



# wwPDB X-ray Structure Validation Summary Report

Oct 9, 2014 – 08:00 PM BST

PDB ID : 4U51  
Title : Crystal structure of Narciclasine bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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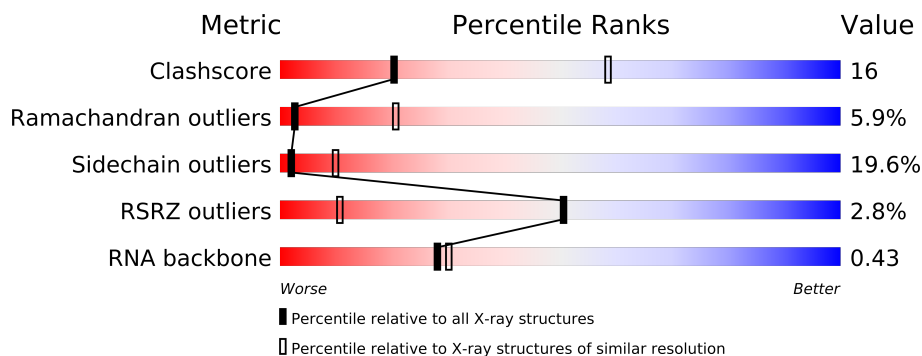
The following versions of software and data (see [references](#)) were used in the production of this report:

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))
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  $\geq 3$ , 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	
7	S5	224	
7	s5	224	

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Mol	Chain	Length	Quality of chain
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	

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Mol	Chain	Length	Quality of chain
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
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	120	
70	o4	120	
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	e0	62	
81	m2	160	
82	p0	311	
83	p1	47	
84	p2	46	

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

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3401	-	X
85	MG	1	3402	-	X
85	MG	1	3403	-	X
85	MG	1	3404	-	X
85	MG	1	3405	-	X
85	MG	1	3406	-	X
85	MG	1	3407	-	X
85	MG	1	3408	-	X
85	MG	1	3409	-	X
85	MG	1	3410	-	X
85	MG	1	3411	-	X
85	MG	1	3412	-	X
85	MG	1	3413	-	X
85	MG	1	3414	-	X
85	MG	1	3416	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3417	-	X
85	MG	1	3418	-	X
85	MG	1	3419	-	X
85	MG	1	3421	-	X
85	MG	1	3423	-	X
85	MG	1	3424	-	X
85	MG	1	3427	-	X
85	MG	1	3429	-	X
85	MG	1	3430	-	X
85	MG	1	3431	-	X
85	MG	1	3432	-	X
85	MG	1	3433	-	X
85	MG	1	3435	-	X
85	MG	1	3437	-	X
85	MG	1	3438	-	X
85	MG	1	3439	-	X
85	MG	1	3440	-	X
85	MG	1	3442	-	X
85	MG	1	3444	-	X
85	MG	1	3445	-	X
85	MG	1	3448	-	X
85	MG	1	3450	-	X
85	MG	1	3451	-	X
85	MG	1	3452	-	X
85	MG	1	3453	-	X
85	MG	1	3454	-	X
85	MG	1	3455	-	X
85	MG	1	3456	-	X
85	MG	1	3457	-	X
85	MG	1	3458	-	X
85	MG	1	3459	-	X
85	MG	1	3460	-	X
85	MG	1	3461	-	X
85	MG	1	3462	-	X
85	MG	1	3463	-	X
85	MG	1	3465	-	X
85	MG	1	3467	-	X
85	MG	1	3468	-	X
85	MG	1	3469	-	X
85	MG	1	3470	-	X
85	MG	1	3471	-	X
85	MG	1	3472	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3473	-	X
85	MG	1	3474	-	X
85	MG	1	3476	-	X
85	MG	1	3477	-	X
85	MG	1	3478	-	X
85	MG	1	3480	-	X
85	MG	1	3481	-	X
85	MG	1	3482	-	X
85	MG	1	3484	-	X
85	MG	1	3485	-	X
85	MG	1	3486	-	X
85	MG	1	3487	-	X
85	MG	1	3488	-	X
85	MG	1	3490	-	X
85	MG	1	3491	-	X
85	MG	1	3492	-	X
85	MG	1	3493	-	X
85	MG	1	3494	-	X
85	MG	1	3495	-	X
85	MG	1	3496	-	X
85	MG	1	3497	-	X
85	MG	1	3498	-	X
85	MG	1	3499	-	X
85	MG	1	3500	-	X
85	MG	1	3501	-	X
85	MG	1	3502	-	X
85	MG	1	3503	-	X
85	MG	1	3504	-	X
85	MG	1	3505	-	X
85	MG	1	3506	-	X
85	MG	1	3507	-	X
85	MG	1	3508	-	X
85	MG	1	3509	-	X
85	MG	1	3510	-	X
85	MG	1	3511	-	X
85	MG	1	3512	-	X
85	MG	1	3513	-	X
85	MG	1	3514	-	X
85	MG	1	3515	-	X
85	MG	1	3516	-	X
85	MG	1	3517	-	X
85	MG	1	3518	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3519	-	X
85	MG	1	3521	-	X
85	MG	1	3522	-	X
85	MG	1	3523	-	X
85	MG	1	3524	-	X
85	MG	1	3525	-	X
85	MG	1	3526	-	X
85	MG	1	3527	-	X
85	MG	1	3528	-	X
85	MG	1	3529	-	X
85	MG	1	3530	-	X
85	MG	1	3531	-	X
85	MG	1	3532	-	X
85	MG	1	3533	-	X
85	MG	1	3534	-	X
85	MG	1	3535	-	X
85	MG	1	3536	-	X
85	MG	1	3537	-	X
85	MG	1	3538	-	X
85	MG	1	3539	-	X
85	MG	1	3540	-	X
85	MG	1	3541	-	X
85	MG	1	3542	-	X
85	MG	1	3543	-	X
85	MG	1	3544	-	X
85	MG	1	3545	-	X
85	MG	1	3546	-	X
85	MG	1	3547	-	X
85	MG	1	3548	-	X
85	MG	1	3549	-	X
85	MG	1	3550	-	X
85	MG	1	3551	-	X
85	MG	1	3552	-	X
85	MG	1	3553	-	X
85	MG	1	3554	-	X
85	MG	1	3555	-	X
85	MG	1	3556	-	X
85	MG	1	3557	-	X
85	MG	1	3559	-	X
85	MG	1	3560	-	X
85	MG	1	3561	-	X
85	MG	1	3562	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3563	-	X
85	MG	1	3564	-	X
85	MG	1	3565	-	X
85	MG	1	3566	-	X
85	MG	1	3567	-	X
85	MG	1	3568	-	X
85	MG	1	3569	-	X
85	MG	1	3570	-	X
85	MG	1	3571	-	X
85	MG	1	3572	-	X
85	MG	1	3573	-	X
85	MG	1	3574	-	X
85	MG	1	3575	-	X
85	MG	1	3576	-	X
85	MG	1	3577	-	X
85	MG	1	3578	-	X
85	MG	1	3579	-	X
85	MG	1	3580	-	X
85	MG	1	3581	-	X
85	MG	1	3582	-	X
85	MG	1	3584	-	X
85	MG	1	3585	-	X
85	MG	1	3586	-	X
85	MG	1	3587	-	X
85	MG	1	3588	-	X
85	MG	1	3589	-	X
85	MG	1	3590	-	X
85	MG	1	3591	-	X
85	MG	1	3592	-	X
85	MG	1	3593	-	X
85	MG	1	3595	-	X
85	MG	1	3596	-	X
85	MG	1	3597	-	X
85	MG	1	3598	-	X
85	MG	1	3599	-	X
85	MG	1	3600	-	X
85	MG	1	3602	-	X
85	MG	1	3603	-	X
85	MG	1	3605	-	X
85	MG	1	3606	-	X
85	MG	1	3608	-	X
85	MG	1	3609	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3610	-	X
85	MG	1	3611	-	X
85	MG	1	3613	-	X
85	MG	1	3615	-	X
85	MG	1	3616	-	X
85	MG	1	3617	-	X
85	MG	1	3619	-	X
85	MG	1	3620	-	X
85	MG	1	3621	-	X
85	MG	1	3622	-	X
85	MG	1	3623	-	X
85	MG	1	3624	-	X
85	MG	1	3625	-	X
85	MG	1	3628	-	X
85	MG	1	3629	-	X
85	MG	1	3630	-	X
85	MG	1	3631	-	X
85	MG	1	3632	-	X
85	MG	1	3633	-	X
85	MG	1	3635	-	X
85	MG	1	3636	-	X
85	MG	1	3640	-	X
85	MG	1	3642	-	X
85	MG	1	3643	-	X
85	MG	1	3646	-	X
85	MG	1	3647	-	X
85	MG	1	3648	-	X
85	MG	1	3649	-	X
85	MG	1	3650	-	X
85	MG	1	3651	-	X
85	MG	1	3652	-	X
85	MG	1	3653	-	X
85	MG	1	3654	-	X
85	MG	1	3655	-	X
85	MG	1	3656	-	X
85	MG	1	3657	-	X
85	MG	1	3658	-	X
85	MG	1	3659	-	X
85	MG	1	3660	-	X
85	MG	1	3661	-	X
85	MG	1	3662	-	X
85	MG	1	3664	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3665	-	X
85	MG	1	3666	-	X
85	MG	1	3667	-	X
85	MG	1	3668	-	X
85	MG	1	3669	-	X
85	MG	1	3670	-	X
85	MG	1	3671	-	X
85	MG	1	3672	-	X
85	MG	1	3673	-	X
85	MG	1	3675	-	X
85	MG	1	3676	-	X
85	MG	1	3678	-	X
85	MG	1	3679	-	X
85	MG	1	3680	-	X
85	MG	1	3682	-	X
85	MG	1	3683	-	X
85	MG	1	3684	-	X
85	MG	1	3685	-	X
85	MG	1	3686	-	X
85	MG	1	3687	-	X
85	MG	1	3688	-	X
85	MG	1	3689	-	X
85	MG	1	3690	-	X
85	MG	1	3691	-	X
85	MG	1	3692	-	X
85	MG	1	3693	-	X
85	MG	1	3694	-	X
85	MG	1	3695	-	X
85	MG	1	3696	-	X
85	MG	1	3697	-	X
85	MG	1	3698	-	X
85	MG	1	3699	-	X
85	MG	1	3700	-	X
85	MG	1	3701	-	X
85	MG	1	3702	-	X
85	MG	1	3703	-	X
85	MG	1	3704	-	X
85	MG	1	3705	-	X
85	MG	1	3706	-	X
85	MG	1	3707	-	X
85	MG	1	3708	-	X
85	MG	1	3709	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3710	-	X
85	MG	1	3711	-	X
85	MG	1	3712	-	X
85	MG	1	3713	-	X
85	MG	1	3715	-	X
85	MG	1	3716	-	X
85	MG	1	3717	-	X
85	MG	1	3720	-	X
85	MG	1	3722	-	X
85	MG	1	3723	-	X
85	MG	1	3724	-	X
85	MG	1	3725	-	X
85	MG	1	3727	-	X
85	MG	1	3729	-	X
85	MG	1	3730	-	X
85	MG	1	3732	-	X
85	MG	1	3734	-	X
85	MG	1	3738	-	X
85	MG	1	3739	-	X
85	MG	1	3740	-	X
85	MG	1	3741	-	X
85	MG	1	3743	-	X
85	MG	1	3744	-	X
85	MG	1	3745	-	X
85	MG	1	3746	-	X
85	MG	1	3747	-	X
85	MG	1	3748	-	X
85	MG	1	3749	-	X
85	MG	1	3751	-	X
85	MG	1	3754	-	X
85	MG	1	3756	-	X
85	MG	1	3757	-	X
85	MG	1	3758	-	X
85	MG	1	3759	-	X
85	MG	1	3760	-	X
85	MG	1	3761	-	X
85	MG	1	3762	-	X
85	MG	1	3763	-	X
85	MG	1	3765	-	X
85	MG	1	3766	-	X
85	MG	1	3767	-	X
85	MG	1	3769	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3771	-	X
85	MG	1	3772	-	X
85	MG	1	3773	-	X
85	MG	1	3774	-	X
85	MG	1	3775	-	X
85	MG	1	3777	-	X
85	MG	1	3778	-	X
85	MG	1	3779	-	X
85	MG	1	3780	-	X
85	MG	1	3781	-	X
85	MG	1	3782	-	X
85	MG	1	3784	-	X
85	MG	1	3785	-	X
85	MG	1	3786	-	X
85	MG	1	3787	-	X
85	MG	1	3788	-	X
85	MG	1	3791	-	X
85	MG	1	3793	-	X
85	MG	1	3794	-	X
85	MG	1	3795	-	X
85	MG	1	3796	-	X
85	MG	1	3798	-	X
85	MG	1	3801	-	X
85	MG	1	3803	-	X
85	MG	1	3804	-	X
85	MG	1	3805	-	X
85	MG	1	3808	-	X
85	MG	1	3811	-	X
85	MG	1	3812	-	X
85	MG	1	3813	-	X
85	MG	1	3814	-	X
85	MG	1	3815	-	X
85	MG	1	3817	-	X
85	MG	1	3818	-	X
85	MG	1	3819	-	X
85	MG	1	3820	-	X
85	MG	1	3821	-	X
85	MG	1	3822	-	X
85	MG	1	3823	-	X
85	MG	1	3824	-	X
85	MG	1	3825	-	X
85	MG	1	3828	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3830	-	X
85	MG	1	3831	-	X
85	MG	1	3832	-	X
85	MG	1	3833	-	X
85	MG	1	3835	-	X
85	MG	1	3836	-	X
85	MG	1	3838	-	X
85	MG	1	3839	-	X
85	MG	1	3841	-	X
85	MG	1	3842	-	X
85	MG	1	3843	-	X
85	MG	1	3844	-	X
85	MG	1	3846	-	X
85	MG	1	3847	-	X
85	MG	1	3849	-	X
85	MG	1	3850	-	X
85	MG	1	3851	-	X
85	MG	1	3852	-	X
85	MG	1	3853	-	X
85	MG	1	3855	-	X
85	MG	1	3857	-	X
85	MG	1	3858	-	X
85	MG	1	3859	-	X
85	MG	1	3860	-	X
85	MG	1	3861	-	X
85	MG	1	3862	-	X
85	MG	1	3863	-	X
85	MG	1	3864	-	X
85	MG	1	4213	-	X
85	MG	1	4214	-	X
85	MG	1	4215	-	X
85	MG	1	4217	-	X
85	MG	1	4218	-	X
85	MG	1	4219	-	X
85	MG	1	4220	-	X
85	MG	2	1901	-	X
85	MG	2	1902	-	X
85	MG	2	1903	-	X
85	MG	2	1904	-	X
85	MG	2	1905	-	X
85	MG	2	1906	-	X
85	MG	2	1907	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1908	-	X
85	MG	2	1909	-	X
85	MG	2	1910	-	X
85	MG	2	1911	-	X
85	MG	2	1912	-	X
85	MG	2	1913	-	X
85	MG	2	1914	-	X
85	MG	2	1915	-	X
85	MG	2	1916	-	X
85	MG	2	1917	-	X
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1921	-	X
85	MG	2	1922	-	X
85	MG	2	1923	-	X
85	MG	2	1924	-	X
85	MG	2	1925	-	X
85	MG	2	1926	-	X
85	MG	2	1928	-	X
85	MG	2	1929	-	X
85	MG	2	1930	-	X
85	MG	2	1931	-	X
85	MG	2	1932	-	X
85	MG	2	1933	-	X
85	MG	2	1934	-	X
85	MG	2	1935	-	X
85	MG	2	1936	-	X
85	MG	2	1937	-	X
85	MG	2	1938	-	X
85	MG	2	1939	-	X
85	MG	2	1940	-	X
85	MG	2	1941	-	X
85	MG	2	1942	-	X
85	MG	2	1943	-	X
85	MG	2	1944	-	X
85	MG	2	1945	-	X
85	MG	2	1947	-	X
85	MG	2	1948	-	X
85	MG	2	1949	-	X
85	MG	2	1950	-	X
85	MG	2	1951	-	X
85	MG	2	1952	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1953	-	X
85	MG	2	1954	-	X
85	MG	2	1955	-	X
85	MG	2	1956	-	X
85	MG	2	1957	-	X
85	MG	2	1958	-	X
85	MG	2	1959	-	X
85	MG	2	1960	-	X
85	MG	2	1961	-	X
85	MG	2	1962	-	X
85	MG	2	1964	-	X
85	MG	2	1965	-	X
85	MG	2	1966	-	X
85	MG	2	1967	-	X
85	MG	2	1968	-	X
85	MG	2	1969	-	X
85	MG	2	1970	-	X
85	MG	2	1971	-	X
85	MG	2	1972	-	X
85	MG	2	1973	-	X
85	MG	2	1974	-	X
85	MG	2	1975	-	X
85	MG	2	1976	-	X
85	MG	2	1977	-	X
85	MG	2	1978	-	X
85	MG	2	1979	-	X
85	MG	2	1980	-	X
85	MG	2	1981	-	X
85	MG	2	1982	-	X
85	MG	2	1983	-	X
85	MG	2	1984	-	X
85	MG	2	1985	-	X
85	MG	2	1986	-	X
85	MG	2	1987	-	X
85	MG	2	1989	-	X
85	MG	2	1990	-	X
85	MG	2	1991	-	X
85	MG	2	1993	-	X
85	MG	2	1994	-	X
85	MG	2	1995	-	X
85	MG	2	1996	-	X
85	MG	2	2001	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	2002	-	X
85	MG	2	2003	-	X
85	MG	2	2004	-	X
85	MG	2	2006	-	X
85	MG	2	2007	-	X
85	MG	2	2008	-	X
85	MG	2	2009	-	X
85	MG	2	2010	-	X
85	MG	2	2011	-	X
85	MG	2	2012	-	X
85	MG	2	2013	-	X
85	MG	2	2014	-	X
85	MG	2	2015	-	X
85	MG	2	2016	-	X
85	MG	2	2017	-	X
85	MG	2	2018	-	X
85	MG	2	2019	-	X
85	MG	2	2020	-	X
85	MG	2	2021	-	X
85	MG	2	2022	-	X
85	MG	2	2182	-	X
85	MG	2	2184	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	206	-	X
85	MG	3	207	-	X
85	MG	3	208	-	X
85	MG	3	209	-	X
85	MG	3	210	-	X
85	MG	3	211	-	X
85	MG	3	212	-	X
85	MG	3	213	-	X
85	MG	4	201	-	X
85	MG	4	202	-	X
85	MG	4	203	-	X
85	MG	4	204	-	X
85	MG	4	205	-	X
85	MG	4	206	-	X
85	MG	4	209	-	X
85	MG	4	210	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	4	211	-	X
85	MG	4	212	-	X
85	MG	4	214	-	X
85	MG	4	215	-	X
85	MG	4	217	-	X
85	MG	4	218	-	X
85	MG	4	219	-	X
85	MG	4	220	-	X
85	MG	5	3402	-	X
85	MG	5	3403	-	X
85	MG	5	3405	-	X
85	MG	5	3406	-	X
85	MG	5	3409	-	X
85	MG	5	3410	-	X
85	MG	5	3411	-	X
85	MG	5	3412	-	X
85	MG	5	3413	-	X
85	MG	5	3414	-	X
85	MG	5	3415	-	X
85	MG	5	3416	-	X
85	MG	5	3417	-	X
85	MG	5	3418	-	X
85	MG	5	3420	-	X
85	MG	5	3421	-	X
85	MG	5	3422	-	X
85	MG	5	3424	-	X
85	MG	5	3425	-	X
85	MG	5	3427	-	X
85	MG	5	3428	-	X
85	MG	5	3429	-	X
85	MG	5	3432	-	X
85	MG	5	3434	-	X
85	MG	5	3436	-	X
85	MG	5	3437	-	X
85	MG	5	3438	-	X
85	MG	5	3439	-	X
85	MG	5	3440	-	X
85	MG	5	3441	-	X
85	MG	5	3442	-	X
85	MG	5	3443	-	X
85	MG	5	3444	-	X
85	MG	5	3445	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3446	-	X
85	MG	5	3448	-	X
85	MG	5	3449	-	X
85	MG	5	3450	-	X
85	MG	5	3451	-	X
85	MG	5	3452	-	X
85	MG	5	3453	-	X
85	MG	5	3454	-	X
85	MG	5	3455	-	X
85	MG	5	3456	-	X
85	MG	5	3457	-	X
85	MG	5	3458	-	X
85	MG	5	3459	-	X
85	MG	5	3460	-	X
85	MG	5	3461	-	X
85	MG	5	3462	-	X
85	MG	5	3463	-	X
85	MG	5	3464	-	X
85	MG	5	3465	-	X
85	MG	5	3467	-	X
85	MG	5	3468	-	X
85	MG	5	3470	-	X
85	MG	5	3471	-	X
85	MG	5	3472	-	X
85	MG	5	3473	-	X
85	MG	5	3474	-	X
85	MG	5	3475	-	X
85	MG	5	3476	-	X
85	MG	5	3477	-	X
85	MG	5	3478	-	X
85	MG	5	3479	-	X
85	MG	5	3480	-	X
85	MG	5	3481	-	X
85	MG	5	3482	-	X
85	MG	5	3483	-	X
85	MG	5	3484	-	X
85	MG	5	3486	-	X
85	MG	5	3487	-	X
85	MG	5	3488	-	X
85	MG	5	3489	-	X
85	MG	5	3490	-	X
85	MG	5	3491	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3492	-	X
85	MG	5	3493	-	X
85	MG	5	3494	-	X
85	MG	5	3495	-	X
85	MG	5	3496	-	X
85	MG	5	3497	-	X
85	MG	5	3498	-	X
85	MG	5	3499	-	X
85	MG	5	3500	-	X
85	MG	5	3501	-	X
85	MG	5	3502	-	X
85	MG	5	3503	-	X
85	MG	5	3504	-	X
85	MG	5	3505	-	X
85	MG	5	3506	-	X
85	MG	5	3507	-	X
85	MG	5	3508	-	X
85	MG	5	3509	-	X
85	MG	5	3510	-	X
85	MG	5	3511	-	X
85	MG	5	3512	-	X
85	MG	5	3514	-	X
85	MG	5	3515	-	X
85	MG	5	3516	-	X
85	MG	5	3517	-	X
85	MG	5	3518	-	X
85	MG	5	3519	-	X
85	MG	5	3520	-	X
85	MG	5	3521	-	X
85	MG	5	3522	-	X
85	MG	5	3523	-	X
85	MG	5	3524	-	X
85	MG	5	3525	-	X
85	MG	5	3526	-	X
85	MG	5	3527	-	X
85	MG	5	3528	-	X
85	MG	5	3529	-	X
85	MG	5	3530	-	X
85	MG	5	3531	-	X
85	MG	5	3532	-	X
85	MG	5	3533	-	X
85	MG	5	3534	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3535	-	X
85	MG	5	3536	-	X
85	MG	5	3537	-	X
85	MG	5	3538	-	X
85	MG	5	3539	-	X
85	MG	5	3540	-	X
85	MG	5	3541	-	X
85	MG	5	3542	-	X
85	MG	5	3543	-	X
85	MG	5	3544	-	X
85	MG	5	3545	-	X
85	MG	5	3546	-	X
85	MG	5	3547	-	X
85	MG	5	3548	-	X
85	MG	5	3549	-	X
85	MG	5	3550	-	X
85	MG	5	3551	-	X
85	MG	5	3552	-	X
85	MG	5	3553	-	X
85	MG	5	3554	-	X
85	MG	5	3555	-	X
85	MG	5	3556	-	X
85	MG	5	3557	-	X
85	MG	5	3558	-	X
85	MG	5	3559	-	X
85	MG	5	3560	-	X
85	MG	5	3561	-	X
85	MG	5	3562	-	X
85	MG	5	3563	-	X
85	MG	5	3564	-	X
85	MG	5	3565	-	X
85	MG	5	3566	-	X
85	MG	5	3568	-	X
85	MG	5	3569	-	X
85	MG	5	3570	-	X
85	MG	5	3571	-	X
85	MG	5	3572	-	X
85	MG	5	3573	-	X
85	MG	5	3574	-	X
85	MG	5	3575	-	X
85	MG	5	3576	-	X
85	MG	5	3577	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3578	-	X
85	MG	5	3579	-	X
85	MG	5	3580	-	X
85	MG	5	3581	-	X
85	MG	5	3582	-	X
85	MG	5	3583	-	X
85	MG	5	3584	-	X
85	MG	5	3585	-	X
85	MG	5	3586	-	X
85	MG	5	3587	-	X
85	MG	5	3588	-	X
85	MG	5	3589	-	X
85	MG	5	3590	-	X
85	MG	5	3591	-	X
85	MG	5	3592	-	X
85	MG	5	3593	-	X
85	MG	5	3594	-	X
85	MG	5	3595	-	X
85	MG	5	3596	-	X
85	MG	5	3597	-	X
85	MG	5	3598	-	X
85	MG	5	3599	-	X
85	MG	5	3600	-	X
85	MG	5	3602	-	X
85	MG	5	3603	-	X
85	MG	5	3605	-	X
85	MG	5	3606	-	X
85	MG	5	3608	-	X
85	MG	5	3609	-	X
85	MG	5	3610	-	X
85	MG	5	3611	-	X
85	MG	5	3612	-	X
85	MG	5	3613	-	X
85	MG	5	3614	-	X
85	MG	5	3615	-	X
85	MG	5	3617	-	X
85	MG	5	3618	-	X
85	MG	5	3622	-	X
85	MG	5	3623	-	X
85	MG	5	3624	-	X
85	MG	5	3625	-	X
85	MG	5	3626	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3627	-	X
85	MG	5	3628	-	X
85	MG	5	3629	-	X
85	MG	5	3630	-	X
85	MG	5	3631	-	X
85	MG	5	3632	-	X
85	MG	5	3633	-	X
85	MG	5	3635	-	X
85	MG	5	3636	-	X
85	MG	5	3638	-	X
85	MG	5	3639	-	X
85	MG	5	3640	-	X
85	MG	5	3641	-	X
85	MG	5	3642	-	X
85	MG	5	3643	-	X
85	MG	5	3644	-	X
85	MG	5	3645	-	X
85	MG	5	3646	-	X
85	MG	5	3648	-	X
85	MG	5	3649	-	X
85	MG	5	3650	-	X
85	MG	5	3654	-	X
85	MG	5	3655	-	X
85	MG	5	3656	-	X
85	MG	5	3658	-	X
85	MG	5	3659	-	X
85	MG	5	3660	-	X
85	MG	5	3661	-	X
85	MG	5	3662	-	X
85	MG	5	3663	-	X
85	MG	5	3664	-	X
85	MG	5	3665	-	X
85	MG	5	3666	-	X
85	MG	5	3667	-	X
85	MG	5	3668	-	X
85	MG	5	3669	-	X
85	MG	5	3670	-	X
85	MG	5	3671	-	X
85	MG	5	3672	-	X
85	MG	5	3673	-	X
85	MG	5	3674	-	X
85	MG	5	3675	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3676	-	X
85	MG	5	3680	-	X
85	MG	5	3681	-	X
85	MG	5	3682	-	X
85	MG	5	3685	-	X
85	MG	5	3686	-	X
85	MG	5	3687	-	X
85	MG	5	3690	-	X
85	MG	5	3691	-	X
85	MG	5	3692	-	X
85	MG	5	3693	-	X
85	MG	5	3694	-	X
85	MG	5	3695	-	X
85	MG	5	3696	-	X
85	MG	5	3698	-	X
85	MG	5	3704	-	X
85	MG	5	3705	-	X
85	MG	5	3707	-	X
85	MG	5	3708	-	X
85	MG	5	3709	-	X
85	MG	5	3710	-	X
85	MG	5	3711	-	X
85	MG	5	3713	-	X
85	MG	5	3714	-	X
85	MG	5	3715	-	X
85	MG	5	3716	-	X
85	MG	5	3717	-	X
85	MG	5	3718	-	X
85	MG	5	3719	-	X
85	MG	5	3720	-	X
85	MG	5	3721	-	X
85	MG	5	3722	-	X
85	MG	5	3724	-	X
85	MG	5	3725	-	X
85	MG	5	3727	-	X
85	MG	5	3728	-	X
85	MG	5	3729	-	X
85	MG	5	3730	-	X
85	MG	5	3731	-	X
85	MG	5	3732	-	X
85	MG	5	3733	-	X
85	MG	5	3734	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3735	-	X
85	MG	5	3736	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3740	-	X
85	MG	5	3741	-	X
85	MG	5	3742	-	X
85	MG	5	3744	-	X
85	MG	5	3746	-	X
85	MG	5	3747	-	X
85	MG	5	3748	-	X
85	MG	5	3749	-	X
85	MG	5	3750	-	X
85	MG	5	3751	-	X
85	MG	5	3752	-	X
85	MG	5	3754	-	X
85	MG	5	3756	-	X
85	MG	5	3757	-	X
85	MG	5	3760	-	X
85	MG	5	3761	-	X
85	MG	5	3762	-	X
85	MG	5	3763	-	X
85	MG	5	3766	-	X
85	MG	5	3768	-	X
85	MG	5	3769	-	X
85	MG	5	3771	-	X
85	MG	5	3772	-	X
85	MG	5	3773	-	X
85	MG	5	3774	-	X
85	MG	5	3775	-	X
85	MG	5	3776	-	X
85	MG	5	3778	-	X
85	MG	5	3779	-	X
85	MG	5	3780	-	X
85	MG	5	3781	-	X
85	MG	5	3782	-	X
85	MG	5	3783	-	X
85	MG	5	3784	-	X
85	MG	5	3786	-	X
85	MG	5	3788	-	X
85	MG	5	3789	-	X
85	MG	5	3790	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3791	-	X
85	MG	5	3792	-	X
85	MG	5	3793	-	X
85	MG	5	3794	-	X
85	MG	5	3795	-	X
85	MG	5	3796	-	X
85	MG	5	3797	-	X
85	MG	5	3798	-	X
85	MG	5	3800	-	X
85	MG	5	3802	-	X
85	MG	5	3807	-	X
85	MG	5	3808	-	X
85	MG	5	3809	-	X
85	MG	5	3810	-	X
85	MG	5	3811	-	X
85	MG	5	3812	-	X
85	MG	5	3813	-	X
85	MG	5	3814	-	X
85	MG	5	3815	-	X
85	MG	5	3817	-	X
85	MG	5	3819	-	X
85	MG	5	3821	-	X
85	MG	5	3823	-	X
85	MG	5	3824	-	X
85	MG	5	3825	-	X
85	MG	5	3826	-	X
85	MG	5	3828	-	X
85	MG	5	3829	-	X
85	MG	5	3831	-	X
85	MG	5	3833	-	X
85	MG	5	3834	-	X
85	MG	5	3835	-	X
85	MG	5	3837	-	X
85	MG	5	3841	-	X
85	MG	5	3842	-	X
85	MG	5	3843	-	X
85	MG	5	3844	-	X
85	MG	5	3845	-	X
85	MG	5	3849	-	X
85	MG	5	3851	-	X
85	MG	5	3852	-	X
85	MG	5	3855	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3857	-	X
85	MG	5	3858	-	X
85	MG	5	3860	-	X
85	MG	5	3861	-	X
85	MG	5	3862	-	X
85	MG	5	3863	-	X
85	MG	5	3864	-	X
85	MG	5	3865	-	X
85	MG	5	3867	-	X
85	MG	5	3868	-	X
85	MG	5	3869	-	X
85	MG	5	3870	-	X
85	MG	5	3871	-	X
85	MG	5	3872	-	X
85	MG	5	3873	-	X
85	MG	5	3874	-	X
85	MG	5	3876	-	X
85	MG	5	3877	-	X
85	MG	5	3878	-	X
85	MG	5	3879	-	X
85	MG	5	3880	-	X
85	MG	5	3881	-	X
85	MG	5	3882	-	X
85	MG	5	3883	-	X
85	MG	5	3884	-	X
85	MG	5	3885	-	X
85	MG	5	3886	-	X
85	MG	5	3887	-	X
85	MG	5	3888	-	X
85	MG	5	3889	-	X
85	MG	5	3890	-	X
85	MG	5	3891	-	X
85	MG	5	3892	-	X
85	MG	5	3893	-	X
85	MG	5	3894	-	X
85	MG	5	3895	-	X
85	MG	5	3896	-	X
85	MG	5	4250	-	X
85	MG	5	4251	-	X
85	MG	5	4252	-	X
85	MG	5	4253	-	X
85	MG	6	1901	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1902	-	X
85	MG	6	1903	-	X
85	MG	6	1904	-	X
85	MG	6	1905	-	X
85	MG	6	1906	-	X
85	MG	6	1907	-	X
85	MG	6	1908	-	X
85	MG	6	1909	-	X
85	MG	6	1910	-	X
85	MG	6	1911	-	X
85	MG	6	1912	-	X
85	MG	6	1913	-	X
85	MG	6	1915	-	X
85	MG	6	1916	-	X
85	MG	6	1917	-	X
85	MG	6	1918	-	X
85	MG	6	1919	-	X
85	MG	6	1920	-	X
85	MG	6	1921	-	X
85	MG	6	1922	-	X
85	MG	6	1923	-	X
85	MG	6	1924	-	X
85	MG	6	1925	-	X
85	MG	6	1926	-	X
85	MG	6	1927	-	X
85	MG	6	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1930	-	X
85	MG	6	1931	-	X
85	MG	6	1932	-	X
85	MG	6	1934	-	X
85	MG	6	1935	-	X
85	MG	6	1936	-	X
85	MG	6	1937	-	X
85	MG	6	1938	-	X
85	MG	6	1939	-	X
85	MG	6	1941	-	X
85	MG	6	1942	-	X
85	MG	6	1943	-	X
85	MG	6	1944	-	X
85	MG	6	1945	-	X
85	MG	6	1946	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1947	-	X
85	MG	6	1948	-	X
85	MG	6	1949	-	X
85	MG	6	1950	-	X
85	MG	6	1951	-	X
85	MG	6	1952	-	X
85	MG	6	1953	-	X
85	MG	6	1954	-	X
85	MG	6	1955	-	X
85	MG	6	1956	-	X
85	MG	6	1957	-	X
85	MG	6	1958	-	X
85	MG	6	1959	-	X
85	MG	6	1960	-	X
85	MG	6	1961	-	X
85	MG	6	1962	-	X
85	MG	6	1963	-	X
85	MG	6	1964	-	X
85	MG	6	1965	-	X
85	MG	6	1966	-	X
85	MG	6	1967	-	X
85	MG	6	1968	-	X
85	MG	6	1970	-	X
85	MG	6	1971	-	X
85	MG	6	1972	-	X
85	MG	6	1973	-	X
85	MG	6	1974	-	X
85	MG	6	1975	-	X
85	MG	6	1976	-	X
85	MG	6	1977	-	X
85	MG	6	1978	-	X
85	MG	6	1979	-	X
85	MG	6	1980	-	X
85	MG	6	1981	-	X
85	MG	6	1982	-	X
85	MG	6	1983	-	X
85	MG	6	1985	-	X
85	MG	6	1986	-	X
85	MG	6	1987	-	X
85	MG	6	1988	-	X
85	MG	6	1989	-	X
85	MG	6	1990	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1991	-	X
85	MG	6	1992	-	X
85	MG	6	1995	-	X
85	MG	6	1998	-	X
85	MG	6	2002	-	X
85	MG	6	2003	-	X
85	MG	6	2005	-	X
85	MG	6	2006	-	X
85	MG	6	2007	-	X
85	MG	6	2008	-	X
85	MG	6	2011	-	X
85	MG	6	2014	-	X
85	MG	6	2015	-	X
85	MG	6	2016	-	X
85	MG	6	2017	-	X
85	MG	6	2018	-	X
85	MG	6	2019	-	X
85	MG	6	2020	-	X
85	MG	6	2021	-	X
85	MG	6	2023	-	X
85	MG	6	2024	-	X
85	MG	6	2025	-	X
85	MG	6	2026	-	X
85	MG	6	2027	-	X
85	MG	6	2028	-	X
85	MG	6	2029	-	X
85	MG	6	2030	-	X
85	MG	6	2031	-	X
85	MG	6	2032	-	X
85	MG	6	2033	-	X
85	MG	6	2034	-	X
85	MG	6	2036	-	X
85	MG	6	2038	-	X
85	MG	6	2039	-	X
85	MG	6	2040	-	X
85	MG	6	2041	-	X
85	MG	6	2201	-	X
85	MG	6	2202	-	X
85	MG	7	201	-	X
85	MG	7	202	-	X
85	MG	7	203	-	X
85	MG	7	204	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	7	205	-	X
85	MG	7	206	-	X
85	MG	7	209	-	X
85	MG	7	210	-	X
85	MG	7	211	-	X
85	MG	7	213	-	X
85	MG	7	214	-	X
85	MG	7	215	-	X
85	MG	7	216	-	X
85	MG	7	217	-	X
85	MG	8	201	-	X
85	MG	8	202	-	X
85	MG	8	203	-	X
85	MG	8	204	-	X
85	MG	8	205	-	X
85	MG	8	206	-	X
85	MG	8	208	-	X
85	MG	8	210	-	X
85	MG	8	211	-	X
85	MG	8	212	-	X
85	MG	8	213	-	X
85	MG	D0	201	-	X
85	MG	L2	301	-	X
85	MG	L3	401	-	X
85	MG	L7	301	-	X
85	MG	L7	304	-	X
85	MG	M0	301	-	X
85	MG	M1	201	-	X
85	MG	M3	203	-	X
85	MG	M5	301	-	X
85	MG	M5	302	-	X
85	MG	M6	202	-	X
85	MG	M7	201	-	X
85	MG	M7	202	-	X
85	MG	M7	203	-	X
85	MG	N0	201	-	X
85	MG	N3	201	-	X
85	MG	N5	201	-	X
85	MG	N5	202	-	X
85	MG	N8	201	-	X
85	MG	N8	203	-	X
85	MG	O2	201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	O7	102	-	X
85	MG	O7	103	-	X
85	MG	O7	104	-	X
85	MG	S2	301	-	X
85	MG	c1	201	-	X
85	MG	c4	201	-	X
85	MG	c8	201	-	X
85	MG	d3	201	-	X
85	MG	d3	202	-	X
85	MG	d4	201	-	X
85	MG	l2	301	-	X
85	MG	l2	302	-	X
85	MG	l3	401	-	X
85	MG	l3	402	-	X
85	MG	l4	401	-	X
85	MG	l7	301	-	X
85	MG	l9	201	-	X
85	MG	m5	301	-	X
85	MG	m5	302	-	X
85	MG	m5	303	-	X
85	MG	m6	201	-	X
85	MG	m6	202	-	X
85	MG	m7	201	-	X
85	MG	n0	201	-	X
85	MG	n0	202	-	X
85	MG	n0	203	-	X
85	MG	n3	201	-	X
85	MG	n3	202	-	X
85	MG	n6	201	-	X
85	MG	n6	202	-	X
85	MG	n8	202	-	X
85	MG	n8	203	-	X
85	MG	n9	101	-	X
85	MG	o1	201	-	X
85	MG	o3	201	-	X
85	MG	o4	201	-	X
85	MG	o7	502	-	X
85	MG	o9	101	-	X
85	MG	q0	202	-	X
85	MG	q1	101	-	X
85	MG	q3	502	-	X
85	MG	s6	301	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	s8	301	-	X
85	MG	s8	302	-	X
85	MG	sM	301	-	X
86	OHX	1	3971	-	X
86	OHX	1	3976	-	X
86	OHX	1	3983	-	X
86	OHX	1	3989	-	X
86	OHX	1	3990	-	X
86	OHX	1	4000	-	X
86	OHX	1	4004	-	X
86	OHX	1	4005	-	X
86	OHX	1	4027	-	X
86	OHX	1	4033	-	X
86	OHX	1	4038	-	X
86	OHX	1	4043	-	X
86	OHX	1	4045	-	X
86	OHX	1	4046	-	X
86	OHX	1	4054	-	X
86	OHX	1	4056	-	X
86	OHX	1	4057	-	X
86	OHX	1	4059	-	X
86	OHX	1	4061	-	X
86	OHX	1	4062	-	X
86	OHX	1	4063	-	X
86	OHX	1	4064	-	X
86	OHX	1	4066	-	X
86	OHX	1	4067	-	X
86	OHX	1	4069	-	X
86	OHX	1	4070	-	X
86	OHX	1	4071	-	X
86	OHX	1	4072	-	X
86	OHX	1	4074	-	X
86	OHX	1	4075	-	X
86	OHX	1	4077	-	X
86	OHX	1	4078	-	X
86	OHX	1	4079	-	X
86	OHX	1	4081	-	X
86	OHX	1	4082	-	X
86	OHX	1	4086	-	X
86	OHX	1	4087	-	X
86	OHX	1	4091	-	X
86	OHX	1	4094	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4097	-	X
86	OHX	1	4099	-	X
86	OHX	1	4107	-	X
86	OHX	1	4108	-	X
86	OHX	1	4109	-	X
86	OHX	1	4110	-	X
86	OHX	1	4111	-	X
86	OHX	1	4112	-	X
86	OHX	1	4114	-	X
86	OHX	1	4116	-	X
86	OHX	1	4118	-	X
86	OHX	1	4119	-	X
86	OHX	1	4121	-	X
86	OHX	1	4122	-	X
86	OHX	1	4125	-	X
86	OHX	1	4126	-	X
86	OHX	1	4127	-	X
86	OHX	1	4128	-	X
86	OHX	1	4129	-	X
86	OHX	1	4130	-	X
86	OHX	1	4133	-	X
86	OHX	1	4134	-	X
86	OHX	1	4135	-	X
86	OHX	1	4137	-	X
86	OHX	1	4138	-	X
86	OHX	1	4139	-	X
86	OHX	1	4140	-	X
86	OHX	1	4141	-	X
86	OHX	1	4142	-	X
86	OHX	1	4143	-	X
86	OHX	1	4146	-	X
86	OHX	1	4149	-	X
86	OHX	1	4151	-	X
86	OHX	1	4153	-	X
86	OHX	1	4154	-	X
86	OHX	1	4157	-	X
86	OHX	1	4158	-	X
86	OHX	1	4159	-	X
86	OHX	1	4160	-	X
86	OHX	1	4162	-	X
86	OHX	1	4163	-	X
86	OHX	1	4166	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4167	-	X
86	OHX	1	4168	-	X
86	OHX	1	4169	-	X
86	OHX	1	4170	-	X
86	OHX	1	4171	-	X
86	OHX	1	4174	-	X
86	OHX	1	4175	-	X
86	OHX	1	4176	-	X
86	OHX	1	4177	-	X
86	OHX	1	4179	-	X
86	OHX	1	4180	-	X
86	OHX	1	4182	-	X
86	OHX	1	4183	-	X
86	OHX	1	4184	-	X
86	OHX	1	4185	-	X
86	OHX	1	4188	-	X
86	OHX	1	4189	-	X
86	OHX	1	4190	-	X
86	OHX	1	4192	-	X
86	OHX	1	4194	-	X
86	OHX	1	4195	-	X
86	OHX	1	4196	-	X
86	OHX	1	4197	-	X
86	OHX	1	4198	-	X
86	OHX	1	4199	-	X
86	OHX	1	4201	-	X
86	OHX	1	4202	-	X
86	OHX	1	4203	-	X
86	OHX	1	4204	-	X
86	OHX	1	4205	-	X
86	OHX	1	4206	-	X
86	OHX	1	4207	-	X
86	OHX	1	4208	-	X
86	OHX	1	4209	-	X
86	OHX	1	4210	-	X
86	OHX	1	4211	-	X
86	OHX	2	2062	-	X
86	OHX	2	2074	-	X
86	OHX	2	2075	-	X
86	OHX	2	2079	-	X
86	OHX	2	2084	-	X
86	OHX	2	2091	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2092	-	X
86	OHX	2	2103	-	X
86	OHX	2	2105	-	X
86	OHX	2	2108	-	X
86	OHX	2	2112	-	X
86	OHX	2	2113	-	X
86	OHX	2	2116	-	X
86	OHX	2	2117	-	X
86	OHX	2	2119	-	X
86	OHX	2	2120	-	X
86	OHX	2	2122	-	X
86	OHX	2	2123	-	X
86	OHX	2	2126	-	X
86	OHX	2	2128	-	X
86	OHX	2	2129	-	X
86	OHX	2	2132	-	X
86	OHX	2	2135	-	X
86	OHX	2	2136	-	X
86	OHX	2	2137	-	X
86	OHX	2	2138	-	X
86	OHX	2	2140	-	X
86	OHX	2	2141	-	X
86	OHX	2	2144	-	X
86	OHX	2	2146	-	X
86	OHX	2	2147	-	X
86	OHX	2	2148	-	X
86	OHX	2	2149	-	X
86	OHX	2	2153	-	X
86	OHX	2	2154	-	X
86	OHX	2	2155	-	X
86	OHX	2	2156	-	X
86	OHX	2	2158	-	X
86	OHX	2	2160	-	X
86	OHX	2	2161	-	X
86	OHX	2	2163	-	X
86	OHX	2	2164	-	X
86	OHX	2	2165	-	X
86	OHX	2	2169	-	X
86	OHX	2	2170	-	X
86	OHX	2	2171	-	X
86	OHX	2	2172	-	X
86	OHX	2	2173	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2174	-	X
86	OHX	2	2175	-	X
86	OHX	2	2177	-	X
86	OHX	2	2179	-	X
86	OHX	2	2180	-	X
86	OHX	3	221	-	X
86	OHX	3	222	-	X
86	OHX	3	223	-	X
86	OHX	3	224	-	X
86	OHX	3	225	-	X
86	OHX	4	228	-	X
86	OHX	4	229	-	X
86	OHX	4	230	-	X
86	OHX	4	233	-	X
86	OHX	4	234	-	X
86	OHX	4	235	-	X
86	OHX	4	236	-	X
86	OHX	4	237	-	X
86	OHX	4	238	-	X
86	OHX	5	3908	-	X
86	OHX	5	3989	-	X
86	OHX	5	3997	-	X
86	OHX	5	4022	-	X
86	OHX	5	4035	-	X
86	OHX	5	4038	-	X
86	OHX	5	4040	-	X
86	OHX	5	4041	-	X
86	OHX	5	4045	-	X
86	OHX	5	4047	-	X
86	OHX	5	4050	-	X
86	OHX	5	4052	-	X
86	OHX	5	4055	-	X
86	OHX	5	4058	-	X
86	OHX	5	4061	-	X
86	OHX	5	4065	-	X
86	OHX	5	4066	-	X
86	OHX	5	4067	-	X
86	OHX	5	4068	-	X
86	OHX	5	4069	-	X
86	OHX	5	4072	-	X
86	OHX	5	4075	-	X
86	OHX	5	4078	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4081	-	X
86	OHX	5	4082	-	X
86	OHX	5	4084	-	X
86	OHX	5	4085	-	X
86	OHX	5	4086	-	X
86	OHX	5	4088	-	X
86	OHX	5	4089	-	X
86	OHX	5	4092	-	X
86	OHX	5	4093	-	X
86	OHX	5	4095	-	X
86	OHX	5	4096	-	X
86	OHX	5	4098	-	X
86	OHX	5	4101	-	X
86	OHX	5	4102	-	X
86	OHX	5	4103	-	X
86	OHX	5	4105	-	X
86	OHX	5	4107	-	X
86	OHX	5	4109	-	X
86	OHX	5	4110	-	X
86	OHX	5	4112	-	X
86	OHX	5	4114	-	X
86	OHX	5	4115	-	X
86	OHX	5	4117	-	X
86	OHX	5	4120	-	X
86	OHX	5	4121	-	X
86	OHX	5	4122	-	X
86	OHX	5	4127	-	X
86	OHX	5	4129	-	X
86	OHX	5	4130	-	X
86	OHX	5	4131	-	X
86	OHX	5	4132	-	X
86	OHX	5	4133	-	X
86	OHX	5	4134	-	X
86	OHX	5	4135	-	X
86	OHX	5	4136	-	X
86	OHX	5	4138	-	X
86	OHX	5	4140	-	X
86	OHX	5	4141	-	X
86	OHX	5	4142	-	X
86	OHX	5	4143	-	X
86	OHX	5	4144	-	X
86	OHX	5	4145	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4146	-	X
86	OHX	5	4147	-	X
86	OHX	5	4148	-	X
86	OHX	5	4150	-	X
86	OHX	5	4151	-	X
86	OHX	5	4152	-	X
86	OHX	5	4153	-	X
86	OHX	5	4154	-	X
86	OHX	5	4156	-	X
86	OHX	5	4157	-	X
86	OHX	5	4158	-	X
86	OHX	5	4159	-	X
86	OHX	5	4160	-	X
86	OHX	5	4161	-	X
86	OHX	5	4164	-	X
86	OHX	5	4167	-	X
86	OHX	5	4168	-	X
86	OHX	5	4170	-	X
86	OHX	5	4171	-	X
86	OHX	5	4173	-	X
86	OHX	5	4174	-	X
86	OHX	5	4176	-	X
86	OHX	5	4178	-	X
86	OHX	5	4179	-	X
86	OHX	5	4180	-	X
86	OHX	5	4181	-	X
86	OHX	5	4182	-	X
86	OHX	5	4183	-	X
86	OHX	5	4186	-	X
86	OHX	5	4187	-	X
86	OHX	5	4188	-	X
86	OHX	5	4190	-	X
86	OHX	5	4191	-	X
86	OHX	5	4192	-	X
86	OHX	5	4195	-	X
86	OHX	5	4196	-	X
86	OHX	5	4197	-	X
86	OHX	5	4198	-	X
86	OHX	5	4199	-	X
86	OHX	5	4200	-	X
86	OHX	5	4202	-	X
86	OHX	5	4204	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4205	-	X
86	OHX	5	4206	-	X
86	OHX	5	4207	-	X
86	OHX	5	4208	-	X
86	OHX	5	4209	-	X
86	OHX	5	4211	-	X
86	OHX	5	4213	-	X
86	OHX	5	4214	-	X
86	OHX	5	4215	-	X
86	OHX	5	4216	-	X
86	OHX	5	4217	-	X
86	OHX	5	4218	-	X
86	OHX	5	4219	-	X
86	OHX	5	4220	-	X
86	OHX	5	4222	-	X
86	OHX	5	4224	-	X
86	OHX	5	4225	-	X
86	OHX	5	4226	-	X
86	OHX	5	4227	-	X
86	OHX	5	4229	-	X
86	OHX	5	4230	-	X
86	OHX	5	4231	-	X
86	OHX	5	4232	-	X
86	OHX	5	4234	-	X
86	OHX	5	4236	-	X
86	OHX	5	4237	-	X
86	OHX	5	4239	-	X
86	OHX	5	4241	-	X
86	OHX	5	4242	-	X
86	OHX	5	4243	-	X
86	OHX	5	4244	-	X
86	OHX	5	4245	-	X
86	OHX	5	4247	-	X
86	OHX	6	2068	-	X
86	OHX	6	2099	-	X
86	OHX	6	2109	-	X
86	OHX	6	2111	-	X
86	OHX	6	2113	-	X
86	OHX	6	2116	-	X
86	OHX	6	2119	-	X
86	OHX	6	2120	-	X
86	OHX	6	2122	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2123	-	X
86	OHX	6	2128	-	X
86	OHX	6	2129	-	X
86	OHX	6	2130	-	X
86	OHX	6	2132	-	X
86	OHX	6	2136	-	X
86	OHX	6	2137	-	X
86	OHX	6	2140	-	X
86	OHX	6	2143	-	X
86	OHX	6	2145	-	X
86	OHX	6	2147	-	X
86	OHX	6	2148	-	X
86	OHX	6	2152	-	X
86	OHX	6	2153	-	X
86	OHX	6	2156	-	X
86	OHX	6	2157	-	X
86	OHX	6	2159	-	X
86	OHX	6	2161	-	X
86	OHX	6	2164	-	X
86	OHX	6	2165	-	X
86	OHX	6	2166	-	X
86	OHX	6	2167	-	X
86	OHX	6	2169	-	X
86	OHX	6	2170	-	X
86	OHX	6	2171	-	X
86	OHX	6	2172	-	X
86	OHX	6	2173	-	X
86	OHX	6	2174	-	X
86	OHX	6	2176	-	X
86	OHX	6	2177	-	X
86	OHX	6	2179	-	X
86	OHX	6	2180	-	X
86	OHX	6	2182	-	X
86	OHX	6	2183	-	X
86	OHX	6	2185	-	X
86	OHX	6	2186	-	X
86	OHX	6	2187	-	X
86	OHX	6	2191	-	X
86	OHX	6	2193	-	X
86	OHX	6	2194	-	X
86	OHX	6	2195	-	X
86	OHX	6	2196	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2199	-	X
86	OHX	6	2200	-	X
86	OHX	7	226	-	X
86	OHX	7	227	-	X
86	OHX	7	228	-	X
86	OHX	8	221	-	X
86	OHX	8	223	-	X
86	OHX	8	227	-	X
86	OHX	8	228	-	X
86	OHX	8	230	-	X
86	OHX	D9	102	-	X
86	OHX	L4	402	-	X
86	OHX	M7	206	-	X
86	OHX	M7	207	-	X
86	OHX	M9	202	-	X
86	OHX	d9	102	-	X
86	OHX	l4	403	-	X
86	OHX	l5	304	-	X
86	OHX	s1	303	-	X
86	OHX	s4	301	-	X
86	OHX	s9	201	-	X
87	ZN	d7	101	-	X

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411178 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 *Saccharomyces cerevisiae* chromosome XII cosmid 9634.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			892	562	156	172	2			

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			

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

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

- Molecule 36 is a RNA chain called 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			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	121	LYS	-	expression tag	UNP P87262
o4	121	LYS	-	expression tag	UNP P87262

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 81 is a protein called unknown protein chain m2.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

- Molecule 83 is a protein called unknown protein chain p1.

