.35	9.99	247,247,247,247	0
87	MG	1	3651	1/1	0.35	9.98	33,33,33,33	0
88	OHX	M7	205	7/7	0.39	9.95	351,351,351,351	0
87	MG	5	3691	1/1	0.28	9.95	54,54,54,54	0
87	MG	1	3668	1/1	0.33	9.94	43,43,43,43	0
87	MG	5	3424	1/1	0.45	9.93	34,34,34,34	0
87	MG	5	3411	1/1	0.22	9.93	41,41,41,41	0
87	MG	2	1916	1/1	0.38	9.93	37,37,37,37	0
87	MG	5	3667	1/1	0.29	9.89	34,34,34,34	0
88	OHX	2	2159	7/7	0.28	9.85	293,293,293,293	0
88	OHX	5	4197	7/7	0.26	9.85	315,315,315,315	0
87	MG	6	1962	1/1	0.24	9.80	26,26,26,26	0
88	OHX	1	4180	7/7	0.32	9.78	315,315,315,315	0
87	MG	1	3838	1/1	0.29	9.76	28,28,28,28	0
88	OHX	1	4085	7/7	0.27	9.74	241,241,241,241	0
87	MG	1	3681	1/1	0.29	9.66	36,36,36,36	0
87	MG	5	3609	1/1	0.21	9.63	22,22,22,22	0
87	MG	6	1961	1/1	0.33	9.54	35,35,35,35	0
88	OHX	15	306	7/7	0.69	9.52	382,382,382,382	0
87	MG	5	3752	1/1	0.28	9.51	4,4,4,4	0
87	MG	1	3608	1/1	0.30	9.51	27,27,27,27	0
87	MG	5	3539	1/1	0.47	9.51	22,22,22,22	0
87	MG	5	3798	1/1	0.35	9.48	30,30,30,30	0
87	MG	6	1952	1/1	0.45	9.47	29,29,29,29	0
87	MG	5	3657	1/1	0.25	9.47	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	4244	7/7	0.30	9.46	280,280,280,280	0
87	MG	5	3795	1/1	0.29	9.45	42,42,42,42	0
88	OHX	1	4090	7/7	0.37	9.41	220,220,220,220	0
87	MG	n0	203	1/1	0.31	9.39	41,41,41,41	0
87	MG	5	3734	1/1	0.26	9.39	33,33,33,33	0
88	OHX	5	4183	7/7	0.34	9.37	224,224,224,224	0
87	MG	5	3788	1/1	0.18	9.34	50,50,50,50	0
87	MG	1	3574	1/1	0.31	9.31	20,20,20,20	0
87	MG	2	1915	1/1	0.35	9.30	36,36,36,36	0
87	MG	1	3545	1/1	0.33	9.29	17,17,17,17	0
87	MG	1	3538	1/1	0.38	9.21	40,40,40,40	0
88	OHX	1	4160	7/7	0.26	9.20	288,288,288,288	0
87	MG	1	3643	1/1	0.28	9.18	44,44,44,44	0
87	MG	6	1919	1/1	0.35	9.17	21,21,21,21	0
87	MG	5	3484	1/1	0.36	9.14	21,21,21,21	0
87	MG	1	3488	1/1	0.29	9.14	32,32,32,32	0
87	MG	n8	202	1/1	0.41	9.11	38,38,38,38	0
87	MG	O2	201	1/1	0.26	9.10	33,33,33,33	0
87	MG	1	3832	1/1	0.31	9.10	41,41,41,41	0
87	MG	1	3671	1/1	0.28	9.08	45,45,45,45	0
87	MG	1	3493	1/1	0.31	9.07	16,16,16,16	0
88	OHX	5	4204	7/7	0.19	9.07	227,227,227,227	0
88	OHX	4	229	7/7	0.27	8.99	206,206,206,206	0
87	MG	1	3728	1/1	0.26	8.99	33,33,33,33	0
87	MG	1	3562	1/1	0.24	8.98	11,11,11,11	0
87	MG	5	3562	1/1	0.36	8.97	5,5,5,5	0
87	MG	5	3831	1/1	0.25	8.97	10,10,10,10	0
87	MG	2	1936	1/1	0.36	8.93	21,21,21,21	0
87	MG	6	1957	1/1	0.58	8.92	17,17,17,17	0
87	MG	1	3787	1/1	0.34	8.92	27,27,27,27	0
88	OHX	5	4229	7/7	0.45	8.91	370,370,370,370	0
87	MG	1	3827	1/1	0.28	8.88	49,49,49,49	0
87	MG	2	1973	1/1	0.29	8.83	47,47,47,47	0
87	MG	5	3669	1/1	0.38	8.83	30,30,30,30	0
87	MG	5	3571	1/1	0.22	8.80	0,0,0,0	0
87	MG	8	211	1/1	0.29	8.77	37,37,37,37	0
88	OHX	1	4057	7/7	0.23	8.76	193,193,193,193	0
87	MG	1	3786	1/1	0.19	8.75	39,39,39,39	0
88	OHX	5	4209	7/7	0.33	8.75	258,258,258,258	0
88	OHX	1	4190	7/7	0.22	8.72	270,270,270,270	0
87	MG	5	3518	1/1	0.28	8.69	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	N0	201	1/1	0.34	8.68	35,35,35,35	0
87	MG	5	3460	1/1	0.21	8.62	97,97,97,97	0
87	MG	5	3585	1/1	0.44	8.61	17,17,17,17	0
87	MG	L7	302	1/1	0.30	8.57	49,49,49,49	0
87	MG	5	3496	1/1	0.37	8.55	26,26,26,26	0
88	OHX	1	4125	7/7	0.28	8.51	244,244,244,244	0
87	MG	M7	202	1/1	0.36	8.51	34,34,34,34	0
87	MG	o1	201	1/1	1.00	8.43	87,87,87,87	0
87	MG	5	3595	1/1	0.34	8.43	2,2,2,2	0
87	MG	1	3534	1/1	0.28	8.42	13,13,13,13	0
87	MG	5	3900	1/1	0.24	8.42	26,26,26,26	0
87	MG	1	3415	1/1	0.33	8.40	11,11,11,11	0
88	OHX	2	2173	7/7	0.27	8.39	237,237,237,237	0
87	MG	5	3431	1/1	0.34	8.36	53,53,53,53	0
88	OHX	1	4127	7/7	0.25	8.28	208,208,208,208	0
87	MG	1	3749	1/1	0.25	8.26	4,4,4,4	0
87	MG	5	3592	1/1	0.30	8.24	2,2,2,2	0
87	MG	5	3661	1/1	0.33	8.23	41,41,41,41	0
87	MG	5	3535	1/1	0.36	8.22	27,27,27,27	0
87	MG	1	3571	1/1	0.29	8.20	14,14,14,14	0
87	MG	6	1989	1/1	0.25	8.20	37,37,37,37	0
87	MG	1	3656	1/1	0.28	8.19	59,59,59,59	0
87	MG	5	3889	1/1	0.38	8.18	37,37,37,37	0
88	OHX	1	4058	7/7	0.22	8.16	174,174,174,174	0
88	OHX	2	2171	7/7	0.28	8.15	254,254,254,254	0
87	MG	1	3682	1/1	0.23	8.15	46,46,46,46	0
88	OHX	5	4207	7/7	0.26	8.11	273,273,273,273	0
87	MG	O5	201	1/1	0.28	8.10	48,48,48,48	0
88	OHX	5	4158	7/7	0.27	8.07	253,253,253,253	0
87	MG	1	3696	1/1	0.41	8.05	26,26,26,26	0
87	MG	5	3414	1/1	0.44	8.02	28,28,28,28	0
87	MG	5	3482	1/1	0.19	7.96	23,23,23,23	0
87	MG	m6	202	1/1	0.34	7.94	48,48,48,48	0
87	MG	m5	303	1/1	0.35	7.92	51,51,51,51	0
87	MG	1	3744	1/1	0.36	7.90	45,45,45,45	0
88	OHX	2	2131	7/7	0.35	7.86	317,317,317,317	0
87	MG	1	3753	1/1	0.28	7.85	54,54,54,54	0
87	MG	1	3418	1/1	0.26	7.84	4,4,4,4	0
87	MG	1	3797	1/1	0.24	7.77	75,75,75,75	0
87	MG	7	203	1/1	0.25	7.77	48,48,48,48	0
87	MG	1	3705	1/1	0.31	7.77	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3855	1/1	0.30	7.74	33,33,33,33	0
88	OHX	1	4198	7/7	0.27	7.73	275,275,275,275	0
87	MG	6	1987	1/1	0.26	7.71	43,43,43,43	0
87	MG	1	3431	1/1	0.41	7.70	23,23,23,23	0
87	MG	1	3480	1/1	0.27	7.69	30,30,30,30	0
87	MG	1	3677	1/1	0.33	7.67	32,32,32,32	0
87	MG	1	3613	1/1	0.43	7.61	36,36,36,36	0
87	MG	5	3821	1/1	0.22	7.60	40,40,40,40	0
87	MG	5	3692	1/1	0.37	7.59	42,42,42,42	0
88	OHX	1	4152	7/7	0.37	7.59	276,276,276,276	0
87	MG	1	3637	1/1	0.31	7.59	30,30,30,30	0
87	MG	6	1935	1/1	0.74	7.58	41,41,41,41	0
88	OHX	5	4150	7/7	0.24	7.56	216,216,216,216	0
87	MG	5	3640	1/1	0.18	7.55	38,38,38,38	0
87	MG	5	3874	1/1	0.39	7.51	15,15,15,15	0
87	MG	4	210	1/1	0.25	7.50	30,30,30,30	0
87	MG	5	3898	1/1	0.23	7.50	32,32,32,32	0
87	MG	1	3863	1/1	0.21	7.49	73,73,73,73	0
87	MG	3	201	1/1	0.22	7.48	30,30,30,30	0
87	MG	6	2008	1/1	0.32	7.47	56,56,56,56	0
87	MG	1	3575	1/1	0.34	7.45	7,7,7,7	0
87	MG	5	3895	1/1	0.23	7.43	41,41,41,41	0
87	MG	1	3823	1/1	0.43	7.41	44,44,44,44	0
87	MG	6	2043	1/1	0.27	7.37	35,35,35,35	0
88	OHX	5	4163	7/7	0.20	7.36	236,236,236,236	0
88	OHX	2	2162	7/7	0.28	7.35	256,256,256,256	0
87	MG	2	1935	1/1	0.35	7.35	27,27,27,27	0
87	MG	2	1925	1/1	0.53	7.34	41,41,41,41	0
87	MG	6	1992	1/1	0.27	7.33	57,57,57,57	0
88	OHX	6	2188	7/7	0.29	7.32	265,265,265,265	0
87	MG	1	3570	1/1	0.45	7.31	16,16,16,16	0
87	MG	5	3662	1/1	0.22	7.29	10,10,10,10	0
87	MG	1	3568	1/1	0.34	7.23	25,25,25,25	0
87	MG	5	3837	1/1	0.25	7.22	58,58,58,58	0
87	MG	5	3843	1/1	0.23	7.22	93,93,93,93	0
88	OHX	5	4224	7/7	0.26	7.18	288,288,288,288	0
87	MG	5	3591	1/1	0.31	7.18	23,23,23,23	0
87	MG	5	3664	1/1	0.24	7.18	15,15,15,15	0
87	MG	5	3611	1/1	0.25	7.16	2,2,2,2	0
87	MG	1	3675	1/1	0.34	7.13	48,48,48,48	0
87	MG	5	3555	1/1	0.34	7.13	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3486	1/1	0.49	7.12	12,12,12,12	0
87	MG	6	1908	1/1	0.24	7.11	34,34,34,34	0
88	OHX	1	4155	7/7	0.32	7.11	280,280,280,280	0
87	MG	2	1910	1/1	0.37	7.09	39,39,39,39	0
88	OHX	5	4170	7/7	0.25	7.06	247,247,247,247	0
87	MG	5	3525	1/1	0.34	7.06	8,8,8,8	0
87	MG	5	3504	1/1	0.26	6.96	10,10,10,10	0
88	OHX	5	4160	7/7	0.34	6.94	231,231,231,231	0
87	MG	2	1908	1/1	0.23	6.93	40,40,40,40	0
87	MG	6	1933	1/1	0.26	6.93	35,35,35,35	0
87	MG	1	3860	1/1	0.24	6.93	101,101,101,101	0
88	OHX	1	4132	7/7	0.22	6.92	180,180,180,180	0
88	OHX	3	224	7/7	0.23	6.91	248,248,248,248	0
88	OHX	2	2143	7/7	0.38	6.91	260,260,260,260	0
87	MG	6	1937	1/1	0.25	6.89	18,18,18,18	0
87	MG	5	3656	1/1	0.26	6.87	34,34,34,34	0
87	MG	5	3789	1/1	0.28	6.87	10,10,10,10	0
88	OHX	5	4145	7/7	0.21	6.86	216,216,216,216	0
88	OHX	1	4153	7/7	0.20	6.85	244,244,244,244	0
87	MG	1	3615	1/1	0.33	6.85	51,51,51,51	0
88	OHX	5	4046	7/7	0.23	6.84	160,160,160,160	0
88	OHX	1	4140	7/7	0.37	6.82	298,298,298,298	0
87	MG	5	3836	1/1	0.23	6.78	28,28,28,28	0
87	MG	1	3641	1/1	0.30	6.77	36,36,36,36	0
87	MG	1	3723	1/1	0.42	6.71	48,48,48,48	0
87	MG	1	3729	1/1	0.33	6.70	52,52,52,52	0
87	MG	6	1978	1/1	0.26	6.70	47,47,47,47	0
87	MG	5	3799	1/1	0.27	6.69	44,44,44,44	0
87	MG	5	3503	1/1	0.33	6.69	15,15,15,15	0
87	MG	L7	301	1/1	0.25	6.68	32,32,32,32	0
88	OHX	1	4173	7/7	0.38	6.68	264,264,264,264	0
87	MG	6	2004	1/1	0.53	6.66	54,54,54,54	0
88	OHX	6	2201	7/7	0.26	6.62	244,244,244,244	0
87	MG	5	3686	1/1	0.29	6.60	35,35,35,35	0
87	MG	5	3634	1/1	0.21	6.60	39,39,39,39	0
87	MG	5	3857	1/1	0.26	6.59	80,80,80,80	0
87	MG	5	3516	1/1	0.28	6.56	27,27,27,27	0
87	MG	5	3429	1/1	0.23	6.55	5,5,5,5	0
87	MG	5	3455	1/1	0.34	6.54	34,34,34,34	0
87	MG	6	1965	1/1	0.20	6.53	26,26,26,26	0
87	MG	5	3617	1/1	0.22	6.52	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3615	1/1	0.26	6.50	36,36,36,36	0
87	MG	6	2042	1/1	0.36	6.46	51,51,51,51	0
87	MG	1	3605	1/1	0.27	6.46	21,21,21,21	0
87	MG	1	3531	1/1	0.21	6.46	11,11,11,11	0
87	MG	6	1999	1/1	0.36	6.46	46,46,46,46	0
87	MG	5	3756	1/1	0.21	6.44	38,38,38,38	0
87	MG	1	3487	1/1	0.26	6.43	26,26,26,26	0
88	OHX	1	4206	7/7	0.34	6.42	275,275,275,275	0
87	MG	5	3462	1/1	0.30	6.42	18,18,18,18	0
88	OHX	1	3991	7/7	0.26	6.41	162,162,162,162	0
88	OHX	6	2182	7/7	0.29	6.40	264,264,264,264	0
87	MG	1	3767	1/1	0.24	6.40	53,53,53,53	0
87	MG	1	3725	1/1	0.21	6.40	21,21,21,21	0
87	MG	2	1932	1/1	0.43	6.39	33,33,33,33	0
87	MG	1	3712	1/1	0.26	6.37	41,41,41,41	0
87	MG	5	3442	1/1	0.29	6.36	1,1,1,1	0
88	OHX	1	4183	7/7	0.28	6.35	350,350,350,350	0
88	OHX	6	2161	7/7	0.24	6.32	251,251,251,251	0
88	OHX	1	4156	7/7	0.26	6.29	234,234,234,234	0
88	OHX	1	3989	7/7	0.27	6.28	147,147,147,147	0
87	MG	2	2012	1/1	0.36	6.28	40,40,40,40	0
87	MG	6	1984	1/1	0.33	6.24	56,56,56,56	0
88	OHX	5	4166	7/7	0.33	6.24	204,204,204,204	0
87	MG	1	3433	1/1	0.33	6.22	17,17,17,17	0
87	MG	5	3464	1/1	0.36	6.21	6,6,6,6	0
87	MG	1	3836	1/1	0.43	6.17	46,46,46,46	0
87	MG	q3	502	1/1	0.25	6.15	48,48,48,48	0
88	OHX	6	2123	7/7	0.19	6.13	188,188,188,188	0
87	MG	5	3520	1/1	0.22	6.13	13,13,13,13	0
87	MG	6	1902	1/1	0.35	6.12	44,44,44,44	0
87	MG	6	2012	1/1	0.31	6.11	33,33,33,33	0
87	MG	1	3799	1/1	0.27	6.10	45,45,45,45	0
87	MG	1	3766	1/1	0.24	6.10	40,40,40,40	0
87	MG	l3	401	1/1	0.41	6.09	4,4,4,4	0
87	MG	5	3479	1/1	0.29	6.09	9,9,9,9	0
87	MG	6	1904	1/1	0.38	6.08	27,27,27,27	0
87	MG	4	209	1/1	0.20	6.07	51,51,51,51	0
88	OHX	5	4221	7/7	0.26	6.05	256,256,256,256	0
87	MG	5	3594	1/1	0.24	6.05	19,19,19,19	0
87	MG	6	1953	1/1	0.31	6.01	27,27,27,27	0
87	MG	2	1955	1/1	0.34	6.01	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3411	1/1	0.28	6.00	20,20,20,20	0
87	MG	m1	202	1/1	0.18	5.98	41,41,41,41	0
87	MG	6	1968	1/1	0.21	5.98	28,28,28,28	0
87	MG	1	3409	1/1	0.26	5.97	7,7,7,7	0
87	MG	L7	303	1/1	0.26	5.97	56,56,56,56	0
87	MG	2	2007	1/1	0.35	5.96	30,30,30,30	0
87	MG	6	1932	1/1	0.28	5.96	29,29,29,29	0
87	MG	1	3512	1/1	0.32	5.95	13,13,13,13	0
87	MG	2	1929	1/1	0.32	5.93	19,19,19,19	0
87	MG	2	1984	1/1	0.24	5.92	37,37,37,37	0
87	MG	1	3477	1/1	0.26	5.91	21,21,21,21	0
87	MG	5	3508	1/1	0.26	5.90	29,29,29,29	0
87	MG	5	3849	1/1	0.31	5.89	30,30,30,30	0
88	OHX	5	4211	7/7	0.33	5.89	277,277,277,277	0
88	OHX	1	4220	7/7	0.34	5.89	239,239,239,239	0
87	MG	6	1942	1/1	0.19	5.84	10,10,10,10	0
87	MG	2	1963	1/1	0.30	5.82	46,46,46,46	0
88	OHX	1	4080	7/7	0.20	5.82	216,216,216,216	0
87	MG	6	1927	1/1	0.30	5.81	23,23,23,23	0
88	OHX	1	4223	7/7	0.26	5.81	222,222,222,222	0
87	MG	5	3897	1/1	0.22	5.81	22,22,22,22	0
87	MG	5	3878	1/1	0.35	5.78	16,16,16,16	0
87	MG	1	3673	1/1	0.16	5.71	61,61,61,61	0
88	OHX	5	4212	7/7	0.31	5.70	270,270,270,270	0
