wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2014 – 11:09 PM BST

PDB ID	:	4U53
Title	:	Crystal structure of Deoxynivalenol bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	3.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

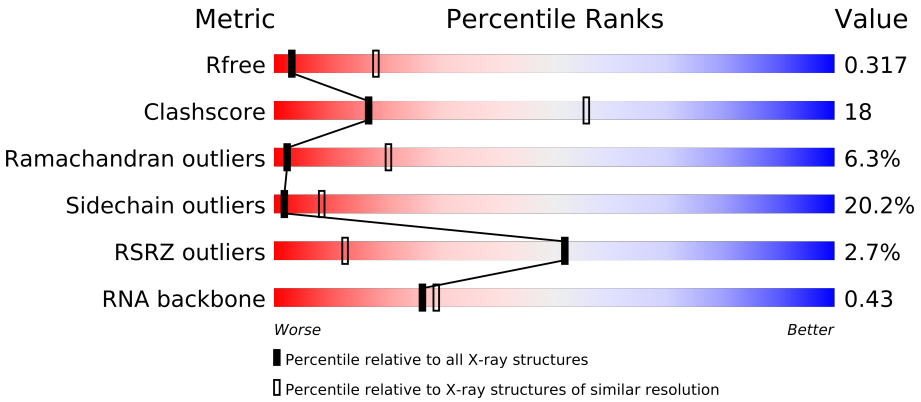
The following versions of software and data (see references) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

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Mol	Chain	Length	Quality of chain
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	

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Mol	Chain	Length	Quality of chain
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	60	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	

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Mol	Chain	Length	Quality of chain
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	

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

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

Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3401	-	X
85	MG	1	3402	-	X
85	MG	1	3403	-	X
85	MG	1	3404	-	X
85	MG	1	3405	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3415	-	X
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	3426	-	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	3443	-	X
85	MG	1	3444	-	X
85	MG	1	3446	-	X
85	MG	1	3447	-	X
85	MG	1	3449	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3469	-	X
85	MG	1	3470	-	X
85	MG	1	3471	-	X
85	MG	1	3473	-	X
85	MG	1	3474	-	X
85	MG	1	3475	-	X
85	MG	1	3476	-	X
85	MG	1	3477	-	X
85	MG	1	3479	-	X
85	MG	1	3480	-	X
85	MG	1	3481	-	X
85	MG	1	3483	-	X
85	MG	1	3484	-	X
85	MG	1	3485	-	X
85	MG	1	3486	-	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	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	3547	-	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	3558	-	X
85	MG	1	3559	-	X
85	MG	1	3560	-	X
85	MG	1	3561	-	X
85	MG	1	3562	-	X
85	MG	1	3563	-	X
85	MG	1	3564	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	3583	-	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	3594	-	X
85	MG	1	3595	-	X
85	MG	1	3596	-	X
85	MG	1	3597	-	X
85	MG	1	3598	-	X
85	MG	1	3599	-	X
85	MG	1	3600	-	X
85	MG	1	3601	-	X
85	MG	1	3602	-	X
85	MG	1	3604	-	X
85	MG	1	3605	-	X
85	MG	1	3607	-	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	3612	-	X
85	MG	1	3613	-	X
85	MG	1	3614	-	X
85	MG	1	3615	-	X
85	MG	1	3617	-	X
85	MG	1	3618	-	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	3626	-	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	3634	-	X
85	MG	1	3635	-	X
85	MG	1	3637	-	X
85	MG	1	3639	-	X
85	MG	1	3640	-	X
85	MG	1	3644	-	X
85	MG	1	3645	-	X
85	MG	1	3646	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3661	-	X
85	MG	1	3664	-	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	3674	-	X
85	MG	1	3676	-	X
85	MG	1	3677	-	X
85	MG	1	3679	-	X
85	MG	1	3680	-	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	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
85	MG	1	3711	-	X
85	MG	1	3712	-	X
85	MG	1	3713	-	X
85	MG	1	3714	-	X
85	MG	1	3715	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3716	-	X
85	MG	1	3717	-	X
85	MG	1	3719	-	X
85	MG	1	3723	-	X
85	MG	1	3725	-	X
85	MG	1	3726	-	X
85	MG	1	3728	-	X
85	MG	1	3730	-	X
85	MG	1	3732	-	X
85	MG	1	3733	-	X
85	MG	1	3734	-	X
85	MG	1	3735	-	X
85	MG	1	3737	-	X
85	MG	1	3738	-	X
85	MG	1	3741	-	X
85	MG	1	3742	-	X
85	MG	1	3743	-	X
85	MG	1	3744	-	X
85	MG	1	3746	-	X
85	MG	1	3747	-	X
85	MG	1	3748	-	X
85	MG	1	3750	-	X
85	MG	1	3751	-	X
85	MG	1	3752	-	X
85	MG	1	3753	-	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	3764	-	X
85	MG	1	3765	-	X
85	MG	1	3768	-	X
85	MG	1	3769	-	X
85	MG	1	3772	-	X
85	MG	1	3773	-	X
85	MG	1	3774	-	X
85	MG	1	3775	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	3783	-	X
85	MG	1	3784	-	X
85	MG	1	3785	-	X
85	MG	1	3787	-	X
85	MG	1	3790	-	X
85	MG	1	3791	-	X
85	MG	1	3792	-	X
85	MG	1	3795	-	X
85	MG	1	3796	-	X
85	MG	1	3798	-	X
85	MG	1	3799	-	X
85	MG	1	3801	-	X
85	MG	1	3803	-	X
85	MG	1	3807	-	X
85	MG	1	3808	-	X
85	MG	1	3811	-	X
85	MG	1	3813	-	X
85	MG	1	3814	-	X
85	MG	1	3815	-	X
85	MG	1	3816	-	X
85	MG	1	3817	-	X
85	MG	1	3818	-	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	3826	-	X
85	MG	1	3827	-	X
85	MG	1	3829	-	X
85	MG	1	3830	-	X
85	MG	1	3831	-	X
85	MG	1	3832	-	X
85	MG	1	3833	-	X
85	MG	1	3834	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	1	3835	-	X
85	MG	1	3837	-	X
85	MG	1	3840	-	X
85	MG	1	3841	-	X
85	MG	1	3843	-	X
85	MG	1	3844	-	X
85	MG	1	3845	-	X
85	MG	1	3846	-	X
85	MG	1	3847	-	X
85	MG	1	3848	-	X
85	MG	1	3850	-	X
85	MG	1	3851	-	X
85	MG	1	3852	-	X
85	MG	1	3853	-	X
85	MG	1	3854	-	X
85	MG	1	3855	-	X
85	MG	1	3856	-	X
85	MG	1	3857	-	X
85	MG	1	3859	-	X
85	MG	1	3860	-	X
85	MG	1	3861	-	X
85	MG	1	3863	-	X
85	MG	1	3865	-	X
85	MG	1	4214	-	X
85	MG	1	4215	-	X
85	MG	1	4218	-	X
85	MG	1	4219	-	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
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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1916	-	X
85	MG	2	1917	-	X
85	MG	2	1918	-	X
85	MG	2	1919	-	X
85	MG	2	1920	-	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	1943	-	X
85	MG	2	1944	-	X
85	MG	2	1945	-	X
85	MG	2	1946	-	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
85	MG	2	1953	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	2	1961	-	X
85	MG	2	1963	-	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	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	1987	-	X
85	MG	2	1988	-	X
85	MG	2	1989	-	X
85	MG	2	1991	-	X
85	MG	2	1993	-	X
85	MG	2	1994	-	X
85	MG	2	1997	-	X
85	MG	2	2000	-	X
85	MG	2	2001	-	X
85	MG	2	2002	-	X
85	MG	2	2003	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
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	2021	-	X
85	MG	2	2022	-	X
85	MG	2	2180	-	X
85	MG	3	201	-	X
85	MG	3	202	-	X
85	MG	3	203	-	X
85	MG	3	204	-	X
85	MG	3	205	-	X
85	MG	3	206	-	X
85	MG	3	207	-	X
85	MG	3	208	-	X
85	MG	3	209	-	X
85	MG	3	211	-	X
85	MG	3	212	-	X
85	MG	3	213	-	X
85	MG	3	214	-	X
85	MG	4	201	-	X
85	MG	4	202	-	X
85	MG	4	203	-	X
85	MG	4	205	-	X
85	MG	4	206	-	X
85	MG	4	207	-	X
85	MG	4	208	-	X
85	MG	4	209	-	X
85	MG	4	210	-	X
85	MG	4	211	-	X
85	MG	4	212	-	X
85	MG	4	213	-	X
85	MG	4	215	-	X
85	MG	4	217	-	X
85	MG	4	218	-	X
85	MG	4	219	-	X
85	MG	5	3402	-	X
85	MG	5	3403	-	X
85	MG	5	3405	-	X
85	MG	5	3406	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3408	-	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	3416	-	X
85	MG	5	3417	-	X
85	MG	5	3418	-	X
85	MG	5	3419	-	X
85	MG	5	3420	-	X
85	MG	5	3422	-	X
85	MG	5	3423	-	X
85	MG	5	3425	-	X
85	MG	5	3426	-	X
85	MG	5	3427	-	X
85	MG	5	3430	-	X
85	MG	5	3432	-	X
85	MG	5	3434	-	X
85	MG	5	3435	-	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
85	MG	5	3447	-	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	3459	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	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	3485	-	X
85	MG	5	3486	-	X
85	MG	5	3487	-	X
85	MG	5	3488	-	X
85	MG	5	3490	-	X
85	MG	5	3491	-	X
85	MG	5	3492	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
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	3513	-	X
85	MG	5	3514	-	X
85	MG	5	3515	-	X
85	MG	5	3516	-	X
85	MG	5	3517	-	X
85	MG	5	3518	-	X
85	MG	5	3519	-	X
85	MG	5	3520	-	X
85	MG	5	3521	-	X
85	MG	5	3522	-	X
85	MG	5	3523	-	X
85	MG	5	3524	-	X
85	MG	5	3525	-	X
85	MG	5	3526	-	X
85	MG	5	3528	-	X
85	MG	5	3529	-	X
85	MG	5	3530	-	X
85	MG	5	3531	-	X
85	MG	5	3532	-	X
85	MG	5	3533	-	X
85	MG	5	3534	-	X
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	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

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Mol	Type	Chain	Res	Geometry	Electron density
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	3565	-	X
85	MG	5	3566	-	X
85	MG	5	3567	-	X
85	MG	5	3568	-	X
85	MG	5	3569	-	X
85	MG	5	3570	-	X
85	MG	5	3571	-	X
85	MG	5	3572	-	X
85	MG	5	3573	-	X
85	MG	5	3574	-	X
85	MG	5	3575	-	X
85	MG	5	3576	-	X
85	MG	5	3577	-	X
85	MG	5	3578	-	X
85	MG	5	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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3596	-	X
85	MG	5	3597	-	X
85	MG	5	3602	-	X
85	MG	5	3604	-	X
85	MG	5	3605	-	X
85	MG	5	3606	-	X
85	MG	5	3607	-	X
85	MG	5	3608	-	X
85	MG	5	3609	-	X
85	MG	5	3610	-	X
85	MG	5	3613	-	X
85	MG	5	3615	-	X
85	MG	5	3617	-	X
85	MG	5	3619	-	X
85	MG	5	3620	-	X
85	MG	5	3621	-	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
85	MG	5	3627	-	X
85	MG	5	3629	-	X
85	MG	5	3630	-	X
85	MG	5	3632	-	X
85	MG	5	3633	-	X
85	MG	5	3637	-	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	3647	-	X
85	MG	5	3648	-	X
85	MG	5	3653	-	X
85	MG	5	3655	-	X
85	MG	5	3656	-	X
85	MG	5	3657	-	X
85	MG	5	3658	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	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
85	MG	5	3676	-	X
85	MG	5	3677	-	X
85	MG	5	3679	-	X
85	MG	5	3680	-	X
85	MG	5	3681	-	X
85	MG	5	3682	-	X
85	MG	5	3683	-	X
85	MG	5	3684	-	X
85	MG	5	3685	-	X
85	MG	5	3687	-	X
85	MG	5	3688	-	X
85	MG	5	3689	-	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	3697	-	X
85	MG	5	3698	-	X
85	MG	5	3700	-	X
85	MG	5	3702	-	X
85	MG	5	3703	-	X
85	MG	5	3704	-	X
85	MG	5	3705	-	X
85	MG	5	3706	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3707	-	X
85	MG	5	3708	-	X
85	MG	5	3709	-	X
85	MG	5	3711	-	X
85	MG	5	3712	-	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	3720	-	X
85	MG	5	3722	-	X
85	MG	5	3725	-	X
85	MG	5	3726	-	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	3734	-	X
85	MG	5	3735	-	X
85	MG	5	3736	-	X
85	MG	5	3737	-	X
85	MG	5	3738	-	X
85	MG	5	3739	-	X
85	MG	5	3740	-	X
85	MG	5	3741	-	X
85	MG	5	3742	-	X
85	MG	5	3743	-	X
85	MG	5	3744	-	X
85	MG	5	3746	-	X
85	MG	5	3747	-	X
85	MG	5	3749	-	X
85	MG	5	3751	-	X
85	MG	5	3754	-	X
85	MG	5	3756	-	X
85	MG	5	3757	-	X
85	MG	5	3759	-	X
85	MG	5	3761	-	X
85	MG	5	3763	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3764	-	X
85	MG	5	3765	-	X
85	MG	5	3766	-	X
85	MG	5	3767	-	X
85	MG	5	3770	-	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	3777	-	X
85	MG	5	3778	-	X
85	MG	5	3780	-	X
85	MG	5	3781	-	X
85	MG	5	3782	-	X
85	MG	5	3783	-	X
85	MG	5	3786	-	X
85	MG	5	3787	-	X
85	MG	5	3788	-	X
85	MG	5	3789	-	X
85	MG	5	3790	-	X
85	MG	5	3791	-	X
85	MG	5	3792	-	X
85	MG	5	3794	-	X
85	MG	5	3795	-	X
85	MG	5	3799	-	X
85	MG	5	3800	-	X
85	MG	5	3801	-	X
85	MG	5	3803	-	X
85	MG	5	3805	-	X
85	MG	5	3806	-	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	3814	-	X
85	MG	5	3816	-	X
85	MG	5	3818	-	X
85	MG	5	3821	-	X
85	MG	5	3822	-	X
85	MG	5	3823	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	5	3824	-	X
85	MG	5	3825	-	X
85	MG	5	3826	-	X
85	MG	5	3828	-	X
85	MG	5	3830	-	X
85	MG	5	3831	-	X
85	MG	5	3832	-	X
85	MG	5	3834	-	X
85	MG	5	3835	-	X
85	MG	5	3836	-	X
85	MG	5	3838	-	X
85	MG	5	3840	-	X
85	MG	5	3841	-	X
85	MG	5	3842	-	X
85	MG	5	3843	-	X
85	MG	5	3846	-	X
85	MG	5	3848	-	X
85	MG	5	3849	-	X
85	MG	5	3850	-	X
85	MG	5	3851	-	X
85	MG	5	3853	-	X
85	MG	5	3855	-	X
85	MG	5	3856	-	X
85	MG	5	3858	-	X
85	MG	5	3859	-	X
85	MG	5	3860	-	X
85	MG	5	3862	-	X
85	MG	5	3864	-	X
85	MG	5	3865	-	X
85	MG	5	3866	-	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	3873	-	X
85	MG	5	3874	-	X
85	MG	5	3875	-	X
85	MG	5	3876	-	X
85	MG	5	3877	-	X
85	MG	5	3878	-	X
85	MG	5	3879	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	3889	-	X
85	MG	5	3890	-	X
85	MG	5	3891	-	X
85	MG	5	3892	-	X
85	MG	5	4248	-	X
85	MG	5	4249	-	X
85	MG	5	4250	-	X
85	MG	6	1901	-	X
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	1914	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1928	-	X
85	MG	6	1929	-	X
85	MG	6	1931	-	X
85	MG	6	1932	-	X
85	MG	6	1933	-	X
85	MG	6	1934	-	X
85	MG	6	1935	-	X
85	MG	6	1936	-	X
85	MG	6	1937	-	X
85	MG	6	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
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	1967	-	X
85	MG	6	1968	-	X
85	MG	6	1969	-	X
85	MG	6	1970	-	X
85	MG	6	1971	-	X
85	MG	6	1972	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	1973	-	X
85	MG	6	1974	-	X
85	MG	6	1975	-	X
85	MG	6	1976	-	X
85	MG	6	1978	-	X
85	MG	6	1979	-	X
85	MG	6	1980	-	X
85	MG	6	1981	-	X
85	MG	6	1984	-	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
85	MG	6	1991	-	X
85	MG	6	1992	-	X
85	MG	6	1993	-	X
85	MG	6	1994	-	X
85	MG	6	1997	-	X
85	MG	6	1999	-	X
85	MG	6	2001	-	X
85	MG	6	2002	-	X
85	MG	6	2004	-	X
85	MG	6	2008	-	X
85	MG	6	2009	-	X
85	MG	6	2010	-	X
85	MG	6	2011	-	X
85	MG	6	2012	-	X
85	MG	6	2013	-	X
85	MG	6	2015	-	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	2022	-	X
85	MG	6	2023	-	X
85	MG	6	2024	-	X
85	MG	6	2027	-	X
85	MG	6	2028	-	X
85	MG	6	2029	-	X
85	MG	6	2030	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	6	2031	-	X
85	MG	6	2032	-	X
85	MG	6	2033	-	X
85	MG	6	2034	-	X
85	MG	6	2035	-	X
85	MG	6	2036	-	X
85	MG	6	2038	-	X
85	MG	6	2039	-	X
85	MG	6	2041	-	X
85	MG	6	2042	-	X
85	MG	6	2043	-	X
85	MG	6	2206	-	X
85	MG	6	2207	-	X
85	MG	7	201	-	X
85	MG	7	202	-	X
85	MG	7	203	-	X
85	MG	7	204	-	X
85	MG	7	205	-	X
85	MG	7	206	-	X
85	MG	7	207	-	X
85	MG	7	209	-	X
85	MG	7	210	-	X
85	MG	7	211	-	X
85	MG	7	212	-	X
85	MG	7	213	-	X
85	MG	7	215	-	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	207	-	X
85	MG	8	209	-	X
85	MG	8	210	-	X
85	MG	8	211	-	X
85	MG	8	212	-	X
85	MG	8	214	-	X
85	MG	8	215	-	X
85	MG	C3	201	-	X
85	MG	D0	201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	L2	301	-	X
85	MG	L2	302	-	X
85	MG	L2	303	-	X
85	MG	L3	401	-	X
85	MG	L3	403	-	X
85	MG	L5	301	-	X
85	MG	L7	301	-	X
85	MG	L7	302	-	X
85	MG	M3	203	-	X
85	MG	M5	302	-	X
85	MG	M7	201	-	X
85	MG	M7	202	-	X
85	MG	M7	203	-	X
85	MG	M7	204	-	X
85	MG	N0	201	-	X
85	MG	N0	202	-	X
85	MG	N3	201	-	X
85	MG	N5	201	-	X
85	MG	N8	201	-	X
85	MG	N8	202	-	X
85	MG	N8	203	-	X
85	MG	N8	204	-	X
85	MG	O2	201	-	X
85	MG	O3	201	-	X
85	MG	O7	102	-	X
85	MG	S2	301	-	X
85	MG	S8	301	-	X
85	MG	c1	201	-	X
85	MG	c8	201	-	X
85	MG	d3	201	-	X
85	MG	d3	202	-	X
85	MG	l2	301	-	X
85	MG	l2	302	-	X
85	MG	l3	401	-	X
85	MG	l3	402	-	X
85	MG	l3	403	-	X
85	MG	l4	401	-	X
85	MG	l5	302	-	X
85	MG	l7	301	-	X
85	MG	l7	302	-	X
85	MG	l9	201	-	X
85	MG	m0	301	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
85	MG	m1	201	-	X
85	MG	m5	302	-	X
85	MG	m6	201	-	X
85	MG	m7	201	-	X
85	MG	m7	204	-	X
85	MG	n0	201	-	X
85	MG	n0	202	-	X
85	MG	n3	201	-	X
85	MG	n3	202	-	X
85	MG	n6	201	-	X
85	MG	n6	202	-	X
85	MG	n8	201	-	X
85	MG	n9	101	-	X
85	MG	o3	201	-	X
85	MG	o3	202	-	X
85	MG	o4	201	-	X
85	MG	q0	202	-	X
85	MG	q3	502	-	X
85	MG	s8	301	-	X
85	MG	s9	201	-	X
86	OHX	1	3898	-	X
86	OHX	1	3978	-	X
86	OHX	1	3985	-	X
86	OHX	1	3991	-	X
86	OHX	1	3992	-	X
86	OHX	1	4004	-	X
86	OHX	1	4005	-	X
86	OHX	1	4006	-	X
86	OHX	1	4008	-	X
86	OHX	1	4009	-	X
86	OHX	1	4014	-	X
86	OHX	1	4015	-	X
86	OHX	1	4025	-	X
86	OHX	1	4026	-	X
86	OHX	1	4028	-	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	4047	-	X
86	OHX	1	4050	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4052	-	X
86	OHX	1	4055	-	X
86	OHX	1	4057	-	X
86	OHX	1	4058	-	X
86	OHX	1	4062	-	X
86	OHX	1	4063	-	X
86	OHX	1	4064	-	X
86	OHX	1	4065	-	X
86	OHX	1	4067	-	X
86	OHX	1	4068	-	X
86	OHX	1	4069	-	X
86	OHX	1	4070	-	X
86	OHX	1	4071	-	X
86	OHX	1	4072	-	X
86	OHX	1	4073	-	X
86	OHX	1	4075	-	X
86	OHX	1	4078	-	X
86	OHX	1	4079	-	X
86	OHX	1	4080	-	X
86	OHX	1	4081	-	X
86	OHX	1	4082	-	X
86	OHX	1	4086	-	X
86	OHX	1	4091	-	X
86	OHX	1	4092	-	X
86	OHX	1	4094	-	X
86	OHX	1	4095	-	X
86	OHX	1	4096	-	X
86	OHX	1	4097	-	X
86	OHX	1	4099	-	X
86	OHX	1	4104	-	X
86	OHX	1	4106	-	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	4115	-	X
86	OHX	1	4116	-	X
86	OHX	1	4118	-	X
86	OHX	1	4119	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4120	-	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	4145	-	X
86	OHX	1	4146	-	X
86	OHX	1	4147	-	X
86	OHX	1	4148	-	X
86	OHX	1	4150	-	X
86	OHX	1	4152	-	X
86	OHX	1	4153	-	X
86	OHX	1	4154	-	X
86	OHX	1	4158	-	X
86	OHX	1	4159	-	X
86	OHX	1	4162	-	X
86	OHX	1	4163	-	X
86	OHX	1	4164	-	X
86	OHX	1	4166	-	X
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	4173	-	X
86	OHX	1	4174	-	X
86	OHX	1	4175	-	X
86	OHX	1	4176	-	X
86	OHX	1	4177	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	1	4179	-	X
86	OHX	1	4181	-	X
86	OHX	1	4182	-	X
86	OHX	1	4183	-	X
86	OHX	1	4184	-	X
86	OHX	1	4185	-	X
86	OHX	1	4187	-	X
86	OHX	1	4188	-	X
86	OHX	1	4189	-	X
86	OHX	1	4191	-	X
86	OHX	1	4193	-	X
86	OHX	1	4194	-	X
86	OHX	1	4195	-	X
86	OHX	1	4196	-	X
86	OHX	1	4198	-	X
86	OHX	1	4200	-	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	4211	-	X
86	OHX	1	4212	-	X
86	OHX	2	2051	-	X
86	OHX	2	2062	-	X
86	OHX	2	2069	-	X
86	OHX	2	2074	-	X
86	OHX	2	2075	-	X
86	OHX	2	2079	-	X
86	OHX	2	2084	-	X
86	OHX	2	2086	-	X
86	OHX	2	2088	-	X
86	OHX	2	2090	-	X
86	OHX	2	2091	-	X
86	OHX	2	2092	-	X
86	OHX	2	2096	-	X
86	OHX	2	2103	-	X
86	OHX	2	2105	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2106	-	X
86	OHX	2	2108	-	X
86	OHX	2	2109	-	X
86	OHX	2	2113	-	X
86	OHX	2	2116	-	X
86	OHX	2	2117	-	X
86	OHX	2	2118	-	X
86	OHX	2	2119	-	X
86	OHX	2	2122	-	X
86	OHX	2	2123	-	X
86	OHX	2	2125	-	X
86	OHX	2	2127	-	X
86	OHX	2	2128	-	X
86	OHX	2	2131	-	X
86	OHX	2	2134	-	X
86	OHX	2	2135	-	X
86	OHX	2	2136	-	X
86	OHX	2	2137	-	X
86	OHX	2	2139	-	X
86	OHX	2	2143	-	X
86	OHX	2	2145	-	X
86	OHX	2	2146	-	X
86	OHX	2	2148	-	X
86	OHX	2	2149	-	X
86	OHX	2	2150	-	X
86	OHX	2	2152	-	X
86	OHX	2	2153	-	X
86	OHX	2	2154	-	X
86	OHX	2	2157	-	X
86	OHX	2	2159	-	X
86	OHX	2	2160	-	X
86	OHX	2	2161	-	X
86	OHX	2	2162	-	X
86	OHX	2	2163	-	X
86	OHX	2	2167	-	X
86	OHX	2	2168	-	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
86	OHX	2	2174	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	2	2177	-	X
86	OHX	2	2178	-	X
86	OHX	3	222	-	X
86	OHX	3	223	-	X
86	OHX	3	224	-	X
86	OHX	3	225	-	X
86	OHX	3	226	-	X
86	OHX	4	228	-	X
86	OHX	4	229	-	X
86	OHX	4	232	-	X
86	OHX	4	233	-	X
86	OHX	4	235	-	X
86	OHX	4	236	-	X
86	OHX	5	3894	-	X
86	OHX	5	3903	-	X
86	OHX	5	3986	-	X
86	OHX	5	3996	-	X
86	OHX	5	4009	-	X
86	OHX	5	4014	-	X
86	OHX	5	4018	-	X
86	OHX	5	4021	-	X
86	OHX	5	4024	-	X
86	OHX	5	4034	-	X
86	OHX	5	4037	-	X
86	OHX	5	4039	-	X
86	OHX	5	4040	-	X
86	OHX	5	4041	-	X
86	OHX	5	4042	-	X
86	OHX	5	4044	-	X
86	OHX	5	4046	-	X
86	OHX	5	4047	-	X
86	OHX	5	4050	-	X
86	OHX	5	4053	-	X
86	OHX	5	4055	-	X
86	OHX	5	4056	-	X
86	OHX	5	4062	-	X
86	OHX	5	4064	-	X
86	OHX	5	4065	-	X
86	OHX	5	4066	-	X
86	OHX	5	4067	-	X
86	OHX	5	4073	-	X
86	OHX	5	4076	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	5	4079	-	X
86	OHX	5	4080	-	X
86	OHX	5	4083	-	X
86	OHX	5	4085	-	X
86	OHX	5	4086	-	X
86	OHX	5	4090	-	X
86	OHX	5	4091	-	X
86	OHX	5	4093	-	X
86	OHX	5	4094	-	X
86	OHX	5	4099	-	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	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	4127	-	X
86	OHX	5	4128	-	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	4136	-	X
86	OHX	5	4138	-	X
86	OHX	5	4139	-	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
86	OHX	5	4146	-	X
86	OHX	5	4147	-	X
86	OHX	5	4148	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	4159	-	X
86	OHX	5	4160	-	X
86	OHX	5	4161	-	X
86	OHX	5	4163	-	X
86	OHX	5	4164	-	X
86	OHX	5	4166	-	X
86	OHX	5	4167	-	X
86	OHX	5	4168	-	X
86	OHX	5	4170	-	X
86	OHX	5	4172	-	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	4185	-	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	4194	-	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	4201	-	X
86	OHX	5	4203	-	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	4210	-	X
86	OHX	5	4212	-	X
86	OHX	5	4213	-	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	4221	-	X
86	OHX	5	4223	-	X
86	OHX	5	4224	-	X
86	OHX	5	4225	-	X
86	OHX	5	4226	-	X
86	OHX	5	4229	-	X
86	OHX	5	4230	-	X
86	OHX	5	4231	-	X
86	OHX	5	4233	-	X
86	OHX	5	4234	-	X
86	OHX	5	4237	-	X
86	OHX	5	4239	-	X
86	OHX	5	4240	-	X
86	OHX	5	4241	-	X
86	OHX	5	4242	-	X
86	OHX	5	4243	-	X
86	OHX	5	4245	-	X
86	OHX	6	2070	-	X
86	OHX	6	2101	-	X
86	OHX	6	2106	-	X
86	OHX	6	2108	-	X
86	OHX	6	2113	-	X
86	OHX	6	2115	-	X
86	OHX	6	2118	-	X
86	OHX	6	2121	-	X
86	OHX	6	2124	-	X
86	OHX	6	2125	-	X
86	OHX	6	2131	-	X
86	OHX	6	2132	-	X
86	OHX	6	2134	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2138	-	X
86	OHX	6	2139	-	X
86	OHX	6	2142	-	X
86	OHX	6	2145	-	X
86	OHX	6	2147	-	X
86	OHX	6	2149	-	X
86	OHX	6	2154	-	X
86	OHX	6	2155	-	X
86	OHX	6	2156	-	X
86	OHX	6	2158	-	X
86	OHX	6	2159	-	X
86	OHX	6	2161	-	X
86	OHX	6	2163	-	X
86	OHX	6	2166	-	X
86	OHX	6	2167	-	X
86	OHX	6	2168	-	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	2175	-	X
86	OHX	6	2176	-	X
86	OHX	6	2177	-	X
86	OHX	6	2178	-	X
86	OHX	6	2180	-	X
86	OHX	6	2181	-	X
86	OHX	6	2183	-	X
86	OHX	6	2184	-	X
86	OHX	6	2186	-	X
86	OHX	6	2187	-	X
86	OHX	6	2188	-	X
86	OHX	6	2189	-	X
86	OHX	6	2190	-	X
86	OHX	6	2191	-	X
86	OHX	6	2195	-	X
86	OHX	6	2197	-	X
86	OHX	6	2198	-	X
86	OHX	6	2199	-	X
86	OHX	6	2200	-	X
86	OHX	6	2203	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
86	OHX	6	2204	-	X
86	OHX	7	225	-	X
86	OHX	7	227	-	X
86	OHX	8	222	-	X
86	OHX	8	224	-	X
86	OHX	8	227	-	X
86	OHX	8	228	-	X
86	OHX	8	230	-	X
86	OHX	D9	102	-	X
86	OHX	M7	205	-	X
86	OHX	M7	206	-	X
86	OHX	M9	203	-	X
86	OHX	O3	202	-	X
86	OHX	O4	201	-	X
86	OHX	O9	101	-	X
86	OHX	l4	403	-	X
86	OHX	l5	306	-	X
86	OHX	l5	307	-	X
86	OHX	m4	201	-	X
86	OHX	o7	503	-	X
86	OHX	s1	303	-	X
87	ZN	d7	101	-	X
88	3J6	5	4246	-	X

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 411183 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
			1214	775	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O	0	0	0
			1105	708	203	194			

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

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

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

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

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

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

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

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

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

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

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

- 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			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	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	0	0	0
			796	516	131	149			
58	n2	98	Total	C	N	O	0	0	0
			778	505	127	146			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 81 is a protein called Unknown Protein m2.

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

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

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

- Molecule 83 is a protein called Unknown Protein p1.

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

- Molecule 84 is a protein called Unknown Protein p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L7	2	Total 2	Mg 2	0	0
85	m6	2	Total 2	Mg 2	0	0
85	n8	2	Total 2	Mg 2	0	0
85	q3	2	Total 2	Mg 2	0	0
85	o1	1	Total 1	Mg 1	0	0
85	N5	1	Total 1	Mg 1	0	0
85	6	147	Total 147	Mg 147	0	0
85	sM	2	Total 2	Mg 2	0	0
85	m5	2	Total 2	Mg 2	0	0
85	l3	3	Total 3	Mg 3	0	0
85	M1	1	Total 1	Mg 1	0	0
85	n0	2	Total 2	Mg 2	0	0
85	d6	1	Total 1	Mg 1	0	0
85	2	123	Total 123	Mg 123	0	0
85	O3	1	Total 1	Mg 1	0	0
85	L4	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	l7	2	Total Mg 2 2	0	0
85	M5	2	Total Mg 2 2	0	0
85	o0	1	Total Mg 1 1	0	0
85	S2	1	Total Mg 1 1	0	0
85	L8	1	Total Mg 1 1	0	0
85	D3	1	Total Mg 1 1	0	0
85	o4	1	Total Mg 1 1	0	0
85	M9	2	Total Mg 2 2	0	0
85	q0	1	Total Mg 1 1	0	0
85	c8	2	Total Mg 2 2	0	0
85	M0	3	Total Mg 3 3	0	0
85	c1	1	Total Mg 1 1	0	0
85	5	496	Total Mg 496 496	0	0
85	L5	1	Total Mg 1 1	0	0
85	O7	1	Total Mg 1 1	0	0
85	l4	1	Total Mg 1 1	0	0
85	n9	1	Total Mg 1 1	0	0
85	1	471	Total Mg 471 471	0	0
85	D0	1	Total Mg 1 1	0	0
85	S8	1	Total Mg 1 1	0	0
85	m1	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	O2	2	Total Mg 2 2	0	0
85	s9	1	Total Mg 1 1	0	0
85	o3	2	Total Mg 2 2	0	0
85	d3	3	Total Mg 3 3	0	0
85	M3	3	Total Mg 3 3	0	0
85	N3	3	Total Mg 3 3	0	0
85	4	20	Total Mg 20 20	0	0
85	n6	2	Total Mg 2 2	0	0
85	L2	3	Total Mg 3 3	0	0
85	l5	3	Total Mg 3 3	0	0
85	C3	1	Total Mg 1 1	0	0
85	M7	4	Total Mg 4 4	0	0
85	N8	5	Total Mg 5 5	0	0
85	s1	1	Total Mg 1 1	0	0
85	l9	1	Total Mg 1 1	0	0
85	s8	2	Total Mg 2 2	0	0
85	c7	1	Total Mg 1 1	0	0
85	7	18	Total Mg 18 18	0	0
85	n3	2	Total Mg 2 2	0	0
85	L3	3	Total Mg 3 3	0	0
85	l2	2	Total Mg 2 2	0	0

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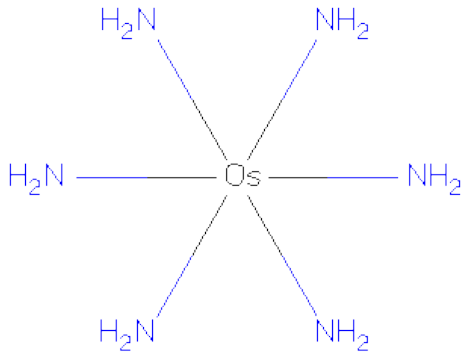
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	8	15	Total Mg 15 15	0	0
85	m0	1	Total Mg 1 1	0	0
85	M6	1	Total Mg 1 1	0	0
85	N0	2	Total Mg 2 2	0	0
85	3	14	Total Mg 14 14	0	0
85	m7	5	Total Mg 5 5	0	0

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



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

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

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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		
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		
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		
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		
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		
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		
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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 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	2	1	Total N Os 7 6 1	0	0
86	S6	1	Total N Os 7 6 1	0	0
86	S8	1	Total N Os 7 6 1	0	0
86	C3	1	Total N Os 7 6 1	0	0
86	C5	1	Total N Os 7 6 1	0	0
86	C8	1	Total N Os 7 6 1	0	0
86	D3	1	Total N Os 7 6 1	0	0
86	D9	1	Total N Os 7 6 1	0	0
86	SR	1	Total N Os 7 6 1	0	0
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86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0
86	1	1	Total N Os 7 6 1	0	0

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

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

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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
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86	1	1	Total	N	Os	0	0
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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
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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		

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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
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86	1	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
			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	L3	1	Total	N	Os	0	0
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86	L3	1	Total	N	Os	0	0
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86	L4	1	Total	N	Os	0	0
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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
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86	M9	1	Total	N	Os	0	0
			7	6	1		
86	N9	1	Total	N	Os	0	0
			7	6	1		
86	O1	1	Total	N	Os	0	0
			7	6	1		
86	O3	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	O4	1	Total N Os 7 6 1	0	0
86	O6	1	Total N Os 7 6 1	0	0
86	O7	1	Total N Os 7 6 1	0	0
86	O9	1	Total N Os 7 6 1	0	0
86	Q2	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	0	0
86	6	1	Total N Os 7 6 1	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
			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
			7	6	1		

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

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

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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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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
			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
			7	6	1		
86	s1	1	Total	N	Os	0	0
			7	6	1		
86	s1	1	Total	N	Os	0	0
			7	6	1		
86	s8	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
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
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			7	6	1		
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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
			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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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	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		
86	5	1	Total	N	Os	0	0
			7	6	1		

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	8	1	Total N Os 7 6 1	0	0
86	l3	1	Total N Os 7 6 1	0	0
86	l3	1	Total N Os 7 6 1	0	0
86	l4	1	Total N Os 7 6 1	0	0
86	l4	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l5	1	Total N Os 7 6 1	0	0
86	l9	1	Total N Os 7 6 1	0	0
86	m0	1	Total N Os 7 6 1	0	0
86	m0	1	Total N Os 7 6 1	0	0
86	m1	1	Total N Os 7 6 1	0	0
86	m4	1	Total N Os 7 6 1	0	0
86	m5	1	Total N Os 7 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	m6	1	Total N Os 7 6 1	0	0
86	m7	1	Total N Os 7 6 1	0	0
86	m8	1	Total N Os 7 6 1	0	0
86	n3	1	Total N Os 7 6 1	0	0
86	n3	1	Total N Os 7 6 1	0	0
86	n6	1	Total N Os 7 6 1	0	0
86	n9	1	Total N Os 7 6 1	0	0
86	o2	1	Total N Os 7 6 1	0	0
86	o3	1	Total N Os 7 6 1	0	0
86	o7	1	Total N Os 7 6 1	0	0
86	o7	1	Total N Os 7 6 1	0	0
86	q2	1	Total N Os 7 6 1	0	0

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

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

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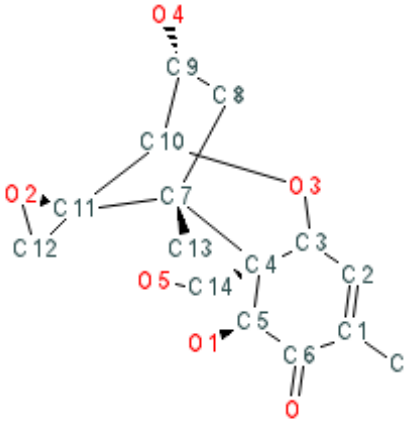
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	Q0	1	Total Zn 1 1	0	0
87	d7	1	Total Zn 1 1	0	0
87	q3	1	Total Zn 1 1	0	0
87	d9	1	Total Zn 1 1	0	0
87	D7	1	Total Zn 1 1	0	0
87	d6	1	Total Zn 1 1	0	0
87	o7	1	Total Zn 1 1	0	0
87	O7	1	Total Zn 1 1	0	0
87	q2	1	Total Zn 1 1	0	0

- Molecule 88 is (3beta,7alpha)-3,7,15-trihydroxy-12,13-epoxytrichothec-9-en-8-one (three-letter code: 3J6) (formula: $C_{15}H_{20}O_6$).



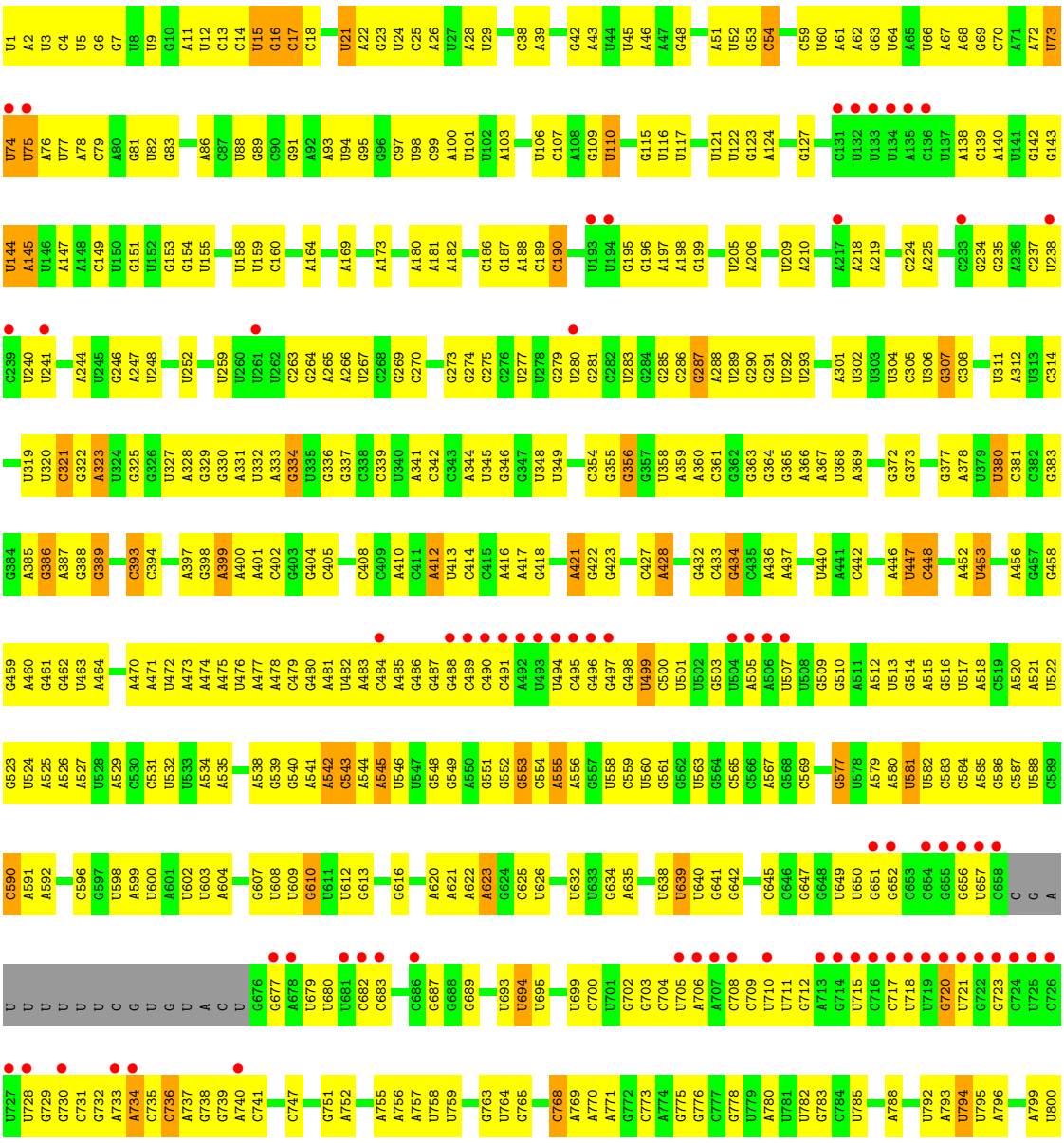
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	1	1	Total C O 21 15 6	0	0
88	5	1	Total C O 21 15 6	0	0

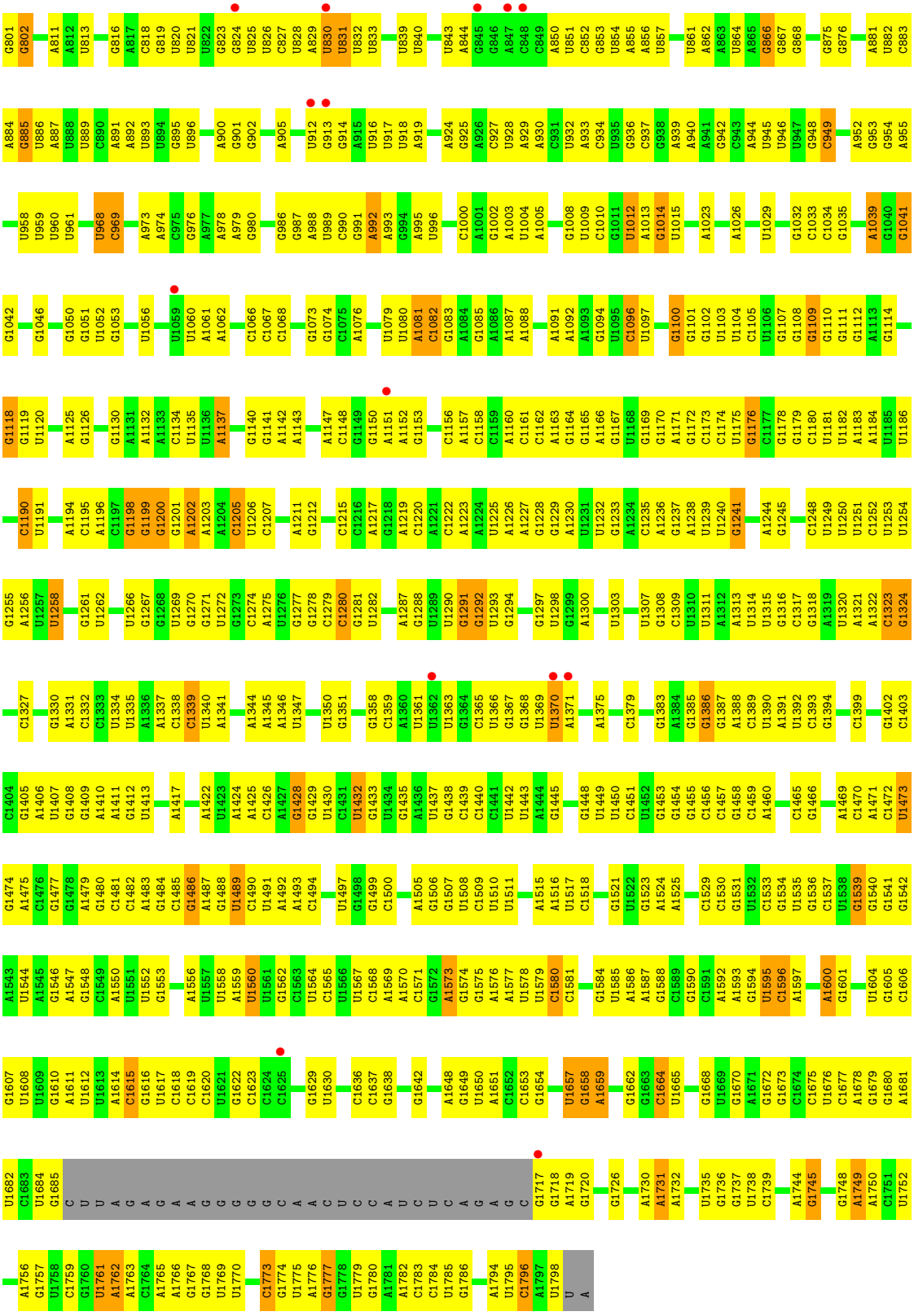
3 Residue-property plots (i)

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

- Molecule 1: Saccharomyces cerevisiae chromosome XII cosmid 9634

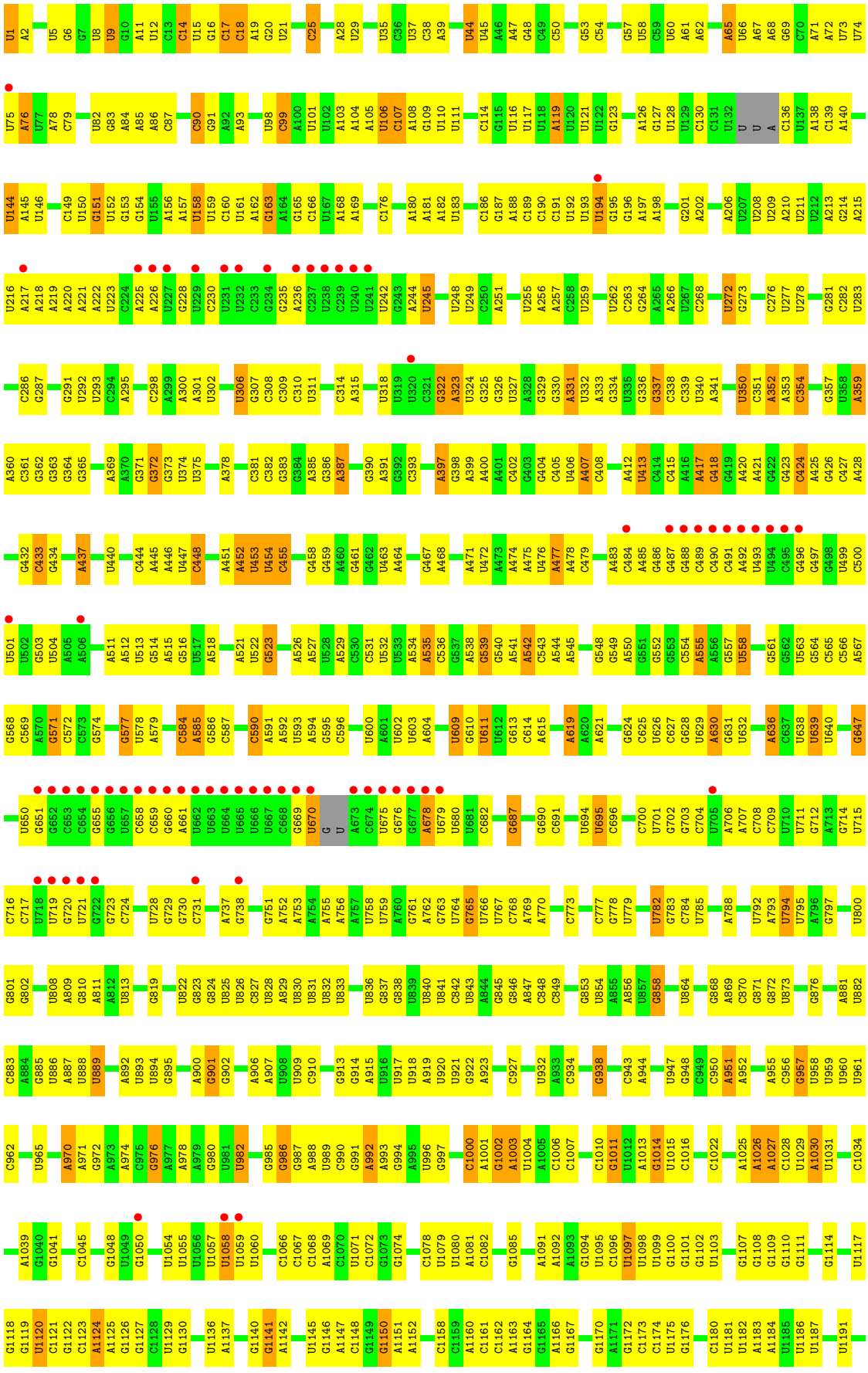
Chain 2:

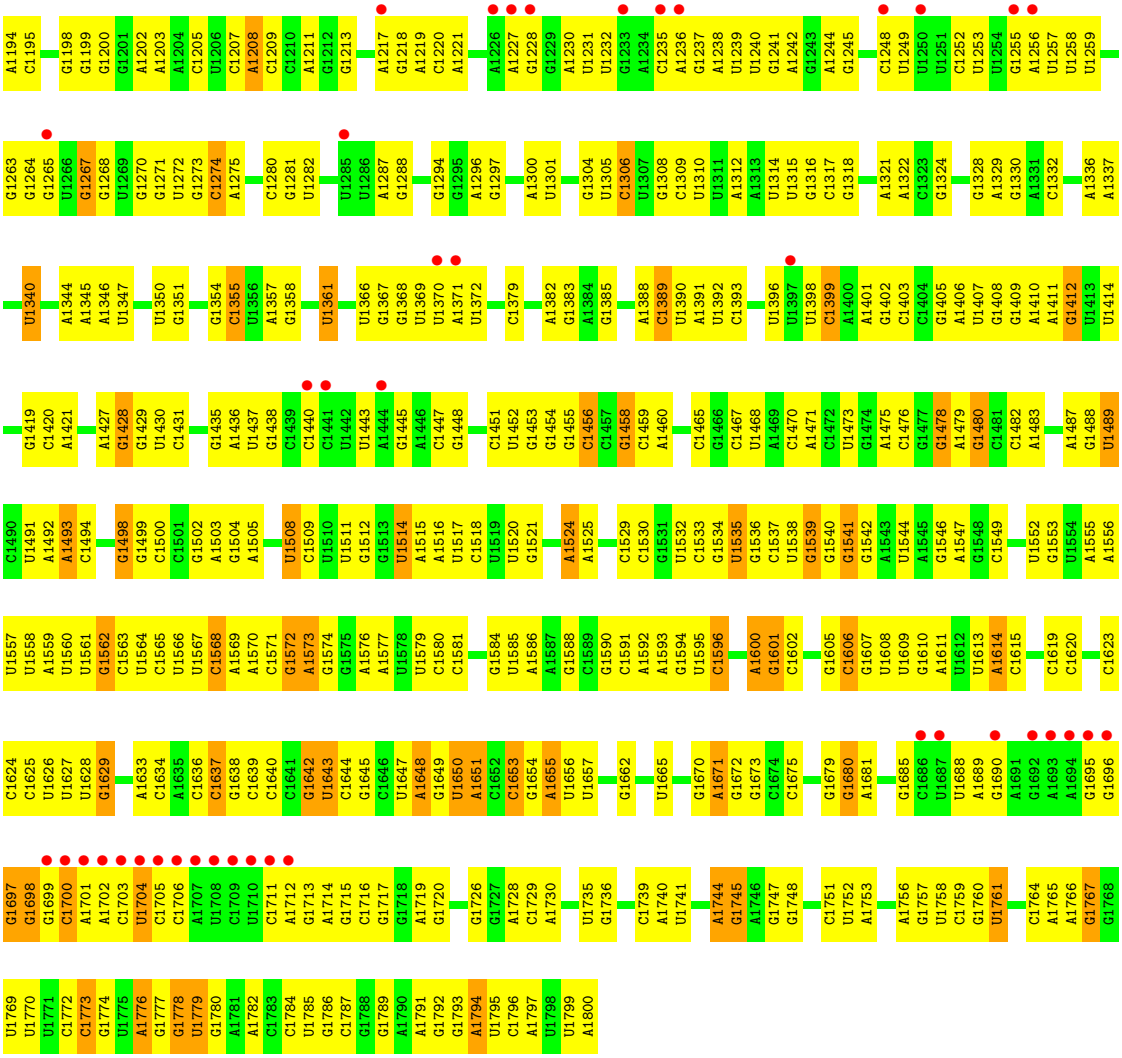




• Molecule 1: Saccharomyces cerevisiae chromosome XII cosmid 9634

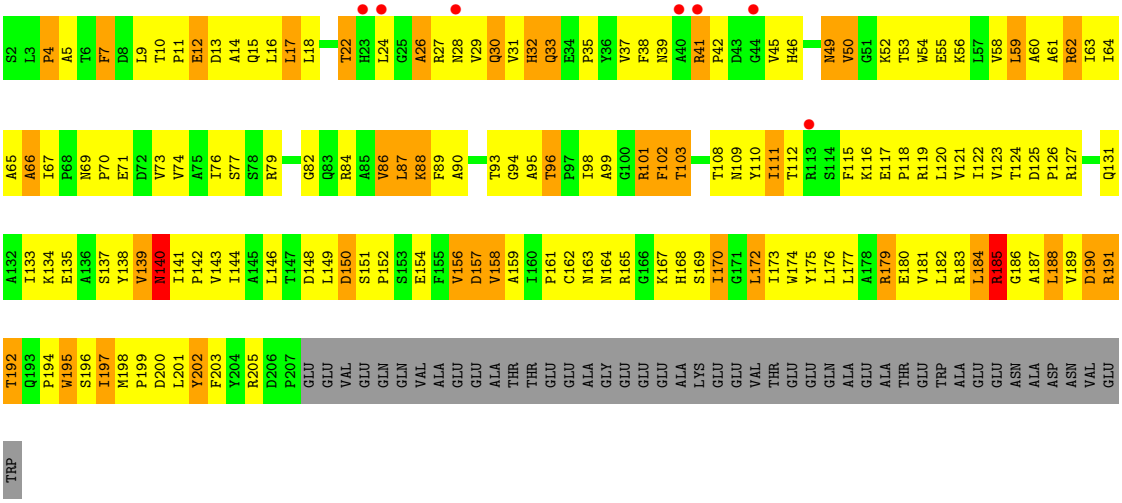
Chain 6:





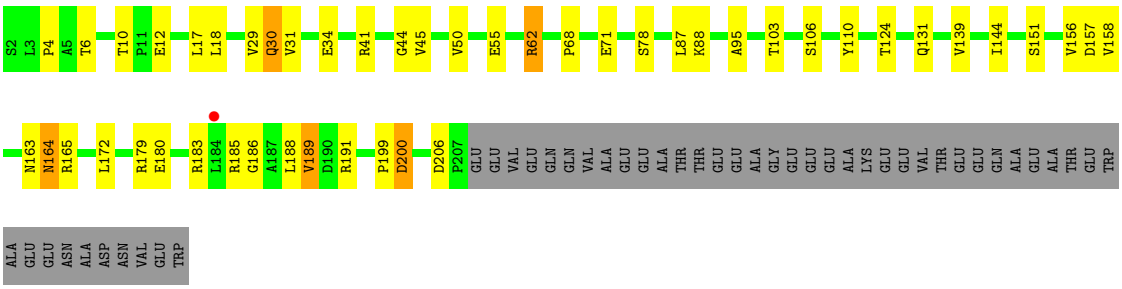
• Molecule 2: 40S ribosomal protein S0-A

Chain S0:



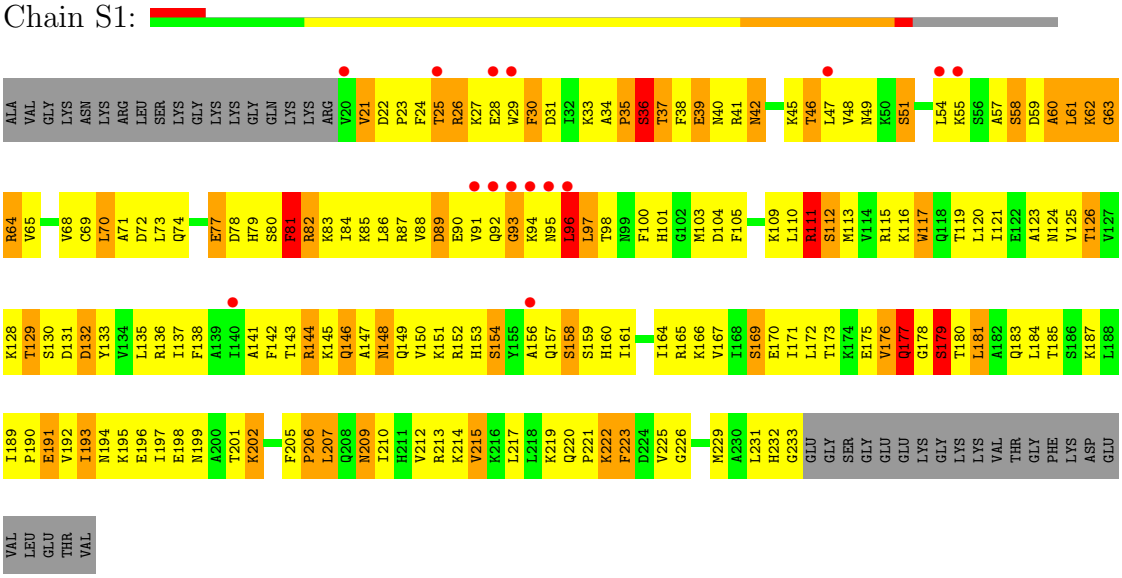
• Molecule 2: 40S ribosomal protein S0-A

Chain s0:



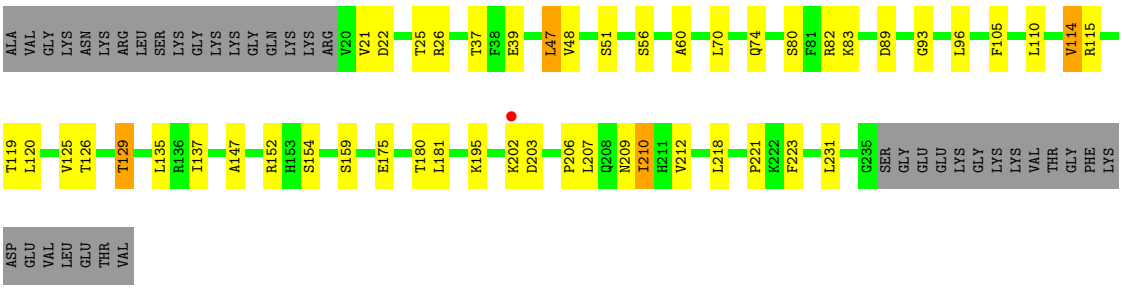
• Molecule 3: 40S ribosomal protein S1-A

Chain S1:



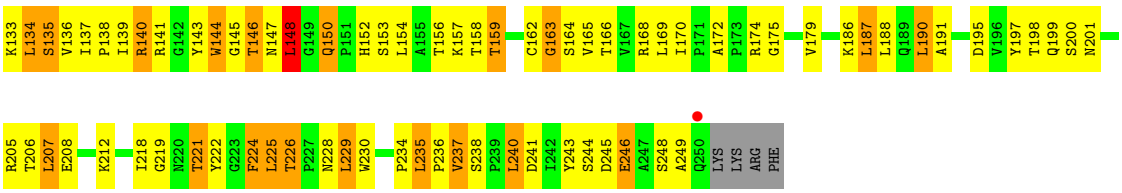
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



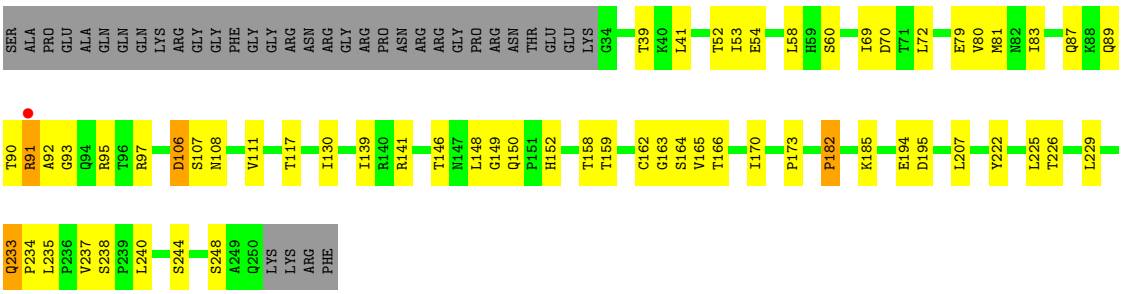
• Molecule 4: 40S ribosomal protein S2

Chain S2:



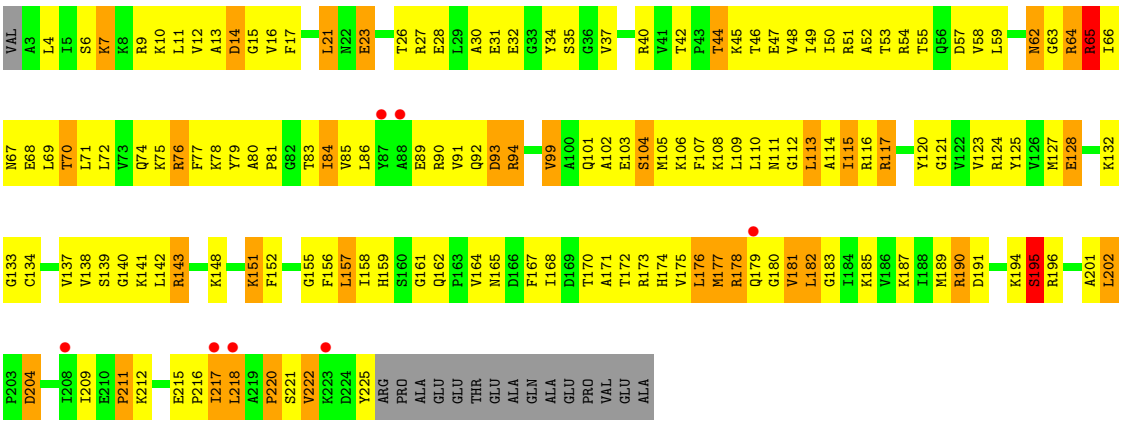
• Molecule 4: 40S ribosomal protein S2

Chain s2:



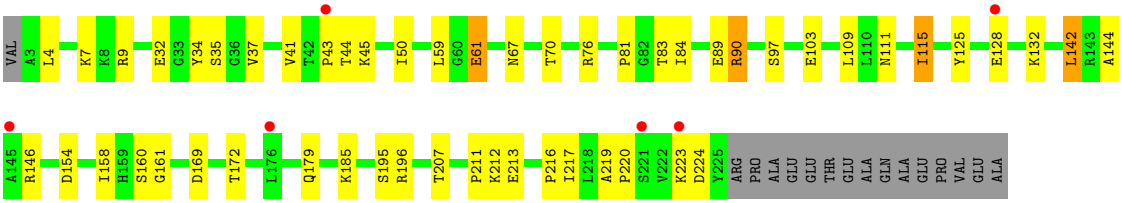
• Molecule 5: 40S ribosomal protein S3

Chain S3:



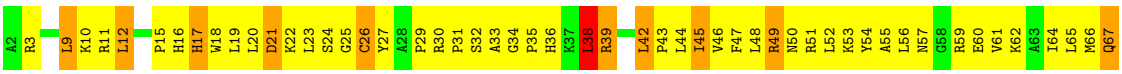
• Molecule 5: 40S ribosomal protein S3

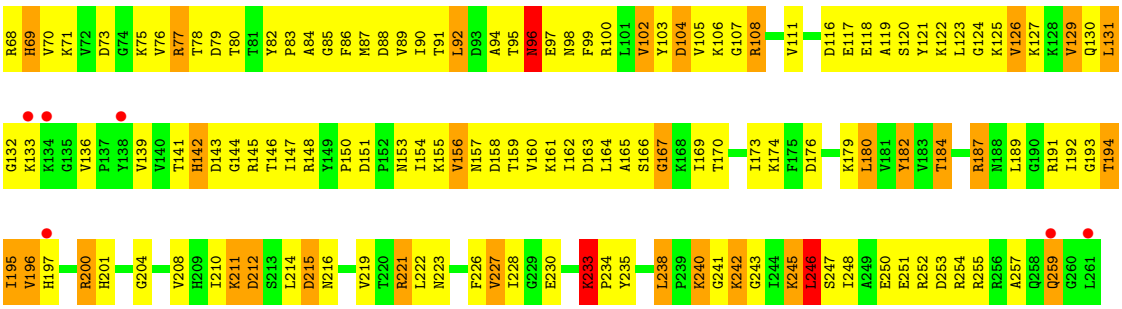
Chain s3:



• Molecule 6: 40S ribosomal protein S4-A

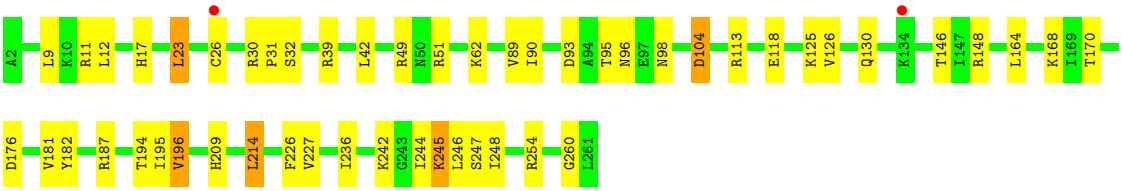
Chain S4:





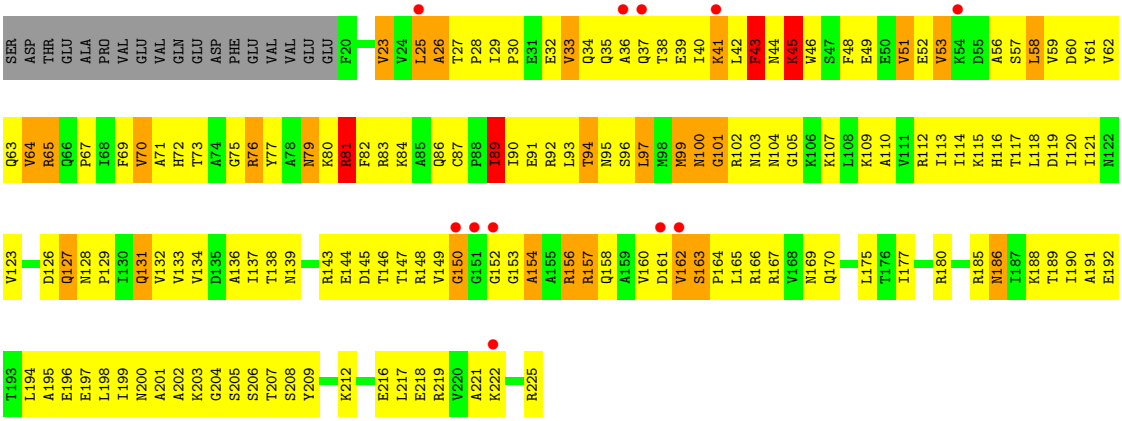
• Molecule 6: 40S ribosomal protein S4-A

Chain s4:



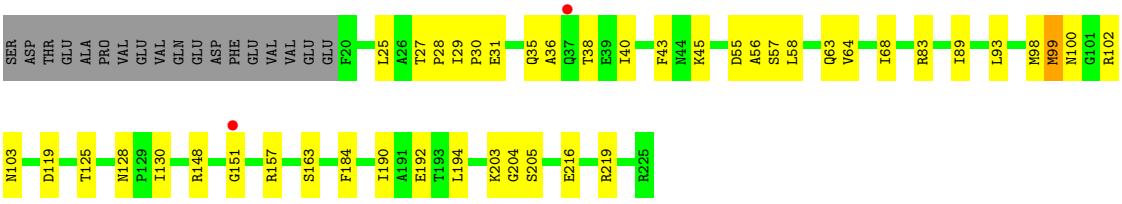
• Molecule 7: 40S ribosomal protein S5

Chain S5:



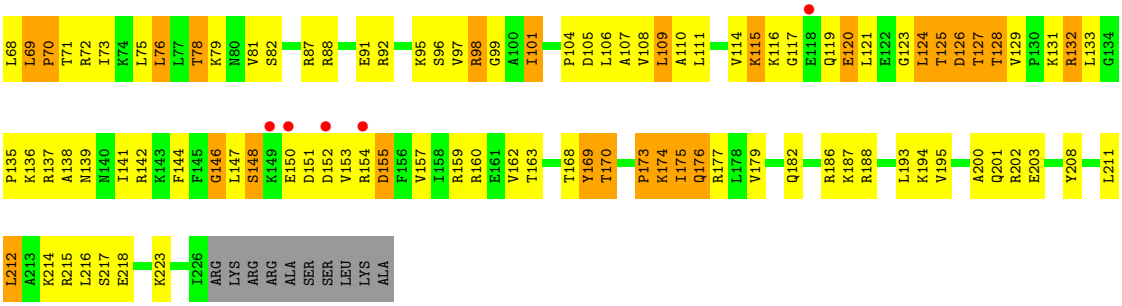
• Molecule 7: 40S ribosomal protein S5

Chain s5:



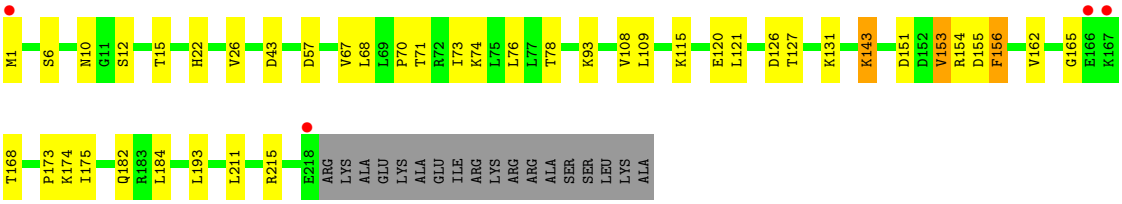
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



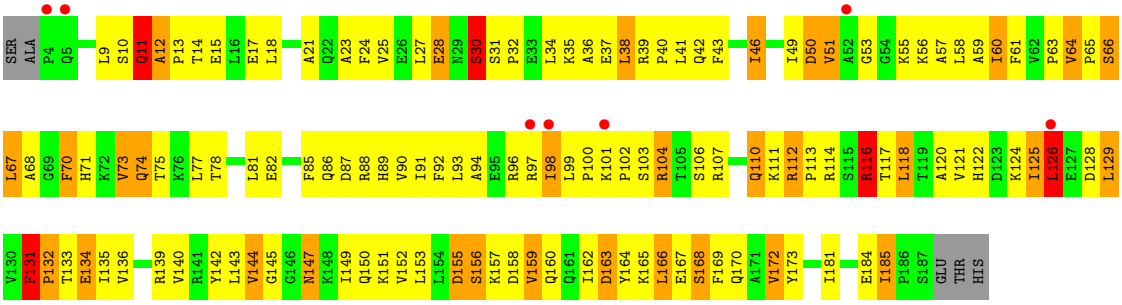
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



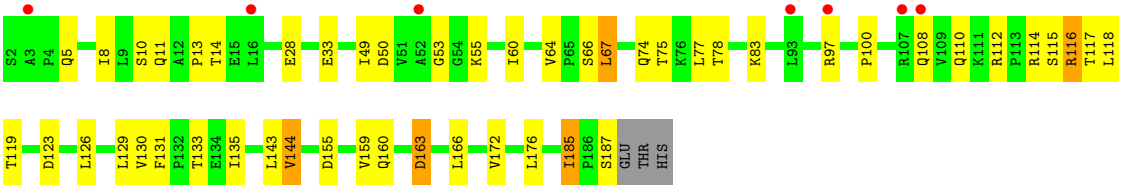
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



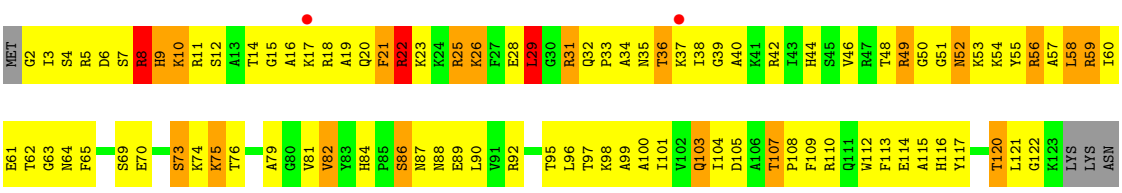
• Molecule 9: 40S ribosomal protein S7-A

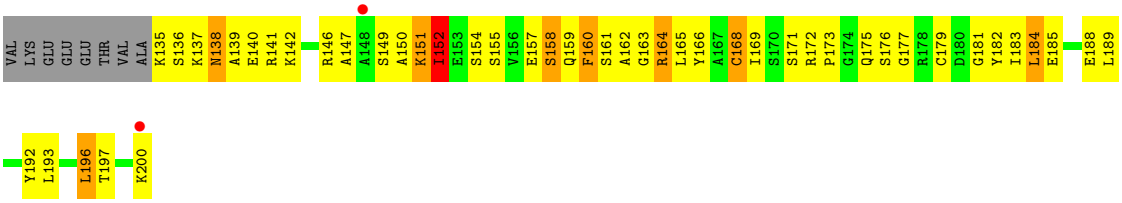
Chain s7:



• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



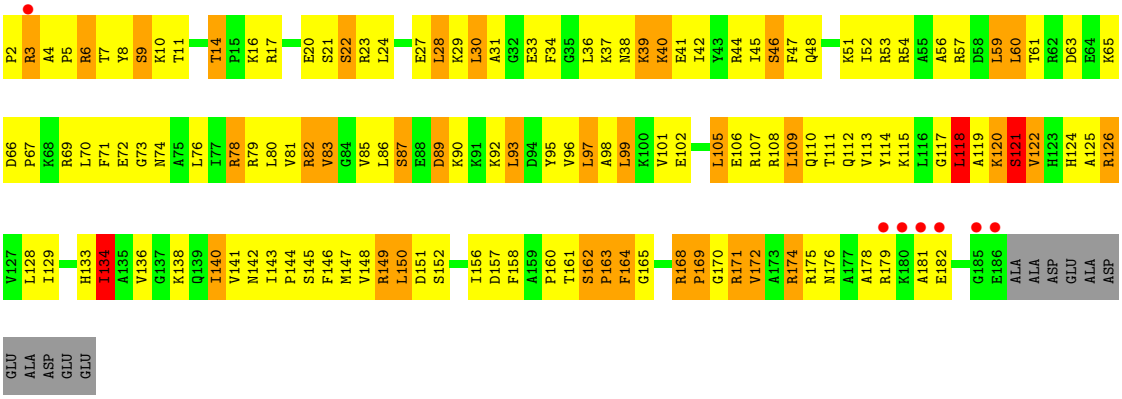


• Molecule 10: 40S ribosomal protein S8-A

Chain s8:

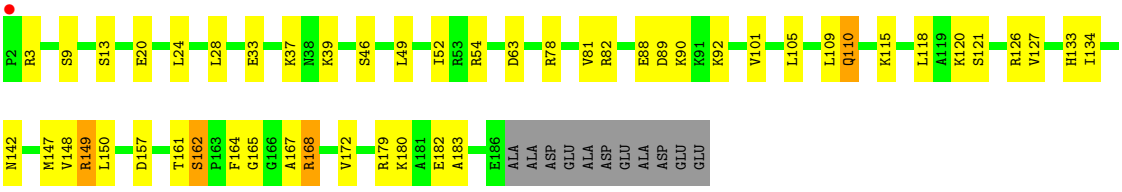
• Molecule 11: 40S ribosomal protein S9-A

Chain S9:



• Molecule 11: 40S ribosomal protein S9-A

Chain s9:

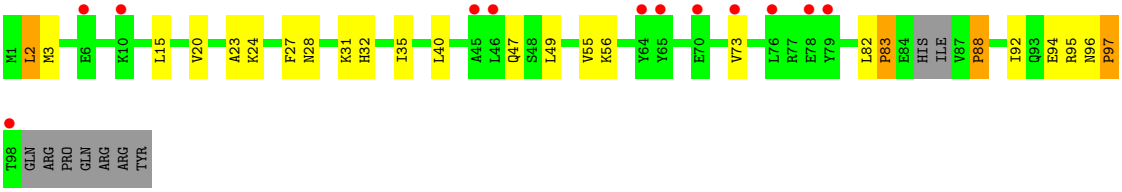


• Molecule 12: 40S ribosomal protein S10-A

Chain C0:

• Molecule 12: 40S ribosomal protein S10-A

Chain c0:

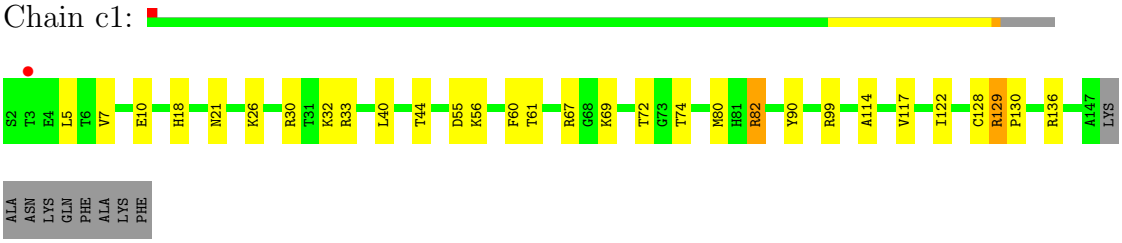


• Molecule 13: 40S ribosomal protein S11-A

Chain C1:

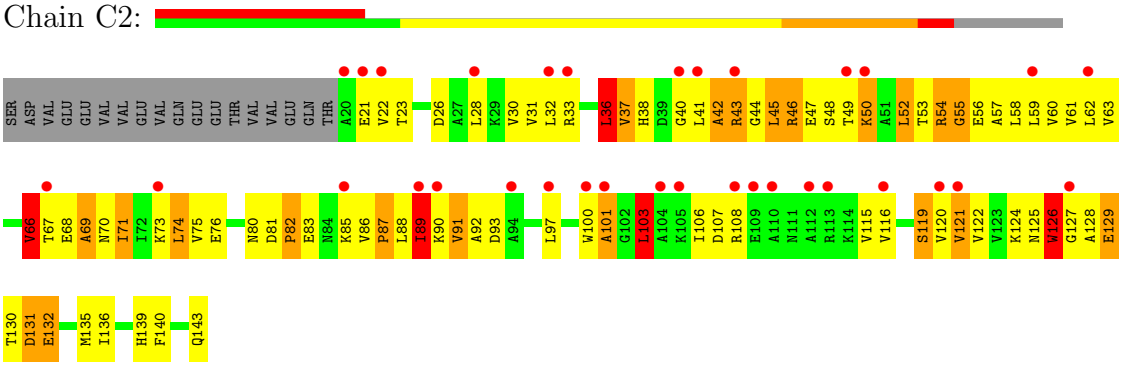
• Molecule 13: 40S ribosomal protein S11-A

Chain c1:



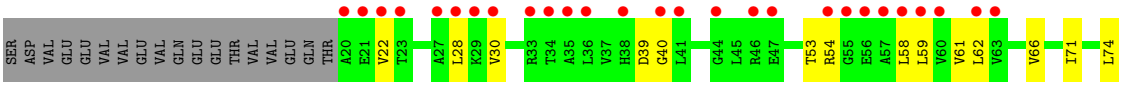
• Molecule 14: 40S ribosomal protein S12

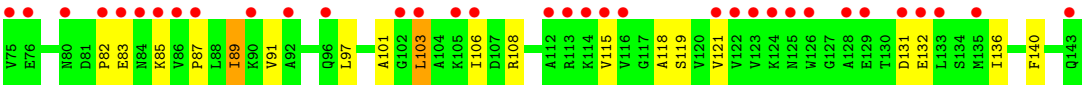
Chain C2:



• Molecule 14: 40S ribosomal protein S12

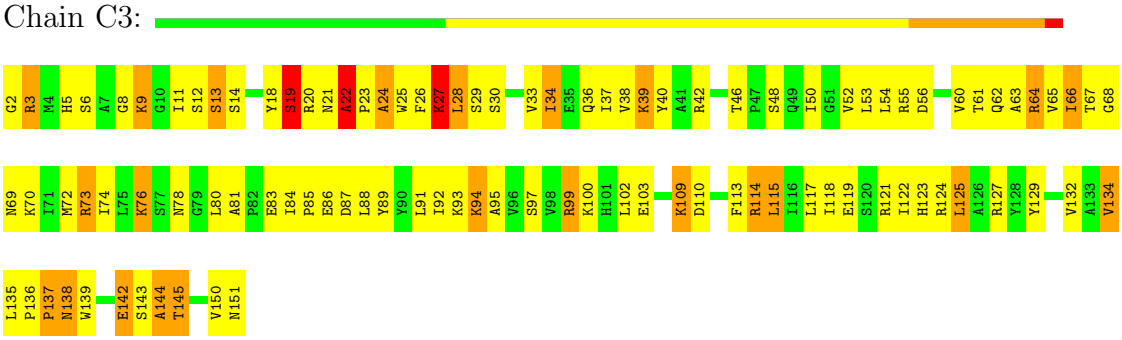
Chain c2:





• Molecule 15: 40S ribosomal protein S13

Chain C3:

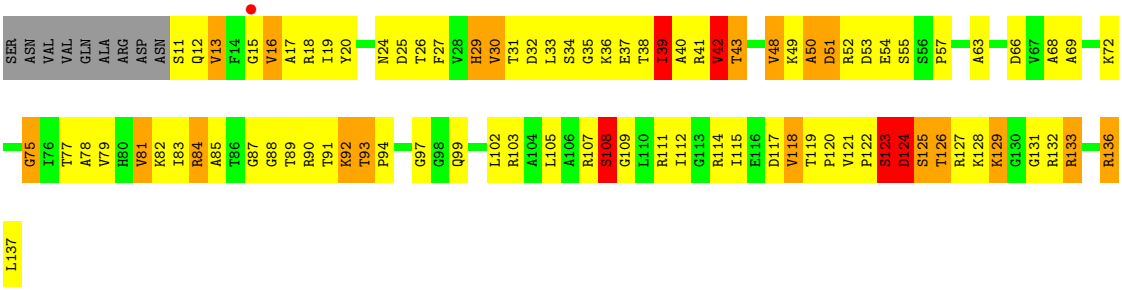


• Molecule 15: 40S ribosomal protein S13

Chain c3:

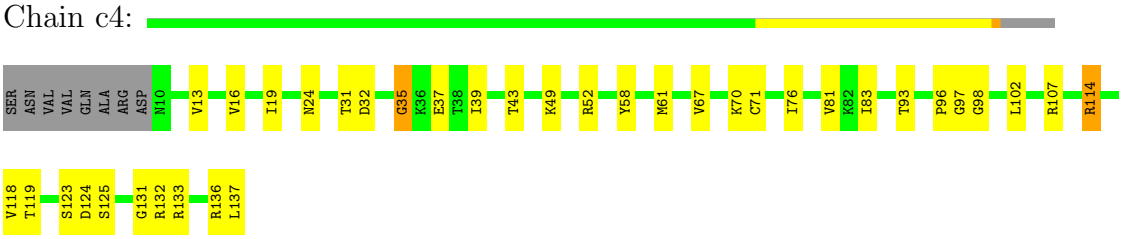
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



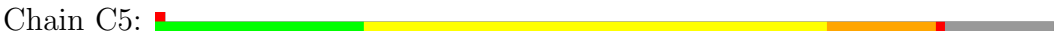
• Molecule 16: 40S ribosomal protein S14-A

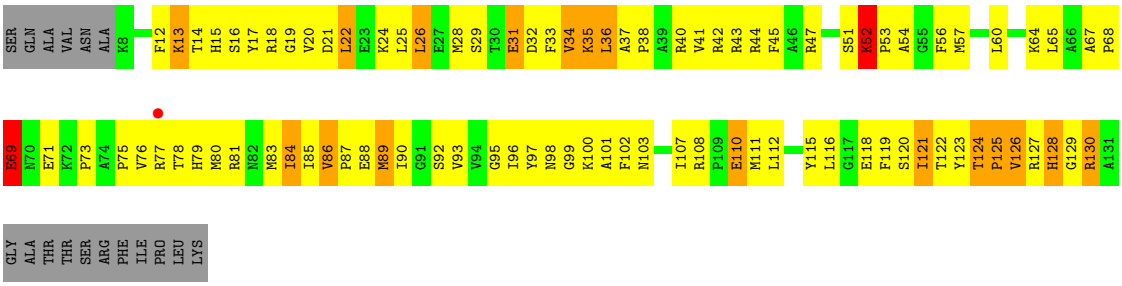
Chain c4:



• Molecule 17: 40S ribosomal protein S15

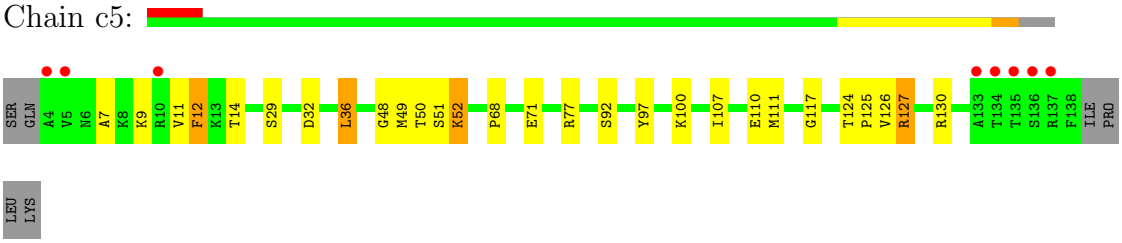
Chain C5:





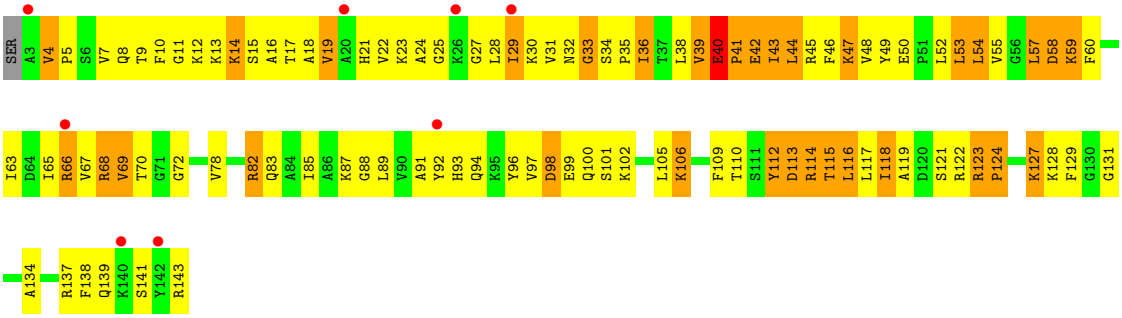
• Molecule 17: 40S ribosomal protein S15

Chain c5:



• Molecule 18: 40S ribosomal protein S16-A

Chain C6:

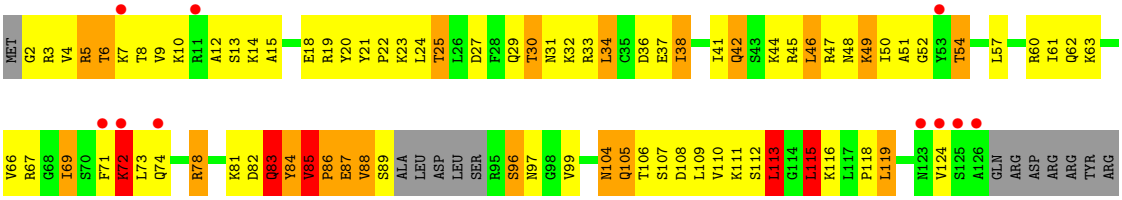


• Molecule 18: 40S ribosomal protein S16-A

Chain c6:

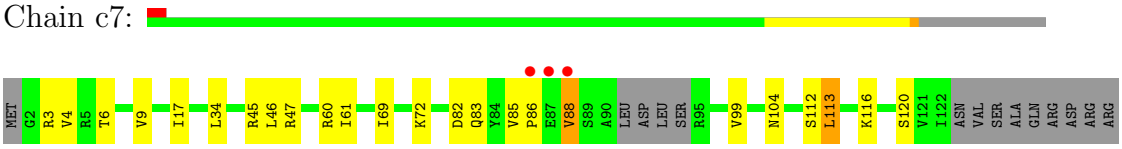
• Molecule 19: 40S ribosomal protein S17-A

Chain C7:



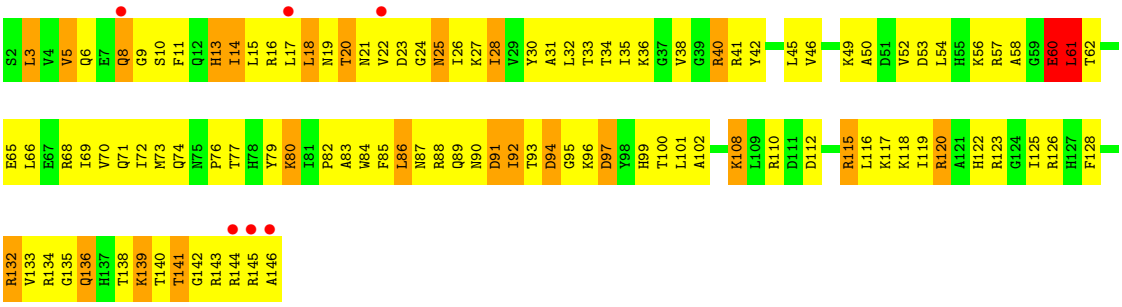
• Molecule 19: 40S ribosomal protein S17-A

Chain c7:



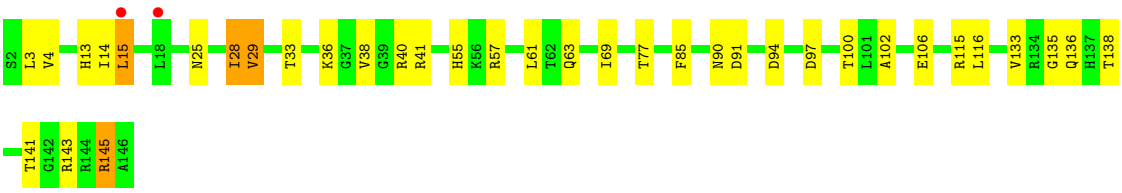
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



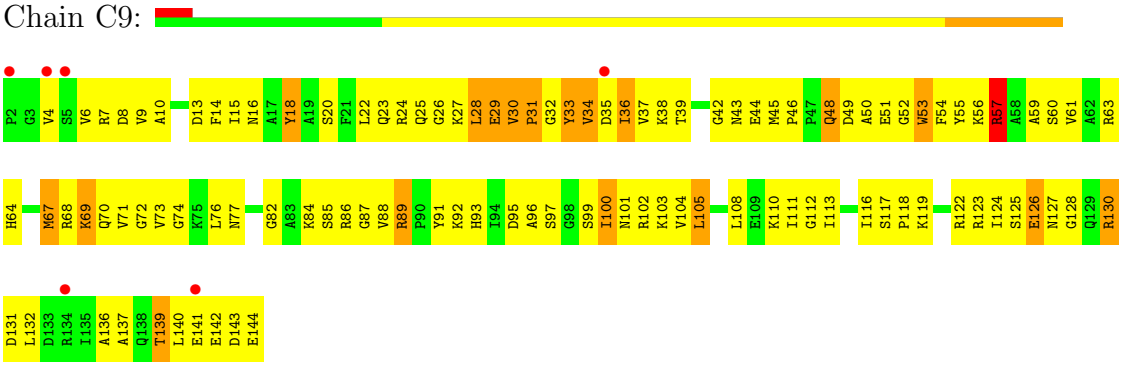
• Molecule 20: 40S ribosomal protein S18-A

Chain c8:



• Molecule 21: 40S ribosomal protein S19-A

Chain C9:

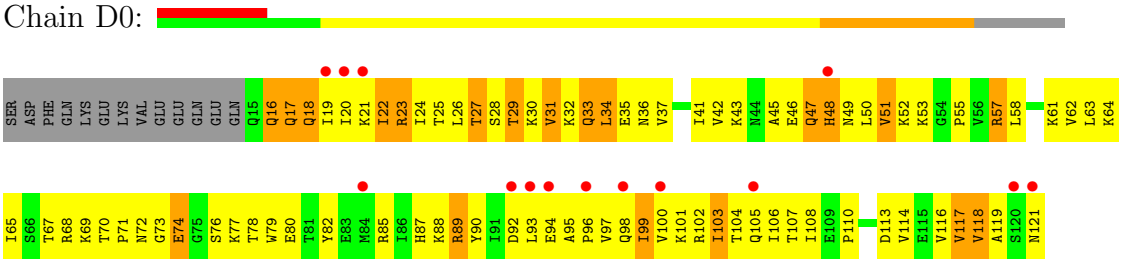


• Molecule 21: 40S ribosomal protein S19-A

Chain c9:

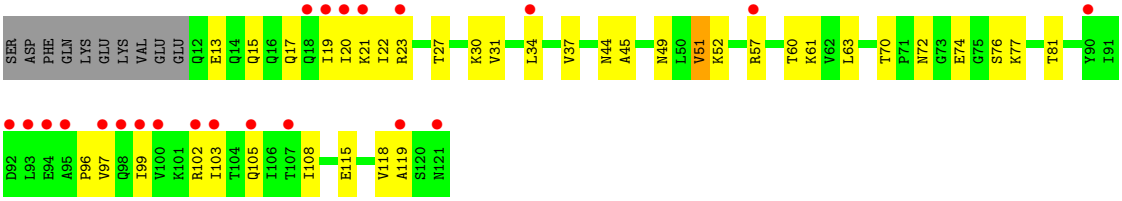
• Molecule 22: 40S ribosomal protein S20

Chain D0:



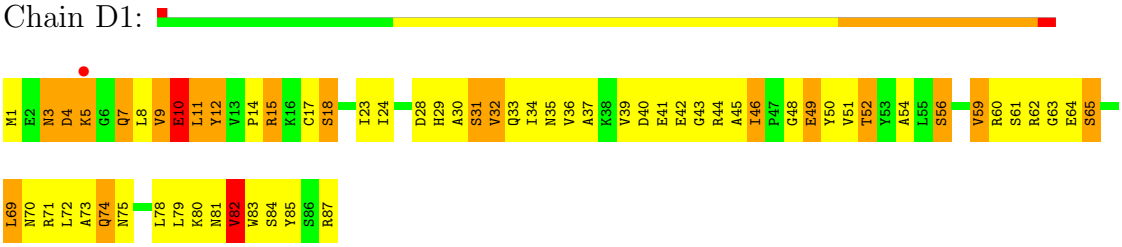
• Molecule 22: 40S ribosomal protein S20

Chain d0:



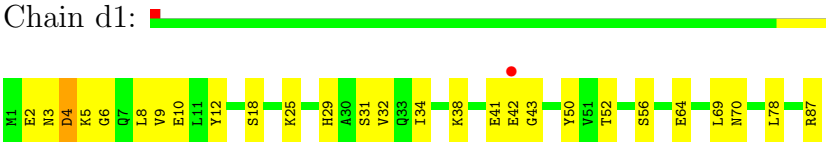
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



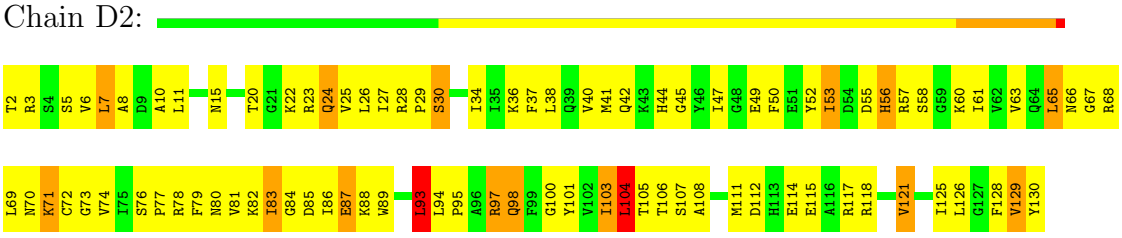
• Molecule 23: 40S ribosomal protein S21-A

Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

Chain D2:

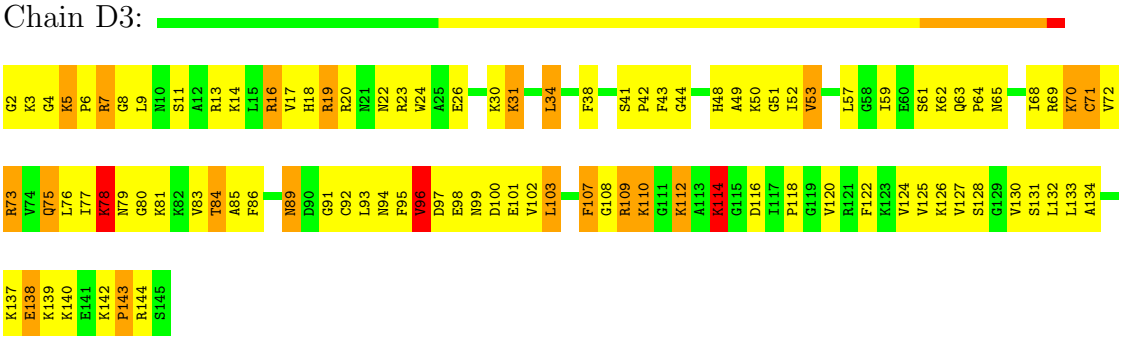


• Molecule 24: 40S ribosomal protein S22-A

Chain d2:

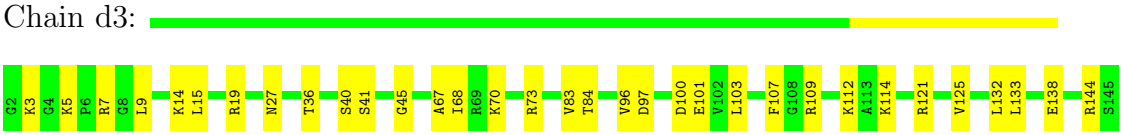
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



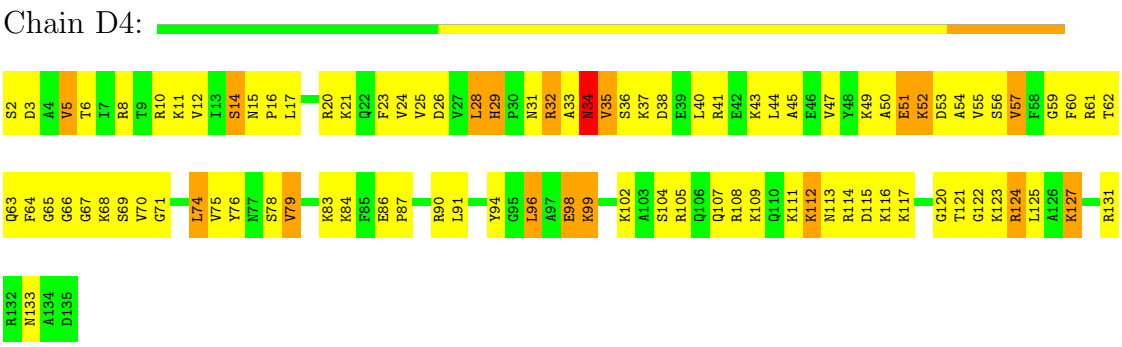
• Molecule 25: 40S ribosomal protein S23-A