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

- Molecule 84 is a protein called unknown protein chain p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	4	Total	Mg	0	0
			4	4		
85	m6	3	Total	Mg	0	0
			3	3		
85	n8	4	Total	Mg	0	0
			4	4		
85	o1	2	Total	Mg	0	0
			2	2		
85	N5	2	Total	Mg	0	0
			2	2		
85	6	144	Total	Mg	0	0
			144	144		
85	sM	2	Total	Mg	0	0
			2	2		
85	m5	3	Total	Mg	0	0
			3	3		
85	l3	2	Total	Mg	0	0
			2	2		
85	M1	1	Total	Mg	0	0
			1	1		
85	d6	1	Total	Mg	0	0
			1	1		
85	2	125	Total	Mg	0	0
			125	125		
85	n0	3	Total	Mg	0	0
			3	3		
85	L4	1	Total	Mg	0	0
			1	1		
85	l7	1	Total	Mg	0	0
			1	1		
85	M5	2	Total	Mg	0	0
			2	2		
85	o9	1	Total	Mg	0	0
			1	1		
85	S2	1	Total	Mg	0	0
			1	1		
85	L8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	D3	1	Total 1	Mg 1	0	0
85	o4	1	Total 1	Mg 1	0	0
85	M9	1	Total 1	Mg 1	0	0
85	q0	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	c8	2	Total 2	Mg 2	0	0
85	M0	2	Total 2	Mg 2	0	0
85	c1	1	Total 1	Mg 1	0	0
85	5	501	Total 501	Mg 501	0	0
85	L5	1	Total 1	Mg 1	0	0
85	O7	3	Total 3	Mg 3	0	0
85	s6	1	Total 1	Mg 1	0	0
85	l4	1	Total 1	Mg 1	0	0
85	n9	1	Total 1	Mg 1	0	0
85	1	472	Total 472	Mg 472	0	0
85	c4	1	Total 1	Mg 1	0	0
85	D0	1	Total 1	Mg 1	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	l2	2	Total 2	Mg 2	0	0
85	O2	1	Total 1	Mg 1	0	0
85	q3	2	Total 2	Mg 2	0	0

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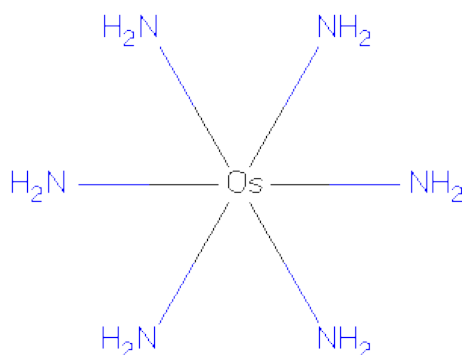
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	o3	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	M3	3	Total 3	Mg 3	0	0
85	N3	3	Total 3	Mg 3	0	0
85	4	20	Total 20	Mg 20	0	0
85	n6	2	Total 2	Mg 2	0	0
85	L2	1	Total 1	Mg 1	0	0
85	o7	1	Total 1	Mg 1	0	0
85	l5	1	Total 1	Mg 1	0	0
85	m7	5	Total 5	Mg 5	0	0
85	M7	5	Total 5	Mg 5	0	0
85	N8	4	Total 4	Mg 4	0	0
85	s1	1	Total 1	Mg 1	0	0
85	l9	1	Total 1	Mg 1	0	0
85	s8	3	Total 3	Mg 3	0	0
85	c7	1	Total 1	Mg 1	0	0
85	7	17	Total 17	Mg 17	0	0
85	n3	2	Total 2	Mg 2	0	0
85	q1	1	Total 1	Mg 1	0	0
85	L3	1	Total 1	Mg 1	0	0
85	d4	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	N6	1	Total	Mg	0	0
			1	1		
85	8	13	Total	Mg	0	0
			13	13		
85	M6	2	Total	Mg	0	0
			2	2		
85	N0	1	Total	Mg	0	0
			1	1		
85	3	14	Total	Mg	0	0
			14	14		

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



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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
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86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	4	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L3	1	Total	N	Os	0	0
			7	6	1		
86	L4	1	Total	N	Os	0	0
			7	6	1		
86	M0	1	Total	N	Os	0	0
			7	6	1		
86	M5	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M7	1	Total	N	Os	0	0
			7	6	1		
86	M8	1	Total	N	Os	0	0
			7	6	1		
86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	N9	1	Total	N	Os	0	0
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86	O3	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	O7	1	Total	N	Os	0	0
			7	6	1		
86	Q2	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
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86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		
86	6	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	c3	1	Total	N	Os	0	0
			7	6	1		
86	c5	1	Total	N	Os	0	0
			7	6	1		
86	c8	1	Total	N	Os	0	0
			7	6	1		
86	d4	1	Total	N	Os	0	0
			7	6	1		
86	d9	1	Total	N	Os	0	0
			7	6	1		
86	sR	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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86	7	1	Total	N	Os	0	0
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86	8	1	Total	N	Os	0	0
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86	8	1	Total	N	Os	0	0
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86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
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86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	13	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	14	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	15	1	Total	N	Os	0	0
			7	6	1		
86	19	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n3	1	Total	N	Os	0	0
			7	6	1		
86	n5	1	Total	N	Os	0	0
			7	6	1		
86	n9	1	Total	N	Os	0	0
			7	6	1		
86	o2	1	Total	N	Os	0	0
			7	6	1		
86	o3	1	Total	N	Os	0	0
			7	6	1		
86	q1	1	Total	N	Os	0	0
			7	6	1		
86	q2	1	Total	N	Os	0	0
			7	6	1		

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

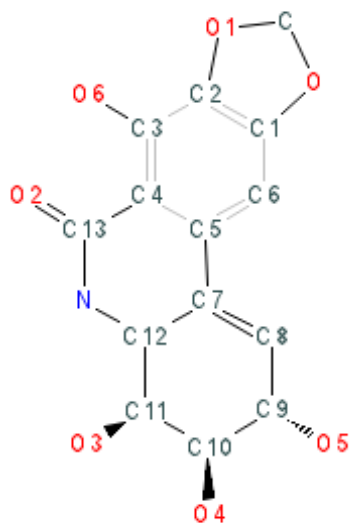
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	q0	1	Total	Zn	0	0
			1	1		
87	D6	1	Total	Zn	0	0
			1	1		
87	Q2	1	Total	Zn	0	0
			1	1		
87	e1	1	Total	Zn	0	0
			1	1		
87	Q3	1	Total	Zn	0	0
			1	1		
87	D9	1	Total	Zn	0	0
			1	1		
87	E1	1	Total	Zn	0	0
			1	1		
87	Q0	1	Total	Zn	0	0
			1	1		
87	d7	1	Total	Zn	0	0
			1	1		

*Continued on next page...*

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

- Molecule 88 is (2S,3R,4S,4aR)-2,3,4,7-tetrahydroxy-3,4,4a,5-tetrahydro[1,3]dioxolo[4,5-j]phenanthridin-6(2H)-one (three-letter code: 3KF) (formula: C<sub>14</sub>H<sub>13</sub>NO<sub>7</sub>).

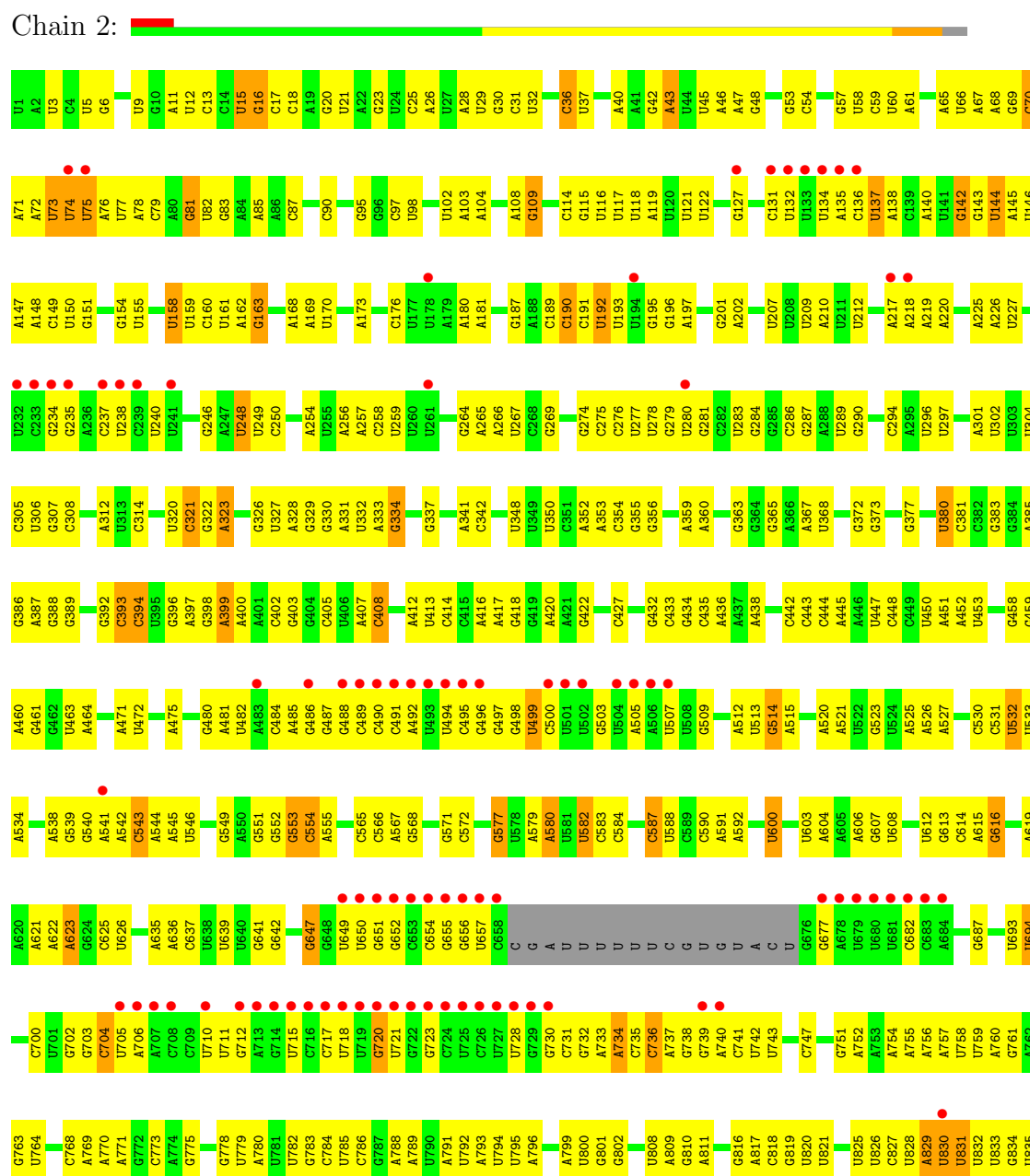


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
88	1	1	Total	C	N	O	0	0
			22	14	1	7		
88	5	1	Total	C	N	O	0	0
			22	14	1	7		

### 3 Residue-property plots

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

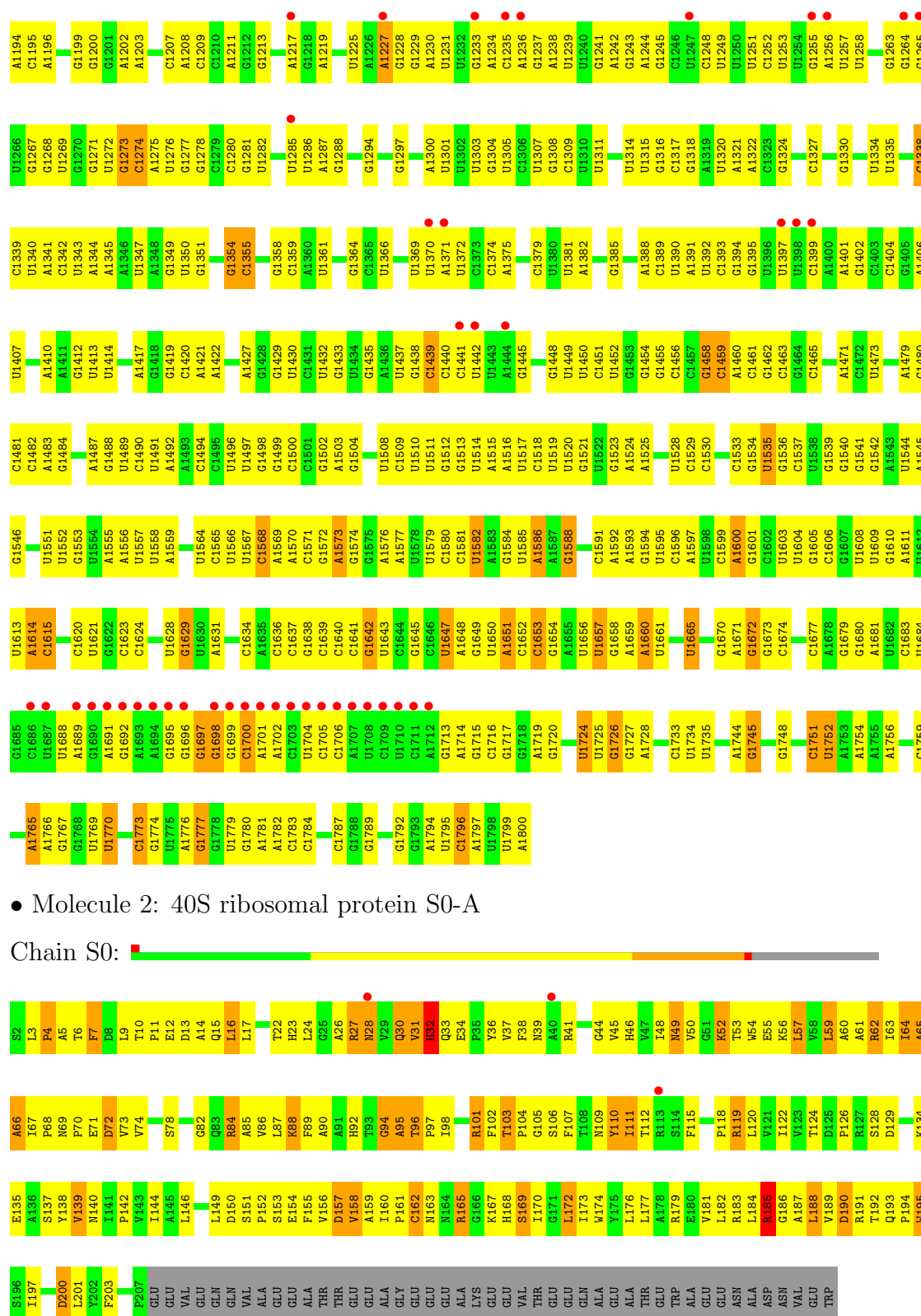
- Molecule 1: *Saccharomyces cerevisiae* chromosome XII cosmid 9634







G1122	C969	U825	A754	U	U602	G516	A451	G371	U297	C224	U150	U74
G1123	A970	U826	A755	A673	U603	U517	A452	G372	A301	A225	G151	U75
A1124	A971	C827	A756	C874	A604	A518	U453	G373	U302	A226	U152	A76
G1125	G972	U830	A757	U675	A605	A521	U454	G383	U303	U227	U77	A78
G1126	A973	U831	U758	U676	A606	U522	C455	G384	U304	G228	U158	C79
G1127	A974	U832	U759	U677	A607	U523	G458	G385	C305	C230	U159	A80
C1128	C975	U833	A760	A678	U608	G523	G459	G386	U306	U231	C160	G81
U1055	G976	U834	G761	U679	U609	C530	G460	G387	C307	G232	U161	U82
G1130	U908	U835	G765	C683	G610	C531	G461	G388	C308	G233	A162	G83
U1058	C910	U836	U766	A684	U611	U532	G462	G389	C309	G234	A163	A84
U1059	U911	G837	U767	C687	G612	U533	U463	G390	C310	G235	A164	A85
A1132	U912	G838	U768	A688	G613	A534	U464	A391	U311	A236	G165	A86
A1133	G913	U839	A769	G688	C614	A615	G465	G392	A312	C237	C166	
U1136	C990	U843	A770	G689	A619		U466	C393	U313	U238	U167	
A1137	G991	A844	A771	G690	A620		G467	C394	C314	C239	U168	
A1138	A992	G845	G772	C691	A621		U470	A397	A315	U240	A169	
A1069	A993	C846	C773	C692	A622		U471	G398	A316	U241		
G1070	G994	A847	A774	U693	A623		U472	A399	C317			
A995	A919	G848	G775	U694			A475	A400				
U996	U920	C849	G776	U695	U626		A476	A401	U320	A244		
G997	U921	C849	G777	U696	C627		A477	A402	A323	U245		
G1073	G922	U852	G778	C697	G628		A478	G403	U324	G246		
G1074	A923	U853		U698	U629		A479	G404	U327	A247		
U1080	A926	U854	U781	U699			A480	G405	U328	U248		
G1081	C927	U855	U782	C700			A481	U406	G329	U249		
C1082	U928	A856	G783	U701			A482	C408	G330	C250		
G1085	A929	U857	C786	U705			A483	C409	A331	A257		
A1086	U930	A858	G787	A706			A484	U412	A332	U258		
A1087	C931	A859	U788	A707			A485	A416	A333	U259		
U1091	C934	A862	A789	C708			G486	A417	G334	U260		
A1092	U935	A863	U790	C709			G487	G418	G337	U261		
A1093	G936	U864	A791	U710			G488	G419	C338	U262		
A1163	C937	U865	U792	U718			G489	G420	C339	C263		
G1095	G938	G867	A793	C717			C490	A421	C340	A266		
U1095	U1016	C868	U794	U719			C491	A425	U340	G269		
C1096	C1017	A868	U795	U720			A492	A426	A341	C270		
U1018	U1018	G871	A799	U721			U493	G426	A342	A271		
A1019	A1019	U872	U800	G722			U494	C430	G346	U272		
A1023	A1023	U873	G801	G723			C495	C431	G347	G273		
A1027	A951	G876	U804	C724			G496	C432	U348	G274		
A1028	A952	G877	U805	U727			G497	C433	C351	C275		
C1028	G953	U878	A806	U728			G498	C434	A352	U277		
U1029	G954	G879	A807	G729			U499	C435	C353	G281		
A1030	A955	G879	A808	U730			C500	G436	A354	U211		
U1031	G956	A884	U808	G731			U501	A437	C354	U212		
G1032	C957	G885	A809	C732			U502	A438	G355	U213		
G1033	G958	U886	G810	U733			G503	U439	C358	G282		
C1034	U959	A887	A811	G734			U504	U440	A359	U283		
G1036	U960	U888	A812	A737			A505	C443	C360	G284		
A1036	U961	A892	U813	G738			A506	C444	A361	A215		
A1039	C962	U893	G819	U739			G510	C445	C362	U216		
A963	U963	U894	U820	A740			A511	A446	G363	A217		
G1041	U964	U895	U821	C741			A512	U447	C364	A218		
G1042	U965	G896	U822	A745			U513	C448	G365	U292		
U966	A967	C897	U823	U745			G514	C449	G366	U293		
C1045	U968		G824	A753			A515	U450	A370	U296		
G1048	G1048											
U1049	U1049											
G1050	G1050											
U1051	A1124											
G1052	G1051											
G1053	A1125											
U1054	G1126											
U1055	G1127											
U1058	C1128											
U1059	U1129											
U1065	G1130											
C1066	A1131											
C1067	A1132											
C1068	A1133											
A1069	U1136											
C1070	A1137											
U1071	A1138											
C1072	G1141											
G1073	A1142											
G1074	A1143											
G1075	U1144											
A1001	A1147											
G1002	C1148											
A1003	G1149											
U1004	G1150											
A1005	A1151											
C1006	A1157											
C1007	C1158											
G1010	G1159											
G1011	A1160											
U1012	C1161											
U1015	A1162											
C1016	G1163											
U1017	G1164											
U1018	C1095											
A1019	A1165											
A1023	G1166											
A1027	U1097											
A1028	U1098											
C1028	U1099											
U1029	G1102											
A1030	U1103											
U1031	U1104											
G1032	G1107											
C1033	G1108											
G1034	G1109											
G1036	G1110											
A1036	G1111											
U960	G1112											
U961	A1113											
C962	G1114											
A963	U1115											
U963	A1116											
G1041	U1117											
G1042	U1118											
U966	G1119											
C1045	U1120											
U968	A1193											



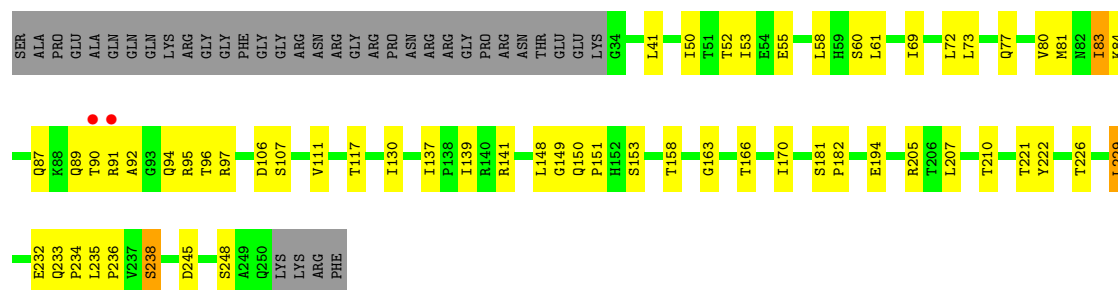
• Molecule 2: 40S ribosomal protein S0-A

Chain s0:



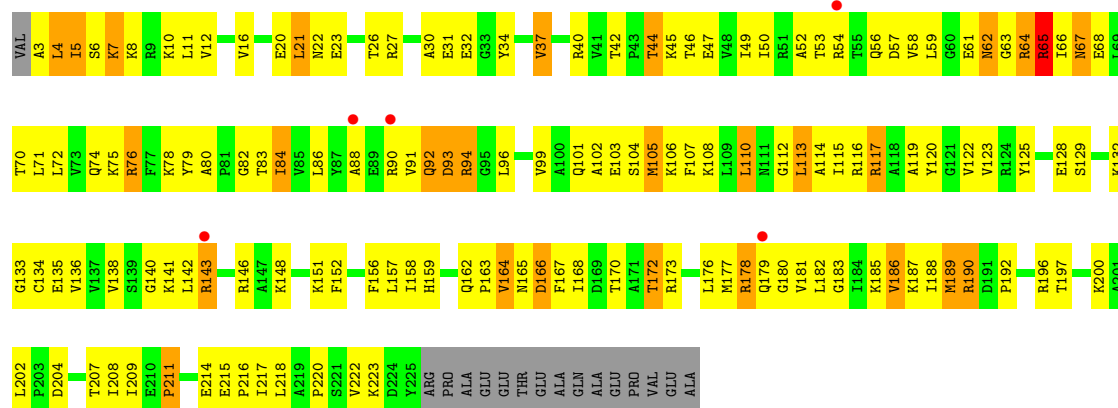
- Molecule 4: 40S ribosomal protein S2

Chain s2:



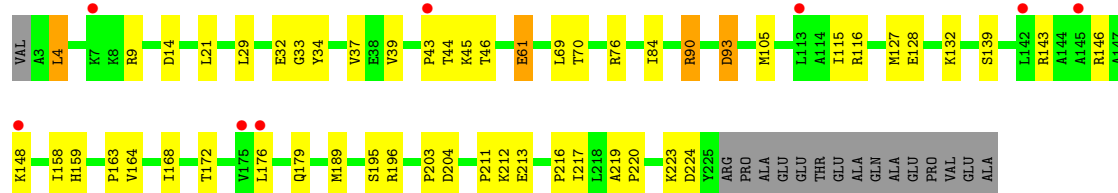
- Molecule 5: 40S ribosomal protein S3

Chain S3:



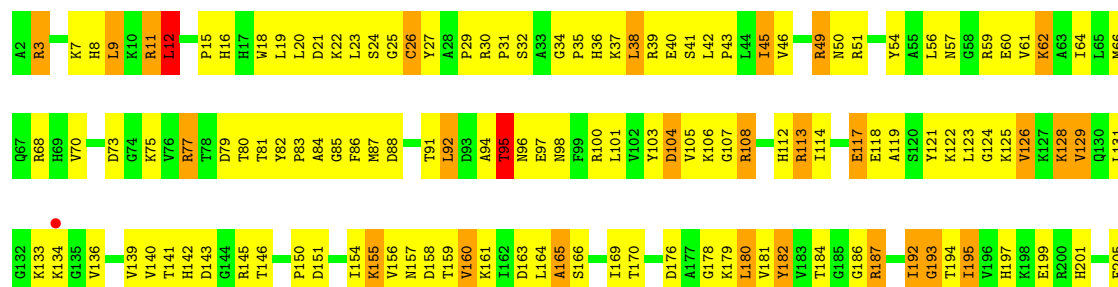
- Molecule 5: 40S ribosomal protein S3

Chain s3:



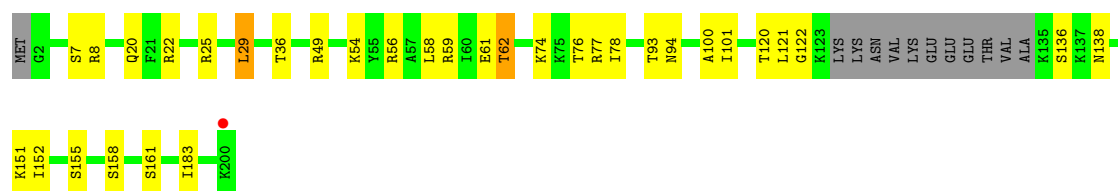
- Molecule 6: 40S ribosomal protein S4-A

Chain S4:



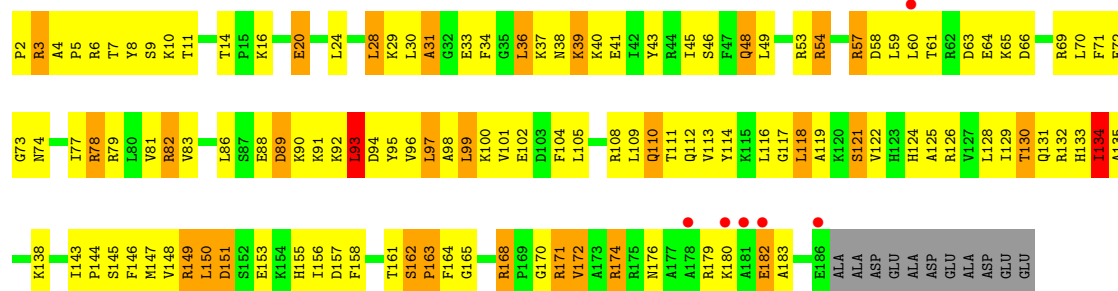






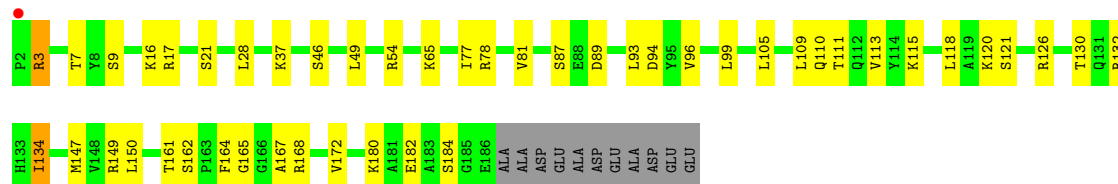
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



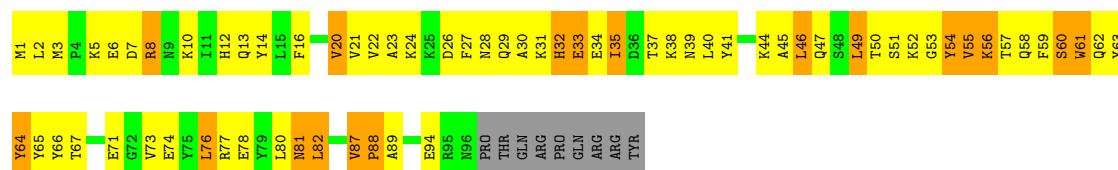
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



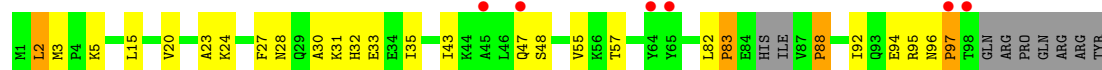
• Molecule 12: 40S ribosomal protein S10-A

Chain C0:



• Molecule 12: 40S ribosomal protein S10-A

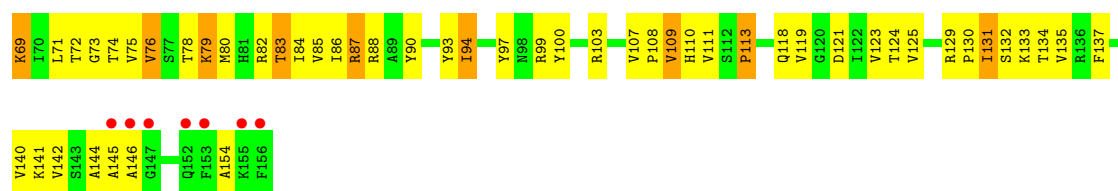
Chain c0:



• Molecule 13: 40S ribosomal protein S11-A

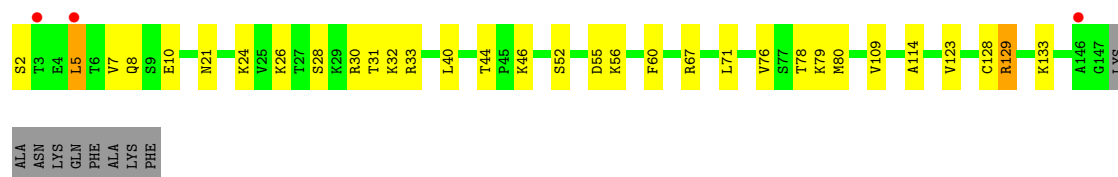
Chain C1:





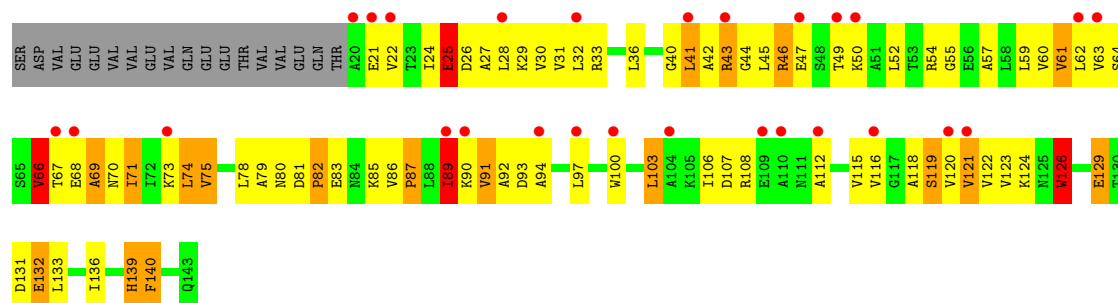
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



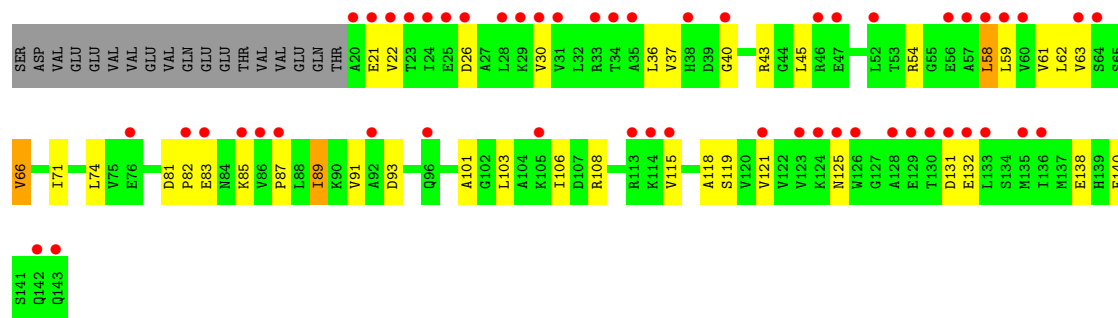
• Molecule 14: 40S ribosomal protein S12

Chain C2:



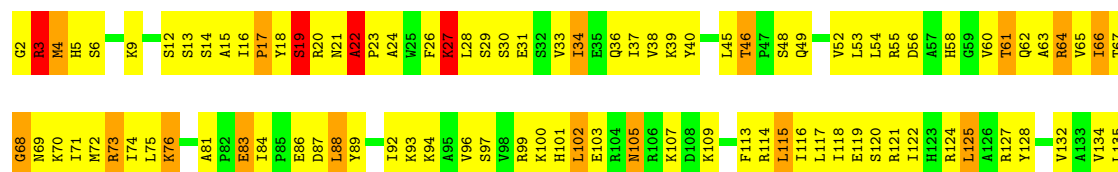
• Molecule 14: 40S ribosomal protein S12

Chain c2:



• Molecule 15: 40S ribosomal protein S13

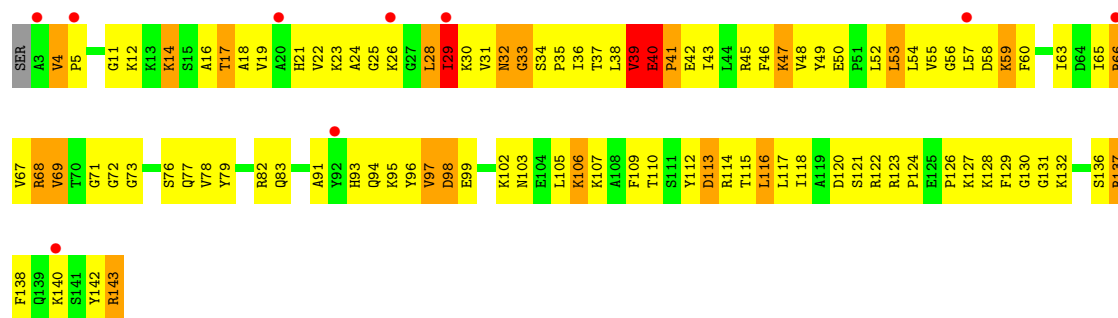
Chain C3:





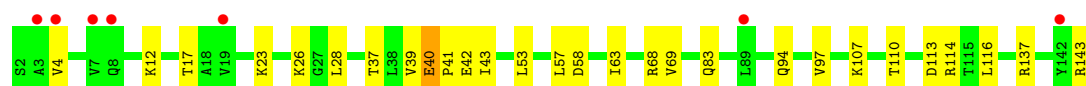


Chain C6: 



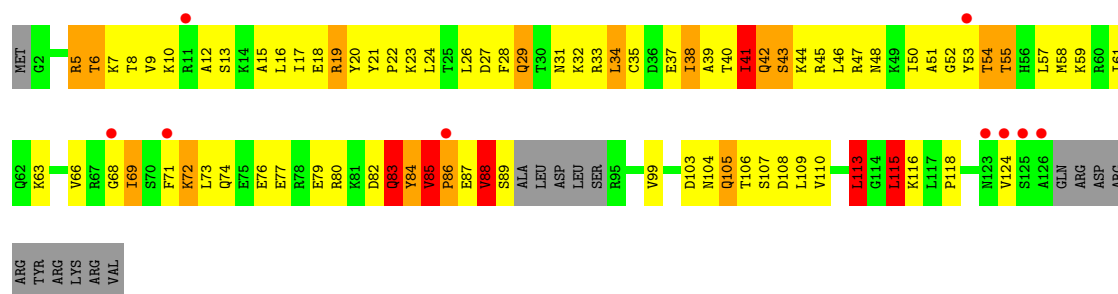
- Molecule 18: 40S ribosomal protein S16-A

Chain c6: 



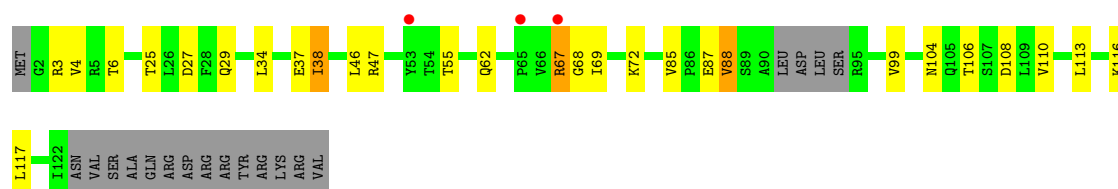
- Molecule 19: 40S ribosomal protein S17-A

Chain C7: 



- Molecule 19: 40S ribosomal protein S17-A

Chain c7: 



- Molecule 20: 40S ribosomal protein S18-A

Chain C8: 





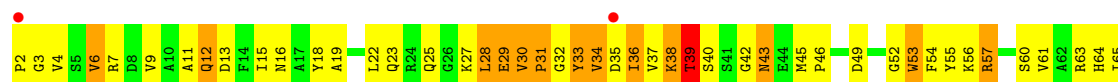
- Molecule 20: 40S ribosomal protein S18-A

Chain c8:



- Molecule 21: 40S ribosomal protein S19-A

Chain C9:



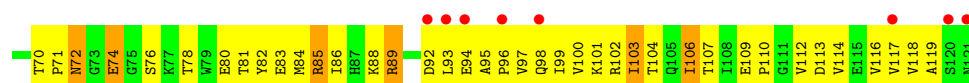
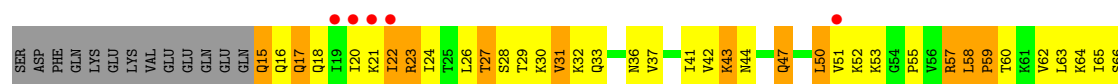
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



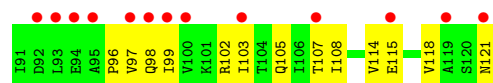
- Molecule 22: 40S ribosomal protein S20

Chain D0:



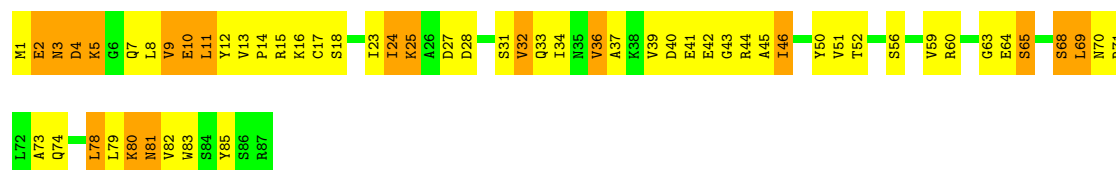
- Molecule 22: 40S ribosomal protein S20

Chain d0:



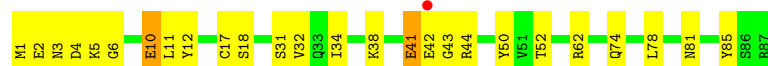
- Molecule 23: 40S ribosomal protein S21-A

Chain D1:



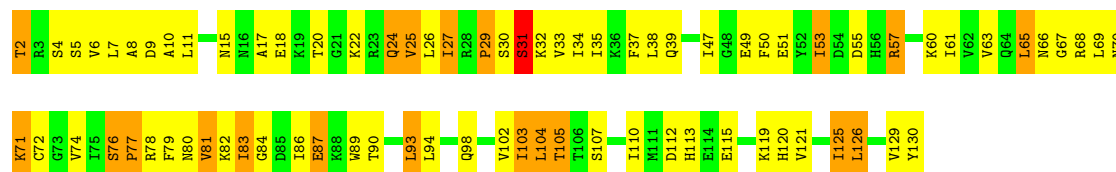
- Molecule 23: 40S ribosomal protein S21-A

Chain d1:



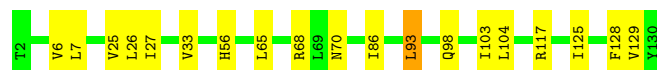
- Molecule 24: 40S ribosomal protein S22-A

Chain D2:



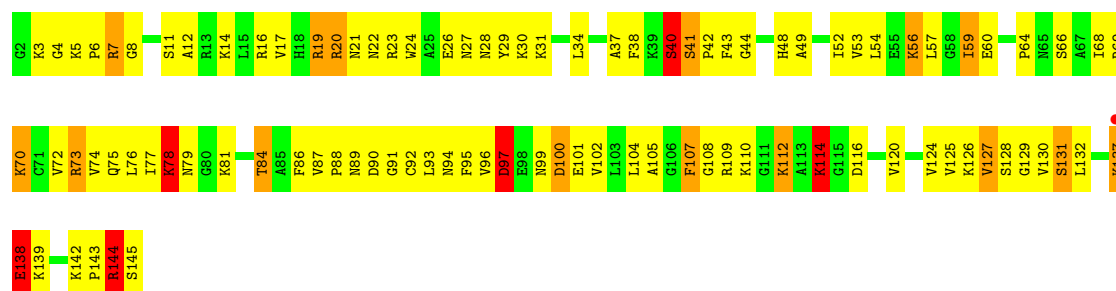
- Molecule 24: 40S ribosomal protein S22-A

Chain d2:



- Molecule 25: 40S ribosomal protein S23-A

Chain D3:



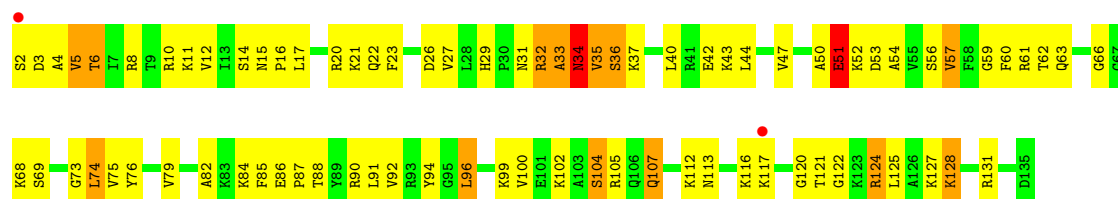
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



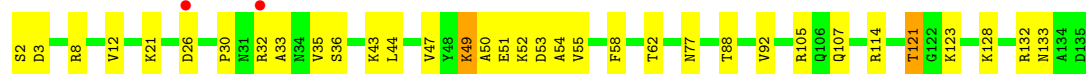
- Molecule 26: 40S ribosomal protein S24-A

Chain D4: 



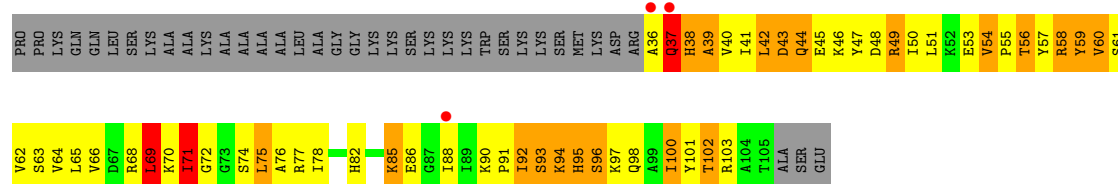
- Molecule 26: 40S ribosomal protein S24-A

Chain d4: 



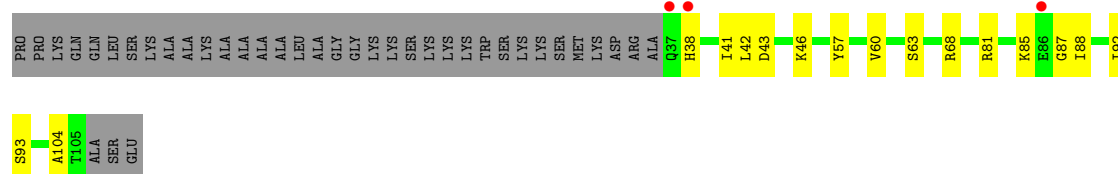
- Molecule 27: 40S ribosomal protein S25-A

Chain D5: 



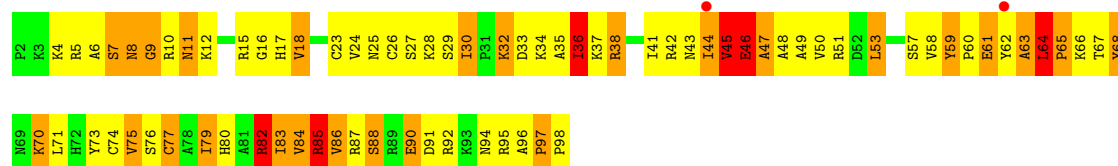
- Molecule 27: 40S ribosomal protein S25-A

Chain d5: 



- Molecule 28: 40S ribosomal protein S26-B

Chain D6: 



- Molecule 28: 40S ribosomal protein S26-B

Chain d6: 



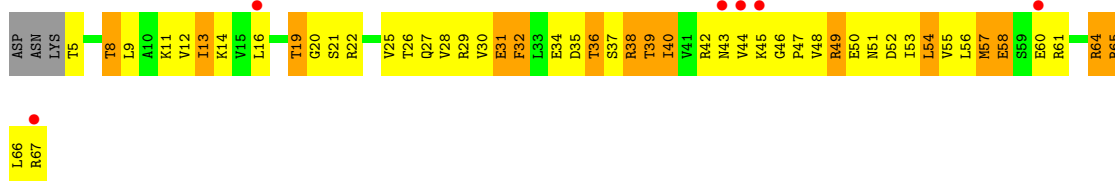
- Molecule 29: 40S ribosomal protein S27-A

V2	L3	V4	Q5	D6	L7	A12	A13	S14	A15	A16	K20	P28	R29	S30	Y31	F32	L33	K36	C37	P38	G39	C40	L41	N42	I43	F47	S48	H49	V54	T55	C56	E57	S58	C59	S60	T61	I62	L63	G64	T65	P66	T67	K70	A71	K72	T77	R81	K82
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- Chain d7:



- Chain D8:



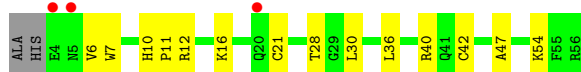
- Chain d8: 



- Chain D9: 



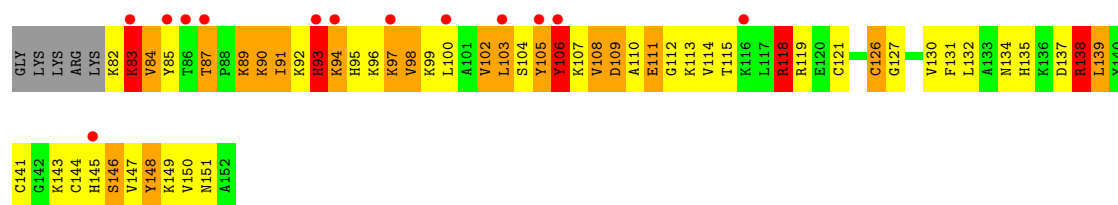
- Chain d9: 



- Chain E0:

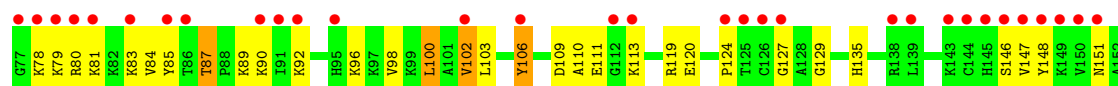


- Chain E1:



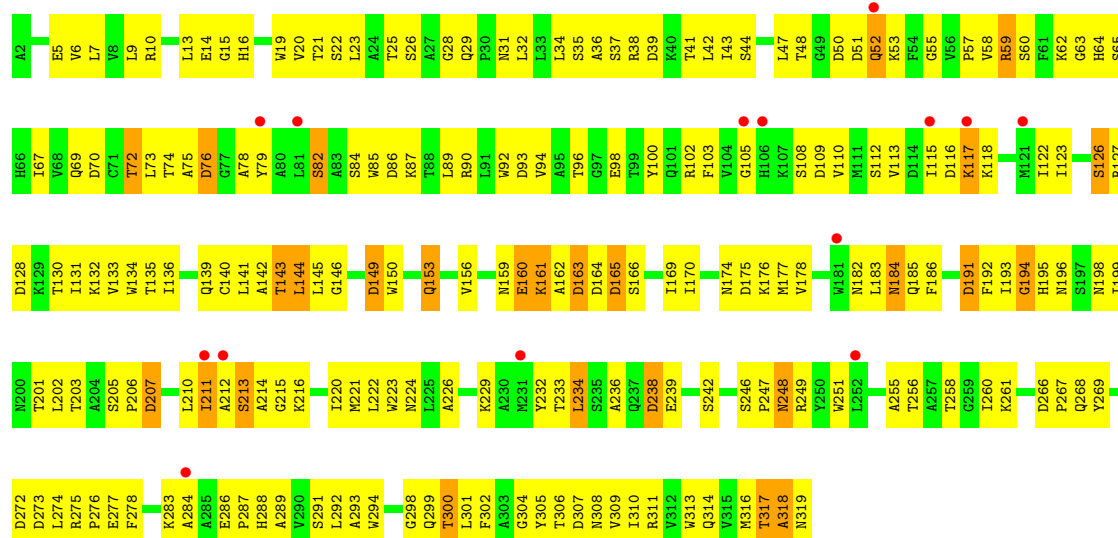
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



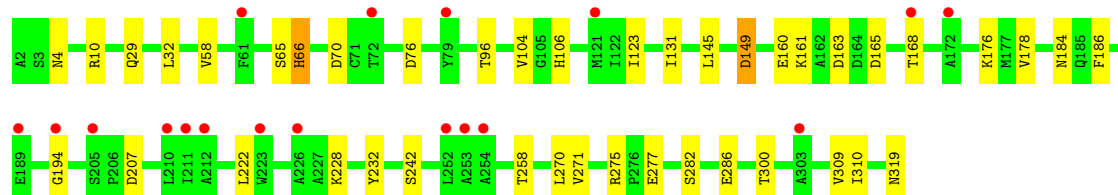
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:



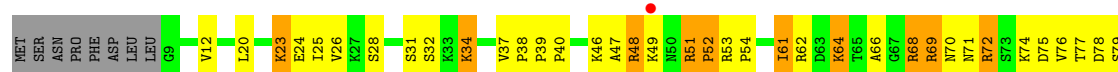
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

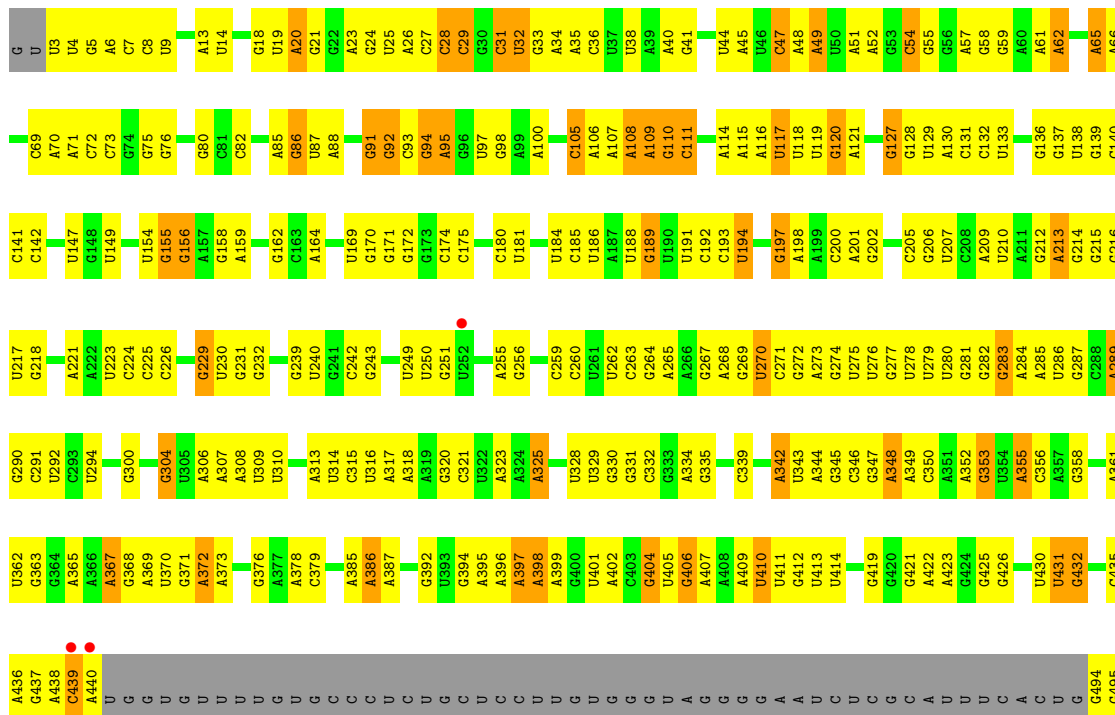
Chain sR:



• Molecule 35: Suppressor protein STM1

Chain SM:

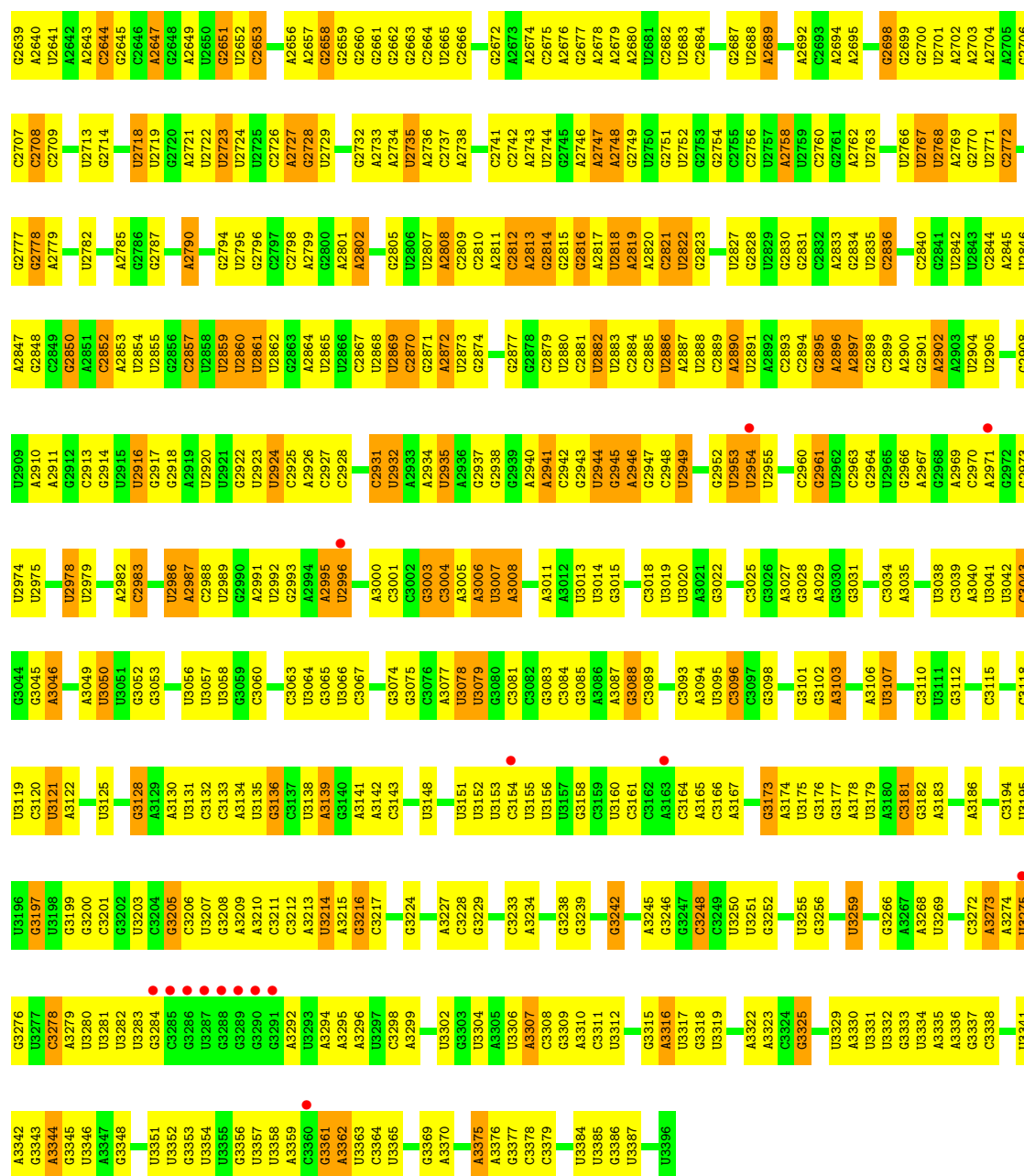






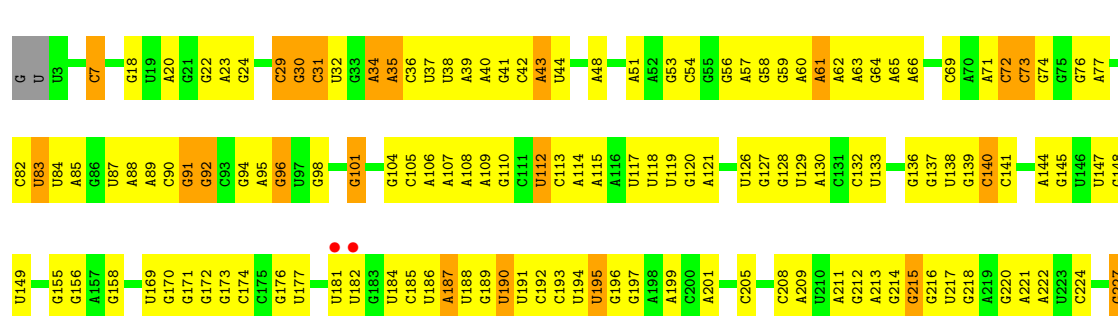






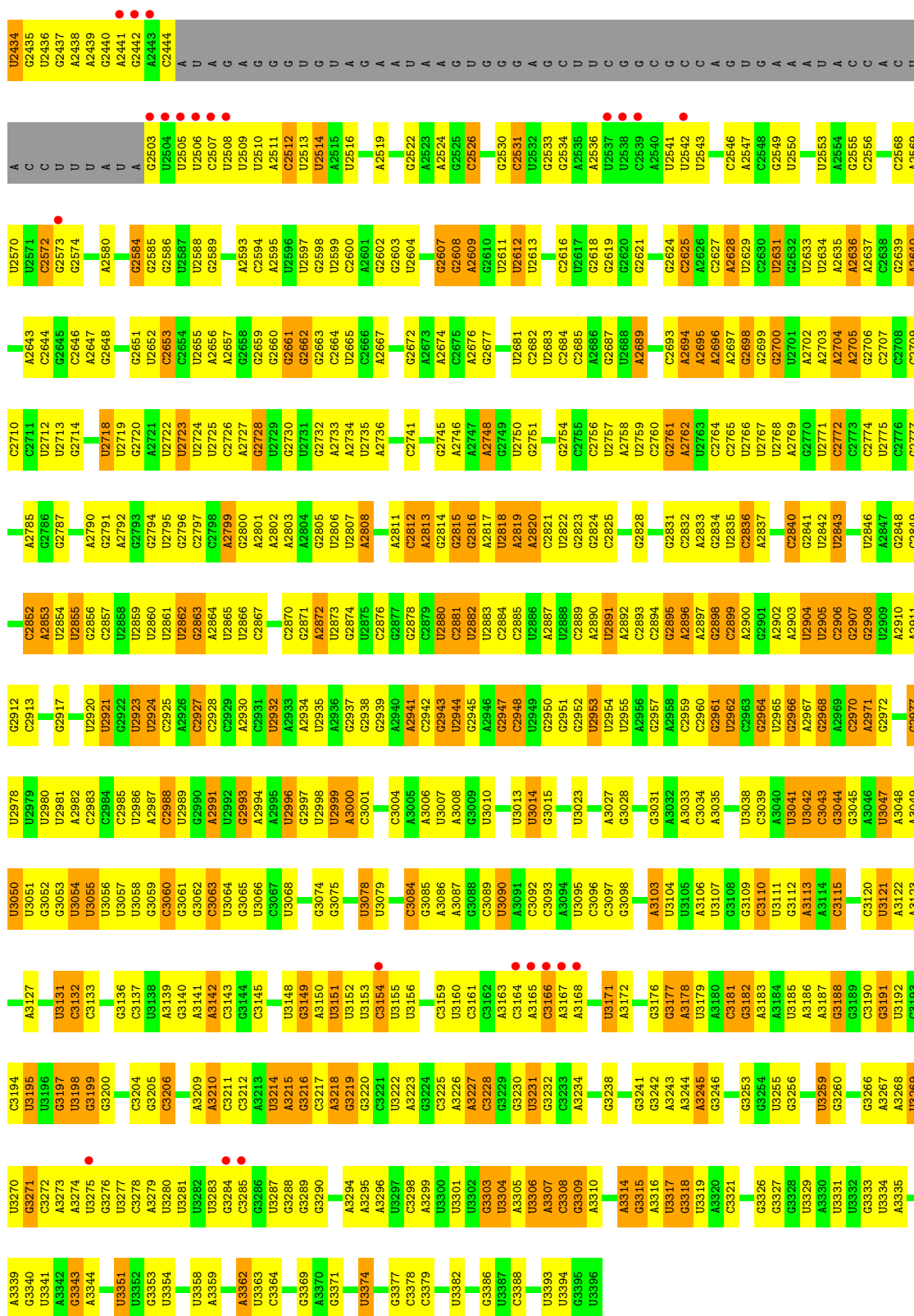
• Molecule 36: TPA\_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 5:



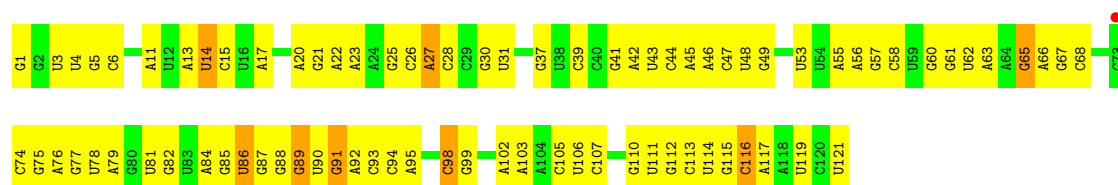
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A1211	G1142	U1073	U1004	U939	C873	U797	A716	G651	C586	U506	U	U382	U506	U230
A1212	G1143	U1074	U1004	G940	U874	C800	C717	G652	U587	U507	G	G383	U314	
G1213	U1144	A1075	G941	C941	C875	A801	G718	A653	G588	U508	U	A384	U316	G236
A1221	U1145	C1076	U1009	U942	C802	C802	U719	G654	A589	U509	U	A385	U316	G236
G1222	C1146	U1077	G1010	U943	C803	C803	A720	G655	G590	G510	U	A386	A317	
A1223	G1147		A1011	C944	C804	C804		A656	G591		U	A318	A319	G239
G1226	G1148	A1080	G1012	C945	G805	G805	G726	A657	A592	G514	G	A389	A319	U240
C1227	G1149	U1081	G1013	C946	A806	A806	G727	G658	C593	C515	U	G390	A323	G241
	G1150	U1082	U1014	U947	A807	A807	G728	G659	U594	A516	G	A391	A324	
	U1151	G1083	U1015	C948	A808	A808	C729	A660	G595	G517	C	G392	A324	G244
	G1152	A1084	U1016	C949	A809	A809	C730	G661	C596	G518	C	U393	A325	
	A1153		C1017	G950	A810	A810	U731	U662	G597	A519	C	G394	U326	C247
A1231	C1154	A1091	G1018	A951	G887	U811		C663	A598	U520	U	A395	U327	U248
C1232	G1155	C1092	G1019	A952	A888	G812	C734	U664	A521	U528	C	U328	U328	U249
G1233	C1156		G1020	G953	U889	G813	A735	A665	A522	A522	U	G397	U329	U250
G1234	G1157	U1095	G1021	U954	C890	A736	A736	A666	U601	G530	G	A398	G330	G251
U1235	A1158	U1096	U1022	U955	G891	A816	G737	C667	A602	U594	C	A399	G330	U252
G1236	A1159	G1097	C1023	U956	U892	A817	A738	G668	A603	C525	U	G400	G333	A253
G1237	C1160	A1098	G1024	C957	C893	G826	G739	U669	G604	U534	C	U401	G341	
C1238	G1161	A1099	A1025	C958	G894	U821	G740	U670	U605	U528	C	A402	A336	A255
C1239	U1162	U1100	C1026	C959	A895	G822	U741	U671	C606	A529	U	C403	G337	G267
A1240	A1163	G1101	A1027	U960	A896	C823	G742	A672	A607	G530	U	G404	A338	U257
U1241	G1164	A1102	U1028	C961	U897	C824	C743	U673	A608		G	U405	G339	G258
G1242	A1165	A1103	G1029	A962	U898	U825	A744		G609	U534	U	G406	C340	C259
	G1166	G1104	A1030	G963	U899	G826		A677	G610		G	A407	G341	
G1246	A1170	A1105	C1031	G964	G900	A830	A747	G678	A611	G538	G	A408	A342	G264
G1249	C1176	C1107	C1032	U965	G901	U831	U748	U679	U612	U541	G	A409	A344	G267
G1250	G1177	U1108	U1033	U966	G902	G832	C749	G680	G613	G542	U	U410	A344	A268
A1251	U1178	U1110	G1034	A967	U903	G833	G750	U681	C614	C543	A	U411	G345	
	A1179	U1111	A1036	C968	U905	G835	A751	U682	C618		G	U412	A348	G269
C1255	G1180	U1112	U1039	C969	U906	G835	G753	G684	A619	C546	G	U413	A349	U270
G1256	U1181	U1113	A1040	A970	G907	A836	C753	G685	U620	G547	G	U414	G349	C271
	A1182	U1114	U1041	A972	G908	A837	U756	G686	A621	G548	A	A416	A352	G272
G1261	C1183	G1115	U1042	A973	G909	G838	C757	U687	A622	U549	A	A417	G353	G274
G1262	A1184		C1043	C974	G910		U764	G688	U623	A550	U	A418	A353	U275
A1263	C1187	C1119	U1044	C975	C911	G845		U689	G624	A551	C	G419	C356	U276
G1264	U1188	A1120	C1045	U976	A914	A945	C768	A690	U629	G552	U	G420	A357	
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A1278	U1190		A1047	U979	A916	A848	G769	A692	C496	G421	C	U359	U359	U280
	U1191	U1124	C1048	A980	A917	U850	G770	C694	U631	U563	C	A423	G360	G281
G1284	C1192	U1125	C1049	U981	C918	C851	U776	C695	G632	G564	A	G424	A361	G282
G1285	A1193	G1126	U1050	C982	U919	G856		C696	C633	U565	U	G425	G384	G283
	G1194	U1127	U1051	A983	A920	G857	G781	A697	G634	G566	U	G426	A365	A284
			U1052	G984	A921	G857	U782	U698	C635	G567	U	C427	A366	A285
G1292	A1197	U1128	U1060	U985	U922	G857	A783		C636	G568	C	A428	A367	U286
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A1294	G1199	U1130	A1062	U990	G924	C861	G785	C702	G639	A570		G432	A369	C291
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C1297	G1203	A1133	A1064	G994	C928	C863	G787		C641	A572		U434	G371	C293
U1298	A1204	G1134	A1065	U995	C928	G864	A706	A706	U642	C573		C435	A372	
A1299	A1205	A1135	A1066	A996	U929	U865	G788	U707	U643	U574		A498	A373	G299
G1300	G1206	A1136	U1067	A997	U930	G867	G789	G708	G644	G499		A436	A374	G300
A1301	C1207	U1137	C1068	A998	U933	C868	A791		A645	C500		A438	A375	G301
A1302	G1207	U1138	C1069	A999	G934	G869	G792	A711	A646	A501		C439	G376	U302
A1303	U1208	G1139	U1070	C1000	G934	G870	C793	U713	C648	G583		U441	A378	G304

G2370	C2146	A2223	G2302	U1890	G1822	A1750	C1669	U1584	G1513	U1442	C1372	A1304
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A2372	U2148	U2225	G	G	G1824	G1752	G1677	G1586	G1517	U1444	G1374	G1306
A2373	G	G	G	G	G1825	G1753	G1677	A1587	G1518	U1445	U1378	G1307
G2374	C	C	G	C	A1896	G1754	G1680	A1588	G1519	A1446	U1379	U1308
G2375	C	C	G	C	G1827	G1755	U1681	A1589	G1520	U1447	G1380	U1309
G2376	U	U	C	C	A1828	G1756	U1681	A1590	U1521	U1448	G1381	G1310
G2377	C	C	C	U	U1831	G1757	C1685	G1591	U1522	A1449	A1382	G1311
G2378	A	A	U	C	G1832	G1758	C1685	G1592	U1523	G1450	G1382	C1312
U2379	G	G	G	G	A1833	C1759	U1688	A1593	G1524	G1451	G1383	G1313
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G2401	C	C	C	C	G1852	U1782	C1708	A1613	U1549	G1473	G1404	U1336
G2402	C	C	C	C	G1853	U1783	C1709	C1614	U1555	A1474	U1405	U1337
G2403	C	C	C	C	G1854	U1784	C1710	C1615	G1552	A1475	U1406	C1338
G2404	C	C	C	C	G1855	U1785	G1711	U1616	U1553	A1476	A1407	C1339
G2405	C	C	C	C	G1856	G1786	G1712	G1617	U1554	G1480	G1408	G1940
G2406	C	C	C	C	G1857	U1787	G1713	G1618	C1556	A1481	U1341	C1342
G2407	C	C	C	C	A1858	C1788	A1715	A1619	C1557	G1482	C1342	C1343
U2408	C	C	C	C	A1859	G1789	U1716	U1627	C1562	G1483	G1344	G1345
G2409	C	C	C	C	U1862	C1793	U1717	C1628	U1563	U1484	U1347	G1346
U2410	C	C	C	C	G1865	G1796	G1718	G1628	G1564	G1486	A1418	U1347
U2411	C	C	C	C	A1866	A1797	U1719	A1632	C1565	U1487	C1420	G1348
G2412	C	C	C	C	C1867	A1798	U1720	C1633	C1566	A1489	U1424	A1350
G2413	C	C	C	C	G1868	G1799	U1721	C1633	U1567	U1490	U1425	U1351
G2414	C	C	C	C	C1869	C1803	U1722	A1637	A1568	G1492	C1426	A1352
G2415	C	C	C	C	U1873	A1804	U1723	A1638	U1569	G1493	U1427	G1353
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G2417	C	C	C	C	G1875	A1806	C1725	G1652	U1569	A1495	G1429	A1355
G2418	C	C	C	C	U1876	G1807	C1726	G1653	U1570	C1496	U1430	U1356
G2419	C	C	C	C	G1877	G1808	A1729	A1654	U1571	U1497	U1431	U1356
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G2421	C	C	C	C	A1879	A1813	G1734	A1656	U1573	C1499	C1432	U1361
G2422	C	C	C	C	U1880	A1814	G1735	C1657	C1574	G1500	A1433	G1362
U2423	C	C	C	C	G1881	U1815	G1736	U1658	A1575	U1501	G1434	G1362
A2424	C	C	C	C	G1882	U1816	U1740	G1659	G1576	C1502	A1435	G1365
G2425	C	C	C	C	A1883	G1817	U1741	C1660	U1577	U1436	U1437	G1366
G2426	C	C	C	C	U1884	U1818	U1742	G1661	C1578	U1438	U1438	G1367
G2427	C	C	C	C	U1885	U1819	G1743	G1662	C1579	U1439	U1439	A1368
G2428	C	C	C	C	U1886	U1820	U1743	C1665	C1580	A1508	G1440	A1369
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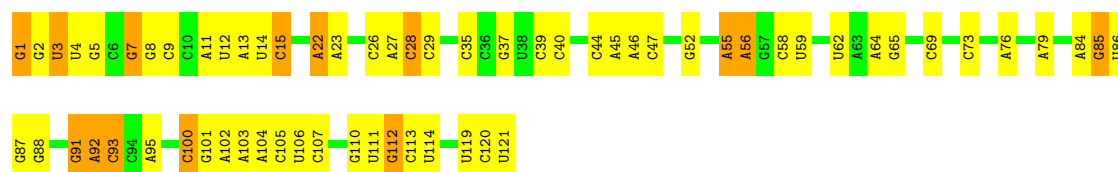
- Molecule 37: TPA\_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 3: 



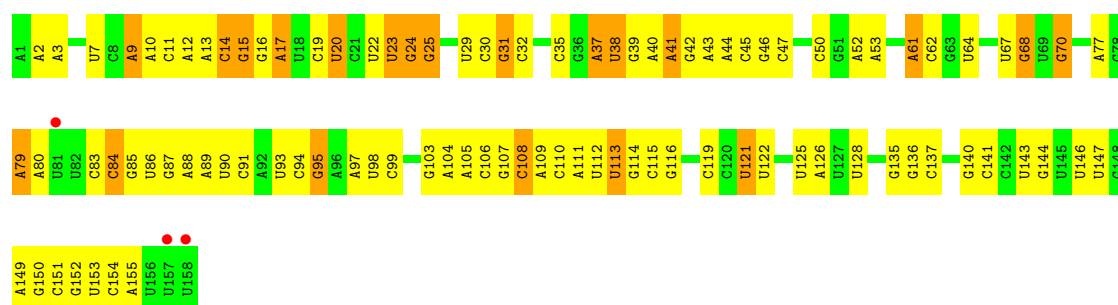
- Molecule 37: TPA\_inf: *Saccharomyces cerevisiae* S288c chromosome XII, complete sequence

Chain 7:



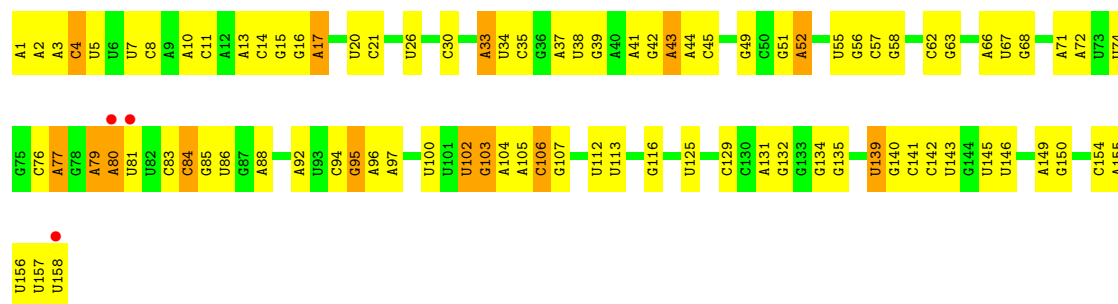
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



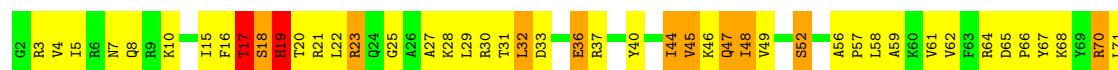
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

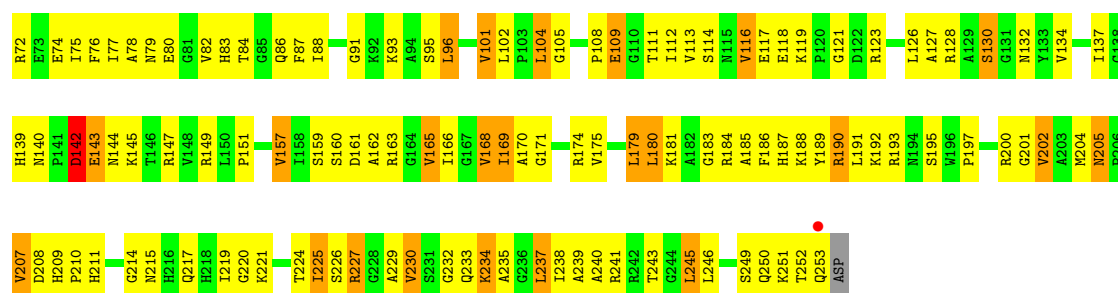
Chain 8:



- Molecule 39: 60S ribosomal protein L2-A

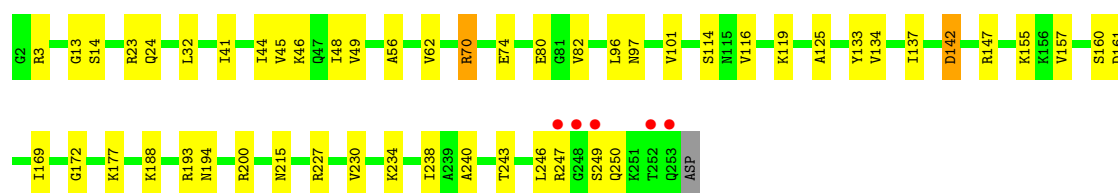
Chain L2:





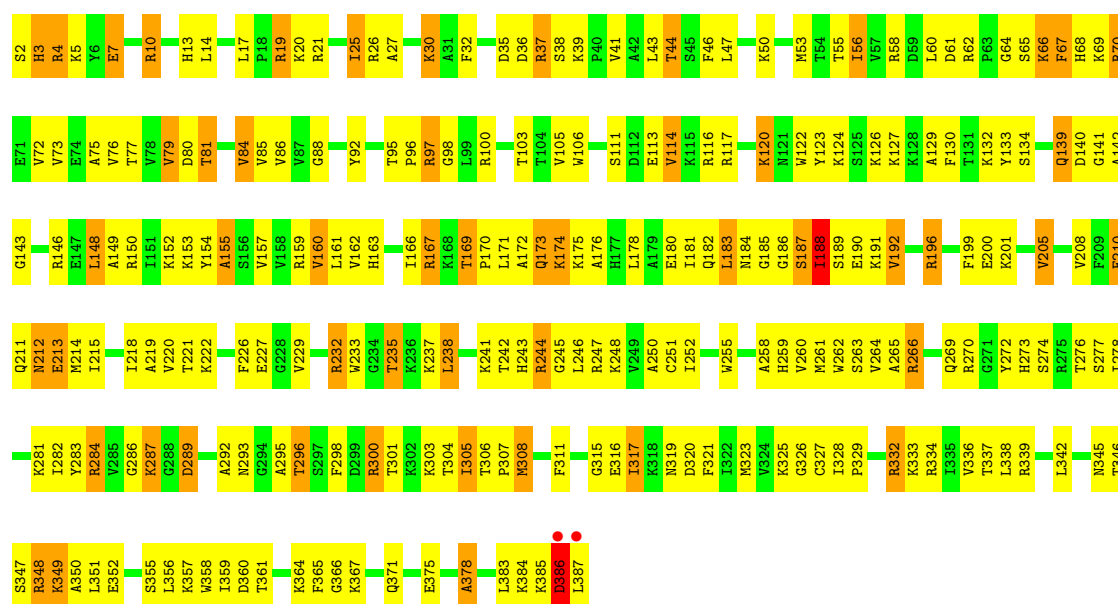
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



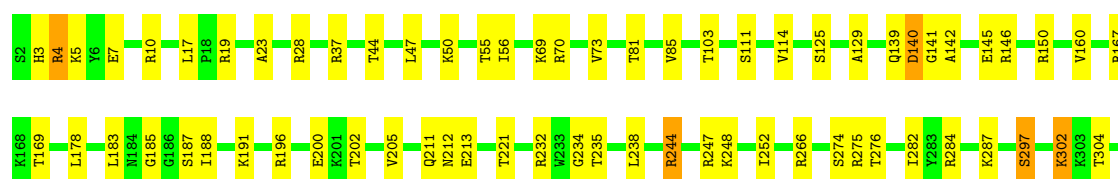
• Molecule 40: 60S ribosomal protein L3

Chain L3:



• Molecule 40: 60S ribosomal protein L3

Chain l3:

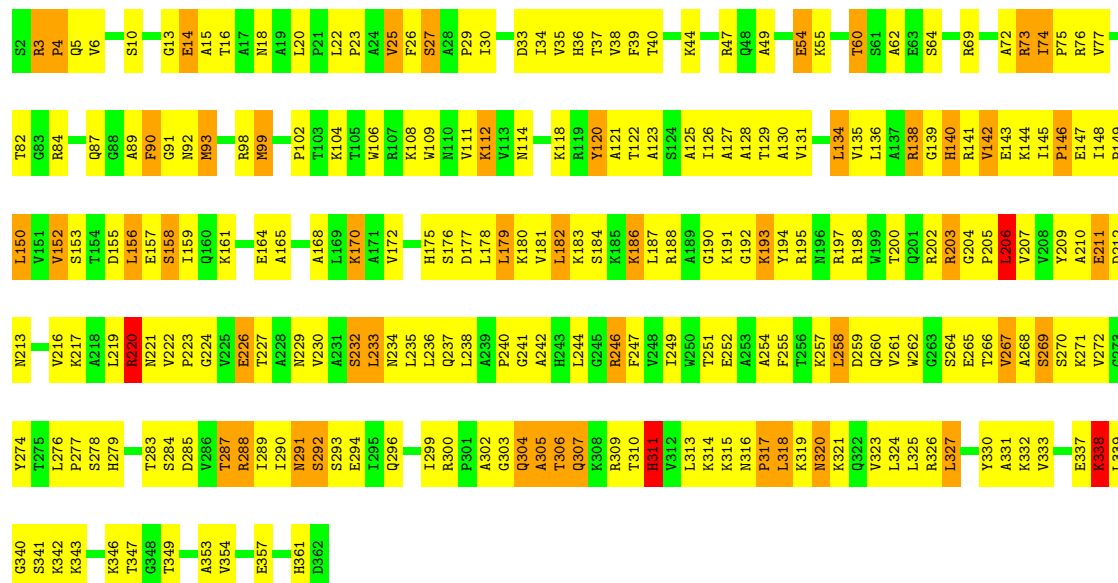






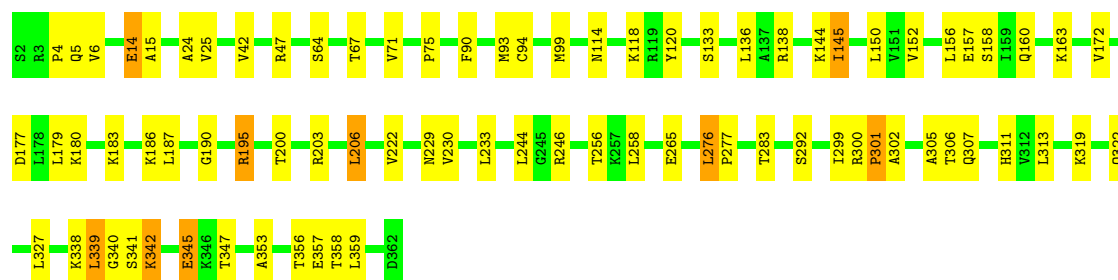
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



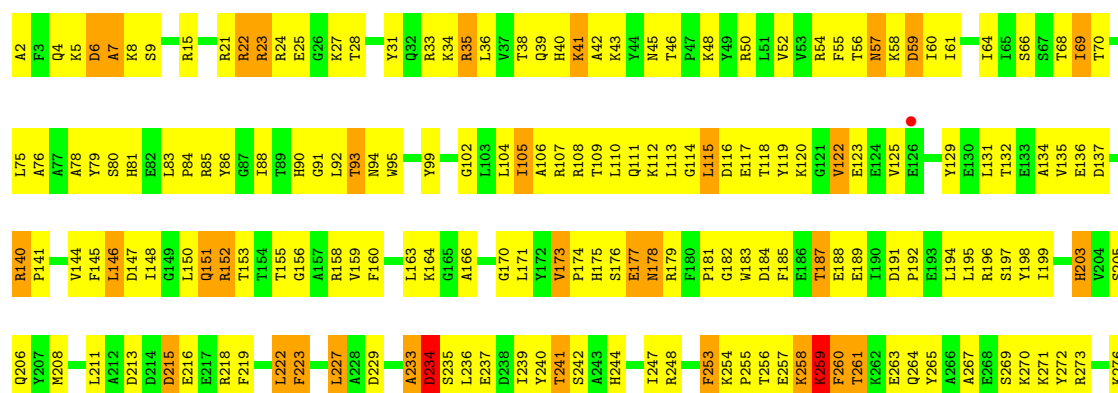
• Molecule 41: 60S ribosomal protein L4-A

Chain L4:



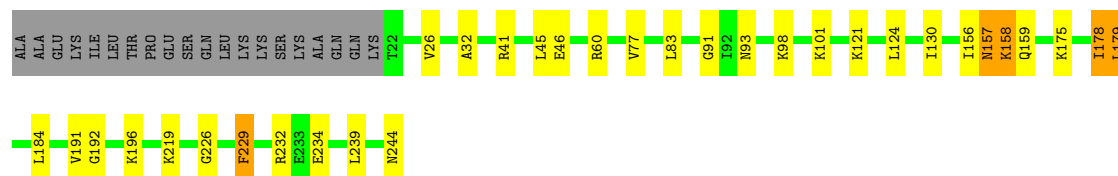
• Molecule 42: 60S ribosomal protein L5

Chain L5:



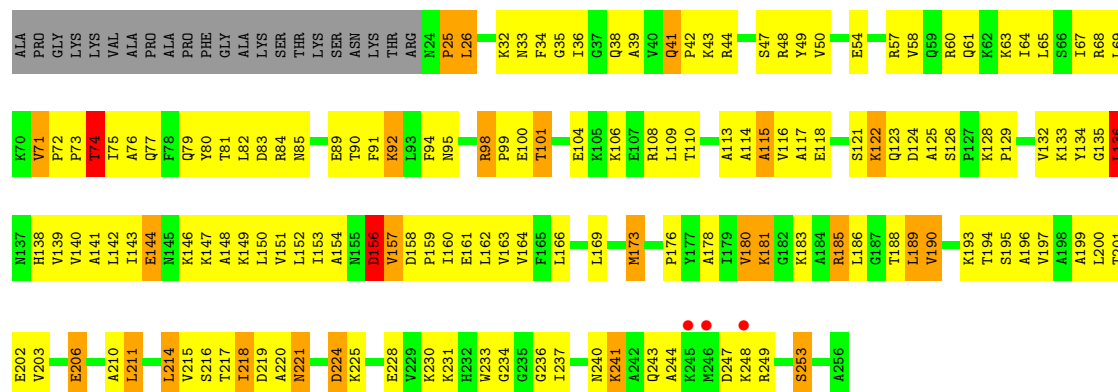


Chain 17:



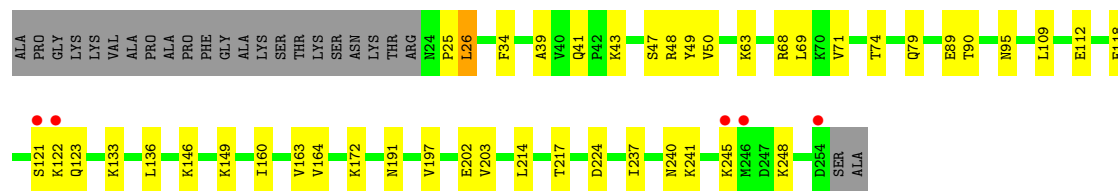
- Molecule 45: 60S ribosomal protein L8-A

Chain L8:



- Molecule 45: 60S ribosomal protein L8-A

Chain 18:



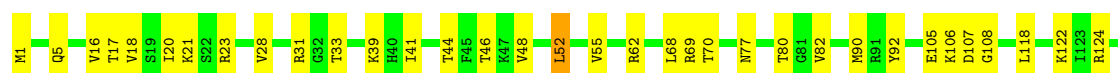
- Molecule 46: 60S ribosomal protein L9-A

Chain L9:



- Molecule 46: 60S ribosomal protein L9-A

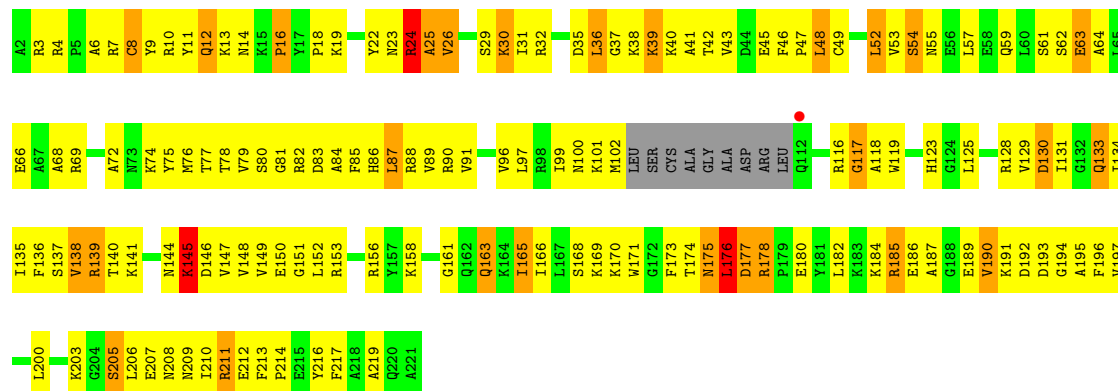
Chain 19:





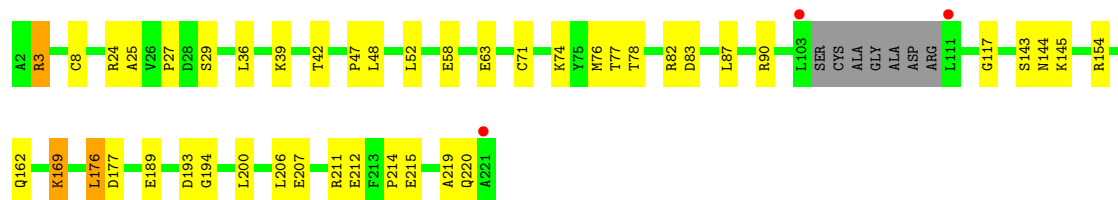
• Molecule 47: 60S ribosomal protein L10

Chain M0:



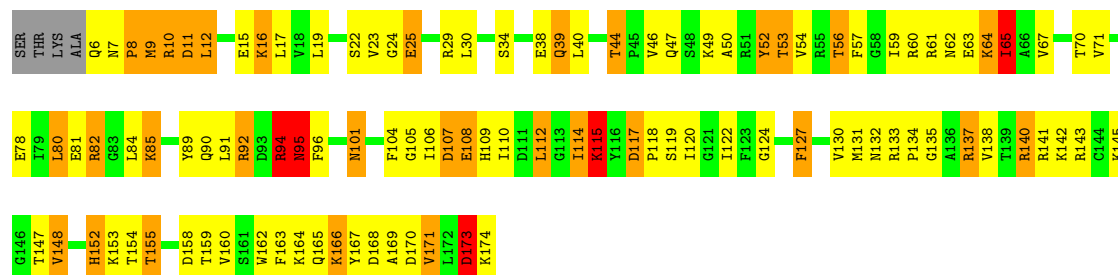
• Molecule 47: 60S ribosomal protein L10

Chain m0:



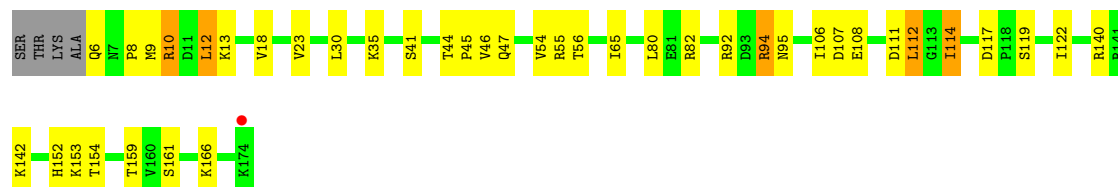
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



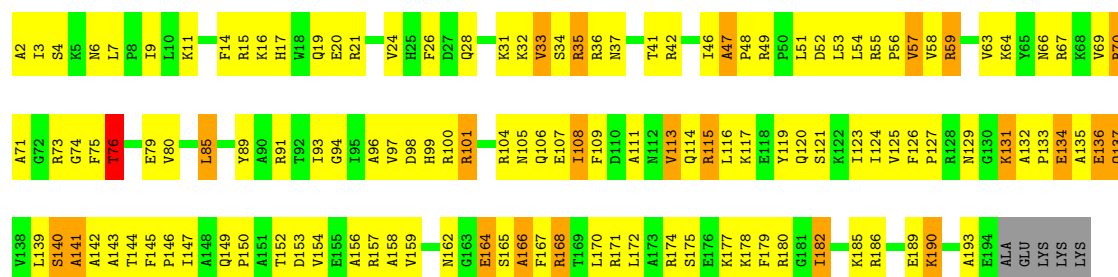
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



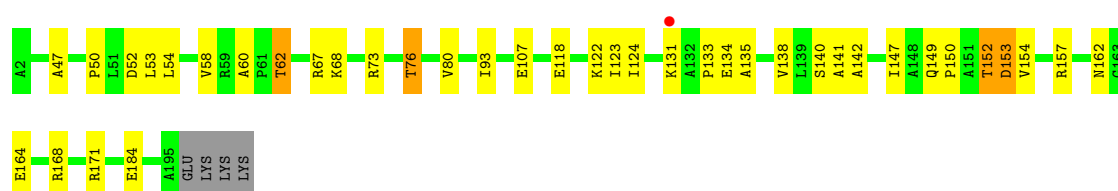
• Molecule 49: 60S ribosomal protein L13-A

## Chain M3:



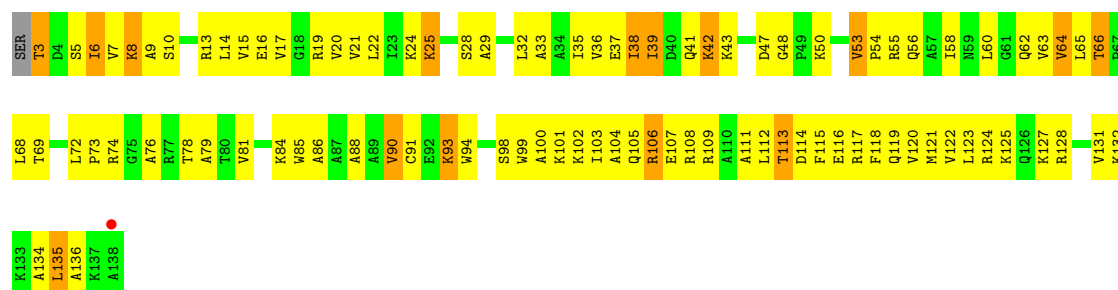
## • Molecule 49: 60S ribosomal protein L13-A

## Chain m3:



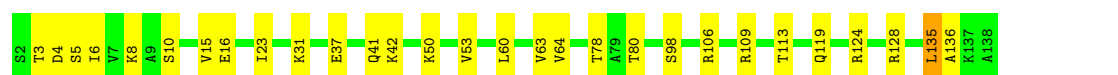
## • Molecule 50: 60S ribosomal protein L14-A

## Chain M4:



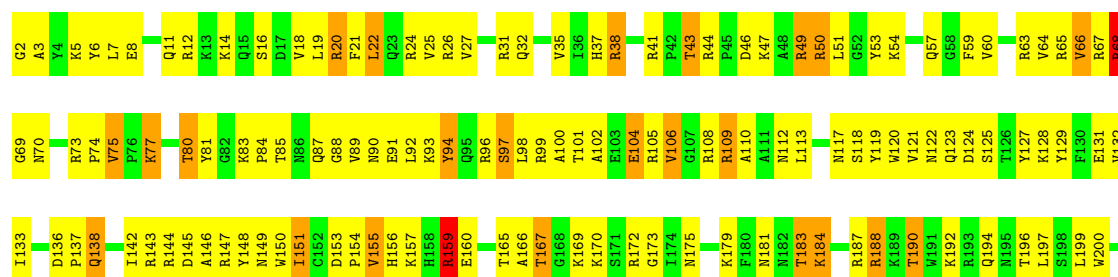
## • Molecule 50: 60S ribosomal protein L14-A

## Chain m4:



## • Molecule 51: 60S ribosomal protein L15-A

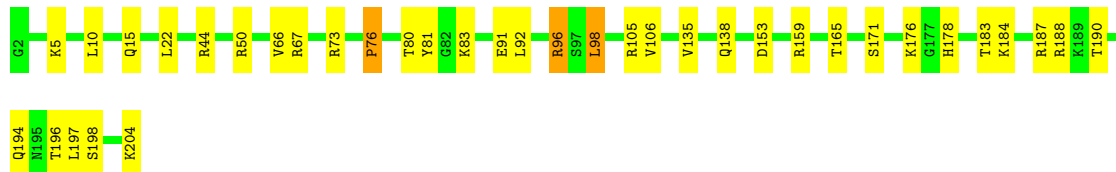
## Chain M5:



K204

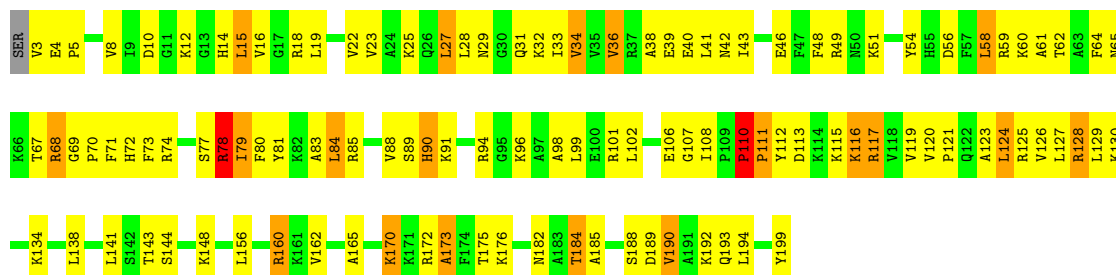
- Molecule 51: 60S ribosomal protein L15-A

Chain m5:



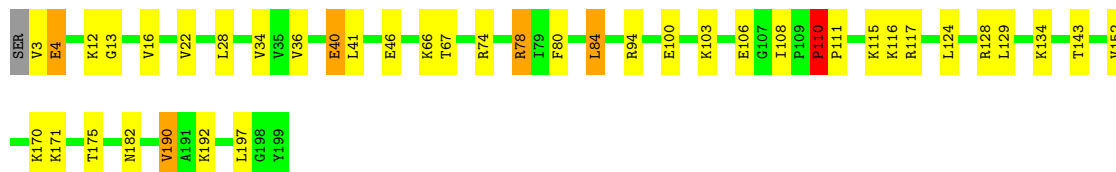
- Molecule 52: 60S ribosomal protein L16-A

Chain M6:



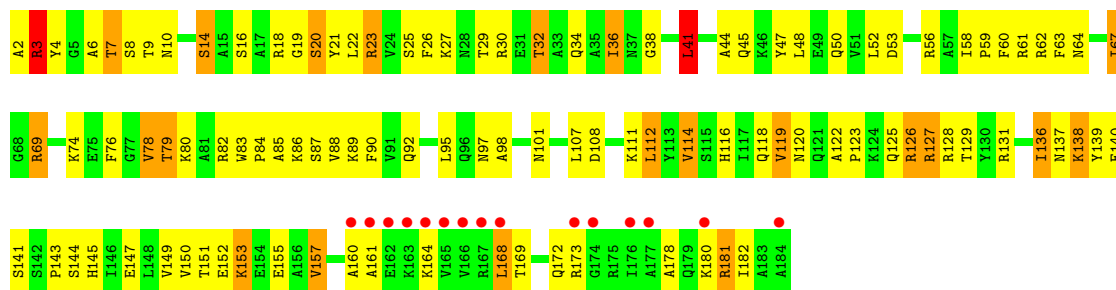
- Molecule 52: 60S ribosomal protein L16-A

Chain m6:



- Molecule 53: 60S ribosomal protein L17-A

Chain M7:

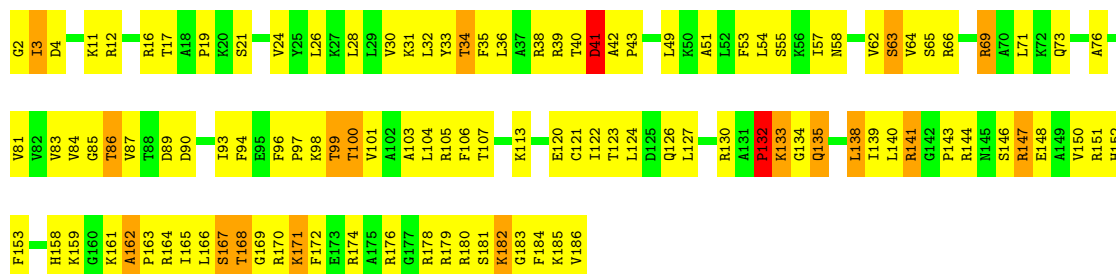


- Molecule 53: 60S ribosomal protein L17-A

Chain m7:

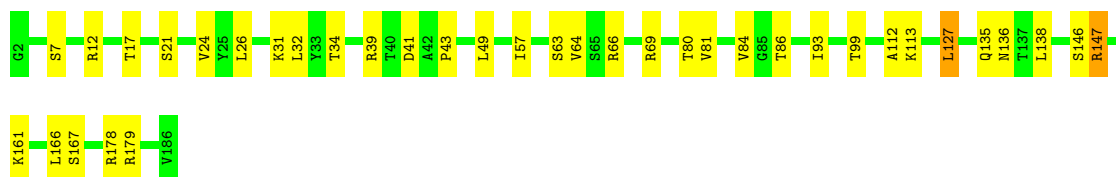


Chain M8:



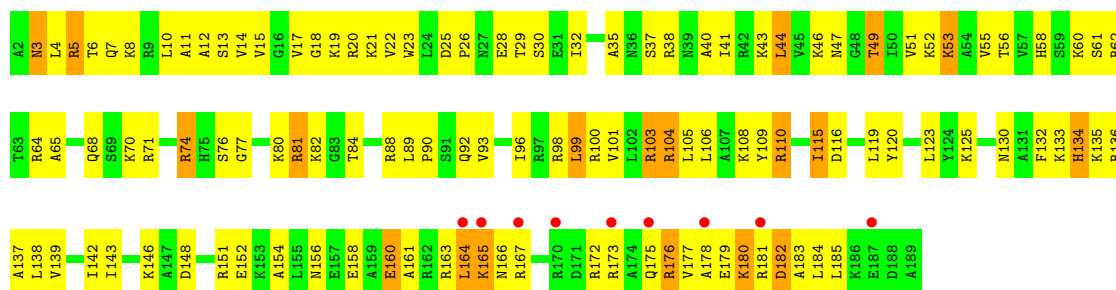
- Molecule 54: 60S ribosomal protein L18-A

Chain m8: 



- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



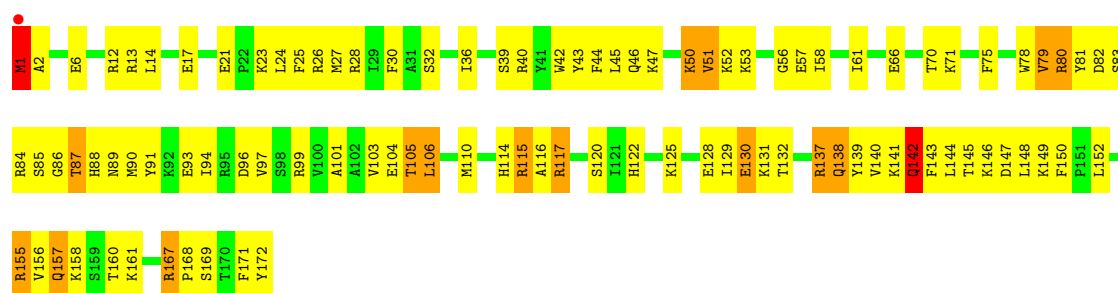
- Molecule 55: 60S ribosomal protein L19-A

Chain m9: 



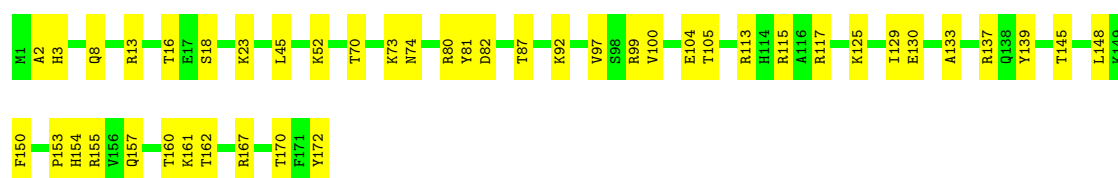
- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



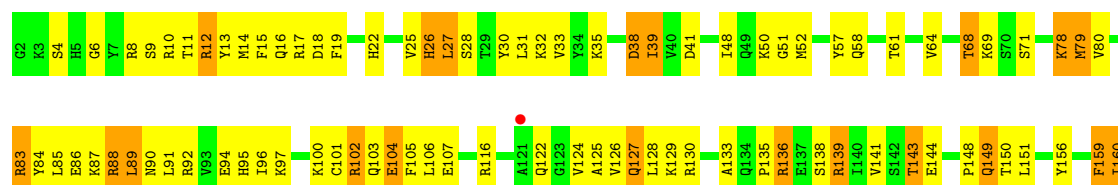
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



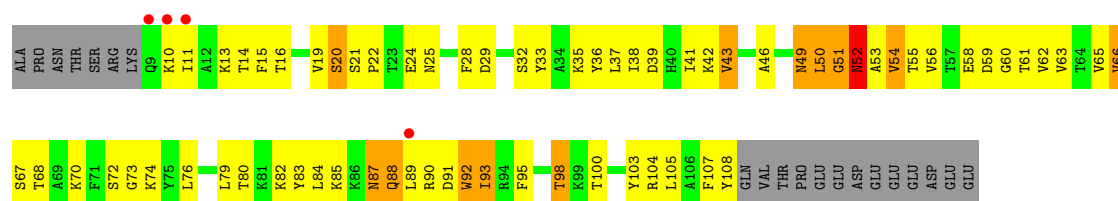
- Molecule 57: 60S ribosomal protein L21-A

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

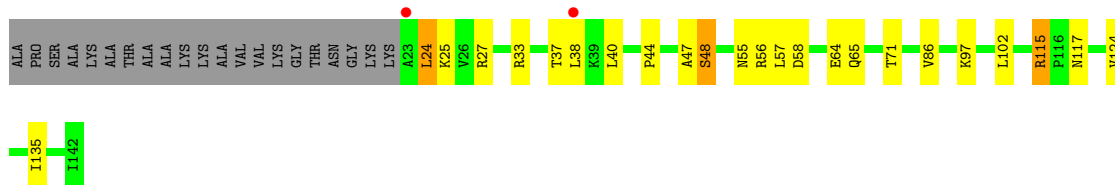
Chain N3:

- Molecule 59: 60S ribosomal protein L23-A

Chain n3:

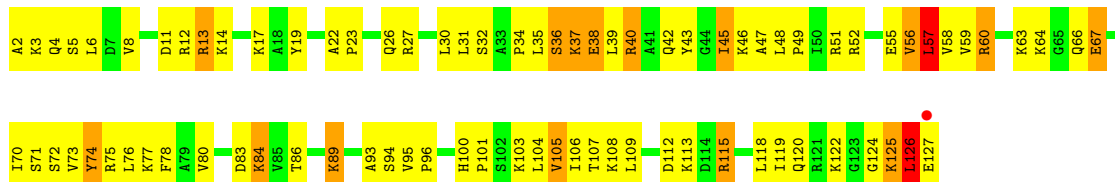
- Molecule 61: 60S ribosomal protein L25

Chain n5:



- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



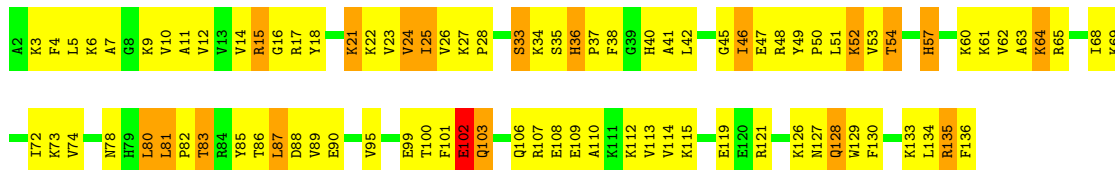
- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



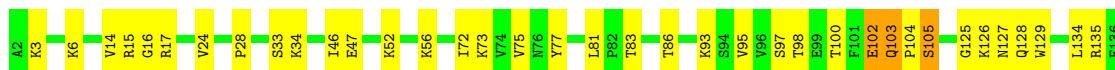
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



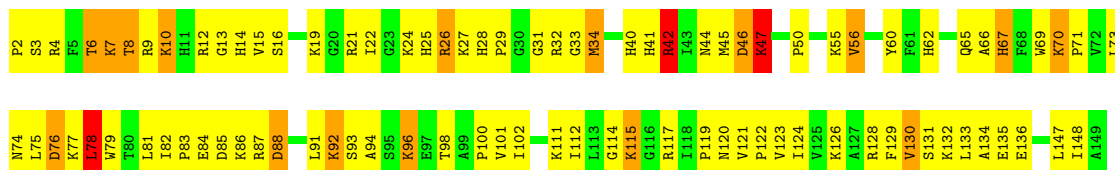
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



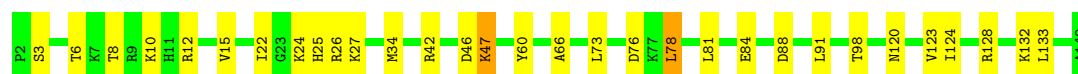
- Molecule 64: 60S ribosomal protein L28

Chain N8:



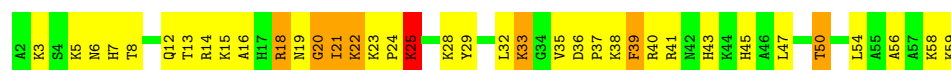
- Molecule 64: 60S ribosomal protein L28

Chain n8: 



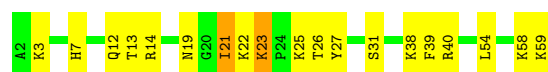
- Molecule 65: 60S ribosomal protein L29

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: 



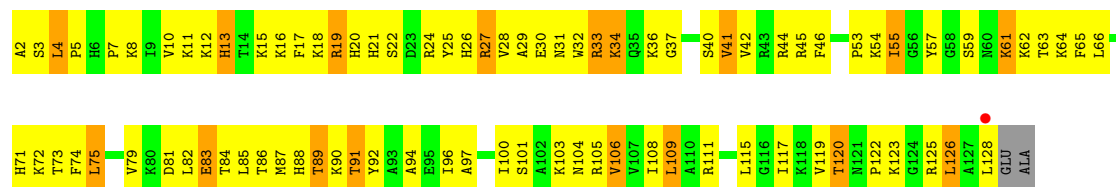
- Molecule 67: 60S ribosomal protein L31-A

Chain o1: 



- Molecule 68: 60S ribosomal protein L32

Chain O2:



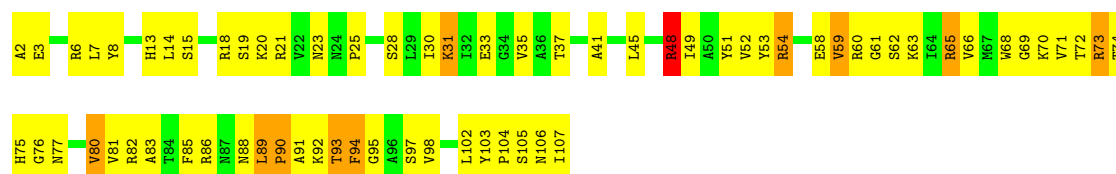
- Molecule 68: 60S ribosomal protein L32

Chain o2:



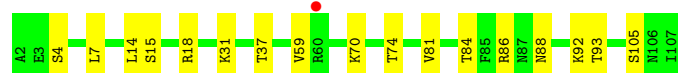
- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



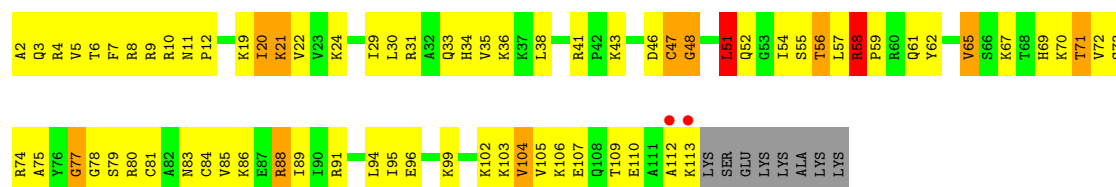
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



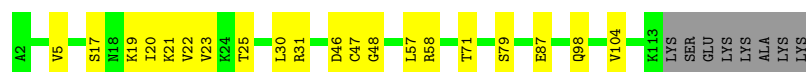
- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



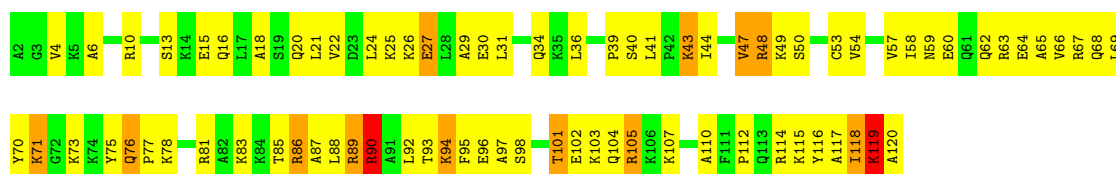
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



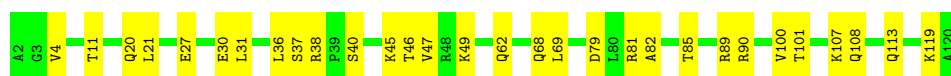
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



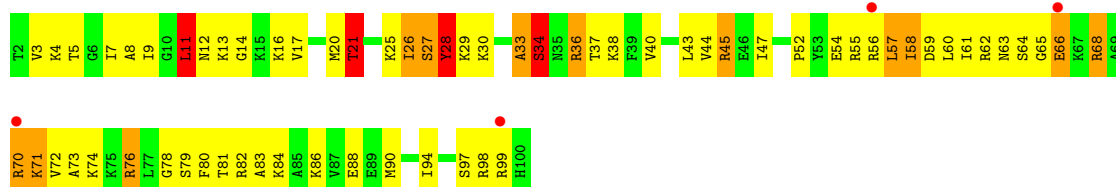
- Molecule 71: 60S ribosomal protein L35-A

Chain o5:



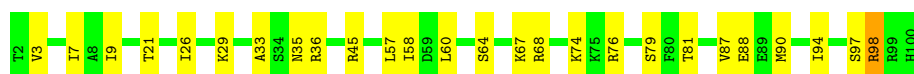
- Molecule 72: 60S ribosomal protein L36-A

Chain O6:



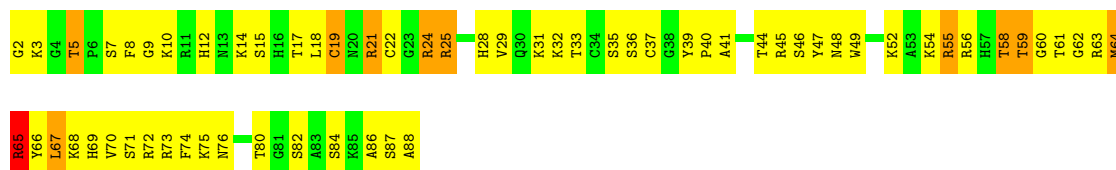
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



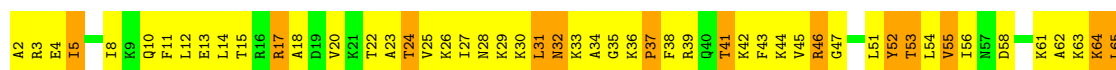
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



- Molecule 74: 60S ribosomal protein L38

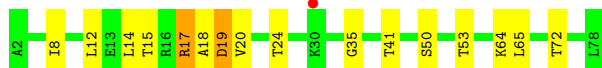
Chain O8:





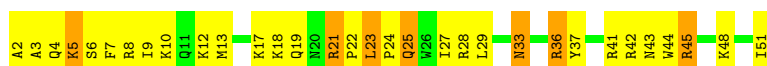
- Molecule 74: 60S ribosomal protein L38

Chain o8:



- Molecule 75: 60S ribosomal protein L39

Chain O9:



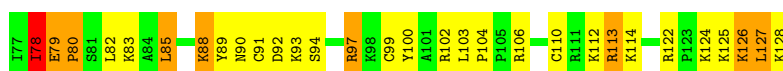
- Molecule 75: 60S ribosomal protein L39

Chain o9:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



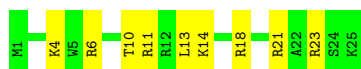
- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



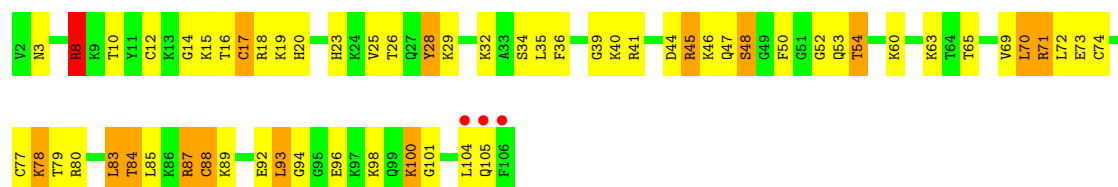
- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



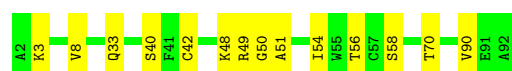
- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



- Molecule 79: 60S ribosomal protein L43-A

Chain q3:



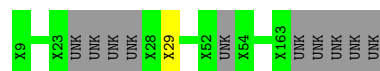
- Molecule 80: 40S ribosomal protein S30-A

Chain e0:



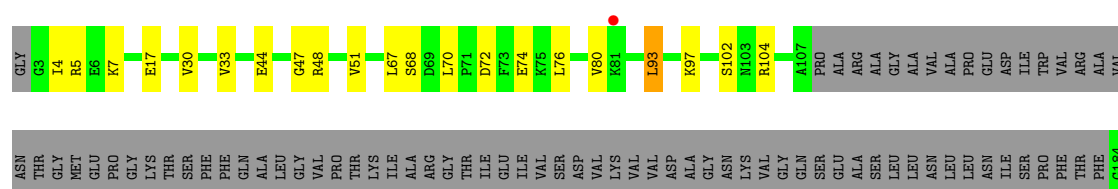
- Molecule 81: unknown protein chain m2

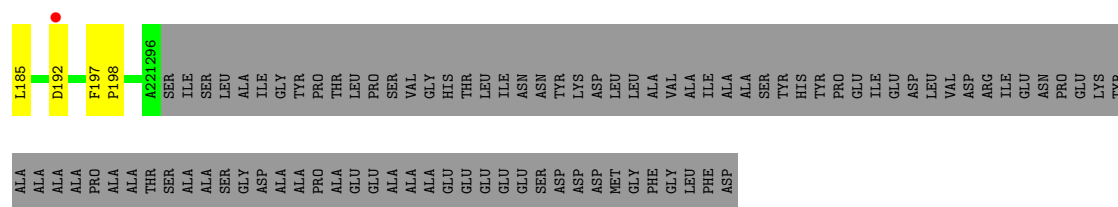
Chain m2:



- Molecule 82: 60S acidic ribosomal protein P0

Chain p0:





- Molecule 83: unknown protein chain p1

Chain p1: 

There are no outlier residues recorded for this chain.