87	MG	c1	201	1/1	0.26	5.68	31,31,31,31	0
87	MG	1	3792	1/1	0.49	5.64	53,53,53,53	0
87	MG	5	3768	1/1	0.19	5.63	49,49,49,49	0
87	MG	5	3519	1/1	0.22	5.61	6,6,6,6	0
88	OHX	2	2164	7/7	0.28	5.61	306,306,306,306	0
88	OHX	5	4186	7/7	0.23	5.61	242,242,242,242	0
87	MG	5	3896	1/1	0.18	5.57	114,114,114,114	0
87	MG	6	1939	1/1	0.24	5.53	20,20,20,20	0
87	MG	7	206	1/1	0.18	5.51	31,31,31,31	0
88	OHX	5	4216	7/7	0.27	5.50	253,253,253,253	0
88	OHX	1	3919	7/7	0.26	5.50	100,100,100,100	0
87	MG	1	3438	1/1	0.26	5.50	20,20,20,20	0
87	MG	1	3553	1/1	0.32	5.49	17,17,17,17	0
87	MG	m5	302	1/1	0.36	5.48	49,49,49,49	0
87	MG	5	3548	1/1	0.25	5.48	11,11,11,11	0
88	OHX	5	4206	7/7	0.25	5.47	224,224,224,224	0
87	MG	5	3614	1/1	0.23	5.47	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	MG	5	3506	1/1	0.27	5.46	19,19,19,19	0
88	OHX	1	4149	7/7	0.20	5.44	144,144,144,144	0
88	OHX	1	4015	7/7	0.20	5.42	202,202,202,202	0
87	MG	6	2032	1/1	0.29	5.41	50,50,50,50	0
88	OHX	5	4245	7/7	0.21	5.36	275,275,275,275	0
88	OHX	5	4227	7/7	0.26	5.36	277,277,277,277	0
87	MG	2	2006	1/1	0.27	5.34	41,41,41,41	0
87	MG	5	3509	1/1	0.32	5.34	15,15,15,15	0
87	MG	2	1952	1/1	0.37	5.32	50,50,50,50	0
87	MG	5	3622	1/1	0.37	5.31	45,45,45,45	0
88	OHX	6	2171	7/7	0.25	5.28	274,274,274,274	0
87	MG	6	1909	1/1	0.31	5.28	41,41,41,41	0
88	OHX	7	226	7/7	0.22	5.26	254,254,254,254	0
87	MG	5	3654	1/1	0.29	5.26	47,47,47,47	0
87	MG	6	1915	1/1	0.50	5.26	56,56,56,56	0
87	MG	1	3618	1/1	0.24	5.23	17,17,17,17	0
88	OHX	5	4029	7/7	0.18	5.17	179,179,179,179	0
87	MG	5	3439	1/1	0.22	5.17	25,25,25,25	0
88	OHX	2	2157	7/7	0.28	5.17	251,251,251,251	0
88	OHX	5	4164	7/7	0.19	5.17	233,233,233,233	0
87	MG	2	1922	1/1	0.28	5.16	31,31,31,31	0
87	MG	1	3439	1/1	0.31	5.16	34,34,34,34	0
87	MG	o4	201	1/1	0.66	5.14	48,48,48,48	0
87	MG	1	3742	1/1	0.21	5.13	49,49,49,49	0
88	OHX	1	4177	7/7	0.28	5.08	322,322,322,322	0
87	MG	1	3811	1/1	0.33	5.08	55,55,55,55	0
87	MG	2	1980	1/1	0.32	5.07	24,24,24,24	0
87	MG	6	1910	1/1	0.26	5.07	44,44,44,44	0
88	OHX	1	4204	7/7	0.23	5.07	246,246,246,246	0
87	MG	1	3550	1/1	0.26	5.06	44,44,44,44	0
87	MG	4	207	1/1	0.25	5.05	42,42,42,42	0
87	MG	1	3816	1/1	0.22	5.03	19,19,19,19	0
88	OHX	5	4232	7/7	0.22	5.03	234,234,234,234	0
87	MG	1	3566	1/1	0.23	5.01	29,29,29,29	0
87	MG	5	3781	1/1	0.17	4.99	39,39,39,39	0
88	OHX	1	4186	7/7	0.20	4.98	171,171,171,171	0
87	MG	5	3473	1/1	0.28	4.95	7,7,7,7	0
87	MG	q1	101	1/1	0.36	4.95	30,30,30,30	0
88	OHX	5	4174	7/7	0.20	4.89	228,228,228,228	0
88	OHX	5	4157	7/7	0.22	4.88	207,207,207,207	0
87	MG	1	3862	1/1	0.25	4.88	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3748	1/1	0.22	4.88	17,17,17,17	0
87	MG	5	3828	1/1	0.28	4.84	39,39,39,39	0
87	MG	1	3795	1/1	0.40	4.82	65,65,65,65	0
87	MG	5	3417	1/1	0.28	4.82	31,31,31,31	0
88	OHX	6	2184	7/7	0.21	4.82	259,259,259,259	0
87	MG	1	3779	1/1	0.23	4.75	40,40,40,40	0
87	MG	5	3658	1/1	0.23	4.74	42,42,42,42	0
87	MG	2	1901	1/1	0.52	4.73	39,39,39,39	0
87	MG	2	1907	1/1	0.41	4.69	26,26,26,26	0
88	OHX	4	231	7/7	0.21	4.69	237,237,237,237	0
88	OHX	5	4075	7/7	0.20	4.69	171,171,171,171	0
87	MG	1	3472	1/1	0.20	4.69	28,28,28,28	0
87	MG	5	3636	1/1	0.21	4.69	26,26,26,26	0
87	MG	5	3582	1/1	0.29	4.66	8,8,8,8	0
87	MG	2	2015	1/1	0.63	4.64	57,57,57,57	0
87	MG	5	4260	1/1	0.26	4.64	37,37,37,37	0
88	OHX	2	2120	7/7	0.23	4.63	230,230,230,230	0
88	OHX	5	4255	7/7	0.21	4.60	249,249,249,249	0
88	OHX	1	4123	7/7	0.27	4.60	224,224,224,224	0
87	MG	6	2203	1/1	0.30	4.59	46,46,46,46	0
87	MG	1	3763	1/1	0.19	4.58	29,29,29,29	0
87	MG	1	3662	1/1	0.34	4.56	24,24,24,24	0
87	MG	1	3634	1/1	0.25	4.56	21,21,21,21	0
87	MG	1	3782	1/1	0.23	4.52	36,36,36,36	0
87	MG	1	4229	1/1	0.25	4.51	20,20,20,20	0
87	MG	1	3685	1/1	0.26	4.51	49,49,49,49	0
88	OHX	1	4209	7/7	0.33	4.50	272,272,272,272	0
87	MG	N8	202	1/1	0.23	4.48	16,16,16,16	0
88	OHX	5	4165	7/7	0.23	4.48	236,236,236,236	0
88	OHX	5	4085	7/7	0.18	4.47	173,173,173,173	0
87	MG	1	3507	1/1	0.24	4.47	26,26,26,26	0
87	MG	2	1945	1/1	0.20	4.47	36,36,36,36	0
87	MG	6	2039	1/1	0.42	4.44	47,47,47,47	0
87	MG	5	3532	1/1	0.20	4.44	16,16,16,16	0
87	MG	5	3502	1/1	0.23	4.43	19,19,19,19	0
87	MG	2	1949	1/1	0.30	4.43	57,57,57,57	0
88	OHX	5	4200	7/7	0.27	4.40	263,263,263,263	0
87	MG	1	3448	1/1	0.28	4.39	23,23,23,23	0
87	MG	2	1948	1/1	0.45	4.39	31,31,31,31	0
87	MG	1	3676	1/1	0.37	4.34	53,53,53,53	0
87	MG	1	3601	1/1	0.29	4.33	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	s8	303	1/1	0.29	4.33	34,34,34,34	0
87	MG	6	1930	1/1	0.22	4.33	35,35,35,35	0
87	MG	6	2037	1/1	0.37	4.31	52,52,52,52	0
88	OHX	1	4146	7/7	0.25	4.30	302,302,302,302	0
87	MG	c8	201	1/1	0.32	4.29	41,41,41,41	0
88	OHX	5	4219	7/7	0.20	4.26	289,289,289,289	0
87	MG	1	3620	1/1	0.24	4.26	42,42,42,42	0
88	OHX	1	4124	7/7	0.25	4.25	277,277,277,277	0
87	MG	1	3868	1/1	0.37	4.25	46,46,46,46	0
87	MG	2	1983	1/1	0.36	4.25	58,58,58,58	0
87	MG	1	3702	1/1	0.27	4.23	32,32,32,32	0
88	OHX	5	4189	7/7	0.22	4.22	222,222,222,222	0
87	MG	2	1981	1/1	0.24	4.20	39,39,39,39	0
87	MG	1	3829	1/1	0.18	4.19	37,37,37,37	0
88	OHX	1	4184	7/7	0.21	4.18	238,238,238,238	0
88	OHX	14	404	7/7	0.35	4.18	286,286,286,286	0
88	OHX	1	4216	7/7	0.45	4.17	285,285,285,285	0
87	MG	N8	205	1/1	0.30	4.16	45,45,45,45	0
87	MG	1	3510	1/1	0.31	4.16	5,5,5,5	0
87	MG	1	3417	1/1	0.28	4.14	32,32,32,32	0
87	MG	6	1980	1/1	0.24	4.13	61,61,61,61	0
87	MG	1	3455	1/1	0.26	4.12	17,17,17,17	0
88	OHX	1	4159	7/7	0.21	4.11	233,233,233,233	0
87	MG	1	3638	1/1	0.33	4.09	40,40,40,40	0
87	MG	5	3750	1/1	0.29	4.07	8,8,8,8	0
88	OHX	5	4208	7/7	0.32	4.06	304,304,304,304	0
87	MG	1	3445	1/1	0.20	4.06	53,53,53,53	0
88	OHX	1	4221	7/7	0.25	4.06	266,266,266,266	0
87	MG	6	1964	1/1	0.21	4.04	34,34,34,34	0
88	OHX	1	4210	7/7	0.20	4.02	277,277,277,277	0
87	MG	1	3661	1/1	0.32	4.01	22,22,22,22	0
87	MG	5	4261	1/1	0.26	4.00	37,37,37,37	0
88	OHX	1	4211	7/7	0.27	4.00	276,276,276,276	0
88	OHX	1	3963	7/7	0.20	3.99	137,137,137,137	0
87	MG	2	1933	1/1	0.23	3.98	39,39,39,39	0
88	OHX	1	4188	7/7	0.23	3.97	258,258,258,258	0
88	OHX	5	4130	7/7	0.21	3.97	209,209,209,209	0
88	OHX	6	2122	7/7	0.27	3.96	209,209,209,209	0
87	MG	5	3477	1/1	0.44	3.94	36,36,36,36	0
87	MG	1	3751	1/1	0.27	3.94	33,33,33,33	0
88	OHX	6	2156	7/7	0.30	3.93	235,235,235,235	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	N8	203	1/1	0.19	3.92	66,66,66,66	0
88	OHX	2	2153	7/7	0.21	3.91	256,256,256,256	0
88	OHX	1	4225	7/7	0.27	3.90	304,304,304,304	0
87	MG	1	3735	1/1	0.19	3.88	92,92,92,92	0
87	MG	1	3625	1/1	0.23	3.88	60,60,60,60	0
87	MG	14	402	1/1	0.26	3.86	41,41,41,41	0
87	MG	5	3529	1/1	0.20	3.84	28,28,28,28	0
87	MG	n6	202	1/1	0.34	3.82	26,26,26,26	0
87	MG	5	3547	1/1	0.32	3.81	36,36,36,36	0
87	MG	3	210	1/1	0.28	3.81	48,48,48,48	0
87	MG	1	3446	1/1	0.42	3.80	27,27,27,27	0
88	OHX	1	4213	7/7	0.18	3.79	202,202,202,202	0
87	MG	6	1934	1/1	0.41	3.77	60,60,60,60	0
87	MG	2	1912	1/1	0.21	3.76	24,24,24,24	0
87	MG	l3	403	1/1	0.23	3.75	59,59,59,59	0
88	OHX	2	2127	7/7	0.21	3.74	239,239,239,239	0
87	MG	m7	201	1/1	0.32	3.73	9,9,9,9	0
87	MG	5	3806	1/1	0.22	3.72	34,34,34,34	0
88	OHX	7	224	7/7	0.20	3.71	201,201,201,201	0
87	MG	5	3839	1/1	0.17	3.68	68,68,68,68	0
87	MG	5	3777	1/1	0.23	3.68	22,22,22,22	0
87	MG	1	3483	1/1	0.30	3.65	20,20,20,20	0
88	OHX	1	4082	7/7	0.21	3.65	213,213,213,213	0
88	OHX	5	4239	7/7	0.55	3.65	313,313,313,313	0
87	MG	d3	201	1/1	0.45	3.64	60,60,60,60	0
87	MG	2	1930	1/1	0.24	3.59	41,41,41,41	0
87	MG	1	3822	1/1	0.17	3.59	21,21,21,21	0
87	MG	1	3595	1/1	0.23	3.55	28,28,28,28	0
87	MG	1	3476	1/1	0.20	3.53	43,43,43,43	0
87	MG	L4	401	1/1	0.25	3.52	35,35,35,35	0
87	MG	1	3557	1/1	0.21	3.51	13,13,13,13	0
87	MG	L3	401	1/1	0.26	3.51	11,11,11,11	0
87	MG	1	3849	1/1	0.19	3.50	20,20,20,20	0
87	MG	1	3623	1/1	0.38	3.49	30,30,30,30	0
88	OHX	1	4059	7/7	0.22	3.45	164,164,164,164	0
87	MG	2	1978	1/1	0.20	3.44	44,44,44,44	0
87	MG	5	3894	1/1	0.26	3.42	87,87,87,87	0
87	MG	5	3689	1/1	0.23	3.42	43,43,43,43	0
87	MG	5	3819	1/1	0.23	3.41	53,53,53,53	0
88	OHX	5	4056	7/7	0.20	3.40	166,166,166,166	0
87	MG	6	1936	1/1	0.21	3.38	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	5	4177	7/7	0.23	3.38	273,273,273,273	0
87	MG	1	3509	1/1	0.26	3.37	6,6,6,6	0
87	MG	1	3556	1/1	0.32	3.36	45,45,45,45	0
88	OHX	6	2107	7/7	0.15	3.35	143,143,143,143	0
88	OHX	7	225	7/7	0.21	3.35	270,270,270,270	0
87	MG	14	401	1/1	0.28	3.34	40,40,40,40	0
88	OHX	2	2172	7/7	0.36	3.33	331,331,331,331	0
88	OHX	1	4166	7/7	0.16	3.32	234,234,234,234	0
87	MG	1	3456	1/1	0.34	3.31	33,33,33,33	0
88	OHX	6	2196	7/7	0.23	3.31	293,293,293,293	0
87	MG	1	3592	1/1	0.24	3.31	5,5,5,5	0
87	MG	5	3892	1/1	0.24	3.29	24,24,24,24	0
88	OHX	5	4076	7/7	0.17	3.29	167,167,167,167	0
87	MG	6	2033	1/1	0.45	3.29	46,46,46,46	0
88	OHX	5	3917	7/7	0.17	3.28	67,67,67,67	0
87	MG	1	3404	1/1	0.21	3.27	30,30,30,30	0
88	OHX	5	4169	7/7	0.22	3.21	244,244,244,244	0
87	MG	s6	301	1/1	0.33	3.21	73,73,73,73	0
87	MG	1	3631	1/1	0.17	3.20	26,26,26,26	0
87	MG	6	1982	1/1	0.28	3.19	46,46,46,46	0
87	MG	1	3489	1/1	0.24	3.17	26,26,26,26	0
88	OHX	5	4188	7/7	0.27	3.17	244,244,244,244	0
87	MG	1	3649	1/1	0.17	3.16	38,38,38,38	0
87	MG	5	3613	1/1	0.22	3.15	18,18,18,18	0
88	OHX	2	2163	7/7	0.21	3.12	279,279,279,279	0
88	OHX	2	2176	7/7	0.25	3.12	252,252,252,252	0
87	MG	1	3688	1/1	0.17	3.11	32,32,32,32	0
87	MG	5	3643	1/1	0.16	3.11	25,25,25,25	0
87	MG	1	3759	1/1	0.20	3.09	9,9,9,9	0
88	OHX	5	4252	7/7	0.17	3.08	237,237,237,237	0
88	OHX	5	4254	7/7	0.22	3.06	269,269,269,269	0
87	MG	5	3847	1/1	0.28	3.05	39,39,39,39	0
87	MG	S8	301	1/1	0.20	3.04	47,47,47,47	0
87	MG	1	3659	1/1	0.16	3.01	5,5,5,5	0
87	MG	5	3697	1/1	0.16	3.01	55,55,55,55	0
87	MG	2	1990	1/1	0.13	3.00	49,49,49,49	0
88	OHX	2	2179	7/7	0.23	2.99	267,267,267,267	0
87	MG	n0	202	1/1	0.26	2.99	42,42,42,42	0
87	MG	5	3767	1/1	0.23	2.98	15,15,15,15	0
87	MG	5	3733	1/1	0.40	2.97	43,43,43,43	0
88	OHX	8	227	7/7	0.22	2.96	233,233,233,233	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3785	1/1	0.26	2.96	43,43,43,43	0
87	MG	5	3403	1/1	0.20	2.94	3,3,3,3	0
88	OHX	5	4141	7/7	0.31	2.94	227,227,227,227	0
87	MG	8	208	1/1	0.17	2.94	42,42,42,42	0
87	MG	5	3441	1/1	0.37	2.91	28,28,28,28	0
87	MG	1	3752	1/1	0.34	2.87	46,46,46,46	0
88	OHX	6	2074	7/7	0.20	2.86	123,123,123,123	0
87	MG	1	3653	1/1	0.20	2.85	30,30,30,30	0
88	OHX	5	4096	7/7	0.20	2.85	181,181,181,181	0
87	MG	2	2005	1/1	0.29	2.84	44,44,44,44	0
87	MG	6	1993	1/1	0.27	2.84	56,56,56,56	0
87	MG	5	3463	1/1	0.22	2.83	26,26,26,26	0
87	MG	5	3596	1/1	0.22	2.80	3,3,3,3	0
88	OHX	5	4253	7/7	0.22	2.79	256,256,256,256	0
88	OHX	5	4152	7/7	0.19	2.78	260,260,260,260	0
88	OHX	5	4223	7/7	0.17	2.77	256,256,256,256	0
88	OHX	1	4142	7/7	0.18	2.77	250,250,250,250	0
87	MG	1	4231	1/1	0.27	2.74	15,15,15,15	0
87	MG	5	3723	1/1	0.20	2.74	69,69,69,69	0
88	OHX	5	3958	7/7	0.25	2.74	100,100,100,100	0
88	OHX	2	2169	7/7	0.20	2.72	221,221,221,221	0
88	OHX	6	2143	7/7	0.20	2.71	233,233,233,233	0
88	OHX	1	4193	7/7	0.42	2.71	290,290,290,290	0
87	MG	5	3537	1/1	0.20	2.70	40,40,40,40	0
88	OHX	5	4215	7/7	0.18	2.70	220,220,220,220	0
88	OHX	1	3943	7/7	0.19	2.69	173,173,173,173	0
88	OHX	6	2176	7/7	0.23	2.67	277,277,277,277	0
87	MG	7	210	1/1	0.20	2.67	66,66,66,66	0