Chain d3:



• Molecule 26: 40S ribosomal protein S24-A

Chain D4:

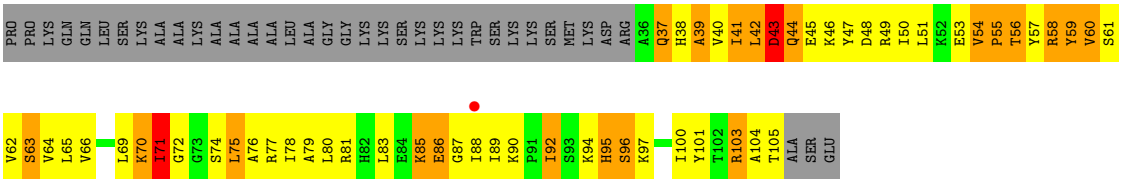


• Molecule 26: 40S ribosomal protein S24-A

Chain d4:

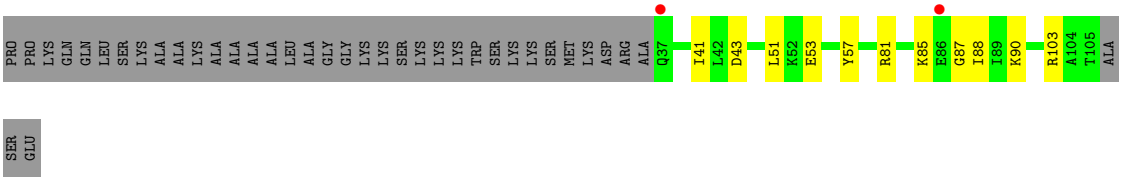
• Molecule 27: 40S ribosomal protein S25-A

Chain D5:



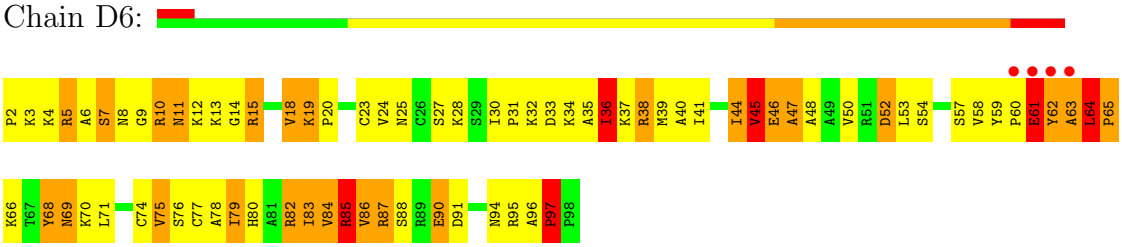
• Molecule 27: 40S ribosomal protein S25-A

Chain d5:



• Molecule 28: 40S ribosomal protein S26-B

Chain D6:

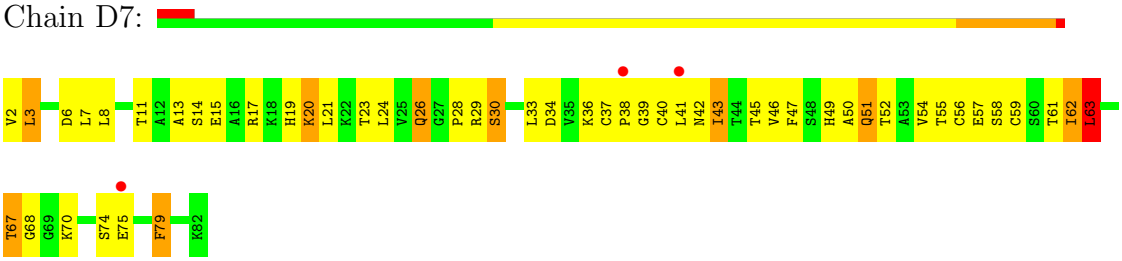


• Molecule 28: 40S ribosomal protein S26-B

Chain d6:

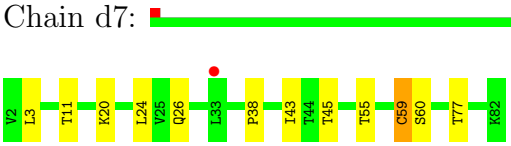
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



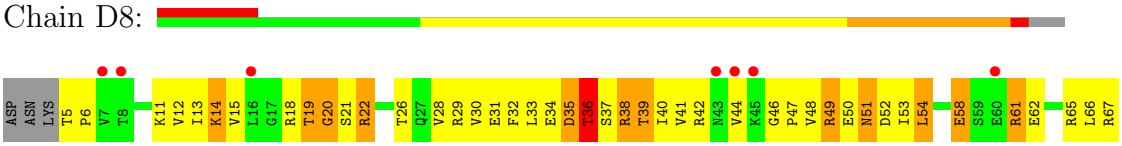
• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



• Molecule 30: 40S ribosomal protein S28-A

Chain D8:

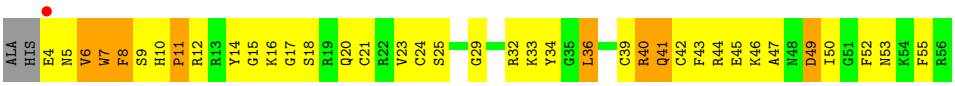


• Molecule 30: 40S ribosomal protein S28-A

Chain d8:

• Molecule 31: 40S ribosomal protein S29-A

Chain D9:

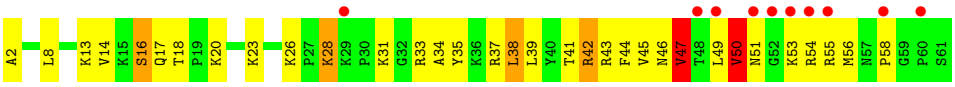


• Molecule 31: 40S ribosomal protein S29-A

Chain d9:

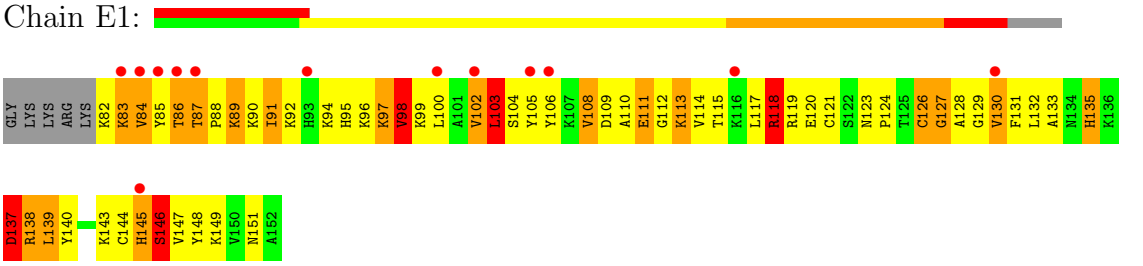
• Molecule 32: 40S ribosomal protein S30-A

Chain E0:



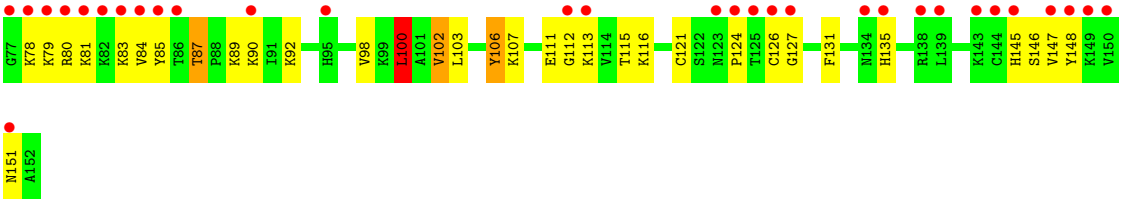
• Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



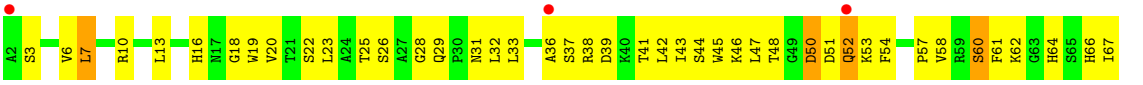
• Molecule 33: Ubiquitin-40S ribosomal protein S31

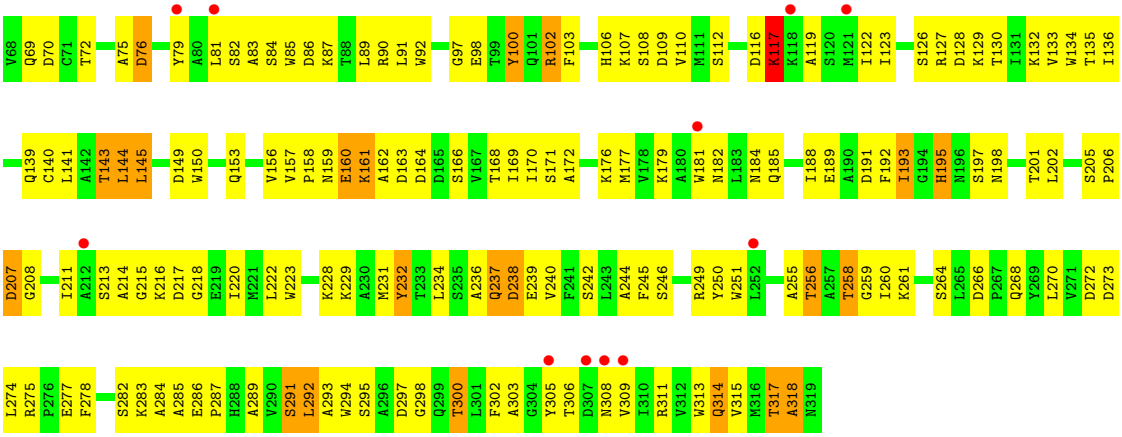
Chain e1:



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

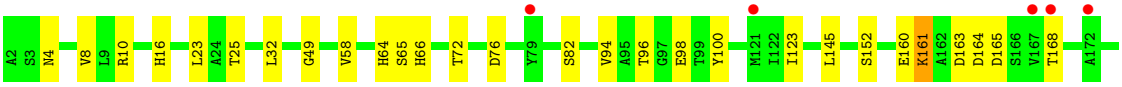
Chain SR:





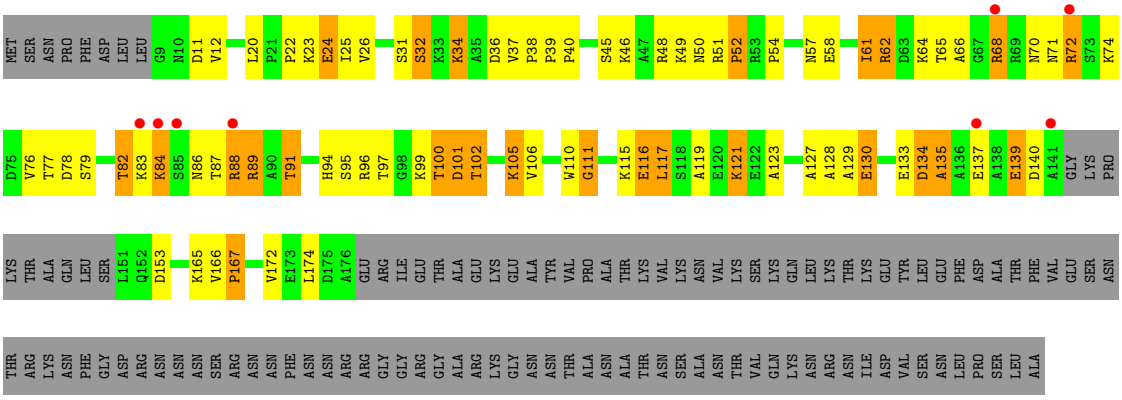
• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain sR:



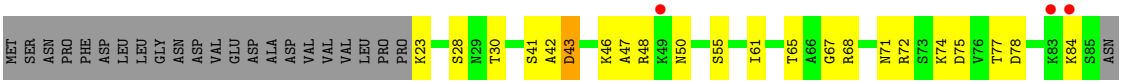
• Molecule 35: Suppressor protein STM1

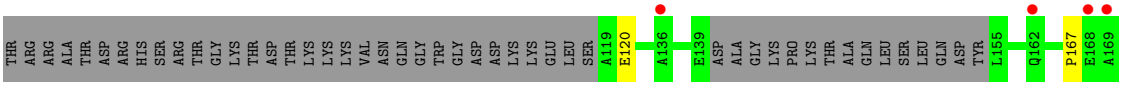
Chain SM:

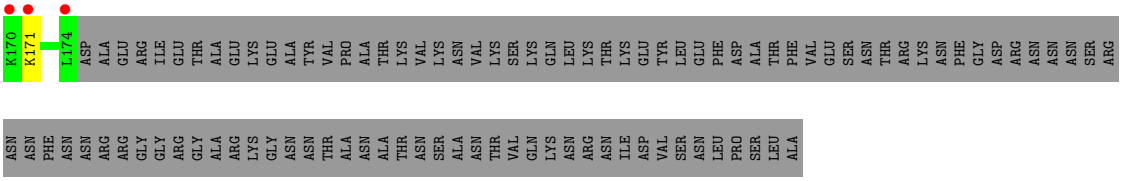


• Molecule 35: Suppressor protein STM1

Chain sM:

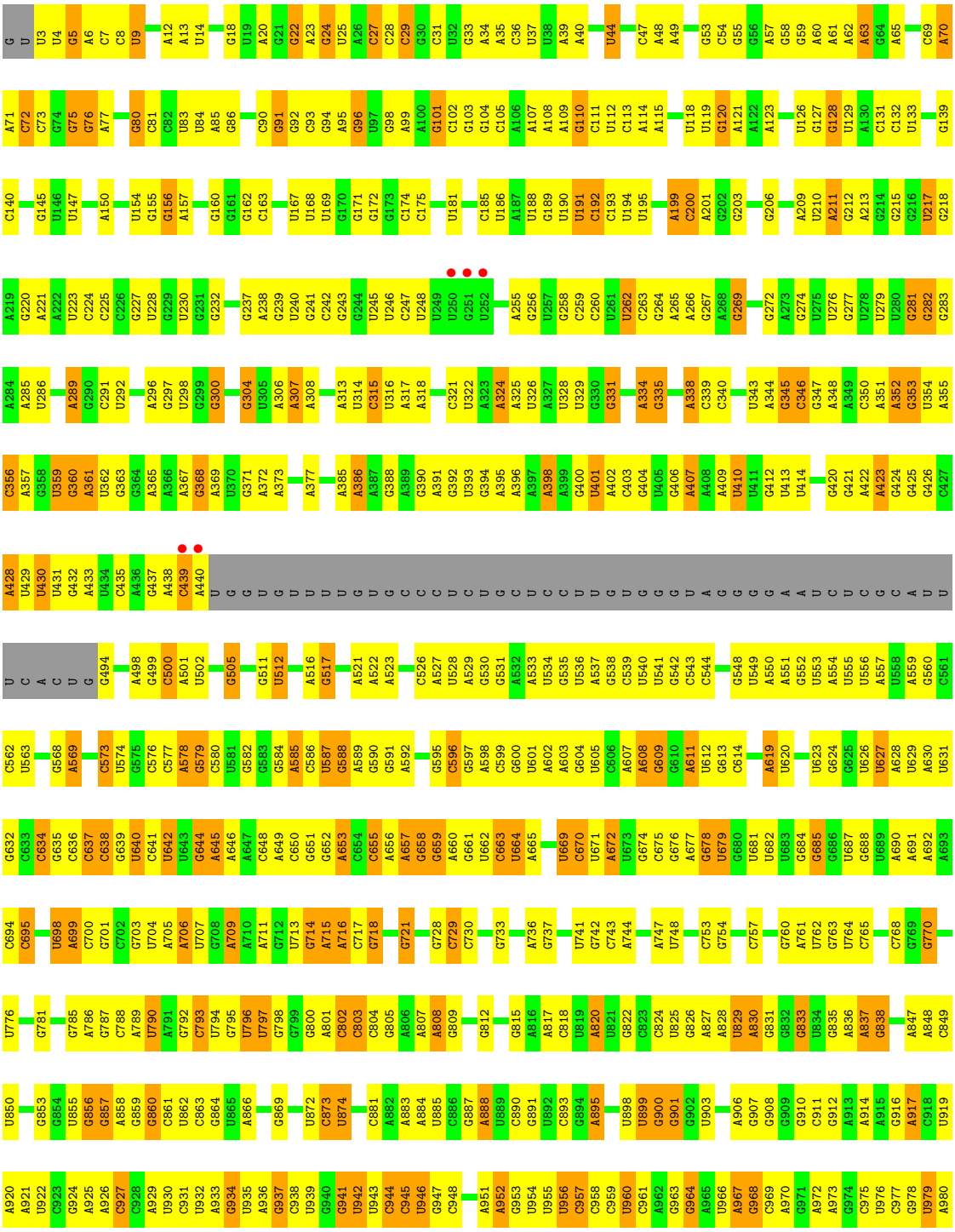


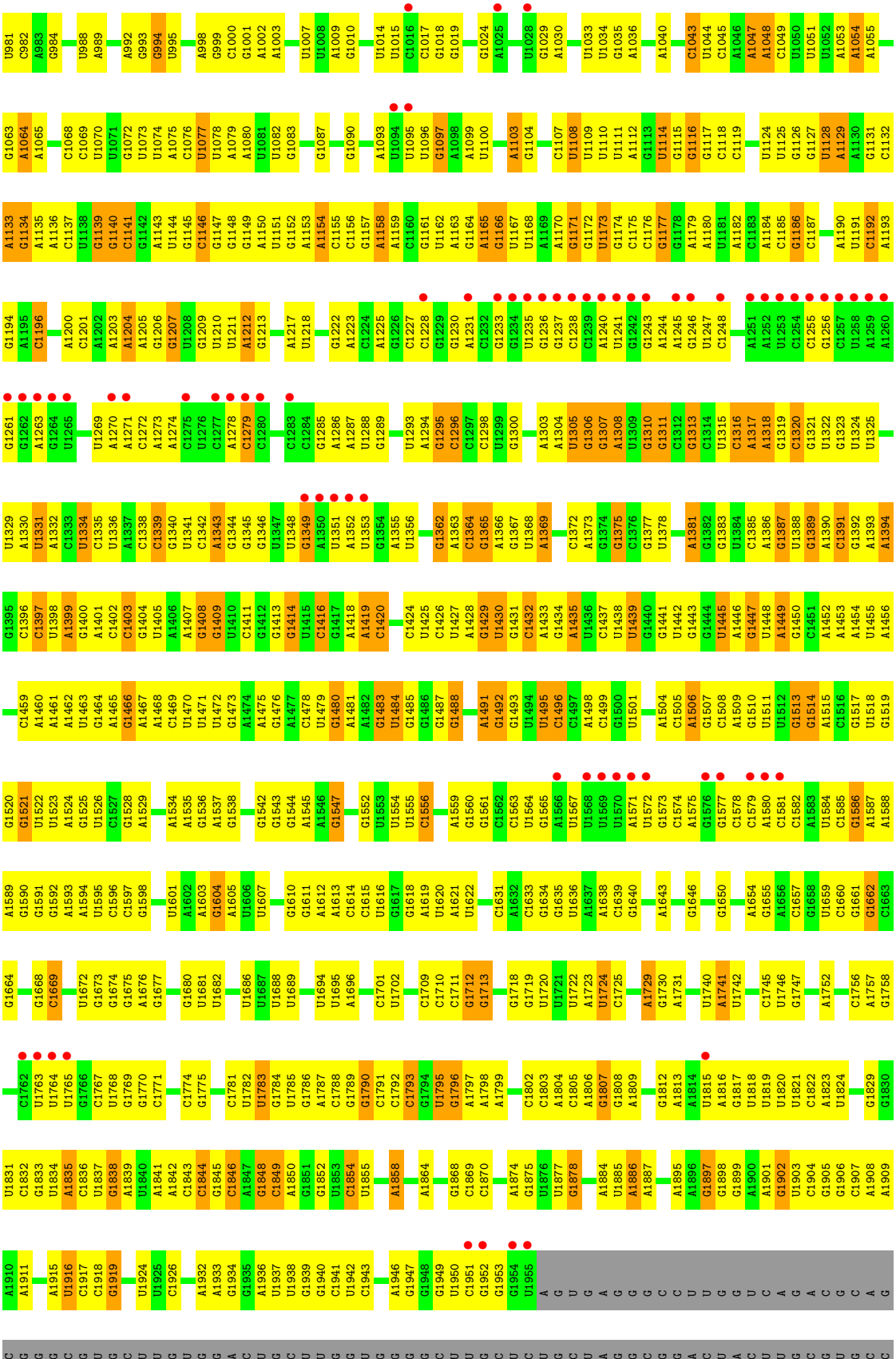


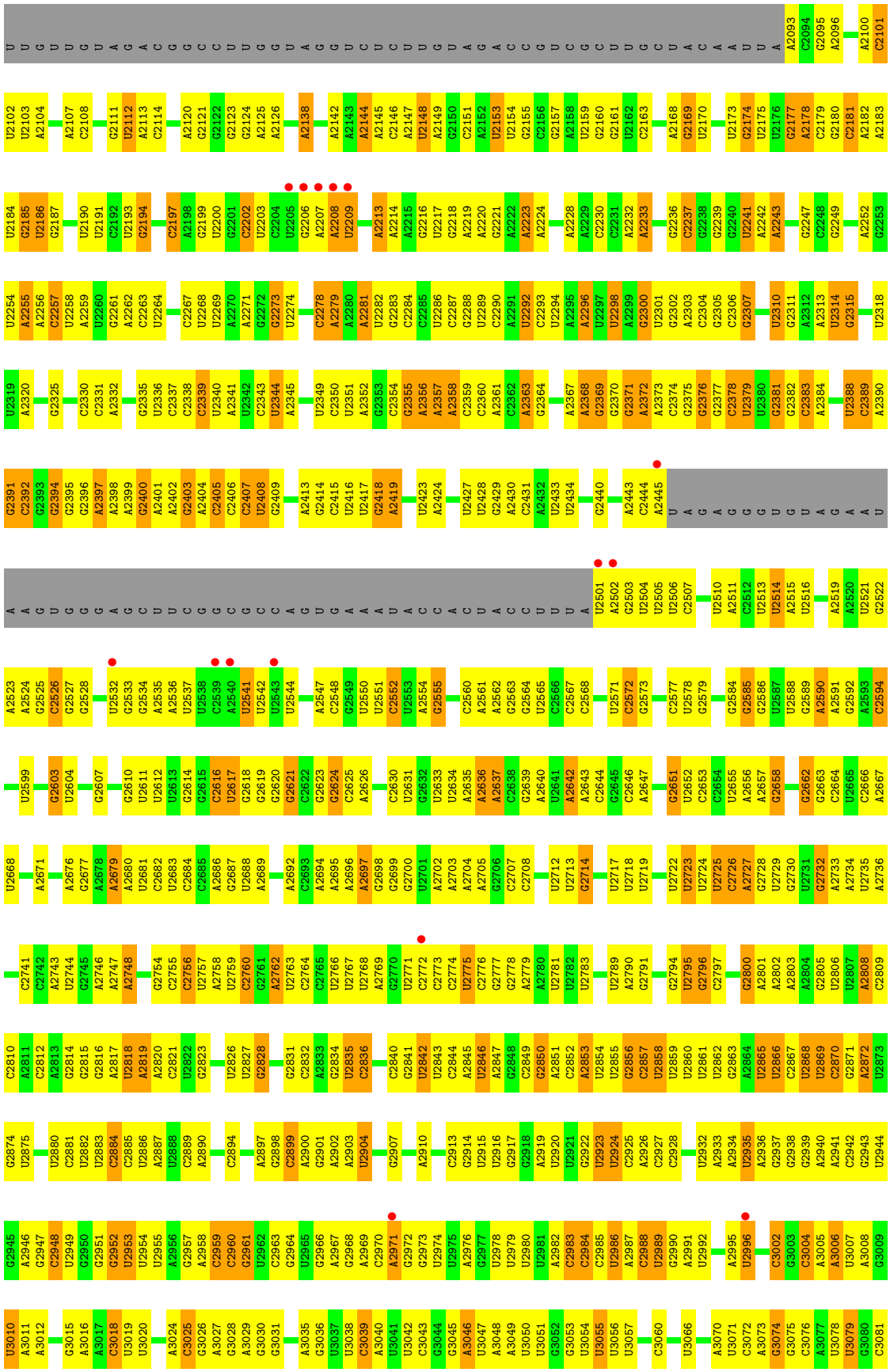


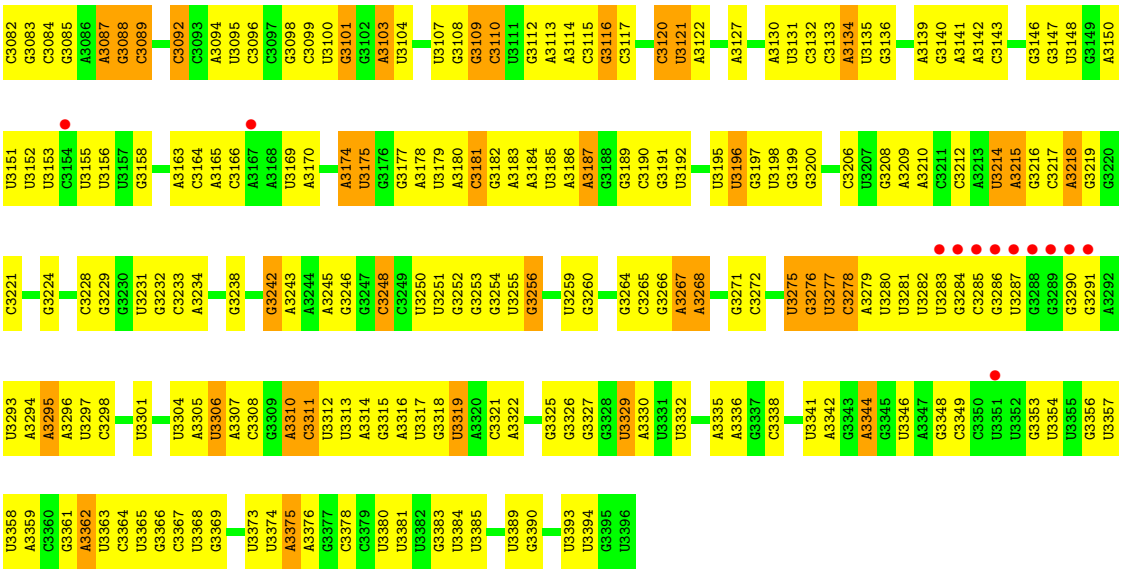
• Molecule 36: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 1:



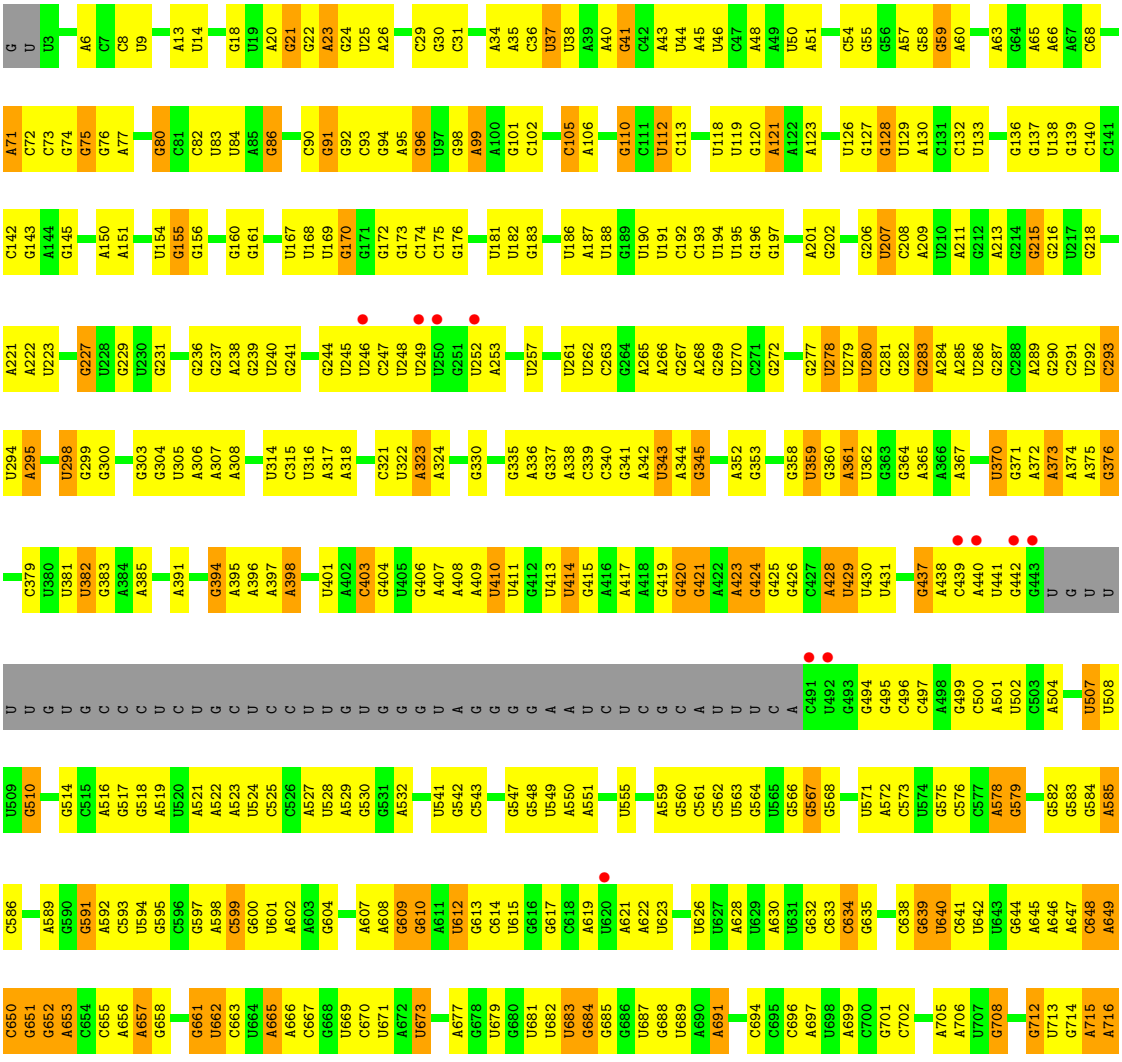


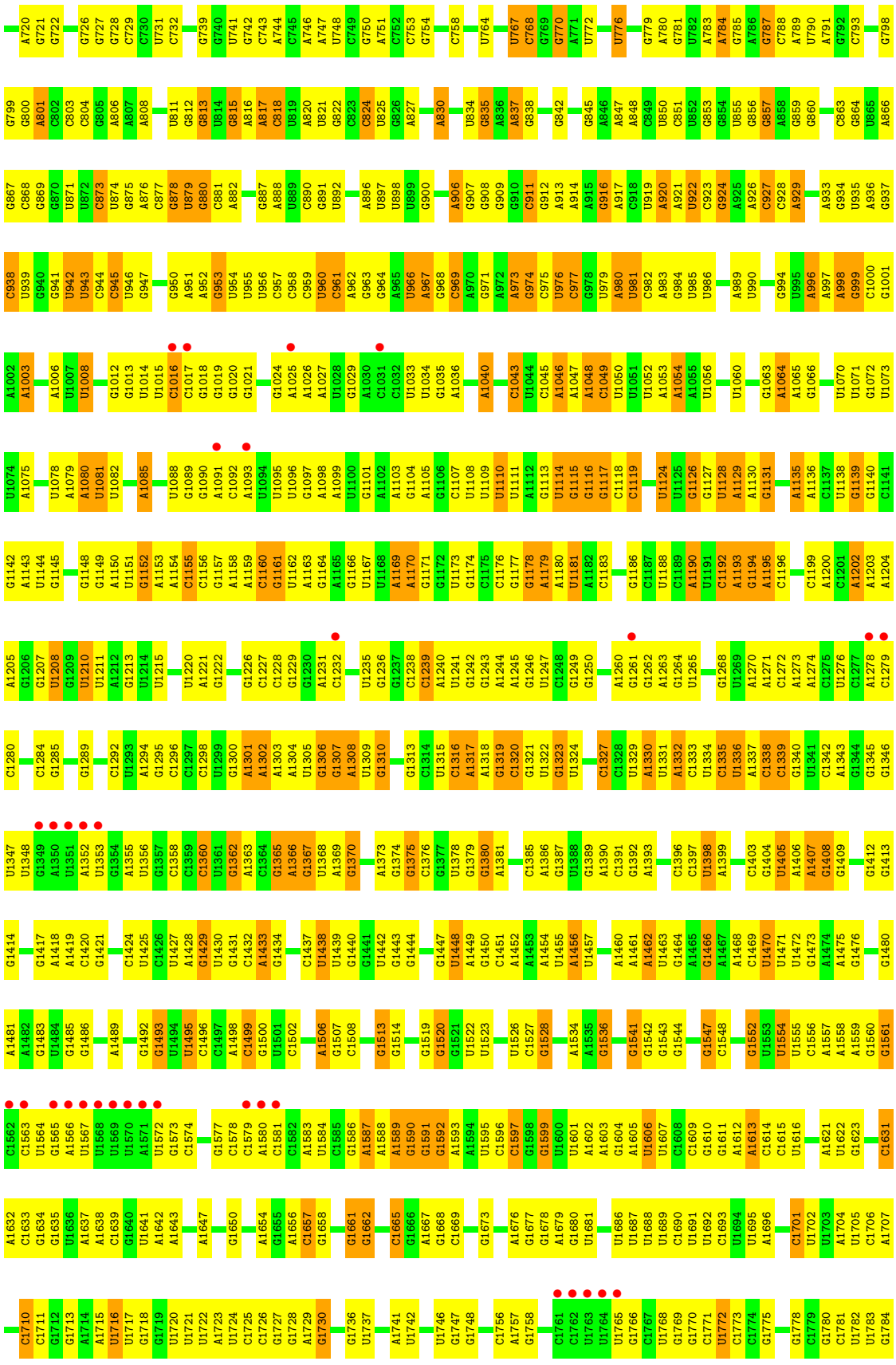


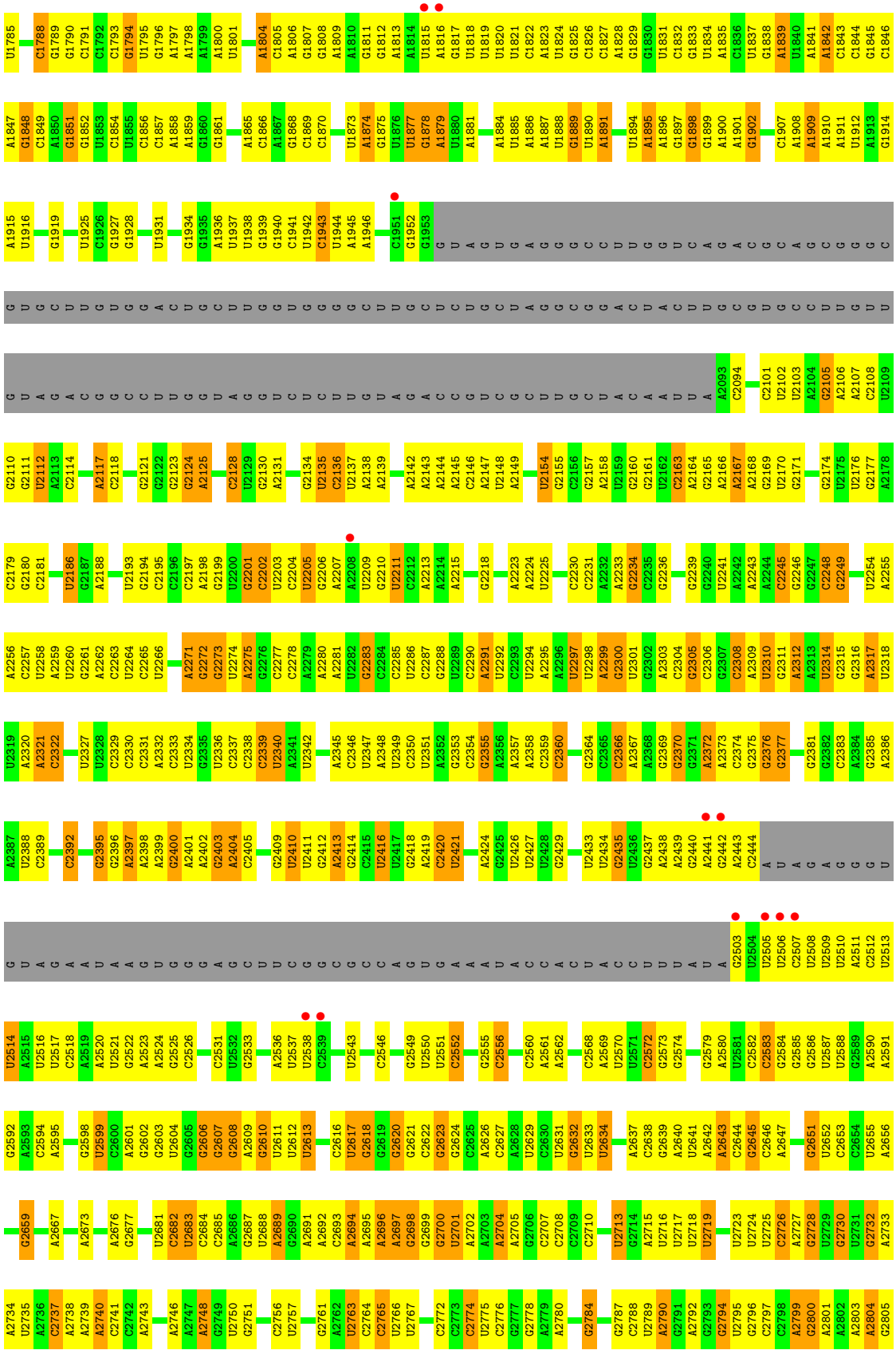


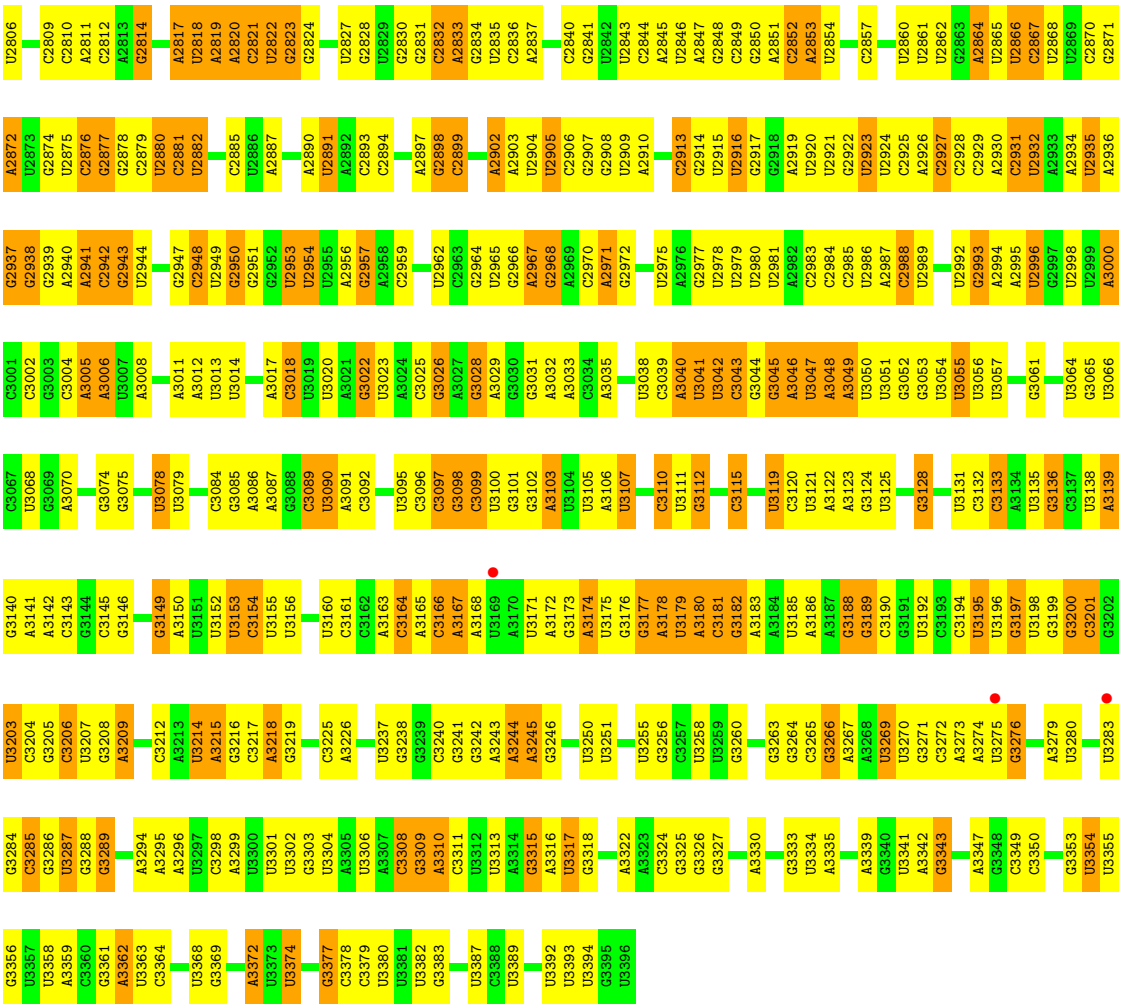
• Molecule 36: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 5:



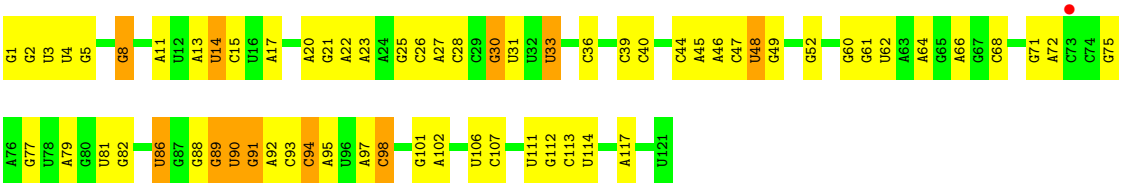






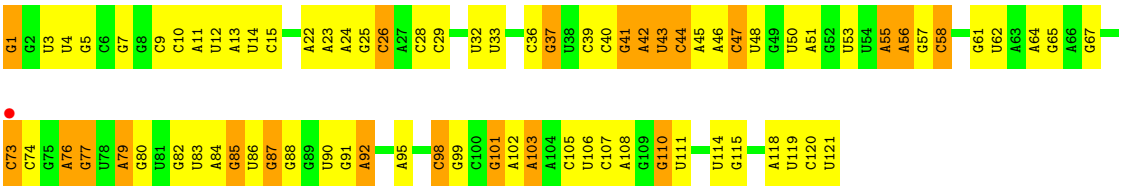
• Molecule 37: TPA_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

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

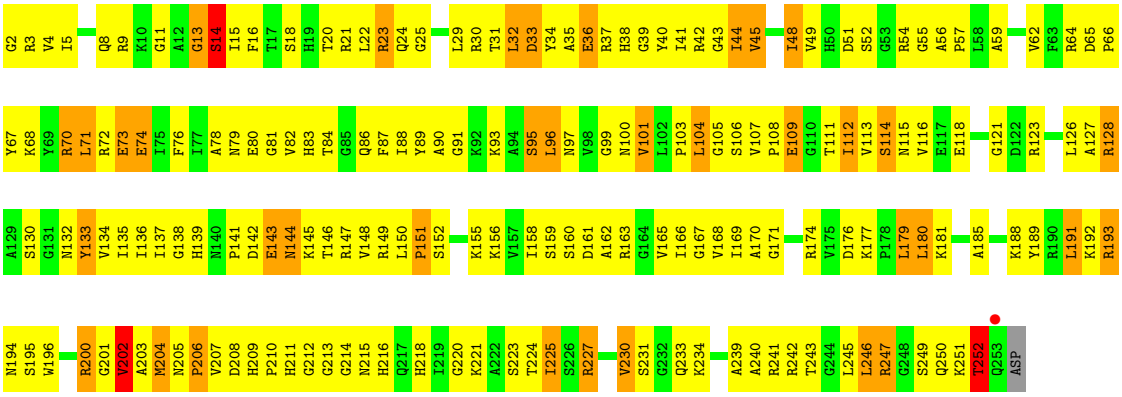
Chain 4:

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

Chain 8:

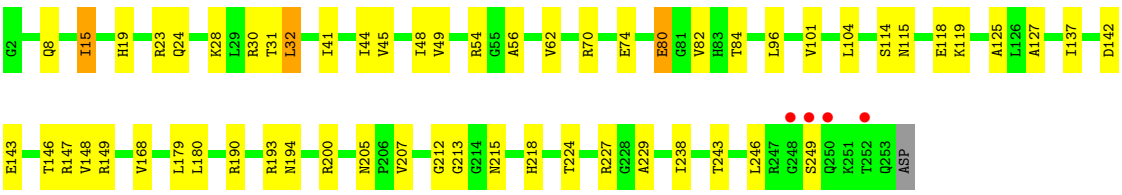
• Molecule 39: 60S ribosomal protein L2-A

Chain L2:



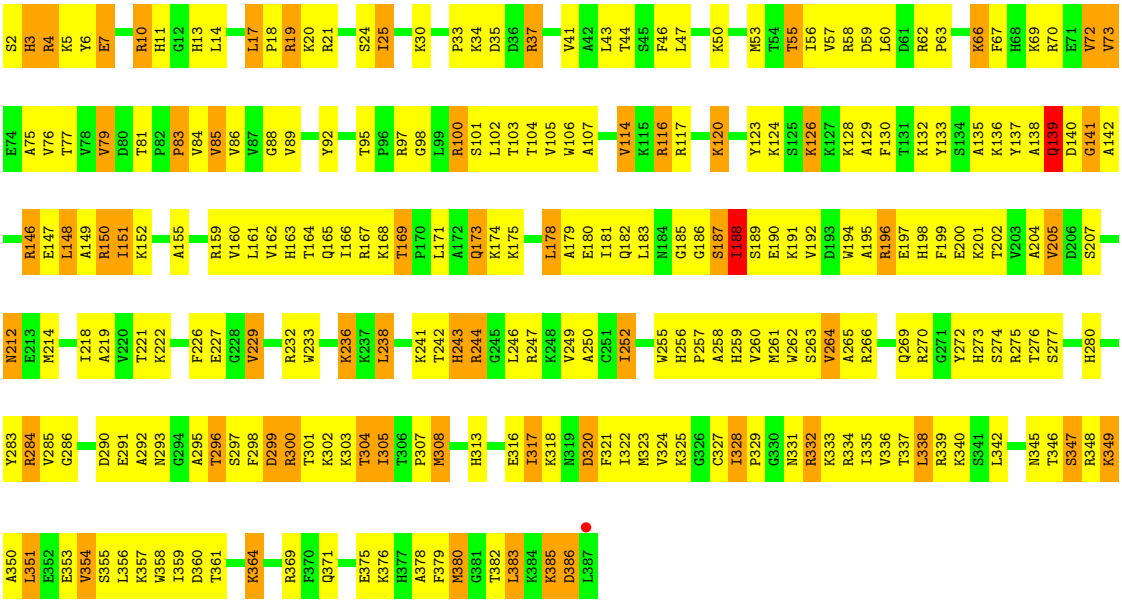
• Molecule 39: 60S ribosomal protein L2-A

Chain l2:



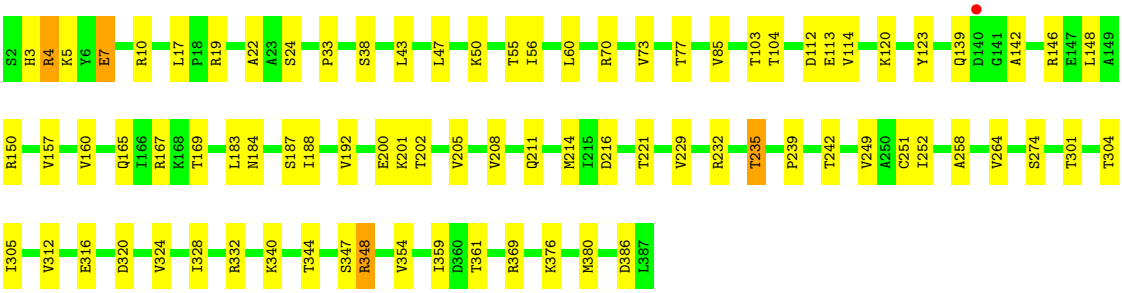
• Molecule 40: 60S ribosomal protein L3

Chain L3:



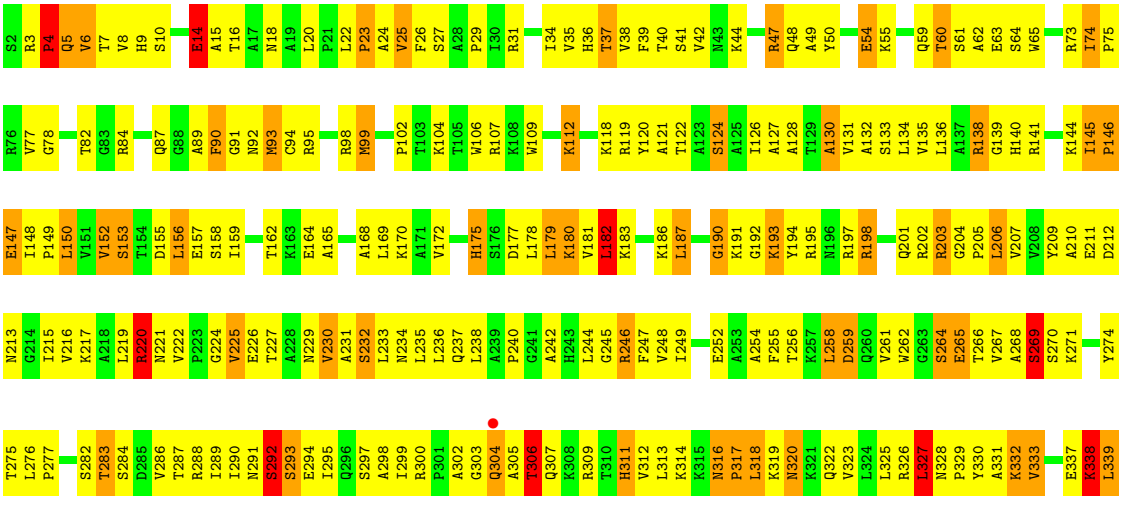
• Molecule 40: 60S ribosomal protein L3

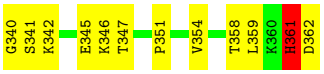
Chain l3:



• Molecule 41: 60S ribosomal protein L4-A

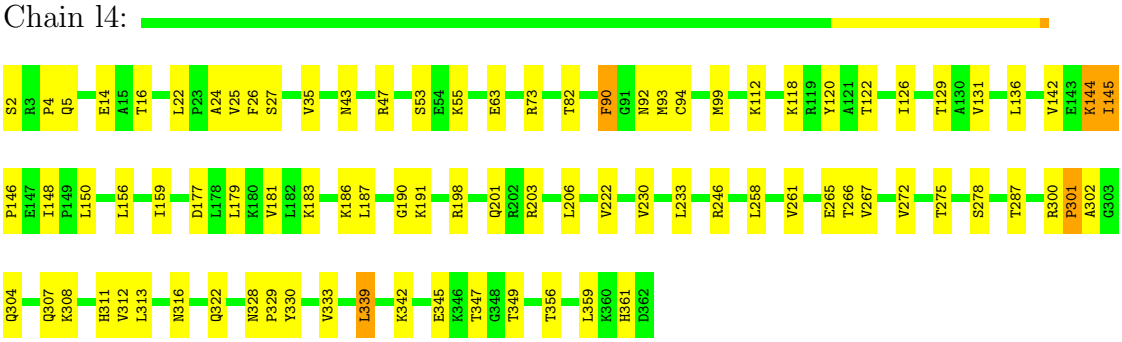
Chain L4:





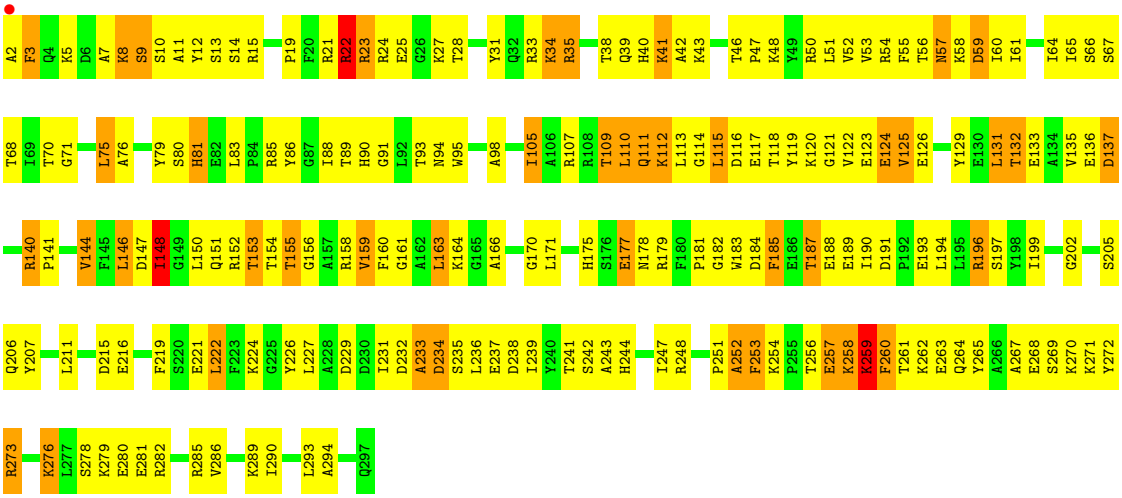
• Molecule 41: 60S ribosomal protein L4-A

Chain l4:



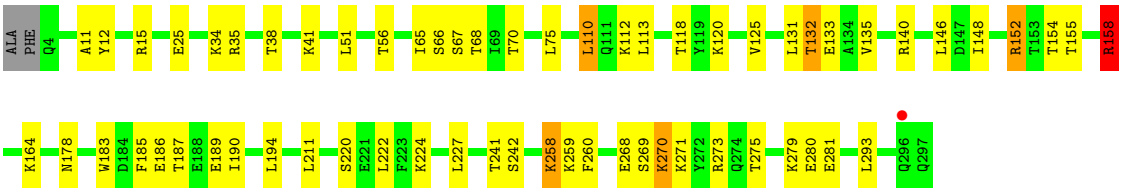
• Molecule 42: 60S ribosomal protein L5

Chain L5:



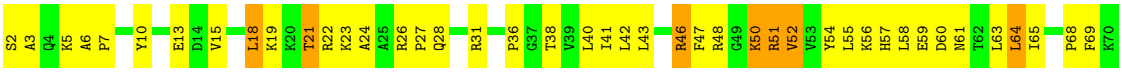
• Molecule 42: 60S ribosomal protein L5

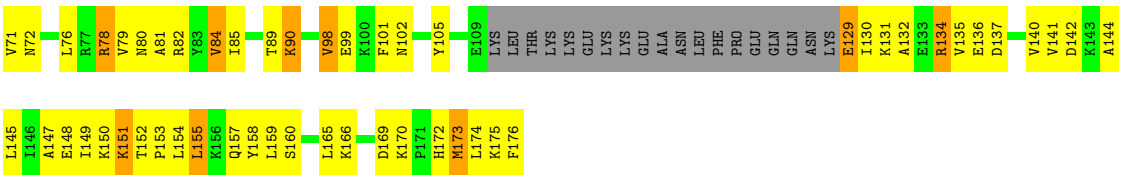
Chain l5:



• Molecule 43: 60S ribosomal protein L6-A

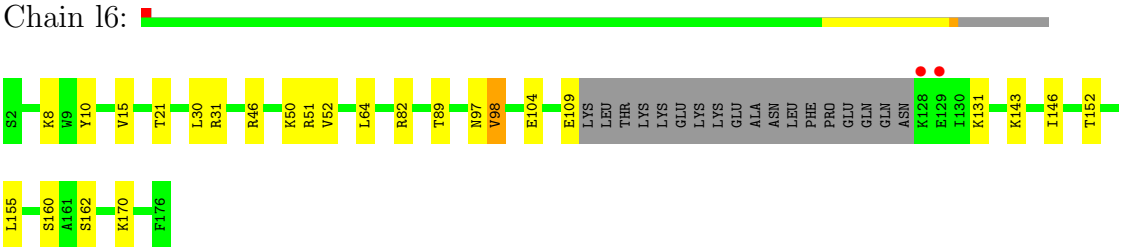
Chain L6:





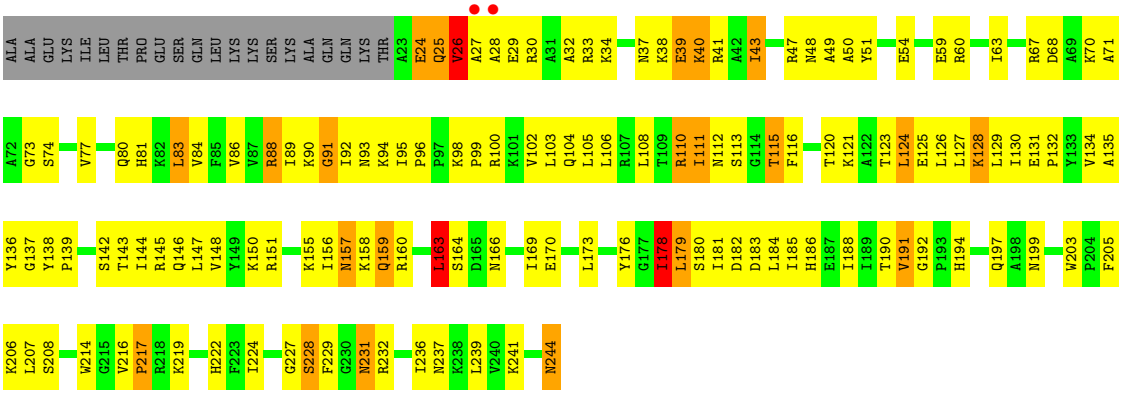
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



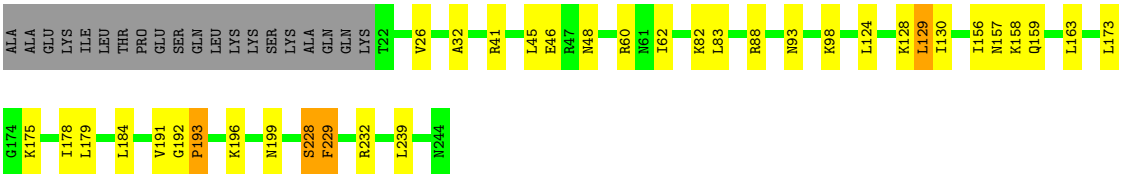
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



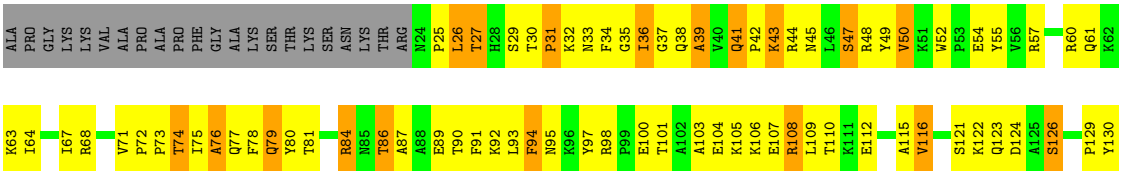
• Molecule 44: 60S ribosomal protein L7-A

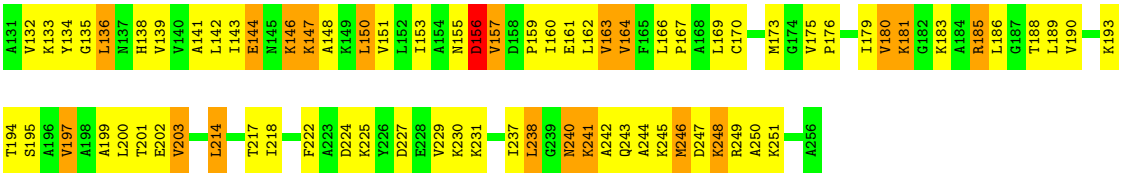
Chain l7:



• Molecule 45: 60S ribosomal protein L8-A

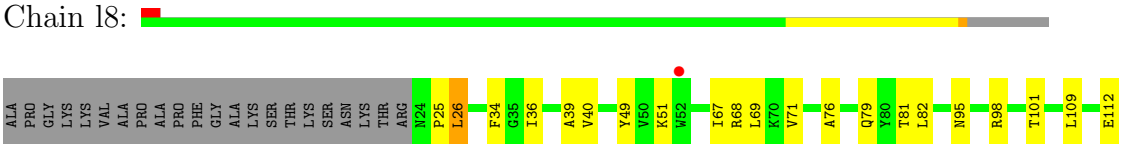
Chain L8:





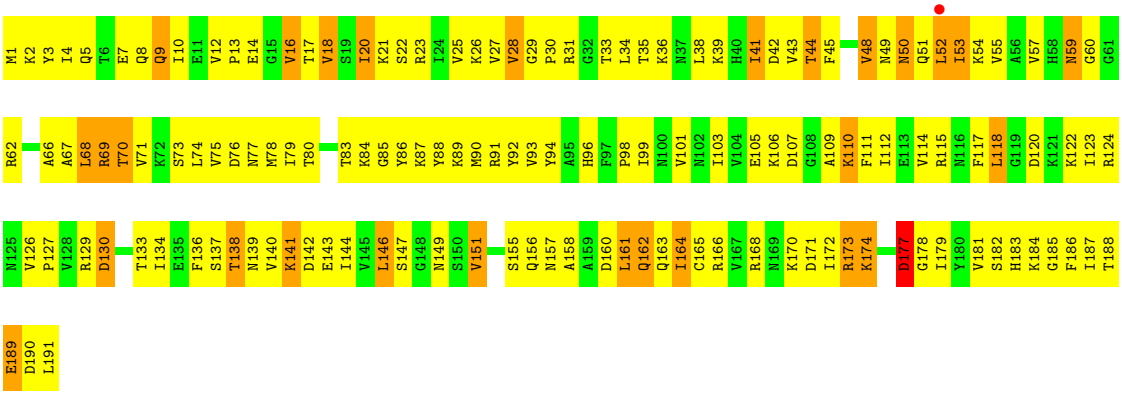
• Molecule 45: 60S ribosomal protein L8-A

Chain l8:



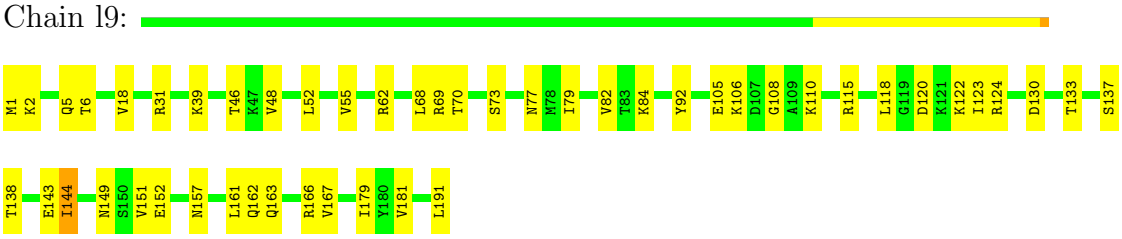
• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



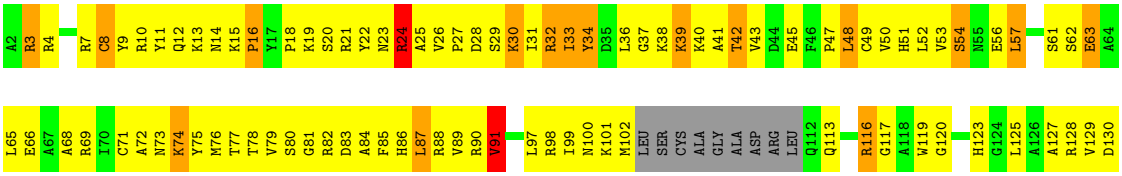
• Molecule 46: 60S ribosomal protein L9-A

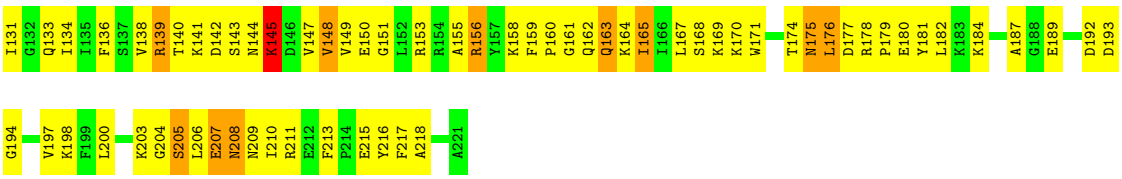
Chain l9:



• Molecule 47: 60S ribosomal protein L10

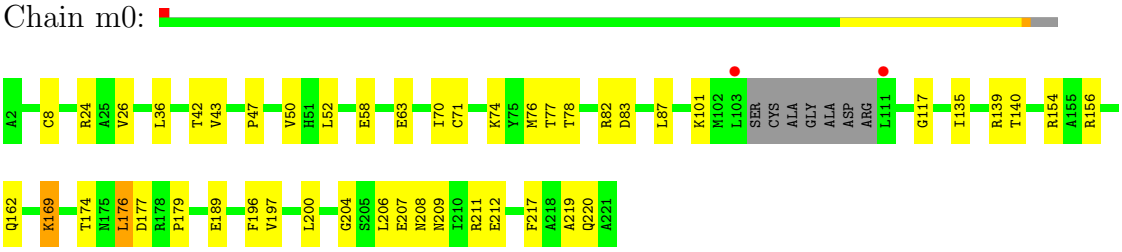
Chain M0:





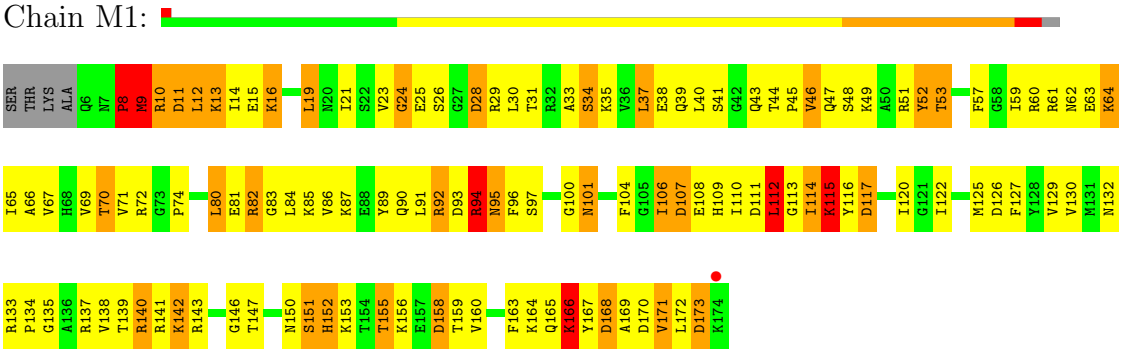
• Molecule 47: 60S ribosomal protein L10

Chain m0:



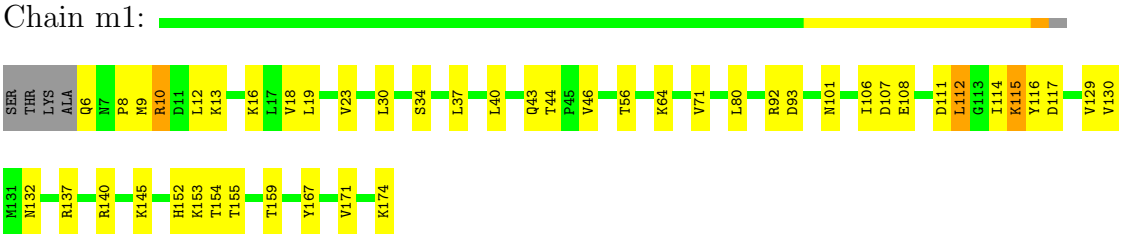
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



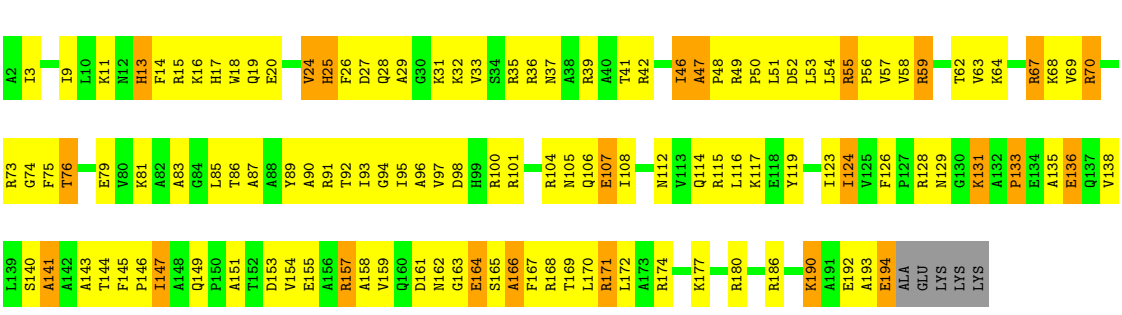
• Molecule 48: 60S ribosomal protein L11-B

Chain m1:



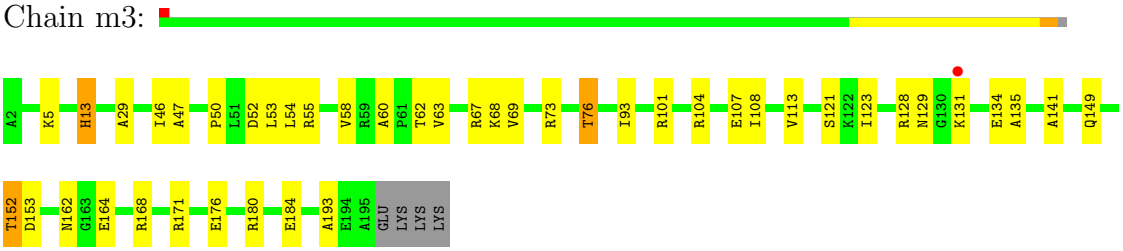
• Molecule 49: 60S ribosomal protein L13-A

Chain M3:



• Molecule 49: 60S ribosomal protein L13-A

Chain m3:

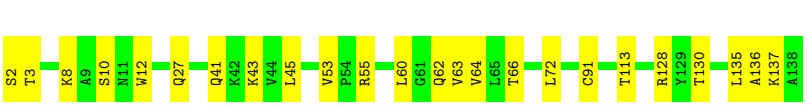


• Molecule 50: 60S ribosomal protein L14-A

Chain M4:

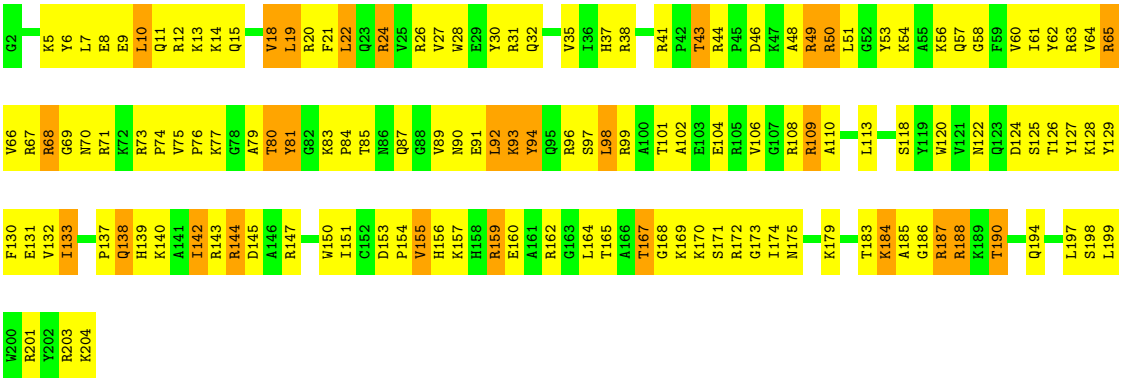
• Molecule 50: 60S ribosomal protein L14-A

Chain m4:



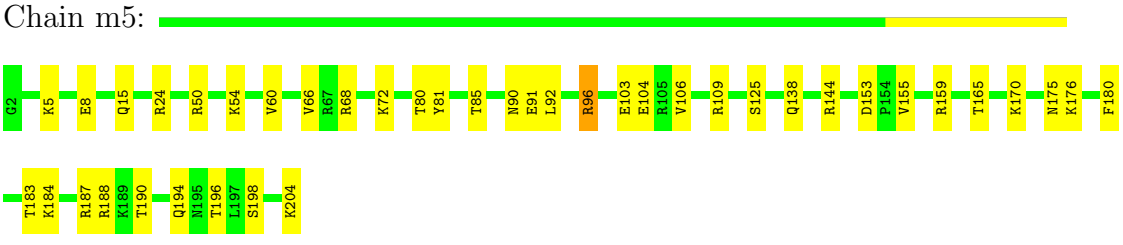
• Molecule 51: 60S ribosomal protein L15-A

Chain M5:



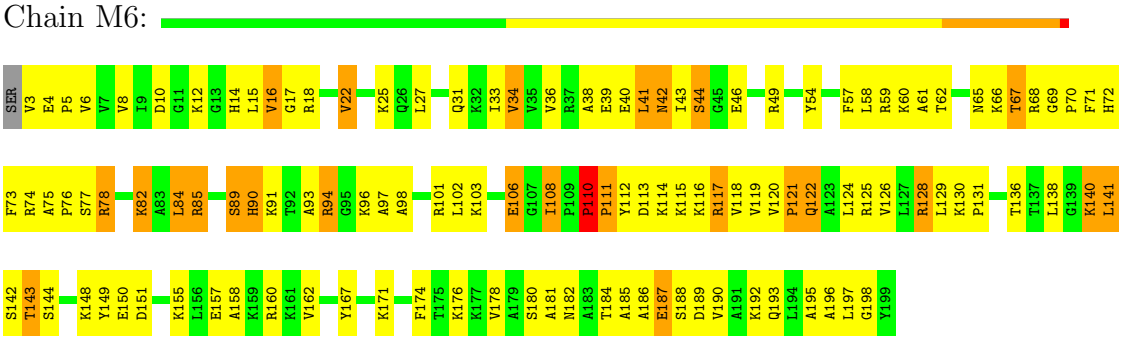
• Molecule 51: 60S ribosomal protein L15-A

Chain m5:



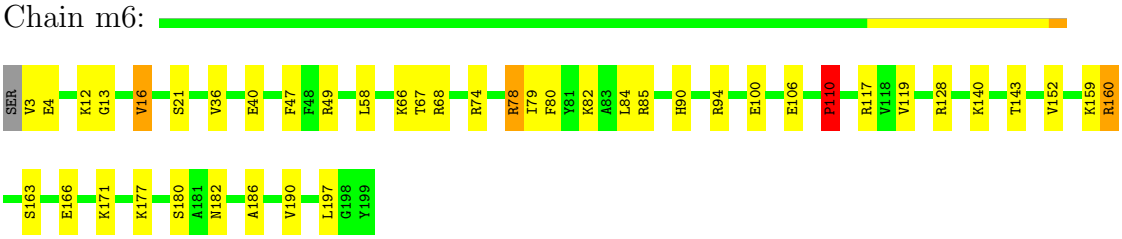
• Molecule 52: 60S ribosomal protein L16-A

Chain M6:



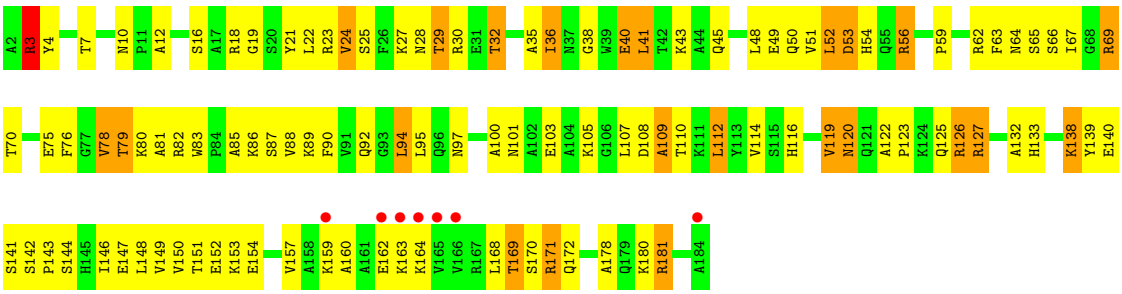
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



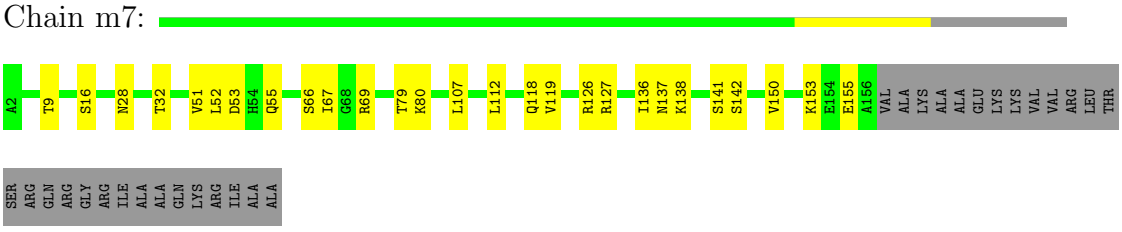
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



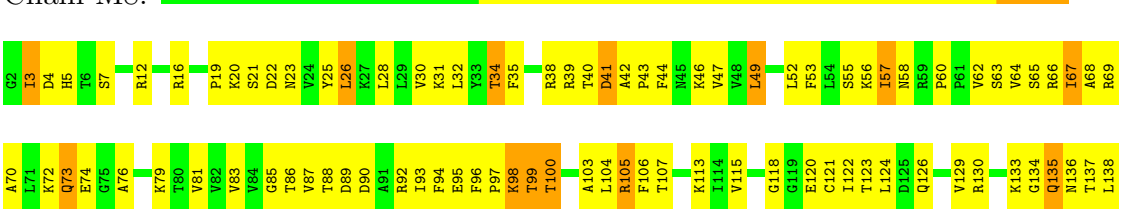
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



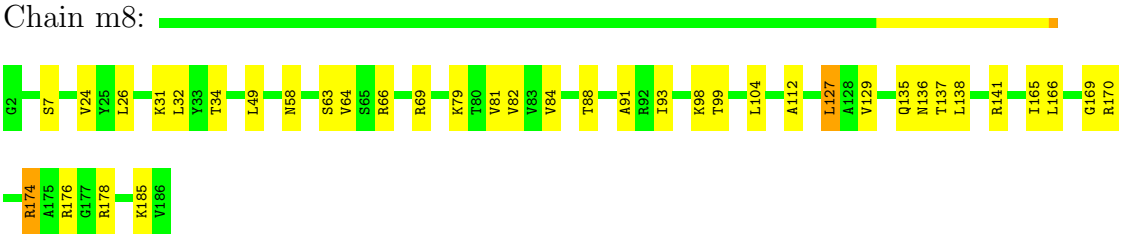
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



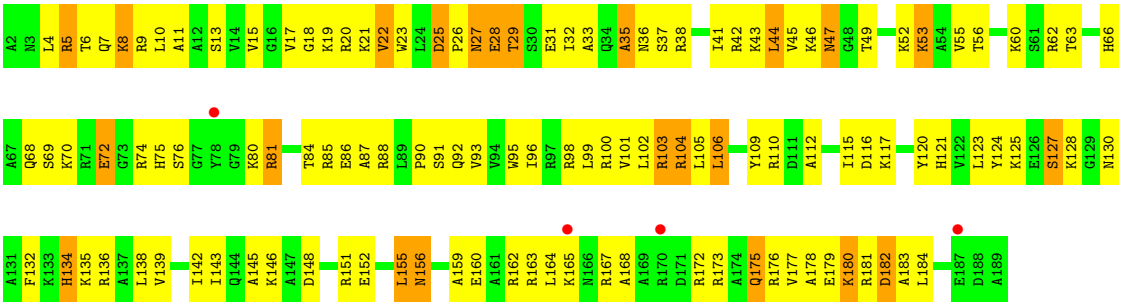
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



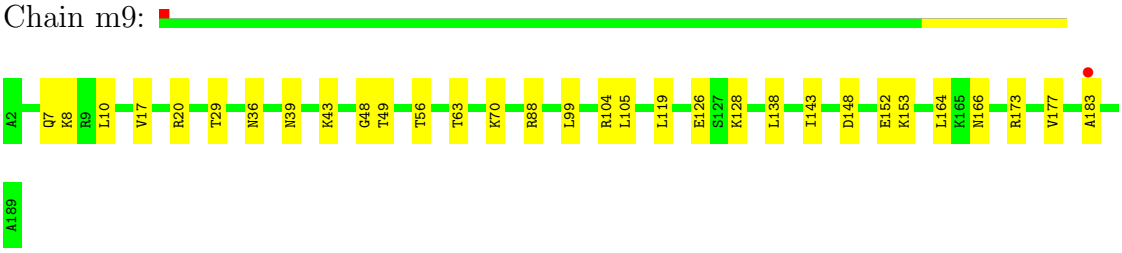
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



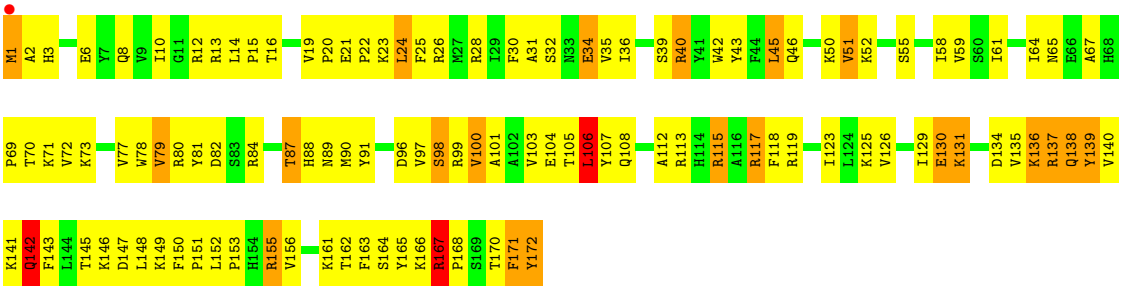
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



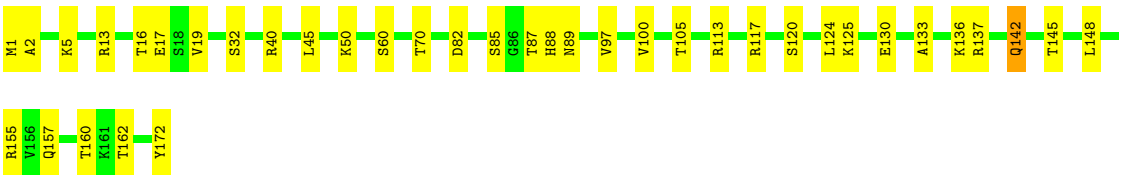
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



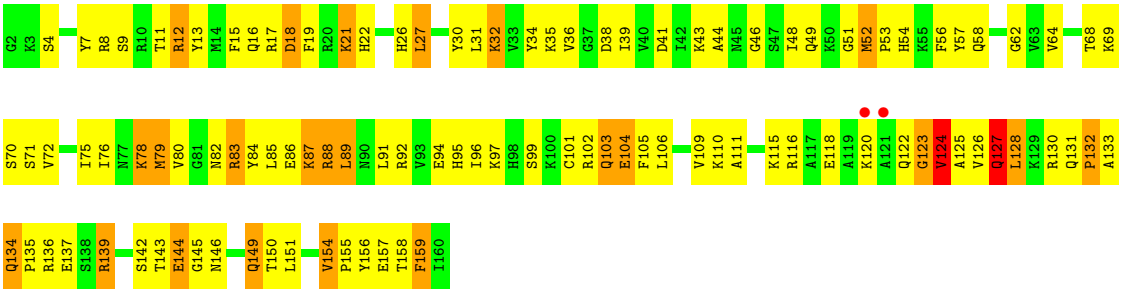
• Molecule 56: 60S ribosomal protein L20-A

Chain n0:



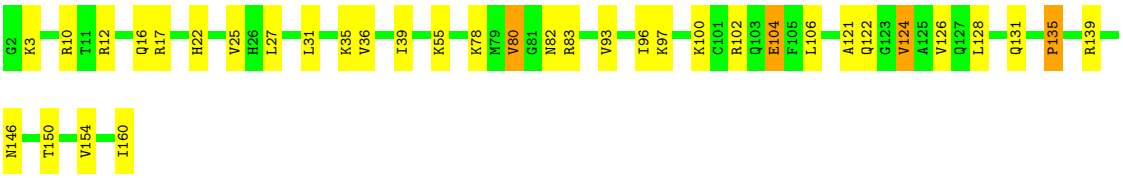
• Molecule 57: 60S ribosomal protein L21-A

Chain N1:



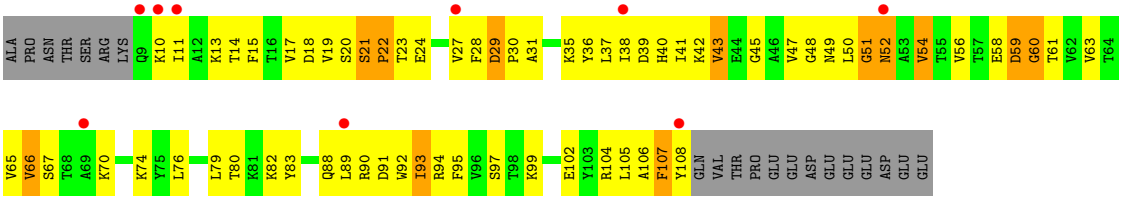
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



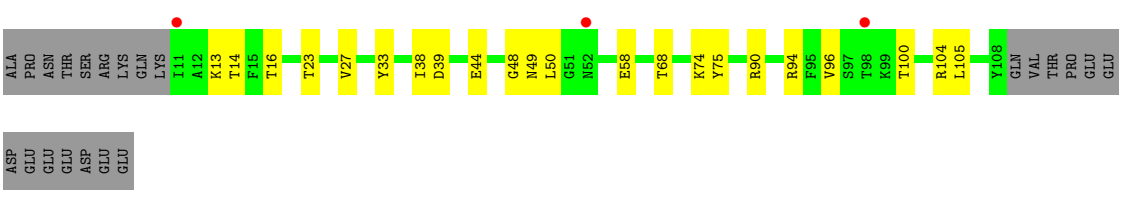
• Molecule 58: 60S ribosomal protein L22-A

Chain N2:



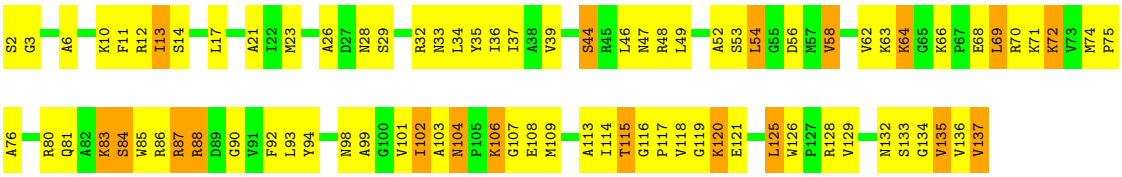
• Molecule 58: 60S ribosomal protein L22-A

Chain n2:



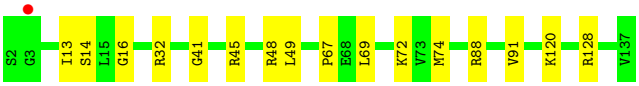
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



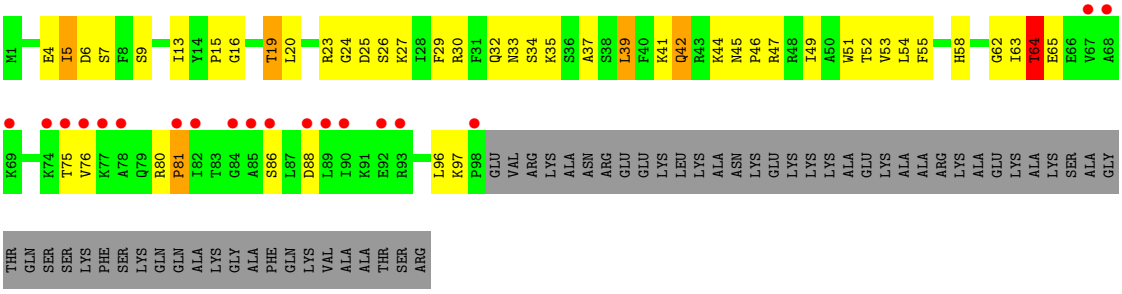
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



• Molecule 60: 60S ribosomal protein L24-A

Chain N4:

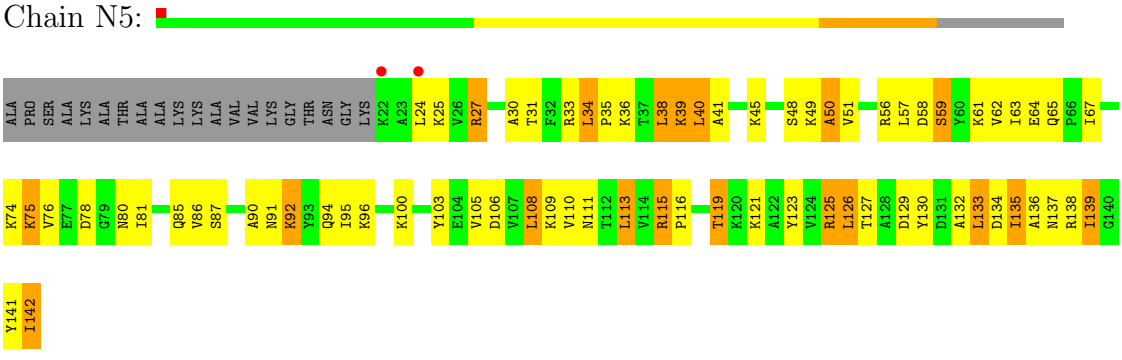


• Molecule 60: 60S ribosomal protein L24-A

Chain n4:

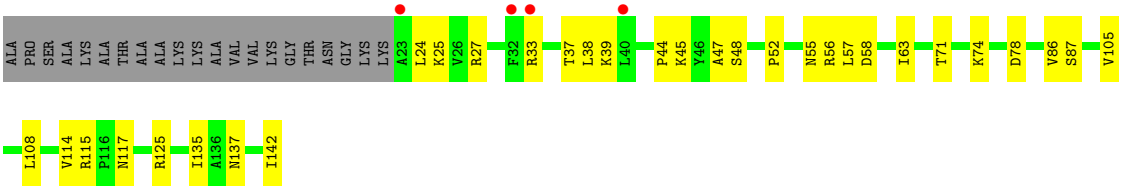
• Molecule 61: 60S ribosomal protein L25

Chain N5:



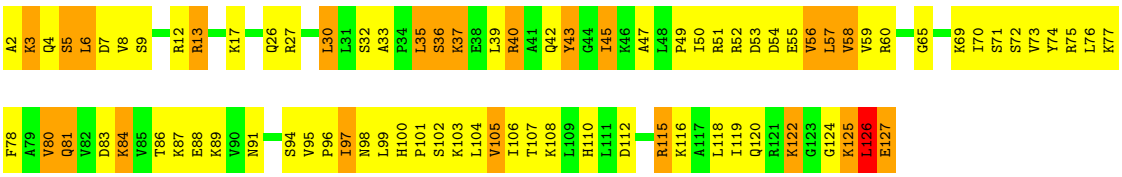
• Molecule 61: 60S ribosomal protein L25

Chain n5:



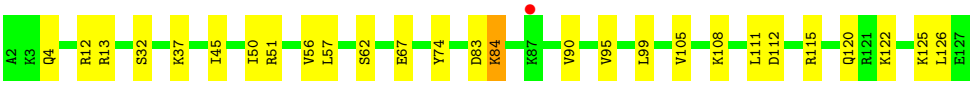
• Molecule 62: 60S ribosomal protein L26-A

Chain N6:



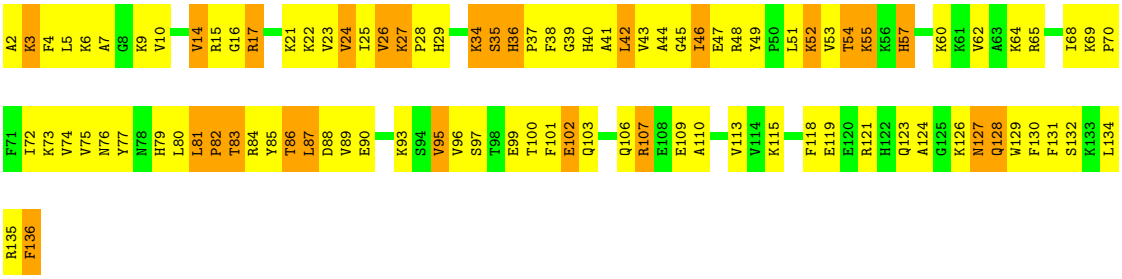
• Molecule 62: 60S ribosomal protein L26-A

Chain n6:



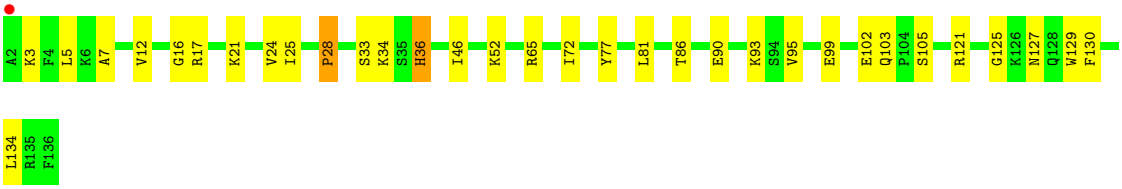
• Molecule 63: 60S ribosomal protein L27-A

Chain N7:



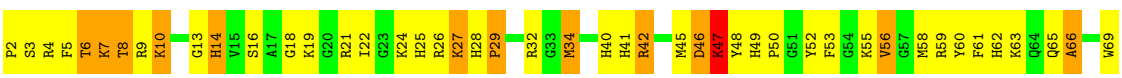
• Molecule 63: 60S ribosomal protein L27-A

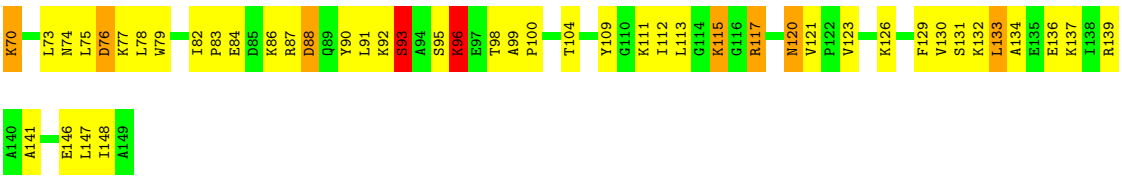
Chain n7:



• Molecule 64: 60S ribosomal protein L28

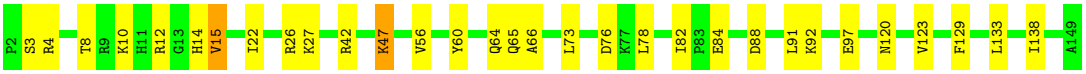
Chain N8:





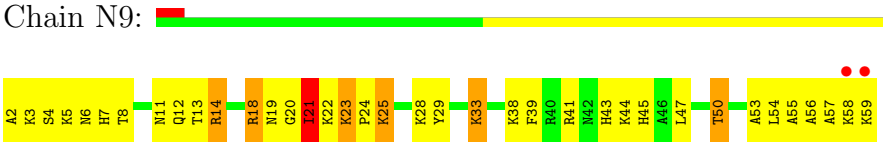
• Molecule 64: 60S ribosomal protein L28

Chain n8:



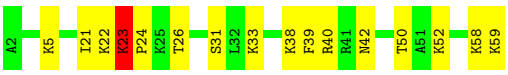
• Molecule 65: 60S ribosomal protein L29

Chain N9:



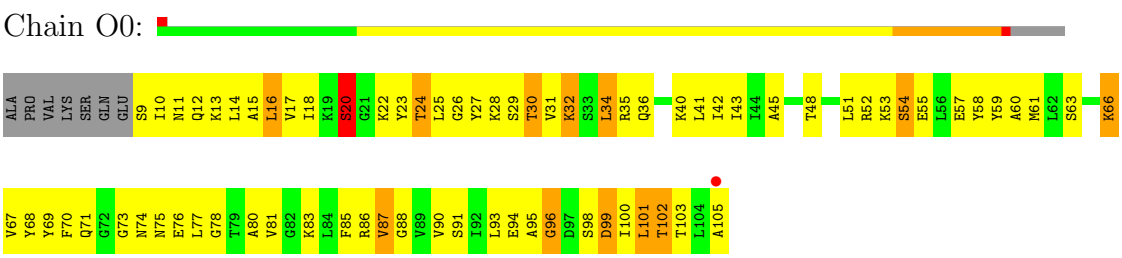
• Molecule 65: 60S ribosomal protein L29

Chain n9:



• Molecule 66: 60S ribosomal protein L30

Chain O0:

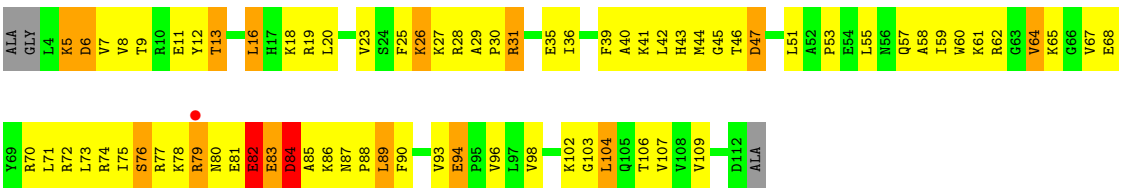


• Molecule 66: 60S ribosomal protein L30

Chain o0:

• Molecule 67: 60S ribosomal protein L31-A

Chain O1:

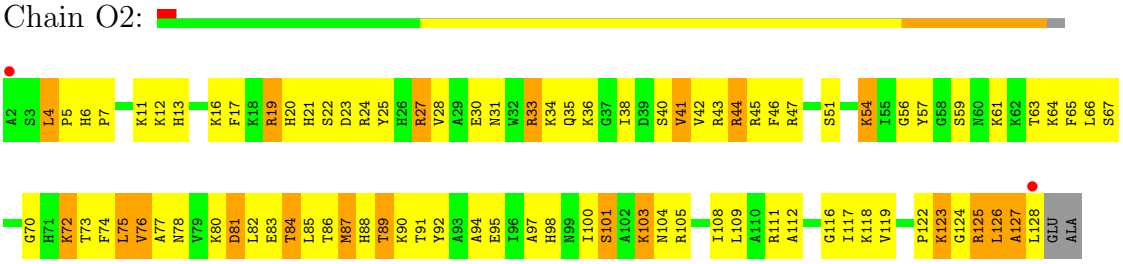


• Molecule 67: 60S ribosomal protein L31-A

Chain o1:

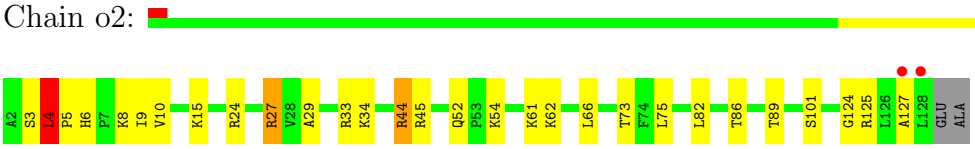
• Molecule 68: 60S ribosomal protein L32

Chain O2:



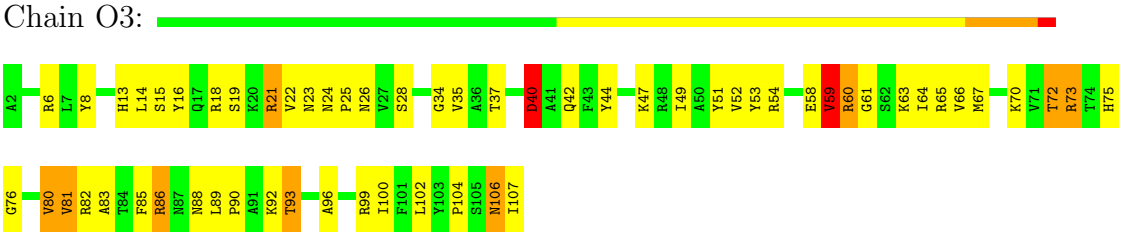
• Molecule 68: 60S ribosomal protein L32