- Molecule 84: unknown protein chain 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, $\alpha$ , $\beta$ , $\gamma$	435.34Å 287.00Å 303.36Å 90.00° 98.98° 90.00°	Depositor
Resolution (Å)	49.18 – 3.20 49.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.18-3.20) 99.9 (49.85-3.20)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.204 , 0.253 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	80.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 1205567 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	411178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, 3KF, 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	0.71	5/41698 (0.0%)	1.31	312/64972 (0.5%)
1	6	0.78	12/42765 (0.0%)	1.35	404/66634 (0.6%)
2	S0	0.44	0/1617	0.66	0/2215
2	s0	0.44	0/1623	0.65	0/2222
3	S1	0.39	0/1735	0.66	2/2335 (0.1%)
3	s1	0.49	0/1748	0.68	0/2352
4	S2	0.51	1/1665 (0.1%)	0.66	0/2263
4	s2	0.56	0/1665	0.75	1/2263 (0.0%)
5	S3	0.49	0/1759	0.68	0/2368
5	s3	0.41	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.72	2/2839 (0.1%)
6	s4	0.49	0/2109	0.72	0/2839
7	S5	0.38	0/1629	0.60	0/2202
7	s5	0.41	0/1629	0.61	0/2202
8	S6	0.47	0/1823	0.66	0/2439
8	s6	0.53	0/1779	0.69	0/2379
9	S7	0.43	0/1506	0.64	0/2028
9	s7	0.44	0/1516	0.63	0/2043
10	S8	0.54	0/1514	0.70	0/2021
10	s8	0.59	0/1514	0.75	3/2021 (0.1%)
11	S9	0.49	0/1519	0.69	1/2035 (0.0%)
11	s9	0.52	0/1519	0.72	2/2035 (0.1%)
12	C0	0.45	0/790	0.71	1/1069 (0.1%)
12	c0	0.36	0/777	0.64	3/1049 (0.3%)
13	C1	0.56	0/1239	0.66	0/1673
13	c1	0.57	0/1194	0.74	1/1610 (0.1%)
14	C2	0.37	0/900	0.66	0/1224
14	c2	0.31	0/900	0.58	0/1224
15	C3	0.50	0/1215	0.66	2/1638 (0.1%)
15	c3	0.53	0/1215	0.70	0/1638
16	C4	0.40	0/901	0.66	0/1217
16	c4	0.51	0/960	0.73	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	C5	0.46	0/998	0.66	0/1341
17	c5	0.47	0/1060	0.69	0/1426
18	C6	0.44	0/1125	0.68	2/1510 (0.1%)
18	c6	0.44	0/1131	0.65	0/1518
19	C7	0.43	0/935	0.65	0/1254
19	c7	0.45	0/914	0.68	0/1224
20	C8	0.43	0/1211	0.65	1/1628 (0.1%)
20	c8	0.45	0/1211	0.66	1/1628 (0.1%)
21	C9	0.41	0/1130	0.60	0/1517
21	c9	0.46	0/1130	0.66	0/1517
22	D0	0.43	0/865	0.65	0/1169
22	d0	0.43	0/892	0.65	0/1205
23	D1	0.42	0/693	0.63	0/935
23	d1	0.50	0/693	0.70	0/935
24	D2	0.53	0/1038	0.72	0/1395
24	d2	0.56	0/1038	0.73	1/1395 (0.1%)
25	D3	0.60	0/1139	0.77	0/1518
25	d3	0.66	0/1139	0.81	2/1518 (0.1%)
26	D4	0.45	0/1087	0.61	0/1449
26	d4	0.51	0/1087	0.71	0/1449
27	D5	0.39	0/571	0.72	0/768
27	d5	0.41	0/566	0.65	0/761
28	D6	0.46	0/782	0.71	0/1047
28	d6	0.57	0/782	0.73	0/1047
29	D7	0.44	0/620	0.66	0/838
29	d7	0.47	0/620	0.74	0/838
30	D8	0.37	0/499	0.60	0/670
30	d8	0.40	0/499	0.64	0/670
31	D9	0.53	0/452	0.70	1/600 (0.2%)
31	d9	0.46	0/452	0.61	0/600
32	E0	0.47	0/483	0.62	0/643
33	E1	0.47	0/577	0.79	0/770
33	e1	0.39	0/619	0.71	0/822
34	SR	0.36	0/2494	0.57	0/3393
34	sR	0.35	0/2495	0.56	0/3395
35	SM	0.51	0/1113	0.71	2/1502 (0.1%)
35	sM	0.46	0/683	0.68	1/923 (0.1%)
36	1	1.08	102/75394 (0.1%)	1.68	1977/117545 (1.7%)
36	5	1.10	107/75414 (0.1%)	1.70	2076/117575 (1.8%)
37	3	0.91	3/2883 (0.1%)	1.45	38/4491 (0.8%)
37	7	1.04	3/2883 (0.1%)	1.64	63/4491 (1.4%)
38	4	1.03	0/3746	1.64	78/5832 (1.3%)
38	8	0.95	0/3746	1.54	62/5832 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.70	0/1948	0.84	1/2617 (0.0%)
39	l2	0.65	0/1946	0.85	1/2614 (0.0%)
40	L3	0.72	1/3146 (0.0%)	0.80	0/4228
40	l3	0.78	0/3146	0.86	2/4228 (0.0%)
41	L4	0.76	0/2800	0.90	3/3790 (0.1%)
41	l4	0.75	1/2800 (0.0%)	0.92	5/3790 (0.1%)
42	L5	0.56	0/2425	0.69	0/3271
42	l5	0.70	0/2408	0.80	1/3248 (0.0%)
43	L6	0.72	0/1260	0.81	1/1694 (0.1%)
43	l6	0.77	0/1269	0.82	2/1705 (0.1%)
44	L7	0.79	0/1821	0.87	2/2451 (0.1%)
44	l7	0.83	0/1828	0.91	4/2461 (0.2%)
45	L8	0.54	0/1836	0.68	0/2481
45	l8	0.49	0/1795	0.65	0/2429
46	L9	0.68	0/1539	0.79	0/2073
46	l9	0.77	0/1539	0.83	1/2073 (0.0%)
47	M0	0.71	1/1741 (0.1%)	0.84	3/2335 (0.1%)
47	m0	0.72	1/1758 (0.1%)	0.81	1/2358 (0.0%)
48	M1	0.50	0/1374	0.72	0/1842
48	m1	0.63	0/1374	0.80	2/1842 (0.1%)
49	M3	0.74	0/1568	0.84	0/2106
49	m3	0.69	0/1573	0.79	0/2113
50	M4	0.74	0/1068	0.83	0/1438
50	m4	0.78	0/1074	0.81	1/1446 (0.1%)
51	M5	0.73	0/1757	0.90	2/2354 (0.1%)
51	m5	0.65	0/1757	0.83	3/2354 (0.1%)
52	M6	0.84	0/1585	0.88	3/2128 (0.1%)
52	m6	0.95	2/1585 (0.1%)	0.94	4/2128 (0.2%)
53	M7	0.77	0/1443	0.86	2/1944 (0.1%)
53	m7	0.91	0/1250	0.88	0/1683
54	M8	0.75	0/1465	0.88	1/1965 (0.1%)
54	m8	0.75	0/1465	0.88	1/1965 (0.1%)
55	M9	0.56	0/1538	0.65	0/2050
55	m9	0.56	0/1538	0.67	0/2050
56	N0	0.75	0/1481	0.81	0/1990
56	n0	0.86	0/1481	0.89	1/1990 (0.1%)
57	N1	0.72	0/1300	0.78	0/1743
57	n1	0.79	1/1300 (0.1%)	0.84	1/1743 (0.1%)
58	N2	0.45	0/812	0.59	0/1099
58	n2	0.46	0/794	0.69	0/1076
59	N3	0.69	0/1018	0.82	0/1369
59	n3	0.78	0/1018	0.85	1/1369 (0.1%)
60	N4	0.56	0/712	0.68	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	n4	0.62	0/1052	0.73	0/1398
61	N5	0.65	0/979	0.82	1/1321 (0.1%)
61	n5	0.64	0/974	0.80	1/1314 (0.1%)
62	N6	0.68	0/1004	0.87	1/1341 (0.1%)
62	n6	0.67	0/1004	0.84	0/1341
63	N7	0.53	0/1118	0.65	0/1497
63	n7	0.53	0/1118	0.68	0/1497
64	N8	0.76	0/1204	0.90	2/1612 (0.1%)
64	n8	0.77	0/1204	0.86	1/1612 (0.1%)
65	N9	0.66	0/473	0.75	0/629
65	n9	0.71	0/473	0.96	1/629 (0.2%)
66	O0	0.50	0/751	0.69	0/1008
66	o0	0.49	0/775	0.66	0/1040
67	O1	0.63	0/890	0.72	0/1196
67	o1	0.73	0/897	0.86	0/1205
68	O2	0.82	0/1041	0.90	0/1394
68	o2	0.81	0/1041	0.90	1/1394 (0.1%)
69	O3	0.87	0/868	0.94	2/1168 (0.2%)
69	o3	0.87	0/868	0.91	2/1168 (0.2%)
70	O4	0.60	0/890	0.77	2/1189 (0.2%)
70	o4	0.58	0/890	0.79	0/1189
71	O5	0.71	0/978	0.81	1/1301 (0.1%)
71	o5	0.58	0/974	0.72	1/1297 (0.1%)
72	O6	0.63	0/778	0.77	0/1034
72	o6	0.56	0/777	0.68	0/1033
73	O7	0.76	0/696	0.95	2/923 (0.2%)
73	o7	0.68	0/696	0.84	0/923
74	O8	0.55	0/618	0.67	0/826
74	o8	0.53	0/614	0.66	0/822
75	O9	0.77	0/443	0.91	0/588
75	o9	0.67	0/443	0.85	0/588
76	Q0	0.72	0/423	0.82	0/562
76	q0	0.86	0/423	0.93	0/562
77	Q1	0.62	0/234	0.81	0/300
77	q1	0.80	0/234	1.02	0/300
78	Q2	0.80	1/860 (0.1%)	0.84	2/1136 (0.2%)
78	q2	0.75	1/860 (0.1%)	0.82	2/1136 (0.2%)
79	Q3	0.70	0/701	0.80	0/934
79	q3	0.70	0/701	0.82	1/934 (0.1%)
80	e0	0.53	0/499	0.74	0/665
82	p0	0.45	0/978	0.62	0/1316
All	All	0.84	242/429959 (0.1%)	1.32	5111/631204 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	s3	0	1
7	s5	0	2
9	S7	0	1
10	S8	0	1
11	s9	0	1
16	C4	0	2
18	c6	0	1
19	C7	0	1
19	c7	0	1
22	d0	0	1
25	D3	0	1
27	D5	0	2
33	E1	0	1
39	L2	0	2
40	l3	0	1
41	L4	0	1
44	l7	0	2
45	L8	0	1
48	M1	0	1
50	m4	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
56	n0	0	3
64	n8	0	1
65	N9	0	1
69	o3	0	1
72	O6	0	1
75	O9	0	1
81	m2	0	1
All	All	0	37

The worst 5 of 242 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	12.79	2.04	1.82
36	5	1152	G	N9-C4	-11.94	1.28	1.38
36	1	3181	C	N3-C4	-9.75	1.27	1.33
36	1	895	A	C5-C6	-9.41	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	9.34	1.98	1.82

The worst 5 of 5111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-26.30	110.22	126.00
36	5	1152	G	N3-C4-C5	25.75	141.47	128.60
36	5	1152	G	C2-N3-C4	-18.79	102.51	111.90
36	5	929	A	O5'-P-OP2	-14.22	92.90	105.70
36	1	2420	C	O5'-P-OP1	-13.73	93.34	105.70

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	38	THR	Peptide
19	C7	85	VAL	Peptide
9	S7	131	PHE	Peptide
10	S8	147	ALA	Peptide

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18758	957	0
1	6	38238	0	19241	989	0
2	S0	1577	0	1567	160	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	166	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	146	0
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	142	0
5	s3	1734	0	1817	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S4	2068	0	2154	153	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	158	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	130	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	119	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	139	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	134	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	63	0
12	c0	762	0	699	0	0
13	C1	1213	0	1257	83	0
13	c1	1168	0	1233	0	0
14	C2	892	0	891	68	0
14	c2	892	0	891	0	0
15	C3	1192	0	1255	98	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	96	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	105	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	93	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	127	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	97	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	70	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	76	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	94	0
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	99	0
26	d4	1073	0	1132	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	D5	563	0	603	67	0
27	d5	558	0	598	0	0
28	D6	769	0	814	112	0
28	d6	769	0	814	0	0
29	D7	610	0	631	39	0
29	d7	610	0	632	0	0
30	D8	497	0	535	46	0
30	d8	497	0	535	0	0
31	D9	442	0	429	44	0
31	d9	442	0	428	0	0
32	E0	475	0	525	28	0
33	E1	566	0	602	59	0
33	e1	608	0	656	0	0
34	SR	2441	0	2397	176	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	62	0
35	sM	680	0	607	0	0
36	1	67355	0	33847	1359	1
36	5	67376	0	33860	1383	0
37	3	2579	0	1304	63	0
37	7	2579	0	1303	55	1
38	4	3353	0	1695	69	0
38	8	3353	0	1695	65	0
39	L2	1914	0	1981	184	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	251	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	237	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	208	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	109	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	130	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	133	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	152	0
46	l9	1518	0	1587	0	0
47	M0	1705	0	1735	155	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	141	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	97	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	158	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	125	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	111	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	125	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	133	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	97	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	107	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	52	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	90	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	38	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	78	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	90	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	82	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1214	105	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	43	0
65	n9	462	0	491	0	0
66	O0	743	0	797	66	0
66	o0	767	0	816	0	0
67	O1	876	0	912	59	0
67	o1	883	0	918	0	0
68	O2	1020	0	1090	94	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	o3	850	0	880	0	0
70	O4	880	0	945	73	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	79	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	78	0
72	o6	770	0	846	0	0
73	O7	681	0	683	61	0
73	o7	681	0	683	0	0
74	O8	612	0	682	61	0
74	o8	608	0	671	0	0
75	O9	436	0	475	45	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	30	0
76	q0	417	0	455	0	0
77	Q1	233	0	284	23	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	53	0
78	q2	847	0	917	0	0
79	Q3	694	0	734	51	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	177	0	0
82	p0	1076	0	989	0	0
83	p1	235	0	51	0	0
84	p2	230	0	50	0	0
85	1	472	0	0	0	0
85	2	125	0	0	0	0
85	3	14	0	0	0	0
85	4	20	0	0	0	0
85	5	501	0	0	0	0
85	6	144	0	0	0	0
85	7	17	0	0	0	0
85	8	13	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	1	0	0	0	0
85	L3	1	0	0	0	0
85	L4	1	0	0	0	0
85	L5	1	0	0	0	0
85	L7	4	0	0	0	0
85	L8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	M0	2	0	0	0	0
85	M1	1	0	0	0	0
85	M3	3	0	0	0	0
85	M5	2	0	0	0	0
85	M6	2	0	0	0	0
85	M7	5	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	3	0	0	0	0
85	N5	2	0	0	0	0
85	N6	1	0	0	0	0
85	N8	4	0	0	0	0
85	O2	1	0	0	0	0
85	O7	3	0	0	0	0
85	Q2	1	0	0	0	0
85	S2	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c4	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	2	0	0	0	0
85	d3	2	0	0	0	0
85	d4	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	2	0	0	0	0
85	l3	2	0	0	0	0
85	l4	1	0	0	0	0
85	l5	1	0	0	0	0
85	l7	1	0	0	0	0
85	l9	1	0	0	0	0
85	m5	3	0	0	0	0
85	m6	3	0	0	0	0
85	m7	5	0	0	0	0
85	n0	3	0	0	0	0
85	n3	2	0	0	0	0
85	n6	2	0	0	0	0
85	n8	4	0	0	0	0
85	n9	1	0	0	0	0
85	o1	2	0	0	0	0
85	o3	1	0	0	0	0
85	o4	1	0	0	0	0
85	o7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	o9	1	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	2	0	0	0	0
85	s1	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	3	0	0	0	0
85	sM	2	0	0	0	0
86	1	2429	0	0	195	0
86	2	1113	0	0	109	1
86	3	84	0	0	3	0
86	4	126	0	0	12	0
86	5	2457	0	0	215	1
86	6	1106	0	0	107	0
86	7	77	0	0	4	0
86	8	119	0	0	23	0
86	C3	7	0	0	0	0
86	C5	7	0	0	4	0
86	C8	7	0	0	0	0
86	D9	7	0	0	0	0
86	L3	14	0	0	2	0
86	L4	7	0	0	2	0
86	M0	7	0	0	1	0
86	M5	7	0	0	1	0
86	M7	14	0	0	3	0
86	M8	7	0	0	0	0
86	M9	7	0	0	0	0
86	N1	7	0	0	1	0
86	N9	7	0	0	0	0
86	O3	7	0	0	1	0
86	O7	14	0	0	4	0
86	Q2	7	0	0	4	0
86	S8	7	0	0	0	0
86	SR	7	0	0	0	0
86	c3	7	0	0	0	0
86	c5	7	0	0	0	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	14	0	0	0	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	n3	14	0	0	0	0
86	n5	7	0	0	0	0
86	n9	7	0	0	0	0
86	o2	7	0	0	0	0
86	o3	7	0	0	0	0
86	q1	7	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s4	7	0	0	0	0
86	s8	7	0	0	0	0
86	s9	7	0	0	0	0
86	sR	7	0	0	0	0
87	D6	1	0	0	0	0
87	D7	1	0	0	0	0
87	D9	1	0	0	0	0
87	E1	1	0	0	0	0
87	O7	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	1	0	0	0	0
87	Q3	1	0	0	0	0
87	d6	1	0	0	0	0
87	d7	1	0	0	0	0
87	d9	1	0	0	0	0
87	e1	1	0	0	0	0
87	o7	1	0	0	0	0
87	q0	1	0	0	0	0
87	q2	1	0	0	0	0
87	q3	1	0	0	0	0
88	1	22	0	0	2	0
88	5	22	0	0	1	0
All	All	411178	0	297243	10849	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 10849 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
78:Q2:17:CYS:CB	78:Q2:17:CYS:SG	2.04	1.46
40:L3:41:VAL:HA	40:L3:185:GLY:HA3	1.30	1.09
36:5:2273:G:O6	86:5:4193:OHX:N5	1.92	1.02
1:2:1595:U:H3	1:2:1600:A:H2	1.07	1.00
36:5:1231:A:H5''	36:5:1232:C:H5'	1.44	0.99

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:7:52:G:OP1	86:5:3939:OHX:N2[2_647]	2.15	0.05
36:1:531:G:OP1	86:2:2162:OHX:N1[2_545]	2.18	0.02

## 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%)	140 (69%)	38 (19%)	26 (13%)	0	3
2	s0	204/251 (81%)	148 (72%)	33 (16%)	23 (11%)	1	4
3	S1	212/254 (84%)	149 (70%)	39 (18%)	24 (11%)	1	4
3	s1	214/254 (84%)	173 (81%)	32 (15%)	9 (4%)	4	31
4	S2	215/253 (85%)	175 (81%)	27 (13%)	13 (6%)	2	20
4	s2	215/253 (85%)	176 (82%)	26 (12%)	13 (6%)	2	20
5	S3	221/239 (92%)	177 (80%)	30 (14%)	14 (6%)	2	18
5	s3	221/239 (92%)	168 (76%)	35 (16%)	18 (8%)	1	10
6	S4	258/260 (99%)	206 (80%)	42 (16%)	10 (4%)	5	33
6	s4	258/260 (99%)	212 (82%)	26 (10%)	20 (8%)	1	11
7	S5	204/224 (91%)	158 (78%)	30 (15%)	16 (8%)	1	11
7	s5	204/224 (91%)	144 (71%)	45 (22%)	15 (7%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S6	224/236 (95%)	194 (87%)	18 (8%)	12 (5%)	3	24
8	s6	216/236 (92%)	189 (88%)	17 (8%)	10 (5%)	4	28
9	S7	182/189 (96%)	142 (78%)	25 (14%)	15 (8%)	1	10
9	s7	184/189 (97%)	144 (78%)	23 (12%)	17 (9%)	1	8
10	S8	184/200 (92%)	155 (84%)	19 (10%)	10 (5%)	3	24
10	s8	184/200 (92%)	158 (86%)	18 (10%)	8 (4%)	4	30
11	S9	183/196 (93%)	135 (74%)	36 (20%)	12 (7%)	2	16
11	s9	183/196 (93%)	149 (81%)	25 (14%)	9 (5%)	3	26
12	C0	94/105 (90%)	66 (70%)	20 (21%)	8 (8%)	1	9
12	c0	92/105 (88%)	64 (70%)	12 (13%)	16 (17%)	0	1
13	C1	153/155 (99%)	124 (81%)	18 (12%)	11 (7%)	2	13
13	c1	144/155 (93%)	118 (82%)	17 (12%)	9 (6%)	2	18
14	C2	122/142 (86%)	71 (58%)	32 (26%)	19 (16%)	0	1
14	c2	122/142 (86%)	69 (57%)	31 (25%)	22 (18%)	0	1
15	C3	148/150 (99%)	119 (80%)	21 (14%)	8 (5%)	3	24
15	c3	148/150 (99%)	110 (74%)	27 (18%)	11 (7%)	2	12
16	C4	125/136 (92%)	87 (70%)	24 (19%)	14 (11%)	1	4
16	c4	126/136 (93%)	95 (75%)	16 (13%)	15 (12%)	1	4
17	C5	122/141 (86%)	86 (70%)	26 (21%)	10 (8%)	1	10
17	c5	133/141 (94%)	88 (66%)	25 (19%)	20 (15%)	0	1
18	C6	139/142 (98%)	114 (82%)	14 (10%)	11 (8%)	1	11
18	c6	140/142 (99%)	113 (81%)	21 (15%)	6 (4%)	4	30
19	C7	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	1	6
19	c7	113/136 (83%)	89 (79%)	15 (13%)	9 (8%)	1	10
20	C8	143/145 (99%)	111 (78%)	20 (14%)	12 (8%)	1	9
20	c8	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1	11
21	C9	141/143 (99%)	109 (77%)	23 (16%)	9 (6%)	2	17
21	c9	141/143 (99%)	117 (83%)	17 (12%)	7 (5%)	3	26
22	D0	105/120 (88%)	78 (74%)	23 (22%)	4 (4%)	5	34
22	d0	108/120 (90%)	82 (76%)	19 (18%)	7 (6%)	2	17
23	D1	85/87 (98%)	59 (69%)	19 (22%)	7 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	d1	85/87 (98%)	65 (76%)	13 (15%)	7 (8%)	1	10
24	D2	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	5	33
24	d2	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	27	77
25	D3	142/144 (99%)	108 (76%)	20 (14%)	14 (10%)	1	7
25	d3	142/144 (99%)	121 (85%)	16 (11%)	5 (4%)	6	37
26	D4	132/134 (98%)	108 (82%)	14 (11%)	10 (8%)	2	12
26	d4	132/134 (98%)	101 (76%)	17 (13%)	14 (11%)	1	5
27	D5	68/107 (64%)	46 (68%)	12 (18%)	10 (15%)	0	2
27	d5	67/107 (63%)	50 (75%)	13 (19%)	4 (6%)	2	20
28	D6	95/97 (98%)	55 (58%)	21 (22%)	19 (20%)	0	0
28	d6	95/97 (98%)	69 (73%)	19 (20%)	7 (7%)	2	12
29	D7	79/81 (98%)	59 (75%)	17 (22%)	3 (4%)	5	34
29	d7	79/81 (98%)	58 (73%)	14 (18%)	7 (9%)	1	8
30	D8	61/66 (92%)	46 (75%)	12 (20%)	3 (5%)	3	26
30	d8	61/66 (92%)	44 (72%)	15 (25%)	2 (3%)	6	38
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	2	20
31	d9	51/55 (93%)	38 (74%)	8 (16%)	5 (10%)	1	7
32	E0	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	8
33	E1	69/76 (91%)	32 (46%)	17 (25%)	20 (29%)	0	0
33	e1	74/76 (97%)	39 (53%)	17 (23%)	18 (24%)	0	0
34	SR	316/318 (99%)	265 (84%)	43 (14%)	8 (2%)	9	49
34	sR	316/318 (99%)	263 (83%)	40 (13%)	13 (4%)	4	32
35	SM	155/273 (57%)	105 (68%)	32 (21%)	18 (12%)	1	4
35	sM	98/273 (36%)	60 (61%)	21 (21%)	17 (17%)	0	1
39	L2	250/253 (99%)	222 (89%)	21 (8%)	7 (3%)	8	44
39	l2	250/253 (99%)	205 (82%)	27 (11%)	18 (7%)	2	13
40	L3	384/386 (100%)	316 (82%)	52 (14%)	16 (4%)	4	31
40	l3	384/386 (100%)	334 (87%)	32 (8%)	18 (5%)	4	27
41	L4	359/361 (99%)	299 (83%)	38 (11%)	22 (6%)	2	19
41	l4	359/361 (99%)	299 (83%)	37 (10%)	23 (6%)	2	17
42	L5	294/296 (99%)	243 (83%)	35 (12%)	16 (5%)	3	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	l5	292/296 (99%)	255 (87%)	28 (10%)	9 (3%)	7	41
43	L6	152/175 (87%)	142 (93%)	8 (5%)	2 (1%)	18	68
43	l6	153/175 (87%)	136 (89%)	13 (8%)	4 (3%)	8	47
44	L7	220/243 (90%)	189 (86%)	22 (10%)	9 (4%)	4	32
44	l7	221/243 (91%)	190 (86%)	25 (11%)	6 (3%)	8	46
45	L8	231/255 (91%)	182 (79%)	34 (15%)	15 (6%)	2	17
45	l8	229/255 (90%)	180 (79%)	32 (14%)	17 (7%)	2	12
46	L9	189/191 (99%)	158 (84%)	20 (11%)	11 (6%)	3	21
46	l9	189/191 (99%)	166 (88%)	18 (10%)	5 (3%)	8	47
47	M0	207/220 (94%)	177 (86%)	21 (10%)	9 (4%)	4	30
47	m0	209/220 (95%)	160 (77%)	31 (15%)	18 (9%)	1	8
48	M1	167/173 (96%)	127 (76%)	23 (14%)	17 (10%)	1	6
48	m1	167/173 (96%)	136 (81%)	21 (13%)	10 (6%)	2	20
49	M3	191/198 (96%)	156 (82%)	28 (15%)	7 (4%)	5	34
49	m3	192/198 (97%)	153 (80%)	23 (12%)	16 (8%)	1	9
50	M4	134/137 (98%)	118 (88%)	10 (8%)	6 (4%)	4	29
50	m4	135/137 (98%)	119 (88%)	13 (10%)	3 (2%)	10	53
51	M5	201/203 (99%)	178 (89%)	20 (10%)	3 (2%)	15	64
51	m5	201/203 (99%)	171 (85%)	24 (12%)	6 (3%)	7	42
52	M6	195/198 (98%)	174 (89%)	17 (9%)	4 (2%)	11	55
52	m6	195/198 (98%)	170 (87%)	19 (10%)	6 (3%)	7	41
53	M7	181/183 (99%)	151 (83%)	23 (13%)	7 (4%)	5	33
53	m7	153/183 (84%)	135 (88%)	16 (10%)	2 (1%)	18	68
54	M8	183/185 (99%)	153 (84%)	22 (12%)	8 (4%)	4	29
54	m8	183/185 (99%)	152 (83%)	25 (14%)	6 (3%)	6	38
55	M9	186/188 (99%)	162 (87%)	22 (12%)	2 (1%)	21	72
55	m9	186/188 (99%)	159 (86%)	24 (13%)	3 (2%)	14	63
56	N0	170/172 (99%)	149 (88%)	15 (9%)	6 (4%)	6	37
56	n0	170/172 (99%)	153 (90%)	13 (8%)	4 (2%)	9	51
57	N1	157/159 (99%)	136 (87%)	18 (12%)	3 (2%)	12	59
57	n1	157/159 (99%)	137 (87%)	15 (10%)	5 (3%)	6	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	N2	98/120 (82%)	82 (84%)	11 (11%)	5 (5%)	3	25
58	n2	96/120 (80%)	79 (82%)	13 (14%)	4 (4%)	4	31
59	N3	134/136 (98%)	119 (89%)	12 (9%)	3 (2%)	10	53
59	n3	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	10	53
60	N4	96/155 (62%)	73 (76%)	14 (15%)	9 (9%)	1	7
60	n4	133/155 (86%)	106 (80%)	15 (11%)	12 (9%)	1	8
61	N5	119/141 (84%)	105 (88%)	12 (10%)	2 (2%)	14	62
61	n5	118/141 (84%)	92 (78%)	15 (13%)	11 (9%)	1	8
62	N6	124/126 (98%)	113 (91%)	9 (7%)	2 (2%)	14	63
62	n6	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	5	32
63	N7	133/135 (98%)	112 (84%)	16 (12%)	5 (4%)	5	34
63	n7	133/135 (98%)	109 (82%)	13 (10%)	11 (8%)	1	9
64	N8	146/148 (99%)	118 (81%)	21 (14%)	7 (5%)	4	27
64	n8	146/148 (99%)	119 (82%)	21 (14%)	6 (4%)	4	32
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	5	36
65	n9	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	1	5
66	O0	95/104 (91%)	83 (87%)	9 (10%)	3 (3%)	6	39
66	o0	98/104 (94%)	84 (86%)	14 (14%)	0	100	100
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	3	23
67	o1	107/112 (96%)	93 (87%)	9 (8%)	5 (5%)	4	27
68	O2	125/129 (97%)	111 (89%)	10 (8%)	4 (3%)	6	39
68	o2	125/129 (97%)	100 (80%)	18 (14%)	7 (6%)	3	23
69	O3	104/106 (98%)	90 (86%)	10 (10%)	4 (4%)	5	34
69	o3	104/106 (98%)	92 (88%)	10 (10%)	2 (2%)	12	59
70	O4	110/120 (92%)	88 (80%)	18 (16%)	4 (4%)	5	36
70	o4	110/120 (92%)	97 (88%)	10 (9%)	3 (3%)	8	46
71	O5	117/119 (98%)	100 (86%)	11 (9%)	6 (5%)	3	25
71	o5	117/119 (98%)	97 (83%)	17 (14%)	3 (3%)	8	47
72	O6	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	2	13
72	o6	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	4	32
73	O7	85/87 (98%)	70 (82%)	13 (15%)	2 (2%)	9	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	o7	85/87 (98%)	65 (76%)	17 (20%)	3 (4%)	6	37
74	O8	75/77 (97%)	59 (79%)	12 (16%)	4 (5%)	3	24
74	o8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	3	24
75	O9	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
75	o9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	11	55
76	Q0	50/52 (96%)	46 (92%)	1 (2%)	3 (6%)	2	20
76	q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	5	32
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
77	q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
78	Q2	103/105 (98%)	82 (80%)	15 (15%)	6 (6%)	3	21
78	q2	103/105 (98%)	90 (87%)	9 (9%)	4 (4%)	5	33
79	Q3	89/91 (98%)	76 (85%)	9 (10%)	4 (4%)	4	29
79	q3	89/91 (98%)	77 (86%)	11 (12%)	1 (1%)	21	72
80	e0	60/62 (97%)	42 (70%)	11 (18%)	7 (12%)	1	4
82	p0	117/311 (38%)	98 (84%)	12 (10%)	7 (6%)	2	20
All	All	22311/24143 (92%)	18107 (81%)	2886 (13%)	1318 (6%)	2	20

5 of 1318 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	32	HIS
2	S0	66	ALA
2	S0	68	PRO
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%)	134 (82%)	30 (18%)	2	12
2	s0	165/209 (79%)	137 (83%)	28 (17%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S1	191/223 (86%)	147 (77%)	44 (23%)	1	5
3	s1	192/223 (86%)	154 (80%)	38 (20%)	2	9
4	S2	176/204 (86%)	140 (80%)	36 (20%)	2	8
4	s2	176/204 (86%)	127 (72%)	49 (28%)	0	2
5	S3	182/194 (94%)	149 (82%)	33 (18%)	2	12
5	s3	182/194 (94%)	144 (79%)	38 (21%)	1	8
6	S4	221/221 (100%)	177 (80%)	44 (20%)	2	9
6	s4	221/221 (100%)	179 (81%)	42 (19%)	2	11
7	S5	173/190 (91%)	145 (84%)	28 (16%)	3	15
7	s5	173/190 (91%)	140 (81%)	33 (19%)	2	11
8	S6	188/201 (94%)	152 (81%)	36 (19%)	2	11
8	s6	187/201 (93%)	158 (84%)	29 (16%)	4	17
9	S7	165/169 (98%)	135 (82%)	30 (18%)	2	12
9	s7	165/169 (98%)	131 (79%)	34 (21%)	2	8
10	S8	150/161 (93%)	123 (82%)	27 (18%)	2	12
10	s8	150/161 (93%)	125 (83%)	25 (17%)	3	14
11	S9	158/165 (96%)	121 (77%)	37 (23%)	1	5
11	s9	158/165 (96%)	121 (77%)	37 (23%)	1	5
12	C0	77/98 (79%)	62 (80%)	15 (20%)	2	10
12	c0	73/98 (74%)	61 (84%)	12 (16%)	3	15
13	C1	129/136 (95%)	108 (84%)	21 (16%)	3	15
13	c1	129/136 (95%)	105 (81%)	24 (19%)	2	11
14	C2	88/118 (75%)	70 (80%)	18 (20%)	2	8
14	c2	88/118 (75%)	68 (77%)	20 (23%)	1	6
15	C3	127/127 (100%)	101 (80%)	26 (20%)	2	8
15	c3	127/127 (100%)	104 (82%)	23 (18%)	2	12
16	C4	81/104 (78%)	63 (78%)	18 (22%)	1	6
16	c4	97/104 (93%)	72 (74%)	25 (26%)	1	2
17	C5	101/117 (86%)	80 (79%)	21 (21%)	2	8
17	c5	103/117 (88%)	85 (82%)	18 (18%)	3	13
18	C6	117/118 (99%)	96 (82%)	21 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	c6	118/118 (100%)	96 (81%)	22 (19%)	2	11
19	C7	94/124 (76%)	74 (79%)	20 (21%)	1	7
19	c7	92/124 (74%)	71 (77%)	21 (23%)	1	6
20	C8	128/128 (100%)	92 (72%)	36 (28%)	0	2
20	c8	128/128 (100%)	99 (77%)	29 (23%)	1	6
21	C9	115/115 (100%)	89 (77%)	26 (23%)	1	6
21	c9	115/115 (100%)	95 (83%)	20 (17%)	3	13
22	D0	100/113 (88%)	83 (83%)	17 (17%)	3	14
22	d0	103/113 (91%)	74 (72%)	29 (28%)	0	2
23	D1	74/74 (100%)	57 (77%)	17 (23%)	1	5
23	d1	74/74 (100%)	53 (72%)	21 (28%)	0	2
24	D2	110/110 (100%)	86 (78%)	24 (22%)	1	7
24	d2	110/110 (100%)	92 (84%)	18 (16%)	3	15
25	D3	119/119 (100%)	103 (87%)	16 (13%)	6	26
25	d3	119/119 (100%)	98 (82%)	21 (18%)	3	13
26	D4	112/112 (100%)	101 (90%)	11 (10%)	12	43
26	d4	112/112 (100%)	90 (80%)	22 (20%)	2	10
27	D5	61/88 (69%)	42 (69%)	19 (31%)	0	1
27	d5	61/88 (69%)	49 (80%)	12 (20%)	2	10
28	D6	83/83 (100%)	63 (76%)	20 (24%)	1	4
28	d6	83/83 (100%)	67 (81%)	16 (19%)	2	10
29	D7	70/70 (100%)	61 (87%)	9 (13%)	6	28
29	d7	70/70 (100%)	58 (83%)	12 (17%)	3	14
30	D8	56/59 (95%)	40 (71%)	16 (29%)	0	1
30	d8	56/59 (95%)	43 (77%)	13 (23%)	1	5
31	D9	47/48 (98%)	35 (74%)	12 (26%)	1	3
31	d9	47/48 (98%)	38 (81%)	9 (19%)	2	11
32	E0	51/51 (100%)	44 (86%)	7 (14%)	5	25
33	E1	62/66 (94%)	47 (76%)	15 (24%)	1	4
33	e1	66/66 (100%)	49 (74%)	17 (26%)	1	2
34	SR	260/261 (100%)	225 (86%)	35 (14%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	sR	260/261 (100%)	229 (88%)	31 (12%)	8	33
35	SM	97/228 (42%)	75 (77%)	22 (23%)	1	6
35	sM	54/228 (24%)	44 (82%)	10 (18%)	2	11
39	L2	193/195 (99%)	150 (78%)	43 (22%)	1	6
39	l2	192/195 (98%)	157 (82%)	35 (18%)	2	12
40	L3	319/322 (99%)	254 (80%)	65 (20%)	2	8
40	l3	320/322 (99%)	249 (78%)	71 (22%)	1	6
41	L4	288/288 (100%)	235 (82%)	53 (18%)	2	11
41	l4	288/288 (100%)	227 (79%)	61 (21%)	1	8
42	L5	244/244 (100%)	203 (83%)	41 (17%)	3	14
42	l5	243/244 (100%)	200 (82%)	43 (18%)	3	13
43	L6	134/152 (88%)	110 (82%)	24 (18%)	2	12
43	l6	135/152 (89%)	112 (83%)	23 (17%)	3	14
44	L7	186/204 (91%)	161 (87%)	25 (13%)	6	26
44	l7	187/204 (92%)	160 (86%)	27 (14%)	5	22
45	L8	187/207 (90%)	154 (82%)	33 (18%)	3	13
45	l8	177/207 (86%)	148 (84%)	29 (16%)	3	15
46	L9	171/171 (100%)	139 (81%)	32 (19%)	2	11
46	l9	171/171 (100%)	125 (73%)	46 (27%)	1	2
47	M0	177/186 (95%)	143 (81%)	34 (19%)	2	10
47	m0	179/186 (96%)	152 (85%)	27 (15%)	4	19
48	M1	147/150 (98%)	116 (79%)	31 (21%)	1	8
48	m1	147/150 (98%)	113 (77%)	34 (23%)	1	5
49	M3	154/158 (98%)	123 (80%)	31 (20%)	2	9
49	m3	154/158 (98%)	127 (82%)	27 (18%)	3	13
50	M4	107/108 (99%)	87 (81%)	20 (19%)	2	11
50	m4	108/108 (100%)	83 (77%)	25 (23%)	1	5
51	M5	175/175 (100%)	145 (83%)	30 (17%)	3	14
51	m5	175/175 (100%)	144 (82%)	31 (18%)	3	13
52	M6	160/161 (99%)	139 (87%)	21 (13%)	6	28
52	m6	160/161 (99%)	125 (78%)	35 (22%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	M7	140/145 (97%)	109 (78%)	31 (22%)	1	7
53	m7	125/145 (86%)	94 (75%)	31 (25%)	1	3
54	M8	150/150 (100%)	129 (86%)	21 (14%)	5	23
54	m8	150/150 (100%)	118 (79%)	32 (21%)	1	7
55	M9	153/153 (100%)	128 (84%)	25 (16%)	3	15
55	m9	153/153 (100%)	127 (83%)	26 (17%)	3	14
56	N0	156/156 (100%)	126 (81%)	30 (19%)	2	10
56	n0	156/156 (100%)	120 (77%)	36 (23%)	1	5
57	N1	136/136 (100%)	106 (78%)	30 (22%)	1	7
57	n1	136/136 (100%)	105 (77%)	31 (23%)	1	6
58	N2	87/106 (82%)	66 (76%)	21 (24%)	1	4
58	n2	85/106 (80%)	71 (84%)	14 (16%)	3	14
59	N3	104/104 (100%)	81 (78%)	23 (22%)	1	7
59	n3	104/104 (100%)	88 (85%)	16 (15%)	4	18
60	N4	57/129 (44%)	51 (90%)	6 (10%)	10	39
60	n4	100/129 (78%)	80 (80%)	20 (20%)	2	9
61	N5	104/117 (89%)	79 (76%)	25 (24%)	1	4
61	n5	104/117 (89%)	89 (86%)	15 (14%)	5	22
62	N6	109/109 (100%)	89 (82%)	20 (18%)	2	12
62	n6	109/109 (100%)	89 (82%)	20 (18%)	2	12
63	N7	115/115 (100%)	90 (78%)	25 (22%)	1	7
63	n7	115/115 (100%)	86 (75%)	29 (25%)	1	3
64	N8	118/118 (100%)	98 (83%)	20 (17%)	3	14
64	n8	118/118 (100%)	93 (79%)	25 (21%)	1	8
65	N9	46/46 (100%)	36 (78%)	10 (22%)	1	7
65	n9	46/46 (100%)	32 (70%)	14 (30%)	0	1
66	O0	81/87 (93%)	70 (86%)	11 (14%)	5	25
66	o0	84/87 (97%)	65 (77%)	19 (23%)	1	6
67	O1	92/96 (96%)	76 (83%)	16 (17%)	3	13
67	o1	94/96 (98%)	66 (70%)	28 (30%)	0	1
68	O2	109/110 (99%)	89 (82%)	20 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	o2	109/110 (99%)	88 (81%)	21 (19%)	2	10
69	O3	90/90 (100%)	74 (82%)	16 (18%)	2	13
69	o3	90/90 (100%)	78 (87%)	12 (13%)	6	27
70	O4	95/102 (93%)	81 (85%)	14 (15%)	4	21
70	o4	95/102 (93%)	78 (82%)	17 (18%)	2	12
71	O5	104/104 (100%)	85 (82%)	19 (18%)	2	12
71	o5	103/104 (99%)	77 (75%)	26 (25%)	1	3
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1	8
72	o6	80/81 (99%)	57 (71%)	23 (29%)	0	1
73	O7	70/70 (100%)	53 (76%)	17 (24%)	1	3
73	o7	70/70 (100%)	62 (89%)	8 (11%)	8	35
74	O8	68/68 (100%)	46 (68%)	22 (32%)	0	0
74	o8	67/68 (98%)	53 (79%)	14 (21%)	1	8
75	O9	45/45 (100%)	37 (82%)	8 (18%)	2	13
75	o9	45/45 (100%)	34 (76%)	11 (24%)	1	3
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	3	14
76	q0	47/47 (100%)	34 (72%)	13 (28%)	0	2
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	1	2
77	q1	23/23 (100%)	14 (61%)	9 (39%)	0	0
78	Q2	90/90 (100%)	67 (74%)	23 (26%)	1	2
78	q2	90/90 (100%)	68 (76%)	22 (24%)	1	3
79	Q3	71/71 (100%)	56 (79%)	15 (21%)	1	8
79	q3	71/71 (100%)	59 (83%)	12 (17%)	3	14
80	e0	53/53 (100%)	43 (81%)	10 (19%)	2	11
82	p0	105/253 (42%)	86 (82%)	19 (18%)	2	12
All	All	18727/20241 (92%)	15053 (80%)	3674 (20%)	2	10

5 of 3674 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	O5	76	GLN
9	s7	60	ILE
64	n8	73	LEU

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Mol	Chain	Res	Type
74	O8	24	THR
4	s2	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
75	O9	32	ASN
11	s9	124	HIS
59	n3	132	ASN
78	Q2	82	GLN
3	s1	209	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 2555 ligands modelled in this entry, 1424 are monoatomic - leaving 1131 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	OHX	1	3865	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3866	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3867	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3868	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3869	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3870	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3871	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3872	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3873	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3874	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3875	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3876	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3877	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3878	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3879	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3880	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3881	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3882	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3883	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3884	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3885	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3886	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3887	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3888	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3889	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3890	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3891	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3892	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3895	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3896	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3906	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3938	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3949	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3981	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3992	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4024	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4067	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4110	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4153	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4196	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	1	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3KF	1	4212	85	25,25,25	0.81	0	39,39,39	1.19	4 (10%)
86	OHX	2	2023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2035	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2049	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2078	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2092	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2121	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2135	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2164	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2178	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	2	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	2	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3897	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3898	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3899	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3900	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3901	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3902	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3903	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3904	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3905	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3906	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3907	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3908	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3909	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3910	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3911	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3912	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3913	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3914	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3915	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3916	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3917	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3918	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3919	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3920	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3921	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3922	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3923	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3924	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3925	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3926	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3927	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3928	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3929	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3930	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3931	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3932	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3933	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3934	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3935	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3936	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3937	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3938	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3939	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3940	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3941	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3942	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3943	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3944	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3945	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3946	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3947	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3948	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3949	-	0,6,6	0.00	-	0,15,15	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3950	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3951	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3952	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3953	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3954	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3955	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3956	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3957	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3958	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3959	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3960	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3961	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3962	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3963	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3964	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3965	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3966	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3967	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3968	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3969	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3970	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3971	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3972	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3973	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3974	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3975	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3976	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3977	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3978	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3979	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3980	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3981	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3982	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3983	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3984	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3985	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3986	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3987	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3988	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3989	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3990	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3991	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3992	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	3993	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3994	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3995	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3996	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3997	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3998	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3999	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4000	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4001	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4002	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4003	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4004	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4005	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4006	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4007	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4008	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4009	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4010	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4011	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4012	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4013	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4014	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4015	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4016	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4017	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4018	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4019	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4020	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4021	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4022	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4023	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4024	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4025	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4026	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4027	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4028	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4029	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4030	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4031	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4032	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4033	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4034	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4035	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4036	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4037	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4038	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4039	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4040	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4041	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4042	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4044	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4045	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4046	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4047	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4048	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4049	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4050	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4051	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4052	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4053	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4054	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4055	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4056	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4057	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4058	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4059	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4060	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4061	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4062	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4063	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4064	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4065	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4066	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4067	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4068	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4069	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4070	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4071	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4072	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4073	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4074	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4075	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4076	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4077	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4078	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4079	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4080	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4081	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4082	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4083	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4084	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4085	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4086	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4087	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4088	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4089	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4090	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4091	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4092	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4093	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4094	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4095	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4096	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4097	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4098	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4099	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4100	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4104	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4107	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4108	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4109	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4110	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4111	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4112	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4113	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4114	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4115	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4116	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4117	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4118	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4119	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4120	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4121	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4122	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4123	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4124	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4125	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4126	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4127	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4128	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4129	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4130	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4131	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4132	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4133	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4134	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4135	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4136	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4137	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4138	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4139	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4140	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4141	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4142	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4143	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4144	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4145	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4146	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4147	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4148	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4149	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4150	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4151	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4152	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4153	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4154	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4155	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4156	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4157	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4158	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4159	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4160	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4161	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4162	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4163	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4164	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4165	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4166	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4167	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4168	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4169	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4170	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4171	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4172	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4173	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4207	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	5	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4213	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4232	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4233	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4234	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4235	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4236	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4237	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4238	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4239	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4240	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4241	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4242	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4243	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4244	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4245	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4246	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	4247	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3KF	5	4248	85	25,25,25	0.59	0	39,39,39	1.07	2 (5%)
86	OHX	6	2043	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2044	-	0,6,6	0.00	-	0,15,15	0.00	-