88	OHX	5	4143	7/7	0.28	2.67	243,243,243,243	0
87	MG	1	3452	1/1	0.31	2.67	27,27,27,27	0
87	MG	1	3648	1/1	0.25	2.66	33,33,33,33	0
88	OHX	5	4190	7/7	0.19	2.66	208,208,208,208	0
87	MG	2	1993	1/1	0.25	2.65	64,64,64,64	0
88	OHX	1	4138	7/7	0.20	2.64	223,223,223,223	0
87	MG	2	1974	1/1	0.20	2.61	55,55,55,55	0
87	MG	6	1973	1/1	0.20	2.59	33,33,33,33	0
88	OHX	5	4218	7/7	0.16	2.59	255,255,255,255	0
88	OHX	5	4065	7/7	0.18	2.56	167,167,167,167	0
87	MG	2	1986	1/1	0.21	2.56	43,43,43,43	0
87	MG	2	1931	1/1	0.38	2.55	51,51,51,51	0
88	OHX	2	2136	7/7	0.28	2.53	238,238,238,238	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	1918	1/1	0.26	2.53	41,41,41,41	0
88	OHX	5	4086	7/7	0.18	2.52	145,145,145,145	0
87	MG	1	3533	1/1	0.29	2.50	28,28,28,28	0
87	MG	M6	201	1/1	0.31	2.48	43,43,43,43	0
88	OHX	6	2045	7/7	0.18	2.47	67,67,67,67	0
87	MG	1	3636	1/1	0.34	2.46	49,49,49,49	0
87	MG	2	1965	1/1	0.20	2.46	42,42,42,42	0
88	OHX	6	2144	7/7	0.22	2.46	243,243,243,243	0
88	OHX	5	4079	7/7	0.22	2.45	194,194,194,194	0
87	MG	6	1990	1/1	0.21	2.40	35,35,35,35	0
88	OHX	5	4201	7/7	0.18	2.40	232,232,232,232	0
87	MG	1	3437	1/1	0.24	2.40	26,26,26,26	0
88	OHX	6	2202	7/7	0.20	2.39	266,266,266,266	0
88	OHX	1	4133	7/7	0.17	2.38	208,208,208,208	0
88	OHX	6	2174	7/7	0.21	2.38	223,223,223,223	0
87	MG	2	1942	1/1	0.24	2.37	39,39,39,39	0
88	OHX	1	3973	7/7	0.18	2.37	129,129,129,129	0
87	MG	6	2003	1/1	0.16	2.37	55,55,55,55	0
88	OHX	6	2117	7/7	0.23	2.37	186,186,186,186	0
87	MG	5	3635	1/1	0.18	2.36	26,26,26,26	0
87	MG	6	1954	1/1	0.21	2.36	11,11,11,11	0
87	MG	1	3781	1/1	0.17	2.35	37,37,37,37	0
88	OHX	5	4104	7/7	0.21	2.35	197,197,197,197	0
87	MG	4	205	1/1	0.27	2.34	19,19,19,19	0
87	MG	5	3627	1/1	0.24	2.34	15,15,15,15	0
88	OHX	5	4006	7/7	0.16	2.33	145,145,145,145	0
87	MG	2	1970	1/1	0.18	2.33	65,65,65,65	0
88	OHX	5	4094	7/7	0.24	2.32	227,227,227,227	0
87	MG	6	1912	1/1	0.22	2.32	44,44,44,44	0
88	OHX	5	4155	7/7	0.21	2.31	220,220,220,220	0
87	MG	5	3813	1/1	0.20	2.30	51,51,51,51	0
88	OHX	1	4191	7/7	0.19	2.27	245,245,245,245	0
88	OHX	5	4047	7/7	0.17	2.27	163,163,163,163	0
88	OHX	2	2119	7/7	0.16	2.26	205,205,205,205	0
88	OHX	2	2128	7/7	0.21	2.26	221,221,221,221	0
88	OHX	5	4142	7/7	0.20	2.25	223,223,223,223	0
88	OHX	1	4099	7/7	0.18	2.25	193,193,193,193	0
87	MG	O7	102	1/1	0.27	2.24	30,30,30,30	0
87	MG	n3	202	1/1	0.31	2.23	60,60,60,60	0
87	MG	5	3451	1/1	0.20	2.22	7,7,7,7	0
87	MG	5	3468	1/1	0.25	2.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3843	1/1	0.32	2.21	50,50,50,50	0
87	MG	5	3866	1/1	0.18	2.20	35,35,35,35	0
87	MG	5	3498	1/1	0.23	2.19	8,8,8,8	0
87	MG	1	3760	1/1	0.17	2.18	54,54,54,54	0
88	OHX	6	2189	7/7	0.21	2.17	266,266,266,266	0
88	OHX	1	4139	7/7	0.17	2.16	213,213,213,213	0
88	OHX	M7	206	7/7	0.27	2.16	282,282,282,282	0
87	MG	1	3658	1/1	0.22	2.16	27,27,27,27	0
87	MG	5	3745	1/1	0.23	2.15	39,39,39,39	0
87	MG	1	3425	1/1	0.21	2.14	30,30,30,30	0
87	MG	1	3733	1/1	0.25	2.14	15,15,15,15	0
87	MG	5	3830	1/1	0.27	2.14	32,32,32,32	0
88	OHX	1	4148	7/7	0.19	2.14	209,209,209,209	0
88	OHX	5	4054	7/7	0.17	2.11	156,156,156,156	0
87	MG	5	3885	1/1	0.16	2.10	38,38,38,38	0
88	OHX	1	4185	7/7	0.20	2.10	302,302,302,302	0
88	OHX	2	2160	7/7	0.32	2.09	246,246,246,246	0
88	OHX	5	4162	7/7	0.17	2.08	208,208,208,208	0
88	OHX	8	229	7/7	0.20	2.08	219,219,219,219	0
87	MG	1	3737	1/1	0.25	2.08	49,49,49,49	0
88	OHX	5	4240	7/7	0.26	2.08	306,306,306,306	0
87	MG	1	3604	1/1	0.19	2.05	14,14,14,14	0
88	OHX	6	2187	7/7	0.26	2.05	317,317,317,317	0
87	MG	5	3527	1/1	0.21	2.02	5,5,5,5	0
87	MG	M0	301	1/1	0.22	2.01	30,30,30,30	0
87	MG	5	3859	1/1	0.30	2.01	38,38,38,38	0
88	OHX	5	4228	7/7	0.27	2.00	251,251,251,251	0
88	OHX	6	2114	7/7	0.21	2.00	209,209,209,209	0
87	MG	5	3569	1/1	0.29	2.00	18,18,18,18	0
87	MG	m7	204	1/1	0.25	2.00	33,33,33,33	0
87	MG	1	3678	1/1	0.19	1.99	5,5,5,5	0
88	OHX	5	4097	7/7	0.19	1.99	175,175,175,175	0
87	MG	m1	201	1/1	0.24	1.98	51,51,51,51	0
88	OHX	6	2197	7/7	0.21	1.98	220,220,220,220	0
87	MG	4	208	1/1	0.16	1.96	44,44,44,44	0
87	MG	1	3768	1/1	0.21	1.96	46,46,46,46	0
87	MG	s8	302	1/1	0.24	1.95	38,38,38,38	0
87	MG	5	3628	1/1	0.19	1.95	35,35,35,35	0
88	OHX	1	4182	7/7	0.17	1.94	253,253,253,253	0
87	MG	5	3655	1/1	0.18	1.92	11,11,11,11	0
87	MG	1	3666	1/1	0.36	1.91	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3616	1/1	0.14	1.91	36,36,36,36	0
88	OHX	6	2165	7/7	0.21	1.91	226,226,226,226	0
87	MG	5	3629	1/1	0.19	1.88	12,12,12,12	0
88	OHX	2	2137	7/7	0.20	1.85	271,271,271,271	0
88	OHX	5	4139	7/7	0.23	1.83	198,198,198,198	0
87	MG	5	3818	1/1	0.19	1.82	42,42,42,42	0
87	MG	2	1956	1/1	0.20	1.81	33,33,33,33	0
87	MG	5	3711	1/1	0.17	1.79	29,29,29,29	0
88	OHX	5	4092	7/7	0.19	1.79	211,211,211,211	0
87	MG	2	1969	1/1	0.44	1.77	61,61,61,61	0
87	MG	2	2016	1/1	0.26	1.77	37,37,37,37	0
88	OHX	6	2179	7/7	0.20	1.76	254,254,254,254	0
88	OHX	5	4178	7/7	0.22	1.74	194,194,194,194	0
88	OHX	1	4070	7/7	0.21	1.73	216,216,216,216	0
88	OHX	6	2159	7/7	0.16	1.73	215,215,215,215	0
87	MG	2	1943	1/1	0.18	1.72	33,33,33,33	0
88	OHX	1	4076	7/7	0.20	1.71	226,226,226,226	0
87	MG	3	207	1/1	0.20	1.71	33,33,33,33	0
87	MG	m5	301	1/1	0.23	1.71	24,24,24,24	0
88	OHX	l5	305	7/7	0.31	1.68	286,286,286,286	0
88	OHX	1	4094	7/7	0.18	1.67	212,212,212,212	0
88	OHX	2	2175	7/7	0.19	1.63	250,250,250,250	0
88	OHX	5	4117	7/7	0.19	1.62	172,172,172,172	0
88	OHX	5	4151	7/7	0.19	1.60	215,215,215,215	0
88	OHX	1	4172	7/7	0.17	1.60	232,232,232,232	0
87	MG	2	1927	1/1	0.36	1.59	19,19,19,19	0
87	MG	7	212	1/1	0.18	1.57	41,41,41,41	0
88	OHX	2	2116	7/7	0.27	1.56	280,280,280,280	0
87	MG	M7	201	1/1	0.40	1.56	35,35,35,35	0
87	MG	5	3488	1/1	0.19	1.56	49,49,49,49	0
87	MG	5	3492	1/1	0.18	1.56	12,12,12,12	0
87	MG	1	3852	1/1	0.24	1.56	20,20,20,20	0
88	OHX	1	4075	7/7	0.17	1.56	235,235,235,235	0
87	MG	M3	201	1/1	0.19	1.55	36,36,36,36	0
87	MG	c7	202	1/1	0.23	1.55	35,35,35,35	0
87	MG	5	3790	1/1	0.17	1.55	26,26,26,26	0
87	MG	5	3416	1/1	0.19	1.55	24,24,24,24	0
88	OHX	1	4088	7/7	0.19	1.55	187,187,187,187	0
88	OHX	5	3998	7/7	0.17	1.53	130,130,130,130	0
87	MG	1	3665	1/1	0.21	1.52	34,34,34,34	0
88	OHX	5	4241	7/7	0.17	1.52	258,258,258,258	0
87	MG	5	3690	1/1	0.16	1.51	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	2	2079	7/7	0.18	1.51	194,194,194,194	0
88	OHX	4	233	7/7	0.18	1.51	275,275,275,275	0
87	MG	1	3442	1/1	0.19	1.51	33,33,33,33	0
88	OHX	5	3912	7/7	0.17	1.49	64,64,64,64	0
88	OHX	2	2113	7/7	0.20	1.49	194,194,194,194	0
88	OHX	6	2140	7/7	0.19	1.49	205,205,205,205	0
88	OHX	1	4117	7/7	0.19	1.49	213,213,213,213	0
87	MG	6	1923	1/1	0.22	1.48	39,39,39,39	0
88	OHX	1	4048	7/7	0.20	1.45	216,216,216,216	0
87	MG	5	3807	1/1	0.14	1.45	35,35,35,35	0
88	OHX	6	2186	7/7	0.28	1.44	295,295,295,295	0
87	MG	1	3642	1/1	0.18	1.43	42,42,42,42	0
88	OHX	5	4168	7/7	0.16	1.41	229,229,229,229	0
87	MG	1	3596	1/1	0.16	1.41	25,25,25,25	0
88	OHX	2	2135	7/7	0.20	1.40	215,215,215,215	0
87	MG	1	3813	1/1	0.17	1.39	23,23,23,23	0
87	MG	5	3631	1/1	0.19	1.39	45,45,45,45	0
88	OHX	6	2157	7/7	0.18	1.39	197,197,197,197	0
88	OHX	5	4115	7/7	0.20	1.38	204,204,204,204	0
88	OHX	6	2130	7/7	0.17	1.38	179,179,179,179	0
87	MG	5	3608	1/1	0.23	1.38	21,21,21,21	0
87	MG	8	210	1/1	0.18	1.37	12,12,12,12	0
87	MG	1	3758	1/1	0.17	1.36	36,36,36,36	0
87	MG	6	1976	1/1	0.20	1.35	28,28,28,28	0
88	OHX	1	3879	7/7	0.15	1.35	59,59,59,59	0
88	OHX	1	4181	7/7	0.17	1.34	252,252,252,252	0
87	MG	S4	301	1/1	0.18	1.33	41,41,41,41	0
87	MG	M7	203	1/1	0.19	1.33	16,16,16,16	0
87	MG	6	1981	1/1	0.19	1.33	29,29,29,29	0
88	OHX	2	2103	7/7	0.15	1.33	215,215,215,215	0
88	OHX	5	4153	7/7	0.19	1.33	217,217,217,217	0
87	MG	2	1944	1/1	0.24	1.33	49,49,49,49	0
88	OHX	1	4107	7/7	0.16	1.32	228,228,228,228	0
87	MG	2	2022	1/1	0.22	1.32	69,69,69,69	0
87	MG	6	1977	1/1	0.20	1.32	17,17,17,17	0
88	OHX	2	2099	7/7	0.17	1.31	208,208,208,208	0
88	OHX	2	2086	7/7	0.17	1.31	207,207,207,207	0
87	MG	6	2019	1/1	0.20	1.30	39,39,39,39	0
88	OHX	1	4131	7/7	0.21	1.30	227,227,227,227	0
87	MG	2	1998	1/1	0.18	1.29	40,40,40,40	0
88	OHX	1	4178	7/7	0.22	1.29	276,276,276,276	0
87	MG	1	3630	1/1	0.18	1.28	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	3915	7/7	0.13	1.28	58,58,58,58	0
88	OHX	5	4042	7/7	0.19	1.27	135,135,135,135	0
88	OHX	1	3996	7/7	0.17	1.26	143,143,143,143	0
88	OHX	1	4214	7/7	0.18	1.26	241,241,241,241	0
87	MG	5	3450	1/1	0.17	1.24	31,31,31,31	0
88	OHX	6	2173	7/7	0.21	1.24	193,193,193,193	0
87	MG	1	3584	1/1	0.25	1.24	29,29,29,29	0
88	OHX	2	2025	7/7	0.19	1.22	82,82,82,82	0
88	OHX	1	4079	7/7	0.20	1.22	183,183,183,183	0
87	MG	1	3773	1/1	0.21	1.22	35,35,35,35	0
87	MG	1	3486	1/1	0.20	1.22	37,37,37,37	0
88	OHX	1	4208	7/7	0.27	1.20	288,288,288,288	0
87	MG	4	214	1/1	0.23	1.20	46,46,46,46	0
88	OHX	1	4222	7/7	0.25	1.20	268,268,268,268	0
88	OHX	1	4199	7/7	0.20	1.20	242,242,242,242	0
87	MG	5	3872	1/1	0.29	1.19	29,29,29,29	0
88	OHX	5	4205	7/7	0.22	1.19	185,185,185,185	0
87	MG	1	3825	1/1	0.16	1.19	32,32,32,32	0
88	OHX	1	3883	7/7	0.16	1.18	62,62,62,62	0
88	OHX	1	4121	7/7	0.14	1.16	190,190,190,190	0
88	OHX	5	4112	7/7	0.21	1.15	225,225,225,225	0
88	OHX	5	3929	7/7	0.18	1.15	77,77,77,77	0
88	OHX	2	2148	7/7	0.18	1.14	225,225,225,225	0
87	MG	q0	202	1/1	0.21	1.13	38,38,38,38	0
88	OHX	1	3908	7/7	0.18	1.13	83,83,83,83	0
88	OHX	1	4187	7/7	0.25	1.12	250,250,250,250	0
88	OHX	2	2152	7/7	0.20	1.11	239,239,239,239	0
88	OHX	6	2170	7/7	0.21	1.11	255,255,255,255	0
88	OHX	5	4235	7/7	0.22	1.11	249,249,249,249	0
88	OHX	5	4055	7/7	0.15	1.10	151,151,151,151	0
87	MG	5	3850	1/1	0.33	1.09	50,50,50,50	0
87	MG	5	3823	1/1	0.17	1.07	28,28,28,28	0
87	MG	1	3523	1/1	0.18	1.07	45,45,45,45	0
88	OHX	5	4176	7/7	0.21	1.07	250,250,250,250	0
88	OHX	1	4147	7/7	0.20	1.07	166,166,166,166	0
87	MG	1	3497	1/1	0.19	1.07	41,41,41,41	0
87	MG	5	3747	1/1	0.15	1.06	29,29,29,29	0
88	OHX	1	3905	7/7	0.18	1.06	84,84,84,84	0
88	OHX	5	4109	7/7	0.20	1.05	167,167,167,167	0
88	OHX	5	4167	7/7	0.16	1.05	189,189,189,189	0
87	MG	6	2001	1/1	0.20	1.04	54,54,54,54	0
88	OHX	4	232	7/7	0.18	1.04	249,249,249,249	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	5	4149	7/7	0.21	1.03	210,210,210,210	0
88	OHX	5	4203	7/7	0.19	1.02	143,143,143,143	0
88	OHX	1	4110	7/7	0.19	1.02	233,233,233,233	0
88	OHX	6	2129	7/7	0.18	1.01	191,191,191,191	0
88	OHX	5	3946	7/7	0.16	1.01	88,88,88,88	0
87	MG	5	3409	1/1	0.19	1.01	32,32,32,32	0
88	OHX	5	4124	7/7	0.18	1.01	185,185,185,185	0
88	OHX	2	2142	7/7	0.18	1.01	172,172,172,172	0
88	OHX	5	4258	7/7	0.24	1.00	245,245,245,245	0
88	OHX	1	4025	7/7	0.17	1.00	160,160,160,160	0
88	OHX	5	4118	7/7	0.20	0.98	193,193,193,193	0
88	OHX	1	4168	7/7	0.20	0.95	257,257,257,257	0
87	MG	5	3444	1/1	0.16	0.94	7,7,7,7	0
88	OHX	5	4091	7/7	0.19	0.93	188,188,188,188	0
87	MG	1	3810	1/1	0.31	0.93	52,52,52,52	0
88	OHX	5	4194	7/7	0.24	0.92	227,227,227,227	0
88	OHX	N9	101	7/7	0.15	0.92	67,67,67,67	0
87	MG	M1	201	1/1	0.19	0.91	64,64,64,64	0
88	OHX	5	4210	7/7	0.32	0.90	304,304,304,304	0
87	MG	n8	203	1/1	0.18	0.90	23,23,23,23	0
88	OHX	6	2109	7/7	0.17	0.89	166,166,166,166	0
88	OHX	6	2185	7/7	0.16	0.88	244,244,244,244	0
87	MG	1	3684	1/1	0.23	0.88	27,27,27,27	0
87	MG	1	3683	1/1	0.15	0.87	21,21,21,21	0