Chain o2:



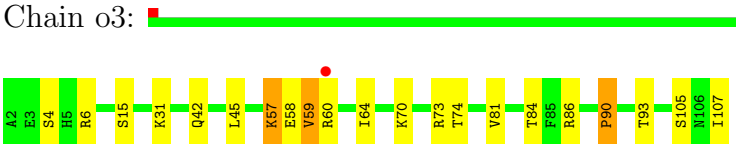
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



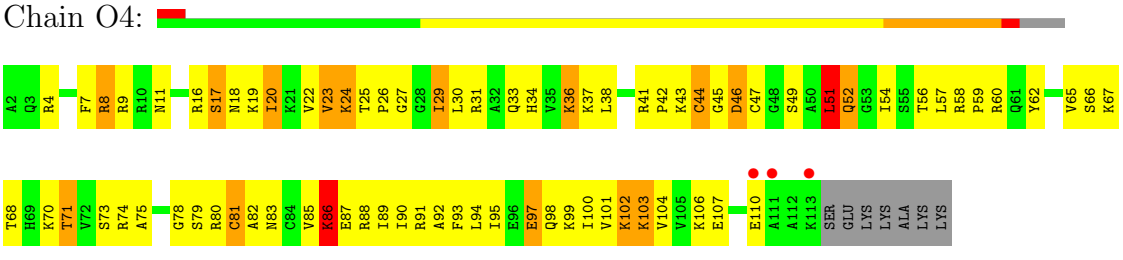
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



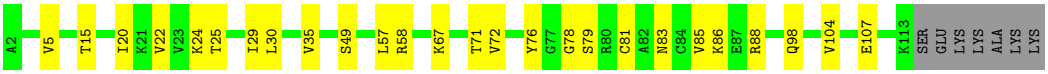
• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



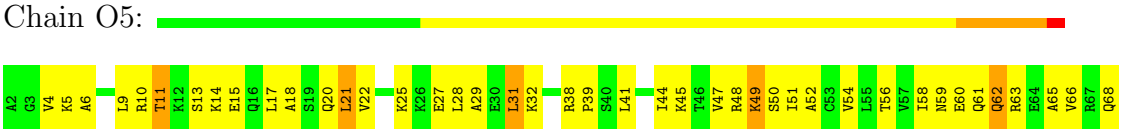
• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



• Molecule 71: 60S ribosomal protein L35-A

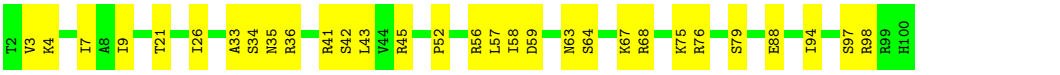
Chain o5:

• Molecule 72: 60S ribosomal protein L36-A

Chain O6:

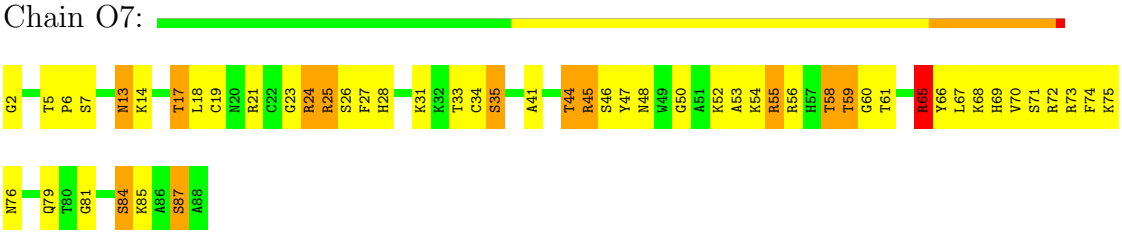
• Molecule 72: 60S ribosomal protein L36-A

Chain o6:



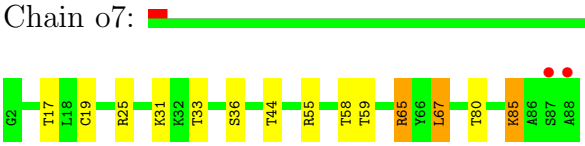
• Molecule 73: 60S ribosomal protein L37-A

Chain O7:



• Molecule 73: 60S ribosomal protein L37-A

Chain o7:

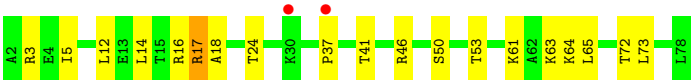


• Molecule 74: 60S ribosomal protein L38

Chain O8:

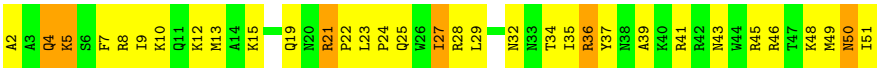
• Molecule 74: 60S ribosomal protein L38

Chain o8:



• Molecule 75: 60S ribosomal protein L39

Chain O9:

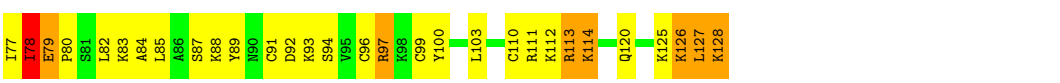


• Molecule 75: 60S ribosomal protein L39

Chain o9:

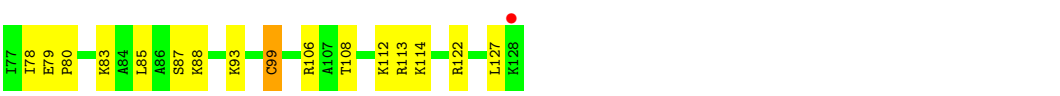
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:

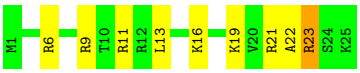


• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:

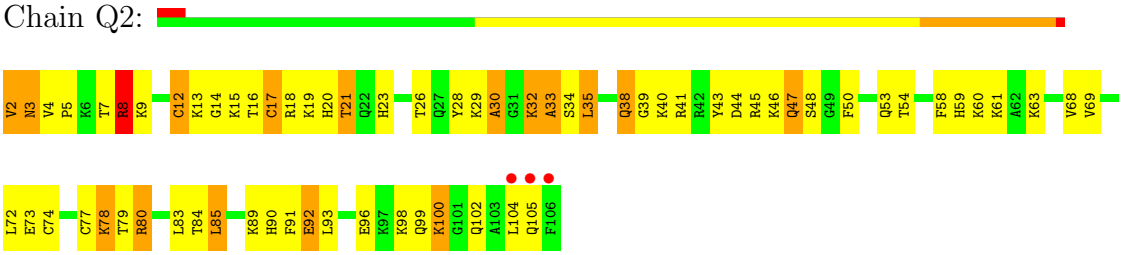
• Molecule 77: 60S ribosomal protein L41-A

Chain q1:



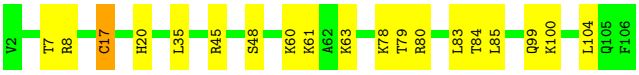
• Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



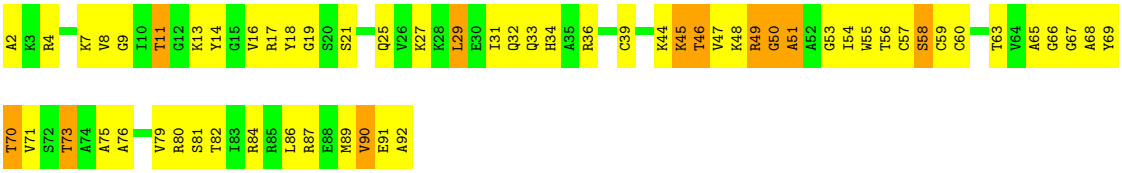
• Molecule 78: 60S ribosomal protein L42-A

Chain q2:



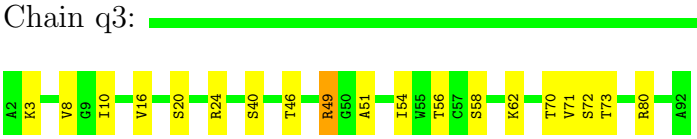
• Molecule 79: 60S ribosomal protein L43-A

Chain Q3:



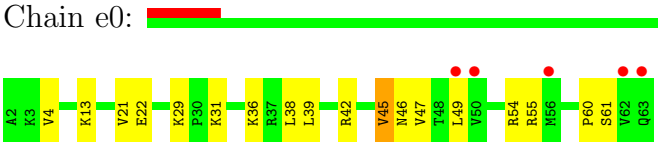
• Molecule 79: 60S ribosomal protein L43-A

Chain q3:



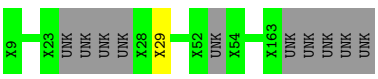
• Molecule 80: 40S ribosomal protein S30-A

Chain e0:



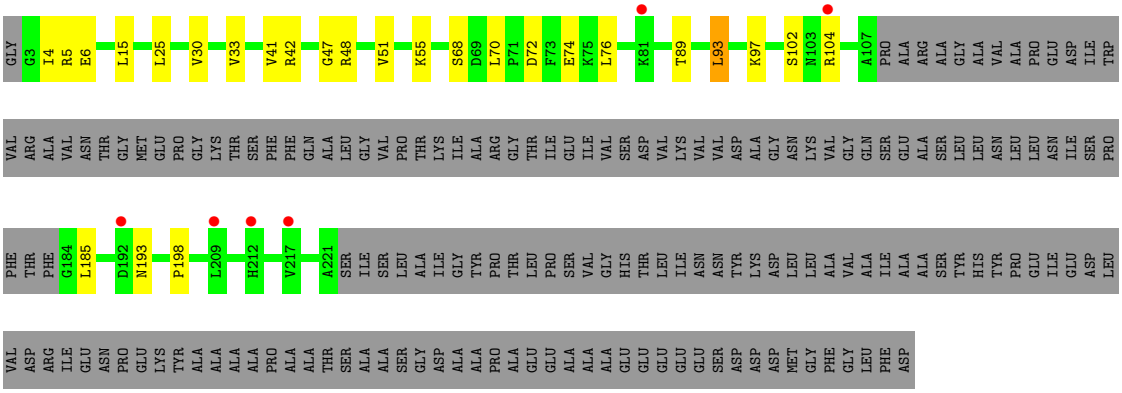
• Molecule 81: Unknown Protein m2

Chain m2:



• Molecule 82: 60S acidic ribosomal protein P0

Chain p0:



• Molecule 83: Unknown Protein p1

Chain p1:

There are no outlier residues recorded for this chain.

• Molecule 84: Unknown Protein p2

Chain p2:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	435.84Å 286.77Å 303.77Å 90.00° 99.03° 90.00°	Depositor
Resolution (Å)	49.70 – 3.30 49.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.70-3.30) 99.4 (49.82-3.30)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.202 , 0.255 0.274 , 0.317	Depositor DCC
R_{free} test set	21781 reflections (1.99%)	DCC
Wilson B-factor (Å^2)	90.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 1095529 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	411183	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

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

[1] 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: 3J6, ZN, OHX, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.74	6/41698 (0.0%)	1.29	289/64972 (0.4%)
1	6	0.88	18/42765 (0.0%)	1.38	477/66634 (0.7%)
2	S0	0.46	0/1617	0.66	0/2215
2	s0	0.48	0/1623	0.69	0/2222
3	S1	0.39	0/1735	0.65	1/2335 (0.0%)
3	s1	0.50	0/1748	0.70	1/2352 (0.0%)
4	S2	0.50	0/1665	0.66	0/2263
4	s2	0.58	0/1665	0.72	0/2263
5	S3	0.50	0/1759	0.66	0/2368
5	s3	0.42	0/1759	0.60	0/2368
6	S4	0.47	0/2109	0.70	1/2839 (0.0%)
6	s4	0.53	0/2109	0.73	0/2839
7	S5	0.40	0/1629	0.59	0/2202
7	s5	0.46	0/1629	0.69	0/2202
8	S6	0.44	0/1823	0.64	0/2439
8	s6	0.55	0/1779	0.70	0/2379
9	S7	0.43	0/1506	0.65	0/2028
9	s7	0.44	0/1516	0.65	0/2043
10	S8	0.54	0/1514	0.71	2/2021 (0.1%)
10	s8	0.60	0/1514	0.74	0/2021
11	S9	0.47	0/1519	0.65	0/2035
11	s9	0.56	0/1519	0.78	1/2035 (0.0%)
12	C0	0.42	0/790	0.64	1/1069 (0.1%)
12	c0	0.37	0/777	0.66	3/1049 (0.3%)
13	C1	0.58	0/1240	0.70	0/1675
13	c1	0.63	0/1194	0.76	0/1610
14	C2	0.38	0/900	0.64	1/1224 (0.1%)
14	c2	0.29	0/900	0.57	0/1224
15	C3	0.47	0/1215	0.68	2/1638 (0.1%)
15	c3	0.54	0/1215	0.71	0/1638
16	C4	0.40	0/901	0.68	0/1217
16	c4	0.52	0/960	0.74	1/1290 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.46	0/998	0.65	0/1341
17	c5	0.48	0/1060	0.70	1/1426 (0.1%)
18	C6	0.45	0/1125	0.68	1/1510 (0.1%)
18	c6	0.51	0/1131	0.70	0/1518
19	C7	0.44	0/935	0.63	0/1254
19	c7	0.47	0/914	0.69	0/1224
20	C8	0.42	0/1211	0.64	0/1628
20	c8	0.50	0/1211	0.71	1/1628 (0.1%)
21	C9	0.45	0/1130	0.65	1/1517 (0.1%)
21	c9	0.50	0/1130	0.67	1/1517 (0.1%)
22	D0	0.46	0/865	0.65	0/1169
22	d0	0.48	0/892	0.68	0/1205
23	D1	0.46	0/693	0.65	0/935
23	d1	0.52	0/693	0.68	0/935
24	D2	0.50	0/1038	0.75	2/1395 (0.1%)
24	d2	0.61	0/1038	0.76	1/1395 (0.1%)
25	D3	0.61	0/1139	0.75	0/1518
25	d3	0.75	0/1139	0.86	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	0.40	0/571	0.72	0/768
27	d5	0.46	0/566	0.71	0/761
28	D6	0.48	0/782	0.71	0/1047
28	d6	0.65	0/782	0.79	1/1047 (0.1%)
29	D7	0.43	0/620	0.67	0/838
29	d7	0.49	0/620	0.64	0/838
30	D8	0.36	0/499	0.56	0/670
30	d8	0.46	0/499	0.63	0/670
31	D9	0.54	0/452	0.70	1/600 (0.2%)
31	d9	0.48	0/452	0.65	0/600
32	E0	0.48	0/483	0.61	0/643
33	E1	0.43	0/577	0.77	0/770
33	e1	0.39	0/619	0.69	1/822 (0.1%)
34	SR	0.37	0/2494	0.58	0/3393
34	sR	0.42	0/2495	0.59	0/3395
35	SM	0.53	0/1113	0.80	4/1502 (0.3%)
35	sM	0.50	0/683	0.73	1/923 (0.1%)
36	1	1.15	144/75394 (0.2%)	1.64	1754/117545 (1.5%)
36	5	1.19	180/75414 (0.2%)	1.67	1900/117575 (1.6%)
37	3	0.94	1/2883 (0.0%)	1.44	31/4491 (0.7%)
37	7	1.14	3/2883 (0.1%)	1.67	68/4491 (1.5%)
38	4	1.06	2/3746 (0.1%)	1.55	59/5832 (1.0%)
38	8	0.98	1/3746 (0.0%)	1.42	27/5832 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	0.70	0/1948	0.85	4/2617 (0.2%)
39	l2	0.67	0/1946	0.84	0/2614
40	L3	0.73	0/3146	0.82	1/4228 (0.0%)
40	l3	0.83	2/3146 (0.1%)	0.90	2/4228 (0.0%)
41	L4	0.81	2/2800 (0.1%)	0.91	3/3790 (0.1%)
41	l4	0.72	1/2800 (0.0%)	0.87	0/3790
42	L5	0.57	0/2425	0.71	0/3271
42	l5	0.70	0/2408	0.82	4/3248 (0.1%)
43	L6	0.74	0/1260	0.79	0/1694
43	l6	0.75	0/1269	0.82	1/1705 (0.1%)
44	L7	0.76	0/1821	0.88	2/2451 (0.1%)
44	l7	0.84	0/1828	0.88	4/2461 (0.2%)
45	L8	0.56	0/1836	0.69	0/2481
45	l8	0.51	0/1795	0.64	0/2429
46	L9	0.64	0/1539	0.77	0/2073
46	l9	0.80	0/1539	0.84	0/2073
47	M0	0.77	1/1741 (0.1%)	0.83	1/2335 (0.0%)
47	m0	0.77	1/1758 (0.1%)	0.83	0/2358
48	M1	0.51	0/1374	0.70	0/1842
48	m1	0.67	0/1374	0.85	2/1842 (0.1%)
49	M3	0.75	0/1568	0.84	1/2106 (0.0%)
49	m3	0.68	0/1573	0.80	0/2113
50	M4	0.73	0/1068	0.76	0/1438
50	m4	0.82	0/1074	0.82	1/1446 (0.1%)
51	M5	0.72	0/1757	0.84	0/2354
51	m5	0.66	0/1757	0.80	2/2354 (0.1%)
52	M6	0.82	0/1585	0.85	1/2128 (0.0%)
52	m6	0.98	2/1585 (0.1%)	0.96	2/2128 (0.1%)
53	M7	0.80	1/1443 (0.1%)	0.84	2/1944 (0.1%)
53	m7	0.84	0/1250	0.84	0/1683
54	M8	0.78	0/1465	0.91	1/1965 (0.1%)
54	m8	0.71	0/1465	0.94	5/1965 (0.3%)
55	M9	0.56	0/1538	0.66	0/2050
55	m9	0.62	0/1538	0.72	0/2050
56	N0	0.74	0/1481	0.84	3/1990 (0.2%)
56	n0	0.89	0/1481	0.89	0/1990
57	N1	0.76	0/1300	0.78	0/1743
57	n1	0.83	2/1300 (0.2%)	0.82	1/1743 (0.1%)
58	N2	0.46	0/812	0.63	0/1099
58	n2	0.50	0/794	0.67	0/1076
59	N3	0.69	0/1018	0.83	1/1369 (0.1%)
59	n3	0.81	0/1018	0.87	0/1369
60	N4	0.55	0/712	0.66	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	n4	0.67	0/1052	0.79	0/1398
61	N5	0.63	0/979	0.77	1/1321 (0.1%)
61	n5	0.67	0/974	0.79	0/1314
62	N6	0.74	0/1004	0.87	1/1341 (0.1%)
62	n6	0.63	0/1004	0.79	0/1341
63	N7	0.54	0/1118	0.70	0/1497
63	n7	0.49	0/1118	0.65	0/1497
64	N8	0.75	0/1204	0.90	0/1612
64	n8	0.77	0/1204	0.87	0/1612
65	N9	0.65	0/473	0.77	1/629 (0.2%)
65	n9	0.79	0/473	0.97	1/629 (0.2%)
66	O0	0.50	0/751	0.66	0/1008
66	o0	0.52	0/775	0.69	0/1040
67	O1	0.63	0/890	0.72	0/1196
67	o1	0.72	0/897	0.84	0/1205
68	O2	0.84	0/1041	0.90	1/1394 (0.1%)
68	o2	0.81	0/1041	0.90	2/1394 (0.1%)
69	O3	0.89	0/868	0.87	1/1168 (0.1%)
69	o3	0.90	0/868	0.90	0/1168
70	O4	0.59	0/890	0.79	1/1189 (0.1%)
70	o4	0.56	0/890	0.76	0/1189
71	O5	0.71	0/978	0.78	0/1301
71	o5	0.56	0/974	0.68	0/1297
72	O6	0.66	0/778	0.76	0/1034
72	o6	0.55	0/777	0.73	0/1033
73	O7	0.75	0/696	0.99	3/923 (0.3%)
73	o7	0.70	0/696	0.86	1/923 (0.1%)
74	O8	0.52	0/618	0.68	0/826
74	o8	0.50	0/614	0.68	0/822
75	O9	0.74	0/443	0.88	0/588
75	o9	0.66	0/443	0.79	0/588
76	Q0	0.69	0/423	0.82	0/562
76	q0	0.94	1/423 (0.2%)	0.92	0/562
77	Q1	0.61	0/234	0.78	0/300
77	q1	0.78	0/234	1.00	0/300
78	Q2	0.88	1/860 (0.1%)	0.90	0/1136
78	q2	0.79	1/860 (0.1%)	0.77	1/1136 (0.1%)
79	Q3	0.71	0/701	0.81	1/934 (0.1%)
79	q3	0.71	0/701	0.80	0/934
80	e0	0.58	0/499	0.74	0/665
82	p0	0.46	0/1092	0.61	0/1474
All	All	0.90	370/430074 (0.1%)	1.30	4696/631364 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S4	0	1
7	s5	0	1
9	S7	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
25	D3	0	1
27	D5	0	1
28	D6	0	1
33	E1	0	1
39	L2	0	1
39	l2	0	1
40	L3	0	1
43	L6	0	1
43	l6	0	1
44	l7	0	1
45	L8	0	1
46	L9	0	1
48	M1	0	1
52	M6	0	1
52	m6	0	1
54	m8	0	1
56	N0	0	1
56	n0	0	1
59	n3	0	1
64	n8	0	1
65	N9	0	2
67	O1	0	1
72	O6	0	1
81	m2	0	1
All	All	0	36

The worst 5 of 370 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	12.26	2.03	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	1152	G	N9-C4	-11.12	1.29	1.38
36	5	2726	C	N3-C4	-9.57	1.27	1.33
78	q2	17	CYS	CB-SG	9.14	1.97	1.82
36	1	3181	C	N3-C4	-8.78	1.27	1.33

The worst 5 of 4696 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	1116	G	O5'-P-OP1	-18.97	87.94	110.70
36	5	1152	G	C2-N3-C4	-18.00	102.90	111.90
36	5	1152	G	N3-C4-C5	17.23	137.22	128.60
36	5	1152	G	N3-C4-N9	-15.73	116.56	126.00
36	1	1495	U	C5-C6-N1	-15.66	114.87	122.70

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
16	C4	124	ASP	Peptide
6	S4	167	GLY	Peptide
9	S7	131	PHE	Peptide
9	S7	30	SER	Peptide

5.2 Close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	1102	0
1	6	38238	0	19240	1042	0
2	S0	1577	0	1567	189	0
2	s0	1583	0	1578	0	0
3	S1	1709	0	1784	187	0
3	s1	1722	0	1793	0	0
4	S2	1635	0	1723	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	s2	1635	0	1723	0	0
5	S3	1734	0	1817	151	0
5	s3	1734	0	1817	0	0
6	S4	2068	0	2154	214	0
6	s4	2068	0	2154	0	0
7	S5	1609	0	1675	187	0
7	s5	1609	0	1675	0	0
8	S6	1799	0	1879	135	0
8	s6	1755	0	1846	0	0
9	S7	1481	0	1572	133	0
9	s7	1491	0	1578	0	0
10	S8	1489	0	1525	154	0
10	s8	1489	0	1525	0	0
11	S9	1494	0	1573	154	0
11	s9	1494	0	1573	0	0
12	C0	773	0	729	84	0
12	c0	762	0	699	0	0
13	C1	1214	0	1259	107	0
13	c1	1168	0	1231	0	0
14	C2	892	0	891	71	0
14	c2	892	0	891	0	0
15	C3	1192	0	1254	111	0
15	c3	1192	0	1255	0	0
16	C4	891	0	883	98	0
16	c4	949	0	985	0	0
17	C5	977	0	1002	112	0
17	c5	1039	0	1050	0	0
18	C6	1105	0	1166	137	0
18	c6	1111	0	1171	0	0
19	C7	926	0	930	96	0
19	c7	906	0	909	0	0
20	C8	1192	0	1222	137	0
20	c8	1192	0	1222	0	0
21	C9	1112	0	1124	113	0
21	c9	1112	0	1124	0	0
22	D0	855	0	917	95	0
22	d0	882	0	939	0	0
23	D1	684	0	672	81	0
23	d1	684	0	672	0	0
24	D2	1021	0	1060	105	0
24	d2	1021	0	1060	0	0
25	D3	1121	0	1196	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	d3	1121	0	1196	0	0
26	D4	1073	0	1132	101	0
26	d4	1073	0	1132	0	0
27	D5	563	0	603	74	0
27	d5	558	0	598	0	0
28	D6	769	0	814	119	0
28	d6	769	0	814	0	0
29	D7	610	0	631	49	0
29	d7	610	0	633	0	0
30	D8	497	0	535	58	0
30	d8	497	0	535	0	0
31	D9	442	0	428	48	0
31	d9	442	0	429	0	0
32	E0	475	0	525	38	0
33	E1	566	0	602	73	0
33	e1	608	0	657	0	0
34	SR	2441	0	2397	163	0
34	sR	2442	0	2392	0	0
35	SM	1104	0	996	82	0
35	sM	680	0	607	0	0
36	1	67355	0	33845	1581	1
36	5	67376	0	33858	1538	0
37	3	2579	0	1304	62	0
37	7	2579	0	1304	63	0
38	4	3353	0	1695	82	0
38	8	3353	0	1695	95	0
39	L2	1914	0	1981	220	0
39	l2	1912	0	1976	0	0
40	L3	3075	0	3142	272	0
40	l3	3075	0	3142	0	0
41	L4	2748	0	2859	247	0
41	l4	2748	0	2859	0	0
42	L5	2375	0	2325	231	0
42	l5	2359	0	2311	0	0
43	L6	1239	0	1326	97	0
43	l6	1248	0	1339	0	0
44	L7	1784	0	1862	165	0
44	l7	1791	0	1869	0	0
45	L8	1804	0	1877	140	0
45	l8	1763	0	1819	0	0
46	L9	1518	0	1587	160	0
46	l9	1518	0	1587	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	M0	1705	0	1735	170	0
47	m0	1722	0	1755	0	0
48	M1	1353	0	1383	117	0
48	m1	1353	0	1383	0	0
49	M3	1543	0	1608	158	0
49	m3	1548	0	1613	0	0
50	M4	1053	0	1149	104	0
50	m4	1059	0	1154	0	0
51	M5	1720	0	1779	184	0
51	m5	1720	0	1779	0	0
52	M6	1555	0	1659	150	0
52	m6	1555	0	1659	0	0
53	M7	1420	0	1437	114	0
53	m7	1227	0	1236	0	0
54	M8	1441	0	1543	132	0
54	m8	1441	0	1543	0	0
55	M9	1521	0	1617	123	0
55	m9	1521	0	1617	0	0
56	N0	1445	0	1487	135	0
56	n0	1445	0	1487	0	0
57	N1	1276	0	1323	123	0
57	n1	1276	0	1323	0	0
58	N2	796	0	812	58	0
58	n2	778	0	791	0	0
59	N3	1003	0	1048	86	0
59	n3	1003	0	1048	0	0
60	N4	699	0	640	36	0
60	n4	1038	0	1071	0	0
61	N5	964	0	1025	75	0
61	n5	959	0	1023	0	0
62	N6	993	0	1081	94	0
62	n6	993	0	1081	0	0
63	N7	1092	0	1155	120	0
63	n7	1092	0	1155	0	0
64	N8	1173	0	1214	111	0
64	n8	1173	0	1215	0	0
65	N9	462	0	491	44	0
65	n9	462	0	491	0	0
66	O0	743	0	797	72	0
66	o0	767	0	816	0	0
67	O1	876	0	912	72	0
67	o1	883	0	918	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	O2	1020	0	1090	87	0
68	o2	1020	0	1090	0	0
69	O3	850	0	880	58	0
69	o3	850	0	880	0	0
70	O4	880	0	945	97	0
70	o4	880	0	945	0	0
71	O5	969	0	1078	107	0
71	o5	965	0	1067	0	0
72	O6	771	0	849	73	0
72	o6	770	0	846	0	0
73	O7	681	0	683	52	0
73	o7	681	0	682	0	0
74	O8	612	0	682	64	0
74	o8	608	0	671	0	0
75	O9	436	0	475	44	0
75	o9	436	0	475	0	0
76	Q0	417	0	455	32	0
76	q0	417	0	456	0	0
77	Q1	233	0	284	21	0
77	q1	233	0	284	0	0
78	Q2	847	0	916	58	0
78	q2	847	0	917	0	0
79	Q3	694	0	734	61	0
79	q3	694	0	734	0	0
80	e0	491	0	542	0	0
81	m2	750	0	175	0	0
82	p0	1077	0	1041	0	0
83	p1	235	0	50	0	0
84	p2	230	0	51	0	0
85	1	471	0	0	0	0
85	2	123	0	0	0	0
85	3	14	0	0	0	0
85	4	20	0	0	0	0
85	5	496	0	0	0	0
85	6	147	0	0	0	0
85	7	18	0	0	0	0
85	8	15	0	0	0	0
85	C3	1	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	3	0	0	0	0
85	L3	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L4	2	0	0	0	0
85	L5	1	0	0	0	0
85	L7	2	0	0	0	0
85	L8	1	0	0	0	0
85	M0	3	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	1	0	0	0	0
85	M7	4	0	0	0	0
85	M9	2	0	0	0	0
85	N0	2	0	0	0	0
85	N3	3	0	0	0	0
85	N5	1	0	0	0	0
85	N8	5	0	0	0	0
85	O2	2	0	0	0	0
85	O3	1	0	0	0	0
85	O7	1	0	0	0	0
85	S2	1	0	0	0	0
85	S8	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	2	0	0	0	0
85	d3	3	0	0	0	0
85	d6	1	0	0	0	0
85	l2	2	0	0	0	0
85	l3	3	0	0	0	0
85	l4	1	0	0	0	0
85	l5	3	0	0	0	0
85	l7	2	0	0	0	0
85	l9	1	0	0	0	0
85	m0	1	0	0	0	0
85	m1	1	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	n0	2	0	0	0	0
85	n3	2	0	0	0	0
85	n6	2	0	0	0	0
85	n8	2	0	0	0	0
85	n9	1	0	0	0	0
85	o0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	o1	1	0	0	0	0
85	o3	2	0	0	0	0
85	o4	1	0	0	0	0
85	q0	1	0	0	0	0
85	q3	2	0	0	0	0
85	s1	1	0	0	0	0
85	s8	2	0	0	0	0
85	s9	1	0	0	0	0
85	sM	2	0	0	0	0
86	1	2429	0	0	223	0
86	2	1099	0	0	115	0
86	3	84	0	0	5	0
86	4	112	0	0	10	0
86	5	2471	0	0	247	0
86	6	1120	0	0	126	0
86	7	70	0	0	4	0
86	8	112	0	0	16	0
86	C3	7	0	0	0	0
86	C5	7	0	0	2	0
86	C8	7	0	0	0	0
86	D3	7	0	0	1	0
86	D9	7	0	0	0	0
86	L3	14	0	0	3	0
86	L4	7	0	0	1	0
86	M0	7	0	0	0	0
86	M5	7	0	0	0	0
86	M7	14	0	0	1	0
86	M9	7	0	0	1	0
86	N9	7	0	0	0	0
86	O1	7	0	0	8	0
86	O3	7	0	0	1	0
86	O4	7	0	0	0	0
86	O6	7	0	0	1	0
86	O7	7	0	0	3	0
86	O9	7	0	0	1	0
86	Q2	7	0	0	5	0
86	S6	7	0	0	1	1
86	S8	7	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	28	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	0	0
86	m1	7	0	0	0	0
86	m4	7	0	0	0	0
86	m5	7	0	0	0	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	n3	14	0	0	0	0
86	n6	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	o7	14	0	0	0	0
86	q2	7	0	0	0	0
86	s1	14	0	0	0	0
86	s8	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	21	0	0	0	0
88	5	21	0	0	3	0
All	All	411183	0	297289	12124	1

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 18.

The worst 5 of 12124 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.03	1.47
78:Q2:17:CYS:SG	78:Q2:77:CYS:HB3	2.03	1.07
36:5:3274:A:H3'	36:5:3275:U:H5"	1.36	1.07
78:Q2:17:CYS:SG	78:Q2:77:CYS:CB	2.70	1.05
36:1:3182:G:OP1	52:M6:160:ARG:NH2	1.90	1.03

All (1) 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)
36:1:531:G:OP1	86:S6:301:OHX:N1[2_545]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S0	204/251 (81%)	139 (68%)	40 (20%)	25 (12%)	1 4
2	s0	204/251 (81%)	148 (72%)	37 (18%)	19 (9%)	1 9
3	S1	212/254 (84%)	147 (69%)	38 (18%)	27 (13%)	0 3
3	s1	214/254 (84%)	164 (77%)	34 (16%)	16 (8%)	2 15
4	S2	215/253 (85%)	177 (82%)	26 (12%)	12 (6%)	3 25
4	s2	215/253 (85%)	171 (80%)	27 (13%)	17 (8%)	1 13
5	S3	221/239 (92%)	176 (80%)	32 (14%)	13 (6%)	2 23
5	s3	221/239 (92%)	172 (78%)	30 (14%)	19 (9%)	1 11
6	S4	258/260 (99%)	205 (80%)	39 (15%)	14 (5%)	3 26
6	s4	258/260 (99%)	206 (80%)	34 (13%)	18 (7%)	2 17
7	S5	204/224 (91%)	149 (73%)	38 (19%)	17 (8%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	s5	204/224 (91%)	145 (71%)	44 (22%)	15 (7%)	2 15
8	S6	224/236 (95%)	194 (87%)	20 (9%)	10 (4%)	4 32
8	s6	216/236 (92%)	184 (85%)	20 (9%)	12 (6%)	3 25
9	S7	182/189 (96%)	132 (72%)	33 (18%)	17 (9%)	1 9
9	s7	184/189 (97%)	142 (77%)	23 (12%)	19 (10%)	1 7
10	S8	184/200 (92%)	150 (82%)	23 (12%)	11 (6%)	2 22
10	s8	184/200 (92%)	155 (84%)	21 (11%)	8 (4%)	4 34
11	S9	183/196 (93%)	146 (80%)	24 (13%)	13 (7%)	2 17
11	s9	183/196 (93%)	144 (79%)	25 (14%)	14 (8%)	1 14
12	C0	94/105 (90%)	68 (72%)	17 (18%)	9 (10%)	1 9
12	c0	92/105 (88%)	60 (65%)	16 (17%)	16 (17%)	0 1
13	C1	153/155 (99%)	118 (77%)	22 (14%)	13 (8%)	1 11
13	c1	144/155 (93%)	112 (78%)	25 (17%)	7 (5%)	3 29
14	C2	122/142 (86%)	70 (57%)	28 (23%)	24 (20%)	0 1
14	c2	122/142 (86%)	68 (56%)	36 (30%)	18 (15%)	0 2
15	C3	148/150 (99%)	120 (81%)	16 (11%)	12 (8%)	1 13
15	c3	148/150 (99%)	112 (76%)	23 (16%)	13 (9%)	1 11
16	C4	125/136 (92%)	92 (74%)	22 (18%)	11 (9%)	1 11
16	c4	126/136 (93%)	94 (75%)	22 (18%)	10 (8%)	1 13
17	C5	122/141 (86%)	89 (73%)	24 (20%)	9 (7%)	2 15
17	c5	133/141 (94%)	87 (65%)	28 (21%)	18 (14%)	0 3
18	C6	139/142 (98%)	108 (78%)	18 (13%)	13 (9%)	1 9
18	c6	140/142 (99%)	111 (79%)	19 (14%)	10 (7%)	2 17
19	C7	116/136 (85%)	86 (74%)	19 (16%)	11 (10%)	1 9
19	c7	113/136 (83%)	84 (74%)	21 (19%)	8 (7%)	2 17
20	C8	143/145 (99%)	110 (77%)	22 (15%)	11 (8%)	1 14
20	c8	143/145 (99%)	112 (78%)	21 (15%)	10 (7%)	2 17
21	C9	141/143 (99%)	114 (81%)	20 (14%)	7 (5%)	3 28
21	c9	141/143 (99%)	109 (77%)	27 (19%)	5 (4%)	6 41
22	D0	105/120 (88%)	87 (83%)	13 (12%)	5 (5%)	4 30
22	d0	108/120 (90%)	83 (77%)	13 (12%)	12 (11%)	1 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	D1	85/87 (98%)	54 (64%)	21 (25%)	10 (12%)	1 4
23	d1	85/87 (98%)	66 (78%)	12 (14%)	7 (8%)	1 13
24	D2	127/129 (98%)	103 (81%)	20 (16%)	4 (3%)	7 45
24	d2	127/129 (98%)	111 (87%)	14 (11%)	2 (2%)	14 64
25	D3	142/144 (99%)	107 (75%)	22 (16%)	13 (9%)	1 9
25	d3	142/144 (99%)	120 (84%)	16 (11%)	6 (4%)	4 34
26	D4	132/134 (98%)	107 (81%)	20 (15%)	5 (4%)	5 37
26	d4	132/134 (98%)	101 (76%)	22 (17%)	9 (7%)	2 18
27	D5	68/107 (64%)	39 (57%)	18 (26%)	11 (16%)	0 1
27	d5	67/107 (63%)	51 (76%)	13 (19%)	3 (4%)	4 32
28	D6	95/97 (98%)	55 (58%)	21 (22%)	19 (20%)	0 1
28	d6	95/97 (98%)	72 (76%)	14 (15%)	9 (10%)	1 9
29	D7	79/81 (98%)	58 (73%)	16 (20%)	5 (6%)	2 20
29	d7	79/81 (98%)	64 (81%)	10 (13%)	5 (6%)	2 20
30	D8	61/66 (92%)	45 (74%)	11 (18%)	5 (8%)	1 13
30	d8	61/66 (92%)	40 (66%)	15 (25%)	6 (10%)	1 8
31	D9	51/55 (93%)	43 (84%)	6 (12%)	2 (4%)	5 37
31	d9	51/55 (93%)	41 (80%)	4 (8%)	6 (12%)	1 4
32	E0	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	3 27
33	E1	69/76 (91%)	31 (45%)	22 (32%)	16 (23%)	0 0
33	e1	74/76 (97%)	35 (47%)	18 (24%)	21 (28%)	0 0
34	SR	316/318 (99%)	263 (83%)	41 (13%)	12 (4%)	5 37
34	sR	316/318 (99%)	269 (85%)	37 (12%)	10 (3%)	6 43
35	SM	155/273 (57%)	101 (65%)	33 (21%)	21 (14%)	0 3
35	sM	98/273 (36%)	56 (57%)	29 (30%)	13 (13%)	0 3
39	L2	250/253 (99%)	208 (83%)	30 (12%)	12 (5%)	4 30
39	l2	250/253 (99%)	206 (82%)	26 (10%)	18 (7%)	2 16
40	L3	384/386 (100%)	319 (83%)	46 (12%)	19 (5%)	3 29
40	l3	384/386 (100%)	331 (86%)	40 (10%)	13 (3%)	6 42
41	L4	359/361 (99%)	289 (80%)	42 (12%)	28 (8%)	1 14
41	l4	359/361 (99%)	290 (81%)	44 (12%)	25 (7%)	2 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	L5	294/296 (99%)	235 (80%)	42 (14%)	17 (6%)	3 23
42	l5	292/296 (99%)	244 (84%)	36 (12%)	12 (4%)	4 35
43	L6	152/175 (87%)	126 (83%)	21 (14%)	5 (3%)	6 43
43	l6	153/175 (87%)	129 (84%)	21 (14%)	3 (2%)	11 58
44	L7	220/243 (90%)	175 (80%)	35 (16%)	10 (4%)	4 32
44	l7	221/243 (91%)	179 (81%)	34 (15%)	8 (4%)	5 40
45	L8	231/255 (91%)	176 (76%)	42 (18%)	13 (6%)	3 25
45	l8	229/255 (90%)	179 (78%)	32 (14%)	18 (8%)	1 13
46	L9	189/191 (99%)	159 (84%)	23 (12%)	7 (4%)	5 39
46	l9	189/191 (99%)	159 (84%)	24 (13%)	6 (3%)	6 43
47	M0	207/220 (94%)	165 (80%)	27 (13%)	15 (7%)	2 16
47	m0	209/220 (95%)	155 (74%)	39 (19%)	15 (7%)	2 16
48	M1	167/173 (96%)	120 (72%)	27 (16%)	20 (12%)	1 4
48	m1	167/173 (96%)	134 (80%)	22 (13%)	11 (7%)	2 19
49	M3	191/198 (96%)	151 (79%)	29 (15%)	11 (6%)	3 23
49	m3	192/198 (97%)	159 (83%)	17 (9%)	16 (8%)	1 12
50	M4	134/137 (98%)	108 (81%)	17 (13%)	9 (7%)	2 18
50	m4	135/137 (98%)	113 (84%)	18 (13%)	4 (3%)	7 46
51	M5	201/203 (99%)	176 (88%)	20 (10%)	5 (2%)	9 51
51	m5	201/203 (99%)	167 (83%)	26 (13%)	8 (4%)	5 36
52	M6	195/198 (98%)	172 (88%)	18 (9%)	5 (3%)	8 50
52	m6	195/198 (98%)	164 (84%)	22 (11%)	9 (5%)	4 31
53	M7	181/183 (99%)	139 (77%)	32 (18%)	10 (6%)	3 25
53	m7	153/183 (84%)	134 (88%)	17 (11%)	2 (1%)	18 69
54	M8	183/185 (99%)	154 (84%)	24 (13%)	5 (3%)	8 49
54	m8	183/185 (99%)	151 (82%)	27 (15%)	5 (3%)	8 49
55	M9	186/188 (99%)	157 (84%)	25 (13%)	4 (2%)	10 55
55	m9	186/188 (99%)	154 (83%)	28 (15%)	4 (2%)	10 55
56	N0	170/172 (99%)	151 (89%)	13 (8%)	6 (4%)	6 41
56	n0	170/172 (99%)	157 (92%)	11 (6%)	2 (1%)	19 71
57	N1	157/159 (99%)	134 (85%)	16 (10%)	7 (4%)	4 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
57	n1	157/159 (99%)	128 (82%)	23 (15%)	6 (4%)	5 37
58	N2	98/120 (82%)	74 (76%)	16 (16%)	8 (8%)	1 13
58	n2	96/120 (80%)	79 (82%)	11 (12%)	6 (6%)	2 20
59	N3	134/136 (98%)	119 (89%)	12 (9%)	3 (2%)	10 55
59	n3	134/136 (98%)	124 (92%)	9 (7%)	1 (1%)	30 81
60	N4	96/155 (62%)	69 (72%)	19 (20%)	8 (8%)	1 12
60	n4	133/155 (86%)	108 (81%)	14 (10%)	11 (8%)	1 12
61	N5	119/141 (84%)	107 (90%)	11 (9%)	1 (1%)	27 78
61	n5	118/141 (84%)	92 (78%)	17 (14%)	9 (8%)	2 15
62	N6	124/126 (98%)	107 (86%)	13 (10%)	4 (3%)	6 43
62	n6	124/126 (98%)	109 (88%)	11 (9%)	4 (3%)	6 43
63	N7	133/135 (98%)	105 (79%)	20 (15%)	8 (6%)	2 22
63	n7	133/135 (98%)	99 (74%)	24 (18%)	10 (8%)	2 15
64	N8	146/148 (99%)	112 (77%)	25 (17%)	9 (6%)	2 21
64	n8	146/148 (99%)	114 (78%)	24 (16%)	8 (6%)	3 25
65	N9	56/58 (97%)	48 (86%)	7 (12%)	1 (2%)	13 61
65	n9	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	1 6
66	O0	95/104 (91%)	81 (85%)	12 (13%)	2 (2%)	11 56
66	o0	98/104 (94%)	90 (92%)	7 (7%)	1 (1%)	22 74
67	O1	107/112 (96%)	92 (86%)	8 (8%)	7 (6%)	2 19
67	o1	107/112 (96%)	83 (78%)	12 (11%)	12 (11%)	1 5
68	O2	125/129 (97%)	109 (87%)	12 (10%)	4 (3%)	6 43
68	o2	125/129 (97%)	101 (81%)	17 (14%)	7 (6%)	3 25
69	O3	104/106 (98%)	88 (85%)	14 (14%)	2 (2%)	12 60
69	o3	104/106 (98%)	90 (86%)	10 (10%)	4 (4%)	5 37
70	O4	110/119 (92%)	87 (79%)	19 (17%)	4 (4%)	5 40
70	o4	110/119 (92%)	93 (84%)	13 (12%)	4 (4%)	5 40
71	O5	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	6 42
71	o5	117/119 (98%)	93 (80%)	20 (17%)	4 (3%)	6 42
72	O6	97/99 (98%)	80 (82%)	9 (9%)	8 (8%)	1 13
72	o6	97/99 (98%)	77 (79%)	12 (12%)	8 (8%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
73	O7	85/87 (98%)	69 (81%)	15 (18%)	1 (1%)	19 71
73	o7	85/87 (98%)	67 (79%)	15 (18%)	3 (4%)	6 41
74	O8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	5 36
74	o8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	3 26
75	O9	48/50 (96%)	38 (79%)	8 (17%)	2 (4%)	4 34
75	o9	48/50 (96%)	40 (83%)	8 (17%)	0	100 100
76	Q0	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	5 36
76	q0	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	5 36
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100 100
77	q1	23/25 (92%)	19 (83%)	2 (9%)	2 (9%)	1 11
78	Q2	103/105 (98%)	72 (70%)	23 (22%)	8 (8%)	1 14
78	q2	103/105 (98%)	93 (90%)	8 (8%)	2 (2%)	12 60
79	Q3	89/91 (98%)	76 (85%)	8 (9%)	5 (6%)	3 25
79	q3	89/91 (98%)	75 (84%)	10 (11%)	4 (4%)	4 32
80	e0	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	2 18
82	p0	139/311 (45%)	119 (86%)	14 (10%)	6 (4%)	4 34
All	All	22333/24141 (92%)	17773 (80%)	3160 (14%)	1400 (6%)	2 20

5 of 1400 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	102	PHE
2	S0	103	THR