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



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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	6	2174	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2175	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2176	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2177	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2178	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2179	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2180	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2181	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2182	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2183	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2184	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2185	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2186	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2187	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2188	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2189	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	214	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	227	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	228	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	229	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	230	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M0	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M7	207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	M9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	N9	101	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	105	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	106	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	Q2	503	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c3	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	c8	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d4	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	d9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	402	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l4	403	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	302	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
86	OHX	l5	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l9	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m0	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m1	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m7	206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n3	204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	n9	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o2	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q1	102	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	q2	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s1	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s4	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s8	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	s9	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	sR	401	-	0,6,6	0.00	-	0,15,15	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3865	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3866	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3867	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3868	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3869	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3870	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3871	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3872	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3873	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3874	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3875	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3876	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3877	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3878	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3879	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3880	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3881	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3882	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3883	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3884	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3885	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3886	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3887	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3888	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3889	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3890	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3891	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3892	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3896	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3917	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3958	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3959	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	1	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4000	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4001	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4042	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4043	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4084	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4085	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4126	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4127	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4168	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4169	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	1	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	1	4211	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	3KF	1	4212	85	-	0/0/38/38	0/4/4/4
86	OHX	2	2023	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2024	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2025	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2026	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2027	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2028	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2029	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2030	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2031	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2032	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2033	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2034	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2035	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2036	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2037	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2038	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2039	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2040	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2041	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2042	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2046	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2063	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2088	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2105	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2130	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2147	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	3	214	-	-	0/0/0/0	0/0/0/0
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	3	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	221	-	-	0/0/0/0	0/0/0/0
86	OHX	4	222	-	-	0/0/0/0	0/0/0/0
86	OHX	4	223	-	-	0/0/0/0	0/0/0/0
86	OHX	4	224	-	-	0/0/0/0	0/0/0/0
86	OHX	4	225	-	-	0/0/0/0	0/0/0/0
86	OHX	4	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	227	-	-	0/0/0/0	0/0/0/0
86	OHX	4	228	-	-	0/0/0/0	0/0/0/0
86	OHX	4	229	-	-	0/0/0/0	0/0/0/0
86	OHX	4	230	-	-	0/0/0/0	0/0/0/0
86	OHX	4	231	-	-	0/0/0/0	0/0/0/0
86	OHX	4	232	-	-	0/0/0/0	0/0/0/0
86	OHX	4	233	-	-	0/0/0/0	0/0/0/0
86	OHX	4	234	-	-	0/0/0/0	0/0/0/0
86	OHX	4	235	-	-	0/0/0/0	0/0/0/0
86	OHX	4	236	-	-	0/0/0/0	0/0/0/0
86	OHX	4	237	-	-	0/0/0/0	0/0/0/0
86	OHX	4	238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3897	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3898	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3899	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3900	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3901	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3902	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3903	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3904	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3905	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3906	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3907	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3908	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3909	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3910	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3911	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3912	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3913	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3914	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3915	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3942	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3943	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3944	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3945	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3946	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3947	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3948	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3949	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3950	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3951	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3952	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3953	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3954	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3955	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3956	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3957	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3958	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3959	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3960	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3961	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3962	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3963	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3964	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3965	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3966	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3967	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3968	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3969	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3970	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3971	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3972	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3973	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3974	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3975	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3976	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3977	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3978	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3979	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3980	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3981	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3982	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3983	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3984	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3985	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3986	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3987	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3988	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3989	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3990	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3991	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3992	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3993	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3994	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3995	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3996	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3997	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3998	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3999	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4000	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4001	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4002	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4003	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4004	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4005	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4006	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4007	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4008	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4009	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4010	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4011	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4012	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4013	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4014	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4015	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4016	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4017	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4018	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4019	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4020	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4021	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4022	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4023	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4024	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4025	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4026	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4027	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4028	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4029	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4030	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4031	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4032	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4033	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4034	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4035	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4036	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4037	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4038	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4039	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4040	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4041	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4042	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4043	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4044	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4045	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4046	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4047	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4048	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4049	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4050	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4051	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4052	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4053	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4054	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4055	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4056	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4057	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4058	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4059	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4060	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4061	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4062	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4063	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4064	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4065	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4066	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4067	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4068	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4069	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4070	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4071	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4072	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4073	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4074	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4075	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4076	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4077	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4078	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4079	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4080	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4081	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4082	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4083	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4084	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4085	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4086	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4087	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4088	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4089	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4090	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4091	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4092	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4093	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4094	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4095	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4096	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4097	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4098	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4099	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4100	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4101	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4102	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4103	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4104	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4105	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4106	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4107	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4108	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4109	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4110	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4111	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4112	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4113	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4114	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4115	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4116	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4117	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4118	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4119	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4120	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4121	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4122	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4123	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4124	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4125	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4126	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4127	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4128	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4129	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4130	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4131	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4132	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4133	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4134	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4135	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4136	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4137	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4138	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4139	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4140	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4141	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4142	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4143	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4144	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4145	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4146	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4147	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4148	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4149	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4150	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4151	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4152	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4153	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4154	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4155	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4156	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4157	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4158	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4159	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4160	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4161	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4162	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4163	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4164	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4165	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4166	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4167	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4168	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4169	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4170	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4171	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4172	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4173	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4174	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4175	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4176	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4177	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4178	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4179	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4180	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4181	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4182	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4183	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4184	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4185	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4186	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4187	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4188	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4189	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4190	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4191	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4192	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4193	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4194	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4195	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4196	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4197	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4198	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4199	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4200	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4201	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4202	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4203	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4204	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4205	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4206	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4207	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4208	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4209	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4210	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4233	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4234	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4235	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4236	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4237	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4238	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4239	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4240	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4241	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4242	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4243	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4244	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4245	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4246	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4247	-	-	0/0/0/0	0/0/0/0
88	3KF	5	4248	85	-	0/0/38/38	0/4/4/4
86	OHX	6	2043	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2044	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2046	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2047	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2048	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2049	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2050	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2051	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2052	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2053	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2054	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2055	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2056	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2057	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2058	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2059	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2060	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2061	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2062	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2063	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2064	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2065	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2066	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2067	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2068	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2069	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2070	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2071	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2072	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2073	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2074	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2075	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2076	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2077	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2078	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2079	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2080	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2081	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2082	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2083	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2084	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2085	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2086	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2087	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2088	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2089	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2090	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2091	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2092	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2093	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2094	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2095	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2096	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2097	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2098	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2099	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2100	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2101	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2102	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2103	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2104	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2105	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2106	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2107	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2108	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2109	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2110	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2111	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2112	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2113	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2114	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2115	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2116	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2117	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2118	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2119	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2120	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2121	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2122	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2123	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2124	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2125	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2126	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2127	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2128	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2129	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2130	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2131	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2132	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2133	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2134	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2135	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2136	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2137	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2138	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2139	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2140	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2141	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2142	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2143	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2144	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2145	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2146	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2172	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	6	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2180	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2181	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2182	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2183	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2184	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2185	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2186	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2187	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2188	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2189	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	7	218	-	-	0/0/0/0	0/0/0/0
86	OHX	7	219	-	-	0/0/0/0	0/0/0/0
86	OHX	7	220	-	-	0/0/0/0	0/0/0/0
86	OHX	7	221	-	-	0/0/0/0	0/0/0/0
86	OHX	7	222	-	-	0/0/0/0	0/0/0/0
86	OHX	7	223	-	-	0/0/0/0	0/0/0/0
86	OHX	7	224	-	-	0/0/0/0	0/0/0/0
86	OHX	7	225	-	-	0/0/0/0	0/0/0/0
86	OHX	7	226	-	-	0/0/0/0	0/0/0/0
86	OHX	7	227	-	-	0/0/0/0	0/0/0/0
86	OHX	7	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	214	-	-	0/0/0/0	0/0/0/0
86	OHX	8	215	-	-	0/0/0/0	0/0/0/0
86	OHX	8	216	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0
86	OHX	8	219	-	-	0/0/0/0	0/0/0/0
86	OHX	8	220	-	-	0/0/0/0	0/0/0/0
86	OHX	8	221	-	-	0/0/0/0	0/0/0/0
86	OHX	8	222	-	-	0/0/0/0	0/0/0/0
86	OHX	8	223	-	-	0/0/0/0	0/0/0/0
86	OHX	8	224	-	-	0/0/0/0	0/0/0/0
86	OHX	8	225	-	-	0/0/0/0	0/0/0/0
86	OHX	8	226	-	-	0/0/0/0	0/0/0/0
86	OHX	8	227	-	-	0/0/0/0	0/0/0/0
86	OHX	8	228	-	-	0/0/0/0	0/0/0/0
86	OHX	8	229	-	-	0/0/0/0	0/0/0/0
86	OHX	8	230	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	402	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	207	-	-	0/0/0/0	0/0/0/0
86	OHX	M8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	N1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	105	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	106	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	503	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	301	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	202	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	302	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	301	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	204	-	-	0/0/0/0	0/0/0/0
86	OHX	m7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	m8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	203	-	-	0/0/0/0	0/0/0/0
86	OHX	n3	204	-	-	0/0/0/0	0/0/0/0
86	OHX	n5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	n9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	o2	201	-	-	0/0/0/0	0/0/0/0
86	OHX	o3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	q1	102	-	-	0/0/0/0	0/0/0/0
86	OHX	q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	302	-	-	0/0/0/0	0/0/0/0
86	OHX	s1	303	-	-	0/0/0/0	0/0/0/0
86	OHX	s4	301	-	-	0/0/0/0	0/0/0/0
86	OHX	s8	304	-	-	0/0/0/0	0/0/0/0
86	OHX	s9	201	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4212	3KF	C3-C4-C13	4.07	120.86	118.00
88	5	4248	3KF	C10-C11-C12	-3.88	102.66	110.56
88	1	4212	3KF	C10-C11-C12	-2.99	104.46	110.56
88	1	4212	3KF	O3-C11-C12	-2.66	103.48	109.16
88	5	4248	3KF	O4-C10-C11	-2.16	105.53	110.36

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	2	1750/1800 (97%)	0.14	97 (5%) 24 5	55, 92, 172, 255	0
1	6	1795/1800 (99%)	0.21	129 (7%) 15 3	45, 84, 196, 261	0
2	S0	206/251 (82%)	0.07	3 (1%) 70 21	95, 110, 122, 146	0
2	s0	206/251 (82%)	-0.04	0 100 100	82, 103, 120, 125	0
3	S1	214/254 (84%)	0.47	15 (7%) 16 4	97, 126, 148, 155	0
3	s1	216/254 (85%)	-0.05	0 100 100	74, 89, 113, 123	0
4	S2	217/253 (85%)	-0.07	0 100 100	73, 89, 109, 123	0
4	s2	217/253 (85%)	-0.09	2 (0%) 81 32	61, 77, 97, 109	0
5	S3	223/239 (93%)	0.11	5 (2%) 59 14	78, 96, 129, 143	0
5	s3	223/239 (93%)	0.38	8 (3%) 41 8	82, 124, 147, 154	0
6	S4	260/260 (100%)	0.16	6 (2%) 57 13	67, 92, 106, 136	0
6	s4	260/260 (100%)	-0.04	0 100 100	56, 85, 99, 121	0
7	S5	206/224 (91%)	0.19	6 (2%) 49 10	100, 122, 137, 151	0
7	s5	206/224 (91%)	0.06	2 (0%) 79 29	80, 105, 128, 138	0
8	S6	226/236 (95%)	0.33	3 (1%) 74 24	67, 100, 124, 150	0
8	s6	218/236 (92%)	0.24	1 (0%) 88 46	57, 88, 112, 134	0
9	S7	184/189 (97%)	0.26	4 (2%) 59 14	87, 117, 141, 148	0
9	s7	186/189 (98%)	0.44	8 (4%) 34 7	80, 117, 146, 155	0
10	S8	188/200 (94%)	0.07	1 (0%) 88 46	58, 76, 121, 135	0
10	s8	188/200 (94%)	0.11	1 (0%) 88 46	51, 73, 125, 139	0
11	S9	185/196 (94%)	0.21	6 (3%) 45 9	85, 100, 135, 164	0
11	s9	185/196 (94%)	0.04	1 (0%) 88 46	73, 90, 124, 157	0
12	C0	96/105 (91%)	-0.07	0 100 100	84, 105, 142, 160	0
12	c0	96/105 (91%)	0.53	6 (6%) 19 4	117, 151, 165, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	C1	155/155 (100%)	0.31	7 (4%) 32 6	62, 75, 130, 142	0
13	c1	146/155 (94%)	0.08	3 (2%) 60 15	54, 73, 107, 131	0
14	C2	124/142 (87%)	1.17	27 (21%) 1 1	132, 146, 161, 169	0
14	c2	124/142 (87%)	2.09	53 (42%) 1 0	195, 206, 215, 218	0
15	C3	150/150 (100%)	-0.11	0 100 100	69, 89, 106, 113	0
15	c3	150/150 (100%)	-0.06	0 100 100	64, 82, 102, 120	0
16	C4	127/136 (93%)	0.15	2 (1%) 68 20	68, 117, 132, 138	0
16	c4	128/136 (94%)	0.04	0 100 100	54, 87, 94, 101	0
17	C5	124/141 (87%)	0.03	0 100 100	81, 98, 134, 150	0
17	c5	135/141 (95%)	0.32	6 (4%) 33 7	92, 114, 138, 148	0
18	C6	141/142 (99%)	0.28	9 (6%) 19 4	85, 114, 120, 123	0
18	c6	142/142 (100%)	0.34	7 (4%) 28 6	74, 99, 118, 143	0
19	C7	120/136 (88%)	0.46	9 (7%) 14 3	98, 114, 138, 143	0
19	c7	117/136 (86%)	0.18	3 (2%) 53 11	88, 105, 128, 133	0
20	C8	145/145 (100%)	0.28	1 (0%) 84 38	79, 109, 137, 144	0
20	c8	145/145 (100%)	0.15	2 (1%) 72 22	79, 100, 125, 138	0
21	C9	143/143 (100%)	0.15	3 (2%) 60 15	93, 110, 127, 141	0
21	c9	143/143 (100%)	0.04	0 100 100	75, 87, 111, 131	0
22	D0	107/120 (89%)	0.71	13 (12%) 5 1	78, 116, 146, 147	0
22	d0	110/120 (91%)	1.05	24 (21%) 1 1	80, 122, 156, 164	0
23	D1	87/87 (100%)	-0.10	0 100 100	92, 99, 119, 128	0
23	d1	87/87 (100%)	-0.01	1 (1%) 77 27	75, 88, 114, 129	0
24	D2	129/129 (100%)	-0.17	0 100 100	72, 83, 94, 107	0
24	d2	129/129 (100%)	-0.15	0 100 100	60, 73, 82, 94	0
25	D3	144/144 (100%)	-0.01	1 (0%) 84 38	58, 65, 75, 86	0
25	d3	144/144 (100%)	-0.08	0 100 100	48, 55, 70, 85	0
26	D4	134/134 (100%)	0.34	2 (1%) 70 21	76, 103, 120, 129	0
26	d4	134/134 (100%)	0.21	2 (1%) 70 21	66, 90, 108, 140	0
27	D5	70/107 (65%)	0.35	3 (4%) 34 7	119, 135, 143, 148	0
27	d5	69/107 (64%)	0.29	3 (4%) 34 7	94, 122, 139, 142	0
28	D6	97/97 (100%)	0.20	2 (2%) 60 15	74, 88, 137, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	d6	97/97 (100%)	-0.09	0 100 100	58, 69, 104, 111	0
29	D7	81/81 (100%)	0.10	1 (1%) 75 26	85, 101, 133, 141	0
29	d7	81/81 (100%)	0.23	2 (2%) 54 12	77, 91, 132, 140	0
30	D8	63/66 (95%)	0.85	6 (9%) 8 2	114, 131, 145, 152	0
30	d8	63/66 (95%)	0.66	1 (1%) 68 20	98, 116, 138, 151	0
31	D9	53/55 (96%)	-0.02	1 (1%) 64 18	78, 85, 110, 123	0
31	d9	53/55 (96%)	0.52	3 (5%) 23 5	79, 98, 147, 161	0
32	E0	60/60 (100%)	0.54	4 (6%) 17 4	67, 96, 136, 137	0
33	E1	71/76 (93%)	0.96	13 (18%) 2 1	111, 129, 146, 149	0
33	e1	76/76 (100%)	1.96	31 (40%) 1 0	144, 182, 193, 195	0
34	SR	318/318 (100%)	0.39	14 (4%) 33 7	71, 123, 144, 164	0
34	sR	318/318 (100%)	0.45	18 (5%) 23 5	110, 132, 145, 159	0
35	SM	159/273 (58%)	0.27	6 (3%) 38 7	63, 90, 148, 153	0
35	sM	104/273 (38%)	0.50	10 (9%) 8 2	75, 116, 194, 203	0
36	1	3149/3396 (92%)	-0.09	119 (3%) 38 7	26, 52, 142, 262	0
36	5	3150/3396 (92%)	-0.15	75 (2%) 56 13	27, 52, 128, 246	0
37	3	121/121 (100%)	-0.23	1 (0%) 83 35	40, 71, 87, 93	0
37	7	121/121 (100%)	-0.35	0 100 100	35, 55, 70, 81	0
38	4	158/158 (100%)	-0.32	3 (1%) 64 18	34, 53, 97, 144	0
38	8	158/158 (100%)	-0.24	3 (1%) 64 18	38, 62, 106, 134	0
39	L2	252/253 (99%)	-0.20	1 (0%) 90 51	35, 49, 66, 79	0
39	l2	252/253 (99%)	-0.10	5 (1%) 62 17	35, 57, 75, 86	0
40	L3	386/386 (100%)	-0.25	2 (0%) 88 46	32, 55, 70, 109	0
40	l3	386/386 (100%)	-0.29	0 100 100	27, 43, 58, 95	0
41	L4	361/361 (100%)	-0.28	0 100 100	30, 45, 66, 78	0
41	l4	361/361 (100%)	-0.21	0 100 100	33, 49, 69, 88	0
42	L5	296/296 (100%)	-0.04	1 (0%) 91 58	52, 78, 97, 122	0
42	l5	294/296 (99%)	-0.14	0 100 100	42, 61, 90, 132	0
43	L6	156/175 (89%)	-0.18	1 (0%) 86 41	40, 48, 71, 95	0
43	l6	157/175 (89%)	-0.23	2 (1%) 74 24	42, 48, 72, 87	0
44	L7	222/243 (91%)	-0.34	0 100 100	32, 41, 77, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	l7	223/243 (91%)	-0.33	0 100 100	30, 39, 78, 123	0
45	L8	233/255 (91%)	0.02	3 (1%) 74 24	58, 73, 110, 123	0
45	l8	231/255 (90%)	0.29	5 (2%) 59 14	72, 86, 118, 129	0
46	L9	191/191 (100%)	-0.10	0 100 100	48, 59, 73, 94	0
46	l9	191/191 (100%)	-0.29	0 100 100	36, 48, 68, 85	0
47	M0	211/220 (95%)	-0.16	1 (0%) 88 46	40, 54, 93, 133	0
47	m0	213/220 (96%)	-0.13	3 (1%) 72 22	40, 64, 89, 106	0
48	M1	169/173 (97%)	0.13	0 100 100	60, 83, 95, 102	0
48	m1	169/173 (97%)	-0.19	1 (0%) 86 41	43, 63, 78, 89	0
49	M3	193/198 (97%)	-0.17	0 100 100	35, 54, 105, 131	0
49	m3	194/198 (97%)	-0.07	1 (0%) 88 46	42, 65, 107, 128	0
50	M4	136/137 (99%)	-0.16	1 (0%) 84 38	42, 50, 65, 75	0
50	m4	137/137 (100%)	-0.33	0 100 100	37, 44, 67, 83	0
51	M5	203/203 (100%)	-0.24	0 100 100	35, 48, 59, 65	0
51	m5	203/203 (100%)	-0.15	0 100 100	41, 58, 71, 76	0
52	M6	197/198 (99%)	-0.26	0 100 100	32, 41, 60, 65	0
52	m6	197/198 (99%)	-0.29	0 100 100	29, 33, 60, 67	0
53	M7	183/183 (100%)	0.15	15 (8%) 12 3	36, 45, 123, 151	0
53	m7	155/183 (84%)	-0.21	0 100 100	32, 40, 56, 85	0
54	M8	185/185 (100%)	-0.32	0 100 100	36, 45, 61, 89	0
54	m8	185/185 (100%)	-0.30	0 100 100	35, 49, 60, 65	0
55	M9	188/188 (100%)	0.29	9 (4%) 29 6	52, 69, 158, 163	0
55	m9	188/188 (100%)	0.16	1 (0%) 88 46	48, 63, 148, 156	0
56	N0	172/172 (100%)	-0.27	1 (0%) 86 41	41, 48, 64, 71	0
56	n0	172/172 (100%)	-0.28	0 100 100	33, 40, 52, 65	0
57	N1	159/159 (100%)	-0.19	1 (0%) 86 41	39, 50, 93, 101	0
57	n1	159/159 (100%)	-0.24	0 100 100	36, 43, 79, 88	0
58	N2	100/120 (83%)	0.41	4 (4%) 36 7	83, 100, 116, 131	0
58	n2	98/120 (81%)	0.23	3 (3%) 47 10	74, 89, 101, 106	0
59	N3	136/136 (100%)	-0.12	3 (2%) 59 14	38, 49, 63, 73	0
59	n3	136/136 (100%)	-0.16	1 (0%) 84 38	28, 41, 58, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
60	N4	98/155 (63%)	0.84	17 (17%) 2 1	47, 66, 166, 170	0
60	n4	135/155 (87%)	0.33	13 (9%) 8 2	41, 97, 129, 147	0
61	N5	121/141 (85%)	-0.03	2 (1%) 67 19	46, 59, 78, 114	0
61	n5	120/141 (85%)	0.20	2 (1%) 67 19	52, 67, 91, 98	0
62	N6	126/126 (100%)	-0.10	1 (0%) 83 35	43, 57, 69, 82	0
62	n6	126/126 (100%)	-0.11	0 100 100	44, 59, 79, 85	0
63	N7	135/135 (100%)	0.14	0 100 100	70, 85, 99, 110	0
63	n7	135/135 (100%)	0.13	0 100 100	80, 95, 117, 130	0
64	N8	148/148 (100%)	-0.24	0 100 100	29, 46, 73, 87	0
64	n8	148/148 (100%)	-0.29	0 100 100	33, 51, 72, 76	0
65	N9	58/58 (100%)	0.16	0 100 100	40, 56, 105, 124	0
65	n9	58/58 (100%)	-0.03	0 100 100	33, 55, 87, 100	0
66	O0	97/104 (93%)	0.09	2 (2%) 60 15	68, 78, 101, 107	0
66	o0	100/104 (96%)	-0.07	0 100 100	76, 85, 112, 124	0
67	O1	109/112 (97%)	0.03	2 (1%) 65 18	49, 63, 98, 114	0
67	o1	109/112 (97%)	-0.09	1 (0%) 81 32	42, 54, 96, 115	0
68	O2	127/129 (98%)	-0.13	1 (0%) 83 35	28, 42, 56, 87	0
68	o2	127/129 (98%)	-0.19	2 (1%) 68 20	27, 46, 58, 89	0
69	O3	106/106 (100%)	-0.24	0 100 100	33, 40, 68, 82	0
69	o3	106/106 (100%)	-0.20	1 (0%) 81 32	31, 38, 67, 84	0
70	O4	112/120 (93%)	0.14	2 (1%) 65 18	46, 66, 107, 120	0
70	o4	112/120 (93%)	0.02	0 100 100	49, 71, 114, 127	0
71	O5	119/119 (100%)	-0.04	0 100 100	46, 62, 73, 78	0
71	o5	119/119 (100%)	-0.03	0 100 100	54, 69, 85, 93	0
72	O6	99/99 (100%)	0.12	4 (4%) 36 7	54, 62, 97, 122	0
72	o6	99/99 (100%)	-0.04	0 100 100	61, 75, 98, 118	0
73	O7	87/87 (100%)	-0.14	0 100 100	35, 41, 66, 95	0
73	o7	87/87 (100%)	0.10	2 (2%) 57 13	38, 46, 76, 115	0
74	O8	77/77 (100%)	0.22	0 100 100	72, 85, 113, 122	0
74	o8	77/77 (100%)	0.40	1 (1%) 74 24	77, 90, 105, 109	0
75	O9	50/50 (100%)	-0.22	0 100 100	44, 48, 55, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
75	o9	50/50 (100%)	-0.24	0	100	100	49, 52, 63, 78	0
76	Q0	52/52 (100%)	-0.07	0	100	100	42, 50, 68, 86	0
76	q0	52/52 (100%)	-0.25	0	100	100	34, 39, 50, 59	0
77	Q1	25/25 (100%)	0.12	0	100	100	55, 57, 59, 62	0
77	q1	25/25 (100%)	-0.20	0	100	100	46, 50, 64, 71	0
78	Q2	105/105 (100%)	0.25	3 (2%)	49	10	37, 57, 83, 124	0
78	q2	105/105 (100%)	0.23	0	100	100	42, 55, 79, 110	0
79	Q3	91/91 (100%)	-0.12	0	100	100	43, 52, 72, 92	0
79	q3	91/91 (100%)	-0.22	0	100	100	43, 57, 72, 84	0
80	e0	62/62 (100%)	0.46	4 (6%)	18	4	63, 87, 126, 138	0
81	m2	0/160	-	-	-	-	-	-
82	p0	120/311 (38%)	0.34	2 (1%)	67	19	90, 106, 126, 135	0
83	p1	0/47	-	-	-	-	-	-
84	p2	0/46	-	-	-	-	-	-
All	All	33040/35346 (93%)	0.03	925 (2%)	50	11	26, 71, 139, 262	0