88	OHX	1	4095	7/7	0.17	0.87	207,207,207,207	0
88	OHX	1	3915	7/7	0.18	0.86	98,98,98,98	0
87	MG	n6	201	1/1	0.24	0.86	25,25,25,25	0
87	MG	6	2005	1/1	0.15	0.86	41,41,41,41	0
87	MG	5	3840	1/1	0.17	0.86	12,12,12,12	0
87	MG	8	212	1/1	0.20	0.85	65,65,65,65	0
88	OHX	6	2175	7/7	0.25	0.84	241,241,241,241	0
88	OHX	1	4151	7/7	0.18	0.84	259,259,259,259	0
88	OHX	D9	102	7/7	0.19	0.84	234,234,234,234	0
88	OHX	1	3891	7/7	0.16	0.84	71,71,71,71	0
87	MG	5	3675	1/1	0.19	0.84	15,15,15,15	0
87	MG	1	3436	1/1	0.16	0.83	33,33,33,33	0
87	MG	1	3762	1/1	0.23	0.83	28,28,28,28	0
88	OHX	1	4115	7/7	0.15	0.81	215,215,215,215	0
87	MG	5	3435	1/1	0.16	0.81	62,62,62,62	0
88	OHX	5	4071	7/7	0.17	0.80	151,151,151,151	0
88	OHX	6	2132	7/7	0.18	0.79	196,196,196,196	0
87	MG	5	3573	1/1	0.21	0.79	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	4030	7/7	0.17	0.78	142,142,142,142	0
87	MG	6	2024	1/1	0.17	0.78	40,40,40,40	0
88	OHX	1	4145	7/7	0.19	0.78	256,256,256,256	0
88	OHX	1	4010	7/7	0.15	0.77	161,161,161,161	0
87	MG	2	1953	1/1	0.22	0.77	70,70,70,70	0
87	MG	5	3648	1/1	0.19	0.77	58,58,58,58	0
88	OHX	1	3929	7/7	0.17	0.76	117,117,117,117	0
87	MG	5	3834	1/1	0.17	0.76	37,37,37,37	0
88	OHX	5	4148	7/7	0.15	0.75	208,208,208,208	0
87	MG	2	1992	1/1	0.28	0.75	53,53,53,53	0
87	MG	2	1920	1/1	0.22	0.74	23,23,23,23	0
88	OHX	6	2152	7/7	0.23	0.73	257,257,257,257	0
88	OHX	1	4150	7/7	0.16	0.73	205,205,205,205	0
88	OHX	5	4066	7/7	0.18	0.73	178,178,178,178	0
87	MG	5	3637	1/1	0.19	0.71	36,36,36,36	0
88	OHX	1	4135	7/7	0.17	0.71	232,232,232,232	0
88	OHX	1	4039	7/7	0.15	0.71	226,226,226,226	0
87	MG	5	3676	1/1	0.13	0.71	38,38,38,38	0
87	MG	1	3560	1/1	0.15	0.71	55,55,55,55	0
87	MG	1	3453	1/1	0.16	0.70	22,22,22,22	0
88	OHX	1	4091	7/7	0.13	0.70	167,167,167,167	0
87	MG	1	3828	1/1	0.19	0.69	40,40,40,40	0
88	OHX	1	4136	7/7	0.17	0.69	209,209,209,209	0
87	MG	6	2027	1/1	0.18	0.69	45,45,45,45	0
88	OHX	5	4217	7/7	0.20	0.69	217,217,217,217	0
88	OHX	1	4170	7/7	0.18	0.68	188,188,188,188	0
88	OHX	2	2134	7/7	0.18	0.68	213,213,213,213	0
87	MG	2	1961	1/1	0.21	0.68	38,38,38,38	0
87	MG	m6	201	1/1	0.21	0.67	36,36,36,36	0
88	OHX	2	2105	7/7	0.17	0.66	193,193,193,193	0
88	OHX	5	4035	7/7	0.16	0.65	139,139,139,139	0
88	OHX	5	4113	7/7	0.17	0.64	242,242,242,242	0
87	MG	s8	301	1/1	0.26	0.63	38,38,38,38	0
87	MG	1	3741	1/1	0.16	0.63	53,53,53,53	0
88	OHX	6	2128	7/7	0.20	0.63	183,183,183,183	0
88	OHX	1	4174	7/7	0.24	0.62	279,279,279,279	0
88	OHX	6	2108	7/7	0.16	0.62	158,158,158,158	0
87	MG	5	3797	1/1	0.18	0.62	41,41,41,41	0
88	OHX	6	2118	7/7	0.14	0.61	181,181,181,181	0
87	MG	5	3758	1/1	0.23	0.61	55,55,55,55	0
88	OHX	5	4147	7/7	0.18	0.61	225,225,225,225	0
88	OHX	2	2117	7/7	0.19	0.61	205,205,205,205	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	2	2139	7/7	0.20	0.61	238,238,238,238	0
88	OHX	5	4009	7/7	0.18	0.59	141,141,141,141	0
87	MG	l5	302	1/1	0.17	0.59	49,49,49,49	0
87	MG	d4	201	1/1	0.21	0.58	43,43,43,43	0
88	OHX	5	4173	7/7	0.21	0.55	260,260,260,260	0
88	OHX	5	4154	7/7	0.23	0.55	245,245,245,245	0
87	MG	O4	201	1/1	0.21	0.55	42,42,42,42	0
88	OHX	5	4119	7/7	0.15	0.53	167,167,167,167	0
88	OHX	6	2050	7/7	0.15	0.52	70,70,70,70	0
87	MG	2	1988	1/1	0.19	0.51	60,60,60,60	0
88	OHX	1	3906	7/7	0.14	0.51	81,81,81,81	0
87	MG	1	3496	1/1	0.16	0.51	33,33,33,33	0
88	OHX	1	3946	7/7	0.17	0.50	112,112,112,112	0
88	OHX	8	230	7/7	0.17	0.50	267,267,267,267	0
88	OHX	6	2146	7/7	0.17	0.49	219,219,219,219	0
88	OHX	1	3877	7/7	0.18	0.49	55,55,55,55	0
87	MG	1	3423	1/1	0.14	0.48	35,35,35,35	0
88	OHX	1	3909	7/7	0.13	0.47	97,97,97,97	0
88	OHX	6	2193	7/7	0.21	0.47	244,244,244,244	0
87	MG	5	3860	1/1	0.18	0.47	33,33,33,33	0
87	MG	1	3525	1/1	0.23	0.45	42,42,42,42	0
87	MG	1	3491	1/1	0.23	0.45	25,25,25,25	0
87	MG	6	2030	1/1	0.19	0.44	24,24,24,24	0
87	MG	1	3485	1/1	0.18	0.43	24,24,24,24	0
88	OHX	3	222	7/7	0.16	0.43	228,228,228,228	0
91	C	q2	502	20/21	0.31	0.43	84,141,144,144	0
87	MG	1	3789	1/1	0.15	0.42	50,50,50,50	0
88	OHX	2	2024	7/7	0.15	0.42	81,81,81,81	0
91	C	Q2	503	20/21	0.20	0.42	15,72,75,75	0
88	OHX	5	4198	7/7	0.17	0.42	241,241,241,241	0
88	OHX	1	4036	7/7	0.15	0.41	161,161,161,161	0
88	OHX	7	217	7/7	0.14	0.41	128,128,128,128	0
88	OHX	5	3961	7/7	0.14	0.41	109,109,109,109	0
88	OHX	1	4109	7/7	0.13	0.41	219,219,219,219	0
87	MG	5	3753	1/1	0.18	0.41	41,41,41,41	0
88	OHX	5	4171	7/7	0.14	0.41	208,208,208,208	0
88	OHX	5	4196	7/7	0.16	0.40	208,208,208,208	0
87	MG	6	2010	1/1	0.17	0.39	45,45,45,45	0
87	MG	1	3808	1/1	0.20	0.37	70,70,70,70	0
88	OHX	4	220	7/7	0.16	0.37	62,62,62,62	0
88	OHX	1	3873	7/7	0.17	0.36	43,43,43,43	0
88	OHX	8	217	7/7	0.16	0.36	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	1	4226	7/7	0.17	0.36	250,250,250,250	0
87	MG	1	3585	1/1	0.29	0.36	7,7,7,7	0
87	MG	5	3436	1/1	0.17	0.36	9,9,9,9	0
87	MG	5	3787	1/1	0.21	0.36	57,57,57,57	0
88	OHX	6	2102	7/7	0.16	0.34	166,166,166,166	0
88	OHX	1	3937	7/7	0.16	0.34	107,107,107,107	0
88	OHX	1	4164	7/7	0.16	0.33	201,201,201,201	0
87	MG	8	214	1/1	0.15	0.32	50,50,50,50	0
88	OHX	5	4045	7/7	0.16	0.31	166,166,166,166	0
88	OHX	5	4103	7/7	0.17	0.31	191,191,191,191	0
88	OHX	5	4233	7/7	0.23	0.31	270,270,270,270	0
88	OHX	2	2174	7/7	0.18	0.30	232,232,232,232	0
87	MG	1	3727	1/1	0.15	0.29	42,42,42,42	0
87	MG	L8	301	1/1	0.25	0.29	47,47,47,47	0
88	OHX	5	4032	7/7	0.17	0.29	140,140,140,140	0
91	C	Q2	502	20/21	0.23	0.29	79,136,138,139	0
88	OHX	6	2151	7/7	0.15	0.28	181,181,181,181	0
87	MG	1	3697	1/1	0.21	0.27	52,52,52,52	0
88	OHX	1	4049	7/7	0.14	0.27	174,174,174,174	0
88	OHX	6	2178	7/7	0.18	0.27	262,262,262,262	0
88	OHX	5	4121	7/7	0.22	0.26	187,187,187,187	0
87	MG	1	3784	1/1	0.12	0.25	42,42,42,42	0
88	OHX	5	3926	7/7	0.16	0.25	70,70,70,70	0
88	OHX	6	2120	7/7	0.15	0.23	148,148,148,148	0
88	OHX	1	4055	7/7	0.15	0.22	157,157,157,157	0
88	OHX	n9	101	7/7	0.15	0.21	70,70,70,70	0
87	MG	5	3817	1/1	0.20	0.21	48,48,48,48	0
90	A	1	3401	22/23	0.19	0.21	10,41,44,44	0
87	MG	1	3818	1/1	0.18	0.21	38,38,38,38	0
88	OHX	5	4062	7/7	0.14	0.21	151,151,151,151	0
87	MG	1	3690	1/1	0.15	0.20	29,29,29,29	0
88	OHX	1	3924	7/7	0.15	0.20	107,107,107,107	0
88	OHX	1	4017	7/7	0.15	0.20	152,152,152,152	0
88	OHX	2	2040	7/7	0.16	0.20	108,108,108,108	0
88	OHX	5	4161	7/7	0.16	0.20	231,231,231,231	0
88	OHX	5	4120	7/7	0.13	0.20	199,199,199,199	0
88	OHX	6	2177	7/7	0.15	0.18	227,227,227,227	0
87	MG	1	3655	1/1	0.25	0.18	56,56,56,56	0
88	OHX	1	3896	7/7	0.14	0.18	74,74,74,74	0
88	OHX	1	3888	7/7	0.15	0.18	63,63,63,63	0
88	OHX	m4	201	7/7	0.23	0.17	290,290,290,290	0
88	OHX	5	3959	7/7	0.15	0.16	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	4	203	1/1	0.23	0.16	33,33,33,33	0
87	MG	m7	205	1/1	0.22	0.15	45,45,45,45	0
88	OHX	5	3943	7/7	0.14	0.15	96,96,96,96	0
87	MG	7	211	1/1	0.15	0.15	55,55,55,55	0
88	OHX	5	4083	7/7	0.14	0.15	159,159,159,159	0
88	OHX	1	4050	7/7	0.16	0.15	140,140,140,140	0
88	OHX	1	4111	7/7	0.21	0.14	189,189,189,189	0
88	OHX	5	4088	7/7	0.16	0.13	178,178,178,178	0
88	OHX	5	3949	7/7	0.13	0.12	85,85,85,85	0
87	MG	1	3468	1/1	0.15	0.12	40,40,40,40	0
88	OHX	5	4256	7/7	0.19	0.12	254,254,254,254	0
88	OHX	2	2132	7/7	0.14	0.10	211,211,211,211	0
88	OHX	6	2052	7/7	0.15	0.09	83,83,83,83	0
88	OHX	6	2149	7/7	0.16	0.09	207,207,207,207	0
88	OHX	2	2078	7/7	0.16	0.08	189,189,189,189	0
88	OHX	5	4222	7/7	0.15	0.08	181,181,181,181	0
88	OHX	5	3996	7/7	0.15	0.08	122,122,122,122	0
91	C	q2	503	20/21	0.22	0.07	15,72,74,74	0
87	MG	8	207	1/1	0.18	0.06	41,41,41,41	0
88	OHX	2	2038	7/7	0.15	0.06	113,113,113,113	0
88	OHX	1	3941	7/7	0.15	0.06	107,107,107,107	0
88	OHX	5	4135	7/7	0.13	0.06	167,167,167,167	0
88	OHX	1	4032	7/7	0.17	0.05	163,163,163,163	0
88	OHX	6	2046	7/7	0.14	0.05	60,60,60,60	0
88	OHX	1	4137	7/7	0.17	0.05	207,207,207,207	0
87	MG	5	3605	1/1	0.15	0.04	48,48,48,48	0
88	OHX	1	3882	7/7	0.15	0.03	59,59,59,59	0
88	OHX	5	4059	7/7	0.15	0.02	158,158,158,158	0
88	OHX	3	225	7/7	0.14	0.02	271,271,271,271	0
88	OHX	5	3916	7/7	0.14	0.02	62,62,62,62	0
87	MG	5	3546	1/1	0.16	0.01	1,1,1,1	0
88	OHX	2	2091	7/7	0.14	0.00	192,192,192,192	0
87	MG	5	3561	1/1	0.15	0.00	27,27,27,27	0
88	OHX	2	2081	7/7	0.17	0.00	191,191,191,191	0
88	OHX	6	2048	7/7	0.15	0.00	70,70,70,70	0
87	MG	5	3827	1/1	0.13	0.00	5,5,5,5	0
88	OHX	6	2180	7/7	0.28	-0.00	279,279,279,279	0
88	OHX	1	3944	7/7	0.15	-0.01	125,125,125,125	0
87	MG	N8	204	1/1	0.18	-0.01	43,43,43,43	0
88	OHX	2	2093	7/7	0.18	-0.01	196,196,196,196	0
88	OHX	O3	201	7/7	0.18	-0.01	178,178,178,178	0
87	MG	5	3430	1/1	0.17	-0.01	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3804	1/1	0.16	-0.01	64,64,64,64	0
87	MG	1	3844	1/1	0.18	-0.02	7,7,7,7	0
88	OHX	5	4126	7/7	0.16	-0.02	228,228,228,228	0
88	OHX	5	3908	7/7	0.16	-0.03	64,64,64,64	0
88	OHX	6	2195	7/7	0.16	-0.04	231,231,231,231	0
87	MG	6	2021	1/1	0.18	-0.04	31,31,31,31	0
89	ZN	D7	101	1/1	0.32	-0.05	328,328,328,328	0
88	OHX	5	3978	7/7	0.15	-0.05	102,102,102,102	0
88	OHX	1	4000	7/7	0.14	-0.05	143,143,143,143	0
88	OHX	5	4106	7/7	0.16	-0.05	180,180,180,180	0
88	OHX	6	2198	7/7	0.17	-0.05	241,241,241,241	0
88	OHX	5	3972	7/7	0.13	-0.06	101,101,101,101	0
87	MG	5	3673	1/1	0.15	-0.06	25,25,25,25	0
87	MG	1	3770	1/1	0.15	-0.06	41,41,41,41	0
88	OHX	5	4110	7/7	0.15	-0.06	184,184,184,184	0
88	OHX	6	2049	7/7	0.15	-0.07	74,74,74,74	0
88	OHX	1	4002	7/7	0.15	-0.07	143,143,143,143	0
88	OHX	1	4205	7/7	0.15	-0.07	220,220,220,220	0
90	A	5	3401	22/23	0.17	-0.07	14,45,48,49	0
87	MG	m7	203	1/1	0.19	-0.08	50,50,50,50	0
88	OHX	6	2145	7/7	0.18	-0.08	176,176,176,176	0
88	OHX	5	4181	7/7	0.16	-0.08	219,219,219,219	0
88	OHX	6	2199	7/7	0.23	-0.08	255,255,255,255	0
87	MG	1	3467	1/1	0.19	-0.08	34,34,34,34	0
88	OHX	1	4069	7/7	0.15	-0.08	169,169,169,169	0
87	MG	1	3757	1/1	0.18	-0.09	41,41,41,41	0
88	OHX	6	2153	7/7	0.17	-0.09	241,241,241,241	0
88	OHX	2	2033	7/7	0.17	-0.10	109,109,109,109	0
88	OHX	1	4012	7/7	0.16	-0.10	172,172,172,172	0
88	OHX	1	4018	7/7	0.15	-0.11	162,162,162,162	0
88	OHX	5	4095	7/7	0.17	-0.11	177,177,177,177	0
87	MG	5	3681	1/1	0.18	-0.11	21,21,21,21	0
88	OHX	2	2077	7/7	0.15	-0.12	148,148,148,148	0
87	MG	5	4259	1/1	0.16	-0.12	20,20,20,20	0
88	OHX	1	4030	7/7	0.15	-0.14	164,164,164,164	0
88	OHX	1	4113	7/7	0.21	-0.14	243,243,243,243	0
88	OHX	1	4081	7/7	0.15	-0.15	187,187,187,187	0
88	OHX	5	3906	7/7	0.15	-0.15	51,51,51,51	0
88	OHX	s1	303	7/7	0.23	-0.15	259,259,259,259	0
88	OHX	1	4042	7/7	0.17	-0.16	160,160,160,160	0
88	OHX	5	4023	7/7	0.16	-0.16	177,177,177,177	0
88	OHX	1	4162	7/7	0.17	-0.16	224,224,224,224	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3745	1/1	0.17	-0.16	34,34,34,34	0
88	OHX	5	3909	7/7	0.16	-0.17	61,61,61,61	0
88	OHX	5	3947	7/7	0.12	-0.17	89,89,89,89	0
88	OHX	2	2100	7/7	0.20	-0.17	241,241,241,241	0
88	OHX	1	3956	7/7	0.14	-0.18	121,121,121,121	0
88	OHX	6	2111	7/7	0.16	-0.18	163,163,163,163	0
88	OHX	5	3992	7/7	0.14	-0.18	156,156,156,156	0
87	MG	5	3687	1/1	0.15	-0.18	37,37,37,37	0
88	OHX	8	228	7/7	0.17	-0.18	204,204,204,204	0
88	OHX	2	2085	7/7	0.15	-0.19	198,198,198,198	0
87	MG	2	2182	1/1	0.21	-0.19	86,86,86,86	0
88	OHX	1	4134	7/7	0.16	-0.19	231,231,231,231	0
87	MG	6	2014	1/1	0.19	-0.19	34,34,34,34	0
87	MG	5	3773	1/1	0.17	-0.19	71,71,71,71	0