5.3.2 Protein sidechains (i)

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%)	135 (82%)	29 (18%)	3 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	s0	165/209 (79%)	131 (79%)	34 (21%)	2 8
3	S1	191/223 (86%)	149 (78%)	42 (22%)	1 6
3	s1	192/223 (86%)	156 (81%)	36 (19%)	2 11
4	S2	176/204 (86%)	134 (76%)	42 (24%)	1 4
4	s2	176/204 (86%)	128 (73%)	48 (27%)	0 2
5	S3	182/194 (94%)	141 (78%)	41 (22%)	1 6
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%)	183 (83%)	38 (17%)	3 15
7	S5	173/190 (91%)	143 (83%)	30 (17%)	3 15
7	s5	173/190 (91%)	144 (83%)	29 (17%)	3 16
8	S6	188/201 (94%)	154 (82%)	34 (18%)	2 12
8	s6	187/201 (93%)	153 (82%)	34 (18%)	2 12
9	S7	165/169 (98%)	135 (82%)	30 (18%)	2 12
9	s7	165/169 (98%)	130 (79%)	35 (21%)	1 7
10	S8	150/161 (93%)	117 (78%)	33 (22%)	1 6
10	s8	150/161 (93%)	124 (83%)	26 (17%)	3 15
11	S9	158/165 (96%)	120 (76%)	38 (24%)	1 4
11	s9	158/165 (96%)	120 (76%)	38 (24%)	1 4
12	C0	77/98 (79%)	66 (86%)	11 (14%)	5 23
12	c0	73/98 (74%)	63 (86%)	10 (14%)	5 26
13	C1	129/136 (95%)	109 (84%)	20 (16%)	4 19
13	c1	129/136 (95%)	104 (81%)	25 (19%)	2 10
14	C2	88/118 (75%)	67 (76%)	21 (24%)	1 4
14	c2	88/118 (75%)	71 (81%)	17 (19%)	2 10
15	C3	127/127 (100%)	104 (82%)	23 (18%)	2 12
15	c3	127/127 (100%)	93 (73%)	34 (27%)	1 2
16	C4	81/104 (78%)	61 (75%)	20 (25%)	1 3
16	c4	97/104 (93%)	69 (71%)	28 (29%)	0 2
17	C5	101/117 (86%)	83 (82%)	18 (18%)	2 13
17	c5	103/117 (88%)	90 (87%)	13 (13%)	7 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	C6	117/118 (99%)	92 (79%)	25 (21%)	1 7
18	c6	118/118 (100%)	91 (77%)	27 (23%)	1 5
19	C7	94/124 (76%)	70 (74%)	24 (26%)	1 3
19	c7	92/124 (74%)	74 (80%)	18 (20%)	2 9
20	C8	128/128 (100%)	102 (80%)	26 (20%)	2 8
20	c8	128/128 (100%)	99 (77%)	29 (23%)	1 5
21	C9	115/115 (100%)	93 (81%)	22 (19%)	2 10
21	c9	115/115 (100%)	91 (79%)	24 (21%)	1 8
22	D0	100/113 (88%)	81 (81%)	19 (19%)	2 11
22	d0	103/113 (91%)	76 (74%)	27 (26%)	1 2
23	D1	74/74 (100%)	56 (76%)	18 (24%)	1 3
23	d1	74/74 (100%)	53 (72%)	21 (28%)	0 2
24	D2	110/110 (100%)	92 (84%)	18 (16%)	3 16
24	d2	110/110 (100%)	96 (87%)	14 (13%)	6 30
25	D3	119/119 (100%)	100 (84%)	19 (16%)	3 18
25	d3	119/119 (100%)	94 (79%)	25 (21%)	1 8
26	D4	112/112 (100%)	92 (82%)	20 (18%)	2 13
26	d4	112/112 (100%)	91 (81%)	21 (19%)	2 11
27	D5	61/88 (69%)	42 (69%)	19 (31%)	0 1
27	d5	61/88 (69%)	53 (87%)	8 (13%)	6 28
28	D6	83/83 (100%)	60 (72%)	23 (28%)	0 2
28	d6	83/83 (100%)	62 (75%)	21 (25%)	1 3
29	D7	70/70 (100%)	58 (83%)	12 (17%)	3 15
29	d7	70/70 (100%)	62 (89%)	8 (11%)	8 36
30	D8	56/59 (95%)	44 (79%)	12 (21%)	1 7
30	d8	56/59 (95%)	46 (82%)	10 (18%)	2 13
31	D9	47/48 (98%)	41 (87%)	6 (13%)	6 29
31	d9	47/48 (98%)	35 (74%)	12 (26%)	1 3
32	E0	51/51 (100%)	42 (82%)	9 (18%)	3 13
33	E1	62/66 (94%)	41 (66%)	21 (34%)	0 1
33	e1	66/66 (100%)	50 (76%)	16 (24%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	SR	260/261 (100%)	227 (87%)	33 (13%)	6 30
34	sR	260/261 (100%)	221 (85%)	39 (15%)	4 21
35	SM	97/228 (42%)	75 (77%)	22 (23%)	1 5
35	sM	54/228 (24%)	42 (78%)	12 (22%)	1 6
39	L2	193/195 (99%)	155 (80%)	38 (20%)	2 9
39	l2	192/195 (98%)	150 (78%)	42 (22%)	1 7
40	L3	321/322 (100%)	250 (78%)	71 (22%)	1 6
40	l3	320/322 (99%)	250 (78%)	70 (22%)	1 7
41	L4	288/288 (100%)	224 (78%)	64 (22%)	1 6
41	l4	288/288 (100%)	222 (77%)	66 (23%)	1 5
42	L5	244/244 (100%)	199 (82%)	45 (18%)	2 12
42	l5	243/244 (100%)	190 (78%)	53 (22%)	1 7
43	L6	134/152 (88%)	115 (86%)	19 (14%)	5 24
43	l6	135/152 (89%)	114 (84%)	21 (16%)	4 19
44	L7	186/204 (91%)	162 (87%)	24 (13%)	6 29
44	l7	187/204 (92%)	158 (84%)	29 (16%)	4 19
45	L8	187/207 (90%)	145 (78%)	42 (22%)	1 6
45	l8	177/207 (86%)	143 (81%)	34 (19%)	2 10
46	L9	171/171 (100%)	136 (80%)	35 (20%)	2 8
46	l9	171/171 (100%)	127 (74%)	44 (26%)	1 3
47	M0	177/186 (95%)	143 (81%)	34 (19%)	2 10
47	m0	179/186 (96%)	146 (82%)	33 (18%)	2 12
48	M1	147/150 (98%)	116 (79%)	31 (21%)	1 7
48	m1	147/150 (98%)	110 (75%)	37 (25%)	1 3
49	M3	154/158 (98%)	130 (84%)	24 (16%)	4 19
49	m3	154/158 (98%)	123 (80%)	31 (20%)	2 8
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2 13
50	m4	108/108 (100%)	89 (82%)	19 (18%)	3 13
51	M5	175/175 (100%)	142 (81%)	33 (19%)	2 11
51	m5	175/175 (100%)	142 (81%)	33 (19%)	2 11
52	M6	160/161 (99%)	133 (83%)	27 (17%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	m6	160/161 (99%)	126 (79%)	34 (21%)	1 7
53	M7	140/145 (97%)	110 (79%)	30 (21%)	1 7
53	m7	125/145 (86%)	100 (80%)	25 (20%)	2 9
54	M8	150/150 (100%)	132 (88%)	18 (12%)	7 33
54	m8	150/150 (100%)	120 (80%)	30 (20%)	2 9
55	M9	153/153 (100%)	125 (82%)	28 (18%)	2 12
55	m9	153/153 (100%)	126 (82%)	27 (18%)	3 13
56	N0	156/156 (100%)	125 (80%)	31 (20%)	2 9
56	n0	156/156 (100%)	120 (77%)	36 (23%)	1 5
57	N1	136/136 (100%)	109 (80%)	27 (20%)	2 9
57	n1	136/136 (100%)	104 (76%)	32 (24%)	1 4
58	N2	87/106 (82%)	77 (88%)	10 (12%)	8 35
58	n2	85/106 (80%)	69 (81%)	16 (19%)	2 11
59	N3	104/104 (100%)	84 (81%)	20 (19%)	2 10
59	n3	104/104 (100%)	90 (86%)	14 (14%)	6 27
60	N4	57/129 (44%)	51 (90%)	6 (10%)	10 40
60	n4	100/129 (78%)	83 (83%)	17 (17%)	3 15
61	N5	104/117 (89%)	81 (78%)	23 (22%)	1 6
61	n5	104/117 (89%)	82 (79%)	22 (21%)	1 7
62	N6	109/109 (100%)	83 (76%)	26 (24%)	1 4
62	n6	109/109 (100%)	85 (78%)	24 (22%)	1 6
63	N7	115/115 (100%)	89 (77%)	26 (23%)	1 5
63	n7	115/115 (100%)	90 (78%)	25 (22%)	1 7
64	N8	118/118 (100%)	96 (81%)	22 (19%)	2 11
64	n8	118/118 (100%)	94 (80%)	24 (20%)	2 8
65	N9	46/46 (100%)	37 (80%)	9 (20%)	2 9
65	n9	46/46 (100%)	35 (76%)	11 (24%)	1 4
66	O0	81/87 (93%)	61 (75%)	20 (25%)	1 3
66	o0	84/87 (97%)	67 (80%)	17 (20%)	2 8
67	O1	92/96 (96%)	73 (79%)	19 (21%)	2 8
67	o1	94/96 (98%)	70 (74%)	24 (26%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
68	O2	109/110 (99%)	86 (79%)	23 (21%)	1 7
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1 6
69	O3	90/90 (100%)	74 (82%)	16 (18%)	2 13
69	o3	90/90 (100%)	70 (78%)	20 (22%)	1 6
70	O4	95/101 (94%)	74 (78%)	21 (22%)	1 6
70	o4	95/101 (94%)	73 (77%)	22 (23%)	1 5
71	O5	104/104 (100%)	84 (81%)	20 (19%)	2 10
71	o5	103/104 (99%)	80 (78%)	23 (22%)	1 6
72	O6	81/81 (100%)	64 (79%)	17 (21%)	1 8
72	o6	80/81 (99%)	58 (72%)	22 (28%)	0 2
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1 7
73	o7	70/70 (100%)	57 (81%)	13 (19%)	2 11
74	O8	68/68 (100%)	50 (74%)	18 (26%)	1 2
74	o8	67/68 (98%)	51 (76%)	16 (24%)	1 4
75	O9	45/45 (100%)	38 (84%)	7 (16%)	4 19
75	o9	45/45 (100%)	37 (82%)	8 (18%)	2 13
76	Q0	47/47 (100%)	40 (85%)	7 (15%)	4 21
76	q0	47/47 (100%)	33 (70%)	14 (30%)	0 1
77	Q1	23/23 (100%)	16 (70%)	7 (30%)	0 1
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0 1
78	Q2	90/90 (100%)	68 (76%)	22 (24%)	1 3
78	q2	90/90 (100%)	73 (81%)	17 (19%)	2 11
79	Q3	71/71 (100%)	58 (82%)	13 (18%)	2 12
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1 6
80	e0	53/53 (100%)	38 (72%)	15 (28%)	0 2
82	p0	105/253 (42%)	84 (80%)	21 (20%)	2 9
All	All	18729/20239 (92%)	14954 (80%)	3775 (20%)	2 8

5 of 3775 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	O5	21	LEU
9	s7	129	LEU

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Mol	Chain	Res	Type
64	n8	65	GLN
74	O8	3	ARG
4	s2	90	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
61	N5	111	ASN
11	s9	124	HIS
57	n1	122	GLN
65	N9	48	HIS
79	Q3	33	GLN

5.3.3 RNA (i)

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 (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2554 ligands modelled in this entry, 1422 are monoatomic - leaving 1132 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	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	-
86	OHX	1	3896	-	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	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	-
86	OHX	1	3939	-	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	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	-
86	OHX	1	3982	-	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	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	-
86	OHX	1	4025	-	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	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	-
86	OHX	1	4068	-	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	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	-
86	OHX	1	4111	-	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	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	-
86	OHX	1	4154	-	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	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	-
86	OHX	1	4197	-	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	4198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4205	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4206	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4207	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4208	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4209	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4210	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4211	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	1	4212	-	0,6,6	0.00	-	0,15,15	0.00	-
88	3J6	1	4213	85	24,24,24	1.91	3 (12%)	42,42,42	1.94	13 (30%)
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	3	215	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	221	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	222	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	223	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	224	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	225	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	3	226	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	4	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	5	3893	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3894	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3895	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	5	3896	-	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	-
88	3J6	5	4246	85	24,24,24	1.14	2 (8%)	42,42,42	1.74	8 (19%)
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	1	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2190	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2191	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2192	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2193	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2194	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2195	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2196	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2197	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2198	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2199	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2200	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	6	2204	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	7	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	8	216	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	217	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	218	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	219	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	220	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	8	221	-	0,6,6	0.00	-	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	8	231	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C3	202	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C5	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	C8	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	D3	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	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	L3	405	-	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	M0	304	-	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	205	-	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	M9	203	-	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	O1	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	O4	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O6	201	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O7	103	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	O9	101	-	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	S6	301	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	S8	302	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	SR	401	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	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	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	404	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l3	405	-	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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	l5	304	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	305	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	306	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	l5	307	-	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	302	-	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	m1	202	-	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	303	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	m6	203	-	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	n6	203	-	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	203	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	502	-	0,6,6	0.00	-	0,15,15	0.00	-
86	OHX	o7	503	-	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	s8	303	-	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	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
86	OHX	1	4212	-	-	0/0/0/0	0/0/0/0
88	3J6	1	4213	85	-	0/3/68/68	0/1/4/4
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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	2	2147	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2148	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2149	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2150	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2151	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2152	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2153	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2154	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2155	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2156	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2157	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2158	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2159	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2160	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2161	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2162	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2163	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2164	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2165	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2166	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2167	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2168	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2169	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2170	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2171	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2172	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2173	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2174	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2175	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2176	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2177	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2178	-	-	0/0/0/0	0/0/0/0
86	OHX	2	2179	-	-	0/0/0/0	0/0/0/0
86	OHX	3	215	-	-	0/0/0/0	0/0/0/0
86	OHX	3	216	-	-	0/0/0/0	0/0/0/0
86	OHX	3	217	-	-	0/0/0/0	0/0/0/0
86	OHX	3	218	-	-	0/0/0/0	0/0/0/0
86	OHX	3	219	-	-	0/0/0/0	0/0/0/0
86	OHX	3	220	-	-	0/0/0/0	0/0/0/0
86	OHX	3	221	-	-	0/0/0/0	0/0/0/0
86	OHX	3	222	-	-	0/0/0/0	0/0/0/0
86	OHX	3	223	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	3	224	-	-	0/0/0/0	0/0/0/0
86	OHX	3	225	-	-	0/0/0/0	0/0/0/0
86	OHX	3	226	-	-	0/0/0/0	0/0/0/0
86	OHX	4	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	5	3893	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3894	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3895	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3896	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	3916	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3917	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3918	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3919	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3920	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3921	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3922	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3923	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3924	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3925	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3926	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3927	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3928	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3929	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3930	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3931	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3932	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3933	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3934	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3935	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3936	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3937	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3938	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3939	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3940	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3941	-	-	0/0/0/0	0/0/0/0
86	OHX	5	3942	-	-	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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	5	4210	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4211	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4212	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4213	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4214	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4215	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4216	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4217	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4218	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4219	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4220	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4221	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4222	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4223	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4224	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4225	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4226	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4227	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4228	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4229	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4230	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4231	-	-	0/0/0/0	0/0/0/0
86	OHX	5	4232	-	-	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
88	3J6	5	4246	85	-	0/3/68/68	0/1/4/4
86	OHX	6	2045	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2046	-	-	0/0/0/0	0/0/0/0
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1	-	0/0/0/0	0/0/0/0
86	OHX	6	2190	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2191	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2192	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2193	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2194	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2195	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2196	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2197	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2198	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2199	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2200	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2201	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2202	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2203	-	-	0/0/0/0	0/0/0/0
86	OHX	6	2204	-	-	0/0/0/0	0/0/0/0
86	OHX	7	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	8	216	-	-	0/0/0/0	0/0/0/0
86	OHX	8	217	-	-	0/0/0/0	0/0/0/0
86	OHX	8	218	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	8	231	-	-	0/0/0/0	0/0/0/0
86	OHX	C3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	C5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	C8	201	-	-	0/0/0/0	0/0/0/0
86	OHX	D3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	D9	102	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	L3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	L4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	M0	304	-	-	0/0/0/0	0/0/0/0
86	OHX	M5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	205	-	-	0/0/0/0	0/0/0/0
86	OHX	M7	206	-	-	0/0/0/0	0/0/0/0
86	OHX	M9	203	-	-	0/0/0/0	0/0/0/0
86	OHX	N9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	O1	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O3	202	-	-	0/0/0/0	0/0/0/0
86	OHX	O4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O6	201	-	-	0/0/0/0	0/0/0/0
86	OHX	O7	103	-	-	0/0/0/0	0/0/0/0
86	OHX	O9	101	-	-	0/0/0/0	0/0/0/0
86	OHX	Q2	502	-	-	0/0/0/0	0/0/0/0
86	OHX	S6	301	-	-	0/0/0/0	0/0/0/0
86	OHX	S8	302	-	-	0/0/0/0	0/0/0/0
86	OHX	SR	401	-	-	0/0/0/0	0/0/0/0
86	OHX	c3	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c5	201	-	-	0/0/0/0	0/0/0/0
86	OHX	c8	203	-	-	0/0/0/0	0/0/0/0
86	OHX	d4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	d9	102	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OHX	l3	404	-	-	0/0/0/0	0/0/0/0
86	OHX	l3	405	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	402	-	-	0/0/0/0	0/0/0/0
86	OHX	l4	403	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	304	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	305	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	306	-	-	0/0/0/0	0/0/0/0
86	OHX	l5	307	-	-	0/0/0/0	0/0/0/0
86	OHX	l9	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	302	-	-	0/0/0/0	0/0/0/0
86	OHX	m0	303	-	-	0/0/0/0	0/0/0/0
86	OHX	m1	202	-	-	0/0/0/0	0/0/0/0
86	OHX	m4	201	-	-	0/0/0/0	0/0/0/0
86	OHX	m5	303	-	-	0/0/0/0	0/0/0/0
86	OHX	m6	203	-	-	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	n6	203	-	-	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	203	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	502	-	-	0/0/0/0	0/0/0/0
86	OHX	o7	503	-	-	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	s8	303	-	-	0/0/0/0	0/0/0/0
86	OHX	sR	401	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4213	3J6	C4-C3	6.53	1.66	1.54
88	1	4213	3J6	O2-C11	5.45	1.55	1.44
88	1	4213	3J6	C11-C7	-2.52	1.49	1.56
88	5	4246	3J6	C14-C4	2.29	1.57	1.51
88	5	4246	3J6	C4-C3	2.10	1.58	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	5	4246	3J6	O3-C10-C9	6.85	121.52	112.98
88	1	4213	3J6	C11-C7-C4	-4.68	103.63	106.67
88	1	4213	3J6	O2-C12-C11	4.60	64.68	59.24
88	5	4246	3J6	O1-C5-C6	-3.92	101.39	109.41
88	1	4213	3J6	C5-C6-C1	3.87	123.75	118.08

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	2	1750/1800 (97%)	0.15	84 (4%) 29 7	56, 95, 173, 261	0
1	6	1795/1800 (99%)	0.17	109 (6%) 21 5	45, 81, 195, 270	0
2	S0	206/251 (82%)	0.10	7 (3%) 43 10	95, 112, 128, 144	0
2	s0	206/251 (82%)	-0.14	1 (0%) 88 51	80, 99, 117, 126	0
3	S1	214/254 (84%)	0.59	15 (7%) 16 4	100, 130, 157, 170	0
3	s1	216/254 (85%)	0.06	1 (0%) 88 51	73, 89, 112, 120	0
4	S2	217/253 (85%)	-0.01	1 (0%) 88 51	72, 90, 107, 127	0
4	s2	217/253 (85%)	-0.04	1 (0%) 88 51	58, 75, 93, 98	0
5	S3	223/239 (93%)	0.15	7 (3%) 47 11	82, 94, 130, 144	0
5	s3	223/239 (93%)	0.31	6 (2%) 52 13	80, 123, 149, 162	0
6	S4	260/260 (100%)	0.30	6 (2%) 57 15	67, 95, 108, 128	0
6	s4	260/260 (100%)	-0.01	2 (0%) 83 39	55, 79, 93, 117	0
7	S5	206/224 (91%)	0.30	11 (5%) 25 6	102, 124, 143, 154	0
7	s5	206/224 (91%)	0.05	2 (0%) 79 33	71, 94, 119, 133	0
8	S6	226/236 (95%)	0.49	8 (3%) 42 10	69, 107, 127, 143	0
8	s6	218/236 (92%)	0.36	4 (1%) 65 20	55, 87, 112, 138	0
9	S7	184/189 (97%)	0.43	7 (3%) 38 9	92, 121, 144, 153	0
9	s7	186/189 (98%)	0.15	7 (3%) 38 9	76, 111, 141, 146	0
10	S8	188/200 (94%)	0.20	4 (2%) 60 17	60, 77, 116, 133	0
10	s8	188/200 (94%)	0.24	3 (1%) 68 22	51, 73, 118, 135	0
11	S9	185/196 (94%)	0.28	7 (3%) 38 9	89, 103, 137, 167	0
11	s9	185/196 (94%)	0.08	1 (0%) 88 51	67, 84, 122, 152	0
12	C0	96/105 (91%)	-0.02	0 100 100	87, 109, 134, 158	0
12	c0	96/105 (91%)	0.81	12 (12%) 5 2	119, 159, 174, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	C1	155/155 (100%)	0.17	4 (2%) 53 13	63, 76, 128, 138	0
13	c1	146/155 (94%)	0.07	1 (0%) 84 42	56, 68, 102, 126	0
14	C2	124/142 (87%)	1.35	33 (26%) 1 1	138, 150, 176, 189	0
14	c2	124/142 (87%)	2.20	61 (49%) 1 0	203, 215, 229, 233	0
15	C3	150/150 (100%)	0.11	0 100 100	72, 93, 109, 119	0
15	c3	150/150 (100%)	-0.01	0 100 100	63, 81, 98, 113	0
16	C4	127/136 (93%)	0.11	1 (0%) 83 39	70, 122, 138, 141	0
16	c4	128/136 (94%)	0.04	0 100 100	55, 86, 96, 110	0
17	C5	124/141 (87%)	0.08	1 (0%) 83 39	87, 105, 143, 156	0
17	c5	135/141 (95%)	0.32	8 (5%) 22 5	87, 109, 140, 148	0
18	C6	141/142 (99%)	0.32	8 (5%) 23 5	87, 116, 124, 128	0
18	c6	142/142 (100%)	0.27	5 (3%) 42 10	67, 87, 106, 130	0
19	C7	120/136 (88%)	0.53	10 (8%) 11 3	99, 114, 140, 142	0
19	c7	117/136 (86%)	0.24	3 (2%) 53 13	83, 96, 123, 124	0
20	C8	145/145 (100%)	0.44	6 (4%) 35 8	89, 115, 138, 147	0
20	c8	145/145 (100%)	0.08	2 (1%) 72 25	73, 93, 112, 127	0
21	C9	143/143 (100%)	0.42	6 (4%) 35 8	97, 114, 128, 144	0
21	c9	143/143 (100%)	-0.06	0 100 100	67, 82, 102, 125	0
22	D0	107/120 (89%)	0.87	14 (13%) 4 2	80, 117, 150, 156	0
22	d0	110/120 (91%)	0.92	22 (20%) 2 1	76, 117, 162, 172	0
23	D1	87/87 (100%)	0.03	1 (1%) 77 30	92, 100, 120, 131	0
23	d1	87/87 (100%)	-0.12	1 (1%) 77 30	73, 85, 110, 123	0
24	D2	129/129 (100%)	-0.12	0 100 100	74, 85, 95, 106	0
24	d2	129/129 (100%)	-0.15	0 100 100	56, 70, 79, 87	0
25	D3	144/144 (100%)	0.00	0 100 100	62, 68, 82, 97	0
25	d3	144/144 (100%)	-0.05	0 100 100	48, 53, 66, 86	0
26	D4	134/134 (100%)	0.30	0 100 100	79, 108, 124, 131	0
26	d4	134/134 (100%)	0.08	3 (2%) 59 16	62, 90, 108, 132	0
27	D5	70/107 (65%)	0.26	1 (1%) 72 25	119, 136, 144, 146	0
27	d5	69/107 (64%)	0.36	2 (2%) 49 12	84, 108, 122, 128	0
28	D6	97/97 (100%)	0.34	4 (4%) 35 8	75, 87, 143, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	-0.13	0 100 100	58, 67, 102, 110	0
29	D7	81/81 (100%)	0.15	3 (3%) 39 9	89, 104, 132, 137	0
29	d7	81/81 (100%)	0.12	1 (1%) 75 29	73, 91, 128, 133	0
30	D8	63/66 (95%)	0.98	7 (11%) 6 2	114, 127, 142, 152	0
30	d8	63/66 (95%)	0.47	1 (1%) 68 22	89, 105, 125, 136	0
31	D9	53/55 (96%)	0.06	1 (1%) 64 20	82, 88, 110, 123	0
31	d9	53/55 (96%)	0.54	2 (3%) 38 9	78, 94, 151, 167	0
32	E0	60/60 (100%)	0.87	10 (16%) 2 1	68, 99, 136, 143	0
33	E1	71/76 (93%)	1.12	13 (18%) 2 1	108, 134, 145, 147	0
33	e1	76/76 (100%)	2.09	31 (40%) 1 0	145, 190, 202, 204	0
34	SR	318/318 (100%)	0.36	14 (4%) 33 7	72, 125, 144, 161	0
34	sR	318/318 (100%)	0.35	11 (3%) 42 10	99, 119, 136, 150	0
35	SM	159/273 (58%)	0.31	8 (5%) 28 6	65, 95, 145, 151	0
35	sM	104/273 (38%)	0.48	10 (9%) 8 2	63, 110, 201, 212	0
36	1	3149/3396 (92%)	-0.09	101 (3%) 45 11	31, 55, 142, 259	0
36	5	3150/3396 (92%)	-0.13	59 (1%) 64 20	30, 54, 128, 238	0
37	3	121/121 (100%)	-0.26	1 (0%) 83 39	44, 73, 90, 96	0
37	7	121/121 (100%)	-0.29	1 (0%) 83 39	34, 56, 70, 77	0
38	4	158/158 (100%)	-0.31	2 (1%) 74 27	37, 58, 103, 140	0
38	8	158/158 (100%)	-0.22	3 (1%) 64 20	41, 67, 111, 136	0
39	L2	252/253 (99%)	-0.09	1 (0%) 90 57	36, 54, 72, 82	0
39	l2	252/253 (99%)	-0.07	4 (1%) 68 22	37, 58, 79, 93	0
40	L3	386/386 (100%)	-0.21	1 (0%) 91 63	34, 57, 75, 114	0
40	l3	386/386 (100%)	-0.25	1 (0%) 91 63	30, 42, 59, 103	0
41	L4	361/361 (100%)	-0.18	1 (0%) 91 63	35, 49, 67, 80	0
41	l4	361/361 (100%)	-0.14	0 100 100	36, 54, 74, 92	0
42	L5	296/296 (100%)	0.04	1 (0%) 91 63	55, 79, 100, 125	0
42	l5	294/296 (99%)	-0.19	1 (0%) 91 63	43, 59, 88, 140	0
43	L6	156/175 (89%)	-0.09	0 100 100	42, 49, 72, 93	0
43	l6	157/175 (89%)	-0.19	2 (1%) 74 27	44, 52, 73, 91	0
44	L7	222/243 (91%)	-0.29	2 (0%) 81 37	34, 43, 75, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	l7	223/243 (91%)	-0.28	0 100 100	32, 41, 80, 131	0
45	L8	233/255 (91%)	0.01	0 100 100	60, 77, 108, 128	0
45	l8	231/255 (90%)	0.46	5 (2%) 59 16	75, 90, 116, 125	0
46	L9	191/191 (100%)	0.06	1 (0%) 88 51	52, 65, 80, 93	0
46	l9	191/191 (100%)	-0.26	0 100 100	37, 48, 67, 81	0
47	M0	211/220 (95%)	-0.04	0 100 100	45, 57, 94, 128	0
47	m0	213/220 (96%)	-0.04	2 (0%) 81 37	43, 64, 88, 110	0
48	M1	169/173 (97%)	0.17	1 (0%) 86 46	63, 85, 100, 110	0
48	m1	169/173 (97%)	0.01	0 100 100	47, 62, 77, 92	0
49	M3	193/198 (97%)	-0.12	0 100 100	37, 56, 99, 126	0
49	m3	194/198 (97%)	-0.06	1 (0%) 88 51	49, 68, 114, 134	0
50	M4	136/137 (99%)	-0.09	1 (0%) 84 42	46, 55, 69, 82	0
50	m4	137/137 (100%)	-0.31	0 100 100	38, 46, 66, 77	0
51	M5	203/203 (100%)	-0.22	0 100 100	38, 52, 63, 71	0
51	m5	203/203 (100%)	-0.06	0 100 100	45, 61, 75, 81	0
52	M6	197/198 (99%)	-0.21	0 100 100	35, 43, 65, 70	0
52	m6	197/198 (99%)	-0.27	0 100 100	29, 33, 64, 71	0
53	M7	183/183 (100%)	0.01	7 (3%) 38 9	40, 47, 107, 140	0
53	m7	155/183 (84%)	-0.20	0 100 100	35, 44, 55, 88	0
54	M8	185/185 (100%)	-0.27	0 100 100	37, 48, 64, 89	0
54	m8	185/185 (100%)	-0.25	0 100 100	39, 52, 62, 68	0
55	M9	188/188 (100%)	0.19	4 (2%) 60 17	56, 73, 155, 162	0
55	m9	188/188 (100%)	0.21	1 (0%) 88 51	53, 66, 139, 150	0
56	N0	172/172 (100%)	-0.21	1 (0%) 86 46	44, 53, 67, 72	0
56	n0	172/172 (100%)	-0.24	0 100 100	35, 42, 54, 68	0
57	N1	159/159 (100%)	-0.10	2 (1%) 74 27	42, 52, 97, 106	0
57	n1	159/159 (100%)	-0.15	0 100 100	39, 44, 80, 84	0
58	N2	100/120 (83%)	0.79	9 (9%) 10 3	86, 102, 117, 131	0
58	n2	98/120 (81%)	0.40	3 (3%) 47 11	77, 92, 106, 108	0
59	N3	136/136 (100%)	-0.12	0 100 100	42, 52, 67, 77	0
59	n3	136/136 (100%)	-0.23	1 (0%) 84 42	34, 41, 57, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	N4	98/155 (63%)	0.82	19 (19%) 2 1	50, 70, 163, 168	0
60	n4	135/155 (87%)	0.34	9 (6%) 17 4	44, 92, 135, 152	0
61	N5	121/141 (85%)	0.01	2 (1%) 67 21	51, 65, 88, 127	0
61	n5	120/141 (85%)	0.29	4 (3%) 44 10	56, 71, 92, 99	0
62	N6	126/126 (100%)	-0.15	0 100 100	52, 59, 69, 79	0
62	n6	126/126 (100%)	0.07	1 (0%) 83 39	58, 66, 84, 92	0
63	N7	135/135 (100%)	0.17	0 100 100	75, 90, 107, 117	0
63	n7	135/135 (100%)	0.04	1 (0%) 84 42	83, 98, 119, 129	0
64	N8	148/148 (100%)	-0.12	0 100 100	34, 48, 72, 84	0
64	n8	148/148 (100%)	-0.09	0 100 100	40, 54, 73, 77	0
65	N9	58/58 (100%)	0.08	2 (3%) 43 10	47, 57, 100, 115	0
65	n9	58/58 (100%)	-0.02	0 100 100	37, 54, 81, 94	0
66	O0	97/104 (93%)	-0.11	1 (1%) 79 33	73, 83, 105, 111	0
66	o0	100/104 (96%)	-0.04	0 100 100	74, 86, 111, 122	0
67	O1	109/112 (97%)	0.21	1 (0%) 81 37	53, 64, 98, 111	0
67	o1	109/112 (97%)	0.04	1 (0%) 81 37	42, 55, 95, 112	0
68	O2	127/129 (98%)	-0.11	2 (1%) 68 22	30, 43, 55, 68	0
68	o2	127/129 (98%)	-0.14	2 (1%) 68 22	32, 52, 65, 82	0
69	O3	106/106 (100%)	-0.20	0 100 100	36, 42, 66, 76	0
69	o3	106/106 (100%)	-0.15	1 (0%) 81 37	34, 41, 68, 84	0
70	O4	112/119 (94%)	0.25	3 (2%) 52 13	55, 70, 115, 131	0
70	o4	112/119 (94%)	0.17	0 100 100	52, 75, 118, 127	0
71	O5	119/119 (100%)	-0.01	0 100 100	50, 67, 76, 77	0
71	o5	119/119 (100%)	0.04	0 100 100	59, 74, 88, 94	0
72	O6	99/99 (100%)	0.03	2 (2%) 62 19	56, 67, 98, 111	0
72	o6	99/99 (100%)	0.02	0 100 100	62, 77, 94, 111	0
73	O7	87/87 (100%)	0.04	0 100 100	41, 46, 72, 92	0
73	o7	87/87 (100%)	0.13	2 (2%) 57 15	46, 51, 85, 129	0
74	O8	77/77 (100%)	0.11	1 (1%) 74 27	81, 90, 113, 119	0
74	o8	77/77 (100%)	0.53	2 (2%) 53 13	81, 92, 108, 112	0
75	O9	50/50 (100%)	-0.22	0 100 100	49, 54, 59, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	o9	50/50 (100%)	-0.11	0 100 100	53, 57, 69, 79	0
76	Q0	52/52 (100%)	-0.08	0 100 100	48, 56, 75, 85	0
76	q0	52/52 (100%)	-0.17	1 (1%) 64 20	33, 38, 49, 58	0
77	Q1	25/25 (100%)	0.24	1 (4%) 36 8	62, 64, 68, 72	0
77	q1	25/25 (100%)	-0.15	0 100 100	47, 51, 64, 73	0
78	Q2	105/105 (100%)	0.31	3 (2%) 49 12	39, 57, 80, 115	0
78	q2	105/105 (100%)	0.37	0 100 100	43, 56, 79, 106	0
79	Q3	91/91 (100%)	-0.10	0 100 100	46, 56, 76, 96	0
79	q3	91/91 (100%)	-0.18	0 100 100	43, 58, 73, 83	0
80	e0	62/62 (100%)	0.56	5 (8%) 12 3	61, 81, 122, 132	0
81	m2	0/160	-	-	-	-
82	p0	143/311 (45%)	0.28	6 (4%) 35 8	88, 107, 168, 173	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35344 (93%)	0.06	907 (2%) 52 13	29, 72, 139, 270	0

The worst 5 of 907 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	1	1237	G	10.1
1	6	662	U	10.0
36	1	1238	C	9.5
60	N4	75	THR	9.3
1	2	718	U	9.3