The worst 5 of 925 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	1	1955	U	9.5
1	2	718	U	9.5
1	6	662	U	9.4
60	N4	75	THR	9.3
36	1	1238	C	9.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
85	MG	5	3857	1/1	0.85	1375.00	85,85,85,85	0
85	MG	6	2005	1/1	0.47	603.16	62,62,62,62	0
85	MG	6	1921	1/1	0.66	493.56	50,50,50,50	0
85	MG	6	1924	1/1	0.91	485.00	112,112,112,112	0
85	MG	6	2011	1/1	0.36	455.00	46,46,46,46	0
85	MG	4	219	1/1	0.78	426.33	93,93,93,93	0
85	MG	8	213	1/1	0.53	382.00	40,40,40,40	0
85	MG	7	211	1/1	0.35	361.00	64,64,64,64	0
85	MG	1	3732	1/1	0.26	283.00	91,91,91,91	0
85	MG	5	3733	1/1	0.45	228.33	71,71,71,71	0
85	MG	3	209	1/1	0.92	202.98	63,63,63,63	0
85	MG	5	3453	1/1	0.59	202.29	49,49,49,49	0
85	MG	6	2039	1/1	0.38	181.47	55,55,55,55	0
85	MG	1	3409	1/1	0.37	168.64	23,23,23,23	0
85	MG	5	3860	1/1	0.49	167.74	39,39,39,39	0
85	MG	6	1945	1/1	0.48	163.00	36,36,36,36	0
85	MG	1	3402	1/1	0.61	159.61	50,50,50,50	0
85	MG	5	3403	1/1	0.57	159.00	42,42,42,42	0
85	MG	6	1975	1/1	0.70	156.62	77,77,77,77	0
85	MG	1	3562	1/1	0.67	136.84	41,41,41,41	0
85	MG	1	3500	1/1	0.71	127.44	74,74,74,74	0
85	MG	5	3884	1/1	1.08	124.87	93,93,93,93	0
85	MG	5	3779	1/1	0.72	123.22	82,82,82,82	0
85	MG	2	1991	1/1	0.98	120.00	107,107,107,107	0
85	MG	5	3421	1/1	0.57	115.00	96,96,96,96	0
85	MG	5	3481	1/1	1.19	110.63	78,78,78,78	0
86	OHX	5	4174	7/7	0.41	108.32	175,175,175,175	0
86	OHX	1	4140	7/7	0.25	106.42	153,153,153,153	0
85	MG	1	3852	1/1	1.19	101.80	93,93,93,93	0
85	MG	1	3784	1/1	0.48	94.43	49,49,49,49	0
85	MG	1	3804	1/1	0.66	94.09	40,40,40,40	0
85	MG	1	3670	1/1	0.61	93.45	54,54,54,54	0
85	MG	2	1934	1/1	0.61	93.42	55,55,55,55	0
85	MG	5	3852	1/1	0.66	92.89	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3821	1/1	1.22	91.82	49,49,49,49	0
85	MG	5	3858	1/1	0.55	87.77	63,63,63,63	0
85	MG	5	3675	1/1	0.30	87.00	58,58,58,58	0
85	MG	2	2001	1/1	0.23	86.96	88,88,88,88	0
85	MG	2	2022	1/1	1.71	85.71	119,119,119,119	0
85	MG	1	3493	1/1	0.69	83.43	73,73,73,73	0
85	MG	5	3708	1/1	0.87	82.62	99,99,99,99	0
86	OHX	2	2123	7/7	0.27	81.67	168,168,168,168	0
85	MG	6	1959	1/1	0.65	81.47	60,60,60,60	0
85	MG	6	2030	1/1	1.44	80.83	74,74,74,74	0
85	MG	1	3619	1/1	0.38	80.00	52,52,52,52	0
85	MG	1	3744	1/1	0.50	79.41	55,55,55,55	0
85	MG	1	3463	1/1	0.20	79.00	50,50,50,50	0
85	MG	2	1905	1/1	0.51	78.99	62,62,62,62	0
85	MG	2	2020	1/1	1.37	77.18	73,73,73,73	0
85	MG	1	3580	1/1	0.67	76.70	31,31,31,31	0
85	MG	5	3555	1/1	0.63	71.09	38,38,38,38	0
85	MG	1	3697	1/1	0.42	70.99	38,38,38,38	0
85	MG	2	1957	1/1	0.93	70.13	74,74,74,74	0
85	MG	5	3718	1/1	0.85	69.84	56,56,56,56	0
85	MG	2	1908	1/1	0.63	69.42	73,73,73,73	0
85	MG	2	1917	1/1	0.67	69.31	54,54,54,54	0
85	MG	7	217	1/1	0.35	68.20	67,67,67,67	0
85	MG	2	2009	1/1	0.54	67.83	53,53,53,53	0
85	MG	1	3559	1/1	0.47	67.44	50,50,50,50	0
85	MG	1	3690	1/1	0.91	65.32	52,52,52,52	0
85	MG	1	3576	1/1	0.64	64.67	22,22,22,22	0
85	MG	2	1984	1/1	0.69	64.63	81,81,81,81	0
85	MG	1	3431	1/1	0.61	60.87	48,48,48,48	0
85	MG	1	3846	1/1	1.04	60.02	50,50,50,50	0
85	MG	5	3649	1/1	0.40	59.51	50,50,50,50	0
85	MG	1	3459	1/1	0.58	59.46	31,31,31,31	0
85	MG	1	3481	1/1	0.48	57.98	44,44,44,44	0
85	MG	2	1989	1/1	0.27	55.50	99,99,99,99	0
85	MG	5	3455	1/1	0.28	55.09	41,41,41,41	0
85	MG	5	3666	1/1	0.65	55.06	43,43,43,43	0
85	MG	6	1926	1/1	0.64	54.98	52,52,52,52	0
85	MG	2	1937	1/1	0.42	54.82	64,64,64,64	0
85	MG	5	3892	1/1	0.40	54.51	54,54,54,54	0
85	MG	1	3525	1/1	0.38	53.92	41,41,41,41	0
85	MG	5	3769	1/1	0.33	53.69	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4224	7/7	0.46	53.58	148,148,148,148	0
85	MG	5	3508	1/1	0.50	52.87	35,35,35,35	0
85	MG	1	3659	1/1	0.58	52.45	39,39,39,39	0
85	MG	5	3510	1/1	0.64	50.89	38,38,38,38	0
85	MG	1	3811	1/1	0.80	50.78	37,37,37,37	0
85	MG	6	1928	1/1	1.14	50.49	81,81,81,81	0
85	MG	1	3599	1/1	0.71	50.21	42,42,42,42	0
85	MG	6	1958	1/1	0.89	50.05	57,57,57,57	0
85	MG	1	3707	1/1	0.69	50.00	54,54,54,54	0
85	MG	2	1906	1/1	0.55	49.95	57,57,57,57	0
85	MG	1	3862	1/1	0.62	49.78	59,59,59,59	0
85	MG	1	3538	1/1	0.81	49.59	32,32,32,32	0
85	MG	2	2018	1/1	1.01	49.46	79,79,79,79	0
85	MG	2	1958	1/1	0.96	49.42	84,84,84,84	0
85	MG	6	1944	1/1	1.18	49.13	82,82,82,82	0
85	MG	8	204	1/1	0.72	49.05	54,54,54,54	0
85	MG	1	3563	1/1	0.56	48.63	26,26,26,26	0
85	MG	1	3692	1/1	0.39	47.94	63,63,63,63	0
85	MG	2	1933	1/1	0.97	47.94	81,81,81,81	0
85	MG	1	3662	1/1	0.37	47.89	34,34,34,34	0
85	MG	5	3872	1/1	0.60	47.52	49,49,49,49	0
85	MG	2	2184	1/1	1.34	47.30	91,91,91,91	0
85	MG	5	3598	1/1	0.50	46.85	17,17,17,17	0
85	MG	6	1915	1/1	0.53	46.77	42,42,42,42	0
85	MG	5	3690	1/1	0.50	46.60	56,56,56,56	0
85	MG	1	3458	1/1	0.46	46.47	72,72,72,72	0
85	MG	5	3696	1/1	1.31	46.41	75,75,75,75	0
85	MG	5	3487	1/1	0.62	46.33	42,42,42,42	0
85	MG	5	3539	1/1	0.45	46.26	34,34,34,34	0
85	MG	6	2028	1/1	0.92	46.12	69,69,69,69	0
85	MG	1	3468	1/1	0.54	46.05	55,55,55,55	0
85	MG	5	3849	1/1	0.83	45.90	59,59,59,59	0
85	MG	1	3542	1/1	0.35	45.81	28,28,28,28	0
85	MG	2	1990	1/1	0.85	45.58	52,52,52,52	0
85	MG	1	3477	1/1	0.75	45.57	47,47,47,47	0
85	MG	4	214	1/1	0.42	45.11	74,74,74,74	0
85	MG	n3	201	1/1	0.47	44.31	21,21,21,21	0
85	MG	5	3618	1/1	0.55	43.94	36,36,36,36	0
85	MG	1	3640	1/1	0.43	43.83	63,63,63,63	0
85	MG	6	1965	1/1	0.61	43.75	76,76,76,76	0
85	MG	5	3623	1/1	0.54	43.75	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3532	1/1	0.60	43.57	20,20,20,20	0
85	MG	1	3499	1/1	0.68	43.45	74,74,74,74	0
85	MG	5	3886	1/1	0.62	43.09	42,42,42,42	0
85	MG	3	213	1/1	0.48	42.88	60,60,60,60	0
85	MG	5	3493	1/1	0.65	42.88	61,61,61,61	0
85	MG	o3	201	1/1	0.93	42.17	37,37,37,37	0
86	OHX	5	4222	7/7	0.25	42.05	152,152,152,152	0
85	MG	1	3835	1/1	0.67	41.61	36,36,36,36	0
85	MG	1	3706	1/1	0.55	41.10	48,48,48,48	0
85	MG	2	2004	1/1	1.27	41.10	89,89,89,89	0
85	MG	2	1982	1/1	0.88	40.88	62,62,62,62	0
85	MG	1	3758	1/1	0.48	40.77	34,34,34,34	0
85	MG	5	3437	1/1	0.56	40.60	42,42,42,42	0
85	MG	5	3731	1/1	0.69	40.60	69,69,69,69	0
85	MG	1	3782	1/1	0.61	40.50	39,39,39,39	0
85	MG	5	3573	1/1	0.61	40.50	27,27,27,27	0
85	MG	1	3404	1/1	0.69	40.44	68,68,68,68	0
85	MG	4	205	1/1	0.54	40.38	45,45,45,45	0
85	MG	1	3597	1/1	0.86	40.36	28,28,28,28	0
85	MG	1	3844	1/1	0.57	40.08	47,47,47,47	0
85	MG	5	3569	1/1	0.55	40.02	26,26,26,26	0
85	MG	5	3451	1/1	0.70	39.85	42,42,42,42	0
85	MG	M5	302	1/1	0.64	39.84	50,50,50,50	0
85	MG	5	3436	1/1	0.33	39.70	34,34,34,34	0
85	MG	5	3682	1/1	0.63	39.27	85,85,85,85	0
85	MG	2	1945	1/1	0.92	39.11	94,94,94,94	0
85	MG	1	3514	1/1	0.41	38.97	26,26,26,26	0
85	MG	1	3549	1/1	0.44	38.60	39,39,39,39	0
85	MG	1	3836	1/1	0.54	38.60	52,52,52,52	0
85	MG	1	3833	1/1	0.41	38.57	30,30,30,30	0
85	MG	1	3406	1/1	0.95	38.54	39,39,39,39	0
85	MG	5	3414	1/1	0.49	38.52	30,30,30,30	0
85	MG	6	1913	1/1	0.48	38.47	37,37,37,37	0
85	MG	5	3633	1/1	0.72	38.30	81,81,81,81	0
86	OHX	1	4163	7/7	0.42	38.17	182,182,182,182	0
85	MG	1	3512	1/1	0.57	37.95	28,28,28,28	0
85	MG	5	3844	1/1	0.21	37.42	41,41,41,41	0
85	MG	5	3560	1/1	0.48	37.40	48,48,48,48	0
85	MG	2	2010	1/1	0.75	37.14	75,75,75,75	0
85	MG	4	218	1/1	0.58	36.85	48,48,48,48	0
85	MG	1	3511	1/1	0.60	36.78	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3832	1/1	0.84	36.68	50,50,50,50	0
85	MG	1	3473	1/1	0.62	36.60	24,24,24,24	0
85	MG	5	3645	1/1	0.83	36.60	51,51,51,51	0
86	OHX	5	4136	7/7	0.40	36.58	150,150,150,150	0
85	MG	2	1995	1/1	0.81	36.40	65,65,65,65	0
85	MG	1	4220	1/1	0.54	36.12	32,32,32,32	0
85	MG	6	1948	1/1	0.55	36.09	40,40,40,40	0
85	MG	5	3834	1/1	0.40	36.08	41,41,41,41	0
85	MG	1	3647	1/1	0.46	35.89	37,37,37,37	0
85	MG	2	1909	1/1	0.84	35.83	71,71,71,71	0
85	MG	6	1911	1/1	1.00	35.47	101,101,101,101	0
85	MG	1	3501	1/1	0.51	35.36	25,25,25,25	0
86	OHX	1	4141	7/7	0.45	35.18	147,147,147,147	0
85	MG	5	3868	1/1	0.67	35.11	38,38,38,38	0
85	MG	2	1913	1/1	1.84	35.11	82,82,82,82	0
85	MG	6	1904	1/1	0.79	34.98	81,81,81,81	0
85	MG	1	3630	1/1	0.40	34.81	57,57,57,57	0
85	MG	2	2013	1/1	0.40	34.80	50,50,50,50	0
85	MG	2	1918	1/1	0.82	34.54	53,53,53,53	0
85	MG	1	3570	1/1	0.41	34.52	26,26,26,26	0
85	MG	6	1939	1/1	0.89	34.46	71,71,71,71	0
85	MG	6	1925	1/1	0.67	34.27	45,45,45,45	0
86	OHX	1	4203	7/7	0.43	34.10	154,154,154,154	0
85	MG	1	3535	1/1	0.59	34.03	22,22,22,22	0
85	MG	6	1946	1/1	0.77	33.88	73,73,73,73	0
85	MG	2	1944	1/1	0.63	33.76	71,71,71,71	0
85	MG	6	1916	1/1	1.54	33.72	67,67,67,67	0
85	MG	6	2026	1/1	0.79	33.62	111,111,111,111	0
85	MG	1	3609	1/1	1.39	33.57	76,76,76,76	0
85	MG	5	3557	1/1	0.72	33.56	43,43,43,43	0
85	MG	5	3593	1/1	0.50	33.29	48,48,48,48	0
85	MG	5	3681	1/1	0.21	32.93	33,33,33,33	0
85	MG	1	3853	1/1	0.51	32.65	23,23,23,23	0
85	MG	N3	201	1/1	0.45	32.63	31,31,31,31	0
85	MG	1	3684	1/1	0.25	32.53	39,39,39,39	0
85	MG	1	3636	1/1	0.48	32.53	72,72,72,72	0
86	OHX	1	4188	7/7	0.44	32.50	141,141,141,141	0
85	MG	1	3694	1/1	0.46	32.48	41,41,41,41	0
85	MG	5	3600	1/1	0.67	32.47	30,30,30,30	0
85	MG	2	2016	1/1	0.70	32.44	64,64,64,64	0
85	MG	1	3461	1/1	0.44	32.43	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	4251	1/1	0.75	32.37	32,32,32,32	0
85	MG	5	3531	1/1	0.39	32.33	30,30,30,30	0
85	MG	5	3591	1/1	0.52	32.32	28,28,28,28	0
85	MG	5	3576	1/1	0.92	32.18	41,41,41,41	0
85	MG	1	3839	1/1	0.75	32.17	63,63,63,63	0
85	MG	2	1994	1/1	1.20	32.08	113,113,113,113	0
85	MG	5	3580	1/1	0.98	31.99	39,39,39,39	0
85	MG	5	3617	1/1	0.66	31.97	45,45,45,45	0
85	MG	5	3473	1/1	0.31	31.79	38,38,38,38	0
85	MG	6	2008	1/1	0.71	31.49	55,55,55,55	0
85	MG	2	1976	1/1	1.22	31.48	83,83,83,83	0
85	MG	5	3851	1/1	0.44	31.47	79,79,79,79	0
85	MG	1	3519	1/1	0.52	31.37	42,42,42,42	0
85	MG	2	1932	1/1	0.54	31.36	59,59,59,59	0
85	MG	5	3528	1/1	0.51	31.34	26,26,26,26	0
85	MG	1	3631	1/1	0.45	31.30	83,83,83,83	0
85	MG	5	3732	1/1	0.40	31.28	45,45,45,45	0
85	MG	q1	101	1/1	0.66	31.22	45,45,45,45	0
85	MG	1	3739	1/1	0.43	31.15	51,51,51,51	0
85	MG	1	3592	1/1	0.69	31.07	42,42,42,42	0
85	MG	4	210	1/1	0.31	31.00	51,51,51,51	0
85	MG	6	1951	1/1	0.80	30.86	85,85,85,85	0
86	OHX	1	4170	7/7	0.46	30.82	179,179,179,179	0
85	MG	2	1954	1/1	0.56	30.81	106,106,106,106	0
85	MG	1	3838	1/1	0.43	30.79	28,28,28,28	0
85	MG	6	1920	1/1	0.54	30.76	61,61,61,61	0
85	MG	2	1914	1/1	0.73	30.64	71,71,71,71	0
85	MG	5	3446	1/1	0.66	30.52	39,39,39,39	0
85	MG	5	3829	1/1	0.88	30.50	58,58,58,58	0
85	MG	1	3492	1/1	0.67	30.49	66,66,66,66	0
85	MG	5	3802	1/1	0.56	30.45	69,69,69,69	0
85	MG	4	203	1/1	0.71	30.27	47,47,47,47	0
85	MG	5	3465	1/1	0.44	30.27	64,64,64,64	0
85	MG	1	3537	1/1	0.49	30.24	47,47,47,47	0
85	MG	1	3678	1/1	0.51	30.21	67,67,67,67	0
85	MG	5	3879	1/1	0.63	30.10	53,53,53,53	0
85	MG	5	3749	1/1	0.50	30.06	42,42,42,42	0
85	MG	1	3556	1/1	0.71	29.87	29,29,29,29	0
85	MG	7	206	1/1	0.40	29.77	40,40,40,40	0
85	MG	1	3418	1/1	0.59	29.77	49,49,49,49	0
85	MG	4	202	1/1	0.55	29.77	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3514	1/1	0.48	29.75	54,54,54,54	0
85	MG	5	3550	1/1	0.53	29.69	49,49,49,49	0
85	MG	1	3550	1/1	0.51	29.69	38,38,38,38	0
85	MG	1	3729	1/1	0.52	29.61	36,36,36,36	0
85	MG	1	3528	1/1	0.68	29.51	31,31,31,31	0
85	MG	3	206	1/1	0.54	29.43	31,31,31,31	0
85	MG	5	3509	1/1	0.53	29.41	24,24,24,24	0
86	OHX	5	4154	7/7	0.43	29.40	143,143,143,143	0
85	MG	2	1912	1/1	0.58	29.32	74,74,74,74	0
85	MG	5	3795	1/1	0.81	29.27	61,61,61,61	0
85	MG	1	3552	1/1	0.74	29.20	38,38,38,38	0
85	MG	1	3858	1/1	0.67	29.07	76,76,76,76	0
85	MG	3	205	1/1	0.50	29.05	30,30,30,30	0
85	MG	1	3596	1/1	0.58	28.98	24,24,24,24	0
85	MG	5	3611	1/1	0.41	28.78	30,30,30,30	0
85	MG	1	3565	1/1	0.40	28.69	33,33,33,33	0
85	MG	1	3526	1/1	0.35	28.52	25,25,25,25	0
85	MG	1	3600	1/1	0.45	28.41	17,17,17,17	0
85	MG	6	1906	1/1	0.60	28.10	49,49,49,49	0
85	MG	5	3789	1/1	0.43	27.95	61,61,61,61	0
85	MG	7	205	1/1	0.53	27.90	26,26,26,26	0
85	MG	5	3584	1/1	0.55	27.69	35,35,35,35	0
85	MG	5	3612	1/1	0.51	27.64	43,43,43,43	0
85	MG	5	3587	1/1	0.59	27.60	26,26,26,26	0
85	MG	2	1928	1/1	0.84	27.57	80,80,80,80	0
85	MG	1	3503	1/1	0.42	27.48	30,30,30,30	0
85	MG	1	4217	1/1	0.87	27.37	37,37,37,37	0
85	MG	1	3460	1/1	0.43	27.30	25,25,25,25	0
85	MG	5	3876	1/1	0.43	27.20	27,27,27,27	0
85	MG	5	4253	1/1	0.39	27.12	36,36,36,36	0
85	MG	6	1922	1/1	0.91	27.11	64,64,64,64	0
85	MG	5	3774	1/1	0.42	27.08	30,30,30,30	0
85	MG	5	3863	1/1	0.55	26.83	68,68,68,68	0
85	MG	8	212	1/1	0.40	26.71	43,43,43,43	0
85	MG	3	212	1/1	0.61	26.68	58,58,58,58	0
85	MG	5	3536	1/1	0.54	26.67	40,40,40,40	0
85	MG	5	3570	1/1	0.37	26.65	25,25,25,25	0
85	MG	5	3538	1/1	0.47	26.58	23,23,23,23	0
85	MG	6	2033	1/1	0.73	26.53	73,73,73,73	0
85	MG	6	1903	1/1	0.92	26.50	54,54,54,54	0
85	MG	1	3540	1/1	0.63	26.45	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2002	1/1	0.51	26.45	96,96,96,96	0
86	OHX	1	4176	7/7	0.50	26.29	132,132,132,132	0
85	MG	2	2011	1/1	0.70	26.25	76,76,76,76	0
85	MG	6	1980	1/1	0.36	26.24	72,72,72,72	0
85	MG	5	3522	1/1	0.48	26.17	44,44,44,44	0
85	MG	6	1972	1/1	0.38	26.07	54,54,54,54	0
85	MG	5	3544	1/1	0.44	25.95	32,32,32,32	0
86	OHX	5	4208	7/7	0.23	25.93	164,164,164,164	0
85	MG	5	3642	1/1	0.41	25.92	45,45,45,45	0
85	MG	1	3412	1/1	0.35	25.79	40,40,40,40	0
85	MG	5	3559	1/1	0.58	25.74	29,29,29,29	0
85	MG	1	3620	1/1	0.34	25.43	70,70,70,70	0
85	MG	5	3664	1/1	0.87	25.39	66,66,66,66	0
85	MG	5	3519	1/1	0.49	25.38	21,21,21,21	0
85	MG	5	3406	1/1	0.51	25.14	41,41,41,41	0
85	MG	5	3713	1/1	0.55	25.05	49,49,49,49	0
85	MG	1	3786	1/1	0.47	25.05	43,43,43,43	0
85	MG	7	201	1/1	0.69	25.00	40,40,40,40	0
85	MG	5	3442	1/1	0.51	25.00	35,35,35,35	0
85	MG	5	3551	1/1	0.72	24.97	44,44,44,44	0
86	OHX	1	4127	7/7	0.49	24.91	164,164,164,164	0
85	MG	5	3672	1/1	0.46	24.86	59,59,59,59	0
85	MG	1	3863	1/1	0.53	24.80	22,22,22,22	0
85	MG	5	3641	1/1	0.40	24.74	32,32,32,32	0
85	MG	1	3557	1/1	0.41	24.67	34,34,34,34	0
86	OHX	5	4148	7/7	0.49	24.57	131,131,131,131	0
85	MG	5	3729	1/1	0.32	24.54	49,49,49,49	0
85	MG	1	3625	1/1	0.44	24.52	50,50,50,50	0
85	MG	5	3448	1/1	0.53	24.48	52,52,52,52	0
85	MG	2	1925	1/1	0.93	24.43	62,62,62,62	0
85	MG	1	3506	1/1	0.51	24.43	33,33,33,33	0
85	MG	1	3502	1/1	1.15	24.39	48,48,48,48	0
85	MG	1	3543	1/1	0.47	24.36	31,31,31,31	0
85	MG	5	3564	1/1	0.78	24.27	21,21,21,21	0
85	MG	6	1986	1/1	0.35	24.27	54,54,54,54	0
85	MG	1	3608	1/1	0.89	24.24	47,47,47,47	0
85	MG	5	3594	1/1	0.62	24.21	25,25,25,25	0
85	MG	5	3610	1/1	0.45	24.11	32,32,32,32	0
85	MG	3	204	1/1	0.60	24.09	53,53,53,53	0
85	MG	5	3595	1/1	0.35	24.05	26,26,26,26	0
85	MG	5	3658	1/1	0.39	24.00	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	S2	301	1/1	0.80	23.78	70,70,70,70	0
85	MG	5	3624	1/1	0.48	23.77	60,60,60,60	0
85	MG	2	1959	1/1	0.68	23.76	97,97,97,97	0
85	MG	1	3667	1/1	0.58	23.64	53,53,53,53	0
85	MG	1	3584	1/1	0.44	23.62	26,26,26,26	0
85	MG	6	2025	1/1	0.76	23.50	95,95,95,95	0
85	MG	5	3638	1/1	0.41	23.47	53,53,53,53	0
85	MG	6	1961	1/1	0.80	23.41	97,97,97,97	0
85	MG	1	3527	1/1	0.47	23.39	26,26,26,26	0
85	MG	2	1962	1/1	0.57	23.34	76,76,76,76	0
85	MG	1	3850	1/1	0.37	23.25	46,46,46,46	0
85	MG	2	2019	1/1	0.64	23.20	81,81,81,81	0
85	MG	1	3643	1/1	0.52	23.15	41,41,41,41	0
86	OHX	6	2177	7/7	0.37	23.08	150,150,150,150	0
85	MG	1	3857	1/1	0.51	22.88	55,55,55,55	0
85	MG	L7	304	1/1	0.51	22.87	41,41,41,41	0
85	MG	1	3775	1/1	0.52	22.85	66,66,66,66	0
85	MG	1	3691	1/1	0.61	22.83	36,36,36,36	0
85	MG	6	1931	1/1	0.52	22.70	64,64,64,64	0
85	MG	1	3700	1/1	0.43	22.55	59,59,59,59	0
85	MG	5	3526	1/1	0.48	22.49	27,27,27,27	0
85	MG	4	209	1/1	0.53	22.44	54,54,54,54	0
85	MG	2	1924	1/1	0.80	22.43	86,86,86,86	0
85	MG	1	3595	1/1	0.60	22.37	30,30,30,30	0
85	MG	5	3656	1/1	0.39	22.26	60,60,60,60	0
85	MG	5	3547	1/1	0.61	22.23	51,51,51,51	0
85	MG	2	1953	1/1	0.65	22.21	111,111,111,111	0
85	MG	5	3606	1/1	0.29	22.21	30,30,30,30	0
86	OHX	5	4227	7/7	0.40	22.20	144,144,144,144	0
85	MG	5	3605	1/1	0.61	22.16	36,36,36,36	0
85	MG	2	1902	1/1	0.36	22.14	51,51,51,51	0
85	MG	5	3888	1/1	0.44	22.09	25,25,25,25	0
85	MG	1	3513	1/1	0.52	22.08	22,22,22,22	0
85	MG	5	3736	1/1	0.27	22.07	44,44,44,44	0
85	MG	1	3455	1/1	0.85	22.05	55,55,55,55	0
85	MG	1	3448	1/1	0.34	21.95	27,27,27,27	0
85	MG	1	3818	1/1	0.39	21.92	55,55,55,55	0
85	MG	1	3715	1/1	0.44	21.91	77,77,77,77	0
85	MG	1	3462	1/1	0.40	21.90	24,24,24,24	0
85	MG	5	3456	1/1	0.39	21.82	28,28,28,28	0
86	OHX	5	4217	7/7	0.40	21.79	177,177,177,177	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3882	1/1	0.62	21.79	58,58,58,58	0
85	MG	1	3551	1/1	0.51	21.76	40,40,40,40	0
85	MG	2	1970	1/1	0.61	21.74	89,89,89,89	0
85	MG	5	3579	1/1	0.35	21.73	32,32,32,32	0
85	MG	5	3411	1/1	0.76	21.67	40,40,40,40	0
85	MG	3	202	1/1	0.44	21.60	49,49,49,49	0
85	MG	6	2040	1/1	0.37	21.54	50,50,50,50	0
85	MG	1	3515	1/1	0.65	21.52	33,33,33,33	0
85	MG	1	3490	1/1	0.68	21.51	58,58,58,58	0
86	OHX	5	4214	7/7	0.46	21.46	148,148,148,148	0
85	MG	5	3552	1/1	0.59	21.45	55,55,55,55	0
85	MG	1	3575	1/1	0.58	21.40	38,38,38,38	0
85	MG	5	3537	1/1	0.75	21.38	35,35,35,35	0
85	MG	D0	201	1/1	0.58	21.38	76,76,76,76	0
85	MG	4	212	1/1	0.41	21.37	58,58,58,58	0
85	MG	1	3751	1/1	0.37	21.22	42,42,42,42	0
85	MG	6	1935	1/1	1.08	21.21	65,65,65,65	0
86	OHX	1	4171	7/7	0.53	21.12	151,151,151,151	0
85	MG	1	3474	1/1	0.37	21.03	78,78,78,78	0
85	MG	1	3759	1/1	0.44	21.03	57,57,57,57	0
85	MG	1	3617	1/1	0.40	21.01	33,33,33,33	0
85	MG	2	2012	1/1	0.54	20.97	76,76,76,76	0
85	MG	5	3429	1/1	0.36	20.96	30,30,30,30	0
85	MG	1	3553	1/1	0.66	20.95	36,36,36,36	0
85	MG	6	1992	1/1	0.34	20.92	48,48,48,48	0
85	MG	1	3655	1/1	0.56	20.81	43,43,43,43	0
86	OHX	M9	202	7/7	0.32	20.78	182,182,182,182	0
85	MG	5	3546	1/1	0.33	20.73	34,34,34,34	0
85	MG	1	3766	1/1	0.41	20.72	56,56,56,56	0
86	OHX	1	4027	7/7	0.36	20.72	134,134,134,134	0
85	MG	5	3474	1/1	0.42	20.70	58,58,58,58	0
85	MG	5	3583	1/1	0.51	20.69	31,31,31,31	0
85	MG	1	3860	1/1	0.47	20.68	49,49,49,49	0
85	MG	6	1983	1/1	0.29	20.65	103,103,103,103	0
85	MG	1	3760	1/1	0.37	20.61	29,29,29,29	0
85	MG	2	1919	1/1	0.56	20.48	67,67,67,67	0
85	MG	1	3518	1/1	0.57	20.43	28,28,28,28	0
85	MG	5	3562	1/1	0.52	20.42	36,36,36,36	0
85	MG	5	3622	1/1	0.46	20.29	39,39,39,39	0
85	MG	5	3725	1/1	0.32	20.29	36,36,36,36	0
85	MG	5	3788	1/1	0.62	20.26	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	2008	1/1	0.94	20.25	55,55,55,55	0
85	MG	2	1940	1/1	0.42	20.22	71,71,71,71	0
85	MG	1	3589	1/1	0.55	20.13	22,22,22,22	0
85	MG	1	3530	1/1	0.85	20.06	26,26,26,26	0
85	MG	5	3648	1/1	0.61	20.06	35,35,35,35	0
85	MG	1	4218	1/1	0.40	20.03	35,35,35,35	0
85	MG	L3	401	1/1	0.48	19.99	35,35,35,35	0
86	OHX	1	4198	7/7	0.28	19.95	149,149,149,149	0
85	MG	2	1911	1/1	0.69	19.88	55,55,55,55	0
85	MG	1	3408	1/1	0.33	19.83	36,36,36,36	0
85	MG	5	3704	1/1	0.51	19.80	51,51,51,51	0
85	MG	1	3586	1/1	0.90	19.79	51,51,51,51	0
86	OHX	5	4181	7/7	0.38	19.77	149,149,149,149	0
85	MG	1	3572	1/1	0.55	19.68	39,39,39,39	0
86	OHX	1	4196	7/7	0.37	19.66	176,176,176,176	0
85	MG	2	1903	1/1	0.63	19.57	48,48,48,48	0
85	MG	7	210	1/1	0.58	19.56	36,36,36,36	0
85	MG	1	3524	1/1	0.42	19.52	28,28,28,28	0
85	MG	5	3541	1/1	0.41	19.49	18,18,18,18	0
85	MG	2	2014	1/1	0.49	19.39	72,72,72,72	0
85	MG	5	3751	1/1	0.40	19.37	40,40,40,40	0
85	MG	1	3727	1/1	0.70	19.36	37,37,37,37	0
85	MG	5	3563	1/1	0.58	19.33	26,26,26,26	0
85	MG	4	206	1/1	0.50	19.32	35,35,35,35	0
85	MG	5	3565	1/1	0.69	19.32	34,34,34,34	0
85	MG	6	1943	1/1	0.35	19.28	42,42,42,42	0
85	MG	2	1947	1/1	0.77	19.24	59,59,59,59	0
85	MG	5	3457	1/1	0.38	19.23	31,31,31,31	0
85	MG	1	3442	1/1	0.44	19.22	24,24,24,24	0
85	MG	1	3821	1/1	0.28	19.20	56,56,56,56	0
85	MG	5	3709	1/1	0.44	19.16	45,45,45,45	0
85	MG	1	3541	1/1	0.63	19.13	62,62,62,62	0
85	MG	6	1971	1/1	0.36	19.08	84,84,84,84	0
85	MG	5	3589	1/1	0.33	19.06	24,24,24,24	0
85	MG	1	3522	1/1	0.60	19.04	34,34,34,34	0
85	MG	5	3491	1/1	0.49	19.03	42,42,42,42	0
85	MG	2	1926	1/1	0.56	19.01	92,92,92,92	0
85	MG	n9	101	1/1	0.29	18.92	31,31,31,31	0
85	MG	5	3548	1/1	0.56	18.85	46,46,46,46	0
85	MG	1	3561	1/1	0.55	18.84	36,36,36,36	0
85	MG	1	3660	1/1	0.54	18.84	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	1983	1/1	0.54	18.76	81,81,81,81	0
85	MG	5	3773	1/1	0.28	18.65	31,31,31,31	0
85	MG	5	3516	1/1	0.72	18.59	41,41,41,41	0
85	MG	L7	301	1/1	0.35	18.55	35,35,35,35	0
85	MG	1	3485	1/1	0.42	18.52	42,42,42,42	0
85	MG	1	4214	1/1	0.53	18.49	39,39,39,39	0
85	MG	5	3877	1/1	0.66	18.48	30,30,30,30	0
85	MG	6	1978	1/1	0.28	18.44	81,81,81,81	0
85	MG	1	3725	1/1	0.33	18.43	49,49,49,49	0
85	MG	1	3564	1/1	0.43	18.39	47,47,47,47	0
85	MG	5	3599	1/1	0.54	18.38	35,35,35,35	0
85	MG	1	3781	1/1	0.42	18.35	46,46,46,46	0
85	MG	5	3864	1/1	0.17	18.33	40,40,40,40	0
85	MG	5	3588	1/1	0.73	18.31	23,23,23,23	0
85	MG	5	3586	1/1	0.51	18.25	26,26,26,26	0
85	MG	5	3714	1/1	0.39	18.24	47,47,47,47	0
85	MG	5	3680	1/1	0.40	18.17	46,46,46,46	0
85	MG	1	3656	1/1	0.26	18.12	34,34,34,34	0
86	OHX	5	4241	7/7	0.47	17.91	183,183,183,183	0
85	MG	d3	202	1/1	0.78	17.91	59,59,59,59	0
86	OHX	2	2144	7/7	0.49	17.89	134,134,134,134	0
85	MG	1	3476	1/1	0.23	17.86	49,49,49,49	0
85	MG	5	3525	1/1	0.45	17.85	38,38,38,38	0
85	MG	N5	201	1/1	0.43	17.85	42,42,42,42	0
85	MG	1	3830	1/1	0.42	17.82	26,26,26,26	0
85	MG	5	3477	1/1	0.43	17.82	40,40,40,40	0
85	MG	3	208	1/1	0.38	17.80	45,45,45,45	0
85	MG	1	3413	1/1	0.58	17.80	57,57,57,57	0
86	OHX	5	4164	7/7	0.34	17.78	137,137,137,137	0
85	MG	1	3574	1/1	0.51	17.72	23,23,23,23	0
85	MG	5	3895	1/1	0.50	17.67	45,45,45,45	0
85	MG	5	3418	1/1	0.54	17.61	21,21,21,21	0
85	MG	4	215	1/1	0.45	17.60	55,55,55,55	0
85	MG	5	3885	1/1	0.62	17.54	47,47,47,47	0
85	MG	q0	202	1/1	0.28	17.52	52,52,52,52	0
85	MG	6	2015	1/1	0.31	17.50	55,55,55,55	0
86	OHX	5	4132	7/7	0.33	17.49	135,135,135,135	0
85	MG	1	3438	1/1	0.54	17.48	49,49,49,49	0
85	MG	5	3542	1/1	0.48	17.45	31,31,31,31	0
85	MG	5	3833	1/1	0.34	17.42	42,42,42,42	0
85	MG	5	3432	1/1	0.30	17.29	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3689	1/1	0.29	17.24	90,90,90,90	0
85	MG	1	3453	1/1	0.40	17.19	49,49,49,49	0
85	MG	1	3539	1/1	0.31	17.17	41,41,41,41	0
85	MG	5	3459	1/1	0.39	17.17	32,32,32,32	0
85	MG	6	1912	1/1	0.72	17.17	58,58,58,58	0
85	MG	5	3566	1/1	0.55	17.15	30,30,30,30	0
85	MG	5	3520	1/1	0.45	17.12	26,26,26,26	0
85	MG	1	3745	1/1	0.42	17.11	28,28,28,28	0
85	MG	5	3650	1/1	0.29	17.09	48,48,48,48	0
85	MG	17	301	1/1	0.64	17.00	40,40,40,40	0
85	MG	5	3828	1/1	0.36	16.99	28,28,28,28	0
86	OHX	1	4057	7/7	0.44	16.96	126,126,126,126	0
85	MG	5	3517	1/1	0.36	16.87	28,28,28,28	0
85	MG	5	3495	1/1	0.39	16.87	44,44,44,44	0
86	OHX	1	4169	7/7	0.52	16.83	168,168,168,168	0
85	MG	6	1989	1/1	0.59	16.83	90,90,90,90	0
85	MG	m5	303	1/1	0.53	16.78	56,56,56,56	0
85	MG	1	3440	1/1	0.52	16.77	37,37,37,37	0
85	MG	1	3649	1/1	0.57	16.76	45,45,45,45	0
85	MG	5	3896	1/1	0.36	16.74	24,24,24,24	0
85	MG	1	3403	1/1	0.42	16.73	35,35,35,35	0
86	OHX	1	4211	7/7	0.46	16.73	173,173,173,173	0
85	MG	5	3475	1/1	0.46	16.72	49,49,49,49	0
85	MG	6	1917	1/1	0.55	16.69	64,64,64,64	0
85	MG	5	3757	1/1	0.56	16.66	63,63,63,63	0
85	MG	1	3487	1/1	0.39	16.64	32,32,32,32	0
85	MG	5	3608	1/1	0.26	16.64	41,41,41,41	0
85	MG	2	1972	1/1	0.52	16.61	73,73,73,73	0
85	MG	6	1955	1/1	0.56	16.56	41,41,41,41	0
85	MG	5	3527	1/1	0.49	16.53	45,45,45,45	0
85	MG	5	3626	1/1	0.34	16.52	37,37,37,37	0
85	MG	1	3855	1/1	0.52	16.52	48,48,48,48	0
85	MG	2	1948	1/1	0.82	16.51	92,92,92,92	0
85	MG	5	3440	1/1	0.42	16.48	40,40,40,40	0
85	MG	7	202	1/1	0.41	16.48	17,17,17,17	0
85	MG	5	3585	1/1	0.53	16.47	41,41,41,41	0
85	MG	1	3486	1/1	0.48	16.44	35,35,35,35	0
85	MG	1	3841	1/1	0.47	16.37	52,52,52,52	0
85	MG	5	3524	1/1	0.57	16.35	36,36,36,36	0
85	MG	7	209	1/1	0.53	16.34	50,50,50,50	0
85	MG	3	211	1/1	0.63	16.29	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3463	1/1	0.39	16.29	43,43,43,43	0
86	OHX	1	4125	7/7	0.44	16.28	133,133,133,133	0
85	MG	2	1965	1/1	0.75	16.23	54,54,54,54	0
85	MG	5	3470	1/1	0.58	16.22	43,43,43,43	0
85	MG	12	302	1/1	0.63	16.20	45,45,45,45	0
86	OHX	5	4170	7/7	0.43	16.18	162,162,162,162	0
86	OHX	4	230	7/7	0.32	16.17	120,120,120,120	0
85	MG	1	3831	1/1	0.45	16.14	21,21,21,21	0
86	OHX	6	2122	7/7	0.45	16.10	123,123,123,123	0
85	MG	5	3497	1/1	0.42	16.10	32,32,32,32	0
86	OHX	2	2160	7/7	0.40	16.09	174,174,174,174	0
86	OHX	1	4108	7/7	0.33	16.05	131,131,131,131	0
86	OHX	4	238	7/7	0.45	16.04	155,155,155,155	0
85	MG	1	3815	1/1	0.26	15.99	50,50,50,50	0
86	OHX	5	4143	7/7	0.36	15.87	153,153,153,153	0
85	MG	1	3688	1/1	0.37	15.85	40,40,40,40	0
86	OHX	6	2179	7/7	0.47	15.82	166,166,166,166	0
85	MG	5	3862	1/1	1.04	15.80	66,66,66,66	0
85	MG	5	3521	1/1	0.33	15.70	32,32,32,32	0
85	MG	2	1964	1/1	0.49	15.69	98,98,98,98	0
85	MG	5	3800	1/1	0.23	15.67	36,36,36,36	0
86	OHX	1	4204	7/7	0.48	15.64	130,130,130,130	0
85	MG	5	3578	1/1	0.68	15.63	34,34,34,34	0
85	MG	2	1961	1/1	0.63	15.60	59,59,59,59	0
85	MG	6	2027	1/1	0.65	15.60	80,80,80,80	0
85	MG	N8	203	1/1	0.58	15.56	31,31,31,31	0
85	MG	5	3512	1/1	0.55	15.54	23,23,23,23	0
85	MG	5	3890	1/1	0.41	15.53	58,58,58,58	0
85	MG	5	3762	1/1	0.38	15.46	42,42,42,42	0
86	OHX	5	4093	7/7	0.29	15.35	138,138,138,138	0
85	MG	6	1908	1/1	0.25	15.34	53,53,53,53	0
85	MG	5	3746	1/1	0.36	15.33	41,41,41,41	0
85	MG	5	3543	1/1	0.49	15.31	31,31,31,31	0
85	MG	6	2024	1/1	0.53	15.26	62,62,62,62	0
85	MG	5	3748	1/1	0.24	15.25	54,54,54,54	0
85	MG	5	3597	1/1	0.78	15.22	40,40,40,40	0
86	OHX	4	234	7/7	0.35	15.18	163,163,163,163	0
85	MG	2	1938	1/1	0.43	15.17	70,70,70,70	0
85	MG	1	3419	1/1	0.52	15.13	89,89,89,89	0
85	MG	2	1974	1/1	0.25	14.95	79,79,79,79	0
85	MG	1	3622	1/1	0.38	14.94	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2199	7/7	0.48	14.93	174,174,174,174	0
85	MG	6	1907	1/1	0.36	14.88	82,82,82,82	0
85	MG	5	3507	1/1	0.54	14.88	34,34,34,34	0
86	OHX	5	4085	7/7	0.53	14.85	133,133,133,133	0
85	MG	1	3629	1/1	0.22	14.84	35,35,35,35	0
85	MG	2	1907	1/1	0.69	14.78	56,56,56,56	0
85	MG	5	3571	1/1	0.64	14.72	34,34,34,34	0
85	MG	5	3710	1/1	0.31	14.69	93,93,93,93	0
85	MG	1	3798	1/1	0.53	14.59	63,63,63,63	0
86	OHX	5	4199	7/7	0.44	14.59	158,158,158,158	0
85	MG	6	1985	1/1	0.59	14.59	74,74,74,74	0
85	MG	5	3640	1/1	0.39	14.57	40,40,40,40	0
85	MG	5	3425	1/1	0.33	14.55	37,37,37,37	0
85	MG	1	3544	1/1	0.38	14.53	35,35,35,35	0
85	MG	5	3553	1/1	0.44	14.51	29,29,29,29	0
85	MG	5	3824	1/1	0.28	14.49	50,50,50,50	0
85	MG	5	3663	1/1	0.33	14.46	48,48,48,48	0
86	OHX	5	4182	7/7	0.48	14.44	129,129,129,129	0
86	OHX	1	4195	7/7	0.56	14.42	161,161,161,161	0
86	OHX	5	4187	7/7	0.37	14.38	133,133,133,133	0
85	MG	1	3445	1/1	0.37	14.35	32,32,32,32	0
85	MG	1	3435	1/1	0.39	14.33	37,37,37,37	0
85	MG	5	3511	1/1	0.62	14.33	31,31,31,31	0
85	MG	1	3796	1/1	0.42	14.33	33,33,33,33	0
85	MG	5	3737	1/1	0.47	14.32	72,72,72,72	0
85	MG	1	3828	1/1	0.56	14.32	56,56,56,56	0
85	MG	1	3588	1/1	0.47	14.31	33,33,33,33	0
85	MG	1	3722	1/1	0.33	14.30	47,47,47,47	0
85	MG	6	1934	1/1	0.42	14.28	88,88,88,88	0
86	OHX	2	2179	7/7	0.47	14.26	187,187,187,187	0
85	MG	1	3669	1/1	0.43	14.24	76,76,76,76	0
85	MG	1	3467	1/1	0.30	14.24	43,43,43,43	0
85	MG	1	3532	1/1	0.41	14.23	26,26,26,26	0
85	MG	5	3791	1/1	0.25	14.21	91,91,91,91	0
85	MG	6	2021	1/1	0.56	14.19	70,70,70,70	0
86	OHX	3	222	7/7	0.43	14.15	177,177,177,177	0
86	OHX	1	4142	7/7	0.41	14.12	144,144,144,144	0
85	MG	1	3469	1/1	0.43	14.12	56,56,56,56	0
85	MG	2	2015	1/1	0.68	14.12	63,63,63,63	0
85	MG	1	3571	1/1	0.33	14.11	23,23,23,23	0
86	OHX	2	2170	7/7	0.38	14.09	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3598	1/1	0.50	14.08	26,26,26,26	0
85	MG	5	3661	1/1	0.43	14.07	43,43,43,43	0
86	OHX	1	4134	7/7	0.39	14.05	129,129,129,129	0
86	OHX	1	4168	7/7	0.32	14.00	124,124,124,124	0
85	MG	1	3812	1/1	0.24	13.97	50,50,50,50	0
85	MG	5	3554	1/1	0.46	13.95	50,50,50,50	0
85	MG	1	3606	1/1	0.33	13.92	43,43,43,43	0
85	MG	n0	202	1/1	0.34	13.90	41,41,41,41	0
85	MG	1	3687	1/1	0.77	13.89	44,44,44,44	0
85	MG	6	1949	1/1	0.80	13.89	57,57,57,57	0
85	MG	1	3429	1/1	0.45	13.87	43,43,43,43	0
85	MG	2	1950	1/1	0.58	13.86	72,72,72,72	0
85	MG	5	3776	1/1	0.76	13.85	52,52,52,52	0
85	MG	1	3709	1/1	0.26	13.84	44,44,44,44	0
85	MG	1	3427	1/1	0.60	13.81	43,43,43,43	0
85	MG	5	3575	1/1	0.46	13.79	31,31,31,31	0
85	MG	2	1916	1/1	0.47	13.79	54,54,54,54	0
85	MG	5	3867	1/1	0.51	13.77	27,27,27,27	0
85	MG	2	1929	1/1	0.62	13.77	73,73,73,73	0
85	MG	2	1931	1/1	0.53	13.77	60,60,60,60	0
85	MG	1	3484	1/1	0.38	13.76	46,46,46,46	0
86	OHX	1	4111	7/7	0.46	13.76	160,160,160,160	0
86	OHX	1	4201	7/7	0.36	13.68	154,154,154,154	0
85	MG	1	3602	1/1	0.33	13.67	31,31,31,31	0
86	OHX	1	4197	7/7	0.33	13.67	147,147,147,147	0
85	MG	1	3444	1/1	0.28	13.65	51,51,51,51	0
85	MG	2	1981	1/1	0.65	13.61	66,66,66,66	0
85	MG	5	3413	1/1	0.69	13.60	39,39,39,39	0
85	MG	2	1936	1/1	0.47	13.58	57,57,57,57	0
85	MG	5	3558	1/1	0.53	13.57	35,35,35,35	0
85	MG	6	1991	1/1	0.40	13.56	62,62,62,62	0
85	MG	6	1910	1/1	0.49	13.52	56,56,56,56	0
85	MG	1	3568	1/1	0.60	13.50	28,28,28,28	0
85	MG	1	3762	1/1	0.63	13.47	42,42,42,42	0
85	MG	6	1967	1/1	0.34	13.44	99,99,99,99	0
85	MG	5	3478	1/1	0.39	13.39	26,26,26,26	0
85	MG	1	3675	1/1	0.34	13.33	41,41,41,41	0
85	MG	5	3646	1/1	0.48	13.32	41,41,41,41	0
85	MG	5	3861	1/1	0.31	13.29	42,42,42,42	0
85	MG	1	3632	1/1	0.39	13.29	30,30,30,30	0
85	MG	2	1915	1/1	0.54	13.26	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	M7	203	1/1	0.44	13.25	31,31,31,31	0
86	OHX	5	4196	7/7	0.43	13.25	131,131,131,131	0
85	MG	1	3591	1/1	0.78	13.20	43,43,43,43	0
85	MG	2	1987	1/1	0.45	13.20	101,101,101,101	0
85	MG	7	213	1/1	0.45	13.20	60,60,60,60	0
86	OHX	1	4162	7/7	0.37	13.20	167,167,167,167	0
86	OHX	1	4199	7/7	0.38	13.18	143,143,143,143	0
85	MG	1	3822	1/1	0.45	13.18	41,41,41,41	0
86	OHX	5	4107	7/7	0.32	13.16	125,125,125,125	0
85	MG	5	3625	1/1	0.42	13.15	43,43,43,43	0
85	MG	1	3491	1/1	0.36	13.15	32,32,32,32	0
85	MG	6	1954	1/1	0.44	13.12	57,57,57,57	0
85	MG	5	3405	1/1	0.47	13.08	31,31,31,31	0
86	OHX	5	4069	7/7	0.30	13.07	123,123,123,123	0
85	MG	2	1985	1/1	0.34	13.07	58,58,58,58	0
85	MG	5	3643	1/1	0.39	13.07	65,65,65,65	0
85	MG	1	3757	1/1	0.45	13.04	56,56,56,56	0
85	MG	8	208	1/1	0.24	13.03	64,64,64,64	0
85	MG	2	1951	1/1	1.03	13.01	102,102,102,102	0
85	MG	5	3790	1/1	0.39	12.94	40,40,40,40	0
85	MG	5	3660	1/1	0.30	12.94	23,23,23,23	0
85	MG	5	3752	1/1	0.30	12.94	52,52,52,52	0
85	MG	4	201	1/1	0.33	12.91	45,45,45,45	0
85	MG	6	2007	1/1	0.34	12.87	54,54,54,54	0
85	MG	5	3817	1/1	0.43	12.86	39,39,39,39	0
85	MG	2	1939	1/1	0.41	12.80	67,67,67,67	0
85	MG	6	1938	1/1	0.59	12.79	51,51,51,51	0
86	OHX	2	2165	7/7	0.36	12.78	157,157,157,157	0
85	MG	1	3740	1/1	0.59	12.74	57,57,57,57	0
85	MG	5	3705	1/1	0.57	12.73	47,47,47,47	0
85	MG	2	1968	1/1	0.39	12.71	64,64,64,64	0
86	OHX	5	4152	7/7	0.37	12.69	149,149,149,149	0
85	MG	5	3428	1/1	0.53	12.68	43,43,43,43	0
85	MG	1	3652	1/1	0.28	12.67	76,76,76,76	0
85	MG	n6	201	1/1	0.58	12.67	53,53,53,53	0
85	MG	5	3772	1/1	0.43	12.67	99,99,99,99	0
85	MG	2	1956	1/1	0.65	12.65	66,66,66,66	0
85	MG	1	3817	1/1	0.26	12.65	43,43,43,43	0
85	MG	5	3574	1/1	0.41	12.63	39,39,39,39	0
85	MG	5	3630	1/1	0.45	12.63	60,60,60,60	0
85	MG	1	3546	1/1	0.40	12.62	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	4	237	7/7	0.40	12.61	146,146,146,146	0
85	MG	5	3842	1/1	0.45	12.53	48,48,48,48	0
85	MG	1	3657	1/1	0.56	12.50	42,42,42,42	0
86	OHX	1	4143	7/7	0.31	12.50	151,151,151,151	0
85	MG	1	3567	1/1	0.47	12.49	30,30,30,30	0
86	OHX	5	4145	7/7	0.45	12.48	139,139,139,139	0
85	MG	5	3807	1/1	0.43	12.37	42,42,42,42	0
86	OHX	5	4176	7/7	0.35	12.35	161,161,161,161	0
85	MG	5	3740	1/1	0.31	12.34	25,25,25,25	0
85	MG	2	1966	1/1	0.29	12.33	93,93,93,93	0
85	MG	1	3579	1/1	0.48	12.32	29,29,29,29	0
85	MG	5	3639	1/1	0.26	12.29	45,45,45,45	0
86	OHX	5	4156	7/7	0.38	12.28	130,130,130,130	0
85	MG	5	3483	1/1	0.28	12.26	49,49,49,49	0
86	OHX	1	4112	7/7	0.56	12.26	136,136,136,136	0
85	MG	1	3738	1/1	0.40	12.23	53,53,53,53	0
86	OHX	5	4234	7/7	0.41	12.21	174,174,174,174	0
85	MG	1	3587	1/1	0.67	12.21	41,41,41,41	0
85	MG	1	3794	1/1	0.28	12.18	31,31,31,31	0
85	MG	5	3808	1/1	0.35	12.15	42,42,42,42	0
85	MG	1	3581	1/1	0.45	12.14	40,40,40,40	0
85	MG	1	3497	1/1	0.39	12.14	42,42,42,42	0
85	MG	2	2017	1/1	0.69	12.12	82,82,82,82	0
85	MG	5	3845	1/1	0.35	12.09	34,34,34,34	0
85	MG	2	1901	1/1	1.35	12.07	85,85,85,85	0
85	MG	M3	203	1/1	0.26	12.04	32,32,32,32	0
85	MG	1	3401	1/1	0.66	12.02	39,39,39,39	0
86	OHX	4	233	7/7	0.38	12.01	128,128,128,128	0
85	MG	1	3724	1/1	0.25	12.00	52,52,52,52	0
86	OHX	5	4078	7/7	0.34	12.00	126,126,126,126	0
85	MG	5	3883	1/1	0.25	12.00	69,69,69,69	0
85	MG	5	3503	1/1	0.27	12.00	37,37,37,37	0
85	MG	5	3635	1/1	0.24	11.98	34,34,34,34	0
85	MG	5	3874	1/1	0.50	11.95	48,48,48,48	0
85	MG	1	3529	1/1	0.34	11.91	43,43,43,43	0
85	MG	1	3671	1/1	0.50	11.88	44,44,44,44	0
85	MG	1	3516	1/1	0.58	11.85	42,42,42,42	0
85	MG	5	3505	1/1	0.51	11.81	28,28,28,28	0
86	OHX	1	4159	7/7	0.57	11.75	177,177,177,177	0
85	MG	6	1977	1/1	0.34	11.74	48,48,48,48	0
85	MG	1	3423	1/1	0.40	11.73	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4242	7/7	0.29	11.70	160,160,160,160	0
85	MG	2	1975	1/1	0.38	11.69	77,77,77,77	0
85	MG	O7	103	1/1	0.81	11.62	57,57,57,57	0
85	MG	5	3515	1/1	0.55	11.62	23,23,23,23	0
85	MG	5	3869	1/1	0.49	11.60	26,26,26,26	0
85	MG	1	3730	1/1	0.39	11.58	25,25,25,25	0
85	MG	1	3703	1/1	0.31	11.51	39,39,39,39	0
85	MG	1	3452	1/1	0.38	11.49	37,37,37,37	0
85	MG	5	3750	1/1	0.28	11.49	50,50,50,50	0
85	MG	1	3661	1/1	0.52	11.49	46,46,46,46	0
86	OHX	1	4072	7/7	0.34	11.48	111,111,111,111	0
85	MG	2	1904	1/1	0.58	11.47	75,75,75,75	0
86	OHX	2	2113	7/7	0.30	11.46	143,143,143,143	0
86	OHX	6	2180	7/7	0.46	11.44	159,159,159,159	0
85	MG	1	3439	1/1	0.72	11.43	40,40,40,40	0
85	MG	1	3676	1/1	0.34	11.42	29,29,29,29	0
85	MG	6	2034	1/1	0.73	11.42	75,75,75,75	0
85	MG	1	3533	1/1	0.37	11.40	34,34,34,34	0
85	MG	6	1942	1/1	0.31	11.40	36,36,36,36	0
85	MG	1	3509	1/1	0.32	11.35	48,48,48,48	0
86	OHX	1	4045	7/7	0.26	11.30	118,118,118,118	0
85	MG	1	3545	1/1	0.34	11.30	33,33,33,33	0
85	MG	6	2017	1/1	0.46	11.28	88,88,88,88	0
86	OHX	1	4208	7/7	0.47	11.25	139,139,139,139	0
85	MG	1	3517	1/1	0.50	11.24	35,35,35,35	0
85	MG	1	3720	1/1	0.39	11.24	41,41,41,41	0
86	OHX	5	4236	7/7	0.44	11.21	165,165,165,165	0
86	OHX	2	2154	7/7	0.40	11.20	178,178,178,178	0
85	MG	1	3673	1/1	0.49	11.20	46,46,46,46	0
85	MG	2	1942	1/1	0.31	11.13	71,71,71,71	0
85	MG	6	1918	1/1	0.76	11.11	81,81,81,81	0
85	MG	5	3794	1/1	0.25	11.10	53,53,53,53	0
85	MG	5	3609	1/1	0.35	11.10	47,47,47,47	0
86	OHX	1	4033	7/7	0.27	11.09	118,118,118,118	0
85	MG	8	210	1/1	0.41	11.08	46,46,46,46	0
85	MG	5	3445	1/1	0.34	11.06	40,40,40,40	0
85	MG	5	3797	1/1	0.47	11.06	58,58,58,58	0
85	MG	1	3642	1/1	0.28	11.04	39,39,39,39	0
86	OHX	5	4226	7/7	0.35	11.02	166,166,166,166	0
85	MG	5	3631	1/1	0.34	11.02	41,41,41,41	0
85	MG	5	3482	1/1	0.45	10.99	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3603	1/1	0.51	10.93	33,33,33,33	0
85	MG	6	1970	1/1	0.31	10.92	71,71,71,71	0
85	MG	5	3590	1/1	0.57	10.91	61,61,61,61	0
86	OHX	5	4245	7/7	0.39	10.90	163,163,163,163	0
86	OHX	6	2186	7/7	0.33	10.89	167,167,167,167	0
85	MG	1	3793	1/1	0.54	10.87	41,41,41,41	0
86	OHX	1	4189	7/7	0.51	10.86	158,158,158,158	0
85	MG	1	3510	1/1	0.43	10.84	29,29,29,29	0
86	OHX	6	2140	7/7	0.33	10.83	150,150,150,150	0
85	MG	6	1902	1/1	0.39	10.79	54,54,54,54	0
86	OHX	6	2200	7/7	0.39	10.76	171,171,171,171	0
85	MG	1	3411	1/1	0.32	10.74	30,30,30,30	0
85	MG	1	3457	1/1	0.40	10.73	40,40,40,40	0
85	MG	5	3881	1/1	0.25	10.72	39,39,39,39	0
85	MG	6	1905	1/1	0.93	10.70	56,56,56,56	0
86	OHX	5	4216	7/7	0.40	10.69	154,154,154,154	0
85	MG	1	3590	1/1	0.38	10.68	25,25,25,25	0
85	MG	5	3468	1/1	0.31	10.65	39,39,39,39	0
86	OHX	1	4185	7/7	0.40	10.65	161,161,161,161	0
85	MG	l3	401	1/1	0.45	10.63	22,22,22,22	0
85	MG	c4	201	1/1	0.57	10.60	56,56,56,56	0
86	OHX	5	4190	7/7	0.42	10.58	156,156,156,156	0
86	OHX	6	2170	7/7	0.40	10.58	143,143,143,143	0
86	OHX	1	4128	7/7	0.22	10.50	134,134,134,134	0
85	MG	1	3573	1/1	0.52	10.49	33,33,33,33	0
85	MG	1	3451	1/1	0.34	10.49	42,42,42,42	0
85	MG	5	3730	1/1	0.31	10.48	44,44,44,44	0
85	MG	1	3414	1/1	0.44	10.48	36,36,36,36	0
85	MG	1	3507	1/1	0.40	10.47	31,31,31,31	0
86	OHX	6	2147	7/7	0.35	10.44	136,136,136,136	0
86	OHX	1	4070	7/7	0.25	10.40	149,149,149,149	0
85	MG	5	3464	1/1	0.27	10.34	36,36,36,36	0
85	MG	6	1998	1/1	0.24	10.27	101,101,101,101	0
85	MG	6	2041	1/1	0.54	10.25	82,82,82,82	0
85	MG	5	3894	1/1	0.30	10.25	81,81,81,81	0
85	MG	5	3439	1/1	0.36	10.24	30,30,30,30	0
85	MG	6	1937	1/1	0.30	10.24	45,45,45,45	0
85	MG	1	3713	1/1	0.44	10.23	66,66,66,66	0
85	MG	8	202	1/1	0.53	10.22	36,36,36,36	0
85	MG	1	3861	1/1	0.38	10.21	71,71,71,71	0
85	MG	2	1921	1/1	0.44	10.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2182	7/7	0.38	10.18	164,164,164,164	0
85	MG	5	3707	1/1	0.25	10.18	53,53,53,53	0
85	MG	5	3427	1/1	0.37	10.18	38,38,38,38	0
85	MG	6	1936	1/1	0.42	10.10	90,90,90,90	0
86	OHX	1	4062	7/7	0.41	10.10	136,136,136,136	0
85	MG	5	3720	1/1	0.32	10.09	48,48,48,48	0
85	MG	5	3627	1/1	0.35	10.06	33,33,33,33	0
85	MG	12	301	1/1	0.39	10.02	38,38,38,38	0
85	MG	1	3769	1/1	0.35	9.97	32,32,32,32	0
85	MG	5	4250	1/1	0.76	9.92	43,43,43,43	0
86	OHX	1	4061	7/7	0.35	9.90	156,156,156,156	0
86	OHX	5	4232	7/7	0.40	9.89	147,147,147,147	0
85	MG	1	3787	1/1	0.29	9.89	42,42,42,42	0
86	OHX	14	403	7/7	0.56	9.86	183,183,183,183	0
86	OHX	5	4192	7/7	0.28	9.84	136,136,136,136	0
86	OHX	6	2129	7/7	0.39	9.83	171,171,171,171	0
86	OHX	5	4047	7/7	0.31	9.81	121,121,121,121	0
85	MG	5	3835	1/1	0.43	9.76	41,41,41,41	0
85	MG	5	3662	1/1	0.36	9.74	31,31,31,31	0
85	MG	1	3658	1/1	0.34	9.73	34,34,34,34	0
86	OHX	M7	206	7/7	0.53	9.72	117,117,117,117	0
85	MG	1	3615	1/1	0.38	9.71	36,36,36,36	0
86	OHX	5	4095	7/7	0.33	9.70	137,137,137,137	0
85	MG	5	3855	1/1	0.33	9.70	51,51,51,51	0
86	OHX	2	2158	7/7	0.36	9.69	130,130,130,130	0
86	OHX	2	2180	7/7	0.55	9.68	163,163,163,163	0
86	OHX	5	4066	7/7	0.28	9.66	141,141,141,141	0
85	MG	5	3561	1/1	0.60	9.66	36,36,36,36	0
85	MG	M5	301	1/1	0.40	9.63	34,34,34,34	0
85	MG	1	3864	1/1	0.50	9.60	34,34,34,34	0
86	OHX	5	4230	7/7	0.36	9.57	171,171,171,171	0
85	MG	5	3506	1/1	0.32	9.57	50,50,50,50	0
86	OHX	1	4066	7/7	0.38	9.53	133,133,133,133	0
85	MG	5	3873	1/1	0.37	9.52	42,42,42,42	0
85	MG	5	3722	1/1	0.33	9.48	45,45,45,45	0
86	OHX	6	2164	7/7	0.40	9.44	132,132,132,132	0
85	MG	1	3635	1/1	0.23	9.43	53,53,53,53	0
85	MG	5	3498	1/1	0.37	9.42	27,27,27,27	0
85	MG	5	3735	1/1	0.29	9.40	49,49,49,49	0
85	MG	1	3521	1/1	0.38	9.40	78,78,78,78	0
85	MG	6	1966	1/1	0.34	9.40	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3805	1/1	0.28	9.36	36,36,36,36	0
86	OHX	5	4213	7/7	0.27	9.31	150,150,150,150	0
85	MG	1	3577	1/1	0.43	9.29	28,28,28,28	0
85	MG	1	3450	1/1	0.28	9.28	36,36,36,36	0
86	OHX	5	4110	7/7	0.21	9.25	153,153,153,153	0
86	OHX	6	2176	7/7	0.41	9.23	154,154,154,154	0
85	MG	6	1957	1/1	1.20	9.22	60,60,60,60	0
86	OHX	1	4153	7/7	0.32	9.18	161,161,161,161	0
85	MG	1	3508	1/1	0.44	9.17	20,20,20,20	0
85	MG	1	3708	1/1	0.26	9.17	61,61,61,61	0
85	MG	1	3824	1/1	0.31	9.16	49,49,49,49	0
85	MG	5	3504	1/1	0.33	9.15	44,44,44,44	0