87	MG	1	3490	1/1	0.15	-0.20	5,5,5,5	0
88	OHX	6	2133	7/7	0.22	-0.20	194,194,194,194	0
88	OHX	2	2109	7/7	0.16	-0.20	213,213,213,213	0
87	MG	6	1941	1/1	0.17	-0.21	25,25,25,25	0
87	MG	5	3864	1/1	0.14	-0.21	37,37,37,37	0
87	MG	5	3478	1/1	0.14	-0.22	39,39,39,39	0
88	OHX	5	3910	7/7	0.14	-0.23	54,54,54,54	0
88	OHX	5	4084	7/7	0.16	-0.23	150,150,150,150	0
88	OHX	5	4072	7/7	0.12	-0.23	182,182,182,182	0
88	OHX	1	4116	7/7	0.16	-0.24	209,209,209,209	0
88	OHX	M8	201	7/7	0.16	-0.24	164,164,164,164	0
88	OHX	1	3899	7/7	0.14	-0.25	73,73,73,73	0
88	OHX	6	2068	7/7	0.13	-0.25	119,119,119,119	0
88	OHX	1	3962	7/7	0.16	-0.26	130,130,130,130	0
88	OHX	5	4048	7/7	0.14	-0.26	147,147,147,147	0
87	MG	1	3429	1/1	0.23	-0.26	41,41,41,41	0
88	OHX	1	3887	7/7	0.12	-0.26	66,66,66,66	0
88	OHX	5	4248	7/7	0.31	-0.26	238,238,238,238	0
87	MG	5	3645	1/1	0.19	-0.27	30,30,30,30	0
88	OHX	6	2055	7/7	0.16	-0.28	92,92,92,92	0
88	OHX	5	3980	7/7	0.15	-0.28	114,114,114,114	0
88	OHX	5	4100	7/7	0.13	-0.28	210,210,210,210	0
88	OHX	6	2051	7/7	0.17	-0.28	79,79,79,79	0
88	OHX	1	4105	7/7	0.12	-0.28	221,221,221,221	0
88	OHX	2	2084	7/7	0.15	-0.29	208,208,208,208	0
88	OHX	n3	204	7/7	0.12	-0.29	168,168,168,168	0
87	MG	2	1977	1/1	0.17	-0.29	44,44,44,44	0
88	OHX	1	4027	7/7	0.14	-0.30	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3994	7/7	0.14	-0.30	134,134,134,134	0
87	MG	1	3573	1/1	0.15	-0.31	3,3,3,3	0
88	OHX	5	4002	7/7	0.12	-0.31	123,123,123,123	0
88	OHX	1	4201	7/7	0.18	-0.31	282,282,282,282	0
87	MG	5	3721	1/1	0.19	-0.32	37,37,37,37	0
87	MG	N3	203	1/1	0.16	-0.32	34,34,34,34	0
88	OHX	5	4125	7/7	0.14	-0.32	193,193,193,193	0
88	OHX	5	3973	7/7	0.13	-0.32	103,103,103,103	0
88	OHX	6	2062	7/7	0.13	-0.33	106,106,106,106	0
88	OHX	5	4008	7/7	0.15	-0.33	138,138,138,138	0
88	OHX	1	4175	7/7	0.17	-0.33	210,210,210,210	0
88	OHX	2	2170	7/7	0.17	-0.33	196,196,196,196	0
88	OHX	5	3995	7/7	0.13	-0.35	115,115,115,115	0
88	OHX	5	4225	7/7	0.20	-0.35	269,269,269,269	0
88	OHX	5	4247	7/7	0.15	-0.35	172,172,172,172	0
88	OHX	4	228	7/7	0.15	-0.35	188,188,188,188	0
88	OHX	2	2058	7/7	0.12	-0.35	137,137,137,137	0
87	MG	6	1991	1/1	0.16	-0.36	35,35,35,35	0
87	MG	2	1995	1/1	0.17	-0.36	38,38,38,38	0
88	OHX	2	2108	7/7	0.14	-0.36	199,199,199,199	0
88	OHX	5	4128	7/7	0.14	-0.36	206,206,206,206	0
88	OHX	1	4093	7/7	0.17	-0.36	227,227,227,227	0
87	MG	5	3426	1/1	0.16	-0.36	4,4,4,4	0
88	OHX	5	3977	7/7	0.14	-0.37	114,114,114,114	0
88	OHX	5	4123	7/7	0.15	-0.37	192,192,192,192	0
88	OHX	5	4078	7/7	0.16	-0.37	167,167,167,167	0
88	OHX	1	3928	7/7	0.15	-0.37	96,96,96,96	0
87	MG	5	3670	1/1	0.15	-0.37	12,12,12,12	0
87	MG	2	1987	1/1	0.15	-0.38	40,40,40,40	0
88	OHX	5	3905	7/7	0.16	-0.38	50,50,50,50	0
87	MG	1	3783	1/1	0.16	-0.38	15,15,15,15	0
88	OHX	5	4040	7/7	0.14	-0.39	163,163,163,163	0
88	OHX	2	2161	7/7	0.23	-0.39	312,312,312,312	0
87	MG	6	1969	1/1	0.14	-0.39	35,35,35,35	0
88	OHX	1	4060	7/7	0.13	-0.40	188,188,188,188	0
88	OHX	5	4257	7/7	0.21	-0.40	289,289,289,289	0
88	OHX	5	4251	7/7	0.15	-0.40	243,243,243,243	0
88	OHX	5	4102	7/7	0.14	-0.40	191,191,191,191	0
88	OHX	1	3894	7/7	0.14	-0.40	72,72,72,72	0
88	OHX	1	3976	7/7	0.13	-0.40	144,144,144,144	0
88	OHX	d4	202	7/7	0.18	-0.40	213,213,213,213	0
88	OHX	2	2076	7/7	0.15	-0.41	193,193,193,193	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	4049	7/7	0.16	-0.41	156,156,156,156	0
88	OHX	6	2162	7/7	0.15	-0.41	210,210,210,210	0
88	OHX	5	3903	7/7	0.14	-0.41	43,43,43,43	0
88	OHX	L3	406	7/7	0.29	-0.41	237,237,237,237	0
87	MG	7	207	1/1	0.13	-0.41	54,54,54,54	0
87	MG	5	3846	1/1	0.17	-0.41	18,18,18,18	0
88	OHX	1	4163	7/7	0.21	-0.41	255,255,255,255	0
87	MG	5	3531	1/1	0.17	-0.42	21,21,21,21	0
88	OHX	6	2139	7/7	0.14	-0.42	242,242,242,242	0
87	MG	1	3522	1/1	0.15	-0.42	21,21,21,21	0
88	OHX	6	2044	7/7	0.14	-0.42	55,55,55,55	0
87	MG	1	3775	1/1	0.15	-0.42	34,34,34,34	0
88	OHX	6	2104	7/7	0.15	-0.42	184,184,184,184	0
88	OHX	5	4039	7/7	0.14	-0.43	155,155,155,155	0
87	MG	L5	301	1/1	0.23	-0.45	32,32,32,32	0
88	OHX	1	3960	7/7	0.12	-0.45	118,118,118,118	0
87	MG	6	1988	1/1	0.14	-0.45	47,47,47,47	0
88	OHX	5	4122	7/7	0.14	-0.46	150,150,150,150	0
88	OHX	8	225	7/7	0.23	-0.46	222,222,222,222	0
88	OHX	2	2027	7/7	0.13	-0.46	81,81,81,81	0
87	MG	6	1983	1/1	0.14	-0.47	42,42,42,42	0
87	MG	2	1997	1/1	0.13	-0.47	33,33,33,33	0
87	MG	2	1947	1/1	0.13	-0.48	30,30,30,30	0
87	MG	5	3835	1/1	0.15	-0.48	60,60,60,60	0
88	OHX	2	2075	7/7	0.17	-0.48	209,209,209,209	0
87	MG	5	3457	1/1	0.16	-0.48	44,44,44,44	0
87	MG	1	3718	1/1	0.16	-0.48	27,27,27,27	0
88	OHX	5	4101	7/7	0.14	-0.49	197,197,197,197	0
88	OHX	5	3976	7/7	0.13	-0.49	110,110,110,110	0
88	OHX	7	216	7/7	0.14	-0.49	103,103,103,103	0
87	MG	2	2000	1/1	0.15	-0.49	31,31,31,31	0
88	OHX	3	223	7/7	0.14	-0.49	235,235,235,235	0
88	OHX	6	2158	7/7	0.15	-0.49	193,193,193,193	0
88	OHX	1	4119	7/7	0.15	-0.49	190,190,190,190	0
88	OHX	6	2124	7/7	0.14	-0.50	218,218,218,218	0
88	OHX	2	2110	7/7	0.14	-0.50	203,203,203,203	0
87	MG	2	1940	1/1	0.17	-0.50	39,39,39,39	0
88	OHX	1	4023	7/7	0.14	-0.50	155,155,155,155	0
87	MG	2	1989	1/1	0.23	-0.51	30,30,30,30	0
87	MG	5	3421	1/1	0.13	-0.51	34,34,34,34	0
88	OHX	1	4120	7/7	0.13	-0.51	230,230,230,230	0
87	MG	6	1995	1/1	0.16	-0.51	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3635	1/1	0.14	-0.52	48,48,48,48	0
88	OHX	5	4231	7/7	0.16	-0.53	285,285,285,285	0
88	OHX	5	4250	7/7	0.15	-0.53	233,233,233,233	0
88	OHX	6	2100	7/7	0.14	-0.53	170,170,170,170	0
87	MG	q3	503	1/1	0.24	-0.53	66,66,66,66	0
88	OHX	1	3933	7/7	0.12	-0.54	93,93,93,93	0
87	MG	1	3769	1/1	0.16	-0.55	38,38,38,38	0
88	OHX	1	4047	7/7	0.15	-0.55	143,143,143,143	0
88	OHX	5	4017	7/7	0.14	-0.55	136,136,136,136	0
88	OHX	2	2035	7/7	0.18	-0.56	111,111,111,111	0
88	OHX	1	4104	7/7	0.13	-0.56	194,194,194,194	0
88	OHX	2	2177	7/7	0.15	-0.56	275,275,275,275	0
87	MG	L3	402	1/1	0.15	-0.57	53,53,53,53	0
87	MG	n8	201	1/1	0.15	-0.57	21,21,21,21	0
87	MG	5	3754	1/1	0.16	-0.57	54,54,54,54	0
88	OHX	2	2043	7/7	0.13	-0.57	132,132,132,132	0
88	OHX	6	2105	7/7	0.17	-0.57	196,196,196,196	0
88	OHX	5	3986	7/7	0.13	-0.57	120,120,120,120	0
88	OHX	1	4114	7/7	0.15	-0.58	205,205,205,205	0
88	OHX	5	4014	7/7	0.16	-0.58	142,142,142,142	0
88	OHX	2	2064	7/7	0.14	-0.58	146,146,146,146	0
88	OHX	5	3990	7/7	0.12	-0.58	119,119,119,119	0
88	OHX	5	4179	7/7	0.16	-0.59	218,218,218,218	0
88	OHX	1	4063	7/7	0.15	-0.59	158,158,158,158	0
88	OHX	6	2056	7/7	0.13	-0.59	94,94,94,94	0
88	OHX	1	3876	7/7	0.14	-0.60	52,52,52,52	0
88	OHX	5	4038	7/7	0.13	-0.60	153,153,153,153	0
88	OHX	6	2121	7/7	0.15	-0.60	213,213,213,213	0
88	OHX	1	4171	7/7	0.15	-0.60	247,247,247,247	0
88	OHX	1	3889	7/7	0.14	-0.60	77,77,77,77	0
88	OHX	1	3945	7/7	0.14	-0.60	109,109,109,109	0
88	OHX	5	4098	7/7	0.14	-0.61	178,178,178,178	0
87	MG	5	3759	1/1	0.15	-0.61	41,41,41,41	0
88	OHX	1	4128	7/7	0.13	-0.61	222,222,222,222	0
87	MG	5	3826	1/1	0.20	-0.62	33,33,33,33	0
89	ZN	d7	101	1/1	0.25	-0.62	285,285,285,285	0
88	OHX	D3	202	7/7	0.17	-0.62	201,201,201,201	0
87	MG	5	3776	1/1	0.21	-0.62	50,50,50,50	0
88	OHX	1	3932	7/7	0.14	-0.63	102,102,102,102	0
87	MG	1	3667	1/1	0.16	-0.63	51,51,51,51	0
88	OHX	5	3968	7/7	0.11	-0.63	98,98,98,98	0
88	OHX	7	215	7/7	0.13	-0.63	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	5	3941	7/7	0.13	-0.63	81,81,81,81	0
88	OHX	6	2126	7/7	0.14	-0.63	177,177,177,177	0
88	OHX	1	3947	7/7	0.15	-0.63	115,115,115,115	0
88	OHX	5	4193	7/7	0.15	-0.64	264,264,264,264	0
88	OHX	1	4194	7/7	0.16	-0.64	293,293,293,293	0
87	MG	1	3640	1/1	0.18	-0.64	49,49,49,49	0
88	OHX	6	2103	7/7	0.15	-0.64	146,146,146,146	0
88	OHX	c1	202	7/7	0.14	-0.65	216,216,216,216	0
88	OHX	1	4077	7/7	0.15	-0.65	172,172,172,172	0
88	OHX	1	4019	7/7	0.12	-0.65	149,149,149,149	0
88	OHX	1	3912	7/7	0.14	-0.66	82,82,82,82	0
88	OHX	5	4137	7/7	0.14	-0.66	171,171,171,171	0
88	OHX	d9	102	7/7	0.14	-0.66	235,235,235,235	0
88	OHX	1	4065	7/7	0.14	-0.66	180,180,180,180	0
88	OHX	5	4057	7/7	0.15	-0.66	144,144,144,144	0
87	MG	1	3614	1/1	0.12	-0.67	30,30,30,30	0
88	OHX	5	3901	7/7	0.16	-0.67	43,43,43,43	0
88	OHX	1	3982	7/7	0.14	-0.67	155,155,155,155	0
87	MG	1	3869	1/1	0.13	-0.67	158,158,158,158	0
87	MG	5	3408	1/1	0.11	-0.67	30,30,30,30	0
88	OHX	2	2092	7/7	0.14	-0.67	206,206,206,206	0
88	OHX	2	2178	7/7	0.12	-0.68	277,277,277,277	0
87	MG	1	3416	1/1	0.12	-0.68	20,20,20,20	0
87	MG	5	3793	1/1	0.16	-0.68	17,17,17,17	0
88	OHX	5	4089	7/7	0.12	-0.68	177,177,177,177	0
88	OHX	6	2163	7/7	0.17	-0.69	239,239,239,239	0
88	OHX	4	226	7/7	0.13	-0.69	150,150,150,150	0
88	OHX	7	223	7/7	0.14	-0.70	204,204,204,204	0
88	OHX	1	3988	7/7	0.14	-0.70	130,130,130,130	0
87	MG	M9	201	1/1	0.20	-0.70	58,58,58,58	0
88	OHX	5	4064	7/7	0.14	-0.70	157,157,157,157	0
88	OHX	5	4111	7/7	0.13	-0.71	168,168,168,168	0
88	OHX	l5	304	7/7	0.13	-0.72	239,239,239,239	0
88	OHX	1	4083	7/7	0.14	-0.73	183,183,183,183	0
88	OHX	1	4087	7/7	0.12	-0.73	188,188,188,188	0
88	OHX	2	2067	7/7	0.13	-0.73	171,171,171,171	0
88	OHX	6	2081	7/7	0.13	-0.74	142,142,142,142	0
88	OHX	2	2046	7/7	0.13	-0.74	131,131,131,131	0
88	OHX	1	3948	7/7	0.12	-0.74	122,122,122,122	0
88	OHX	1	4100	7/7	0.17	-0.74	204,204,204,204	0
87	MG	1	3726	1/1	0.15	-0.74	60,60,60,60	0
87	MG	1	3738	1/1	0.14	-0.75	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
87	MG	5	3792	1/1	0.13	-0.75	40,40,40,40	0
88	OHX	2	2095	7/7	0.15	-0.75	183,183,183,183	0
88	OHX	5	4027	7/7	0.13	-0.76	132,132,132,132	0
88	OHX	7	220	7/7	0.11	-0.76	128,128,128,128	0
88	OHX	5	4131	7/7	0.12	-0.77	193,193,193,193	0
88	OHX	1	4089	7/7	0.11	-0.78	187,187,187,187	0
88	OHX	m1	203	7/7	0.17	-0.78	259,259,259,259	0
88	OHX	2	2147	7/7	0.14	-0.78	238,238,238,238	0
88	OHX	1	4101	7/7	0.15	-0.78	136,136,136,136	0
88	OHX	1	3916	7/7	0.13	-0.79	88,88,88,88	0
88	OHX	2	2130	7/7	0.16	-0.79	188,188,188,188	0
88	OHX	5	4028	7/7	0.13	-0.79	143,143,143,143	0
88	OHX	6	2082	7/7	0.14	-0.79	136,136,136,136	0
88	OHX	5	4019	7/7	0.13	-0.80	138,138,138,138	0
87	MG	1	3450	1/1	0.12	-0.80	32,32,32,32	0
87	MG	m5	304	1/1	0.15	-0.81	26,26,26,26	0
88	OHX	2	2115	7/7	0.15	-0.81	184,184,184,184	0
88	OHX	2	2055	7/7	0.13	-0.81	150,150,150,150	0
87	MG	5	3679	1/1	0.15	-0.81	38,38,38,38	0
88	OHX	1	3979	7/7	0.12	-0.81	129,129,129,129	0
87	MG	6	1997	1/1	0.15	-0.81	30,30,30,30	0
88	OHX	5	3966	7/7	0.15	-0.81	108,108,108,108	0
88	OHX	6	2115	7/7	0.13	-0.82	152,152,152,152	0
88	OHX	6	2155	7/7	0.16	-0.82	215,215,215,215	0
88	OHX	1	4051	7/7	0.11	-0.82	184,184,184,184	0
87	MG	1	3721	1/1	0.12	-0.82	51,51,51,51	0
87	MG	1	3815	1/1	0.16	-0.82	59,59,59,59	0
88	OHX	1	3985	7/7	0.15	-0.83	149,149,149,149	0
88	OHX	1	3953	7/7	0.11	-0.83	114,114,114,114	0
88	OHX	2	2149	7/7	0.12	-0.83	256,256,256,256	0
87	MG	5	3604	1/1	0.13	-0.84	19,19,19,19	0
87	MG	d6	102	1/1	0.18	-0.84	33,33,33,33	0
88	OHX	2	2129	7/7	0.19	-0.84	299,299,299,299	0
87	MG	5	3708	1/1	0.13	-0.84	44,44,44,44	0
88	OHX	2	2125	7/7	0.13	-0.85	212,212,212,212	0
88	OHX	3	218	7/7	0.09	-0.85	147,147,147,147	0
88	OHX	5	4051	7/7	0.12	-0.85	150,150,150,150	0
88	OHX	6	2125	7/7	0.12	-0.85	177,177,177,177	0
88	OHX	2	2140	7/7	0.15	-0.85	273,273,273,273	0
88	OHX	5	4114	7/7	0.15	-0.85	132,132,132,132	0