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3445	1/1	0.85	662.00	32,32,32,32	0
85	MG	2	2013	1/1	0.76	588.00	80,80,80,80	0
85	MG	5	3732	1/1	0.59	478.00	79,79,79,79	0
85	MG	2	1956	1/1	1.47	324.25	83,83,83,83	0
85	MG	L3	403	1/1	0.94	303.00	46,46,46,46	0
85	MG	5	3621	1/1	0.76	292.65	49,49,49,49	0
85	MG	4	219	1/1	0.54	274.36	86,86,86,86	0
85	MG	1	3402	1/1	0.83	271.14	75,75,75,75	0
85	MG	5	3457	1/1	0.45	237.60	32,32,32,32	0
85	MG	2	2008	1/1	0.48	223.00	66,66,66,66	0
85	MG	6	1924	1/1	1.18	182.27	105,105,105,105	0
85	MG	7	202	1/1	0.90	177.34	41,41,41,41	0
85	MG	5	3490	1/1	0.50	173.50	49,49,49,49	0
85	MG	8	214	1/1	1.06	156.50	67,67,67,67	0
85	MG	1	3701	1/1	0.38	141.67	65,65,65,65	0
85	MG	1	3738	1/1	0.65	140.71	76,76,76,76	0
85	MG	5	3517	1/1	0.63	137.29	21,21,21,21	0
85	MG	5	3480	1/1	0.84	135.84	87,87,87,87	0
85	MG	1	3410	1/1	0.47	130.81	20,20,20,20	0
85	MG	1	3693	1/1	0.64	127.08	56,56,56,56	0
85	MG	6	2039	1/1	0.83	116.76	66,66,66,66	0
85	MG	5	3465	1/1	0.54	112.94	58,58,58,58	0
85	MG	4	203	1/1	0.70	112.40	49,49,49,49	0
86	OHX	1	4185	7/7	0.60	110.50	194,194,194,194	0
85	MG	6	2043	1/1	0.78	103.83	106,106,106,106	0
85	MG	5	3703	1/1	0.29	101.67	55,55,55,55	0
85	MG	3	202	1/1	0.60	98.65	51,51,51,51	0
85	MG	1	3596	1/1	0.84	98.47	26,26,26,26	0
85	MG	1	3649	1/1	0.49	96.71	34,34,34,34	0
85	MG	8	215	1/1	0.56	95.75	38,38,38,38	0
85	MG	5	3452	1/1	0.67	94.42	40,40,40,40	0
86	OHX	5	4042	7/7	0.25	91.86	142,142,142,142	0
85	MG	6	1933	1/1	0.77	91.62	75,75,75,75	0
85	MG	1	3598	1/1	0.74	89.04	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	2	1973	1/1	1.84	88.91	99,99,99,99	0
85	MG	5	3506	1/1	0.67	87.06	42,42,42,42	0
85	MG	1	3474	1/1	0.69	85.26	78,78,78,78	0
85	MG	1	3758	1/1	0.44	81.86	98,98,98,98	0
85	MG	6	2030	1/1	0.90	78.76	67,67,67,67	0
85	MG	5	3565	1/1	0.49	76.50	43,43,43,43	0
85	MG	5	3552	1/1	0.72	76.34	39,39,39,39	0
85	MG	4	202	1/1	0.88	76.01	51,51,51,51	0
85	MG	5	3883	1/1	0.56	75.55	44,44,44,44	0
86	OHX	1	4163	7/7	0.38	74.60	174,174,174,174	0
85	MG	2	1957	1/1	1.03	74.58	76,76,76,76	0
85	MG	5	3735	1/1	0.46	74.30	43,43,43,43	0
85	MG	5	3581	1/1	1.08	73.81	58,58,58,58	0
85	MG	1	3492	1/1	0.72	73.52	57,57,57,57	0
85	MG	1	3561	1/1	0.58	72.78	37,37,37,37	0
85	MG	1	3458	1/1	0.79	72.50	77,77,77,77	0
85	MG	5	3787	1/1	0.46	72.14	64,64,64,64	0
85	MG	5	3434	1/1	0.57	70.37	36,36,36,36	0
85	MG	1	3661	1/1	0.31	70.00	48,48,48,48	0
85	MG	5	3644	1/1	0.85	69.49	60,60,60,60	0
85	MG	6	1980	1/1	0.89	68.71	64,64,64,64	0
85	MG	1	3846	1/1	0.92	67.88	53,53,53,53	0
85	MG	1	3499	1/1	0.55	67.36	61,61,61,61	0
85	MG	7	211	1/1	0.34	67.00	63,63,63,63	0
85	MG	5	3406	1/1	0.85	65.78	44,44,44,44	0
85	MG	5	3435	1/1	0.75	65.13	45,45,45,45	0
85	MG	4	201	1/1	0.69	65.12	51,51,51,51	0
85	MG	5	3574	1/1	0.61	64.57	27,27,27,27	0
85	MG	5	3712	1/1	0.46	64.45	50,50,50,50	0
85	MG	1	3854	1/1	0.49	64.40	73,73,73,73	0
85	MG	5	3672	1/1	0.48	64.20	54,54,54,54	0
85	MG	3	201	1/1	0.37	64.16	76,76,76,76	0
85	MG	5	3706	1/1	0.60	63.61	104,104,104,104	0
85	MG	1	3742	1/1	0.33	63.52	65,65,65,65	0
85	MG	2	2007	1/1	1.25	62.38	54,54,54,54	0
85	MG	l7	302	1/1	0.55	61.83	41,41,41,41	0
85	MG	1	3493	1/1	0.53	61.62	83,83,83,83	0
85	MG	1	3865	1/1	0.65	61.50	70,70,70,70	0
85	MG	6	1926	1/1	0.61	60.73	53,53,53,53	0
85	MG	6	1973	1/1	0.60	60.61	48,48,48,48	0
85	MG	2	1991	1/1	0.39	60.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3770	1/1	0.53	60.02	72,72,72,72	0
85	MG	1	3468	1/1	0.64	59.17	47,47,47,47	0
85	MG	5	4249	1/1	0.55	58.24	49,49,49,49	0
85	MG	5	3826	1/1	0.99	58.23	51,51,51,51	0
85	MG	2	1917	1/1	0.76	58.12	52,52,52,52	0
85	MG	5	3801	1/1	0.65	58.08	50,50,50,50	0
85	MG	1	3512	1/1	0.75	57.85	26,26,26,26	0
85	MG	5	3689	1/1	0.78	57.76	66,66,66,66	0
85	MG	1	3536	1/1	0.83	57.52	63,63,63,63	0
86	OHX	5	4198	7/7	0.58	57.48	159,159,159,159	0
85	MG	5	3576	1/1	0.51	57.17	29,29,29,29	0
85	MG	1	3707	1/1	0.94	57.03	51,51,51,51	0
85	MG	2	1909	1/1	0.87	56.80	73,73,73,73	0
85	MG	5	3560	1/1	0.66	56.46	32,32,32,32	0
85	MG	5	3622	1/1	0.65	56.34	39,39,39,39	0
85	MG	6	1915	1/1	0.85	56.01	47,47,47,47	0
85	MG	5	3563	1/1	0.62	55.31	32,32,32,32	0
86	OHX	1	4194	7/7	0.51	55.03	148,148,148,148	0
85	MG	6	1918	1/1	0.81	54.62	78,78,78,78	0
85	MG	5	3562	1/1	0.86	53.88	36,36,36,36	0
85	MG	2	2012	1/1	0.59	53.81	65,65,65,65	0
85	MG	1	3418	1/1	0.79	53.71	60,60,60,60	0
85	MG	2	1994	1/1	0.80	53.01	57,57,57,57	0
85	MG	2	1967	1/1	0.36	53.00	95,95,95,95	0
85	MG	5	3871	1/1	0.74	52.82	44,44,44,44	0
85	MG	5	3626	1/1	0.57	52.67	38,38,38,38	0
85	MG	6	2010	1/1	0.44	52.67	55,55,55,55	0
85	MG	1	3670	1/1	0.64	51.99	50,50,50,50	0
85	MG	5	3737	1/1	0.77	51.69	32,32,32,32	0
85	MG	7	215	1/1	0.48	51.67	47,47,47,47	0
85	MG	6	1958	1/1	0.75	51.61	60,60,60,60	0
85	MG	2	1934	1/1	0.59	51.02	58,58,58,58	0
85	MG	N3	201	1/1	0.52	50.93	40,40,40,40	0
85	MG	5	3876	1/1	0.81	50.55	59,59,59,59	0
85	MG	1	3637	1/1	0.72	50.26	78,78,78,78	0
85	MG	6	1910	1/1	0.64	50.03	53,53,53,53	0
85	MG	5	3695	1/1	1.05	49.74	81,81,81,81	0
85	MG	2	2017	1/1	1.09	49.43	80,80,80,80	0
85	MG	1	3685	1/1	0.48	49.38	45,45,45,45	0
85	MG	5	3765	1/1	1.20	49.34	31,31,31,31	0
85	MG	5	3716	1/1	1.08	49.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3418	1/1	0.92	49.16	29,29,29,29	0
85	MG	1	4215	1/1	0.64	48.85	48,48,48,48	0
85	MG	1	3623	1/1	0.55	48.65	48,48,48,48	0
86	OHX	5	4216	7/7	0.49	48.15	189,189,189,189	0
85	MG	2	1937	1/1	0.69	48.13	65,65,65,65	0
85	MG	5	3704	1/1	0.92	47.93	51,51,51,51	0
85	MG	5	3501	1/1	0.55	47.82	45,45,45,45	0
85	MG	1	3790	1/1	0.54	47.77	49,49,49,49	0
85	MG	1	3583	1/1	0.47	47.69	22,22,22,22	0
85	MG	5	3584	1/1	0.80	47.29	27,27,27,27	0
85	MG	6	1956	1/1	0.76	46.69	44,44,44,44	0
85	MG	2	1987	1/1	0.39	46.45	101,101,101,101	0
85	MG	5	3548	1/1	0.83	46.21	46,46,46,46	0
85	MG	5	3885	1/1	0.61	45.30	26,26,26,26	0
85	MG	5	3881	1/1	0.83	45.00	68,68,68,68	0
85	MG	1	3558	1/1	0.71	44.92	61,61,61,61	0
85	MG	5	3486	1/1	0.57	44.87	46,46,46,46	0
85	MG	5	3577	1/1	1.18	44.80	45,45,45,45	0
85	MG	1	3414	1/1	0.77	43.99	59,59,59,59	0
85	MG	5	3545	1/1	0.67	43.81	45,45,45,45	0
85	MG	1	3698	1/1	0.60	43.16	45,45,45,45	0
85	MG	5	3494	1/1	0.47	43.00	37,37,37,37	0
85	MG	2	1936	1/1	0.49	42.95	57,57,57,57	0
85	MG	5	3530	1/1	0.70	42.94	20,20,20,20	0
85	MG	1	3834	1/1	0.97	42.65	59,59,59,59	0
85	MG	5	3860	1/1	1.18	42.51	62,62,62,62	0
85	MG	8	204	1/1	0.90	42.04	58,58,58,58	0
85	MG	1	3708	1/1	1.40	41.94	73,73,73,73	0
85	MG	5	3604	1/1	0.39	41.68	35,35,35,35	0
85	MG	1	3754	1/1	0.57	41.18	58,58,58,58	0
85	MG	5	3891	1/1	0.71	41.04	86,86,86,86	0
85	MG	2	1918	1/1	0.90	41.00	51,51,51,51	0
85	MG	6	2036	1/1	0.79	40.90	74,74,74,74	0
85	MG	2	1903	1/1	0.86	40.55	45,45,45,45	0
85	MG	2	1988	1/1	1.12	40.48	63,63,63,63	0
85	MG	1	3419	1/1	1.32	40.35	95,95,95,95	0
85	MG	5	3681	1/1	0.37	40.07	46,46,46,46	0
85	MG	2	1979	1/1	1.05	40.02	60,60,60,60	0
85	MG	3	204	1/1	0.67	39.87	52,52,52,52	0
85	MG	1	3774	1/1	0.42	39.43	58,58,58,58	0
85	MG	1	3514	1/1	0.51	39.26	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	7	206	1/1	0.65	39.25	29,29,29,29	0
85	MG	1	3837	1/1	0.73	39.25	34,34,34,34	0
86	OHX	5	4176	7/7	0.45	39.22	159,159,159,159	0
85	MG	6	1931	1/1	0.57	39.03	64,64,64,64	0
85	MG	M5	302	1/1	0.94	39.01	53,53,53,53	0
85	MG	1	3549	1/1	0.75	38.73	38,38,38,38	0
85	MG	1	3522	1/1	0.75	38.72	34,34,34,34	0
85	MG	1	3460	1/1	0.66	38.45	24,24,24,24	0
85	MG	1	3405	1/1	1.07	38.43	64,64,64,64	0
85	MG	1	3449	1/1	0.44	38.42	36,36,36,36	0
85	MG	1	3413	1/1	0.42	38.39	44,44,44,44	0
85	MG	5	3879	1/1	0.73	38.33	63,63,63,63	0
85	MG	6	2033	1/1	1.16	38.27	64,64,64,64	0
85	MG	5	3666	1/1	0.79	38.24	43,43,43,43	0
85	MG	1	3497	1/1	0.48	38.13	52,52,52,52	0
85	MG	5	3536	1/1	0.61	38.08	34,34,34,34	0
85	MG	5	3865	1/1	0.72	38.08	40,40,40,40	0
85	MG	1	3728	1/1	0.56	38.07	49,49,49,49	0
85	MG	1	3741	1/1	0.50	37.56	57,57,57,57	0
85	MG	5	3403	1/1	1.02	37.14	66,66,66,66	0
85	MG	2	1907	1/1	0.80	37.06	60,60,60,60	0
85	MG	6	1904	1/1	0.86	36.94	75,75,75,75	0
85	MG	1	3712	1/1	0.32	36.75	59,59,59,59	0
85	MG	1	3851	1/1	0.44	36.62	41,41,41,41	0
85	MG	1	3486	1/1	0.63	36.38	32,32,32,32	0
85	MG	1	3860	1/1	0.30	36.26	78,78,78,78	0
85	MG	1	3500	1/1	0.80	36.08	84,84,84,84	0
86	OHX	1	4169	7/7	0.51	35.88	178,178,178,178	0
85	MG	5	3566	1/1	0.57	35.71	29,29,29,29	0
85	MG	5	3496	1/1	0.36	35.67	38,38,38,38	0
85	MG	3	209	1/1	0.63	35.58	62,62,62,62	0
85	MG	2	2022	1/1	1.06	35.55	128,128,128,128	0
85	MG	5	3846	1/1	0.65	35.54	51,51,51,51	0
85	MG	1	3671	1/1	1.17	35.52	46,46,46,46	0
85	MG	6	1913	1/1	0.53	35.47	41,41,41,41	0
85	MG	5	3583	1/1	0.56	35.35	32,32,32,32	0
86	OHX	1	4202	7/7	0.42	35.34	147,147,147,147	0
85	MG	5	3414	1/1	0.54	35.29	29,29,29,29	0
85	MG	5	3882	1/1	0.82	35.26	62,62,62,62	0
85	MG	2	1914	1/1	0.86	35.12	76,76,76,76	0
85	MG	5	3488	1/1	0.55	34.90	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	6	1951	1/1	0.72	34.68	80,80,80,80	0
85	MG	1	3407	1/1	0.86	34.63	43,43,43,43	0
85	MG	4	210	1/1	0.26	34.50	57,57,57,57	0
85	MG	1	3607	1/1	1.14	34.35	50,50,50,50	0
85	MG	1	3668	1/1	0.48	34.23	44,44,44,44	0
85	MG	1	3575	1/1	0.66	33.85	25,25,25,25	0
85	MG	5	3856	1/1	0.46	33.82	70,70,70,70	0
85	MG	5	3520	1/1	0.62	33.77	41,41,41,41	0
85	MG	1	3829	1/1	0.38	33.67	32,32,32,32	0
85	MG	2	1980	1/1	0.99	33.63	67,67,67,67	0
85	MG	5	3444	1/1	0.30	33.50	48,48,48,48	0
85	MG	5	3638	1/1	0.56	33.47	65,65,65,65	0
85	MG	6	1945	1/1	0.42	33.45	38,38,38,38	0
85	MG	1	3423	1/1	0.44	33.44	40,40,40,40	0
85	MG	1	3591	1/1	0.65	33.37	34,34,34,34	0
85	MG	1	3659	1/1	0.76	33.36	45,45,45,45	0
85	MG	5	3590	1/1	0.40	33.31	47,47,47,47	0
85	MG	5	3862	1/1	0.24	33.10	44,44,44,44	0
85	MG	6	2028	1/1	0.93	32.98	91,91,91,91	0
85	MG	5	3608	1/1	0.43	32.96	34,34,34,34	0
85	MG	5	3454	1/1	0.34	32.88	42,42,42,42	0
85	MG	1	3644	1/1	0.37	32.83	42,42,42,42	0
85	MG	1	3588	1/1	0.56	32.65	25,25,25,25	0
85	MG	3	206	1/1	0.62	32.61	31,31,31,31	0
85	MG	5	3447	1/1	0.34	32.44	46,46,46,46	0
85	MG	5	3675	1/1	0.82	32.28	58,58,58,58	0
85	MG	1	3571	1/1	0.75	32.26	48,48,48,48	0
85	MG	5	3513	1/1	0.64	32.10	30,30,30,30	0
85	MG	5	3596	1/1	0.70	32.03	33,33,33,33	0
85	MG	1	3523	1/1	0.40	32.00	29,29,29,29	0
85	MG	1	3534	1/1	0.64	31.95	24,24,24,24	0
85	MG	1	3599	1/1	0.67	31.93	23,23,23,23	0
85	MG	5	3818	1/1	0.78	31.91	51,51,51,51	0
85	MG	6	1944	1/1	0.89	31.87	65,65,65,65	0
85	MG	1	3551	1/1	0.64	31.78	39,39,39,39	0
85	MG	S2	301	1/1	1.08	31.75	64,64,64,64	0
85	MG	2	1925	1/1	1.02	31.62	57,57,57,57	0
85	MG	5	3597	1/1	0.74	31.56	33,33,33,33	0
85	MG	1	3435	1/1	0.33	31.55	43,43,43,43	0
85	MG	5	3682	1/1	0.70	31.47	91,91,91,91	0
85	MG	1	3617	1/1	0.62	31.46	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3850	1/1	0.68	31.38	47,47,47,47	0
85	MG	5	3570	1/1	0.76	31.35	28,28,28,28	0
85	MG	5	3749	1/1	0.93	31.32	47,47,47,47	0
85	MG	5	3730	1/1	0.59	31.18	76,76,76,76	0
85	MG	5	3539	1/1	0.58	31.07	26,26,26,26	0
85	MG	1	3785	1/1	0.70	31.04	37,37,37,37	0
85	MG	1	3579	1/1	0.80	30.93	32,32,32,32	0
85	MG	5	3529	1/1	0.51	30.92	31,31,31,31	0
85	MG	5	3544	1/1	0.76	30.74	51,51,51,51	0
85	MG	1	3832	1/1	0.40	30.63	29,29,29,29	0
86	OHX	5	4146	7/7	0.27	30.60	167,167,167,167	0
85	MG	1	3537	1/1	0.88	30.49	35,35,35,35	0
86	OHX	6	2183	7/7	0.50	30.46	168,168,168,168	0
85	MG	6	1922	1/1	0.81	30.45	63,63,63,63	0
85	MG	6	1905	1/1	0.72	30.42	47,47,47,47	0
85	MG	8	209	1/1	0.21	30.41	67,67,67,67	0
85	MG	5	3561	1/1	0.93	30.22	22,22,22,22	0
85	MG	1	3473	1/1	0.68	30.22	26,26,26,26	0
85	MG	7	210	1/1	0.67	30.18	41,41,41,41	0
86	OHX	1	4170	7/7	0.47	30.14	190,190,190,190	0
85	MG	2	2015	1/1	0.83	30.09	67,67,67,67	0
85	MG	7	212	1/1	0.50	30.06	42,42,42,42	0
85	MG	l2	301	1/1	0.68	29.91	44,44,44,44	0
85	MG	1	3452	1/1	0.38	29.86	44,44,44,44	0
85	MG	6	2020	1/1	0.47	29.70	118,118,118,118	0
85	MG	6	1948	1/1	0.60	29.59	37,37,37,37	0
85	MG	1	3653	1/1	0.40	29.57	79,79,79,79	0
85	MG	1	3585	1/1	0.87	29.51	55,55,55,55	0
85	MG	5	3751	1/1	0.52	29.40	33,33,33,33	0
85	MG	5	3538	1/1	0.43	29.40	23,23,23,23	0
85	MG	1	3645	1/1	0.42	29.24	42,42,42,42	0
85	MG	2	1940	1/1	0.52	29.19	70,70,70,70	0
85	MG	5	3792	1/1	0.60	28.94	53,53,53,53	0
86	OHX	1	4203	7/7	0.36	28.92	152,152,152,152	0
85	MG	5	3889	1/1	0.75	28.88	58,58,58,58	0
85	MG	5	3512	1/1	0.59	28.86	60,60,60,60	0
85	MG	1	3814	1/1	0.54	28.79	51,51,51,51	0
85	MG	1	3527	1/1	0.70	28.78	31,31,31,31	0
85	MG	1	3803	1/1	0.53	28.77	51,51,51,51	0
85	MG	1	3506	1/1	0.59	28.74	36,36,36,36	0
85	MG	1	3461	1/1	0.42	28.71	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3595	1/1	0.55	28.57	17,17,17,17	0
85	MG	5	3764	1/1	0.32	28.50	62,62,62,62	0
85	MG	1	3574	1/1	0.61	28.43	42,42,42,42	0
85	MG	5	3587	1/1	0.62	28.40	58,58,58,58	0
85	MG	6	1921	1/1	0.43	28.38	46,46,46,46	0
85	MG	2	1913	1/1	1.32	28.37	87,87,87,87	0
85	MG	2	2019	1/1	1.40	28.33	89,89,89,89	0
85	MG	5	3585	1/1	0.58	28.20	25,25,25,25	0
85	MG	1	3564	1/1	0.54	28.13	45,45,45,45	0
85	MG	5	3459	1/1	0.33	28.07	32,32,32,32	0
85	MG	5	3869	1/1	0.72	27.91	51,51,51,51	0
85	MG	1	3779	1/1	0.45	27.80	60,60,60,60	0
85	MG	1	3850	1/1	0.84	27.62	61,61,61,61	0
85	MG	1	3679	1/1	0.47	27.57	68,68,68,68	0
85	MG	2	1904	1/1	0.57	27.54	74,74,74,74	0
85	MG	2	1978	1/1	1.06	27.51	71,71,71,71	0
85	MG	5	3664	1/1	0.89	27.38	50,50,50,50	0
85	MG	4	218	1/1	0.67	27.08	58,58,58,58	0
85	MG	1	3835	1/1	0.56	27.03	24,24,24,24	0
85	MG	1	3691	1/1	0.67	26.98	52,52,52,52	0
85	MG	5	3537	1/1	0.56	26.71	35,35,35,35	0
85	MG	6	2031	1/1	0.52	26.39	71,71,71,71	0
85	MG	2	1981	1/1	0.70	26.28	78,78,78,78	0
85	MG	2	1926	1/1	0.70	26.21	96,96,96,96	0
85	MG	5	3472	1/1	0.44	26.01	41,41,41,41	0
85	MG	1	3544	1/1	0.52	25.96	40,40,40,40	0
85	MG	6	1912	1/1	0.76	25.93	53,53,53,53	0
85	MG	6	1955	1/1	0.89	25.91	40,40,40,40	0
85	MG	2	1952	1/1	0.69	25.90	115,115,115,115	0
85	MG	5	3482	1/1	0.23	25.89	57,57,57,57	0
85	MG	1	3640	1/1	0.43	25.86	51,51,51,51	0
85	MG	6	1928	1/1	0.79	25.78	78,78,78,78	0
85	MG	5	3778	1/1	0.37	25.75	92,92,92,92	0
85	MG	3	205	1/1	0.48	25.75	41,41,41,41	0
85	MG	6	1925	1/1	0.70	25.67	42,42,42,42	0
85	MG	1	3552	1/1	0.82	25.66	40,40,40,40	0
85	MG	1	3513	1/1	0.53	25.60	23,23,23,23	0
85	MG	1	3824	1/1	0.52	25.46	49,49,49,49	0
85	MG	6	1976	1/1	0.76	25.45	68,68,68,68	0
85	MG	1	3859	1/1	0.40	25.35	55,55,55,55	0
85	MG	O3	201	1/1	0.32	25.32	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	6	2181	7/7	0.38	25.29	150,150,150,150	0
86	OHX	5	4174	7/7	0.51	25.20	167,167,167,167	0
85	MG	1	3467	1/1	0.63	25.19	44,44,44,44	0
85	MG	5	3623	1/1	0.69	25.18	61,61,61,61	0
85	MG	1	3573	1/1	0.77	25.17	25,25,25,25	0
85	MG	6	2009	1/1	0.58	25.09	59,59,59,59	0
85	MG	5	3736	1/1	0.68	25.08	76,76,76,76	0
85	MG	1	3593	1/1	0.58	25.06	72,72,72,72	0
85	MG	2	2014	1/1	1.01	24.97	65,65,65,65	0
85	MG	2	1905	1/1	0.56	24.93	58,58,58,58	0
85	MG	1	3843	1/1	0.35	24.78	57,57,57,57	0
85	MG	6	2027	1/1	0.62	24.75	73,73,73,73	0
85	MG	1	3511	1/1	0.59	24.69	41,41,41,41	0
85	MG	1	3590	1/1	0.99	24.65	46,46,46,46	0
85	MG	5	3568	1/1	0.61	24.60	35,35,35,35	0
86	OHX	5	4134	7/7	0.24	24.56	158,158,158,158	0
85	MG	c8	201	1/1	1.12	24.54	81,81,81,81	0
85	MG	1	3503	1/1	0.50	24.52	29,29,29,29	0
85	MG	5	3726	1/1	0.53	24.52	29,29,29,29	0
85	MG	5	3580	1/1	0.61	24.34	34,34,34,34	0
85	MG	5	3535	1/1	0.71	24.32	39,39,39,39	0
86	OHX	6	2167	7/7	0.50	24.31	132,132,132,132	0
85	MG	5	3766	1/1	0.70	24.26	37,37,37,37	0
85	MG	1	3863	1/1	0.62	24.25	51,51,51,51	0
85	MG	1	3699	1/1	0.34	24.20	46,46,46,46	0
85	MG	5	3426	1/1	1.15	24.15	50,50,50,50	0
85	MG	5	3632	1/1	0.44	24.14	97,97,97,97	0
85	MG	2	1902	1/1	0.40	24.11	52,52,52,52	0
85	MG	2	1912	1/1	0.72	24.06	72,72,72,72	0
85	MG	5	3639	1/1	0.54	23.80	45,45,45,45	0
85	MG	2	1935	1/1	0.69	23.66	52,52,52,52	0
85	MG	5	3794	1/1	0.51	23.64	56,56,56,56	0
86	OHX	1	4188	7/7	0.57	23.60	149,149,149,149	0
85	MG	5	3573	1/1	0.90	23.59	38,38,38,38	0
85	MG	6	2002	1/1	0.80	23.56	83,83,83,83	0
86	OHX	3	224	7/7	0.32	23.52	176,176,176,176	0
85	MG	1	3462	1/1	0.53	23.47	27,27,27,27	0
85	MG	2	2018	1/1	0.68	23.45	78,78,78,78	0
85	MG	1	3857	1/1	0.58	23.44	44,44,44,44	0
85	MG	6	2011	1/1	0.77	23.32	68,68,68,68	0
85	MG	1	3525	1/1	0.42	23.29	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3637	1/1	0.48	23.29	56,56,56,56	0
86	OHX	5	4223	7/7	0.46	23.25	131,131,131,131	0
85	MG	1	3431	1/1	0.53	23.23	52,52,52,52	0
85	MG	1	3447	1/1	0.50	22.94	31,31,31,31	0
85	MG	5	3554	1/1	0.69	22.92	47,47,47,47	0
85	MG	5	3518	1/1	0.49	22.91	27,27,27,27	0
85	MG	5	3540	1/1	0.61	22.88	32,32,32,32	0
85	MG	1	3587	1/1	0.67	22.88	39,39,39,39	0
85	MG	1	3476	1/1	0.22	22.83	53,53,53,53	0
85	MG	N8	203	1/1	0.58	22.82	34,34,34,34	0
85	MG	5	3858	1/1	0.80	22.71	58,58,58,58	0
86	OHX	1	4079	7/7	0.27	22.69	144,144,144,144	0
85	MG	5	3756	1/1	0.38	22.68	59,59,59,59	0
85	MG	1	3801	1/1	0.42	22.60	37,37,37,37	0
85	MG	2	1945	1/1	0.54	22.56	98,98,98,98	0
85	MG	1	3655	1/1	0.63	22.53	71,71,71,71	0
85	MG	6	1959	1/1	0.66	22.45	57,57,57,57	0
85	MG	5	3443	1/1	0.44	22.45	35,35,35,35	0
85	MG	1	3795	1/1	0.33	22.37	62,62,62,62	0
85	MG	1	3635	1/1	0.48	22.33	59,59,59,59	0
85	MG	2	1982	1/1	0.35	22.25	77,77,77,77	0
85	MG	1	3515	1/1	0.98	22.24	40,40,40,40	0
85	MG	5	3693	1/1	0.41	22.23	52,52,52,52	0
85	MG	6	1916	1/1	1.48	22.13	58,58,58,58	0
85	MG	1	3808	1/1	0.63	22.05	39,39,39,39	0
85	MG	1	3562	1/1	0.44	21.94	24,24,24,24	0
85	MG	5	3508	1/1	0.55	21.91	38,38,38,38	0
85	MG	1	3715	1/1	0.46	21.88	62,62,62,62	0
85	MG	5	3541	1/1	0.57	21.88	33,33,33,33	0
85	MG	1	3535	1/1	0.72	21.81	50,50,50,50	0
85	MG	2	1938	1/1	0.63	21.77	72,72,72,72	0
85	MG	5	3427	1/1	0.39	21.69	32,32,32,32	0
85	MG	6	1968	1/1	0.59	21.68	70,70,70,70	0
85	MG	1	3455	1/1	0.85	21.67	59,59,59,59	0
85	MG	5	3790	1/1	0.32	21.67	73,73,73,73	0
86	OHX	5	4093	7/7	0.38	21.63	135,135,135,135	0
85	MG	5	3641	1/1	0.44	21.58	55,55,55,55	0
85	MG	1	3569	1/1	0.47	21.41	29,29,29,29	0
85	MG	8	211	1/1	0.57	21.35	65,65,65,65	0
85	MG	4	205	1/1	0.58	21.28	52,52,52,52	0
85	MG	6	1965	1/1	0.63	21.26	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3842	1/1	0.39	21.26	41,41,41,41	0
86	OHX	5	4065	7/7	0.26	21.25	139,139,139,139	0
85	MG	6	1987	1/1	0.70	21.22	76,76,76,76	0
85	MG	2	1964	1/1	0.61	21.15	56,56,56,56	0
85	MG	5	3524	1/1	0.44	21.14	29,29,29,29	0
85	MG	l2	302	1/1	0.67	21.14	28,28,28,28	0
85	MG	5	3549	1/1	0.85	21.12	59,59,59,59	0
86	OHX	1	4095	7/7	0.27	21.11	161,161,161,161	0
85	MG	1	3761	1/1	0.70	21.10	39,39,39,39	0
85	MG	5	3836	1/1	0.21	21.00	55,55,55,55	0
85	MG	6	1906	1/1	0.50	20.93	50,50,50,50	0
85	MG	5	3413	1/1	0.61	20.92	35,35,35,35	0
86	OHX	5	4148	7/7	0.57	20.91	130,130,130,130	0
85	MG	1	3695	1/1	0.64	20.68	42,42,42,42	0
85	MG	5	3809	1/1	0.41	20.65	37,37,37,37	0
86	OHX	2	2137	7/7	0.29	20.58	185,185,185,185	0
85	MG	5	3835	1/1	0.55	20.39	48,48,48,48	0
85	MG	5	3507	1/1	0.63	20.35	25,25,25,25	0
85	MG	1	3529	1/1	0.91	20.26	33,33,33,33	0
85	MG	1	3518	1/1	0.55	20.25	27,27,27,27	0
85	MG	1	3502	1/1	0.81	20.21	50,50,50,50	0
85	MG	1	3440	1/1	0.61	20.19	36,36,36,36	0
85	MG	1	3469	1/1	0.37	20.17	47,47,47,47	0
85	MG	5	3523	1/1	0.53	20.11	40,40,40,40	0
85	MG	6	1939	1/1	0.70	20.11	69,69,69,69	0
85	MG	1	3750	1/1	0.38	20.05	56,56,56,56	0
85	MG	5	3799	1/1	0.28	19.88	48,48,48,48	0
86	OHX	1	4108	7/7	0.31	19.84	132,132,132,132	0
85	MG	1	3760	1/1	0.57	19.77	55,55,55,55	0
86	OHX	6	2187	7/7	0.42	19.76	169,169,169,169	0
86	OHX	5	4067	7/7	0.30	19.64	128,128,128,128	0
85	MG	1	3576	1/1	0.64	19.52	29,29,29,29	0
85	MG	1	3586	1/1	0.92	19.48	52,52,52,52	0
85	MG	L2	303	1/1	0.54	19.46	44,44,44,44	0
85	MG	5	3411	1/1	0.82	19.44	44,44,44,44	0
85	MG	1	3784	1/1	0.46	19.39	52,52,52,52	0
85	MG	5	3526	1/1	0.46	19.31	24,24,24,24	0
85	MG	1	3791	1/1	0.38	19.22	47,47,47,47	0
86	OHX	4	236	7/7	0.50	19.22	149,149,149,149	0
86	OHX	O9	101	7/7	0.51	19.13	142,142,142,142	0
85	MG	1	3519	1/1	0.70	19.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	1	3735	1/1	0.24	19.00	90,90,90,90	0
85	MG	8	207	1/1	0.57	18.95	74,74,74,74	0
85	MG	2	1958	1/1	0.66	18.94	100,100,100,100	0
85	MG	1	3409	1/1	0.42	18.93	34,34,34,34	0
85	MG	2	1977	1/1	0.71	18.92	61,61,61,61	0
85	MG	1	3429	1/1	0.49	18.89	44,44,44,44	0
85	MG	5	3874	1/1	0.63	18.85	29,29,29,29	0
85	MG	1	3498	1/1	0.48	18.83	35,35,35,35	0
85	MG	1	3856	1/1	1.55	18.81	67,67,67,67	0
85	MG	1	3438	1/1	0.50	18.79	51,51,51,51	0
85	MG	7	207	1/1	0.39	18.79	34,34,34,34	0
86	OHX	1	4152	7/7	0.44	18.77	162,162,162,162	0
85	MG	3	213	1/1	0.56	18.75	65,65,65,65	0
85	MG	1	3543	1/1	0.41	18.75	37,37,37,37	0
85	MG	5	3450	1/1	0.64	18.70	38,38,38,38	0
85	MG	1	3815	1/1	0.45	18.63	51,51,51,51	0
85	MG	1	3509	1/1	0.46	18.60	56,56,56,56	0
85	MG	6	1943	1/1	0.46	18.58	38,38,38,38	0
85	MG	1	3459	1/1	0.39	18.57	37,37,37,37	0
85	MG	1	3594	1/1	0.63	18.51	34,34,34,34	0
85	MG	1	3763	1/1	0.37	18.47	34,34,34,34	0
86	OHX	2	2123	7/7	0.27	18.40	161,161,161,161	0
86	OHX	5	4164	7/7	0.44	18.40	151,151,151,151	0
85	MG	5	3816	1/1	0.43	18.39	70,70,70,70	0
85	MG	1	3526	1/1	0.46	18.38	23,23,23,23	0
85	MG	5	3831	1/1	0.44	18.37	40,40,40,40	0
85	MG	1	3633	1/1	0.34	18.31	37,37,37,37	0
85	MG	1	3676	1/1	0.40	18.21	43,43,43,43	0
85	MG	1	3669	1/1	0.57	18.20	81,81,81,81	0
85	MG	1	3841	1/1	0.36	18.18	67,67,67,67	0
85	MG	1	3541	1/1	0.43	18.17	30,30,30,30	0
85	MG	5	3555	1/1	0.51	18.13	35,35,35,35	0
85	MG	6	1938	1/1	0.64	18.05	48,48,48,48	0
85	MG	o4	201	1/1	0.72	18.04	64,64,64,64	0
85	MG	1	3657	1/1	0.56	18.03	45,45,45,45	0
85	MG	1	3501	1/1	0.51	18.00	27,27,27,27	0
85	MG	6	1903	1/1	0.68	17.99	51,51,51,51	0
85	MG	5	3551	1/1	0.44	17.98	53,53,53,53	0
85	MG	6	1991	1/1	0.91	17.83	89,89,89,89	0
86	OHX	5	4191	7/7	0.32	17.81	169,169,169,169	0
85	MG	6	1981	1/1	0.41	17.69	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	4198	7/7	0.34	17.65	142,142,142,142	0
85	MG	5	3864	1/1	0.53	17.65	30,30,30,30	0
85	MG	5	3594	1/1	1.03	17.64	37,37,37,37	0
85	MG	5	3763	1/1	0.59	17.61	48,48,48,48	0
85	MG	3	208	1/1	0.49	17.60	51,51,51,51	0
85	MG	1	3602	1/1	0.60	17.60	37,37,37,37	0
85	MG	1	3403	1/1	0.51	17.50	40,40,40,40	0
85	MG	4	209	1/1	0.42	17.49	55,55,55,55	0
85	MG	1	3485	1/1	0.53	17.47	42,42,42,42	0
85	MG	1	3542	1/1	0.47	17.40	35,35,35,35	0
85	MG	1	3566	1/1	0.53	17.38	27,27,27,27	0
86	OHX	5	4154	7/7	0.37	17.33	144,144,144,144	0
86	OHX	5	4226	7/7	0.38	17.33	152,152,152,152	0
85	MG	5	3571	1/1	0.43	17.32	44,44,44,44	0
85	MG	2	1975	1/1	0.48	17.25	89,89,89,89	0
85	MG	5	3773	1/1	0.44	17.25	32,32,32,32	0
86	OHX	1	4195	7/7	0.40	17.18	171,171,171,171	0
85	MG	5	3547	1/1	0.71	17.17	59,59,59,59	0
86	OHX	5	4239	7/7	0.41	17.14	182,182,182,182	0
85	MG	1	3567	1/1	0.69	17.14	30,30,30,30	0
85	MG	5	3806	1/1	0.55	17.14	43,43,43,43	0
85	MG	2	1911	1/1	0.69	17.11	59,59,59,59	0
86	OHX	6	2125	7/7	0.34	17.04	134,134,134,134	0
85	MG	6	1972	1/1	0.51	17.01	73,73,73,73	0
85	MG	N0	202	1/1	0.66	16.97	45,45,45,45	0
85	MG	5	3567	1/1	0.38	16.93	29,29,29,29	0
85	MG	7	201	1/1	0.61	16.92	42,42,42,42	0
86	OHX	5	4213	7/7	0.46	16.85	150,150,150,150	0
85	MG	1	3700	1/1	0.34	16.75	51,51,51,51	0
85	MG	5	3775	1/1	1.03	16.64	55,55,55,55	0
85	MG	6	2004	1/1	0.37	16.64	99,99,99,99	0
86	OHX	1	4142	7/7	0.34	16.62	155,155,155,155	0
85	MG	1	3778	1/1	0.44	16.60	61,61,61,61	0
85	MG	5	3855	1/1	0.50	16.54	91,91,91,91	0
85	MG	5	3868	1/1	0.55	16.52	35,35,35,35	0
86	OHX	5	4136	7/7	0.40	16.51	139,139,139,139	0
85	MG	1	3427	1/1	0.71	16.50	45,45,45,45	0
85	MG	5	3477	1/1	0.44	16.50	27,27,27,27	0
85	MG	1	3629	1/1	0.33	16.47	33,33,33,33	0
85	MG	1	3798	1/1	0.54	16.40	47,47,47,47	0
85	MG	1	3674	1/1	0.34	16.38	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	7	217	1/1	0.33	16.38	56,56,56,56	0
85	MG	1	3833	1/1	0.49	16.30	20,20,20,20	0
85	MG	1	3556	1/1	0.48	16.30	39,39,39,39	0
85	MG	6	1994	1/1	0.43	16.29	50,50,50,50	0
86	OHX	1	4209	7/7	0.60	16.25	149,149,149,149	0
85	MG	5	3708	1/1	0.28	16.25	97,97,97,97	0
85	MG	8	203	1/1	0.46	16.24	69,69,69,69	0
85	MG	2	1944	1/1	0.54	16.22	75,75,75,75	0
86	OHX	1	4063	7/7	0.49	16.21	143,143,143,143	0
85	MG	1	3823	1/1	0.37	16.20	55,55,55,55	0
85	MG	n0	202	1/1	0.41	16.13	45,45,45,45	0
85	MG	7	203	1/1	0.49	16.11	30,30,30,30	0
86	OHX	5	4224	7/7	0.34	15.97	206,206,206,206	0
85	MG	5	3593	1/1	0.73	15.96	45,45,45,45	0
85	MG	1	3646	1/1	0.55	15.95	46,46,46,46	0
85	MG	1	3769	1/1	0.39	15.93	53,53,53,53	0
85	MG	1	3711	1/1	0.34	15.86	57,57,57,57	0
85	MG	1	3479	1/1	0.35	15.75	44,44,44,44	0
85	MG	5	3848	1/1	0.55	15.71	75,75,75,75	0
86	OHX	5	4233	7/7	0.56	15.71	167,167,167,167	0
85	MG	1	3545	1/1	0.49	15.66	58,58,58,58	0
85	MG	1	3538	1/1	0.25	15.64	42,42,42,42	0
85	MG	5	3412	1/1	0.45	15.61	33,33,33,33	0
86	OHX	1	4107	7/7	0.27	15.59	149,149,149,149	0
85	MG	5	3525	1/1	0.48	15.58	54,54,54,54	0
85	MG	5	3811	1/1	0.55	15.57	58,58,58,58	0
85	MG	4	215	1/1	0.46	15.48	63,63,63,63	0
85	MG	1	3787	1/1	0.58	15.45	41,41,41,41	0
85	MG	1	3453	1/1	0.55	15.42	37,37,37,37	0
85	MG	5	3473	1/1	0.28	15.35	67,67,67,67	0
85	MG	1	3555	1/1	0.54	15.28	22,22,22,22	0
85	MG	1	3540	1/1	0.48	15.27	65,65,65,65	0
85	MG	2	2010	1/1	0.66	15.26	53,53,53,53	0
85	MG	6	1917	1/1	0.62	15.24	58,58,58,58	0
85	MG	1	3442	1/1	0.44	15.23	27,27,27,27	0
86	OHX	5	4243	7/7	0.49	15.21	164,164,164,164	0
85	MG	5	3875	1/1	0.42	15.21	32,32,32,32	0
85	MG	2	1916	1/1	0.54	15.16	46,46,46,46	0
85	MG	5	3588	1/1	0.49	15.14	26,26,26,26	0
85	MG	5	3629	1/1	0.47	15.05	64,64,64,64	0
86	OHX	5	4181	7/7	0.34	15.05	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	1	3811	1/1	0.36	15.04	48,48,48,48	0
85	MG	2	1931	1/1	0.70	14.98	66,66,66,66	0
86	OHX	1	4205	7/7	0.49	14.96	141,141,141,141	0
85	MG	5	3481	1/1	0.51	14.93	45,45,45,45	0
85	MG	1	3508	1/1	0.53	14.89	20,20,20,20	0
86	OHX	5	4107	7/7	0.36	14.87	131,131,131,131	0
85	MG	6	1908	1/1	0.40	14.85	46,46,46,46	0
86	OHX	1	4168	7/7	0.37	14.85	126,126,126,126	0
85	MG	1	3605	1/1	0.42	14.83	47,47,47,47	0
85	MG	2	1972	1/1	0.55	14.83	74,74,74,74	0
85	MG	O2	201	1/1	0.32	14.77	30,30,30,30	0
85	MG	1	3631	1/1	0.38	14.76	58,58,58,58	0
85	MG	5	3870	1/1	0.40	14.71	45,45,45,45	0
85	MG	2	1960	1/1	0.44	14.68	61,61,61,61	0
85	MG	5	3671	1/1	0.39	14.63	35,35,35,35	0
85	MG	5	3460	1/1	0.38	14.58	30,30,30,30	0
85	MG	5	3479	1/1	0.38	14.52	68,68,68,68	0
85	MG	1	3688	1/1	0.57	14.50	45,45,45,45	0
85	MG	5	3661	1/1	0.60	14.49	43,43,43,43	0
86	OHX	1	4127	7/7	0.54	14.49	170,170,170,170	0
86	OHX	1	4111	7/7	0.45	14.46	175,175,175,175	0
85	MG	1	3608	1/1	0.96	14.45	85,85,85,85	0
86	OHX	5	4170	7/7	0.39	14.45	163,163,163,163	0
85	MG	1	3532	1/1	0.43	14.42	25,25,25,25	0
85	MG	1	3597	1/1	0.49	14.40	26,26,26,26	0
85	MG	1	3614	1/1	0.40	14.38	31,31,31,31	0
86	OHX	5	4132	7/7	0.34	14.38	138,138,138,138	0
85	MG	5	3532	1/1	0.38	14.38	31,31,31,31	0
85	MG	5	3743	1/1	0.53	14.34	48,48,48,48	0
85	MG	2	1969	1/1	0.53	14.30	72,72,72,72	0
86	OHX	1	4046	7/7	0.30	14.28	131,131,131,131	0
85	MG	5	3759	1/1	0.27	14.23	54,54,54,54	0
85	MG	5	3606	1/1	0.32	14.20	51,51,51,51	0
86	OHX	6	2131	7/7	0.41	14.20	177,177,177,177	0
85	MG	5	3509	1/1	0.70	14.19	39,39,39,39	0
85	MG	2	1933	1/1	0.70	14.19	82,82,82,82	0
85	MG	5	3840	1/1	0.55	14.16	52,52,52,52	0
85	MG	5	3534	1/1	0.49	14.13	42,42,42,42	0
85	MG	1	3799	1/1	0.28	14.03	30,30,30,30	0
86	OHX	1	4206	7/7	0.36	14.03	149,149,149,149	0
85	MG	5	3456	1/1	0.34	14.02	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3717	1/1	0.54	14.00	63,63,63,63	0
85	MG	5	3575	1/1	0.52	13.98	33,33,33,33	0
85	MG	2	1961	1/1	0.48	13.97	80,80,80,80	0
85	MG	1	3777	1/1	0.45	13.97	62,62,62,62	0
85	MG	5	3653	1/1	0.33	13.93	35,35,35,35	0
85	MG	2	1971	1/1	0.36	13.92	74,74,74,74	0
86	OHX	1	4176	7/7	0.40	13.88	137,137,137,137	0
85	MG	1	3470	1/1	0.34	13.85	46,46,46,46	0
85	MG	1	3507	1/1	0.39	13.81	33,33,33,33	0
86	OHX	5	4187	7/7	0.35	13.81	132,132,132,132	0
85	MG	5	3476	1/1	0.63	13.80	43,43,43,43	0
85	MG	5	3521	1/1	0.65	13.80	33,33,33,33	0
86	OHX	1	4187	7/7	0.39	13.79	139,139,139,139	0
85	MG	6	1935	1/1	0.82	13.75	58,58,58,58	0
85	MG	n3	201	1/1	0.53	13.75	27,27,27,27	0
85	MG	1	3660	1/1	0.58	13.74	32,32,32,32	0
86	OHX	1	4125	7/7	0.42	13.73	133,133,133,133	0
85	MG	1	3531	1/1	0.34	13.72	31,31,31,31	0
85	MG	5	3613	1/1	0.36	13.71	35,35,35,35	0
85	MG	1	3417	1/1	0.57	13.69	44,44,44,44	0
85	MG	5	3409	1/1	0.54	13.68	49,49,49,49	0
85	MG	2	1915	1/1	0.70	13.68	79,79,79,79	0
86	OHX	8	230	7/7	0.42	13.66	144,144,144,144	0
85	MG	5	3859	1/1	0.29	13.66	47,47,47,47	0
85	MG	2	1950	1/1	1.17	13.64	106,106,106,106	0
86	OHX	1	4166	7/7	0.41	13.63	120,120,120,120	0
86	OHX	2	2153	7/7	0.38	13.63	191,191,191,191	0
86	OHX	2	2092	7/7	0.43	13.63	135,135,135,135	0
86	OHX	5	4021	7/7	0.33	13.62	120,120,120,120	0
85	MG	5	3625	1/1	0.33	13.60	44,44,44,44	0
85	MG	1	3848	1/1	0.39	13.53	57,57,57,57	0
85	MG	1	4219	1/1	0.50	13.50	35,35,35,35	0
85	MG	l3	402	1/1	0.45	13.50	27,27,27,27	0
85	MG	4	206	1/1	0.51	13.48	38,38,38,38	0
85	MG	6	1946	1/1	0.75	13.42	71,71,71,71	0
85	MG	1	3580	1/1	0.51	13.42	40,40,40,40	0
85	MG	1	3517	1/1	0.50	13.37	36,36,36,36	0
85	MG	1	3572	1/1	0.57	13.36	26,26,26,26	0
85	MG	2	2011	1/1	0.31	13.32	61,61,61,61	0
85	MG	5	3589	1/1	0.41	13.29	32,32,32,32	0
85	MG	5	3423	1/1	0.35	13.29	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3514	1/1	0.58	13.28	48,48,48,48	0
85	MG	5	3504	1/1	0.37	13.27	53,53,53,53	0
85	MG	6	1919	1/1	0.59	13.26	46,46,46,46	0
85	MG	1	3560	1/1	0.54	13.25	40,40,40,40	0
85	MG	3	203	1/1	0.31	13.25	105,105,105,105	0
85	MG	1	3743	1/1	0.45	13.21	62,62,62,62	0
85	MG	1	3621	1/1	0.47	13.17	66,66,66,66	0
85	MG	6	1974	1/1	0.45	13.15	52,52,52,52	0
86	OHX	1	4171	7/7	0.48	13.12	158,158,158,158	0
85	MG	1	3630	1/1	0.36	13.12	57,57,57,57	0
85	MG	1	3626	1/1	0.38	13.07	51,51,51,51	0
86	OHX	5	4197	7/7	0.39	13.04	152,152,152,152	0
85	MG	5	3810	1/1	0.40	13.03	86,86,86,86	0
86	OHX	1	4112	7/7	0.57	13.03	127,127,127,127	0
86	OHX	2	2161	7/7	0.54	13.01	192,192,192,192	0
86	OHX	5	4153	7/7	0.29	13.00	125,125,125,125	0
85	MG	m0	301	1/1	0.38	12.99	36,36,36,36	0
85	MG	5	3630	1/1	0.54	12.97	42,42,42,42	0
85	MG	5	3462	1/1	0.59	12.96	30,30,30,30	0
85	MG	D0	201	1/1	0.53	12.94	78,78,78,78	0
85	MG	5	3624	1/1	0.55	12.93	48,48,48,48	0
85	MG	5	3556	1/1	0.54	12.89	28,28,28,28	0
85	MG	1	3475	1/1	0.36	12.88	37,37,37,37	0
85	MG	2	1906	1/1	0.38	12.88	57,57,57,57	0
85	MG	5	3620	1/1	0.23	12.86	44,44,44,44	0
85	MG	5	3711	1/1	0.31	12.84	51,51,51,51	0
85	MG	1	3752	1/1	0.48	12.79	49,49,49,49	0
85	MG	q0	202	1/1	0.41	12.77	45,45,45,45	0
85	MG	2	1953	1/1	0.54	12.77	110,110,110,110	0
86	OHX	5	4225	7/7	0.35	12.77	176,176,176,176	0
86	OHX	2	2159	7/7	0.42	12.74	165,165,165,165	0
86	OHX	6	2190	7/7	0.32	12.74	163,163,163,163	0
85	MG	1	3830	1/1	0.52	12.72	56,56,56,56	0
86	OHX	5	4120	7/7	0.34	12.71	155,155,155,155	0
86	OHX	1	4140	7/7	0.24	12.70	142,142,142,142	0
86	OHX	5	4167	7/7	0.29	12.69	114,114,114,114	0
86	OHX	5	4230	7/7	0.37	12.68	150,150,150,150	0
85	MG	1	3491	1/1	0.39	12.66	32,32,32,32	0
85	MG	1	3565	1/1	0.57	12.64	35,35,35,35	0
86	OHX	1	4141	7/7	0.41	12.50	154,154,154,154	0
86	OHX	1	4200	7/7	0.43	12.48	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	5	4221	7/7	0.31	12.48	155,155,155,155	0
85	MG	5	3497	1/1	0.47	12.44	37,37,37,37	0
85	MG	5	3586	1/1	0.34	12.40	26,26,26,26	0
86	OHX	1	4139	7/7	0.39	12.35	118,118,118,118	0
85	MG	6	1954	1/1	0.47	12.34	54,54,54,54	0
85	MG	5	3853	1/1	0.35	12.32	49,49,49,49	0
86	OHX	6	2124	7/7	0.52	12.29	120,120,120,120	0
85	MG	5	3789	1/1	0.36	12.28	40,40,40,40	0
85	MG	1	3692	1/1	0.42	12.24	43,43,43,43	0
85	MG	5	3720	1/1	0.51	12.23	42,42,42,42	0
86	OHX	5	4156	7/7	0.41	12.20	128,128,128,128	0
85	MG	5	3781	1/1	0.36	12.20	31,31,31,31	0
85	MG	5	3676	1/1	0.47	12.19	49,49,49,49	0
85	MG	5	3559	1/1	0.47	12.16	36,36,36,36	0
85	MG	1	3821	1/1	0.29	12.16	60,60,60,60	0
85	MG	2	2016	1/1	0.59	12.15	69,69,69,69	0
86	OHX	5	4192	7/7	0.28	12.04	131,131,131,131	0
85	MG	2	1928	1/1	0.69	12.01	86,86,86,86	0
85	MG	5	3492	1/1	0.48	12.00	58,58,58,58	0
85	MG	1	3437	1/1	0.31	11.99	35,35,35,35	0
86	OHX	6	2204	7/7	0.54	11.98	170,170,170,170	0
85	MG	5	3741	1/1	0.38	11.98	38,38,38,38	0
86	OHX	1	4114	7/7	0.34	11.97	133,133,133,133	0
85	MG	1	3589	1/1	0.38	11.97	29,29,29,29	0
85	MG	1	3690	1/1	0.28	11.96	92,92,92,92	0
85	MG	1	3559	1/1	0.33	11.94	26,26,26,26	0
85	MG	5	3866	1/1	0.38	11.93	25,25,25,25	0
85	MG	1	3759	1/1	0.50	11.91	53,53,53,53	0
85	MG	5	3419	1/1	0.22	11.89	96,96,96,96	0
85	MG	5	3658	1/1	0.30	11.89	37,37,37,37	0
86	OHX	2	2119	7/7	0.33	11.88	166,166,166,166	0
85	MG	1	3762	1/1	0.26	11.86	57,57,57,57	0
85	MG	1	3818	1/1	0.38	11.86	53,53,53,53	0
85	MG	1	3667	1/1	0.45	11.85	57,57,57,57	0
85	MG	5	3728	1/1	0.34	11.82	52,52,52,52	0
85	MG	2	1993	1/1	0.68	11.82	121,121,121,121	0
85	MG	o3	202	1/1	0.56	11.81	38,38,38,38	0
85	MG	5	3776	1/1	0.37	11.80	53,53,53,53	0
85	MG	6	1911	1/1	0.44	11.78	100,100,100,100	0
85	MG	1	3456	1/1	0.34	11.77	27,27,27,27	0
85	MG	5	3663	1/1	0.41	11.77	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	2	2157	7/7	0.42	11.76	130,130,130,130	0
85	MG	1	3852	1/1	0.33	11.76	57,57,57,57	0
85	MG	6	2024	1/1	0.47	11.76	56,56,56,56	0
85	MG	6	1960	1/1	0.62	11.74	42,42,42,42	0
85	MG	1	3415	1/1	0.48	11.71	34,34,34,34	0
85	MG	1	3446	1/1	0.33	11.69	45,45,45,45	0
85	MG	2	1924	1/1	0.62	11.69	89,89,89,89	0
85	MG	1	3732	1/1	0.33	11.67	36,36,36,36	0
85	MG	5	3739	1/1	0.32	11.64	58,58,58,58	0
85	MG	5	3515	1/1	0.47	11.62	31,31,31,31	0
85	MG	2	2021	1/1	0.55	11.54	99,99,99,99	0
85	MG	2	1929	1/1	0.58	11.51	79,79,79,79	0
85	MG	1	3584	1/1	0.61	11.50	41,41,41,41	0
85	MG	5	3451	1/1	0.28	11.43	40,40,40,40	0
86	OHX	3	223	7/7	0.39	11.42	133,133,133,133	0
85	MG	2	1989	1/1	1.16	11.42	122,122,122,122	0
86	OHX	5	4143	7/7	0.35	11.39	151,151,151,151	0
85	MG	5	3437	1/1	0.45	11.38	56,56,56,56	0
85	MG	5	3645	1/1	0.35	11.36	41,41,41,41	0
85	MG	8	202	1/1	0.59	11.31	41,41,41,41	0
86	OHX	1	4081	7/7	0.33	11.29	151,151,151,151	0
86	OHX	5	4215	7/7	0.46	11.28	159,159,159,159	0
86	OHX	1	4146	7/7	0.38	11.22	144,144,144,144	0
85	MG	5	3591	1/1	0.45	11.21	30,30,30,30	0
85	MG	5	3432	1/1	0.33	11.18	83,83,83,83	0
85	MG	5	3467	1/1	0.29	11.18	35,35,35,35	0
85	MG	1	3424	1/1	0.38	11.15	53,53,53,53	0
85	MG	3	214	1/1	0.43	11.12	65,65,65,65	0
85	MG	5	3607	1/1	0.39	11.12	33,33,33,33	0
85	MG	d3	202	1/1	0.82	11.09	58,58,58,58	0
85	MG	2	1963	1/1	0.59	11.07	107,107,107,107	0
86	OHX	5	4131	7/7	0.38	11.06	146,146,146,146	0
85	MG	5	3610	1/1	0.45	11.06	37,37,37,37	0
85	MG	5	3878	1/1	0.32	11.03	40,40,40,40	0
85	MG	5	3430	1/1	0.47	11.00	38,38,38,38	0
85	MG	7	213	1/1	0.53	11.00	70,70,70,70	0
85	MG	1	3432	1/1	0.75	11.00	36,36,36,36	0
86	OHX	1	4033	7/7	0.28	10.99	127,127,127,127	0
85	MG	5	3464	1/1	0.30	10.95	39,39,39,39	0
85	MG	1	3650	1/1	0.43	10.94	46,46,46,46	0
85	MG	1	3826	1/1	0.48	10.92	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3707	1/1	0.38	10.91	49,49,49,49	0
86	OHX	5	4066	7/7	0.32	10.91	132,132,132,132	0
85	MG	5	3780	1/1	0.33	10.89	60,60,60,60	0
86	OHX	1	4175	7/7	0.37	10.83	159,159,159,159	0
86	OHX	5	4231	7/7	0.44	10.81	162,162,162,162	0
85	MG	1	3612	1/1	0.23	10.79	42,42,42,42	0
85	MG	6	1920	1/1	0.50	10.79	62,62,62,62	0
86	OHX	2	2113	7/7	0.37	10.79	146,146,146,146	0
85	MG	m6	201	1/1	0.47	10.79	32,32,32,32	0
86	OHX	1	4181	7/7	0.38	10.76	152,152,152,152	0
85	MG	5	3511	1/1	0.37	10.75	36,36,36,36	0
85	MG	5	3503	1/1	0.57	10.71	34,34,34,34	0
85	MG	5	3522	1/1	0.64	10.70	38,38,38,38	0
85	MG	1	3592	1/1	0.43	10.68	54,54,54,54	0
85	MG	1	3807	1/1	0.32	10.66	62,62,62,62	0
85	MG	5	3449	1/1	0.33	10.63	32,32,32,32	0
85	MG	6	2015	1/1	0.28	10.62	58,58,58,58	0
86	OHX	6	2173	7/7	0.36	10.60	140,140,140,140	0
86	OHX	5	4173	7/7	0.55	10.59	127,127,127,127	0
86	OHX	1	4065	7/7	0.30	10.59	124,124,124,124	0
85	MG	1	3463	1/1	0.45	10.53	49,49,49,49	0
85	MG	6	1949	1/1	0.79	10.53	55,55,55,55	0
85	MG	5	3843	1/1	0.52	10.48	40,40,40,40	0