85	MG	M1	201	1/1	0.42	9.11	82,82,82,82	0
85	MG	5	3462	1/1	0.51	9.09	28,28,28,28	0
85	MG	5	3665	1/1	0.43	9.08	66,66,66,66	0
85	MG	o9	101	1/1	0.41	9.07	46,46,46,46	0
85	MG	5	3443	1/1	0.25	9.06	25,25,25,25	0
85	MG	1	3747	1/1	0.42	9.05	54,54,54,54	0
85	MG	5	3577	1/1	0.29	9.05	27,27,27,27	0
86	OHX	5	4173	7/7	0.46	9.04	119,119,119,119	0
85	MG	1	4219	1/1	0.35	9.00	34,34,34,34	0
85	MG	5	3837	1/1	0.31	8.94	34,34,34,34	0
86	OHX	4	229	7/7	0.21	8.92	127,127,127,127	0
85	MG	5	3760	1/1	0.35	8.90	82,82,82,82	0
86	OHX	2	2174	7/7	0.48	8.86	160,160,160,160	0
86	OHX	1	4114	7/7	0.30	8.85	137,137,137,137	0
85	MG	5	3734	1/1	0.31	8.85	40,40,40,40	0
85	MG	5	3549	1/1	0.49	8.84	49,49,49,49	0
85	MG	5	3878	1/1	0.37	8.82	30,30,30,30	0
85	MG	1	3716	1/1	0.25	8.81	34,34,34,34	0
85	MG	5	3819	1/1	0.45	8.78	59,59,59,59	0
85	MG	2	1935	1/1	0.45	8.78	51,51,51,51	0
85	MG	1	3686	1/1	0.26	8.76	46,46,46,46	0
85	MG	1	3803	1/1	0.25	8.71	59,59,59,59	0
85	MG	6	1952	1/1	0.56	8.70	69,69,69,69	0
85	MG	2	2006	1/1	0.31	8.69	65,65,65,65	0
86	OHX	1	4056	7/7	0.30	8.69	107,107,107,107	0
85	MG	2	1977	1/1	0.34	8.67	62,62,62,62	0
85	MG	5	3422	1/1	0.45	8.67	38,38,38,38	0
85	MG	1	3819	1/1	0.34	8.66	62,62,62,62	0
85	MG	1	3421	1/1	0.38	8.64	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	2021	1/1	1.03	8.64	84,84,84,84	0
85	MG	5	3671	1/1	0.36	8.64	30,30,30,30	0
86	OHX	6	2156	7/7	0.41	8.62	146,146,146,146	0
85	MG	1	3531	1/1	0.71	8.62	70,70,70,70	0
85	MG	5	3409	1/1	0.43	8.60	46,46,46,46	0
86	OHX	5	4109	7/7	0.22	8.55	129,129,129,129	0
85	MG	5	3489	1/1	0.39	8.55	26,26,26,26	0
86	OHX	6	2193	7/7	0.38	8.54	151,151,151,151	0
85	MG	1	3610	1/1	0.63	8.52	64,64,64,64	0
86	OHX	8	223	7/7	0.32	8.52	126,126,126,126	0
85	MG	1	3593	1/1	0.47	8.51	45,45,45,45	0
85	MG	1	3472	1/1	0.31	8.50	29,29,29,29	0
85	MG	5	3592	1/1	0.46	8.49	34,34,34,34	0
86	OHX	1	4119	7/7	0.38	8.47	130,130,130,130	0
85	MG	M6	202	1/1	0.56	8.47	69,69,69,69	0
85	MG	2	1967	1/1	0.69	8.47	58,58,58,58	0
85	MG	5	3659	1/1	0.25	8.46	53,53,53,53	0
86	OHX	5	4050	7/7	0.35	8.45	128,128,128,128	0
85	MG	5	3533	1/1	0.38	8.45	45,45,45,45	0
86	OHX	1	4138	7/7	0.38	8.44	151,151,151,151	0
85	MG	2	1980	1/1	0.49	8.42	63,63,63,63	0
85	MG	2	1910	1/1	0.44	8.37	59,59,59,59	0
85	MG	6	2201	1/1	0.58	8.37	65,65,65,65	0
85	MG	1	3585	1/1	0.60	8.36	43,43,43,43	0
85	MG	5	3502	1/1	0.31	8.35	30,30,30,30	0
86	OHX	1	4166	7/7	0.36	8.34	126,126,126,126	0
86	OHX	6	2183	7/7	0.32	8.34	175,175,175,175	0
85	MG	5	3871	1/1	0.35	8.33	40,40,40,40	0
86	OHX	1	4077	7/7	0.57	8.32	145,145,145,145	0
86	OHX	1	4180	7/7	0.28	8.31	145,145,145,145	0
85	MG	5	3717	1/1	0.29	8.31	47,47,47,47	0
86	OHX	1	4210	7/7	0.46	8.30	152,152,152,152	0
86	OHX	2	2153	7/7	0.43	8.27	161,161,161,161	0
85	MG	1	3756	1/1	0.35	8.24	49,49,49,49	0
85	MG	5	3815	1/1	0.41	8.23	43,43,43,43	0
85	MG	1	3664	1/1	0.37	8.17	33,33,33,33	0
85	MG	1	3851	1/1	0.24	8.16	67,67,67,67	0
85	MG	5	3763	1/1	0.31	8.13	44,44,44,44	0
85	MG	5	3744	1/1	0.24	8.11	61,61,61,61	0
86	OHX	2	2149	7/7	0.30	8.11	121,121,121,121	0
85	MG	1	3437	1/1	0.28	8.11	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	4139	7/7	0.41	8.09	123,123,123,123	0
86	OHX	6	2157	7/7	0.25	8.05	139,139,139,139	0
85	MG	6	1941	1/1	0.28	8.05	53,53,53,53	0
85	MG	5	3694	1/1	0.25	8.03	54,54,54,54	0
85	MG	5	3501	1/1	0.39	8.03	40,40,40,40	0
86	OHX	2	2119	7/7	0.31	8.02	157,157,157,157	0
85	MG	1	3704	1/1	0.32	8.02	45,45,45,45	0
86	OHX	1	4205	7/7	0.31	8.02	140,140,140,140	0
85	MG	1	3496	1/1	0.29	8.01	34,34,34,34	0
85	MG	5	3410	1/1	0.25	8.00	62,62,62,62	0
85	MG	1	3410	1/1	0.49	8.00	44,44,44,44	0
85	MG	5	3668	1/1	0.33	7.98	34,34,34,34	0
86	OHX	5	4197	7/7	0.38	7.98	151,151,151,151	0
85	MG	5	3761	1/1	0.43	7.98	38,38,38,38	0
86	OHX	5	4161	7/7	0.26	7.97	150,150,150,150	0
85	MG	6	1995	1/1	0.27	7.93	57,57,57,57	0
85	MG	1	3523	1/1	0.44	7.93	68,68,68,68	0
85	MG	6	2019	1/1	0.34	7.92	63,63,63,63	0
86	OHX	3	223	7/7	0.47	7.91	154,154,154,154	0
86	OHX	1	4174	7/7	0.36	7.91	155,155,155,155	0
85	MG	5	3415	1/1	0.36	7.88	60,60,60,60	0
85	MG	5	3715	1/1	0.36	7.88	50,50,50,50	0
85	MG	6	1960	1/1	0.53	7.87	46,46,46,46	0
86	OHX	1	4167	7/7	0.26	7.86	128,128,128,128	0
85	MG	1	3498	1/1	0.27	7.86	33,33,33,33	0
86	OHX	1	4126	7/7	0.30	7.84	161,161,161,161	0
85	MG	2	1971	1/1	0.41	7.82	81,81,81,81	0
85	MG	5	3792	1/1	0.42	7.82	45,45,45,45	0
86	OHX	5	4082	7/7	0.30	7.80	134,134,134,134	0
86	OHX	1	4158	7/7	0.33	7.77	134,134,134,134	0
85	MG	2	1986	1/1	0.30	7.75	68,68,68,68	0
86	OHX	5	4237	7/7	0.24	7.75	193,193,193,193	0
85	MG	5	3488	1/1	0.24	7.74	51,51,51,51	0
86	OHX	5	4179	7/7	0.44	7.73	136,136,136,136	0
85	MG	1	4213	1/1	0.40	7.72	31,31,31,31	0
85	MG	5	3613	1/1	0.27	7.72	46,46,46,46	0
85	MG	5	3756	1/1	0.19	7.71	61,61,61,61	0
85	MG	6	1923	1/1	0.35	7.69	75,75,75,75	0
85	MG	n0	203	1/1	0.26	7.68	37,37,37,37	0
86	OHX	5	4134	7/7	0.21	7.67	157,157,157,157	0
85	MG	6	2029	1/1	0.45	7.66	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3534	1/1	0.29	7.66	34,34,34,34	0
85	MG	1	3712	1/1	0.36	7.66	31,31,31,31	0
85	MG	5	3412	1/1	0.27	7.65	34,34,34,34	0
85	MG	1	3849	1/1	0.49	7.65	55,55,55,55	0
86	OHX	2	2092	7/7	0.31	7.65	128,128,128,128	0
85	MG	5	3523	1/1	0.54	7.64	34,34,34,34	0
85	MG	6	1919	1/1	0.40	7.63	46,46,46,46	0
85	MG	1	3456	1/1	0.28	7.63	24,24,24,24	0
86	OHX	5	3989	7/7	0.32	7.59	110,110,110,110	0
86	OHX	5	4153	7/7	0.27	7.56	120,120,120,120	0
86	OHX	6	2153	7/7	0.31	7.54	157,157,157,157	0
85	MG	5	3698	1/1	0.36	7.54	54,54,54,54	0
85	MG	1	3847	1/1	0.27	7.52	48,48,48,48	0
85	MG	5	3738	1/1	0.48	7.52	29,29,29,29	0
85	MG	1	3417	1/1	0.40	7.52	43,43,43,43	0
86	OHX	2	2103	7/7	0.28	7.52	157,157,157,157	0
85	MG	5	3438	1/1	0.39	7.51	54,54,54,54	0
85	MG	1	3702	1/1	0.35	7.51	42,42,42,42	0
85	MG	5	3596	1/1	0.39	7.49	39,39,39,39	0
86	OHX	5	4188	7/7	0.25	7.49	133,133,133,133	0
85	MG	1	3621	1/1	0.40	7.47	69,69,69,69	0
86	OHX	1	4184	7/7	0.46	7.46	142,142,142,142	0
85	MG	6	1973	1/1	0.36	7.40	52,52,52,52	0
85	MG	5	3460	1/1	0.31	7.39	29,29,29,29	0
85	MG	1	3788	1/1	0.53	7.38	31,31,31,31	0
86	OHX	2	2172	7/7	0.25	7.37	169,169,169,169	0
86	OHX	5	4159	7/7	0.36	7.37	202,202,202,202	0
86	OHX	8	228	7/7	0.29	7.36	151,151,151,151	0
86	OHX	5	4105	7/7	0.40	7.36	148,148,148,148	0
86	OHX	1	4129	7/7	0.25	7.35	175,175,175,175	0
86	OHX	5	4022	7/7	0.28	7.33	123,123,123,123	0
85	MG	1	3605	1/1	0.28	7.31	37,37,37,37	0
85	MG	8	211	1/1	0.50	7.30	94,94,94,94	0
85	MG	1	3665	1/1	0.27	7.28	47,47,47,47	0
86	OHX	7	226	7/7	0.35	7.27	174,174,174,174	0
85	MG	5	3825	1/1	0.39	7.24	38,38,38,38	0
86	OHX	1	4175	7/7	0.28	7.20	166,166,166,166	0
85	MG	1	3504	1/1	0.45	7.20	46,46,46,46	0
85	MG	5	3614	1/1	0.30	7.18	34,34,34,34	0
86	OHX	2	2163	7/7	0.36	7.17	178,178,178,178	0
86	OHX	5	4211	7/7	0.41	7.16	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3823	1/1	0.22	7.16	77,77,77,77	0
85	MG	n0	201	1/1	0.39	7.10	46,46,46,46	0
85	MG	5	3450	1/1	0.36	7.10	34,34,34,34	0
85	MG	1	3536	1/1	0.27	7.08	39,39,39,39	0
86	OHX	s9	201	7/7	0.45	7.08	149,149,149,149	0
86	OHX	5	4133	7/7	0.42	7.03	145,145,145,145	0
86	OHX	1	4067	7/7	0.25	7.02	148,148,148,148	0
85	MG	7	203	1/1	0.36	7.00	53,53,53,53	0
85	MG	n8	202	1/1	0.33	7.00	46,46,46,46	0
85	MG	5	3870	1/1	0.45	6.98	58,58,58,58	0
86	OHX	6	2165	7/7	0.28	6.98	172,172,172,172	0
85	MG	1	3680	1/1	0.29	6.98	46,46,46,46	0
85	MG	1	3424	1/1	0.40	6.94	49,49,49,49	0
85	MG	5	3782	1/1	0.29	6.93	33,33,33,33	0
86	OHX	1	4109	7/7	0.39	6.91	150,150,150,150	0
86	OHX	6	2161	7/7	0.32	6.90	159,159,159,159	0
85	MG	5	3486	1/1	0.28	6.88	46,46,46,46	0
86	OHX	6	2136	7/7	0.26	6.88	145,145,145,145	0
86	OHX	8	221	7/7	0.21	6.86	129,129,129,129	0
86	OHX	5	4150	7/7	0.34	6.83	155,155,155,155	0
86	OHX	7	228	7/7	0.27	6.78	143,143,143,143	0
85	MG	2	1960	1/1	0.39	6.78	71,71,71,71	0
85	MG	1	3470	1/1	0.25	6.77	41,41,41,41	0
86	OHX	3	225	7/7	0.30	6.77	152,152,152,152	0
85	MG	5	3841	1/1	0.25	6.75	56,56,56,56	0
86	OHX	2	2122	7/7	0.26	6.73	155,155,155,155	0
85	MG	6	1979	1/1	0.34	6.70	63,63,63,63	0
85	MG	1	3801	1/1	0.24	6.69	68,68,68,68	0
85	MG	1	3554	1/1	0.47	6.63	43,43,43,43	0
85	MG	6	1901	1/1	0.38	6.62	47,47,47,47	0
85	MG	5	3500	1/1	0.33	6.62	34,34,34,34	0
85	MG	6	1964	1/1	0.27	6.60	65,65,65,65	0
85	MG	1	3430	1/1	0.60	6.56	51,51,51,51	0
85	MG	5	3471	1/1	0.37	6.54	38,38,38,38	0
85	MG	1	3683	1/1	0.39	6.54	59,59,59,59	0
85	MG	1	3711	1/1	0.26	6.53	53,53,53,53	0
85	MG	1	3771	1/1	0.20	6.52	49,49,49,49	0
86	OHX	1	4081	7/7	0.27	6.52	147,147,147,147	0
85	MG	6	1947	1/1	0.40	6.51	54,54,54,54	0
85	MG	d3	201	1/1	0.42	6.49	54,54,54,54	0
85	MG	8	201	1/1	0.28	6.48	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	8	230	7/7	0.40	6.48	136,136,136,136	0
86	OHX	5	4129	7/7	0.29	6.45	122,122,122,122	0
85	MG	5	3812	1/1	0.27	6.43	78,78,78,78	0
86	OHX	6	2130	7/7	0.27	6.42	149,149,149,149	0
86	OHX	1	4063	7/7	0.33	6.42	150,150,150,150	0
85	MG	5	3673	1/1	0.39	6.40	32,32,32,32	0
85	MG	1	3582	1/1	0.56	6.39	49,49,49,49	0
85	MG	1	3480	1/1	0.32	6.39	54,54,54,54	0
85	MG	6	1950	1/1	0.35	6.38	46,46,46,46	0
86	OHX	6	2123	7/7	0.23	6.38	129,129,129,129	0
86	OHX	5	4121	7/7	0.31	6.36	141,141,141,141	0
85	MG	2	2007	1/1	0.48	6.33	81,81,81,81	0
86	OHX	1	4094	7/7	0.29	6.29	140,140,140,140	0
85	MG	1	3780	1/1	0.24	6.29	49,49,49,49	0
85	MG	6	1956	1/1	0.43	6.27	51,51,51,51	0
85	MG	6	1981	1/1	0.24	6.27	60,60,60,60	0
85	MG	5	3449	1/1	0.34	6.26	56,56,56,56	0
85	MG	5	3615	1/1	0.24	6.25	34,34,34,34	0
85	MG	6	2036	1/1	0.65	6.25	111,111,111,111	0
85	MG	2	1949	1/1	0.36	6.25	55,55,55,55	0
85	MG	m7	201	1/1	0.53	6.24	38,38,38,38	0
85	MG	1	3734	1/1	0.30	6.24	29,29,29,29	0
85	MG	6	1982	1/1	0.31	6.23	83,83,83,83	0
86	OHX	1	4110	7/7	0.32	6.21	120,120,120,120	0
85	MG	s8	302	1/1	0.42	6.20	50,50,50,50	0
85	MG	2	1922	1/1	0.38	6.18	66,66,66,66	0
86	OHX	5	4243	7/7	0.35	6.17	158,158,158,158	0
86	OHX	1	4177	7/7	0.41	6.16	161,161,161,161	0
85	MG	6	1929	1/1	0.30	6.16	64,64,64,64	0
86	OHX	5	4147	7/7	0.34	6.15	130,130,130,130	0
85	MG	5	3441	1/1	0.36	6.14	30,30,30,30	0
86	OHX	1	4086	7/7	0.31	6.12	143,143,143,143	0
86	OHX	1	4075	7/7	0.27	6.11	132,132,132,132	0
85	MG	5	3784	1/1	0.42	6.08	84,84,84,84	0
86	OHX	5	4205	7/7	0.28	6.07	160,160,160,160	0
86	OHX	5	4096	7/7	0.32	6.07	146,146,146,146	0
85	MG	1	3685	1/1	0.23	6.05	39,39,39,39	0
86	OHX	6	2111	7/7	0.31	6.03	142,142,142,142	0
85	MG	2	1941	1/1	0.32	5.95	68,68,68,68	0
85	MG	l3	402	1/1	0.37	5.95	38,38,38,38	0
86	OHX	7	227	7/7	0.27	5.94	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4180	7/7	0.37	5.91	134,134,134,134	0
85	MG	1	3407	1/1	0.25	5.89	41,41,41,41	0
85	MG	6	2003	1/1	0.38	5.89	72,72,72,72	0
85	MG	1	3495	1/1	0.27	5.88	47,47,47,47	0
85	MG	4	217	1/1	0.23	5.87	40,40,40,40	0
85	MG	5	3667	1/1	0.26	5.86	47,47,47,47	0
86	OHX	5	4140	7/7	0.29	5.86	132,132,132,132	0
86	OHX	1	4183	7/7	0.34	5.84	165,165,165,165	0
85	MG	1	3654	1/1	0.33	5.82	74,74,74,74	0
86	OHX	1	4207	7/7	0.40	5.82	146,146,146,146	0
85	MG	5	3742	1/1	0.23	5.80	35,35,35,35	0
85	MG	1	3560	1/1	0.25	5.78	28,28,28,28	0
85	MG	5	4252	1/1	0.43	5.78	29,29,29,29	0
85	MG	5	3499	1/1	0.29	5.77	35,35,35,35	0
85	MG	5	3778	1/1	0.41	5.76	83,83,83,83	0
85	MG	6	1953	1/1	0.38	5.76	69,69,69,69	0
85	MG	5	3887	1/1	0.31	5.73	33,33,33,33	0
86	OHX	1	4154	7/7	0.27	5.72	140,140,140,140	0
85	MG	4	204	1/1	0.61	5.72	63,63,63,63	0
86	OHX	2	2135	7/7	0.28	5.72	152,152,152,152	0
85	MG	7	215	1/1	0.37	5.71	53,53,53,53	0
85	MG	5	3686	1/1	0.46	5.71	53,53,53,53	0
85	MG	1	3842	1/1	0.44	5.70	40,40,40,40	0
85	MG	5	3798	1/1	0.44	5.70	43,43,43,43	0
86	OHX	1	4121	7/7	0.29	5.68	158,158,158,158	0
86	OHX	6	2143	7/7	0.19	5.68	125,125,125,125	0
85	MG	6	1968	1/1	0.37	5.66	76,76,76,76	0
86	OHX	1	4122	7/7	0.30	5.65	116,116,116,116	0
85	MG	1	3505	1/1	0.30	5.65	36,36,36,36	0
85	MG	o1	201	1/1	0.44	5.65	43,43,43,43	0
85	MG	1	3478	1/1	0.29	5.64	42,42,42,42	0
86	OHX	2	2147	7/7	0.33	5.62	153,153,153,153	0
85	MG	5	3654	1/1	0.27	5.62	33,33,33,33	0
86	OHX	1	4146	7/7	0.25	5.61	162,162,162,162	0
86	OHX	2	2108	7/7	0.34	5.59	151,151,151,151	0
86	OHX	15	304	7/7	0.41	5.58	164,164,164,164	0
86	OHX	5	4191	7/7	0.31	5.58	174,174,174,174	0
85	MG	5	3496	1/1	0.35	5.57	32,32,32,32	0
86	OHX	1	4091	7/7	0.23	5.56	122,122,122,122	0
85	MG	5	3747	1/1	0.27	5.54	49,49,49,49	0
86	OHX	6	2116	7/7	0.38	5.50	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3785	1/1	0.44	5.48	58,58,58,58	0
85	MG	2	1979	1/1	0.33	5.45	95,95,95,95	0
85	MG	6	2032	1/1	0.66	5.44	76,76,76,76	0
85	MG	1	3555	1/1	0.27	5.44	36,36,36,36	0
85	MG	5	3479	1/1	0.27	5.44	58,58,58,58	0
85	MG	5	3458	1/1	0.26	5.41	65,65,65,65	0
86	OHX	1	4054	7/7	0.27	5.38	119,119,119,119	0
86	OHX	6	2194	7/7	0.31	5.37	147,147,147,147	0
86	OHX	5	4167	7/7	0.33	5.37	117,117,117,117	0
85	MG	5	3670	1/1	0.24	5.37	45,45,45,45	0
86	OHX	1	4107	7/7	0.27	5.36	146,146,146,146	0
85	MG	5	3711	1/1	0.28	5.35	45,45,45,45	0
85	MG	1	3488	1/1	0.28	5.34	36,36,36,36	0
86	OHX	1	4069	7/7	0.27	5.34	125,125,125,125	0
86	OHX	1	4082	7/7	0.32	5.34	160,160,160,160	0
85	MG	6	2202	1/1	0.44	5.33	85,85,85,85	0
86	OHX	1	4190	7/7	0.32	5.32	152,152,152,152	0
85	MG	2	1978	1/1	0.25	5.32	88,88,88,88	0
85	MG	n8	203	1/1	0.40	5.31	43,43,43,43	0
85	MG	3	201	1/1	0.28	5.30	69,69,69,69	0
85	MG	5	3655	1/1	0.27	5.29	62,62,62,62	0
85	MG	5	3452	1/1	0.17	5.29	32,32,32,32	0
85	MG	5	3674	1/1	0.18	5.28	73,73,73,73	0
86	OHX	1	3990	7/7	0.23	5.28	134,134,134,134	0
85	MG	8	206	1/1	0.26	5.27	67,67,67,67	0
85	MG	5	3814	1/1	0.24	5.26	66,66,66,66	0
86	OHX	5	4195	7/7	0.24	5.25	136,136,136,136	0
85	MG	5	3687	1/1	0.26	5.24	81,81,81,81	0
85	MG	5	3424	1/1	0.50	5.23	67,67,67,67	0
85	MG	5	3775	1/1	0.29	5.22	66,66,66,66	0
86	OHX	5	4045	7/7	0.21	5.22	113,113,113,113	0
85	MG	1	3717	1/1	0.33	5.22	45,45,45,45	0
85	MG	5	3741	1/1	0.24	5.20	38,38,38,38	0
85	MG	1	3534	1/1	0.25	5.20	32,32,32,32	0
86	OHX	5	4244	7/7	0.26	5.20	144,144,144,144	0
85	MG	1	3808	1/1	0.27	5.19	45,45,45,45	0
85	MG	5	3754	1/1	0.27	5.17	63,63,63,63	0
85	MG	L2	301	1/1	0.38	5.11	38,38,38,38	0
85	MG	1	3698	1/1	0.22	5.11	52,52,52,52	0
86	OHX	5	4239	7/7	0.30	5.10	177,177,177,177	0
85	MG	6	2006	1/1	0.34	5.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3774	1/1	0.26	5.07	66,66,66,66	0
85	MG	c8	201	1/1	0.67	5.07	87,87,87,87	0
85	MG	6	1930	1/1	0.28	5.06	62,62,62,62	0
85	MG	6	1974	1/1	0.23	5.05	72,72,72,72	0
86	OHX	2	2137	7/7	0.41	5.05	151,151,151,151	0
86	OHX	5	4215	7/7	0.27	5.03	189,189,189,189	0
85	MG	1	3765	1/1	0.27	5.03	53,53,53,53	0
85	MG	2	1993	1/1	0.26	5.03	66,66,66,66	0
86	OHX	5	4220	7/7	0.37	5.01	164,164,164,164	0
85	MG	5	3494	1/1	0.31	5.01	46,46,46,46	0
86	OHX	1	4137	7/7	0.22	5.01	137,137,137,137	0
86	OHX	5	4144	7/7	0.34	5.00	166,166,166,166	0
86	OHX	5	4114	7/7	0.30	4.99	137,137,137,137	0
86	OHX	2	2155	7/7	0.24	4.98	164,164,164,164	0
85	MG	1	3547	1/1	0.15	4.98	62,62,62,62	0
85	MG	5	3771	1/1	0.27	4.98	37,37,37,37	0
86	OHX	6	2099	7/7	0.22	4.96	130,130,130,130	0
85	MG	1	3749	1/1	0.24	4.95	49,49,49,49	0
86	OHX	1	3989	7/7	0.22	4.94	117,117,117,117	0
85	MG	1	4215	1/1	0.27	4.93	31,31,31,31	0
86	OHX	5	4247	7/7	0.35	4.91	173,173,173,173	0
86	OHX	5	4052	7/7	0.25	4.90	123,123,123,123	0
85	MG	1	3433	1/1	0.27	4.90	42,42,42,42	0
85	MG	6	1927	1/1	0.27	4.88	55,55,55,55	0
86	OHX	5	4131	7/7	0.38	4.88	145,145,145,145	0
85	MG	1	3548	1/1	0.26	4.86	42,42,42,42	0
86	OHX	1	4005	7/7	0.27	4.86	129,129,129,129	0
86	OHX	3	221	7/7	0.33	4.84	136,136,136,136	0
86	OHX	D9	102	7/7	0.34	4.83	165,165,165,165	0
85	MG	5	3454	1/1	0.37	4.83	35,35,35,35	0
85	MG	1	3646	1/1	0.26	4.83	69,69,69,69	0
85	MG	1	3710	1/1	0.24	4.82	55,55,55,55	0
85	MG	5	3766	1/1	0.31	4.82	44,44,44,44	0
85	MG	5	3518	1/1	0.28	4.79	36,36,36,36	0
85	MG	1	3471	1/1	0.29	4.79	40,40,40,40	0
85	MG	6	2014	1/1	0.59	4.78	63,63,63,63	0
85	MG	1	3741	1/1	0.27	4.76	43,43,43,43	0
85	MG	5	3556	1/1	0.43	4.75	33,33,33,33	0
85	MG	2	1952	1/1	0.53	4.74	106,106,106,106	0
86	OHX	5	4186	7/7	0.28	4.74	132,132,132,132	0
86	OHX	1	4206	7/7	0.37	4.72	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	3	224	7/7	0.29	4.72	149,149,149,149	0
86	OHX	6	2152	7/7	0.40	4.72	188,188,188,188	0
85	MG	5	3728	1/1	0.51	4.70	81,81,81,81	0
85	MG	1	3432	1/1	0.40	4.68	38,38,38,38	0
86	OHX	5	4067	7/7	0.18	4.67	144,144,144,144	0
85	MG	19	201	1/1	0.30	4.64	47,47,47,47	0
85	MG	m6	201	1/1	0.44	4.62	75,75,75,75	0
86	OHX	1	3971	7/7	0.21	4.61	117,117,117,117	0
85	MG	1	3777	1/1	0.23	4.61	54,54,54,54	0
85	MG	1	3666	1/1	0.27	4.59	54,54,54,54	0
86	OHX	5	4219	7/7	0.39	4.59	136,136,136,136	0
86	OHX	1	4202	7/7	0.41	4.57	154,154,154,154	0
86	OHX	1	4182	7/7	0.39	4.57	153,153,153,153	0
85	MG	M0	301	1/1	0.31	4.56	42,42,42,42	0
86	OHX	1	4116	7/7	0.32	4.55	144,144,144,144	0
85	MG	1	3778	1/1	0.24	4.55	35,35,35,35	0
85	MG	1	3699	1/1	0.30	4.55	53,53,53,53	0
85	MG	5	3793	1/1	0.23	4.50	49,49,49,49	0
86	OHX	5	4081	7/7	0.26	4.49	130,130,130,130	0
85	MG	5	3724	1/1	0.29	4.49	58,58,58,58	0
85	MG	2	1930	1/1	0.30	4.49	68,68,68,68	0
85	MG	5	3676	1/1	0.25	4.49	44,44,44,44	0
85	MG	1	3795	1/1	0.23	4.48	53,53,53,53	0
86	OHX	2	2138	7/7	0.29	4.44	178,178,178,178	0
86	OHX	6	2173	7/7	0.31	4.44	135,135,135,135	0
85	MG	1	3767	1/1	0.30	4.44	69,69,69,69	0
86	OHX	2	2140	7/7	0.34	4.40	176,176,176,176	0
86	OHX	2	2126	7/7	0.28	4.39	147,147,147,147	0
85	MG	N8	201	1/1	0.23	4.39	31,31,31,31	0
85	MG	d4	201	1/1	0.48	4.39	66,66,66,66	0
85	MG	1	3566	1/1	0.31	4.38	35,35,35,35	0
86	OHX	2	2136	7/7	0.29	4.36	144,144,144,144	0
85	MG	6	1963	1/1	0.42	4.35	114,114,114,114	0
85	MG	5	3490	1/1	0.22	4.35	29,29,29,29	0
85	MG	5	3880	1/1	0.38	4.33	89,89,89,89	0
85	MG	1	3695	1/1	0.42	4.32	46,46,46,46	0
85	MG	6	2023	1/1	0.28	4.31	106,106,106,106	0
85	MG	6	1932	1/1	0.25	4.30	51,51,51,51	0
85	MG	1	3814	1/1	0.18	4.30	53,53,53,53	0
86	OHX	5	4146	7/7	0.21	4.29	171,171,171,171	0
85	MG	2	1923	1/1	0.30	4.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	6	2174	7/7	0.28	4.27	162,162,162,162	0
85	MG	5	3810	1/1	0.24	4.27	31,31,31,31	0
85	MG	2	2002	1/1	0.38	4.27	113,113,113,113	0
85	MG	O7	102	1/1	0.30	4.27	34,34,34,34	0
85	MG	5	3719	1/1	0.27	4.24	69,69,69,69	0
86	OHX	5	4101	7/7	0.29	4.22	113,113,113,113	0
86	OHX	5	4160	7/7	0.35	4.21	145,145,145,145	0
86	OHX	6	2185	7/7	0.17	4.18	148,148,148,148	0
86	OHX	2	2075	7/7	0.28	4.18	155,155,155,155	0
85	MG	5	3582	1/1	0.34	4.18	28,28,28,28	0
85	MG	1	3578	1/1	0.23	4.14	30,30,30,30	0
86	OHX	8	227	7/7	0.21	4.14	151,151,151,151	0
86	OHX	4	228	7/7	0.19	4.13	115,115,115,115	0
85	MG	5	3568	1/1	0.33	4.12	38,38,38,38	0
85	MG	5	3572	1/1	0.35	4.11	34,34,34,34	0
85	MG	5	3467	1/1	0.24	4.09	33,33,33,33	0
85	MG	O7	104	1/1	0.36	4.08	48,48,48,48	0
85	MG	5	3484	1/1	0.60	4.07	17,17,17,17	0
86	OHX	6	2191	7/7	0.40	4.05	168,168,168,168	0
85	MG	1	3616	1/1	0.36	4.04	38,38,38,38	0
85	MG	5	3716	1/1	0.30	4.03	65,65,65,65	0
86	OHX	2	2132	7/7	0.40	4.03	141,141,141,141	0
85	MG	1	3623	1/1	0.29	4.02	40,40,40,40	0
85	MG	5	3796	1/1	0.25	4.02	41,41,41,41	0
86	OHX	5	4055	7/7	0.24	4.01	144,144,144,144	0
85	MG	5	3809	1/1	0.19	4.00	69,69,69,69	0
85	MG	6	1990	1/1	0.27	4.00	61,61,61,61	0
86	OHX	5	4122	7/7	0.23	3.99	152,152,152,152	0
86	OHX	5	4112	7/7	0.25	3.98	145,145,145,145	0
85	MG	m5	302	1/1	0.22	3.96	42,42,42,42	0
85	MG	n6	202	1/1	0.35	3.96	48,48,48,48	0
86	OHX	5	4158	7/7	0.22	3.95	157,157,157,157	0
86	OHX	5	4068	7/7	0.21	3.94	125,125,125,125	0
85	MG	1	3748	1/1	0.35	3.93	52,52,52,52	0
86	OHX	1	4071	7/7	0.23	3.93	157,157,157,157	0
85	MG	5	3632	1/1	0.20	3.92	41,41,41,41	0
85	MG	5	3727	1/1	0.41	3.91	27,27,27,27	0
86	OHX	2	2091	7/7	0.37	3.87	177,177,177,177	0
86	OHX	6	2171	7/7	0.28	3.87	166,166,166,166	0
85	MG	o4	201	1/1	0.42	3.87	60,60,60,60	0
86	OHX	5	4206	7/7	0.26	3.86	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3743	1/1	0.21	3.85	46,46,46,46	0
85	MG	1	3613	1/1	0.17	3.84	43,43,43,43	0
86	OHX	5	4088	7/7	0.23	3.84	126,126,126,126	0
86	OHX	2	2169	7/7	0.30	3.83	141,141,141,141	0
86	OHX	6	2196	7/7	0.29	3.82	162,162,162,162	0
85	MG	1	3820	1/1	0.28	3.81	47,47,47,47	0
85	MG	6	1909	1/1	0.50	3.80	128,128,128,128	0
86	OHX	6	2166	7/7	0.36	3.80	167,167,167,167	0
86	OHX	1	4135	7/7	0.26	3.80	126,126,126,126	0
85	MG	8	203	1/1	0.30	3.79	56,56,56,56	0
86	OHX	5	4178	7/7	0.40	3.79	151,151,151,151	0
85	MG	1	3843	1/1	0.36	3.79	55,55,55,55	0
85	MG	5	3811	1/1	0.19	3.78	39,39,39,39	0
86	OHX	2	2120	7/7	0.23	3.77	152,152,152,152	0
86	OHX	1	4099	7/7	0.24	3.76	135,135,135,135	0
86	OHX	5	4102	7/7	0.23	3.76	126,126,126,126	0
86	OHX	6	2119	7/7	0.27	3.76	118,118,118,118	0
86	OHX	5	4198	7/7	0.33	3.76	140,140,140,140	0
85	MG	5	3417	1/1	0.22	3.75	27,27,27,27	0
86	OHX	2	2161	7/7	0.54	3.75	152,152,152,152	0
85	MG	5	3434	1/1	0.29	3.74	81,81,81,81	0
85	MG	5	3783	1/1	0.23	3.74	35,35,35,35	0
86	OHX	1	4004	7/7	0.20	3.74	129,129,129,129	0
86	OHX	1	4130	7/7	0.29	3.71	160,160,160,160	0
85	MG	O2	201	1/1	0.34	3.71	33,33,33,33	0
85	MG	1	3648	1/1	0.25	3.71	47,47,47,47	0
86	OHX	1	4192	7/7	0.42	3.69	164,164,164,164	0
85	MG	2	1969	1/1	0.52	3.68	131,131,131,131	0
86	OHX	M7	207	7/7	0.30	3.67	159,159,159,159	0
85	MG	4	211	1/1	0.30	3.67	37,37,37,37	0
85	MG	m5	301	1/1	0.38	3.67	56,56,56,56	0
86	OHX	2	2175	7/7	0.40	3.66	174,174,174,174	0
85	MG	s8	301	1/1	0.31	3.65	62,62,62,62	0
85	MG	5	3768	1/1	0.46	3.64	99,99,99,99	0
86	OHX	5	4084	7/7	0.25	3.61	127,127,127,127	0
85	MG	1	3859	1/1	0.34	3.60	121,121,121,121	0
85	MG	1	3746	1/1	0.21	3.60	40,40,40,40	0
86	OHX	2	2156	7/7	0.22	3.59	161,161,161,161	0
85	MG	6	2038	1/1	0.47	3.59	85,85,85,85	0
86	OHX	5	4120	7/7	0.27	3.59	147,147,147,147	0
85	MG	2	1955	1/1	0.31	3.58	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	2	1996	1/1	0.27	3.57	96,96,96,96	0
85	MG	5	3476	1/1	0.19	3.56	83,83,83,83	0
85	MG	5	3535	1/1	0.20	3.53	56,56,56,56	0
85	MG	6	2018	1/1	0.49	3.52	79,79,79,79	0
86	OHX	1	4078	7/7	0.25	3.52	139,139,139,139	0
86	OHX	1	4097	7/7	0.33	3.51	165,165,165,165	0
86	OHX	1	3976	7/7	0.29	3.51	99,99,99,99	0
85	MG	6	1987	1/1	0.28	3.50	104,104,104,104	0
86	OHX	1	4133	7/7	0.25	3.50	152,152,152,152	0
86	OHX	1	3983	7/7	0.25	3.49	118,118,118,118	0
86	OHX	5	4089	7/7	0.26	3.48	125,125,125,125	0
86	OHX	5	4130	7/7	0.28	3.48	150,150,150,150	0
85	MG	5	3692	1/1	0.31	3.43	45,45,45,45	0
86	OHX	2	2129	7/7	0.31	3.43	158,158,158,158	0
85	MG	5	3823	1/1	0.18	3.43	67,67,67,67	0
86	OHX	6	2132	7/7	0.27	3.43	159,159,159,159	0
86	OHX	5	4115	7/7	0.25	3.42	157,157,157,157	0
85	MG	n3	202	1/1	0.42	3.39	48,48,48,48	0
86	OHX	2	2117	7/7	0.31	3.39	154,154,154,154	0
85	MG	5	3781	1/1	0.17	3.39	54,54,54,54	0
85	MG	5	3865	1/1	0.25	3.37	31,31,31,31	0
85	MG	M7	202	1/1	0.32	3.35	28,28,28,28	0
85	MG	5	3402	1/1	0.25	3.35	29,29,29,29	0
85	MG	1	3651	1/1	0.26	3.34	50,50,50,50	0
86	OHX	5	4127	7/7	0.29	3.34	128,128,128,128	0
85	MG	1	3679	1/1	0.24	3.34	41,41,41,41	0
86	OHX	2	2146	7/7	0.36	3.33	154,154,154,154	0
86	OHX	1	4064	7/7	0.30	3.32	124,124,124,124	0
85	MG	6	1988	1/1	0.37	3.31	74,74,74,74	0
86	OHX	5	4038	7/7	0.24	3.31	145,145,145,145	0
85	MG	m6	202	1/1	0.34	3.31	32,32,32,32	0
85	MG	5	3891	1/1	0.27	3.30	124,124,124,124	0
86	OHX	1	4157	7/7	0.37	3.30	158,158,158,158	0
86	OHX	2	2112	7/7	0.29	3.30	176,176,176,176	0
85	MG	N0	201	1/1	0.32	3.29	40,40,40,40	0
85	MG	1	3701	1/1	0.51	3.28	77,77,77,77	0
86	OHX	1	4194	7/7	0.39	3.28	146,146,146,146	0
85	MG	6	2016	1/1	0.26	3.27	118,118,118,118	0
85	MG	2	2182	1/1	0.30	3.26	74,74,74,74	0
85	MG	q3	502	1/1	0.34	3.21	73,73,73,73	0
86	OHX	5	4040	7/7	0.22	3.20	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	4142	7/7	0.27	3.20	145,145,145,145	0
85	MG	5	3444	1/1	0.20	3.20	31,31,31,31	0
85	MG	1	3779	1/1	0.22	3.19	73,73,73,73	0
86	OHX	5	4204	7/7	0.27	3.18	137,137,137,137	0
86	OHX	2	2128	7/7	0.25	3.16	148,148,148,148	0
85	MG	5	3629	1/1	0.26	3.15	46,46,46,46	0
86	OHX	1	4059	7/7	0.18	3.14	144,144,144,144	0
86	OHX	5	3908	7/7	0.19	3.14	66,66,66,66	0
86	OHX	5	4141	7/7	0.23	3.13	123,123,123,123	0
85	MG	1	3624	1/1	0.19	3.12	45,45,45,45	0
86	OHX	6	2068	7/7	0.19	3.11	108,108,108,108	0
86	OHX	5	4138	7/7	0.26	3.10	124,124,124,124	0
85	MG	5	3826	1/1	0.24	3.10	46,46,46,46	0
86	OHX	s1	303	7/7	0.41	3.09	187,187,187,187	0
85	MG	5	3461	1/1	0.26	3.09	44,44,44,44	0
85	MG	5	3416	1/1	0.24	3.09	39,39,39,39	0
86	OHX	2	2173	7/7	0.45	3.08	170,170,170,170	0
85	MG	c1	201	1/1	0.31	3.08	54,54,54,54	0
86	OHX	1	4074	7/7	0.29	3.07	128,128,128,128	0
86	OHX	2	2062	7/7	0.24	3.07	142,142,142,142	0
86	OHX	1	4046	7/7	0.21	3.07	119,119,119,119	0
86	OHX	L4	402	7/7	0.27	3.06	157,157,157,157	0
85	MG	1	3628	1/1	0.28	3.06	36,36,36,36	0
85	MG	5	3581	1/1	0.26	3.06	32,32,32,32	0
86	OHX	6	2167	7/7	0.37	3.05	124,124,124,124	0
86	OHX	5	4117	7/7	0.27	3.05	144,144,144,144	0
86	OHX	6	2113	7/7	0.43	3.03	167,167,167,167	0
86	OHX	1	4079	7/7	0.30	3.03	135,135,135,135	0
85	MG	1	3454	1/1	0.45	3.02	56,56,56,56	0
86	OHX	1	4118	7/7	0.31	3.02	141,141,141,141	0
86	OHX	5	4231	7/7	0.56	3.02	163,163,163,163	0
85	MG	6	2031	1/1	0.51	2.98	92,92,92,92	0
86	OHX	2	2141	7/7	0.24	2.96	169,169,169,169	0
86	OHX	6	2137	7/7	0.23	2.96	202,202,202,202	0
86	OHX	5	4041	7/7	0.28	2.95	136,136,136,136	0
85	MG	6	1962	1/1	0.28	2.94	48,48,48,48	0
86	OHX	2	2164	7/7	0.25	2.93	179,179,179,179	0
86	OHX	2	2105	7/7	0.24	2.93	132,132,132,132	0
85	MG	N5	202	1/1	0.21	2.93	52,52,52,52	0
85	MG	5	3480	1/1	0.45	2.92	60,60,60,60	0
85	MG	M7	201	1/1	0.74	2.91	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3545	1/1	0.43	2.89	66,66,66,66	0
85	MG	5	3540	1/1	0.23	2.86	39,39,39,39	0
85	MG	3	210	1/1	0.29	2.85	64,64,64,64	0
86	OHX	6	2159	7/7	0.23	2.83	146,146,146,146	0
85	MG	1	3405	1/1	0.53	2.83	117,117,117,117	0
86	OHX	2	2177	7/7	0.36	2.83	164,164,164,164	0
85	MG	1	3611	1/1	0.21	2.81	47,47,47,47	0
86	OHX	5	4135	7/7	0.27	2.81	140,140,140,140	0
85	MG	7	214	1/1	0.22	2.81	72,72,72,72	0
85	MG	1	3723	1/1	0.25	2.80	64,64,64,64	0
86	OHX	2	2116	7/7	0.38	2.80	165,165,165,165	0
85	MG	5	3628	1/1	0.23	2.78	62,62,62,62	0
86	OHX	5	4207	7/7	0.28	2.78	156,156,156,156	0
85	MG	7	216	1/1	0.22	2.78	56,56,56,56	0
86	OHX	5	4200	7/7	0.30	2.78	147,147,147,147	0
86	OHX	5	4072	7/7	0.30	2.78	141,141,141,141	0
86	OHX	5	4171	7/7	0.27	2.78	153,153,153,153	0
86	OHX	6	2128	7/7	0.31	2.76	142,142,142,142	0
85	MG	5	3843	1/1	0.31	2.75	54,54,54,54	0
85	MG	1	3668	1/1	0.33	2.75	40,40,40,40	0
85	MG	5	3420	1/1	0.18	2.75	77,77,77,77	0
85	MG	1	3650	1/1	0.23	2.69	27,27,27,27	0
85	MG	1	3705	1/1	0.24	2.68	46,46,46,46	0
86	OHX	5	4092	7/7	0.23	2.66	164,164,164,164	0
86	OHX	5	4218	7/7	0.32	2.65	160,160,160,160	0
86	OHX	5	4035	7/7	0.24	2.65	100,100,100,100	0
85	MG	1	3482	1/1	0.24	2.65	30,30,30,30	0
86	OHX	6	2148	7/7	0.21	2.65	173,173,173,173	0
86	OHX	1	4000	7/7	0.29	2.64	124,124,124,124	0
85	MG	5	3695	1/1	0.16	2.63	51,51,51,51	0
86	OHX	2	2084	7/7	0.20	2.63	133,133,133,133	0
85	MG	1	3416	1/1	0.28	2.63	32,32,32,32	0
85	MG	5	3644	1/1	0.18	2.62	35,35,35,35	0
85	MG	1	3696	1/1	0.34	2.62	48,48,48,48	0
85	MG	1	3773	1/1	0.27	2.62	55,55,55,55	0
86	OHX	5	4065	7/7	0.22	2.61	154,154,154,154	0
86	OHX	2	2079	7/7	0.23	2.58	131,131,131,131	0
86	OHX	6	2195	7/7	0.29	2.58	161,161,161,161	0
85	MG	5	3529	1/1	0.41	2.57	56,56,56,56	0
86	OHX	5	4168	7/7	0.25	2.55	102,102,102,102	0
86	OHX	6	2187	7/7	0.37	2.55	181,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3780	1/1	0.45	2.54	84,84,84,84	0
85	MG	5	3603	1/1	0.20	2.54	50,50,50,50	0
85	MG	1	3825	1/1	0.23	2.52	45,45,45,45	0
86	OHX	5	4061	7/7	0.22	2.51	129,129,129,129	0
85	MG	2	2003	1/1	0.25	2.51	120,120,120,120	0
85	MG	4	220	1/1	0.20	2.50	54,54,54,54	0
87	ZN	d7	101	1/1	0.59	2.49	162,162,162,162	0
86	OHX	5	4209	7/7	0.20	2.48	127,127,127,127	0
86	OHX	1	4087	7/7	0.24	2.48	137,137,137,137	0
86	OHX	1	4160	7/7	0.43	2.47	171,171,171,171	0
85	MG	5	3693	1/1	0.21	2.45	50,50,50,50	0
85	MG	2	1973	1/1	0.39	2.44	90,90,90,90	0
85	MG	1	3653	1/1	0.41	2.43	101,101,101,101	0
85	MG	2	1943	1/1	0.29	2.43	69,69,69,69	0
86	OHX	5	4103	7/7	0.28	2.42	136,136,136,136	0
85	MG	5	3492	1/1	0.32	2.41	51,51,51,51	0
85	MG	1	3761	1/1	0.19	2.41	42,42,42,42	0
85	MG	5	3813	1/1	0.23	2.40	51,51,51,51	0
86	OHX	5	4058	7/7	0.26	2.40	137,137,137,137	0
86	OHX	2	2074	7/7	0.22	2.39	121,121,121,121	0
85	MG	8	205	1/1	0.28	2.39	40,40,40,40	0
86	OHX	5	4098	7/7	0.22	2.38	110,110,110,110	0
85	MG	1	3754	1/1	0.21	2.37	29,29,29,29	0
85	MG	5	3636	1/1	0.29	2.36	81,81,81,81	0
85	MG	5	3786	1/1	0.28	2.34	52,52,52,52	0
86	OHX	1	4043	7/7	0.22	2.34	109,109,109,109	0
85	MG	5	3602	1/1	0.28	2.34	46,46,46,46	0
86	OHX	5	4157	7/7	0.22	2.33	122,122,122,122	0
86	OHX	2	2171	7/7	0.41	2.33	160,160,160,160	0
85	MG	1	3772	1/1	0.21	2.33	51,51,51,51	0
85	MG	6	1976	1/1	0.23	2.32	47,47,47,47	0
86	OHX	s4	301	7/7	0.26	2.31	169,169,169,169	0
85	MG	1	3791	1/1	0.18	2.30	62,62,62,62	0
86	OHX	5	4086	7/7	0.28	2.30	115,115,115,115	0
85	MG	sM	301	1/1	0.37	2.30	48,48,48,48	0
86	OHX	4	235	7/7	0.21	2.29	146,146,146,146	0
85	MG	5	3472	1/1	0.22	2.29	46,46,46,46	0
85	MG	5	3669	1/1	0.24	2.27	31,31,31,31	0
86	OHX	1	4179	7/7	0.46	2.27	150,150,150,150	0
85	MG	1	3633	1/1	0.18	2.26	34,34,34,34	0
86	OHX	5	4183	7/7	0.33	2.26	183,183,183,183	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3569	1/1	0.29	2.26	35,35,35,35	0
86	OHX	1	4038	7/7	0.21	2.24	131,131,131,131	0
86	OHX	4	236	7/7	0.23	2.22	141,141,141,141	0
85	MG	5	3893	1/1	0.25	2.22	53,53,53,53	0
85	MG	1	3494	1/1	0.20	2.22	48,48,48,48	0
85	MG	5	3721	1/1	0.24	2.21	50,50,50,50	0
86	OHX	1	4149	7/7	0.22	2.21	148,148,148,148	0
86	OHX	6	2109	7/7	0.21	2.19	116,116,116,116	0
85	MG	5	3889	1/1	0.22	2.19	88,88,88,88	0
86	OHX	6	2169	7/7	0.33	2.19	170,170,170,170	0
85	MG	1	3672	1/1	0.13	2.17	83,83,83,83	0
86	OHX	6	2172	7/7	0.25	2.17	118,118,118,118	0
85	MG	7	204	1/1	0.22	2.15	84,84,84,84	0
86	OHX	6	2120	7/7	0.30	2.15	150,150,150,150	0
85	MG	6	2020	1/1	0.26	2.14	51,51,51,51	0
85	MG	1	3693	1/1	0.23	2.13	37,37,37,37	0
86	OHX	5	4075	7/7	0.22	2.13	152,152,152,152	0
85	MG	1	3763	1/1	0.27	2.12	49,49,49,49	0
85	MG	14	401	1/1	0.35	2.12	37,37,37,37	0
85	MG	5	3530	1/1	0.20	2.10	24,24,24,24	0
85	MG	5	3685	1/1	0.22	2.09	49,49,49,49	0
86	OHX	5	4202	7/7	0.31	2.09	148,148,148,148	0
86	OHX	1	4209	7/7	0.27	2.09	171,171,171,171	0
85	MG	o7	502	1/1	0.26	2.09	44,44,44,44	0
86	OHX	5	4225	7/7	0.24	2.09	200,200,200,200	0
85	MG	5	3831	1/1	0.27	2.08	54,54,54,54	0
85	MG	1	3813	1/1	0.20	2.08	48,48,48,48	0
85	MG	3	207	1/1	0.27	2.07	64,64,64,64	0
85	MG	1	3465	1/1	0.23	2.07	48,48,48,48	0
86	OHX	2	2148	7/7	0.23	2.07	179,179,179,179	0
86	OHX	6	2145	7/7	0.25	2.06	120,120,120,120	0
86	OHX	5	3997	7/7	0.23	2.05	84,84,84,84	0
85	MG	1	3682	1/1	0.34	2.04	68,68,68,68	0
85	MG	s6	301	1/1	0.33	2.04	83,83,83,83	0
86	OHX	5	4151	7/7	0.28	2.03	147,147,147,147	0
86	OHX	5	4229	7/7	0.32	2.03	124,124,124,124	0
85	MG	5	3691	1/1	0.27	2.02	40,40,40,40	0
86	OHX	1	4151	7/7	0.22	2.00	121,121,121,121	0
85	MG	5	3838	1/1	0.13	2.00	57,57,57,57	0
86	OHX	6	2168	7/7	0.24	1.99	155,155,155,155	0
86	OHX	6	2192	7/7	0.29	1.99	184,184,184,184	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3787	1/1	0.21	1.98	21,21,21,21	0
85	MG	5	3634	1/1	0.28	1.97	46,46,46,46	0
85	MG	2	1927	1/1	0.38	1.96	45,45,45,45	0
86	OHX	1	4148	7/7	0.26	1.95	161,161,161,161	0
86	OHX	m7	206	7/7	0.32	1.94	127,127,127,127	0
86	OHX	5	4228	7/7	0.18	1.94	188,188,188,188	0
86	OHX	6	2154	7/7	0.22	1.92	156,156,156,156	0
85	MG	1	3612	1/1	0.28	1.90	37,37,37,37	0
85	MG	5	3419	1/1	0.27	1.88	34,34,34,34	0
85	MG	2	1920	1/1	0.32	1.87	60,60,60,60	0
86	OHX	3	220	7/7	0.21	1.87	157,157,157,157	0
85	MG	1	3764	1/1	0.21	1.86	34,34,34,34	0
86	OHX	1	4089	7/7	0.16	1.85	141,141,141,141	0
85	MG	5	3799	1/1	0.29	1.85	82,82,82,82	0
86	OHX	5	4137	7/7	0.24	1.85	137,137,137,137	0
85	MG	4	213	1/1	0.25	1.84	46,46,46,46	0
85	MG	5	3621	1/1	0.18	1.82	52,52,52,52	0
85	MG	6	1997	1/1	0.35	1.82	52,52,52,52	0
86	OHX	2	2176	7/7	0.30	1.81	176,176,176,176	0
85	MG	1	3752	1/1	0.29	1.80	60,60,60,60	0
85	MG	M3	202	1/1	0.46	1.79	97,97,97,97	0
86	OHX	1	4186	7/7	0.46	1.78	188,188,188,188	0
85	MG	L4	401	1/1	0.24	1.77	35,35,35,35	0
86	OHX	6	2184	7/7	0.38	1.76	159,159,159,159	0
86	OHX	5	4172	7/7	0.19	1.75	138,138,138,138	0
86	OHX	1	4100	7/7	0.36	1.71	175,175,175,175	0
86	OHX	2	2111	7/7	0.23	1.70	126,126,126,126	0
86	OHX	1	4147	7/7	0.43	1.69	152,152,152,152	0
86	OHX	1	4106	7/7	0.26	1.68	125,125,125,125	0
85	MG	5	3846	1/1	0.37	1.67	53,53,53,53	0
85	MG	L7	303	1/1	0.16	1.67	42,42,42,42	0
86	OHX	1	4020	7/7	0.20	1.67	132,132,132,132	0
86	OHX	2	2076	7/7	0.22	1.67	139,139,139,139	0
86	OHX	5	4025	7/7	0.20	1.65	107,107,107,107	0
86	OHX	5	4163	7/7	0.22	1.63	146,146,146,146	0
86	OHX	6	2124	7/7	0.30	1.61	178,178,178,178	0
85	MG	5	3513	1/1	0.20	1.61	32,32,32,32	0
86	OHX	6	2188	7/7	0.28	1.61	172,172,172,172	0
86	OHX	1	4015	7/7	0.19	1.57	123,123,123,123	0
85	MG	7	207	1/1	0.22	1.55	61,61,61,61	0
85	MG	N8	204	1/1	0.22	1.55	38,38,38,38	0
85	MG	1	3645	1/1	0.29	1.53	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	2	2005	1/1	0.35	1.52	67,67,67,67	0
85	MG	2	1963	1/1	0.35	1.52	156,156,156,156	0
85	MG	5	3827	1/1	0.28	1.52	30,30,30,30	0
86	OHX	6	2106	7/7	0.19	1.52	120,120,120,120	0
86	OHX	1	4173	7/7	0.27	1.51	183,183,183,183	0
85	MG	1	3733	1/1	0.25	1.51	55,55,55,55	0
85	MG	5	3567	1/1	0.19	1.51	25,25,25,25	0
85	MG	1	3663	1/1	0.29	1.50	65,65,65,65	0
85	MG	5	3866	1/1	0.17	1.49	26,26,26,26	0
86	OHX	2	2086	7/7	0.18	1.48	127,127,127,127	0
86	OHX	2	2096	7/7	0.29	1.48	154,154,154,154	0
85	MG	c7	201	1/1	0.43	1.47	77,77,77,77	0
86	OHX	5	4184	7/7	0.39	1.46	137,137,137,137	0
86	OHX	8	229	7/7	0.24	1.45	153,153,153,153	0
86	OHX	m4	201	7/7	0.42	1.44	204,204,204,204	0
86	OHX	5	4155	7/7	0.24	1.43	128,128,128,128	0
85	MG	2	2000	1/1	0.27	1.42	94,94,94,94	0
86	OHX	14	402	7/7	0.28	1.42	199,199,199,199	0
85	MG	1	3601	1/1	0.22	1.40	40,40,40,40	0
85	MG	5	3726	1/1	0.16	1.39	91,91,91,91	0
85	MG	n8	201	1/1	0.20	1.39	31,31,31,31	0
86	OHX	1	4092	7/7	0.17	1.39	156,156,156,156	0
86	OHX	5	4108	7/7	0.21	1.38	125,125,125,125	0
85	MG	1	3827	1/1	0.17	1.38	30,30,30,30	0
86	OHX	6	2144	7/7	0.21	1.37	144,144,144,144	0
85	MG	1	3583	1/1	0.37	1.36	33,33,33,33	0
86	OHX	2	2130	7/7	0.27	1.36	215,215,215,215	0
86	OHX	5	4194	7/7	0.19	1.35	126,126,126,126	0
86	OHX	6	2103	7/7	0.35	1.35	170,170,170,170	0
85	MG	2	1992	1/1	0.33	1.34	60,60,60,60	0
85	MG	1	3726	1/1	0.20	1.30	63,63,63,63	0
85	MG	5	3435	1/1	0.20	1.29	33,33,33,33	0
86	OHX	5	4000	7/7	0.23	1.28	114,114,114,114	0
86	OHX	1	4095	7/7	0.24	1.27	165,165,165,165	0
86	OHX	1	4068	7/7	0.21	1.27	136,136,136,136	0
86	OHX	5	4246	7/7	0.41	1.25	158,158,158,158	0
85	MG	8	209	1/1	0.24	1.25	46,46,46,46	0
86	OHX	1	3871	7/7	0.16	1.24	63,63,63,63	0
85	MG	M7	205	1/1	0.32	1.22	41,41,41,41	0
85	MG	5	3431	1/1	0.25	1.22	76,76,76,76	0
85	MG	5	3743	1/1	0.20	1.22	45,45,45,45	0
86	OHX	5	4128	7/7	0.20	1.21	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3620	1/1	0.34	1.21	43,43,43,43	0
86	OHX	1	3948	7/7	0.12	1.20	128,128,128,128	0
86	OHX	1	4150	7/7	0.41	1.17	178,178,178,178	0
85	MG	5	4249	1/1	0.20	1.17	37,37,37,37	0
86	OHX	1	4007	7/7	0.17	1.16	115,115,115,115	0
85	MG	1	3634	1/1	0.28	1.16	64,64,64,64	0
85	MG	5	3423	1/1	0.19	1.16	43,43,43,43	0
85	MG	1	3447	1/1	0.30	1.14	40,40,40,40	0
86	OHX	1	4164	7/7	0.27	1.14	149,149,149,149	0
86	OHX	2	2127	7/7	0.20	1.14	148,148,148,148	0
85	MG	6	2009	1/1	0.22	1.14	73,73,73,73	0
86	OHX	2	2151	7/7	0.33	1.13	176,176,176,176	0
86	OHX	1	3985	7/7	0.19	1.13	124,124,124,124	0
85	MG	5	3653	1/1	0.30	1.13	68,68,68,68	0
85	MG	L7	302	1/1	0.23	1.12	45,45,45,45	0
86	OHX	5	4185	7/7	0.31	1.12	151,151,151,151	0
86	OHX	6	2181	7/7	0.28	1.11	195,195,195,195	0
86	OHX	5	4240	7/7	0.31	1.11	157,157,157,157	0
85	MG	1	3627	1/1	0.40	1.11	77,77,77,77	0
85	MG	3	226	1/1	0.25	1.11	71,71,71,71	0
85	MG	5	3408	1/1	0.22	1.10	28,28,28,28	0
85	MG	5	3404	1/1	0.20	1.10	53,53,53,53	0
86	OHX	2	2090	7/7	0.24	1.10	133,133,133,133	0
86	OHX	2	2162	7/7	0.35	1.10	162,162,162,162	0
85	MG	5	3647	1/1	0.21	1.09	60,60,60,60	0
86	OHX	5	3925	7/7	0.20	1.08	78,78,78,78	0
86	OHX	1	4013	7/7	0.17	1.07	125,125,125,125	0
85	MG	1	3797	1/1	0.27	1.07	47,47,47,47	0
85	MG	5	3765	1/1	0.32	1.06	43,43,43,43	0
85	MG	5	3777	1/1	0.21	1.06	53,53,53,53	0
86	OHX	1	4014	7/7	0.21	1.06	136,136,136,136	0
86	OHX	5	4201	7/7	0.43	1.06	162,162,162,162	0
86	OHX	d9	102	7/7	0.51	1.05	196,196,196,196	0
86	OHX	1	4181	7/7	0.25	1.05	114,114,114,114	0
86	OHX	1	4104	7/7	0.20	1.03	135,135,135,135	0
85	MG	4	207	1/1	0.21	1.03	44,44,44,44	0
85	MG	5	3803	1/1	0.17	1.02	48,48,48,48	0
85	MG	s8	303	1/1	0.44	1.02	55,55,55,55	0
85	MG	1	3639	1/1	0.25	1.01	53,53,53,53	0
85	MG	1	3719	1/1	0.15	1.00	77,77,77,77	0
86	OHX	1	4172	7/7	0.18	1.00	109,109,109,109	0
86	OHX	5	4139	7/7	0.21	0.98	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3856	1/1	0.20	0.98	102,102,102,102	0
86	OHX	6	2189	7/7	0.24	0.98	183,183,183,183	0
86	OHX	6	2158	7/7	0.27	0.97	138,138,138,138	0
86	OHX	1	4093	7/7	0.15	0.97	152,152,152,152	0
86	OHX	1	4080	7/7	0.33	0.97	129,129,129,129	0
86	OHX	5	3981	7/7	0.21	0.96	99,99,99,99	0
86	OHX	M8	201	7/7	0.23	0.96	151,151,151,151	0
86	OHX	1	4132	7/7	0.20	0.96	129,129,129,129	0
86	OHX	1	4042	7/7	0.18	0.95	136,136,136,136	0
85	MG	5	3407	1/1	0.17	0.95	41,41,41,41	0
86	OHX	5	4042	7/7	0.21	0.95	112,112,112,112	0
85	MG	1	3644	1/1	0.19	0.94	44,44,44,44	0
86	OHX	5	4048	7/7	0.19	0.93	107,107,107,107	0
86	OHX	1	4123	7/7	0.23	0.93	143,143,143,143	0
86	OHX	5	4087	7/7	0.26	0.92	120,120,120,120	0
86	OHX	6	2162	7/7	0.24	0.91	159,159,159,159	0
86	OHX	1	4017	7/7	0.24	0.90	137,137,137,137	0
85	MG	1	3489	1/1	0.31	0.89	52,52,52,52	0
86	OHX	2	2109	7/7	0.21	0.89	167,167,167,167	0
86	OHX	1	4161	7/7	0.21	0.88	158,158,158,158	0
85	MG	5	3701	1/1	0.17	0.88	37,37,37,37	0
86	OHX	5	4233	7/7	0.23	0.87	155,155,155,155	0
86	OHX	8	224	7/7	0.24	0.86	131,131,131,131	0
85	MG	m7	202	1/1	0.26	0.85	28,28,28,28	0
85	MG	5	3723	1/1	0.23	0.85	42,42,42,42	0
86	OHX	2	2145	7/7	0.33	0.83	192,192,192,192	0
86	OHX	2	2106	7/7	0.20	0.83	152,152,152,152	0
85	MG	1	3638	1/1	0.20	0.82	62,62,62,62	0
85	MG	N6	201	1/1	0.25	0.82	41,41,41,41	0
85	MG	5	3426	1/1	0.23	0.82	43,43,43,43	0
85	MG	L5	301	1/1	0.43	0.82	67,67,67,67	0
86	OHX	1	4113	7/7	0.21	0.81	183,183,183,183	0
85	MG	6	2010	1/1	0.40	0.81	166,166,166,166	0
85	MG	1	3483	1/1	0.22	0.80	52,52,52,52	0
85	MG	1	3834	1/1	0.44	0.77	53,53,53,53	0
86	OHX	1	4200	7/7	0.21	0.77	176,176,176,176	0
86	OHX	5	4053	7/7	0.20	0.76	140,140,140,140	0
86	OHX	5	4113	7/7	0.24	0.75	129,129,129,129	0
88	3KF	5	4248	22/22	0.20	0.75	28,28,28,28	0
85	MG	1	3425	1/1	0.24	0.74	32,32,32,32	0
86	OHX	5	4023	7/7	0.17	0.74	111,111,111,111	0
86	OHX	2	2150	7/7	0.19	0.73	181,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3721	1/1	0.30	0.72	48,48,48,48	0
86	OHX	1	3908	7/7	0.24	0.72	93,93,93,93	0
86	OHX	1	3869	7/7	0.22	0.72	62,62,62,62	0
86	OHX	1	4009	7/7	0.19	0.72	139,139,139,139	0
86	OHX	1	4096	7/7	0.24	0.72	168,168,168,168	0
86	OHX	5	4106	7/7	0.20	0.71	134,134,134,134	0
86	OHX	6	2175	7/7	0.17	0.70	159,159,159,159	0