88	OHX	6	2116	7/7	0.13	-0.85	146,146,146,146	0
87	MG	1	4227	1/1	0.15	-0.86	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	4031	7/7	0.15	-0.86	125,125,125,125	0
88	OHX	5	4238	7/7	0.13	-0.87	228,228,228,228	0
88	OHX	2	2124	7/7	0.15	-0.87	213,213,213,213	0
88	OHX	O7	103	7/7	0.13	-0.87	125,125,125,125	0
87	MG	1	3427	1/1	0.13	-0.88	54,54,54,54	0
87	MG	m7	202	1/1	0.14	-0.88	14,14,14,14	0
87	MG	5	3815	1/1	0.12	-0.88	36,36,36,36	0
88	OHX	6	2127	7/7	0.13	-0.88	190,190,190,190	0
88	OHX	1	3993	7/7	0.15	-0.89	141,141,141,141	0
88	OHX	2	2026	7/7	0.13	-0.89	89,89,89,89	0
88	OHX	5	4043	7/7	0.13	-0.89	163,163,163,163	0
88	OHX	1	3995	7/7	0.14	-0.89	140,140,140,140	0
88	OHX	2	2121	7/7	0.09	-0.89	237,237,237,237	0
88	OHX	2	2032	7/7	0.13	-0.90	106,106,106,106	0
88	OHX	l9	600	7/7	0.13	-0.90	219,219,219,219	0
88	OHX	o7	502	7/7	0.10	-0.90	123,123,123,123	0
88	OHX	8	218	7/7	0.10	-0.90	135,135,135,135	0
87	MG	2	1950	1/1	0.14	-0.90	29,29,29,29	0
88	OHX	7	221	7/7	0.10	-0.91	135,135,135,135	0
88	OHX	1	3967	7/7	0.13	-0.91	124,124,124,124	0
88	OHX	l3	406	7/7	0.17	-0.92	200,200,200,200	0
88	OHX	2	2123	7/7	0.12	-0.92	212,212,212,212	0
88	OHX	m0	302	7/7	0.13	-0.92	232,232,232,232	0
88	OHX	1	3954	7/7	0.11	-0.92	112,112,112,112	0
88	OHX	2	2180	7/7	0.15	-0.92	300,300,300,300	0
88	OHX	7	222	7/7	0.11	-0.92	170,170,170,170	0
88	OHX	6	2078	7/7	0.13	-0.93	116,116,116,116	0
88	OHX	2	2069	7/7	0.12	-0.94	154,154,154,154	0
88	OHX	5	4093	7/7	0.13	-0.94	154,154,154,154	0
88	OHX	2	2114	7/7	0.13	-0.94	208,208,208,208	0
87	MG	2	2181	1/1	0.13	-0.94	58,58,58,58	0
87	MG	1	3626	1/1	0.15	-0.94	27,27,27,27	0
87	MG	5	3774	1/1	0.22	-0.95	56,56,56,56	0
88	OHX	1	4224	7/7	0.12	-0.95	281,281,281,281	0
88	OHX	6	2072	7/7	0.12	-0.96	108,108,108,108	0
88	OHX	q2	504	7/7	0.13	-0.97	138,138,138,138	0
87	MG	1	3720	1/1	0.11	-0.98	21,21,21,21	0
88	OHX	1	4037	7/7	0.12	-0.98	161,161,161,161	0
89	ZN	Q0	500	1/1	0.12	-0.99	44,44,44,44	0
87	MG	c9	201	1/1	0.17	-0.99	44,44,44,44	0
87	MG	5	3725	1/1	0.13	-1.00	37,37,37,37	0
87	MG	sM	401	1/1	0.16	-1.00	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	6	2065	7/7	0.12	-1.01	104,104,104,104	0
88	OHX	2	2057	7/7	0.11	-1.02	171,171,171,171	0
88	OHX	5	4133	7/7	0.14	-1.02	196,196,196,196	0
88	OHX	2	2141	7/7	0.13	-1.02	222,222,222,222	0
88	OHX	1	3950	7/7	0.13	-1.02	111,111,111,111	0
88	OHX	1	3895	7/7	0.15	-1.02	76,76,76,76	0
88	OHX	5	4144	7/7	0.10	-1.04	222,222,222,222	0
87	MG	l5	301	1/1	0.11	-1.04	56,56,56,56	0
88	OHX	5	3988	7/7	0.12	-1.04	123,123,123,123	0
88	OHX	2	2138	7/7	0.13	-1.04	203,203,203,203	0
88	OHX	1	4043	7/7	0.14	-1.04	170,170,170,170	0
88	OHX	1	4016	7/7	0.12	-1.04	175,175,175,175	0
88	OHX	1	4092	7/7	0.14	-1.05	205,205,205,205	0
87	MG	1	3421	1/1	0.17	-1.05	43,43,43,43	0
88	OHX	1	4045	7/7	0.14	-1.05	157,157,157,157	0
88	OHX	1	4024	7/7	0.12	-1.06	166,166,166,166	0
88	OHX	5	4004	7/7	0.12	-1.06	129,129,129,129	0
87	MG	5	3705	1/1	0.13	-1.06	50,50,50,50	0
88	OHX	6	2083	7/7	0.13	-1.06	118,118,118,118	0
87	MG	D3	201	1/1	0.11	-1.06	36,36,36,36	0
88	OHX	6	2061	7/7	0.13	-1.06	110,110,110,110	0
87	MG	1	3598	1/1	0.12	-1.06	15,15,15,15	0
88	OHX	6	2191	7/7	0.12	-1.07	282,282,282,282	0
88	OHX	2	2030	7/7	0.14	-1.07	97,97,97,97	0
88	OHX	c8	202	7/7	0.11	-1.07	186,186,186,186	0
88	OHX	2	2089	7/7	0.09	-1.07	168,168,168,168	0
88	OHX	1	3927	7/7	0.11	-1.07	95,95,95,95	0
88	OHX	6	2053	7/7	0.13	-1.08	73,73,73,73	0
87	MG	n0	201	1/1	0.10	-1.08	48,48,48,48	0
88	OHX	2	2122	7/7	0.11	-1.09	222,222,222,222	0
88	OHX	5	3969	7/7	0.12	-1.09	102,102,102,102	0
88	OHX	1	4167	7/7	0.14	-1.09	221,221,221,221	0
88	OHX	1	4144	7/7	0.16	-1.09	273,273,273,273	0
88	OHX	1	4158	7/7	0.10	-1.09	257,257,257,257	0
87	MG	5	3727	1/1	0.12	-1.10	18,18,18,18	0
88	OHX	1	4031	7/7	0.14	-1.10	176,176,176,176	0
87	MG	6	1940	1/1	0.13	-1.11	17,17,17,17	0
88	OHX	2	2096	7/7	0.12	-1.11	185,185,185,185	0
88	OHX	5	3987	7/7	0.13	-1.12	113,113,113,113	0
88	OHX	1	4096	7/7	0.12	-1.12	191,191,191,191	0
88	OHX	6	2172	7/7	0.13	-1.13	240,240,240,240	0
88	OHX	5	4116	7/7	0.14	-1.13	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3406	1/1	0.24	-1.13	38,38,38,38	0
88	OHX	2	2150	7/7	0.16	-1.13	273,273,273,273	0
88	OHX	5	4195	7/7	0.15	-1.14	230,230,230,230	0
88	OHX	5	3913	7/7	0.13	-1.14	64,64,64,64	0
88	OHX	1	3931	7/7	0.10	-1.15	96,96,96,96	0
87	MG	1	3716	1/1	0.17	-1.15	41,41,41,41	0
88	OHX	1	4011	7/7	0.14	-1.15	126,126,126,126	0
88	OHX	5	4105	7/7	0.17	-1.15	188,188,188,188	0
88	OHX	6	2190	7/7	0.12	-1.15	304,304,304,304	0
87	MG	5	3731	1/1	0.12	-1.16	37,37,37,37	0
87	MG	5	3822	1/1	0.14	-1.16	58,58,58,58	0
88	OHX	6	2110	7/7	0.12	-1.16	134,134,134,134	0
89	ZN	d9	101	1/1	0.11	-1.17	61,61,61,61	0
88	OHX	1	4014	7/7	0.12	-1.17	166,166,166,166	0
88	OHX	1	3875	7/7	0.13	-1.17	45,45,45,45	0
89	ZN	q3	501	1/1	0.08	-1.17	65,65,65,65	0
88	OHX	5	4214	7/7	0.13	-1.17	281,281,281,281	0
88	OHX	1	3968	7/7	0.13	-1.18	110,110,110,110	0
88	OHX	L4	402	7/7	0.15	-1.18	252,252,252,252	0
88	OHX	1	3942	7/7	0.09	-1.19	107,107,107,107	0
88	OHX	1	3977	7/7	0.13	-1.19	133,133,133,133	0
88	OHX	5	4159	7/7	0.13	-1.19	178,178,178,178	0
88	OHX	6	2200	7/7	0.15	-1.20	237,237,237,237	0
88	OHX	5	3904	7/7	0.13	-1.20	50,50,50,50	0
88	OHX	5	3963	7/7	0.12	-1.20	94,94,94,94	0
87	MG	2	1999	1/1	0.11	-1.20	85,85,85,85	0
89	ZN	D9	101	1/1	0.10	-1.20	66,66,66,66	0
87	MG	1	3426	1/1	0.14	-1.20	14,14,14,14	0
88	OHX	6	2141	7/7	0.12	-1.21	181,181,181,181	0
88	OHX	2	2036	7/7	0.11	-1.21	105,105,105,105	0
88	OHX	1	4141	7/7	0.10	-1.21	229,229,229,229	0
87	MG	5	3785	1/1	0.14	-1.21	36,36,36,36	0
88	OHX	1	4044	7/7	0.12	-1.21	148,148,148,148	0
87	MG	1	3817	1/1	0.14	-1.21	37,37,37,37	0
88	OHX	1	4035	7/7	0.09	-1.22	189,189,189,189	0
88	OHX	2	2107	7/7	0.11	-1.22	174,174,174,174	0
88	OHX	6	2066	7/7	0.12	-1.23	111,111,111,111	0
88	OHX	5	4140	7/7	0.12	-1.23	179,179,179,179	0
88	OHX	2	2106	7/7	0.14	-1.23	196,196,196,196	0
88	OHX	1	3925	7/7	0.12	-1.24	102,102,102,102	0
88	OHX	5	3982	7/7	0.14	-1.24	105,105,105,105	0
88	OHX	14	403	7/7	0.12	-1.24	317,317,317,317	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	8	219	7/7	0.14	-1.24	128,128,128,128	0
87	MG	2	1971	1/1	0.14	-1.24	26,26,26,26	0
88	OHX	4	224	7/7	0.07	-1.24	166,166,166,166	0
88	OHX	1	3981	7/7	0.12	-1.25	166,166,166,166	0
88	OHX	3	216	7/7	0.13	-1.25	148,148,148,148	0
88	OHX	2	2056	7/7	0.12	-1.25	149,149,149,149	0
88	OHX	1	4129	7/7	0.13	-1.25	194,194,194,194	0
88	OHX	5	4187	7/7	0.17	-1.25	237,237,237,237	0
88	OHX	2	2101	7/7	0.11	-1.25	199,199,199,199	0
88	OHX	2	2042	7/7	0.13	-1.26	108,108,108,108	0
88	OHX	1	3990	7/7	0.11	-1.26	132,132,132,132	0
88	OHX	1	4056	7/7	0.13	-1.26	175,175,175,175	0
87	MG	2	1994	1/1	0.14	-1.26	51,51,51,51	0
88	OHX	5	3936	7/7	0.12	-1.27	82,82,82,82	0
88	OHX	2	2165	7/7	0.14	-1.27	306,306,306,306	0
88	OHX	2	2023	7/7	0.13	-1.27	75,75,75,75	0
88	OHX	5	4052	7/7	0.14	-1.27	155,155,155,155	0
88	OHX	1	3898	7/7	0.13	-1.28	74,74,74,74	0
88	OHX	2	2049	7/7	0.13	-1.28	135,135,135,135	0
88	OHX	1	3959	7/7	0.12	-1.28	132,132,132,132	0
87	MG	5	3829	1/1	0.14	-1.28	33,33,33,33	0
88	OHX	5	3933	7/7	0.14	-1.28	71,71,71,71	0
88	OHX	m0	301	7/7	0.12	-1.28	148,148,148,148	0
88	OHX	8	223	7/7	0.11	-1.28	162,162,162,162	0
88	OHX	L3	405	7/7	0.12	-1.29	157,157,157,157	0
88	OHX	6	2136	7/7	0.12	-1.29	206,206,206,206	0
88	OHX	1	4197	7/7	0.14	-1.30	233,233,233,233	0
88	OHX	5	4005	7/7	0.14	-1.30	114,114,114,114	0
88	OHX	1	4106	7/7	0.12	-1.30	179,179,179,179	0
87	MG	M0	302	1/1	0.17	-1.31	24,24,24,24	0
87	MG	6	1971	1/1	0.14	-1.31	22,22,22,22	0
88	OHX	1	3987	7/7	0.14	-1.32	149,149,149,149	0
88	OHX	6	2166	7/7	0.13	-1.32	235,235,235,235	0
87	MG	5	3716	1/1	0.08	-1.33	67,67,67,67	0
88	OHX	2	2126	7/7	0.14	-1.34	205,205,205,205	0
88	OHX	5	4230	7/7	0.13	-1.35	270,270,270,270	0
87	MG	1	3444	1/1	0.11	-1.35	42,42,42,42	0
88	OHX	5	3935	7/7	0.13	-1.36	83,83,83,83	0
88	OHX	c3	201	7/7	0.16	-1.36	248,248,248,248	0
88	OHX	1	3966	7/7	0.11	-1.36	108,108,108,108	0
88	OHX	6	2091	7/7	0.09	-1.36	139,139,139,139	0
87	MG	8	206	1/1	0.13	-1.37	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	6	1966	1/1	0.14	-1.38	39,39,39,39	0
88	OHX	5	3902	7/7	0.14	-1.38	41,41,41,41	0
88	OHX	2	2051	7/7	0.11	-1.39	123,123,123,123	0
88	OHX	1	3958	7/7	0.11	-1.39	127,127,127,127	0
88	OHX	6	2106	7/7	0.10	-1.39	158,158,158,158	0
88	OHX	6	2160	7/7	0.16	-1.40	233,233,233,233	0
88	OHX	1	3984	7/7	0.09	-1.40	136,136,136,136	0
88	OHX	1	4073	7/7	0.11	-1.40	181,181,181,181	0
87	MG	1	3703	1/1	0.12	-1.40	12,12,12,12	0
88	OHX	5	3939	7/7	0.10	-1.40	83,83,83,83	0
88	OHX	2	2060	7/7	0.12	-1.41	151,151,151,151	0
88	OHX	2	2102	7/7	0.13	-1.42	174,174,174,174	0
88	OHX	1	3957	7/7	0.12	-1.42	124,124,124,124	0
88	OHX	1	3920	7/7	0.12	-1.42	98,98,98,98	0
88	OHX	6	2064	7/7	0.10	-1.43	127,127,127,127	0
88	OHX	6	2088	7/7	0.13	-1.43	176,176,176,176	0
88	OHX	6	2169	7/7	0.14	-1.43	219,219,219,219	0
88	OHX	5	3922	7/7	0.13	-1.44	68,68,68,68	0
88	OHX	2	2072	7/7	0.10	-1.44	158,158,158,158	0
88	OHX	2	2158	7/7	0.14	-1.44	307,307,307,307	0
88	OHX	2	2034	7/7	0.12	-1.44	99,99,99,99	0
87	MG	5	3448	1/1	0.12	-1.44	29,29,29,29	0
88	OHX	5	3981	7/7	0.14	-1.45	110,110,110,110	0
88	OHX	6	2092	7/7	0.11	-1.45	166,166,166,166	0
87	MG	1	3622	1/1	0.08	-1.46	36,36,36,36	0
88	OHX	5	4061	7/7	0.12	-1.46	169,169,169,169	0
88	OHX	5	3954	7/7	0.14	-1.46	99,99,99,99	0
88	OHX	5	3983	7/7	0.13	-1.47	121,121,121,121	0
87	MG	5	3702	1/1	0.14	-1.47	32,32,32,32	0
87	MG	5	3744	1/1	0.12	-1.47	29,29,29,29	0
87	MG	6	1967	1/1	0.12	-1.47	29,29,29,29	0
88	OHX	1	3980	7/7	0.10	-1.48	118,118,118,118	0
87	MG	5	3760	1/1	0.12	-1.48	34,34,34,34	0
88	OHX	1	4041	7/7	0.12	-1.48	169,169,169,169	0
88	OHX	5	4077	7/7	0.14	-1.48	184,184,184,184	0
87	MG	6	2023	1/1	0.09	-1.49	61,61,61,61	0
88	OHX	O7	104	7/7	0.12	-1.50	126,126,126,126	0
87	MG	5	3603	1/1	0.10	-1.50	21,21,21,21	0
88	OHX	1	4195	7/7	0.16	-1.50	259,259,259,259	0
88	OHX	1	4005	7/7	0.13	-1.50	162,162,162,162	0
88	OHX	5	3918	7/7	0.12	-1.50	70,70,70,70	0
88	OHX	5	4220	7/7	0.11	-1.51	248,248,248,248	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	5	3944	7/7	0.12	-1.51	97,97,97,97	0
89	ZN	e1	501	1/1	0.10	-1.52	160,160,160,160	0
88	OHX	5	4036	7/7	0.12	-1.52	162,162,162,162	0
88	OHX	8	226	7/7	0.13	-1.52	259,259,259,259	0
88	OHX	n3	203	7/7	0.10	-1.52	92,92,92,92	0
88	OHX	1	4038	7/7	0.14	-1.53	165,165,165,165	0
87	MG	5	3852	1/1	0.17	-1.53	47,47,47,47	0
88	OHX	6	2075	7/7	0.10	-1.53	124,124,124,124	0
88	OHX	1	4161	7/7	0.14	-1.54	216,216,216,216	0
88	OHX	3	221	7/7	0.11	-1.54	180,180,180,180	0
87	MG	5	3772	1/1	0.11	-1.54	18,18,18,18	0
88	OHX	1	4004	7/7	0.11	-1.54	160,160,160,160	0
89	ZN	Q3	501	1/1	0.06	-1.54	61,61,61,61	0
87	MG	5	3871	1/1	0.11	-1.54	18,18,18,18	0
88	OHX	2	2028	7/7	0.14	-1.55	99,99,99,99	0
88	OHX	1	3921	7/7	0.12	-1.55	93,93,93,93	0
87	MG	5	3487	1/1	0.11	-1.55	28,28,28,28	0
87	MG	5	3680	1/1	0.15	-1.56	51,51,51,51	0
89	ZN	q0	201	1/1	0.12	-1.57	41,41,41,41	0
88	OHX	5	3957	7/7	0.13	-1.57	102,102,102,102	0
89	ZN	o7	501	1/1	0.11	-1.57	40,40,40,40	0
88	OHX	5	3911	7/7	0.13	-1.57	49,49,49,49	0
88	OHX	5	4107	7/7	0.11	-1.57	187,187,187,187	0
88	OHX	2	2031	7/7	0.12	-1.58	99,99,99,99	0
88	OHX	5	4108	7/7	0.14	-1.59	182,182,182,182	0
88	OHX	1	3999	7/7	0.12	-1.59	166,166,166,166	0
88	OHX	1	3878	7/7	0.13	-1.60	52,52,52,52	0
88	OHX	2	2047	7/7	0.08	-1.61	135,135,135,135	0
89	ZN	O7	101	1/1	0.09	-1.61	33,33,33,33	0
88	OHX	1	3884	7/7	0.13	-1.61	63,63,63,63	0
88	OHX	2	2166	7/7	0.12	-1.61	273,273,273,273	0
88	OHX	6	2113	7/7	0.13	-1.61	147,147,147,147	0
88	OHX	2	2111	7/7	0.14	-1.62	197,197,197,197	0
88	OHX	6	2047	7/7	0.13	-1.62	66,66,66,66	0
88	OHX	1	3893	7/7	0.12	-1.62	74,74,74,74	0
88	OHX	5	3934	7/7	0.14	-1.62	82,82,82,82	0
88	OHX	6	2054	7/7	0.11	-1.62	80,80,80,80	0
88	OHX	1	4064	7/7	0.10	-1.63	167,167,167,167	0
88	OHX	1	4007	7/7	0.14	-1.63	159,159,159,159	0
88	OHX	5	4026	7/7	0.10	-1.64	157,157,157,157	0
88	OHX	5	4199	7/7	0.14	-1.65	244,244,244,244	0
88	OHX	2	2074	7/7	0.14	-1.65	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	1	3881	7/7	0.12	-1.66	63,63,63,63	0
88	OHX	2	2059	7/7	0.13	-1.67	146,146,146,146	0
88	OHX	2	2048	7/7	0.07	-1.67	125,125,125,125	0
88	OHX	2	2061	7/7	0.11	-1.67	145,145,145,145	0
88	OHX	1	4046	7/7	0.06	-1.67	172,172,172,172	0
89	ZN	Q2	501	1/1	0.10	-1.67	305,305,305,305	0
88	OHX	1	4112	7/7	0.11	-1.67	198,198,198,198	0
88	OHX	1	4103	7/7	0.18	-1.68	204,204,204,204	0
88	OHX	o3	202	7/7	0.12	-1.68	135,135,135,135	0
88	OHX	1	4013	7/7	0.15	-1.68	138,138,138,138	0
88	OHX	4	225	7/7	0.11	-1.68	159,159,159,159	0
88	OHX	5	4129	7/7	0.12	-1.68	200,200,200,200	0
88	OHX	2	2155	7/7	0.12	-1.69	229,229,229,229	0
88	OHX	1	3917	7/7	0.11	-1.69	92,92,92,92	0
88	OHX	4	227	7/7	0.10	-1.70	186,186,186,186	0
88	OHX	3	215	7/7	0.11	-1.70	114,114,114,114	0
88	OHX	SR	401	7/7	0.10	-1.71	200,200,200,200	0
88	OHX	2	2054	7/7	0.11	-1.71	156,156,156,156	0
88	OHX	6	2119	7/7	0.11	-1.71	187,187,187,187	0
88	OHX	2	2039	7/7	0.11	-1.71	112,112,112,112	0
88	OHX	5	3928	7/7	0.12	-1.71	70,70,70,70	0
88	OHX	1	3918	7/7	0.12	-1.72	80,80,80,80	0
88	OHX	l5	303	7/7	0.09	-1.72	200,200,200,200	0
88	OHX	5	4010	7/7	0.12	-1.72	145,145,145,145	0
88	OHX	6	2137	7/7	0.10	-1.72	212,212,212,212	0
88	OHX	5	3951	7/7	0.11	-1.72	105,105,105,105	0
87	MG	M3	202	1/1	0.17	-1.73	50,50,50,50	0
88	OHX	5	3955	7/7	0.12	-1.73	107,107,107,107	0
88	OHX	6	2183	7/7	0.17	-1.73	256,256,256,256	0
88	OHX	2	2154	7/7	0.14	-1.74	244,244,244,244	0
87	MG	1	3527	1/1	0.15	-1.74	22,22,22,22	0
88	OHX	6	2147	7/7	0.14	-1.74	184,184,184,184	0
88	OHX	2	2080	7/7	0.11	-1.75	174,174,174,174	0
88	OHX	2	2082	7/7	0.09	-1.75	195,195,195,195	0
87	MG	1	3629	1/1	0.21	-1.76	45,45,45,45	0
88	OHX	1	4067	7/7	0.13	-1.76	172,172,172,172	0
88	OHX	1	3922	7/7	0.10	-1.76	99,99,99,99	0
88	OHX	2	2098	7/7	0.10	-1.76	186,186,186,186	0
88	OHX	1	4165	7/7	0.12	-1.76	204,204,204,204	0
88	OHX	2	2144	7/7	0.14	-1.76	222,222,222,222	0
88	OHX	M9	202	7/7	0.21	-1.77	285,285,285,285	0
88	OHX	2	2145	7/7	0.11	-1.77	226,226,226,226	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3720	1/1	0.14	-1.78	36,36,36,36	0
88	OHX	6	2167	7/7	0.11	-1.78	236,236,236,236	0
88	OHX	1	4006	7/7	0.09	-1.78	160,160,160,160	0
88	OHX	2	2066	7/7	0.12	-1.79	157,157,157,157	0
88	OHX	2	2151	7/7	0.12	-1.79	262,262,262,262	0
88	OHX	1	4061	7/7	0.06	-1.79	180,180,180,180	0
88	OHX	1	4053	7/7	0.09	-1.80	173,173,173,173	0
88	OHX	5	4073	7/7	0.12	-1.81	183,183,183,183	0
88	OHX	6	2148	7/7	0.13	-1.81	212,212,212,212	0
87	MG	2	1967	1/1	0.10	-1.82	50,50,50,50	0
88	OHX	6	2086	7/7	0.09	-1.82	135,135,135,135	0
87	MG	1	3435	1/1	0.12	-1.83	23,23,23,23	0
88	OHX	1	3936	7/7	0.10	-1.84	103,103,103,103	0
88	OHX	5	4134	7/7	0.10	-1.85	185,185,185,185	0
88	OHX	L3	404	7/7	0.14	-1.86	157,157,157,157	0
88	OHX	5	3945	7/7	0.12	-1.86	93,93,93,93	0
87	MG	1	3549	1/1	0.12	-1.87	44,44,44,44	0
88	OHX	2	2094	7/7	0.07	-1.87	175,175,175,175	0
88	OHX	1	3964	7/7	0.14	-1.89	114,114,114,114	0
88	OHX	6	2154	7/7	0.11	-1.90	209,209,209,209	0
88	OHX	1	3910	7/7	0.11	-1.90	79,79,79,79	0
88	OHX	1	4022	7/7	0.13	-1.91	180,180,180,180	0
88	OHX	l3	405	7/7	0.11	-1.91	146,146,146,146	0
87	MG	4	212	1/1	0.11	-1.91	36,36,36,36	0
88	OHX	5	4060	7/7	0.10	-1.91	181,181,181,181	0
88	OHX	5	4050	7/7	0.14	-1.92	151,151,151,151	0
88	OHX	1	3890	7/7	0.12	-1.94	76,76,76,76	0
88	OHX	2	2090	7/7	0.12	-1.94	170,170,170,170	0
89	ZN	q2	501	1/1	0.08	-1.95	200,200,200,200	0
87	MG	5	3766	1/1	0.13	-1.95	21,21,21,21	0
87	MG	5	3870	1/1	0.09	-1.95	28,28,28,28	0
88	OHX	5	4090	7/7	0.10	-1.95	175,175,175,175	0
88	OHX	1	4020	7/7	0.13	-1.96	173,173,173,173	0
88	OHX	1	4097	7/7	0.12	-1.97	227,227,227,227	0
88	OHX	6	2138	7/7	0.11	-1.97	187,187,187,187	0
88	OHX	1	3972	7/7	0.09	-1.97	137,137,137,137	0
88	OHX	5	3925	7/7	0.12	-1.98	67,67,67,67	0
87	MG	5	3618	1/1	0.07	-1.98	22,22,22,22	0
87	MG	5	3714	1/1	0.12	-1.98	35,35,35,35	0
88	OHX	6	2060	7/7	0.09	-1.99	88,88,88,88	0
88	OHX	6	2073	7/7	0.12	-1.99	123,123,123,123	0
88	OHX	1	4029	7/7	0.12	-1.99	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	8	222	7/7	0.12	-2.00	166,166,166,166	0
88	OHX	5	3962	7/7	0.13	-2.01	78,78,78,78	0
88	OHX	M0	303	7/7	0.14	-2.01	153,153,153,153	0
87	MG	5	3710	1/1	0.08	-2.01	27,27,27,27	0
88	OHX	1	4071	7/7	0.06	-2.01	203,203,203,203	0
88	OHX	5	4063	7/7	0.11	-2.02	178,178,178,178	0
88	OHX	6	2099	7/7	0.09	-2.02	135,135,135,135	0
89	ZN	E1	501	1/1	0.04	-2.02	102,102,102,102	0
88	OHX	6	2095	7/7	0.10	-2.03	146,146,146,146	0
88	OHX	C8	201	7/7	0.09	-2.03	116,116,116,116	0
88	OHX	sR	401	7/7	0.11	-2.03	220,220,220,220	0
88	OHX	2	2053	7/7	0.10	-2.03	147,147,147,147	0
88	OHX	2	2045	7/7	0.11	-2.03	125,125,125,125	0
87	MG	5	3704	1/1	0.14	-2.04	16,16,16,16	0
89	ZN	D6	500	1/1	0.09	-2.04	77,77,77,77	0
88	OHX	1	4034	7/7	0.09	-2.05	184,184,184,184	0
88	OHX	6	2150	7/7	0.12	-2.05	206,206,206,206	0
88	OHX	5	4022	7/7	0.12	-2.06	152,152,152,152	0
88	OHX	6	2070	7/7	0.10	-2.06	126,126,126,126	0
88	OHX	6	2192	7/7	0.14	-2.07	303,303,303,303	0
88	OHX	1	3911	7/7	0.10	-2.07	83,83,83,83	0
88	OHX	5	3940	7/7	0.11	-2.07	78,78,78,78	0
88	OHX	1	4143	7/7	0.10	-2.07	239,239,239,239	0
88	OHX	5	4003	7/7	0.10	-2.08	134,134,134,134	0
88	OHX	l3	404	7/7	0.09	-2.08	126,126,126,126	0
88	OHX	1	3935	7/7	0.12	-2.09	105,105,105,105	0
88	OHX	5	3932	7/7	0.13	-2.11	98,98,98,98	0
88	OHX	5	4000	7/7	0.10	-2.12	134,134,134,134	0
88	OHX	1	3939	7/7	0.10	-2.13	108,108,108,108	0
87	MG	5	3671	1/1	0.12	-2.13	10,10,10,10	0
87	MG	1	3837	1/1	0.11	-2.14	21,21,21,21	0
88	OHX	4	222	7/7	0.12	-2.14	121,121,121,121	0
87	MG	1	3580	1/1	0.11	-2.14	10,10,10,10	0
87	MG	3	211	1/1	0.10	-2.16	47,47,47,47	0
88	OHX	5	3914	7/7	0.13	-2.16	62,62,62,62	0
88	OHX	5	3950	7/7	0.13	-2.17	97,97,97,97	0
88	OHX	2	2063	7/7	0.12	-2.17	165,165,165,165	0
88	OHX	2	2037	7/7	0.11	-2.17	114,114,114,114	0
88	OHX	6	2164	7/7	0.11	-2.17	211,211,211,211	0
88	OHX	5	3991	7/7	0.09	-2.19	127,127,127,127	0
88	OHX	s1	302	7/7	0.12	-2.19	78,78,78,78	0
88	OHX	5	4034	7/7	0.09	-2.20	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3997	7/7	0.13	-2.22	146,146,146,146	0
88	OHX	5	3965	7/7	0.09	-2.22	100,100,100,100	0
88	OHX	5	4081	7/7	0.14	-2.23	141,141,141,141	0
87	MG	5	3706	1/1	0.09	-2.23	37,37,37,37	0
87	MG	1	4230	1/1	0.10	-2.24	14,14,14,14	0
88	OHX	1	4126	7/7	0.13	-2.25	251,251,251,251	0
88	OHX	5	4082	7/7	0.13	-2.26	194,194,194,194	0
88	OHX	1	3885	7/7	0.12	-2.26	53,53,53,53	0
88	OHX	5	3971	7/7	0.12	-2.27	97,97,97,97	0
88	OHX	5	3924	7/7	0.13	-2.28	60,60,60,60	0
88	OHX	1	3949	7/7	0.12	-2.28	111,111,111,111	0
88	OHX	1	3874	7/7	0.12	-2.28	45,45,45,45	0
87	MG	1	3567	1/1	0.13	-2.29	21,21,21,21	0
88	OHX	6	2135	7/7	0.12	-2.29	183,183,183,183	0
88	OHX	5	4243	7/7	0.17	-2.29	180,180,180,180	0
88	OHX	6	2057	7/7	0.10	-2.30	92,92,92,92	0
88	OHX	6	2076	7/7	0.10	-2.30	125,125,125,125	0
88	OHX	1	4078	7/7	0.07	-2.31	176,176,176,176	0
88	OHX	3	220	7/7	0.10	-2.31	196,196,196,196	0
88	OHX	5	4080	7/7	0.09	-2.31	165,165,165,165	0
88	OHX	5	3937	7/7	0.13	-2.31	87,87,87,87	0
88	OHX	5	4213	7/7	0.13	-2.31	215,215,215,215	0
88	OHX	1	4001	7/7	0.12	-2.32	146,146,146,146	0
88	OHX	2	2073	7/7	0.14	-2.32	169,169,169,169	0
88	OHX	5	4156	7/7	0.12	-2.32	203,203,203,203	0
87	MG	1	3481	1/1	0.07	-2.32	20,20,20,20	0
87	MG	1	3750	1/1	0.12	-2.32	32,32,32,32	0
88	OHX	5	3964	7/7	0.10	-2.33	98,98,98,98	0
88	OHX	1	3986	7/7	0.11	-2.33	155,155,155,155	0
88	OHX	2	2112	7/7	0.17	-2.33	235,235,235,235	0
87	MG	5	3623	1/1	0.13	-2.33	20,20,20,20	0
87	MG	5	3833	1/1	0.07	-2.33	45,45,45,45	0
88	OHX	5	3993	7/7	0.11	-2.33	133,133,133,133	0
88	OHX	1	3969	7/7	0.10	-2.35	120,120,120,120	0
88	OHX	5	4016	7/7	0.08	-2.35	153,153,153,153	0
88	OHX	c5	201	7/7	0.13	-2.36	215,215,215,215	0
88	OHX	5	4068	7/7	0.10	-2.36	160,160,160,160	0
88	OHX	6	2063	7/7	0.12	-2.37	100,100,100,100	0
88	OHX	5	4053	7/7	0.09	-2.39	159,159,159,159	0
88	OHX	6	2194	7/7	0.15	-2.41	263,263,263,263	0
88	OHX	1	4179	7/7	0.11	-2.42	283,283,283,283	0
88	OHX	5	3907	7/7	0.12	-2.42	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	1	3886	7/7	0.13	-2.42	65,65,65,65	0
88	OHX	5	4020	7/7	0.15	-2.43	171,171,171,171	0
87	MG	5	3791	1/1	0.10	-2.43	37,37,37,37	0
88	OHX	S8	302	7/7	0.15	-2.44	247,247,247,247	0
87	MG	1	3805	1/1	0.14	-2.45	30,30,30,30	0
88	OHX	5	4246	7/7	0.26	-2.47	318,318,318,318	0
88	OHX	2	2068	7/7	0.11	-2.48	200,200,200,200	0
88	OHX	C3	201	7/7	0.09	-2.49	238,238,238,238	0
88	OHX	m6	203	7/7	0.12	-2.50	117,117,117,117	0
88	OHX	1	3901	7/7	0.12	-2.50	75,75,75,75	0
87	MG	2	2001	1/1	0.13	-2.51	33,33,33,33	0
89	ZN	d6	101	1/1	0.08	-2.52	55,55,55,55	0
87	MG	1	3408	1/1	0.13	-2.53	17,17,17,17	0
88	OHX	5	4015	7/7	0.12	-2.53	144,144,144,144	0
88	OHX	1	4068	7/7	0.11	-2.54	205,205,205,205	0
88	OHX	5	4069	7/7	0.11	-2.54	163,163,163,163	0
88	OHX	1	4008	7/7	0.10	-2.56	168,168,168,168	0
88	OHX	6	2098	7/7	0.07	-2.57	154,154,154,154	0
88	OHX	1	4157	7/7	0.12	-2.57	213,213,213,213	0
88	OHX	2	2087	7/7	0.12	-2.57	161,161,161,161	0
88	OHX	2	2070	7/7	0.10	-2.57	155,155,155,155	0
88	OHX	2	2065	7/7	0.11	-2.57	165,165,165,165	0
88	OHX	1	4118	7/7	0.11	-2.59	179,179,179,179	0
87	MG	5	3810	1/1	0.11	-2.60	33,33,33,33	0
87	MG	s1	301	1/1	0.11	-2.60	22,22,22,22	0
88	OHX	5	4138	7/7	0.12	-2.62	180,180,180,180	0
88	OHX	s8	304	7/7	0.19	-2.62	255,255,255,255	0
88	OHX	5	4070	7/7	0.09	-2.63	166,166,166,166	0
87	MG	5	3775	1/1	0.13	-2.63	55,55,55,55	0
88	OHX	2	2097	7/7	0.10	-2.63	193,193,193,193	0
88	OHX	1	4052	7/7	0.13	-2.64	159,159,159,159	0
87	MG	1	3754	1/1	0.13	-2.66	46,46,46,46	0
88	OHX	5	4025	7/7	0.11	-2.67	139,139,139,139	0
87	MG	5	3471	1/1	0.10	-2.67	57,57,57,57	0
87	MG	1	3809	1/1	0.12	-2.67	65,65,65,65	0
87	MG	5	3630	1/1	0.11	-2.67	37,37,37,37	0
88	OHX	1	3938	7/7	0.12	-2.68	115,115,115,115	0
88	OHX	1	3975	7/7	0.11	-2.70	125,125,125,125	0
87	MG	5	3405	1/1	0.10	-2.71	17,17,17,17	0
88	OHX	6	2101	7/7	0.10	-2.71	151,151,151,151	0
88	OHX	1	3900	7/7	0.12	-2.72	78,78,78,78	0
88	OHX	1	4086	7/7	0.11	-2.72	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	5	4087	7/7	0.12	-2.74	172,172,172,172	0
88	OHX	5	3956	7/7	0.11	-2.74	95,95,95,95	0
88	OHX	2	2133	7/7	0.13	-2.75	238,238,238,238	0
88	OHX	1	3978	7/7	0.07	-2.75	139,139,139,139	0