86	OHX	5	4015	7/7	0.19	0.68	136,136,136,136	0
85	MG	m7	203	1/1	0.18	0.68	48,48,48,48	0
85	MG	2	1999	1/1	0.40	0.68	75,75,75,75	0
86	OHX	4	232	7/7	0.16	0.67	139,139,139,139	0
86	OHX	1	3970	7/7	0.18	0.67	114,114,114,114	0
85	MG	6	1984	1/1	0.17	0.66	54,54,54,54	0
85	MG	o1	202	1/1	0.27	0.66	84,84,84,84	0
85	MG	N3	203	1/1	0.32	0.66	54,54,54,54	0
86	OHX	1	4039	7/7	0.25	0.65	127,127,127,127	0
85	MG	5	3679	1/1	0.24	0.64	45,45,45,45	0
86	OHX	5	4125	7/7	0.15	0.64	121,121,121,121	0
86	OHX	2	2085	7/7	0.29	0.63	161,161,161,161	0
86	OHX	5	4212	7/7	0.18	0.63	111,111,111,111	0
86	OHX	5	4064	7/7	0.28	0.63	127,127,127,127	0
85	MG	4	208	1/1	0.17	0.63	50,50,50,50	0
86	OHX	1	4049	7/7	0.19	0.63	126,126,126,126	0
85	MG	6	1914	1/1	0.26	0.63	85,85,85,85	0
85	MG	5	3770	1/1	0.28	0.62	74,74,74,74	0
86	OHX	1	4187	7/7	0.28	0.62	147,147,147,147	0
86	OHX	5	4119	7/7	0.22	0.62	167,167,167,167	0
86	OHX	5	4043	7/7	0.22	0.61	142,142,142,142	0
86	OHX	1	4036	7/7	0.23	0.61	143,143,143,143	0
86	OHX	2	2131	7/7	0.21	0.61	124,124,124,124	0
86	OHX	6	2197	7/7	0.35	0.59	161,161,161,161	0
86	OHX	m8	201	7/7	0.22	0.59	149,149,149,149	0
85	MG	2	1946	1/1	0.18	0.58	68,68,68,68	0
86	OHX	6	2102	7/7	0.23	0.57	132,132,132,132	0
85	MG	3	203	1/1	0.20	0.56	97,97,97,97	0
86	OHX	1	4120	7/7	0.19	0.56	146,146,146,146	0
86	OHX	5	4221	7/7	0.27	0.56	169,169,169,169	0
86	OHX	2	2167	7/7	0.25	0.55	165,165,165,165	0
85	MG	5	3466	1/1	0.25	0.54	93,93,93,93	0
86	OHX	5	4166	7/7	0.28	0.53	181,181,181,181	0
85	MG	1	3436	1/1	0.22	0.53	42,42,42,42	0
86	OHX	1	4058	7/7	0.21	0.52	196,196,196,196	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2178	7/7	0.20	0.52	188,188,188,188	0
86	OHX	6	2121	7/7	0.23	0.51	166,166,166,166	0
86	OHX	5	3990	7/7	0.25	0.51	145,145,145,145	0
86	OHX	O3	201	7/7	0.20	0.50	127,127,127,127	0
85	MG	1	3742	1/1	0.15	0.50	41,41,41,41	0
86	OHX	1	4008	7/7	0.17	0.49	135,135,135,135	0
85	MG	1	3728	1/1	0.24	0.49	72,72,72,72	0
86	OHX	5	4116	7/7	0.27	0.48	148,148,148,148	0
86	OHX	2	2100	7/7	0.24	0.48	167,167,167,167	0
86	OHX	1	4098	7/7	0.26	0.48	115,115,115,115	0
85	MG	5	3700	1/1	0.21	0.46	62,62,62,62	0
85	MG	M6	201	1/1	0.22	0.45	43,43,43,43	0
86	OHX	1	4165	7/7	0.26	0.44	230,230,230,230	0
86	OHX	5	3953	7/7	0.23	0.44	103,103,103,103	0
85	MG	1	3731	1/1	0.20	0.42	64,64,64,64	0
85	MG	d6	102	1/1	0.27	0.42	57,57,57,57	0
86	OHX	6	2146	7/7	0.23	0.41	169,169,169,169	0
86	OHX	2	2025	7/7	0.20	0.41	96,96,96,96	0
85	MG	1	3558	1/1	0.18	0.39	53,53,53,53	0
86	OHX	5	4057	7/7	0.18	0.37	117,117,117,117	0
86	OHX	5	4019	7/7	0.15	0.37	117,117,117,117	0
86	OHX	1	3981	7/7	0.22	0.36	122,122,122,122	0
86	OHX	6	2149	7/7	0.17	0.36	155,155,155,155	0
86	OHX	6	2139	7/7	0.29	0.33	167,167,167,167	0
86	OHX	6	2135	7/7	0.16	0.33	154,154,154,154	0
85	MG	5	3469	1/1	0.18	0.32	108,108,108,108	0
85	MG	D3	201	1/1	0.22	0.32	57,57,57,57	0
85	MG	N8	202	1/1	0.25	0.32	49,49,49,49	0
87	ZN	D7	101	1/1	0.26	0.31	155,155,155,155	0
86	OHX	5	4123	7/7	0.28	0.29	171,171,171,171	0
86	OHX	5	4111	7/7	0.23	0.28	112,112,112,112	0
85	MG	1	3807	1/1	0.20	0.28	59,59,59,59	0
86	OHX	5	4071	7/7	0.28	0.28	133,133,133,133	0
86	OHX	2	2087	7/7	0.23	0.27	139,139,139,139	0
85	MG	8	207	1/1	0.22	0.26	50,50,50,50	0
85	MG	1	3802	1/1	0.29	0.26	52,52,52,52	0
86	OHX	5	4090	7/7	0.24	0.26	145,145,145,145	0
86	OHX	1	3882	7/7	0.17	0.25	73,73,73,73	0
86	OHX	6	2178	7/7	0.38	0.23	149,149,149,149	0
86	OHX	6	2044	7/7	0.20	0.22	81,81,81,81	0
86	OHX	5	4203	7/7	0.18	0.22	168,168,168,168	0
86	OHX	1	4191	7/7	0.16	0.21	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2000	1/1	0.21	0.20	85,85,85,85	0
86	OHX	1	4076	7/7	0.15	0.19	152,152,152,152	0
86	OHX	2	2181	7/7	0.23	0.19	179,179,179,179	0
85	MG	2	1988	1/1	0.24	0.18	80,80,80,80	0
87	ZN	Q2	501	1/1	0.23	0.18	89,89,89,89	0
86	OHX	1	4115	7/7	0.20	0.18	136,136,136,136	0
86	OHX	2	2065	7/7	0.20	0.17	122,122,122,122	0
85	MG	1	3415	1/1	0.23	0.17	53,53,53,53	0
86	OHX	8	222	7/7	0.12	0.17	134,134,134,134	0
86	OHX	5	4031	7/7	0.19	0.16	136,136,136,136	0
85	MG	1	3443	1/1	0.16	0.14	82,82,82,82	0
85	MG	6	2035	1/1	0.47	0.14	103,103,103,103	0
85	MG	5	3702	1/1	0.18	0.14	54,54,54,54	0
86	OHX	2	2058	7/7	0.15	0.12	125,125,125,125	0
86	OHX	6	2051	7/7	0.15	0.12	102,102,102,102	0
86	OHX	5	4083	7/7	0.19	0.12	137,137,137,137	0
86	OHX	1	3965	7/7	0.18	0.11	113,113,113,113	0
86	OHX	5	3906	7/7	0.17	0.11	61,61,61,61	0
86	OHX	5	4091	7/7	0.18	0.11	131,131,131,131	0
86	OHX	2	2088	7/7	0.21	0.11	149,149,149,149	0
85	MG	1	3441	1/1	0.18	0.10	44,44,44,44	0
86	OHX	1	4083	7/7	0.23	0.10	160,160,160,160	0
85	MG	6	1940	1/1	0.21	0.09	104,104,104,104	0
85	MG	6	1969	1/1	0.18	0.08	65,65,65,65	0
85	MG	5	3767	1/1	0.21	0.08	51,51,51,51	0
86	OHX	5	4223	7/7	0.22	0.08	170,170,170,170	0
86	OHX	1	4003	7/7	0.17	0.07	112,112,112,112	0
85	MG	m7	205	1/1	0.23	0.06	35,35,35,35	0
86	OHX	6	2086	7/7	0.18	0.05	124,124,124,124	0
86	OHX	1	4131	7/7	0.38	0.05	180,180,180,180	0
85	MG	1	3681	1/1	0.18	0.05	38,38,38,38	0
86	OHX	2	2121	7/7	0.23	0.05	161,161,161,161	0
85	MG	2	2183	1/1	0.24	0.05	108,108,108,108	0
86	OHX	2	2054	7/7	0.17	0.05	151,151,151,151	0
86	OHX	1	4050	7/7	0.18	0.04	121,121,121,121	0
86	OHX	5	4162	7/7	0.17	0.03	157,157,157,157	0
86	OHX	5	4007	7/7	0.18	0.03	120,120,120,120	0
86	OHX	5	3898	7/7	0.16	0.03	48,48,48,48	0
85	MG	1	3810	1/1	0.19	0.02	53,53,53,53	0
86	OHX	S8	301	7/7	0.27	0.01	178,178,178,178	0
86	OHX	d4	202	7/7	0.26	-0.00	184,184,184,184	0
86	OHX	5	4006	7/7	0.17	0.00	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	4025	7/7	0.15	-0.00	136,136,136,136	0
86	OHX	1	4101	7/7	0.21	-0.01	155,155,155,155	0
86	OHX	2	2115	7/7	0.20	-0.01	132,132,132,132	0
86	OHX	L3	403	7/7	0.40	-0.02	174,174,174,174	0
86	OHX	1	4019	7/7	0.18	-0.03	121,121,121,121	0
85	MG	6	2001	1/1	0.23	-0.04	85,85,85,85	0
86	OHX	8	218	7/7	0.19	-0.05	120,120,120,120	0
86	OHX	n3	204	7/7	0.15	-0.05	123,123,123,123	0
86	OHX	2	2080	7/7	0.21	-0.06	195,195,195,195	0
85	MG	1	3422	1/1	0.14	-0.06	32,32,32,32	0
85	MG	5	3745	1/1	0.16	-0.07	64,64,64,64	0
86	OHX	1	4145	7/7	0.24	-0.07	176,176,176,176	0
86	OHX	6	2133	7/7	0.26	-0.07	137,137,137,137	0
86	OHX	6	2127	7/7	0.19	-0.08	161,161,161,161	0
86	OHX	1	4035	7/7	0.18	-0.08	105,105,105,105	0
85	MG	1	3845	1/1	0.18	-0.09	45,45,45,45	0
85	MG	M3	201	1/1	0.19	-0.10	43,43,43,43	0
86	OHX	1	4023	7/7	0.21	-0.11	162,162,162,162	0
86	OHX	l9	202	7/7	0.19	-0.12	140,140,140,140	0
86	OHX	5	4177	7/7	0.26	-0.12	160,160,160,160	0
85	MG	1	3466	1/1	0.16	-0.12	46,46,46,46	0
86	OHX	5	4033	7/7	0.15	-0.13	127,127,127,127	0
86	OHX	s8	304	7/7	0.36	-0.13	181,181,181,181	0
86	OHX	5	4193	7/7	0.18	-0.13	100,100,100,100	0
86	OHX	1	4088	7/7	0.18	-0.13	100,100,100,100	0
86	OHX	l3	404	7/7	0.29	-0.14	153,153,153,153	0
86	OHX	5	3897	7/7	0.19	-0.15	53,53,53,53	0
86	OHX	1	4047	7/7	0.17	-0.17	131,131,131,131	0
86	OHX	3	219	7/7	0.16	-0.17	135,135,135,135	0
86	OHX	6	2101	7/7	0.16	-0.18	139,139,139,139	0
86	OHX	1	4006	7/7	0.20	-0.19	110,110,110,110	0
85	MG	1	3783	1/1	0.18	-0.20	58,58,58,58	0
86	OHX	m1	201	7/7	0.28	-0.22	167,167,167,167	0
86	OHX	sR	401	7/7	0.26	-0.22	175,175,175,175	0
86	OHX	1	4103	7/7	0.20	-0.24	131,131,131,131	0
86	OHX	1	4073	7/7	0.16	-0.24	127,127,127,127	0
86	OHX	6	2163	7/7	0.24	-0.24	210,210,210,210	0
86	OHX	2	2166	7/7	0.19	-0.26	186,186,186,186	0
86	OHX	q1	102	7/7	0.20	-0.26	108,108,108,108	0
86	OHX	6	2115	7/7	0.19	-0.28	141,141,141,141	0
86	OHX	1	3889	7/7	0.14	-0.28	82,82,82,82	0
86	OHX	l5	303	7/7	0.24	-0.28	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2143	7/7	0.19	-0.29	153,153,153,153	0
85	MG	m7	204	1/1	0.22	-0.29	34,34,34,34	0
86	OHX	1	4044	7/7	0.22	-0.30	124,124,124,124	0
86	OHX	1	4156	7/7	0.16	-0.30	125,125,125,125	0
85	MG	1	3806	1/1	0.43	-0.30	203,203,203,203	0
86	OHX	1	3955	7/7	0.19	-0.30	109,109,109,109	0
86	OHX	6	2151	7/7	0.17	-0.32	126,126,126,126	0
85	MG	1	3637	1/1	0.28	-0.33	80,80,80,80	0
85	MG	5	3840	1/1	0.16	-0.34	34,34,34,34	0
85	MG	5	3433	1/1	0.16	-0.34	37,37,37,37	0
85	MG	N3	202	1/1	0.18	-0.34	63,63,63,63	0
86	OHX	5	4169	7/7	0.19	-0.35	123,123,123,123	0
86	OHX	1	4052	7/7	0.23	-0.36	161,161,161,161	0
85	MG	5	3607	1/1	0.17	-0.36	28,28,28,28	0
86	OHX	5	4238	7/7	0.21	-0.36	113,113,113,113	0
86	OHX	6	2104	7/7	0.18	-0.37	122,122,122,122	0
85	MG	1	3604	1/1	0.16	-0.39	38,38,38,38	0
86	OHX	6	2155	7/7	0.17	-0.39	122,122,122,122	0
85	MG	5	3619	1/1	0.16	-0.39	47,47,47,47	0
86	OHX	1	3921	7/7	0.18	-0.40	118,118,118,118	0
86	OHX	5	4165	7/7	0.18	-0.40	193,193,193,193	0
86	OHX	3	217	7/7	0.16	-0.42	129,129,129,129	0
86	OHX	5	4010	7/7	0.16	-0.42	117,117,117,117	0
86	OHX	5	4059	7/7	0.16	-0.42	138,138,138,138	0
86	OHX	2	2093	7/7	0.20	-0.42	162,162,162,162	0
86	OHX	2	2069	7/7	0.16	-0.43	122,122,122,122	0
86	OHX	1	4028	7/7	0.17	-0.43	139,139,139,139	0
86	OHX	5	3963	7/7	0.15	-0.43	102,102,102,102	0
86	OHX	5	4118	7/7	0.17	-0.43	163,163,163,163	0
86	OHX	8	226	7/7	0.22	-0.44	136,136,136,136	0
86	OHX	2	2101	7/7	0.14	-0.44	159,159,159,159	0
86	OHX	2	2124	7/7	0.23	-0.44	155,155,155,155	0
86	OHX	1	4055	7/7	0.16	-0.44	159,159,159,159	0
85	MG	5	3822	1/1	0.23	-0.45	94,94,94,94	0
85	MG	1	3428	1/1	0.18	-0.45	56,56,56,56	0
86	OHX	1	3944	7/7	0.18	-0.45	106,106,106,106	0
86	OHX	2	2099	7/7	0.13	-0.47	125,125,125,125	0
86	OHX	6	2045	7/7	0.14	-0.50	72,72,72,72	0
86	OHX	m0	302	7/7	0.22	-0.50	139,139,139,139	0
87	ZN	q2	501	1/1	0.20	-0.50	88,88,88,88	0
86	OHX	2	2152	7/7	0.20	-0.50	196,196,196,196	0
86	OHX	6	2064	7/7	0.14	-0.51	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2118	7/7	0.15	-0.52	172,172,172,172	0
86	OHX	1	3895	7/7	0.17	-0.52	82,82,82,82	0
85	MG	M0	302	1/1	0.21	-0.53	47,47,47,47	0
86	OHX	5	3971	7/7	0.13	-0.53	119,119,119,119	0
86	OHX	1	4030	7/7	0.18	-0.53	113,113,113,113	0
85	MG	Q2	502	1/1	0.15	-0.54	65,65,65,65	0
86	OHX	5	3905	7/7	0.15	-0.56	66,66,66,66	0
86	OHX	1	3892	7/7	0.13	-0.57	80,80,80,80	0
86	OHX	4	227	7/7	0.13	-0.57	131,131,131,131	0
86	OHX	5	3913	7/7	0.14	-0.57	62,62,62,62	0
85	MG	5	3688	1/1	0.14	-0.58	39,39,39,39	0
85	MG	1	3854	1/1	0.17	-0.58	71,71,71,71	0
86	OHX	1	4018	7/7	0.16	-0.58	142,142,142,142	0
86	OHX	6	2142	7/7	0.17	-0.58	151,151,151,151	0
85	MG	1	3674	1/1	0.26	-0.58	65,65,65,65	0
86	OHX	4	225	7/7	0.15	-0.58	114,114,114,114	0
86	OHX	5	4062	7/7	0.15	-0.58	122,122,122,122	0
86	OHX	N9	101	7/7	0.14	-0.59	71,71,71,71	0
85	MG	5	3485	1/1	0.15	-0.59	74,74,74,74	0
86	OHX	7	224	7/7	0.13	-0.61	114,114,114,114	0
86	OHX	1	3879	7/7	0.14	-0.62	70,70,70,70	0
86	OHX	1	3913	7/7	0.12	-0.62	112,112,112,112	0
86	OHX	5	4018	7/7	0.14	-0.62	121,121,121,121	0
86	OHX	1	4031	7/7	0.18	-0.62	152,152,152,152	0
85	MG	6	1993	1/1	0.19	-0.63	81,81,81,81	0
86	OHX	2	2102	7/7	0.18	-0.63	157,157,157,157	0
86	OHX	1	4048	7/7	0.13	-0.63	155,155,155,155	0
85	MG	7	208	1/1	0.15	-0.64	64,64,64,64	0
86	OHX	5	4149	7/7	0.16	-0.64	123,123,123,123	0
86	OHX	2	2095	7/7	0.18	-0.64	164,164,164,164	0
86	OHX	c5	201	7/7	0.22	-0.65	181,181,181,181	0
85	MG	m6	203	1/1	0.12	-0.65	35,35,35,35	0
86	OHX	6	2125	7/7	0.15	-0.67	156,156,156,156	0
86	OHX	2	2125	7/7	0.17	-0.67	159,159,159,159	0
86	OHX	4	231	7/7	0.10	-0.67	154,154,154,154	0
85	MG	1	3626	1/1	0.16	-0.69	47,47,47,47	0
86	OHX	2	2057	7/7	0.15	-0.69	163,163,163,163	0
86	OHX	5	4099	7/7	0.14	-0.71	163,163,163,163	0
86	OHX	5	4044	7/7	0.15	-0.72	129,129,129,129	0
86	OHX	1	3905	7/7	0.16	-0.72	87,87,87,87	0
86	OHX	1	3967	7/7	0.13	-0.72	114,114,114,114	0
86	OHX	2	2114	7/7	0.16	-0.72	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	C5	201	7/7	0.21	-0.72	178,178,178,178	0
86	OHX	5	4009	7/7	0.16	-0.73	104,104,104,104	0
87	ZN	d9	101	1/1	0.15	-0.73	101,101,101,101	0
86	OHX	2	2089	7/7	0.15	-0.73	126,126,126,126	0
85	MG	1	3641	1/1	0.13	-0.74	64,64,64,64	0
86	OHX	1	3964	7/7	0.12	-0.75	128,128,128,128	0
86	OHX	1	3947	7/7	0.13	-0.75	127,127,127,127	0
85	MG	5	3447	1/1	0.13	-0.75	43,43,43,43	0
86	OHX	2	2067	7/7	0.11	-0.76	150,150,150,150	0
86	OHX	5	4189	7/7	0.25	-0.78	187,187,187,187	0
86	OHX	5	3899	7/7	0.15	-0.80	71,71,71,71	0
85	MG	1	3826	1/1	0.16	-0.81	60,60,60,60	0
86	OHX	1	3865	7/7	0.15	-0.81	48,48,48,48	0
86	OHX	5	4060	7/7	0.17	-0.82	160,160,160,160	0
86	OHX	n5	201	7/7	0.34	-0.82	231,231,231,231	0
86	OHX	6	2150	7/7	0.14	-0.82	153,153,153,153	0
86	OHX	6	2073	7/7	0.14	-0.82	122,122,122,122	0
86	OHX	o2	201	7/7	0.15	-0.83	105,105,105,105	0
86	OHX	2	2134	7/7	0.19	-0.84	169,169,169,169	0
86	OHX	5	4054	7/7	0.12	-0.85	151,151,151,151	0
86	OHX	2	2082	7/7	0.13	-0.85	170,170,170,170	0
85	MG	5	3854	1/1	0.13	-0.87	69,69,69,69	0
86	OHX	6	2063	7/7	0.15	-0.87	101,101,101,101	0
85	MG	5	3706	1/1	0.14	-0.87	47,47,47,47	0
85	MG	SM	301	1/1	0.14	-0.88	56,56,56,56	0
86	OHX	1	3868	7/7	0.14	-0.88	60,60,60,60	0
86	OHX	2	2072	7/7	0.19	-0.88	132,132,132,132	0
86	OHX	1	4022	7/7	0.13	-0.88	142,142,142,142	0
86	OHX	5	3901	7/7	0.17	-0.88	58,58,58,58	0
86	OHX	2	2098	7/7	0.11	-0.88	163,163,163,163	0
85	MG	5	3832	1/1	0.16	-0.89	74,74,74,74	0
86	OHX	1	3878	7/7	0.12	-0.89	70,70,70,70	0
86	OHX	m5	304	7/7	0.16	-0.89	136,136,136,136	0
85	MG	1	3420	1/1	0.21	-0.92	93,93,93,93	0
86	OHX	5	3922	7/7	0.16	-0.93	81,81,81,81	0
86	OHX	5	3972	7/7	0.13	-0.93	109,109,109,109	0
86	OHX	5	4070	7/7	0.16	-0.94	127,127,127,127	0
85	MG	1	3479	1/1	0.15	-0.94	89,89,89,89	0
86	OHX	1	3937	7/7	0.09	-0.96	124,124,124,124	0
85	MG	1	3776	1/1	0.14	-0.96	71,71,71,71	0
86	OHX	6	2043	7/7	0.14	-0.96	61,61,61,61	0
86	OHX	1	3987	7/7	0.17	-0.96	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3430	1/1	0.17	-0.96	31,31,31,31	0
86	OHX	5	4100	7/7	0.15	-0.96	147,147,147,147	0
87	ZN	q0	201	1/1	0.14	-0.96	34,34,34,34	0
86	OHX	2	2142	7/7	0.16	-0.97	187,187,187,187	0
86	OHX	1	4024	7/7	0.16	-0.97	114,114,114,114	0
86	OHX	7	223	7/7	0.08	-0.97	114,114,114,114	0
86	OHX	1	4029	7/7	0.14	-0.97	148,148,148,148	0
86	OHX	1	3993	7/7	0.15	-0.98	109,109,109,109	0
86	OHX	1	3922	7/7	0.13	-0.98	101,101,101,101	0
85	MG	l5	301	1/1	0.11	-0.99	69,69,69,69	0
86	OHX	1	3918	7/7	0.12	-0.99	123,123,123,123	0
86	OHX	2	2073	7/7	0.17	-0.99	158,158,158,158	0
86	OHX	M5	303	7/7	0.20	-0.99	125,125,125,125	0
86	OHX	6	2100	7/7	0.15	-0.99	131,131,131,131	0
86	OHX	1	3886	7/7	0.17	-1.00	73,73,73,73	0
86	OHX	5	4124	7/7	0.12	-1.01	153,153,153,153	0
86	OHX	O7	105	7/7	0.11	-1.01	107,107,107,107	0
86	OHX	2	2023	7/7	0.14	-1.01	76,76,76,76	0
86	OHX	7	218	7/7	0.12	-1.01	96,96,96,96	0
87	ZN	q3	501	1/1	0.09	-1.02	71,71,71,71	0
86	OHX	2	2081	7/7	0.16	-1.02	149,149,149,149	0
86	OHX	1	3874	7/7	0.14	-1.02	63,63,63,63	0
87	ZN	Q0	500	1/1	0.13	-1.02	50,50,50,50	0
86	OHX	1	3867	7/7	0.13	-1.06	60,60,60,60	0
86	OHX	5	4032	7/7	0.14	-1.06	144,144,144,144	0
86	OHX	6	2138	7/7	0.23	-1.06	135,135,135,135	0
86	OHX	6	2052	7/7	0.13	-1.06	81,81,81,81	0
85	MG	5	3739	1/1	0.15	-1.06	62,62,62,62	0
85	MG	6	1999	1/1	0.14	-1.07	60,60,60,60	0
85	MG	M7	204	1/1	0.16	-1.07	36,36,36,36	0
85	MG	q3	503	1/1	0.19	-1.08	65,65,65,65	0
86	OHX	1	4084	7/7	0.16	-1.08	139,139,139,139	0
85	MG	5	3604	1/1	0.12	-1.09	67,67,67,67	0
86	OHX	1	4011	7/7	0.12	-1.09	142,142,142,142	0
86	OHX	2	2068	7/7	0.15	-1.09	181,181,181,181	0
86	OHX	5	4097	7/7	0.16	-1.10	155,155,155,155	0
86	OHX	5	3995	7/7	0.12	-1.10	122,122,122,122	0
85	MG	1	3829	1/1	0.16	-1.10	27,27,27,27	0
86	OHX	1	3933	7/7	0.12	-1.11	108,108,108,108	0
86	OHX	5	4104	7/7	0.15	-1.11	99,99,99,99	0
85	MG	c8	202	1/1	0.21	-1.11	74,74,74,74	0
86	OHX	1	3951	7/7	0.14	-1.11	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3938	7/7	0.11	-1.13	104,104,104,104	0
85	MG	6	1994	1/1	0.14	-1.13	60,60,60,60	0
86	OHX	1	3977	7/7	0.08	-1.14	115,115,115,115	0
86	OHX	6	2048	7/7	0.14	-1.15	76,76,76,76	0
86	OHX	6	2105	7/7	0.12	-1.15	132,132,132,132	0
86	OHX	c3	201	7/7	0.21	-1.16	174,174,174,174	0
86	OHX	1	4012	7/7	0.11	-1.16	150,150,150,150	0
86	OHX	c8	203	7/7	0.15	-1.17	167,167,167,167	0
86	OHX	1	3954	7/7	0.09	-1.18	113,113,113,113	0
86	OHX	7	220	7/7	0.12	-1.18	103,103,103,103	0
86	OHX	6	2087	7/7	0.16	-1.18	125,125,125,125	0
86	OHX	o3	202	7/7	0.13	-1.18	118,118,118,118	0
86	OHX	1	3969	7/7	0.14	-1.19	120,120,120,120	0
86	OHX	1	3896	7/7	0.12	-1.21	81,81,81,81	0
86	OHX	2	2033	7/7	0.12	-1.21	118,118,118,118	0
86	OHX	1	3887	7/7	0.13	-1.21	82,82,82,82	0
86	OHX	6	2049	7/7	0.12	-1.22	86,86,86,86	0
86	OHX	1	3975	7/7	0.14	-1.22	103,103,103,103	0
86	OHX	1	4001	7/7	0.18	-1.22	107,107,107,107	0
86	OHX	2	2060	7/7	0.13	-1.23	113,113,113,113	0
86	OHX	8	216	7/7	0.06	-1.23	120,120,120,120	0
86	OHX	1	3941	7/7	0.07	-1.23	109,109,109,109	0
87	ZN	D9	101	1/1	0.10	-1.24	84,84,84,84	0
86	OHX	1	4060	7/7	0.11	-1.24	163,163,163,163	0
86	OHX	5	3902	7/7	0.14	-1.24	60,60,60,60	0
86	OHX	2	2043	7/7	0.12	-1.26	121,121,121,121	0
87	ZN	D6	500	1/1	0.10	-1.26	77,77,77,77	0
85	MG	1	3434	1/1	0.12	-1.27	48,48,48,48	0
86	OHX	2	2055	7/7	0.11	-1.27	124,124,124,124	0
85	MG	sM	302	1/1	0.13	-1.27	47,47,47,47	0
86	OHX	6	2082	7/7	0.14	-1.28	122,122,122,122	0
86	OHX	1	3986	7/7	0.12	-1.28	128,128,128,128	0
86	OHX	5	3912	7/7	0.13	-1.28	72,72,72,72	0
86	OHX	6	2114	7/7	0.15	-1.28	160,160,160,160	0
86	OHX	6	2198	7/7	0.21	-1.28	211,211,211,211	0
86	OHX	6	2160	7/7	0.24	-1.30	204,204,204,204	0
86	OHX	6	2091	7/7	0.15	-1.31	156,156,156,156	0
86	OHX	5	3976	7/7	0.11	-1.32	100,100,100,100	0
85	MG	5	3677	1/1	0.13	-1.32	38,38,38,38	0
86	OHX	m0	301	7/7	0.10	-1.33	131,131,131,131	0
86	OHX	6	2096	7/7	0.20	-1.34	204,204,204,204	0
86	OHX	5	3931	7/7	0.12	-1.35	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	5	3657	1/1	0.15	-1.36	33,33,33,33	0
86	OHX	2	2168	7/7	0.11	-1.36	167,167,167,167	0
86	OHX	5	3977	7/7	0.12	-1.36	120,120,120,120	0
86	OHX	1	4034	7/7	0.07	-1.37	158,158,158,158	0
85	MG	5	3699	1/1	0.15	-1.37	34,34,34,34	0
87	ZN	o7	501	1/1	0.10	-1.37	46,46,46,46	0
86	OHX	5	3968	7/7	0.10	-1.37	110,110,110,110	0
86	OHX	1	4041	7/7	0.12	-1.38	140,140,140,140	0
87	ZN	e1	501	1/1	0.19	-1.39	192,192,192,192	0
85	MG	1	3618	1/1	0.10	-1.39	65,65,65,65	0
86	OHX	1	4002	7/7	0.13	-1.39	126,126,126,126	0
86	OHX	1	3961	7/7	0.15	-1.41	105,105,105,105	0
86	OHX	l5	302	7/7	0.10	-1.42	148,148,148,148	0
86	OHX	6	2050	7/7	0.17	-1.42	87,87,87,87	0
86	OHX	1	3875	7/7	0.14	-1.42	69,69,69,69	0
86	OHX	5	4034	7/7	0.10	-1.44	140,140,140,140	0
85	MG	5	3848	1/1	0.14	-1.44	71,71,71,71	0
86	OHX	5	4028	7/7	0.12	-1.44	117,117,117,117	0
87	ZN	E1	501	1/1	0.06	-1.45	123,123,123,123	0
86	OHX	5	3958	7/7	0.12	-1.45	94,94,94,94	0
85	MG	5	3816	1/1	0.13	-1.46	47,47,47,47	0
86	OHX	6	2190	7/7	0.31	-1.46	201,201,201,201	0
86	OHX	1	3881	7/7	0.14	-1.46	68,68,68,68	0
85	MG	1	3607	1/1	0.13	-1.47	59,59,59,59	0
86	OHX	1	3870	7/7	0.12	-1.47	58,58,58,58	0
86	OHX	n3	203	7/7	0.10	-1.49	106,106,106,106	0
86	OHX	2	2035	7/7	0.14	-1.49	107,107,107,107	0
85	MG	5	3753	1/1	0.14	-1.51	46,46,46,46	0
86	OHX	6	2054	7/7	0.09	-1.52	101,101,101,101	0
86	OHX	5	3937	7/7	0.13	-1.52	84,84,84,84	0
85	MG	M9	201	1/1	0.14	-1.52	65,65,65,65	0
86	OHX	5	3935	7/7	0.07	-1.53	74,74,74,74	0
87	ZN	Q3	501	1/1	0.09	-1.53	58,58,58,58	0
85	MG	5	3818	1/1	0.08	-1.53	72,72,72,72	0
86	OHX	1	4090	7/7	0.23	-1.56	164,164,164,164	0
86	OHX	1	4032	7/7	0.09	-1.56	107,107,107,107	0
86	OHX	5	4037	7/7	0.07	-1.56	162,162,162,162	0
86	OHX	5	3965	7/7	0.14	-1.56	109,109,109,109	0
85	MG	L8	301	1/1	0.26	-1.59	57,57,57,57	0
86	OHX	2	2048	7/7	0.08	-1.59	125,125,125,125	0
86	OHX	2	2053	7/7	0.10	-1.59	140,140,140,140	0
86	OHX	2	2139	7/7	0.16	-1.59	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	8	219	7/7	0.10	-1.60	137,137,137,137	0
87	ZN	O7	101	1/1	0.08	-1.61	40,40,40,40	0
86	OHX	1	3873	7/7	0.13	-1.62	65,65,65,65	0
86	OHX	2	2029	7/7	0.11	-1.62	113,113,113,113	0
87	ZN	d6	101	1/1	0.12	-1.62	64,64,64,64	0
86	OHX	2	2036	7/7	0.08	-1.62	100,100,100,100	0
85	MG	1	3426	1/1	0.16	-1.62	66,66,66,66	0
86	OHX	6	2069	7/7	0.08	-1.63	159,159,159,159	0
86	OHX	5	3904	7/7	0.17	-1.63	61,61,61,61	0
86	OHX	5	4016	7/7	0.17	-1.63	106,106,106,106	0
86	OHX	1	3945	7/7	0.10	-1.63	125,125,125,125	0
85	MG	1	3816	1/1	0.20	-1.65	144,144,144,144	0
86	OHX	1	4016	7/7	0.08	-1.66	170,170,170,170	0
85	MG	5	3830	1/1	0.14	-1.66	76,76,76,76	0
86	OHX	M0	303	7/7	0.16	-1.66	132,132,132,132	0
86	OHX	O7	106	7/7	0.12	-1.66	112,112,112,112	0
86	OHX	C3	201	7/7	0.13	-1.66	170,170,170,170	0
85	MG	5	3601	1/1	0.14	-1.68	42,42,42,42	0
86	OHX	1	3884	7/7	0.10	-1.68	78,78,78,78	0
86	OHX	6	2098	7/7	0.12	-1.71	126,126,126,126	0
86	OHX	C8	201	7/7	0.07	-1.72	128,128,128,128	0
86	OHX	6	2131	7/7	0.09	-1.72	148,148,148,148	0
86	OHX	2	2064	7/7	0.13	-1.73	121,121,121,121	0
86	OHX	1	4124	7/7	0.11	-1.74	155,155,155,155	0
86	OHX	1	4102	7/7	0.13	-1.75	154,154,154,154	0
86	OHX	1	4193	7/7	0.09	-1.75	178,178,178,178	0
86	OHX	2	2027	7/7	0.12	-1.75	79,79,79,79	0
86	OHX	6	2071	7/7	0.07	-1.76	95,95,95,95	0
86	OHX	n9	102	7/7	0.13	-1.76	74,74,74,74	0
86	OHX	2	2047	7/7	0.07	-1.77	137,137,137,137	0
86	OHX	4	221	7/7	0.14	-1.77	61,61,61,61	0
86	OHX	2	2110	7/7	0.05	-1.78	137,137,137,137	0
86	OHX	6	2093	7/7	0.09	-1.79	177,177,177,177	0
86	OHX	1	3935	7/7	0.14	-1.79	101,101,101,101	0
86	OHX	2	2107	7/7	0.10	-1.80	125,125,125,125	0
86	OHX	5	3916	7/7	0.11	-1.81	67,67,67,67	0
86	OHX	5	4094	7/7	0.12	-1.81	144,144,144,144	0
86	OHX	6	2107	7/7	0.12	-1.82	136,136,136,136	0
86	OHX	1	4051	7/7	0.11	-1.82	149,149,149,149	0
86	OHX	6	2085	7/7	0.05	-1.82	140,140,140,140	0
86	OHX	8	214	7/7	0.13	-1.83	61,61,61,61	0
86	OHX	6	2117	7/7	0.09	-1.83	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3956	7/7	0.10	-1.83	95,95,95,95	0
86	OHX	5	4175	7/7	0.20	-1.83	169,169,169,169	0
86	OHX	1	4105	7/7	0.15	-1.83	146,146,146,146	0
86	OHX	5	4076	7/7	0.11	-1.83	124,124,124,124	0
86	OHX	1	3931	7/7	0.08	-1.85	107,107,107,107	0
86	OHX	L3	402	7/7	0.11	-1.86	119,119,119,119	0
86	OHX	5	3910	7/7	0.14	-1.86	64,64,64,64	0
86	OHX	1	3910	7/7	0.09	-1.86	91,91,91,91	0
86	OHX	2	2031	7/7	0.11	-1.87	120,120,120,120	0
85	MG	1	3718	1/1	0.16	-1.87	39,39,39,39	0
86	OHX	1	3924	7/7	0.09	-1.88	118,118,118,118	0
86	OHX	5	3907	7/7	0.13	-1.89	54,54,54,54	0
86	OHX	1	3991	7/7	0.12	-1.90	144,144,144,144	0
86	OHX	1	3914	7/7	0.09	-1.91	98,98,98,98	0
86	OHX	1	3876	7/7	0.10	-1.91	65,65,65,65	0
86	OHX	5	3911	7/7	0.11	-1.92	66,66,66,66	0
85	MG	5	3689	1/1	0.13	-1.93	46,46,46,46	0
86	OHX	5	3980	7/7	0.14	-1.93	101,101,101,101	0
86	OHX	1	3980	7/7	0.07	-1.94	121,121,121,121	0
86	OHX	5	3934	7/7	0.12	-1.94	84,84,84,84	0
86	OHX	6	2067	7/7	0.10	-1.94	111,111,111,111	0
85	MG	2	1997	1/1	0.15	-1.95	85,85,85,85	0
86	OHX	1	3902	7/7	0.13	-1.95	92,92,92,92	0
86	OHX	6	2060	7/7	0.10	-1.96	108,108,108,108	0
86	OHX	SR	401	7/7	0.11	-1.96	180,180,180,180	0
86	OHX	5	3984	7/7	0.08	-1.96	108,108,108,108	0
86	OHX	5	4013	7/7	0.04	-1.96	133,133,133,133	0
86	OHX	1	3898	7/7	0.16	-1.97	94,94,94,94	0
86	OHX	2	2094	7/7	0.09	-1.97	151,151,151,151	0
86	OHX	1	3920	7/7	0.07	-1.98	103,103,103,103	0
86	OHX	1	4040	7/7	0.16	-1.98	125,125,125,125	0
86	OHX	1	3982	7/7	0.13	-1.98	108,108,108,108	0
86	OHX	4	223	7/7	0.08	-1.98	88,88,88,88	0
86	OHX	4	226	7/7	0.10	-2.00	125,125,125,125	0
86	OHX	5	4063	7/7	0.12	-2.00	129,129,129,129	0
86	OHX	1	3998	7/7	0.12	-2.02	112,112,112,112	0
86	OHX	6	2097	7/7	0.07	-2.03	178,178,178,178	0
86	OHX	2	2040	7/7	0.12	-2.05	109,109,109,109	0
86	OHX	5	4056	7/7	0.09	-2.05	156,156,156,156	0
86	OHX	5	4027	7/7	0.09	-2.05	149,149,149,149	0
86	OHX	2	2133	7/7	0.13	-2.05	164,164,164,164	0
86	OHX	5	4003	7/7	0.13	-2.06	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2037	7/7	0.11	-2.07	150,150,150,150	0
86	OHX	2	2046	7/7	0.08	-2.07	132,132,132,132	0
85	MG	5	3697	1/1	0.10	-2.08	44,44,44,44	0
86	OHX	6	2134	7/7	0.17	-2.08	138,138,138,138	0
85	MG	5	3684	1/1	0.16	-2.10	35,35,35,35	0
86	OHX	5	3998	7/7	0.11	-2.11	117,117,117,117	0
86	OHX	5	4079	7/7	0.14	-2.11	120,120,120,120	0
86	OHX	5	4026	7/7	0.12	-2.14	128,128,128,128	0
86	OHX	5	3918	7/7	0.12	-2.15	73,73,73,73	0
86	OHX	3	215	7/7	0.13	-2.16	123,123,123,123	0
85	MG	6	2022	1/1	0.09	-2.16	89,89,89,89	0
86	OHX	5	4077	7/7	0.14	-2.17	112,112,112,112	0
85	MG	1	3714	1/1	0.18	-2.17	54,54,54,54	0
86	OHX	1	3906	7/7	0.11	-2.17	95,95,95,95	0
86	OHX	5	4235	7/7	0.16	-2.17	154,154,154,154	0
86	OHX	5	3939	7/7	0.11	-2.20	92,92,92,92	0
86	OHX	1	4037	7/7	0.10	-2.21	152,152,152,152	0
86	OHX	1	4136	7/7	0.14	-2.21	118,118,118,118	0
86	OHX	5	3964	7/7	0.10	-2.21	109,109,109,109	0
86	OHX	2	2024	7/7	0.12	-2.22	85,85,85,85	0
86	OHX	6	2126	7/7	0.17	-2.22	133,133,133,133	0
85	MG	5	3853	1/1	0.17	-2.23	85,85,85,85	0
86	OHX	2	2097	7/7	0.10	-2.25	182,182,182,182	0
86	OHX	6	2141	7/7	0.13	-2.27	143,143,143,143	0
86	OHX	1	3943	7/7	0.11	-2.27	112,112,112,112	0
86	OHX	1	4026	7/7	0.11	-2.27	128,128,128,128	0
86	OHX	5	3920	7/7	0.10	-2.27	71,71,71,71	0
86	OHX	5	3959	7/7	0.08	-2.28	103,103,103,103	0
85	MG	1	3449	1/1	0.10	-2.29	38,38,38,38	0
86	OHX	1	4053	7/7	0.12	-2.29	134,134,134,134	0
86	OHX	6	2062	7/7	0.10	-2.30	133,133,133,133	0
85	MG	5	3836	1/1	0.14	-2.31	62,62,62,62	0
86	OHX	3	214	7/7	0.08	-2.31	104,104,104,104	0
85	MG	5	3401	1/1	0.10	-2.31	67,67,67,67	0
86	OHX	2	2039	7/7	0.09	-2.32	103,103,103,103	0
86	OHX	2	2083	7/7	0.10	-2.32	141,141,141,141	0
85	MG	1	3770	1/1	0.14	-2.33	68,68,68,68	0
86	OHX	1	3972	7/7	0.06	-2.33	127,127,127,127	0
86	OHX	1	3899	7/7	0.11	-2.34	94,94,94,94	0
86	OHX	5	4008	7/7	0.06	-2.35	161,161,161,161	0
86	OHX	1	4010	7/7	0.13	-2.37	146,146,146,146	0
88	3KF	1	4212	22/22	0.13	-2.39	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	4117	7/7	0.15	-2.40	136,136,136,136	0
86	OHX	Q2	503	7/7	0.06	-2.41	85,85,85,85	0
86	OHX	4	222	7/7	0.11	-2.41	68,68,68,68	0
86	OHX	2	2077	7/7	0.10	-2.42	127,127,127,127	0
85	MG	s1	301	1/1	0.13	-2.43	86,86,86,86	0
86	OHX	8	225	7/7	0.10	-2.43	153,153,153,153	0
86	OHX	2	2051	7/7	0.11	-2.44	119,119,119,119	0
86	OHX	1	3994	7/7	0.10	-2.44	140,140,140,140	0
86	OHX	1	3930	7/7	0.11	-2.45	116,116,116,116	0
86	OHX	5	3950	7/7	0.12	-2.45	109,109,109,109	0
86	OHX	2	2071	7/7	0.12	-2.47	133,133,133,133	0
86	OHX	1	3890	7/7	0.10	-2.48	70,70,70,70	0
86	OHX	q2	502	7/7	0.08	-2.48	88,88,88,88	0
86	OHX	5	3930	7/7	0.14	-2.48	77,77,77,77	0
86	OHX	5	4046	7/7	0.06	-2.49	138,138,138,138	0
86	OHX	6	2055	7/7	0.11	-2.49	105,105,105,105	0
86	OHX	5	4036	7/7	0.10	-2.52	137,137,137,137	0
86	OHX	1	3927	7/7	0.12	-2.52	102,102,102,102	0
86	OHX	6	2079	7/7	0.11	-2.52	129,129,129,129	0
85	MG	2	1998	1/1	0.11	-2.53	110,110,110,110	0
86	OHX	5	4029	7/7	0.12	-2.54	107,107,107,107	0
86	OHX	1	3926	7/7	0.12	-2.56	103,103,103,103	0
86	OHX	1	3984	7/7	0.15	-2.57	130,130,130,130	0
85	MG	1	3809	1/1	0.10	-2.58	40,40,40,40	0
86	OHX	5	4020	7/7	0.09	-2.58	130,130,130,130	0
86	OHX	5	3967	7/7	0.07	-2.58	108,108,108,108	0
86	OHX	2	2056	7/7	0.11	-2.59	134,134,134,134	0
86	OHX	1	3963	7/7	0.13	-2.59	112,112,112,112	0
86	OHX	5	3982	7/7	0.10	-2.61	88,88,88,88	0
85	MG	1	3475	1/1	0.14	-2.62	36,36,36,36	0
86	OHX	6	2095	7/7	0.17	-2.63	190,190,190,190	0
86	OHX	7	225	7/7	0.08	-2.64	147,147,147,147	0
86	OHX	6	2092	7/7	0.08	-2.67	142,142,142,142	0
86	OHX	2	2032	7/7	0.10	-2.67	106,106,106,106	0
86	OHX	2	2028	7/7	0.13	-2.67	102,102,102,102	0
86	OHX	N1	201	7/7	0.13	-2.68	70,70,70,70	0
86	OHX	5	3929	7/7	0.11	-2.69	68,68,68,68	0
86	OHX	1	3936	7/7	0.10	-2.69	97,97,97,97	0
86	OHX	1	3907	7/7	0.12	-2.71	81,81,81,81	0
86	OHX	5	3947	7/7	0.06	-2.71	97,97,97,97	0
86	OHX	1	4021	7/7	0.10	-2.71	125,125,125,125	0
86	OHX	5	3960	7/7	0.06	-2.72	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3750	1/1	0.15	-2.73	70,70,70,70	0
86	OHX	1	3885	7/7	0.11	-2.75	72,72,72,72	0
86	OHX	7	219	7/7	0.11	-2.76	100,100,100,100	0
85	MG	1	4216	1/1	0.09	-2.77	74,74,74,74	0
86	OHX	1	3992	7/7	0.07	-2.80	132,132,132,132	0
86	OHX	6	2078	7/7	0.05	-2.82	116,116,116,116	0
86	OHX	5	3928	7/7	0.13	-2.82	107,107,107,107	0
86	OHX	2	2157	7/7	0.32	-2.82	251,251,251,251	0
86	OHX	1	3901	7/7	0.08	-2.82	83,83,83,83	0
86	OHX	5	3941	7/7	0.11	-2.83	100,100,100,100	0
86	OHX	2	2030	7/7	0.10	-2.85	103,103,103,103	0
86	OHX	5	4051	7/7	0.07	-2.86	109,109,109,109	0
86	OHX	5	4024	7/7	0.09	-2.87	93,93,93,93	0
86	OHX	1	3891	7/7	0.10	-2.87	72,72,72,72	0
86	OHX	1	3877	7/7	0.11	-2.89	61,61,61,61	0
85	MG	5	3712	1/1	0.08	-2.89	74,74,74,74	0
86	OHX	2	2066	7/7	0.10	-2.90	139,139,139,139	0
86	OHX	2	2049	7/7	0.07	-2.92	136,136,136,136	0
85	MG	5	3805	1/1	0.09	-2.93	30,30,30,30	0
86	OHX	1	3956	7/7	0.12	-2.93	87,87,87,87	0
86	OHX	1	3866	7/7	0.12	-2.93	53,53,53,53	0
86	OHX	5	3973	7/7	0.08	-2.94	112,112,112,112	0
86	OHX	6	2070	7/7	0.08	-2.96	168,168,168,168	0
86	OHX	1	3950	7/7	0.12	-2.98	121,121,121,121	0
86	OHX	13	403	7/7	0.09	-2.99	109,109,109,109	0
85	MG	1	3790	1/1	0.10	-2.99	85,85,85,85	0
86	OHX	5	3954	7/7	0.10	-2.99	96,96,96,96	0
85	MG	5	3856	1/1	0.15	-3.00	77,77,77,77	0
85	MG	7	212	1/1	0.14	-3.01	35,35,35,35	0
86	OHX	s1	302	7/7	0.11	-3.05	96,96,96,96	0
86	OHX	5	3994	7/7	0.08	-3.06	116,116,116,116	0
86	OHX	1	3996	7/7	0.09	-3.07	166,166,166,166	0
85	MG	1	3446	1/1	0.11	-3.09	48,48,48,48	0
86	OHX	5	4005	7/7	0.07	-3.10	113,113,113,113	0
85	MG	5	3637	1/1	0.15	-3.10	57,57,57,57	0
86	OHX	1	3911	7/7	0.07	-3.12	90,90,90,90	0
86	OHX	2	2034	7/7	0.10	-3.13	110,110,110,110	0
86	OHX	6	2094	7/7	0.07	-3.13	134,134,134,134	0
86	OHX	5	3942	7/7	0.09	-3.15	94,94,94,94	0
85	MG	5	3678	1/1	0.08	-3.16	96,96,96,96	0
86	OHX	5	4049	7/7	0.11	-3.16	108,108,108,108	0
86	OHX	1	3925	7/7	0.07	-3.17	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3872	7/7	0.11	-3.17	60,60,60,60	0
86	OHX	5	3914	7/7	0.10	-3.18	77,77,77,77	0
85	MG	1	3520	1/1	0.08	-3.18	38,38,38,38	0
86	OHX	1	3904	7/7	0.11	-3.21	97,97,97,97	0
86	OHX	1	3953	7/7	0.11	-3.23	102,102,102,102	0
86	OHX	6	2066	7/7	0.10	-3.24	102,102,102,102	0
86	OHX	5	4011	7/7	0.10	-3.26	112,112,112,112	0
86	OHX	1	3932	7/7	0.07	-3.27	91,91,91,91	0
86	OHX	2	2026	7/7	0.11	-3.27	93,93,93,93	0
86	OHX	5	4014	7/7	0.12	-3.27	110,110,110,110	0
86	OHX	5	4002	7/7	0.09	-3.28	125,125,125,125	0
86	OHX	5	3903	7/7	0.10	-3.28	62,62,62,62	0
86	OHX	6	2046	7/7	0.12	-3.32	82,82,82,82	0
86	OHX	2	2061	7/7	0.10	-3.32	136,136,136,136	0
86	OHX	1	3966	7/7	0.08	-3.33	143,143,143,143	0
86	OHX	6	2118	7/7	0.12	-3.33	159,159,159,159	0
86	OHX	3	216	7/7	0.07	-3.35	112,112,112,112	0
86	OHX	2	2059	7/7	0.10	-3.37	131,131,131,131	0
85	MG	5	3839	1/1	0.12	-3.38	72,72,72,72	0
86	OHX	5	4021	7/7	0.12	-3.42	122,122,122,122	0
86	OHX	5	3949	7/7	0.11	-3.43	90,90,90,90	0
86	OHX	1	3978	7/7	0.12	-3.43	109,109,109,109	0
86	OHX	2	2063	7/7	0.07	-3.44	142,142,142,142	0
85	MG	1	3753	1/1	0.13	-3.44	37,37,37,37	0
86	OHX	5	4001	7/7	0.11	-3.45	123,123,123,123	0
86	OHX	1	3880	7/7	0.11	-3.47	74,74,74,74	0
86	OHX	6	2065	7/7	0.07	-3.47	110,110,110,110	0
86	OHX	5	4080	7/7	0.11	-3.51	144,144,144,144	0
86	OHX	1	4085	7/7	0.15	-3.52	201,201,201,201	0
86	OHX	6	2088	7/7	0.08	-3.53	129,129,129,129	0
86	OHX	5	3948	7/7	0.08	-3.53	104,104,104,104	0
86	OHX	1	3997	7/7	0.10	-3.53	164,164,164,164	0
86	OHX	5	3993	7/7	0.05	-3.53	126,126,126,126	0
86	OHX	1	3903	7/7	0.12	-3.53	94,94,94,94	0
86	OHX	5	4017	7/7	0.08	-3.54	120,120,120,120	0
86	OHX	5	4012	7/7	0.16	-3.55	155,155,155,155	0
86	OHX	5	3966	7/7	0.09	-3.56	100,100,100,100	0
86	OHX	2	2070	7/7	0.09	-3.58	137,137,137,137	0
86	OHX	5	3996	7/7	0.08	-3.58	116,116,116,116	0
86	OHX	5	3900	7/7	0.10	-3.58	58,58,58,58	0
86	OHX	6	2047	7/7	0.16	-3.64	84,84,84,84	0
86	OHX	5	3936	7/7	0.07	-3.65	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	1	3934	7/7	0.10	-3.65	103,103,103,103	0
85	MG	5	3850	1/1	0.13	-3.66	53,53,53,53	0
86	OHX	5	4073	7/7	0.07	-3.68	159,159,159,159	0
86	OHX	6	2061	7/7	0.09	-3.69	123,123,123,123	0
86	OHX	1	3957	7/7	0.06	-3.77	114,114,114,114	0
86	OHX	1	3916	7/7	0.09	-3.78	107,107,107,107	0
86	OHX	5	4004	7/7	0.09	-3.80	105,105,105,105	0
85	MG	5	3759	1/1	0.16	-3.82	54,54,54,54	0
86	OHX	2	2044	7/7	0.06	-3.86	110,110,110,110	0
86	OHX	5	3921	7/7	0.08	-3.88	74,74,74,74	0
86	OHX	5	3992	7/7	0.15	-3.89	106,106,106,106	0
86	OHX	8	217	7/7	0.08	-3.89	111,111,111,111	0
86	OHX	8	215	7/7	0.07	-3.89	93,93,93,93	0
86	OHX	6	2081	7/7	0.08	-3.89	143,143,143,143	0
86	OHX	1	3929	7/7	0.08	-3.89	97,97,97,97	0
86	OHX	1	3897	7/7	0.09	-3.90	84,84,84,84	0
85	MG	5	3703	1/1	0.14	-3.92	67,67,67,67	0
86	OHX	5	3969	7/7	0.10	-3.92	109,109,109,109	0
85	MG	5	3683	1/1	0.11	-3.96	32,32,32,32	0
86	OHX	1	3894	7/7	0.11	-3.96	100,100,100,100	0
86	OHX	6	2072	7/7	0.07	-3.96	121,121,121,121	0
86	OHX	6	2053	7/7	0.09	-3.96	92,92,92,92	0
86	OHX	5	4210	7/7	0.14	-4.01	199,199,199,199	0
86	OHX	1	3888	7/7	0.12	-4.01	79,79,79,79	0
86	OHX	5	4126	7/7	0.16	-4.03	192,192,192,192	0
86	OHX	5	3979	7/7	0.09	-4.04	91,91,91,91	0
86	OHX	1	3912	7/7	0.08	-4.10	93,93,93,93	0
86	OHX	6	2058	7/7	0.10	-4.10	100,100,100,100	0
86	OHX	5	3952	7/7	0.09	-4.11	98,98,98,98	0
86	OHX	5	3945	7/7	0.09	-4.15	84,84,84,84	0
86	OHX	6	2112	7/7	0.14	-4.17	149,149,149,149	0
85	MG	5	3804	1/1	0.09	-4.20	165,165,165,165	0
86	OHX	2	2045	7/7	0.06	-4.22	111,111,111,111	0
86	OHX	2	2041	7/7	0.08	-4.26	103,103,103,103	0
86	OHX	6	2108	7/7	0.14	-4.26	132,132,132,132	0
86	OHX	1	3968	7/7	0.07	-4.27	114,114,114,114	0
86	OHX	5	3974	7/7	0.10	-4.28	104,104,104,104	0
85	MG	5	3758	1/1	0.09	-4.29	40,40,40,40	0
86	OHX	7	222	7/7	0.09	-4.29	106,106,106,106	0
86	OHX	5	3991	7/7	0.08	-4.34	124,124,124,124	0
86	OHX	6	2084	7/7	0.09	-4.36	135,135,135,135	0
86	OHX	1	3960	7/7	0.07	-4.36	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	2	2078	7/7	0.10	-4.37	136,136,136,136	0
85	MG	5	3764	1/1	0.10	-4.38	63,63,63,63	0
86	OHX	1	3942	7/7	0.08	-4.44	97,97,97,97	0
86	OHX	5	3946	7/7	0.08	-4.44	95,95,95,95	0
86	OHX	5	3909	7/7	0.12	-4.44	58,58,58,58	0
86	OHX	6	2076	7/7	0.09	-4.45	108,108,108,108	0
86	OHX	1	4144	7/7	0.11	-4.46	120,120,120,120	0
85	MG	5	3785	1/1	0.08	-4.47	39,39,39,39	0
86	OHX	1	3973	7/7	0.09	-4.47	110,110,110,110	0
86	OHX	6	2057	7/7	0.08	-4.51	94,94,94,94	0
86	OHX	1	4065	7/7	0.07	-4.53	163,163,163,163	0
86	OHX	3	218	7/7	0.11	-4.56	138,138,138,138	0
86	OHX	5	3970	7/7	0.10	-4.62	88,88,88,88	0
85	MG	1	3737	1/1	0.10	-4.67	61,61,61,61	0
86	OHX	1	3974	7/7	0.11	-4.72	111,111,111,111	0
86	OHX	1	3979	7/7	0.07	-4.72	87,87,87,87	0
86	OHX	5	3924	7/7	0.11	-4.74	65,65,65,65	0
85	MG	5	3806	1/1	0.11	-4.75	89,89,89,89	0
86	OHX	5	3983	7/7	0.08	-4.77	94,94,94,94	0
86	OHX	1	3988	7/7	0.15	-4.81	117,117,117,117	0
86	OHX	1	3915	7/7	0.10	-4.82	103,103,103,103	0
86	OHX	1	3893	7/7	0.07	-4.83	82,82,82,82	0
85	MG	1	3736	1/1	0.12	-4.90	34,34,34,34	0
86	OHX	1	3958	7/7	0.07	-4.90	121,121,121,121	0
85	MG	5	3652	1/1	0.12	-4.90	102,102,102,102	0
86	OHX	5	3940	7/7	0.08	-4.91	90,90,90,90	0
86	OHX	1	3952	7/7	0.10	-4.92	101,101,101,101	0
86	OHX	6	2080	7/7	0.09	-4.95	129,129,129,129	0
86	OHX	5	3975	7/7	0.08	-4.95	92,92,92,92	0
86	OHX	1	3939	7/7	0.08	-4.96	105,105,105,105	0
86	OHX	5	3938	7/7	0.09	-4.97	95,95,95,95	0
86	OHX	1	3900	7/7	0.09	-4.98	72,72,72,72	0
86	OHX	1	3940	7/7	0.12	-5.03	111,111,111,111	0
86	OHX	1	3909	7/7	0.07	-5.05	103,103,103,103	0
86	OHX	5	3927	7/7	0.08	-5.07	91,91,91,91	0
86	OHX	2	2052	7/7	0.09	-5.08	124,124,124,124	0
85	MG	n8	204	1/1	0.12	-5.09	37,37,37,37	0
86	OHX	2	2038	7/7	0.11	-5.11	108,108,108,108	0
86	OHX	6	2056	7/7	0.08	-5.11	99,99,99,99	0
86	OHX	1	4155	7/7	0.10	-5.12	110,110,110,110	0
86	OHX	1	4152	7/7	0.08	-5.14	129,129,129,129	0
86	OHX	6	2110	7/7	0.11	-5.15	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
86	OHX	5	3999	7/7	0.13	-5.15	115,115,115,115	0
86	OHX	5	3932	7/7	0.11	-5.19	75,75,75,75	0
86	OHX	5	3988	7/7	0.09	-5.19	111,111,111,111	0
85	MG	6	2004	1/1	0.11	-5.21	56,56,56,56	0
86	OHX	1	3959	7/7	0.09	-5.25	104,104,104,104	0
86	OHX	5	4074	7/7	0.12	-5.32	100,100,100,100	0
86	OHX	2	2104	7/7	0.28	-5.34	212,212,212,212	0
85	MG	5	3801	1/1	0.12	-5.40	43,43,43,43	0
86	OHX	6	2090	7/7	0.07	-5.45	149,149,149,149	0
85	MG	1	3800	1/1	0.12	-5.55	57,57,57,57	0
86	OHX	2	2042	7/7	0.06	-5.55	112,112,112,112	0
86	OHX	6	2059	7/7	0.06	-5.57	93,93,93,93	0
86	OHX	7	221	7/7	0.10	-5.62	101,101,101,101	0
86	OHX	5	3944	7/7	0.09	-5.63	87,87,87,87	0
86	OHX	5	3957	7/7	0.12	-5.85	75,75,75,75	0
86	OHX	4	224	7/7	0.11	-5.87	93,93,93,93	0
86	OHX	5	3985	7/7	0.07	-5.88	128,128,128,128	0
86	OHX	5	3933	7/7	0.09	-5.97	89,89,89,89	0
86	OHX	5	3919	7/7	0.09	-6.03	78,78,78,78	0
85	MG	5	3820	1/1	0.10	-6.16	58,58,58,58	0
86	OHX	8	220	7/7	0.06	-6.20	123,123,123,123	0
86	OHX	5	3986	7/7	0.04	-6.21	92,92,92,92	0
86	OHX	5	3926	7/7	0.08	-6.39	85,85,85,85	0
86	OHX	5	3987	7/7	0.06	-6.55	105,105,105,105	0
86	OHX	6	2075	7/7	0.07	-6.61	121,121,121,121	0
86	OHX	1	3949	7/7	0.10	-6.63	103,103,103,103	0
86	OHX	5	3923	7/7	0.07	-6.70	74,74,74,74	0
86	OHX	1	3923	7/7	0.06	-6.71	82,82,82,82	0
86	OHX	5	3951	7/7	0.07	-6.82	113,113,113,113	0
86	OHX	6	2077	7/7	0.08	-6.94	110,110,110,110	0
86	OHX	2	2050	7/7	0.06	-6.96	127,127,127,127	0
86	OHX	m6	204	7/7	0.07	-6.98	103,103,103,103	0
85	MG	5	3616	1/1	0.08	-7.05	57,57,57,57	0
86	OHX	5	4030	7/7	0.08	-7.09	119,119,119,119	0
86	OHX	1	4178	7/7	0.29	-7.13	254,254,254,254	0
86	OHX	5	3955	7/7	0.07	-7.22	87,87,87,87	0
86	OHX	5	3943	7/7	0.10	-7.63	89,89,89,89	0
86	OHX	6	2074	7/7	0.08	-7.73	102,102,102,102	0
86	OHX	5	4039	7/7	0.12	-7.74	115,115,115,115	0
85	MG	5	3651	1/1	0.06	-7.80	32,32,32,32	0
86	OHX	1	3999	7/7	0.08	-7.91	95,95,95,95	0
85	MG	6	2013	1/1	0.16	-7.98	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
86	OHX	1	3962	7/7	0.06	-8.05	77,77,77,77	0
86	OHX	1	3883	7/7	0.08	-8.09	67,67,67,67	0
85	MG	1	3768	1/1	0.09	-8.39	93,93,93,93	0
86	OHX	5	3915	7/7	0.08	-8.94	70,70,70,70	0
86	OHX	1	3946	7/7	0.07	-9.02	117,117,117,117	0
86	OHX	1	3995	7/7	0.08	-9.08	105,105,105,105	0
86	OHX	6	2089	7/7	0.07	-9.53	117,117,117,117	0
86	OHX	1	3917	7/7	0.10	-9.55	99,99,99,99	0
86	OHX	5	3978	7/7	0.06	-10.58	89,89,89,89	0
86	OHX	6	2083	7/7	0.07	-10.82	122,122,122,122	0
86	OHX	1	3919	7/7	0.07	-12.54	100,100,100,100	0
86	OHX	5	3961	7/7	0.10	-13.48	103,103,103,103	0
86	OHX	1	3928	7/7	0.07	-15.89	90,90,90,90	0
86	OHX	5	3917	7/7	0.10	-16.67	80,80,80,80	0
86	OHX	5	3962	7/7	0.06	-35.26	88,88,88,88	0
85	MG	5	3875	1/1	0.55	-	41,41,41,41	0
85	MG	1	3799	1/1	0.24	-	87,87,87,87	0
85	MG	4	216	1/1	0.37	-	65,65,65,65	0
85	MG	1	3848	1/1	0.59	-	45,45,45,45	0
85	MG	1	3789	1/1	0.20	-	69,69,69,69	0
85	MG	1	3837	1/1	1.00	-	57,57,57,57	0
85	MG	1	3840	1/1	0.37	-	50,50,50,50	0
85	MG	1	3677	1/1	0.06	-	78,78,78,78	0
85	MG	1	3594	1/1	0.60	-	69,69,69,69	0
85	MG	1	3735	1/1	0.63	-	67,67,67,67	0
85	MG	5	3859	1/1	0.11	-	73,73,73,73	0
85	MG	5	3755	1/1	0.44	-	47,47,47,47	0
86	OHX	2	2159	7/7	0.15	-	277,277,277,277	0
85	MG	6	2012	1/1	0.24	-	74,74,74,74	0
85	MG	1	3464	1/1	0.58	-	51,51,51,51	0
85	MG	6	2042	1/1	0.36	-	81,81,81,81	0
85	MG	6	1996	1/1	0.48	-	107,107,107,107	0
85	MG	6	1933	1/1	1.07	-	80,80,80,80	0
85	MG	6	2037	1/1	0.44	-	55,55,55,55	0
85	MG	1	3792	1/1	0.16	-	58,58,58,58	0
85	MG	1	3614	1/1	0.41	-	54,54,54,54	0
85	MG	5	3847	1/1	0.37	-	41,41,41,41	0
85	MG	1	3755	1/1	0.31	-	88,88,88,88	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.