88	OHX	5	3952	7/7	0.10	-2.75	101,101,101,101	0
88	OHX	1	3961	7/7	0.09	-2.76	112,112,112,112	0
88	OHX	5	3927	7/7	0.12	-2.76	72,72,72,72	0
88	OHX	5	4021	7/7	0.10	-2.77	126,126,126,126	0
88	OHX	5	4037	7/7	0.11	-2.77	135,135,135,135	0
88	OHX	1	3923	7/7	0.12	-2.77	97,97,97,97	0
88	OHX	5	3984	7/7	0.11	-2.79	113,113,113,113	0
88	OHX	1	3930	7/7	0.10	-2.79	95,95,95,95	0
88	OHX	5	4007	7/7	0.11	-2.82	113,113,113,113	0
88	OHX	5	3985	7/7	0.10	-2.83	96,96,96,96	0
88	OHX	6	2134	7/7	0.11	-2.83	183,183,183,183	0
88	OHX	6	2079	7/7	0.08	-2.84	112,112,112,112	0
88	OHX	1	4122	7/7	0.11	-2.84	235,235,235,235	0
88	OHX	5	4172	7/7	0.14	-2.84	236,236,236,236	0
88	OHX	1	4033	7/7	0.10	-2.85	147,147,147,147	0
88	OHX	C5	201	7/7	0.11	-2.85	254,254,254,254	0
88	OHX	1	3965	7/7	0.08	-2.88	104,104,104,104	0
88	OHX	1	4066	7/7	0.12	-2.90	195,195,195,195	0
88	OHX	1	3955	7/7	0.11	-2.91	117,117,117,117	0
88	OHX	5	4018	7/7	0.12	-2.93	143,143,143,143	0
88	OHX	5	3989	7/7	0.11	-2.95	105,105,105,105	0
88	OHX	1	4084	7/7	0.11	-2.95	231,231,231,231	0
88	OHX	2	2041	7/7	0.11	-2.95	102,102,102,102	0
88	OHX	4	221	7/7	0.11	-2.99	86,86,86,86	0
88	OHX	1	3902	7/7	0.11	-3.00	72,72,72,72	0
88	OHX	5	4249	7/7	0.12	-3.00	254,254,254,254	0
88	OHX	1	4169	7/7	0.13	-3.01	161,161,161,161	0
87	MG	5	3699	1/1	0.12	-3.02	38,38,38,38	0
87	MG	1	3814	1/1	0.20	-3.03	47,47,47,47	0
87	MG	1	3484	1/1	0.08	-3.04	0,0,0,0	0
88	OHX	1	4040	7/7	0.12	-3.04	186,186,186,186	0
88	OHX	5	4044	7/7	0.08	-3.06	143,143,143,143	0
88	OHX	2	2029	7/7	0.10	-3.06	100,100,100,100	0
88	OHX	1	3880	7/7	0.12	-3.07	52,52,52,52	0
88	OHX	m5	306	7/7	0.09	-3.07	160,160,160,160	0
88	OHX	6	2080	7/7	0.09	-3.08	122,122,122,122	0
88	OHX	5	3942	7/7	0.11	-3.08	92,92,92,92	0
88	OHX	4	223	7/7	0.08	-3.08	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	5	4011	7/7	0.12	-3.08	88,88,88,88	0
88	OHX	5	4058	7/7	0.11	-3.09	135,135,135,135	0
87	MG	1	3835	1/1	0.12	-3.09	6,6,6,6	0
88	OHX	6	2071	7/7	0.09	-3.10	133,133,133,133	0
88	OHX	1	3904	7/7	0.13	-3.10	97,97,97,97	0
87	MG	SM	301	1/1	0.10	-3.11	32,32,32,32	0
88	OHX	5	3994	7/7	0.10	-3.15	119,119,119,119	0
87	MG	5	3824	1/1	0.10	-3.17	39,39,39,39	0
87	MG	6	2002	1/1	0.12	-3.17	21,21,21,21	0
88	OHX	5	4033	7/7	0.13	-3.18	162,162,162,162	0
88	OHX	2	2167	7/7	0.12	-3.20	254,254,254,254	0
88	OHX	6	2094	7/7	0.08	-3.20	153,153,153,153	0
88	OHX	2	2083	7/7	0.09	-3.21	188,188,188,188	0
88	OHX	1	3892	7/7	0.11	-3.21	68,68,68,68	0
88	OHX	5	3920	7/7	0.12	-3.24	65,65,65,65	0
87	MG	5	3515	1/1	0.09	-3.25	12,12,12,12	0
88	OHX	5	4041	7/7	0.08	-3.25	154,154,154,154	0
88	OHX	5	4024	7/7	0.09	-3.27	134,134,134,134	0
88	OHX	1	4098	7/7	0.10	-3.28	210,210,210,210	0
87	MG	5	3764	1/1	0.09	-3.29	20,20,20,20	0
87	MG	6	2013	1/1	0.09	-3.30	25,25,25,25	0
88	OHX	5	4185	7/7	0.16	-3.31	207,207,207,207	0
88	OHX	6	2058	7/7	0.12	-3.32	86,86,86,86	0
87	MG	5	3418	1/1	0.09	-3.33	5,5,5,5	0
88	OHX	1	3971	7/7	0.11	-3.33	128,128,128,128	0
87	MG	1	3547	1/1	0.14	-3.33	8,8,8,8	0
88	OHX	5	4013	7/7	0.09	-3.34	129,129,129,129	0
88	OHX	6	2084	7/7	0.10	-3.36	129,129,129,129	0
87	MG	1	4228	1/1	0.14	-3.36	42,42,42,42	0
88	OHX	5	4001	7/7	0.09	-3.37	121,121,121,121	0
88	OHX	5	3921	7/7	0.12	-3.37	70,70,70,70	0
88	OHX	6	2142	7/7	0.12	-3.37	185,185,185,185	0
88	OHX	5	3997	7/7	0.09	-3.38	146,146,146,146	0
88	OHX	6	2067	7/7	0.11	-3.38	95,95,95,95	0
88	OHX	1	3952	7/7	0.13	-3.39	124,124,124,124	0
88	OHX	6	2112	7/7	0.13	-3.40	155,155,155,155	0
88	OHX	1	4028	7/7	0.11	-3.42	177,177,177,177	0
88	OHX	2	2050	7/7	0.11	-3.44	143,143,143,143	0
88	OHX	6	2089	7/7	0.09	-3.46	128,128,128,128	0
87	MG	5	3854	1/1	0.10	-3.47	2,2,2,2	0
88	OHX	6	2097	7/7	0.12	-3.47	153,153,153,153	0
88	OHX	1	3926	7/7	0.12	-3.48	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
88	OHX	1	3974	7/7	0.11	-3.48	89,89,89,89	0
88	OHX	1	4054	7/7	0.12	-3.50	168,168,168,168	0
88	OHX	1	3951	7/7	0.09	-3.50	111,111,111,111	0
87	MG	6	1996	1/1	0.07	-3.52	24,24,24,24	0
88	OHX	7	219	7/7	0.10	-3.56	128,128,128,128	0
87	MG	1	3679	1/1	0.07	-3.58	33,33,33,33	0
88	OHX	6	2131	7/7	0.12	-3.59	202,202,202,202	0
88	OHX	3	217	7/7	0.11	-3.60	133,133,133,133	0
87	MG	5	3751	1/1	0.11	-3.61	25,25,25,25	0
87	MG	5	3844	1/1	0.11	-3.63	44,44,44,44	0
88	OHX	1	3913	7/7	0.10	-3.64	89,89,89,89	0
87	MG	1	3746	1/1	0.10	-3.65	32,32,32,32	0
88	OHX	1	4102	7/7	0.09	-3.66	213,213,213,213	0
88	OHX	5	3960	7/7	0.11	-3.66	95,95,95,95	0
87	MG	1	3610	1/1	0.10	-3.67	54,54,54,54	0
87	MG	1	3824	1/1	0.11	-3.70	58,58,58,58	0
88	OHX	5	3953	7/7	0.14	-3.70	89,89,89,89	0
88	OHX	8	220	7/7	0.11	-3.73	152,152,152,152	0
88	OHX	5	3931	7/7	0.09	-3.76	82,82,82,82	0
87	MG	2	1979	1/1	0.10	-3.77	57,57,57,57	0
87	MG	M7	204	1/1	0.10	-3.80	15,15,15,15	0
88	OHX	5	3999	7/7	0.13	-3.80	112,112,112,112	0
88	OHX	5	3930	7/7	0.10	-3.81	81,81,81,81	0
88	OHX	2	2052	7/7	0.11	-3.81	134,134,134,134	0
88	OHX	5	3975	7/7	0.12	-3.81	91,91,91,91	0
88	OHX	1	4003	7/7	0.11	-3.84	144,144,144,144	0
88	OHX	2	2168	7/7	0.10	-3.87	198,198,198,198	0
88	OHX	1	3992	7/7	0.10	-3.88	116,116,116,116	0
87	MG	1	3447	1/1	0.07	-3.89	16,16,16,16	0
87	MG	5	3842	1/1	0.10	-3.91	37,37,37,37	0
88	OHX	5	4127	7/7	0.14	-3.94	201,201,201,201	0
87	MG	6	2011	1/1	0.08	-3.95	46,46,46,46	0
88	OHX	2	2062	7/7	0.12	-3.96	169,169,169,169	0
87	MG	5	3703	1/1	0.10	-4.01	46,46,46,46	0
88	OHX	1	3940	7/7	0.10	-4.05	94,94,94,94	0
88	OHX	7	218	7/7	0.09	-4.07	144,144,144,144	0
87	MG	5	3746	1/1	0.12	-4.08	0,0,0,0	0
87	MG	1	3664	1/1	0.15	-4.13	19,19,19,19	0
88	OHX	8	224	7/7	0.09	-4.15	178,178,178,178	0
88	OHX	5	3938	7/7	0.11	-4.25	83,83,83,83	0
88	OHX	6	2069	7/7	0.12	-4.31	107,107,107,107	0
88	OHX	5	3970	7/7	0.09	-4.32	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	1	3715	1/1	0.09	-4.34	49,49,49,49	0
88	OHX	2	2088	7/7	0.12	-4.35	184,184,184,184	0
87	MG	5	3858	1/1	0.08	-4.43	56,56,56,56	0
87	MG	1	3834	1/1	0.10	-4.44	20,20,20,20	0
88	OHX	5	4175	7/7	0.10	-4.45	243,243,243,243	0
88	OHX	5	4067	7/7	0.11	-4.45	181,181,181,181	0
88	OHX	1	3983	7/7	0.08	-4.47	140,140,140,140	0
88	OHX	5	4099	7/7	0.12	-4.50	172,172,172,172	0
88	OHX	2	2044	7/7	0.08	-4.50	121,121,121,121	0
87	MG	1	3700	1/1	0.10	-4.51	49,49,49,49	0
87	MG	1	3709	1/1	0.08	-4.56	36,36,36,36	0
88	OHX	1	3907	7/7	0.10	-4.56	78,78,78,78	0
88	OHX	1	3897	7/7	0.13	-4.64	75,75,75,75	0
87	MG	2	2003	1/1	0.15	-4.64	50,50,50,50	0
88	OHX	8	221	7/7	0.09	-4.71	157,157,157,157	0
87	MG	5	3638	1/1	0.10	-4.72	29,29,29,29	0
88	OHX	3	219	7/7	0.10	-4.73	158,158,158,158	0
87	MG	1	3731	1/1	0.07	-4.73	32,32,32,32	0
88	OHX	1	4062	7/7	0.14	-4.75	173,173,173,173	0
87	MG	1	3654	1/1	0.06	-4.75	29,29,29,29	0
87	MG	2	1964	1/1	0.06	-4.77	34,34,34,34	0
88	OHX	6	2090	7/7	0.10	-4.81	135,135,135,135	0
88	OHX	6	2087	7/7	0.09	-4.84	131,131,131,131	0
87	MG	5	3616	1/1	0.11	-4.84	19,19,19,19	0
88	OHX	1	4009	7/7	0.10	-4.87	178,178,178,178	0
88	OHX	6	2093	7/7	0.10	-4.98	132,132,132,132	0
88	OHX	1	4207	7/7	0.08	-4.99	191,191,191,191	0
88	OHX	5	3974	7/7	0.11	-5.03	99,99,99,99	0
88	OHX	1	3970	7/7	0.09	-5.03	140,140,140,140	0
87	MG	5	3433	1/1	0.10	-5.12	27,27,27,27	0
87	MG	N5	201	1/1	0.18	-5.12	49,49,49,49	0
88	OHX	2	2156	7/7	0.21	-5.15	290,290,290,290	0
88	OHX	1	3934	7/7	0.10	-5.16	92,92,92,92	0
88	OHX	5	3919	7/7	0.10	-5.20	68,68,68,68	0
87	MG	5	3729	1/1	0.05	-5.29	24,24,24,24	0
87	MG	5	3423	1/1	0.10	-5.33	25,25,25,25	0
88	OHX	1	4108	7/7	0.12	-5.43	210,210,210,210	0
88	OHX	2	2071	7/7	0.11	-5.43	168,168,168,168	0
88	OHX	1	3903	7/7	0.10	-5.48	82,82,82,82	0
88	OHX	6	2096	7/7	0.11	-5.50	164,164,164,164	0
88	OHX	6	2077	7/7	0.11	-5.54	121,121,121,121	0
88	OHX	1	4026	7/7	0.11	-5.60	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
88	OHX	5	4136	7/7	0.09	-5.61	242,242,242,242	0
88	OHX	5	4012	7/7	0.11	-5.67	122,122,122,122	0
87	MG	3	203	1/1	0.10	-5.69	55,55,55,55	0
88	OHX	1	4130	7/7	0.12	-5.73	209,209,209,209	0
88	OHX	1	4192	7/7	0.14	-5.77	270,270,270,270	0
87	MG	1	3807	1/1	0.09	-6.00	30,30,30,30	0
87	MG	1	3474	1/1	0.11	-6.01	5,5,5,5	0
88	OHX	M5	303	7/7	0.14	-6.09	146,146,146,146	0
87	MG	5	3653	1/1	0.07	-6.14	52,52,52,52	0
87	MG	5	3602	1/1	0.10	-6.17	24,24,24,24	0
87	MG	1	3747	1/1	0.08	-6.29	25,25,25,25	0
88	OHX	6	2059	7/7	0.12	-6.35	94,94,94,94	0
88	OHX	2	2118	7/7	0.07	-6.37	206,206,206,206	0
88	OHX	2	2104	7/7	0.14	-6.49	217,217,217,217	0
87	MG	5	3863	1/1	0.12	-6.50	22,22,22,22	0
88	OHX	5	3923	7/7	0.11	-6.55	63,63,63,63	0
88	OHX	1	3914	7/7	0.11	-6.76	91,91,91,91	0
88	OHX	5	4202	7/7	0.11	-7.10	220,220,220,220	0
87	MG	6	2022	1/1	0.14	-7.13	50,50,50,50	0
88	OHX	1	4021	7/7	0.12	-7.16	178,178,178,178	0
87	MG	1	3633	1/1	0.08	-7.21	32,32,32,32	0
87	MG	6	2017	1/1	0.08	-7.38	52,52,52,52	0
87	MG	5	3420	1/1	0.08	-7.63	31,31,31,31	0
87	MG	5	3784	1/1	0.12	-7.70	48,48,48,48	0
87	MG	1	3607	1/1	0.10	-8.26	15,15,15,15	0
87	MG	1	3644	1/1	0.05	-8.28	17,17,17,17	0
88	OHX	5	4182	7/7	0.10	-8.28	212,212,212,212	0
88	OHX	6	2085	7/7	0.10	-8.32	128,128,128,128	0
88	OHX	5	3967	7/7	0.10	-8.54	93,93,93,93	0
87	MG	5	3861	1/1	0.13	-8.67	53,53,53,53	0
87	MG	5	3652	1/1	0.12	-9.50	19,19,19,19	0
88	OHX	5	3948	7/7	0.09	-10.05	80,80,80,80	0
88	OHX	1	4072	7/7	0.10	-10.05	169,169,169,169	0
87	MG	4	216	1/1	0.09	-10.97	23,23,23,23	0
87	MG	1	3740	1/1	0.06	-12.57	15,15,15,15	0
87	MG	1	3774	1/1	0.09	-12.60	54,54,54,54	0
87	MG	5	3811	1/1	0.07	-14.47	48,48,48,48	0
87	MG	5	3770	1/1	0.07	-14.51	62,62,62,62	0
88	OHX	1	3998	7/7	0.11	-18.33	141,141,141,141	0
87	MG	5	3659	1/1	0.09	-21.67	29,29,29,29	0
87	MG	1	3776	1/1	0.13	-29.00	61,61,61,61	0
88	OHX	5	3979	7/7	0.09	-33.74	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
87	MG	5	3809	1/1	0.07	-50.00	70,70,70,70	0
87	MG	7	204	1/1	0.08	-75.00	46,46,46,46	0
87	MG	5	3814	1/1	0.11	-77.00	96,96,96,96	0
87	MG	6	1998	1/1	0.14	-	57,57,57,57	0
87	MG	6	1924	1/1	0.23	-	41,41,41,41	0
87	MG	6	2041	1/1	0.28	-	21,21,21,21	0
87	MG	1	3796	1/1	0.09	-	13,13,13,13	0
87	MG	2	1954	1/1	0.28	-	65,65,65,65	0
87	MG	2	2014	1/1	0.56	-	46,46,46,46	0
87	MG	5	3887	1/1	0.32	-	34,34,34,34	0
87	MG	1	3846	1/1	0.50	-	31,31,31,31	0
87	MG	1	3850	1/1	0.30	-	26,26,26,26	0
87	MG	1	3861	1/1	0.38	-	79,79,79,79	0
87	MG	2	1904	1/1	0.22	-	30,30,30,30	0
87	MG	4	218	1/1	0.39	-	36,36,36,36	0
87	MG	4	215	1/1	0.50	-	32,32,32,32	0
87	MG	5	3620	1/1	0.45	-	21,21,21,21	0
87	MG	6	2036	1/1	0.24	-	37,37,37,37	0
87	MG	7	213	1/1	0.43	-	47,47,47,47	0
87	MG	1	3866	1/1	0.41	-	34,34,34,34	0
87	MG	8	216	1/1	0.40	-	14,14,14,14	0
87	MG	1	3539	1/1	0.45	-	20,20,20,20	0
87	MG	5	3880	1/1	0.70	-	36,36,36,36	0
87	MG	1	3502	1/1	0.39	-	58,58,58,58	0
87	MG	1	3857	1/1	0.61	-	37,37,37,37	0
87	MG	5	3812	1/1	0.74	-	39,39,39,39	0
87	MG	6	1979	1/1	0.57	-	40,40,40,40	0
87	MG	5	3778	1/1	0.13	-	48,48,48,48	0
87	MG	1	3492	1/1	0.44	-	36,36,36,36	0
87	MG	1	3847	1/1	0.86	-	50,50,50,50	0
87	MG	1	3800	1/1	0.17	-	37,37,37,37	0
87	MG	5	3786	1/1	0.15	-	49,49,49,49	0
87	MG	6	2000	1/1	0.08	-	49,49,49,49	0
87	MG	5	3888	1/1	0.21	-	33,33,33,33	0
87	MG	1	3543	1/1	0.65	-	45,45,45,45	0
87	MG	5	3805	1/1	0.19	-	45,45,45,45	0
87	MG	2	1996	1/1	0.49	-	32,32,32,32	0
87	MG	1	3617	1/1	0.39	-	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.