85	MG	1	3516	1/1	0.49	10.43	41,41,41,41	0
85	MG	5	3683	1/1	0.33	10.41	33,33,33,33	0
85	MG	5	3578	1/1	0.40	10.35	37,37,37,37	0
85	MG	5	3502	1/1	0.38	10.34	48,48,48,48	0
86	OHX	1	4211	7/7	0.45	10.32	151,151,151,151	0
86	OHX	5	4240	7/7	0.29	10.30	161,161,161,161	0
85	MG	5	3582	1/1	0.42	10.28	44,44,44,44	0
85	MG	1	3613	1/1	0.43	10.23	56,56,56,56	0
86	OHX	2	2177	7/7	0.43	10.22	198,198,198,198	0
86	OHX	5	4147	7/7	0.36	10.21	127,127,127,127	0
86	OHX	5	4133	7/7	0.48	10.19	158,158,158,158	0
85	MG	1	3610	1/1	0.34	10.15	46,46,46,46	0
85	MG	2	2009	1/1	0.60	10.14	72,72,72,72	0
86	OHX	5	4237	7/7	0.27	10.13	186,186,186,186	0
85	MG	n0	201	1/1	0.43	10.10	43,43,43,43	0
86	OHX	6	2191	7/7	0.42	10.08	172,172,172,172	0
85	MG	1	3792	1/1	0.63	10.07	32,32,32,32	0
85	MG	2	1919	1/1	0.69	10.07	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	6	2042	1/1	0.26	10.05	53,53,53,53	0
85	MG	1	3550	1/1	0.39	10.04	43,43,43,43	0
85	MG	5	3783	1/1	0.53	10.03	89,89,89,89	0
85	MG	1	3840	1/1	0.38	10.00	28,28,28,28	0
86	OHX	1	4073	7/7	0.37	10.00	112,112,112,112	0
86	OHX	5	4179	7/7	0.39	9.99	139,139,139,139	0
85	MG	5	3821	1/1	0.31	9.99	44,44,44,44	0
85	MG	5	3791	1/1	0.47	9.95	47,47,47,47	0
86	OHX	1	4062	7/7	0.40	9.94	165,165,165,165	0
85	MG	1	3689	1/1	0.33	9.91	39,39,39,39	0
85	MG	6	2029	1/1	0.34	9.90	113,113,113,113	0
85	MG	1	3471	1/1	0.37	9.89	40,40,40,40	0
85	MG	2	1946	1/1	0.48	9.88	72,72,72,72	0
85	MG	1	3686	1/1	0.31	9.87	41,41,41,41	0
85	MG	6	1914	1/1	0.69	9.87	89,89,89,89	0
85	MG	1	3730	1/1	0.50	9.86	43,43,43,43	0
86	OHX	4	233	7/7	0.43	9.83	161,161,161,161	0
86	OHX	5	4151	7/7	0.32	9.82	146,146,146,146	0
85	MG	6	1936	1/1	0.43	9.79	80,80,80,80	0
85	MG	8	206	1/1	0.50	9.78	46,46,46,46	0
85	MG	2	2180	1/1	0.43	9.75	74,74,74,74	0
86	OHX	1	4162	7/7	0.42	9.75	165,165,165,165	0
86	OHX	2	2163	7/7	0.32	9.74	148,148,148,148	0
85	MG	5	3572	1/1	0.44	9.73	30,30,30,30	0
85	MG	1	3658	1/1	0.32	9.68	36,36,36,36	0
85	MG	5	3805	1/1	0.46	9.68	41,41,41,41	0
85	MG	1	3457	1/1	0.37	9.68	49,49,49,49	0
86	OHX	8	224	7/7	0.35	9.65	130,130,130,130	0
85	MG	1	3601	1/1	0.34	9.63	31,31,31,31	0
85	MG	5	3558	1/1	0.49	9.62	38,38,38,38	0
85	MG	5	3478	1/1	0.37	9.60	62,62,62,62	0
85	MG	5	3592	1/1	0.37	9.56	33,33,33,33	0
86	OHX	1	4212	7/7	0.46	9.55	174,174,174,174	0
85	MG	1	3401	1/1	0.51	9.55	39,39,39,39	0
85	MG	1	3578	1/1	0.39	9.55	23,23,23,23	0
85	MG	5	3422	1/1	0.66	9.53	66,66,66,66	0
86	OHX	5	4109	7/7	0.22	9.50	132,132,132,132	0
86	OHX	5	4080	7/7	0.27	9.47	140,140,140,140	0
86	OHX	1	4028	7/7	0.34	9.46	140,140,140,140	0
85	MG	6	2206	1/1	0.44	9.46	53,53,53,53	0
85	MG	5	3442	1/1	0.25	9.46	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3543	1/1	0.31	9.46	37,37,37,37	0
85	MG	6	2035	1/1	0.87	9.44	65,65,65,65	0
86	OHX	5	4110	7/7	0.33	9.40	168,168,168,168	0
86	OHX	1	4119	7/7	0.42	9.35	134,134,134,134	0
85	MG	C3	201	1/1	0.75	9.33	70,70,70,70	0
85	MG	1	3844	1/1	0.45	9.32	41,41,41,41	0
85	MG	5	3800	1/1	0.28	9.31	57,57,57,57	0
86	OHX	6	2142	7/7	0.45	9.31	149,149,149,149	0
85	MG	N0	201	1/1	0.23	9.30	54,54,54,54	0
86	OHX	5	4152	7/7	0.34	9.27	153,153,153,153	0
85	MG	1	3510	1/1	0.38	9.23	33,33,33,33	0
85	MG	6	1947	1/1	0.50	9.21	57,57,57,57	0
85	MG	1	3723	1/1	0.34	9.18	39,39,39,39	0
85	MG	5	3782	1/1	0.29	9.17	30,30,30,30	0
85	MG	5	3668	1/1	0.28	9.14	36,36,36,36	0
86	OHX	1	4138	7/7	0.39	9.14	164,164,164,164	0
86	OHX	1	4159	7/7	0.47	9.13	170,170,170,170	0
85	MG	1	3477	1/1	0.34	9.10	45,45,45,45	0
85	MG	6	1942	1/1	0.28	9.09	34,34,34,34	0
85	MG	l9	201	1/1	0.31	9.07	39,39,39,39	0
86	OHX	1	4045	7/7	0.28	9.07	121,121,121,121	0
86	OHX	l4	403	7/7	0.67	9.06	183,183,183,183	0
85	MG	5	3405	1/1	0.29	9.05	32,32,32,32	0
85	MG	1	3714	1/1	0.38	9.02	49,49,49,49	0
85	MG	1	3783	1/1	0.28	9.01	53,53,53,53	0
85	MG	1	3620	1/1	0.48	9.00	61,61,61,61	0
85	MG	5	3777	1/1	0.44	8.96	88,88,88,88	0
85	MG	5	3744	1/1	0.32	8.95	70,70,70,70	0
86	OHX	1	4094	7/7	0.32	8.94	145,145,145,145	0
86	OHX	2	2172	7/7	0.53	8.93	166,166,166,166	0
85	MG	5	3647	1/1	0.41	8.93	33,33,33,33	0
85	MG	5	3550	1/1	0.42	8.93	33,33,33,33	0
85	MG	1	3733	1/1	0.41	8.91	27,27,27,27	0
86	OHX	1	4153	7/7	0.31	8.91	146,146,146,146	0
85	MG	1	3530	1/1	0.60	8.87	75,75,75,75	0
85	MG	5	3439	1/1	0.53	8.87	42,42,42,42	0
86	OHX	4	232	7/7	0.35	8.85	131,131,131,131	0
85	MG	5	3873	1/1	0.39	8.85	27,27,27,27	0
86	OHX	5	4204	7/7	0.34	8.84	168,168,168,168	0
85	MG	2	1901	1/1	1.35	8.83	83,83,83,83	0
85	MG	2	2003	1/1	0.40	8.83	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	5	4190	7/7	0.35	8.82	147,147,147,147	0
86	OHX	5	4196	7/7	0.38	8.80	130,130,130,130	0
85	MG	6	2034	1/1	0.73	8.78	83,83,83,83	0
85	MG	1	3570	1/1	0.37	8.78	25,25,25,25	0
85	MG	5	3440	1/1	0.46	8.78	35,35,35,35	0
85	MG	5	3788	1/1	0.27	8.77	63,63,63,63	0
86	OHX	1	3978	7/7	0.34	8.76	105,105,105,105	0
85	MG	5	3738	1/1	0.47	8.73	42,42,42,42	0
85	MG	5	3420	1/1	0.43	8.72	41,41,41,41	0
85	MG	1	3553	1/1	0.48	8.71	51,51,51,51	0
86	OHX	2	2178	7/7	0.56	8.67	170,170,170,170	0
86	OHX	5	3986	7/7	0.30	8.64	123,123,123,123	0
85	MG	5	3640	1/1	0.35	8.63	35,35,35,35	0
85	MG	1	3747	1/1	0.58	8.62	67,67,67,67	0
85	MG	1	3480	1/1	0.41	8.62	48,48,48,48	0
86	OHX	5	4182	7/7	0.46	8.61	134,134,134,134	0
85	MG	2	1985	1/1	0.27	8.60	106,106,106,106	0
85	MG	5	3487	1/1	0.29	8.59	54,54,54,54	0
85	MG	1	3524	1/1	0.29	8.59	44,44,44,44	0
85	MG	5	3546	1/1	0.52	8.57	49,49,49,49	0
86	OHX	8	228	7/7	0.32	8.56	154,154,154,154	0
85	MG	5	3516	1/1	0.37	8.56	42,42,42,42	0
85	MG	6	1957	1/1	1.32	8.56	56,56,56,56	0
86	OHX	1	4096	7/7	0.27	8.53	161,161,161,161	0
85	MG	2	1910	1/1	0.41	8.52	63,63,63,63	0
85	MG	2	1921	1/1	0.60	8.48	59,59,59,59	0
86	OHX	5	4105	7/7	0.42	8.47	147,147,147,147	0
85	MG	5	3485	1/1	0.34	8.47	53,53,53,53	0
86	OHX	1	4183	7/7	0.43	8.44	150,150,150,150	0
85	MG	6	1901	1/1	0.46	8.41	44,44,44,44	0
86	OHX	1	4126	7/7	0.32	8.39	161,161,161,161	0
85	MG	5	3474	1/1	0.46	8.35	44,44,44,44	0
85	MG	1	3820	1/1	0.31	8.35	46,46,46,46	0
85	MG	6	1929	1/1	0.38	8.34	59,59,59,59	0
85	MG	5	3417	1/1	0.33	8.34	31,31,31,31	0
85	MG	1	3744	1/1	0.37	8.34	48,48,48,48	0
86	OHX	1	4099	7/7	0.27	8.31	138,138,138,138	0
85	MG	5	3662	1/1	0.39	8.31	33,33,33,33	0
85	MG	1	3494	1/1	0.31	8.30	44,44,44,44	0
85	MG	2	1949	1/1	0.80	8.27	80,80,80,80	0
86	OHX	1	4058	7/7	0.38	8.24	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	1	3547	1/1	0.36	8.21	43,43,43,43	0
85	MG	2	1983	1/1	0.33	8.21	64,64,64,64	0
86	OHX	1	4137	7/7	0.23	8.19	143,143,143,143	0
85	MG	5	3499	1/1	0.43	8.18	42,42,42,42	0
86	OHX	6	2154	7/7	0.35	8.18	198,198,198,198	0
85	MG	1	3656	1/1	0.44	8.17	47,47,47,47	0
85	MG	L2	301	1/1	0.54	8.16	38,38,38,38	0
86	OHX	1	4057	7/7	0.30	8.15	106,106,106,106	0
85	MG	1	3404	1/1	0.69	8.14	57,57,57,57	0
86	OHX	2	2174	7/7	0.40	8.10	175,175,175,175	0
85	MG	1	3408	1/1	0.34	8.06	46,46,46,46	0
86	OHX	5	4083	7/7	0.44	8.06	123,123,123,123	0
85	MG	1	3554	1/1	0.37	8.05	38,38,38,38	0
85	MG	1	4214	1/1	0.34	8.05	34,34,34,34	0
86	OHX	1	4050	7/7	0.28	8.04	139,139,139,139	0
85	MG	1	3704	1/1	0.24	8.04	45,45,45,45	0
85	MG	2	2001	1/1	0.64	8.03	121,121,121,121	0
85	MG	6	2008	1/1	0.26	8.02	54,54,54,54	0
85	MG	L7	301	1/1	0.41	8.01	38,38,38,38	0
85	MG	1	3451	1/1	0.35	7.98	37,37,37,37	0
85	MG	1	3817	1/1	0.30	7.96	53,53,53,53	0
85	MG	5	3633	1/1	0.39	7.96	44,44,44,44	0
86	OHX	1	4158	7/7	0.34	7.95	142,142,142,142	0
85	MG	1	3765	1/1	0.42	7.92	47,47,47,47	0
85	MG	1	3563	1/1	0.36	7.90	51,51,51,51	0
85	MG	M7	203	1/1	0.34	7.90	36,36,36,36	0
85	MG	1	3677	1/1	0.28	7.86	31,31,31,31	0
85	MG	1	3748	1/1	0.34	7.85	29,29,29,29	0
86	OHX	6	2186	7/7	0.38	7.85	158,158,158,158	0
85	MG	1	3827	1/1	0.33	7.84	47,47,47,47	0
85	MG	1	3421	1/1	0.37	7.83	44,44,44,44	0
85	MG	5	3410	1/1	0.30	7.83	63,63,63,63	0
85	MG	1	3757	1/1	0.32	7.81	29,29,29,29	0
85	MG	1	3595	1/1	0.63	7.81	24,24,24,24	0
85	MG	1	3484	1/1	0.38	7.79	51,51,51,51	0
85	MG	1	3622	1/1	0.33	7.77	75,75,75,75	0
86	OHX	5	4145	7/7	0.49	7.75	127,127,127,127	0
85	MG	5	3687	1/1	0.41	7.72	46,46,46,46	0
85	MG	6	2041	1/1	0.31	7.70	55,55,55,55	0
85	MG	5	3828	1/1	0.35	7.69	52,52,52,52	0
86	OHX	6	2197	7/7	0.32	7.67	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	6	1961	1/1	0.36	7.66	83,83,83,83	0
85	MG	1	3443	1/1	0.22	7.66	72,72,72,72	0
85	MG	5	3747	1/1	0.31	7.65	51,51,51,51	0
85	MG	6	1934	1/1	0.48	7.63	81,81,81,81	0
85	MG	5	3657	1/1	0.42	7.61	44,44,44,44	0
86	OHX	2	2143	7/7	0.51	7.60	135,135,135,135	0
86	OHX	6	2177	7/7	0.44	7.60	146,146,146,146	0
85	MG	1	3483	1/1	0.44	7.59	51,51,51,51	0
85	MG	1	3694	1/1	0.30	7.57	36,36,36,36	0
85	MG	2	2002	1/1	0.30	7.57	124,124,124,124	0
85	MG	1	3664	1/1	0.36	7.55	44,44,44,44	0
85	MG	1	3577	1/1	0.19	7.55	37,37,37,37	0
85	MG	8	212	1/1	0.40	7.54	57,57,57,57	0
85	MG	6	1907	1/1	0.45	7.54	75,75,75,75	0
86	OHX	5	4114	7/7	0.32	7.53	137,137,137,137	0
86	OHX	2	2125	7/7	0.35	7.51	145,145,145,145	0
86	OHX	1	4080	7/7	0.33	7.51	144,144,144,144	0
85	MG	5	3838	1/1	0.30	7.48	43,43,43,43	0
85	MG	2	1965	1/1	0.39	7.46	95,95,95,95	0
86	OHX	5	4180	7/7	0.34	7.46	137,137,137,137	0
85	MG	1	3504	1/1	0.40	7.45	43,43,43,43	0
85	MG	1	3716	1/1	0.32	7.44	57,57,57,57	0
86	OHX	1	4177	7/7	0.49	7.43	161,161,161,161	0
86	OHX	5	4157	7/7	0.26	7.42	125,125,125,125	0
86	OHX	5	4229	7/7	0.41	7.42	174,174,174,174	0
86	OHX	6	2158	7/7	0.45	7.41	146,146,146,146	0
85	MG	l3	403	1/1	0.34	7.41	36,36,36,36	0
85	MG	5	3740	1/1	0.26	7.41	31,31,31,31	0
86	OHX	2	2154	7/7	0.30	7.37	169,169,169,169	0
86	OHX	1	4078	7/7	0.50	7.36	133,133,133,133	0
86	OHX	1	3991	7/7	0.28	7.34	117,117,117,117	0
86	OHX	1	4189	7/7	0.30	7.32	156,156,156,156	0
86	OHX	5	4207	7/7	0.26	7.32	153,153,153,153	0
86	OHX	2	2108	7/7	0.33	7.31	158,158,158,158	0
85	MG	2	1941	1/1	0.44	7.31	79,79,79,79	0
86	OHX	1	4067	7/7	0.34	7.30	125,125,125,125	0
86	OHX	2	2148	7/7	0.29	7.30	128,128,128,128	0
86	OHX	5	4212	7/7	0.29	7.28	165,165,165,165	0
86	OHX	5	4245	7/7	0.34	7.27	177,177,177,177	0
85	MG	6	1969	1/1	0.45	7.27	46,46,46,46	0
85	MG	5	3673	1/1	0.46	7.25	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	N8	201	1/1	0.29	7.24	32,32,32,32	0
86	OHX	6	2180	7/7	0.38	7.24	150,150,150,150	0
85	MG	1	3781	1/1	0.24	7.24	66,66,66,66	0
86	OHX	1	4145	7/7	0.31	7.23	170,170,170,170	0
85	MG	1	3625	1/1	0.28	7.22	45,45,45,45	0
86	OHX	o7	503	7/7	0.41	7.21	143,143,143,143	0
85	MG	2	1923	1/1	0.37	7.21	63,63,63,63	0
85	MG	1	3521	1/1	0.36	7.21	81,81,81,81	0
85	MG	5	3656	1/1	0.37	7.19	57,57,57,57	0
85	MG	6	2018	1/1	0.72	7.18	61,61,61,61	0
85	MG	6	1902	1/1	0.39	7.18	50,50,50,50	0
85	MG	5	3832	1/1	0.42	7.17	42,42,42,42	0
86	OHX	2	2170	7/7	0.24	7.16	165,165,165,165	0
85	MG	5	3825	1/1	0.32	7.15	29,29,29,29	0
86	OHX	1	4082	7/7	0.24	7.14	149,149,149,149	0
85	MG	1	3624	1/1	0.42	7.14	42,42,42,42	0
85	MG	1	3539	1/1	0.47	7.09	23,23,23,23	0
85	MG	5	3822	1/1	0.36	7.08	33,33,33,33	0
85	MG	5	3643	1/1	0.22	7.07	41,41,41,41	0
86	OHX	2	2128	7/7	0.37	7.05	162,162,162,162	0
85	MG	5	3709	1/1	0.37	7.05	47,47,47,47	0
85	MG	5	3602	1/1	0.40	7.04	44,44,44,44	0
85	MG	6	1950	1/1	0.40	7.00	44,44,44,44	0
85	MG	5	3761	1/1	0.55	7.00	34,34,34,34	0
86	OHX	1	4167	7/7	0.26	6.99	131,131,131,131	0
86	OHX	5	4127	7/7	0.28	6.99	131,131,131,131	0
85	MG	5	3500	1/1	0.34	6.98	30,30,30,30	0
85	MG	1	3450	1/1	0.33	6.93	52,52,52,52	0
85	MG	2	1947	1/1	0.56	6.93	98,98,98,98	0
85	MG	1	3775	1/1	0.32	6.92	49,49,49,49	0
86	OHX	5	4188	7/7	0.25	6.92	130,130,130,130	0
85	MG	1	3651	1/1	0.26	6.91	48,48,48,48	0
86	OHX	6	2118	7/7	0.48	6.91	131,131,131,131	0
85	MG	6	1986	1/1	0.35	6.90	50,50,50,50	0
86	OHX	1	4184	7/7	0.37	6.89	162,162,162,162	0
85	MG	5	3660	1/1	0.23	6.89	27,27,27,27	0
86	OHX	6	2198	7/7	0.37	6.87	152,152,152,152	0
85	MG	1	3533	1/1	0.26	6.86	37,37,37,37	0
85	MG	O7	102	1/1	0.42	6.84	44,44,44,44	0
85	MG	2	1966	1/1	0.74	6.83	123,123,123,123	0
85	MG	1	3703	1/1	0.35	6.83	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	4135	7/7	0.28	6.83	128,128,128,128	0
86	OHX	1	4091	7/7	0.23	6.82	128,128,128,128	0
86	OHX	2	2139	7/7	0.37	6.81	182,182,182,182	0
85	MG	5	4250	1/1	0.42	6.79	35,35,35,35	0
85	MG	4	211	1/1	0.36	6.77	44,44,44,44	0
85	MG	4	213	1/1	0.29	6.76	56,56,56,56	0
86	OHX	1	4064	7/7	0.33	6.76	152,152,152,152	0
85	MG	5	3746	1/1	0.32	6.75	40,40,40,40	0
85	MG	6	1962	1/1	0.37	6.75	41,41,41,41	0
86	OHX	5	4076	7/7	0.38	6.74	121,121,121,121	0
85	MG	5	3834	1/1	0.27	6.74	37,37,37,37	0
85	MG	5	3453	1/1	0.47	6.74	41,41,41,41	0
85	MG	1	3495	1/1	0.33	6.72	49,49,49,49	0
85	MG	s9	201	1/1	0.54	6.71	71,71,71,71	0
86	OHX	5	3996	7/7	0.27	6.68	87,87,87,87	0
86	OHX	5	4183	7/7	0.35	6.66	181,181,181,181	0
86	OHX	3	226	7/7	0.30	6.65	153,153,153,153	0
85	MG	5	3700	1/1	0.36	6.64	43,43,43,43	0
85	MG	6	2021	1/1	0.30	6.62	83,83,83,83	0
86	OHX	5	4094	7/7	0.40	6.62	153,153,153,153	0
85	MG	5	3470	1/1	0.41	6.61	40,40,40,40	0
86	OHX	6	2108	7/7	0.22	6.60	124,124,124,124	0
86	OHX	5	4142	7/7	0.27	6.60	138,138,138,138	0
85	MG	6	1953	1/1	0.33	6.57	66,66,66,66	0
85	MG	1	3825	1/1	0.47	6.55	68,68,68,68	0
85	MG	1	3709	1/1	0.20	6.55	61,61,61,61	0
85	MG	2	1922	1/1	0.38	6.54	66,66,66,66	0
86	OHX	1	4182	7/7	0.22	6.54	157,157,157,157	0
86	OHX	8	222	7/7	0.22	6.53	133,133,133,133	0
85	MG	2	2006	1/1	0.51	6.52	86,86,86,86	0
85	MG	m7	201	1/1	0.53	6.51	36,36,36,36	0
85	MG	5	3774	1/1	0.18	6.47	87,87,87,87	0
85	MG	5	3867	1/1	0.47	6.45	52,52,52,52	0
85	MG	1	3619	1/1	0.33	6.45	57,57,57,57	0
85	MG	2	1932	1/1	0.35	6.43	71,71,71,71	0
85	MG	1	3855	1/1	0.27	6.35	27,27,27,27	0
85	MG	1	3680	1/1	0.33	6.33	47,47,47,47	0
85	MG	6	1988	1/1	0.29	6.33	55,55,55,55	0
86	OHX	1	4006	7/7	0.28	6.31	133,133,133,133	0
85	MG	5	3849	1/1	0.32	6.30	62,62,62,62	0
85	MG	1	3652	1/1	0.40	6.29	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	1	3444	1/1	0.42	6.23	47,47,47,47	0
86	OHX	1	4118	7/7	0.39	6.22	144,144,144,144	0
86	OHX	1	4191	7/7	0.47	6.22	167,167,167,167	0
86	OHX	5	4150	7/7	0.40	6.20	159,159,159,159	0
85	MG	5	3665	1/1	0.34	6.20	62,62,62,62	0
85	MG	5	3742	1/1	0.32	6.20	37,37,37,37	0
85	MG	1	3528	1/1	0.30	6.19	43,43,43,43	0
85	MG	1	3581	1/1	0.46	6.17	53,53,53,53	0
85	MG	5	3416	1/1	0.28	6.15	34,34,34,34	0
85	MG	5	3713	1/1	0.24	6.13	52,52,52,52	0
86	OHX	1	4109	7/7	0.31	6.12	156,156,156,156	0
85	MG	n9	101	1/1	0.29	6.11	37,37,37,37	0
86	OHX	1	4075	7/7	0.35	6.09	139,139,139,139	0
85	MG	o3	201	1/1	0.33	6.09	48,48,48,48	0
85	MG	1	3756	1/1	0.34	6.08	46,46,46,46	0
86	OHX	1	4179	7/7	0.28	6.07	146,146,146,146	0
85	MG	5	3531	1/1	0.45	6.07	44,44,44,44	0
85	MG	5	3674	1/1	0.21	6.07	71,71,71,71	0
86	OHX	6	2200	7/7	0.30	6.03	172,172,172,172	0
85	MG	5	3692	1/1	0.34	6.03	51,51,51,51	0
85	MG	5	3519	1/1	0.42	6.02	33,33,33,33	0
85	MG	5	3714	1/1	0.33	6.01	72,72,72,72	0
86	OHX	5	4159	7/7	0.30	6.00	188,188,188,188	0
85	MG	5	3615	1/1	0.25	6.00	43,43,43,43	0
85	MG	8	201	1/1	0.25	6.00	94,94,94,94	0
85	MG	1	3439	1/1	0.57	5.98	26,26,26,26	0
86	OHX	5	4121	7/7	0.33	5.97	139,139,139,139	0
85	MG	5	3655	1/1	0.35	5.97	63,63,63,63	0
85	MG	1	3737	1/1	0.26	5.94	33,33,33,33	0
85	MG	1	3773	1/1	0.22	5.93	71,71,71,71	0
85	MG	1	3746	1/1	0.26	5.92	44,44,44,44	0
85	MG	1	3496	1/1	0.27	5.90	37,37,37,37	0
85	MG	6	2207	1/1	0.35	5.90	77,77,77,77	0
86	OHX	5	4205	7/7	0.29	5.90	121,121,121,121	0
85	MG	6	2012	1/1	0.45	5.88	62,62,62,62	0
86	OHX	6	2121	7/7	0.27	5.88	117,117,117,117	0
85	MG	5	3830	1/1	0.23	5.87	44,44,44,44	0
85	MG	2	1943	1/1	0.41	5.86	73,73,73,73	0
86	OHX	6	2138	7/7	0.30	5.85	154,154,154,154	0
86	OHX	l5	307	7/7	0.66	5.84	176,176,176,176	0
86	OHX	1	4120	7/7	0.26	5.84	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	6	2163	7/7	0.33	5.84	160,160,160,160	0
86	OHX	5	4053	7/7	0.19	5.84	132,132,132,132	0
85	MG	5	3814	1/1	0.23	5.83	32,32,32,32	0
85	MG	1	3454	1/1	0.63	5.83	65,65,65,65	0
86	OHX	1	4116	7/7	0.40	5.82	149,149,149,149	0
86	OHX	6	2172	7/7	0.34	5.82	176,176,176,176	0
86	OHX	M7	205	7/7	0.58	5.80	122,122,122,122	0
85	MG	6	1979	1/1	0.24	5.79	81,81,81,81	0
86	OHX	5	4046	7/7	0.37	5.78	120,120,120,120	0
85	MG	5	3680	1/1	0.26	5.73	53,53,53,53	0
85	MG	5	3823	1/1	0.35	5.72	40,40,40,40	0
86	OHX	1	4128	7/7	0.26	5.72	132,132,132,132	0
86	OHX	5	4234	7/7	0.28	5.70	199,199,199,199	0
85	MG	2	1976	1/1	0.26	5.65	101,101,101,101	0
85	MG	5	3471	1/1	0.27	5.64	49,49,49,49	0
85	MG	3	212	1/1	0.34	5.63	80,80,80,80	0
86	OHX	2	2171	7/7	0.41	5.60	168,168,168,168	0
86	OHX	1	4174	7/7	0.36	5.58	164,164,164,164	0
85	MG	5	3786	1/1	0.32	5.57	24,24,24,24	0
86	OHX	1	4068	7/7	0.24	5.55	153,153,153,153	0
86	OHX	5	4200	7/7	0.34	5.54	162,162,162,162	0
85	MG	5	3569	1/1	0.44	5.53	34,34,34,34	0
85	MG	6	1952	1/1	0.51	5.52	62,62,62,62	0
86	OHX	1	4129	7/7	0.23	5.52	173,173,173,173	0
85	MG	1	3796	1/1	0.39	5.51	31,31,31,31	0
85	MG	1	3632	1/1	0.38	5.50	39,39,39,39	0
86	OHX	5	4009	7/7	0.19	5.50	122,122,122,122	0
85	MG	1	3609	1/1	0.57	5.48	63,63,63,63	0
86	OHX	1	4134	7/7	0.32	5.48	145,145,145,145	0
85	MG	5	3605	1/1	0.23	5.48	37,37,37,37	0
86	OHX	6	2070	7/7	0.25	5.46	107,107,107,107	0
85	MG	2	1908	1/1	0.40	5.46	77,77,77,77	0
86	OHX	7	225	7/7	0.33	5.46	169,169,169,169	0
85	MG	6	1967	1/1	0.28	5.45	99,99,99,99	0
88	3J6	5	4246	21/21	0.26	5.43	35,35,35,35	0
85	MG	1	3684	1/1	0.24	5.43	67,67,67,67	0
85	MG	7	209	1/1	0.30	5.42	42,42,42,42	0
85	MG	1	3782	1/1	0.29	5.41	42,42,42,42	0
86	OHX	1	4122	7/7	0.31	5.41	116,116,116,116	0
85	MG	6	1923	1/1	0.38	5.40	69,69,69,69	0
85	MG	5	3505	1/1	0.35	5.37	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	6	1941	1/1	0.32	5.36	52,52,52,52	0
85	MG	8	210	1/1	0.38	5.34	47,47,47,47	0
86	OHX	2	2135	7/7	0.31	5.34	152,152,152,152	0
85	MG	1	3654	1/1	0.51	5.33	107,107,107,107	0
85	MG	5	3691	1/1	0.33	5.32	49,49,49,49	0
86	OHX	1	4047	7/7	0.31	5.32	124,124,124,124	0
85	MG	1	3600	1/1	0.30	5.31	40,40,40,40	0
85	MG	1	3726	1/1	0.28	5.29	34,34,34,34	0
86	OHX	1	4110	7/7	0.35	5.28	128,128,128,128	0
86	OHX	5	4014	7/7	0.25	5.28	139,139,139,139	0
86	OHX	6	2161	7/7	0.27	5.28	149,149,149,149	0
86	OHX	1	4196	7/7	0.42	5.28	137,137,137,137	0
86	OHX	5	4064	7/7	0.29	5.27	142,142,142,142	0
86	OHX	5	4037	7/7	0.33	5.27	152,152,152,152	0
85	MG	1	3611	1/1	0.41	5.26	50,50,50,50	0
85	MG	1	3672	1/1	0.20	5.26	83,83,83,83	0
85	MG	6	2017	1/1	0.30	5.26	47,47,47,47	0
86	OHX	2	2131	7/7	0.29	5.24	143,143,143,143	0
85	MG	1	3772	1/1	0.28	5.23	35,35,35,35	0
85	MG	5	3659	1/1	0.31	5.22	50,50,50,50	0
86	OHX	6	2175	7/7	0.30	5.21	116,116,116,116	0
85	MG	1	3725	1/1	0.26	5.21	54,54,54,54	0
86	OHX	1	4070	7/7	0.33	5.19	131,131,131,131	0
85	MG	7	204	1/1	0.25	5.17	61,61,61,61	0
86	OHX	1	4154	7/7	0.39	5.15	147,147,147,147	0
86	OHX	1	4043	7/7	0.25	5.13	113,113,113,113	0
85	MG	m1	201	1/1	0.25	5.12	57,57,57,57	0
85	MG	5	3694	1/1	0.20	5.11	43,43,43,43	0
85	MG	5	3448	1/1	0.35	5.11	59,59,59,59	0
85	MG	5	3461	1/1	0.36	5.10	51,51,51,51	0
86	OHX	l5	306	7/7	0.47	5.09	162,162,162,162	0
85	MG	L2	302	1/1	0.41	5.08	40,40,40,40	0
86	OHX	1	4121	7/7	0.39	5.08	166,166,166,166	0
86	OHX	6	2169	7/7	0.39	5.05	181,181,181,181	0
86	OHX	6	2199	7/7	0.28	5.05	160,160,160,160	0
86	OHX	1	4208	7/7	0.47	5.05	151,151,151,151	0
85	MG	1	3411	1/1	0.39	5.04	50,50,50,50	0
85	MG	6	2001	1/1	0.43	5.04	57,57,57,57	0
85	MG	L7	302	1/1	0.24	5.03	46,46,46,46	0
86	OHX	6	2176	7/7	0.42	5.02	129,129,129,129	0
86	OHX	6	2145	7/7	0.23	5.01	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	6	2184	7/7	0.47	5.00	146,146,146,146	0
86	OHX	1	4148	7/7	0.27	5.00	156,156,156,156	0
86	OHX	6	2203	7/7	0.41	4.98	167,167,167,167	0
86	OHX	O3	202	7/7	0.33	4.96	128,128,128,128	0
85	MG	5	3667	1/1	0.26	4.94	49,49,49,49	0
86	OHX	6	2168	7/7	0.29	4.94	178,178,178,178	0
86	OHX	5	4210	7/7	0.37	4.93	166,166,166,166	0
86	OHX	2	2103	7/7	0.24	4.90	168,168,168,168	0
86	OHX	2	2127	7/7	0.29	4.89	153,153,153,153	0
86	OHX	2	2150	7/7	0.44	4.88	182,182,182,182	0
85	MG	1	3481	1/1	0.31	4.88	34,34,34,34	0
86	OHX	1	4201	7/7	0.58	4.87	159,159,159,159	0
85	MG	5	3642	1/1	0.46	4.86	60,60,60,60	0
85	MG	5	3884	1/1	0.32	4.86	42,42,42,42	0
85	MG	1	3847	1/1	0.31	4.85	48,48,48,48	0
86	OHX	8	227	7/7	0.24	4.84	161,161,161,161	0
86	OHX	5	4242	7/7	0.36	4.81	145,145,145,145	0
85	MG	M7	202	1/1	0.39	4.79	37,37,37,37	0
86	OHX	5	4056	7/7	0.27	4.79	146,146,146,146	0
86	OHX	2	2160	7/7	0.53	4.76	154,154,154,154	0
85	MG	l7	301	1/1	0.37	4.75	42,42,42,42	0
86	OHX	6	2132	7/7	0.28	4.75	150,150,150,150	0
85	MG	1	3853	1/1	0.49	4.75	78,78,78,78	0
86	OHX	7	227	7/7	0.28	4.73	146,146,146,146	0
85	MG	5	3463	1/1	0.30	4.72	52,52,52,52	0
86	OHX	1	4086	7/7	0.25	4.72	142,142,142,142	0
86	OHX	2	2084	7/7	0.28	4.69	139,139,139,139	0
85	MG	1	3813	1/1	0.35	4.68	54,54,54,54	0
86	OHX	2	2090	7/7	0.24	4.67	140,140,140,140	0
86	OHX	2	2167	7/7	0.26	4.64	143,143,143,143	0
85	MG	2	1959	1/1	0.33	4.64	72,72,72,72	0
85	MG	2	1939	1/1	0.31	4.63	72,72,72,72	0
86	OHX	1	4207	7/7	0.47	4.60	133,133,133,133	0
85	MG	5	3619	1/1	0.33	4.58	43,43,43,43	0
86	OHX	5	4034	7/7	0.31	4.58	102,102,102,102	0
86	OHX	5	4161	7/7	0.25	4.57	152,152,152,152	0
85	MG	1	3713	1/1	0.30	4.56	37,37,37,37	0
85	MG	5	3498	1/1	0.33	4.56	36,36,36,36	0
86	OHX	5	4099	7/7	0.29	4.56	119,119,119,119	0
85	MG	5	3510	1/1	0.33	4.52	28,28,28,28	0
86	OHX	4	229	7/7	0.20	4.50	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	6	2178	7/7	0.34	4.48	156,156,156,156	0
85	MG	5	3690	1/1	0.35	4.48	39,39,39,39	0
86	OHX	3	222	7/7	0.20	4.46	162,162,162,162	0
85	MG	5	3757	1/1	0.28	4.46	67,67,67,67	0
85	MG	6	2019	1/1	0.31	4.46	54,54,54,54	0
85	MG	n6	201	1/1	0.62	4.42	54,54,54,54	0
86	OHX	2	2091	7/7	0.44	4.38	182,182,182,182	0
86	OHX	s1	303	7/7	0.38	4.38	180,180,180,180	0
85	MG	5	3648	1/1	0.23	4.37	59,59,59,59	0
86	OHX	5	4055	7/7	0.27	4.37	134,134,134,134	0
85	MG	1	3822	1/1	0.28	4.36	47,47,47,47	0
86	OHX	2	2074	7/7	0.24	4.35	131,131,131,131	0
85	MG	6	1964	1/1	0.32	4.32	60,60,60,60	0
85	MG	5	3734	1/1	0.17	4.32	51,51,51,51	0
86	OHX	5	4186	7/7	0.27	4.32	138,138,138,138	0
85	MG	5	3729	1/1	0.24	4.31	43,43,43,43	0
85	MG	5	3483	1/1	0.65	4.31	19,19,19,19	0
86	OHX	3	225	7/7	0.29	4.29	149,149,149,149	0
86	OHX	5	4091	7/7	0.24	4.28	135,135,135,135	0
86	OHX	6	2106	7/7	0.24	4.27	123,123,123,123	0
86	OHX	1	4193	7/7	0.55	4.27	154,154,154,154	0
86	OHX	5	4178	7/7	0.42	4.26	145,145,145,145	0
86	OHX	6	2115	7/7	0.36	4.25	155,155,155,155	0
85	MG	2	1930	1/1	0.27	4.24	68,68,68,68	0
86	OHX	1	4147	7/7	0.34	4.24	159,159,159,159	0
85	MG	1	3705	1/1	0.21	4.23	46,46,46,46	0
86	OHX	2	2173	7/7	0.41	4.23	186,186,186,186	0
85	MG	6	1963	1/1	0.35	4.22	114,114,114,114	0
86	OHX	6	2139	7/7	0.26	4.20	192,192,192,192	0
86	OHX	5	4050	7/7	0.31	4.20	126,126,126,126	0
85	MG	5	3892	1/1	0.23	4.19	49,49,49,49	0
85	MG	5	3767	1/1	0.30	4.19	48,48,48,48	0
85	MG	5	4248	1/1	0.45	4.19	47,47,47,47	0
86	OHX	6	2159	7/7	0.30	4.19	141,141,141,141	0
85	MG	1	3615	1/1	0.40	4.17	41,41,41,41	0
85	MG	6	2013	1/1	0.23	4.17	77,77,77,77	0
85	MG	6	1909	1/1	0.42	4.16	123,123,123,123	0
85	MG	4	217	1/1	0.24	4.15	45,45,45,45	0
86	OHX	5	4141	7/7	0.25	4.14	128,128,128,128	0
86	OHX	4	228	7/7	0.23	4.12	122,122,122,122	0
85	MG	6	1992	1/1	0.31	4.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	5	4206	7/7	0.29	4.11	159,159,159,159	0
85	MG	1	3433	1/1	0.27	4.11	37,37,37,37	0
86	OHX	5	4128	7/7	0.24	4.10	147,147,147,147	0
86	OHX	5	4044	7/7	0.22	4.10	129,129,129,129	0
85	MG	2	2000	1/1	0.22	4.08	86,86,86,86	0
85	MG	1	3816	1/1	0.30	4.06	49,49,49,49	0
85	MG	5	3795	1/1	0.26	4.05	36,36,36,36	0
85	MG	5	3727	1/1	0.61	4.04	74,74,74,74	0
86	OHX	1	4173	7/7	0.31	4.04	183,183,183,183	0
85	MG	6	2038	1/1	0.59	4.03	113,113,113,113	0
85	MG	4	212	1/1	0.21	4.03	68,68,68,68	0
85	MG	5	3725	1/1	0.20	4.03	103,103,103,103	0
86	OHX	2	2146	7/7	0.35	4.01	157,157,157,157	0
85	MG	2	1984	1/1	0.26	4.00	71,71,71,71	0
86	OHX	5	4168	7/7	0.29	3.99	102,102,102,102	0
86	OHX	1	4055	7/7	0.25	3.99	123,123,123,123	0
86	OHX	5	4201	7/7	0.29	3.98	157,157,157,157	0
85	MG	6	2023	1/1	0.29	3.96	58,58,58,58	0
85	MG	2	1968	1/1	0.34	3.94	84,84,84,84	0
85	MG	5	3491	1/1	0.35	3.94	51,51,51,51	0
85	MG	5	3408	1/1	0.30	3.93	34,34,34,34	0
86	OHX	1	4130	7/7	0.30	3.93	164,164,164,164	0
85	MG	6	1927	1/1	0.37	3.93	48,48,48,48	0
86	OHX	5	4218	7/7	0.38	3.92	140,140,140,140	0
85	MG	1	3719	1/1	0.24	3.89	46,46,46,46	0
85	MG	5	3731	1/1	0.20	3.89	47,47,47,47	0
85	MG	5	3705	1/1	0.20	3.86	51,51,51,51	0
85	MG	1	3639	1/1	0.22	3.86	67,67,67,67	0
86	OHX	1	3985	7/7	0.27	3.85	118,118,118,118	0
86	OHX	2	2134	7/7	0.25	3.85	165,165,165,165	0
86	OHX	5	4018	7/7	0.23	3.85	121,121,121,121	0
85	MG	5	3553	1/1	0.39	3.84	40,40,40,40	0
85	MG	n6	202	1/1	0.51	3.84	56,56,56,56	0
85	MG	1	3734	1/1	0.24	3.83	65,65,65,65	0
86	OHX	D9	102	7/7	0.35	3.83	175,175,175,175	0
85	MG	5	3677	1/1	0.30	3.82	42,42,42,42	0
85	MG	6	1937	1/1	0.31	3.82	45,45,45,45	0
86	OHX	5	4160	7/7	0.37	3.81	153,153,153,153	0
85	MG	5	3772	1/1	0.22	3.80	37,37,37,37	0
85	MG	6	1978	1/1	0.29	3.78	50,50,50,50	0
86	OHX	5	4241	7/7	0.29	3.77	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	4008	7/7	0.24	3.71	121,121,121,121	0
86	OHX	5	4219	7/7	0.31	3.71	160,160,160,160	0
85	MG	5	3808	1/1	0.23	3.71	32,32,32,32	0
85	MG	5	3880	1/1	0.24	3.70	77,77,77,77	0
85	MG	5	3722	1/1	0.30	3.69	42,42,42,42	0
85	MG	M7	204	1/1	0.42	3.68	42,42,42,42	0
85	MG	3	211	1/1	0.26	3.68	80,80,80,80	0
85	MG	s8	301	1/1	0.36	3.67	51,51,51,51	0
86	OHX	5	4217	7/7	0.40	3.65	159,159,159,159	0
86	OHX	M7	206	7/7	0.30	3.64	156,156,156,156	0
86	OHX	6	2134	7/7	0.24	3.64	152,152,152,152	0
85	MG	5	3685	1/1	0.38	3.64	59,59,59,59	0
86	OHX	5	4090	7/7	0.23	3.63	168,168,168,168	0
86	OHX	2	2136	7/7	0.34	3.62	152,152,152,152	0
86	OHX	1	4038	7/7	0.25	3.61	132,132,132,132	0
85	MG	5	3697	1/1	0.29	3.60	61,61,61,61	0
86	OHX	5	4103	7/7	0.29	3.60	140,140,140,140	0
85	MG	4	208	1/1	0.23	3.60	54,54,54,54	0
85	MG	5	3425	1/1	0.37	3.60	40,40,40,40	0
86	OHX	5	4130	7/7	0.23	3.59	152,152,152,152	0
85	MG	1	3706	1/1	0.25	3.58	47,47,47,47	0
85	MG	n8	201	1/1	0.29	3.57	45,45,45,45	0
86	OHX	2	2088	7/7	0.33	3.56	147,147,147,147	0
86	OHX	5	4144	7/7	0.40	3.56	169,169,169,169	0
85	MG	1	3768	1/1	0.24	3.56	53,53,53,53	0
85	MG	2	1948	1/1	0.34	3.56	59,59,59,59	0
85	MG	q3	502	1/1	0.33	3.53	75,75,75,75	0
86	OHX	2	2162	7/7	0.25	3.53	191,191,191,191	0
86	OHX	M9	203	7/7	0.27	3.48	182,182,182,182	0
85	MG	S8	301	1/1	0.31	3.46	62,62,62,62	0
86	OHX	6	2166	7/7	0.23	3.46	156,156,156,156	0
85	MG	5	3438	1/1	0.23	3.45	34,34,34,34	0
86	OHX	5	4208	7/7	0.24	3.42	135,135,135,135	0
85	MG	1	3702	1/1	0.41	3.41	80,80,80,80	0
85	MG	1	3412	1/1	0.28	3.39	31,31,31,31	0
86	OHX	2	2117	7/7	0.35	3.39	158,158,158,158	0
85	MG	5	3455	1/1	0.37	3.39	80,80,80,80	0
86	OHX	2	2062	7/7	0.27	3.38	154,154,154,154	0
86	OHX	1	4164	7/7	0.29	3.36	143,143,143,143	0
85	MG	5	3617	1/1	0.25	3.36	48,48,48,48	0
85	MG	5	3803	1/1	0.22	3.35	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	6	2101	7/7	0.27	3.34	137,137,137,137	0
85	MG	1	3717	1/1	0.45	3.33	86,86,86,86	0
85	MG	5	3715	1/1	0.29	3.33	47,47,47,47	0
86	OHX	1	4014	7/7	0.23	3.32	139,139,139,139	0
86	OHX	1	4025	7/7	0.23	3.31	128,128,128,128	0
85	MG	5	3495	1/1	0.34	3.31	27,27,27,27	0
85	MG	2	1974	1/1	0.30	3.29	66,66,66,66	0
86	OHX	5	4085	7/7	0.32	3.26	113,113,113,113	0
86	OHX	2	2168	7/7	0.30	3.25	163,163,163,163	0
86	OHX	6	2170	7/7	0.36	3.25	122,122,122,122	0
86	OHX	5	4101	7/7	0.22	3.25	131,131,131,131	0
86	OHX	2	2122	7/7	0.29	3.24	153,153,153,153	0
86	OHX	5	4047	7/7	0.23	3.24	109,109,109,109	0
86	OHX	2	2149	7/7	0.28	3.20	179,179,179,179	0
85	MG	5	3670	1/1	0.21	3.17	47,47,47,47	0
86	OHX	5	4102	7/7	0.30	3.17	138,138,138,138	0
85	MG	M7	201	1/1	0.43	3.17	32,32,32,32	0
86	OHX	5	4140	7/7	0.27	3.16	132,132,132,132	0
86	OHX	5	4199	7/7	0.36	3.16	157,157,157,157	0
85	MG	1	3861	1/1	0.35	3.15	76,76,76,76	0
85	MG	6	1971	1/1	0.20	3.13	76,76,76,76	0
85	MG	1	3687	1/1	0.27	3.13	53,53,53,53	0
85	MG	5	3533	1/1	0.22	3.13	56,56,56,56	0
85	MG	8	205	1/1	0.32	3.13	49,49,49,49	0
85	MG	5	3841	1/1	0.38	3.12	51,51,51,51	0
86	OHX	1	4150	7/7	0.26	3.11	122,122,122,122	0
85	MG	2	1997	1/1	0.27	3.10	109,109,109,109	0
86	OHX	1	4071	7/7	0.23	3.10	158,158,158,158	0
85	MG	5	3679	1/1	0.20	3.08	38,38,38,38	0
85	MG	5	3718	1/1	0.26	3.07	51,51,51,51	0
85	MG	7	205	1/1	0.28	3.06	83,83,83,83	0
85	MG	5	3887	1/1	0.22	3.06	79,79,79,79	0
85	MG	1	3780	1/1	0.28	3.06	38,38,38,38	0
86	OHX	6	2189	7/7	0.25	3.04	150,150,150,150	0
85	MG	1	3430	1/1	0.51	3.03	54,54,54,54	0
85	MG	6	1990	1/1	0.35	3.03	68,68,68,68	0
85	MG	1	3568	1/1	0.31	3.02	33,33,33,33	0
86	OHX	5	4138	7/7	0.30	3.02	125,125,125,125	0
85	MG	5	3627	1/1	0.21	3.01	67,67,67,67	0
86	OHX	2	2169	7/7	0.42	2.99	156,156,156,156	0
85	MG	5	3557	1/1	0.23	2.99	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	N5	201	1/1	0.26	2.99	74,74,74,74	0
85	MG	5	3890	1/1	0.22	2.98	62,62,62,62	0
86	OHX	1	4069	7/7	0.27	2.95	138,138,138,138	0
86	OHX	2	2096	7/7	0.30	2.95	153,153,153,153	0
86	OHX	6	2113	7/7	0.29	2.94	136,136,136,136	0
85	MG	1	3634	1/1	0.54	2.93	80,80,80,80	0
86	OHX	5	4040	7/7	0.27	2.91	141,141,141,141	0
86	OHX	1	4015	7/7	0.25	2.90	146,146,146,146	0
85	MG	M3	203	1/1	0.35	2.89	36,36,36,36	0
86	OHX	6	2149	7/7	0.30	2.88	132,132,132,132	0
85	MG	N8	202	1/1	0.28	2.86	35,35,35,35	0
86	OHX	5	4166	7/7	0.35	2.85	185,185,185,185	0
86	OHX	5	4062	7/7	0.37	2.84	129,129,129,129	0
86	OHX	5	4172	7/7	0.21	2.83	147,147,147,147	0
85	MG	5	3609	1/1	0.24	2.82	35,35,35,35	0
85	MG	n3	202	1/1	0.37	2.81	51,51,51,51	0
86	OHX	1	4115	7/7	0.26	2.81	138,138,138,138	0
87	ZN	d7	101	1/1	0.48	2.77	157,157,157,157	0
86	OHX	4	235	7/7	0.31	2.77	149,149,149,149	0
86	OHX	5	4203	7/7	0.32	2.77	139,139,139,139	0
86	OHX	1	4097	7/7	0.40	2.76	168,168,168,168	0
85	MG	1	3426	1/1	0.32	2.75	66,66,66,66	0
86	OHX	6	2147	7/7	0.31	2.74	119,119,119,119	0
86	OHX	2	2116	7/7	0.39	2.74	169,169,169,169	0
85	MG	6	1970	1/1	0.23	2.73	61,61,61,61	0
85	MG	5	3684	1/1	0.23	2.73	35,35,35,35	0
85	MG	5	3824	1/1	0.34	2.71	31,31,31,31	0
86	OHX	5	4039	7/7	0.20	2.71	115,115,115,115	0
86	OHX	2	2086	7/7	0.19	2.70	128,128,128,128	0
86	OHX	1	4092	7/7	0.17	2.70	173,173,173,173	0
85	MG	6	1993	1/1	0.28	2.70	58,58,58,58	0
86	OHX	2	2145	7/7	0.34	2.67	163,163,163,163	0
85	MG	6	1989	1/1	0.23	2.66	103,103,103,103	0
86	OHX	m4	201	7/7	0.42	2.66	221,221,221,221	0
85	MG	N8	204	1/1	0.41	2.66	44,44,44,44	0
85	MG	6	1975	1/1	0.25	2.66	63,63,63,63	0
85	MG	6	1999	1/1	0.35	2.65	54,54,54,54	0
85	MG	6	2032	1/1	0.28	2.65	52,52,52,52	0
85	MG	1	3628	1/1	0.30	2.65	30,30,30,30	0
86	OHX	2	2079	7/7	0.24	2.65	134,134,134,134	0
85	MG	2	1951	1/1	0.41	2.65	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	2	2152	7/7	0.42	2.62	164,164,164,164	0
86	OHX	5	4194	7/7	0.21	2.62	133,133,133,133	0
85	MG	l4	401	1/1	0.39	2.62	41,41,41,41	0
85	MG	1	3465	1/1	0.24	2.60	56,56,56,56	0
85	MG	2	1955	1/1	0.48	2.59	63,63,63,63	0
86	OHX	1	4004	7/7	0.20	2.59	116,116,116,116	0
85	MG	m7	204	1/1	0.35	2.59	37,37,37,37	0
85	MG	1	3618	1/1	0.19	2.58	74,74,74,74	0
85	MG	5	3528	1/1	0.20	2.56	28,28,28,28	0
86	OHX	5	3894	7/7	0.18	2.53	51,51,51,51	0
86	OHX	6	2188	7/7	0.35	2.52	161,161,161,161	0
86	OHX	5	4117	7/7	0.24	2.51	137,137,137,137	0
86	OHX	1	4133	7/7	0.32	2.51	150,150,150,150	0
86	OHX	O4	201	7/7	0.48	2.50	160,160,160,160	0
86	OHX	5	4139	7/7	0.22	2.50	147,147,147,147	0
85	MG	1	4218	1/1	0.24	2.49	40,40,40,40	0
86	OHX	1	4072	7/7	0.23	2.47	159,159,159,159	0
86	OHX	5	3903	7/7	0.21	2.46	75,75,75,75	0
86	OHX	5	4079	7/7	0.27	2.46	128,128,128,128	0
85	MG	d3	201	1/1	0.31	2.45	49,49,49,49	0
85	MG	1	3764	1/1	0.21	2.45	39,39,39,39	0
86	OHX	1	3992	7/7	0.23	2.45	143,143,143,143	0
86	OHX	1	3898	7/7	0.20	2.45	82,82,82,82	0
85	MG	5	3402	1/1	0.25	2.45	29,29,29,29	0
85	MG	1	3831	1/1	0.21	2.44	30,30,30,30	0
85	MG	c1	201	1/1	0.36	2.42	51,51,51,51	0
85	MG	1	3751	1/1	0.41	2.42	48,48,48,48	0
85	MG	5	3688	1/1	0.17	2.42	51,51,51,51	0
85	MG	1	3845	1/1	0.48	2.41	60,60,60,60	0
85	MG	5	3851	1/1	0.21	2.38	82,82,82,82	0
85	MG	5	3754	1/1	0.17	2.37	58,58,58,58	0
85	MG	6	1997	1/1	0.28	2.36	62,62,62,62	0
86	OHX	5	4024	7/7	0.20	2.34	103,103,103,103	0
86	OHX	2	2105	7/7	0.24	2.34	135,135,135,135	0
86	OHX	5	4163	7/7	0.20	2.33	154,154,154,154	0
86	OHX	6	2155	7/7	0.27	2.33	161,161,161,161	0
86	OHX	5	4086	7/7	0.22	2.32	129,129,129,129	0
85	MG	6	1984	1/1	0.24	2.32	87,87,87,87	0
86	OHX	5	4129	7/7	0.29	2.31	131,131,131,131	0
85	MG	m5	302	1/1	0.21	2.30	45,45,45,45	0
85	MG	5	3441	1/1	0.21	2.30	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	2	2075	7/7	0.27	2.29	155,155,155,155	0
86	OHX	1	4204	7/7	0.31	2.29	153,153,153,153	0
86	OHX	5	4185	7/7	0.40	2.29	151,151,151,151	0
86	OHX	5	4041	7/7	0.23	2.27	118,118,118,118	0
86	OHX	6	2171	7/7	0.29	2.27	152,152,152,152	0
86	OHX	2	2051	7/7	0.16	2.27	132,132,132,132	0
85	MG	2	1920	1/1	0.36	2.23	61,61,61,61	0
85	MG	3	207	1/1	0.25	2.22	66,66,66,66	0
85	MG	1	3753	1/1	0.26	2.20	69,69,69,69	0
86	OHX	5	4115	7/7	0.29	2.20	158,158,158,158	0
86	OHX	6	2195	7/7	0.36	2.19	179,179,179,179	0
86	OHX	2	2118	7/7	0.20	2.19	175,175,175,175	0
85	MG	1	3604	1/1	0.23	2.17	39,39,39,39	0
85	MG	5	3886	1/1	0.25	2.16	86,86,86,86	0
86	OHX	1	4026	7/7	0.19	2.16	152,152,152,152	0
86	OHX	1	4009	7/7	0.18	2.16	139,139,139,139	0
85	MG	L3	401	1/1	0.26	2.15	39,39,39,39	0
86	OHX	2	2106	7/7	0.23	2.15	144,144,144,144	0
86	OHX	6	2156	7/7	0.23	2.14	150,150,150,150	0
85	MG	5	3702	1/1	0.24	2.14	72,72,72,72	0
85	MG	5	3812	1/1	0.22	2.13	65,65,65,65	0
85	MG	4	207	1/1	0.22	2.12	49,49,49,49	0
86	OHX	1	4005	7/7	0.20	2.12	133,133,133,133	0
85	MG	5	3698	1/1	0.22	2.10	43,43,43,43	0
86	OHX	1	4106	7/7	0.30	2.09	133,133,133,133	0
86	OHX	1	4104	7/7	0.22	2.09	152,152,152,152	0
86	OHX	6	2174	7/7	0.30	2.07	173,173,173,173	0
85	MG	5	3468	1/1	0.21	2.06	32,32,32,32	0
85	MG	6	1932	1/1	0.24	2.05	43,43,43,43	0
86	OHX	2	2069	7/7	0.23	2.05	128,128,128,128	0
86	OHX	5	4073	7/7	0.21	2.04	153,153,153,153	0
86	OHX	2	2109	7/7	0.21	2.03	172,172,172,172	0
85	MG	l5	302	1/1	0.38	2.03	69,69,69,69	0
85	MG	l3	401	1/1	0.28	2.03	33,33,33,33	0
86	OHX	1	4052	7/7	0.20	2.02	151,151,151,151	0
85	MG	6	2022	1/1	0.39	2.01	72,72,72,72	0
85	MG	5	3579	1/1	0.30	2.00	29,29,29,29	0
85	MG	5	3877	1/1	0.25	2.00	95,95,95,95	0
86	OHX	1	3911	7/7	0.24	1.99	100,100,100,100	0
85	MG	1	3505	1/1	0.23	1.98	38,38,38,38	0
85	MG	5	3628	1/1	0.18	1.98	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3733	1/1	0.20	1.96	40,40,40,40	0
86	OHX	6	2193	7/7	0.30	1.94	193,193,193,193	0
85	MG	5	3564	1/1	0.20	1.91	28,28,28,28	0
86	OHX	1	4157	7/7	0.29	1.90	162,162,162,162	0
86	OHX	1	4093	7/7	0.18	1.88	154,154,154,154	0
85	MG	1	3416	1/1	0.41	1.88	57,57,57,57	0
85	MG	2	2005	1/1	0.22	1.88	73,73,73,73	0
86	OHX	8	231	7/7	0.29	1.88	156,156,156,156	0
86	OHX	2	2155	7/7	0.22	1.86	162,162,162,162	0
86	OHX	5	4171	7/7	0.33	1.86	161,161,161,161	0
86	OHX	1	4098	7/7	0.35	1.85	120,120,120,120	0
85	MG	6	1985	1/1	0.18	1.85	102,102,102,102	0
85	MG	1	3810	1/1	0.33	1.85	64,64,64,64	0
86	OHX	1	4186	7/7	0.27	1.84	151,151,151,151	0
85	MG	1	3770	1/1	0.22	1.84	61,61,61,61	0
86	OHX	5	4135	7/7	0.26	1.84	147,147,147,147	0
86	OHX	7	226	7/7	0.23	1.84	137,137,137,137	0
85	MG	8	213	1/1	0.27	1.83	93,93,93,93	0
86	OHX	1	4076	7/7	0.21	1.83	133,133,133,133	0
85	MG	5	3612	1/1	0.22	1.82	37,37,37,37	0
85	MG	5	3631	1/1	0.18	1.82	43,43,43,43	0
85	MG	1	3767	1/1	0.20	1.82	45,45,45,45	0
85	MG	m5	301	1/1	0.32	1.82	36,36,36,36	0
85	MG	6	1977	1/1	0.23	1.81	51,51,51,51	0
86	OHX	2	2126	7/7	0.21	1.81	151,151,151,151	0
86	OHX	5	4089	7/7	0.20	1.79	142,142,142,142	0
86	OHX	5	4113	7/7	0.27	1.77	130,130,130,130	0
86	OHX	5	4096	7/7	0.21	1.76	108,108,108,108	0
85	MG	m7	205	1/1	0.29	1.76	43,43,43,43	0
85	MG	1	3546	1/1	0.19	1.75	66,66,66,66	0
86	OHX	5	4069	7/7	0.34	1.75	141,141,141,141	0
86	OHX	O6	201	7/7	0.38	1.74	135,135,135,135	0
85	MG	5	3424	1/1	0.25	1.74	49,49,49,49	0
85	MG	O2	202	1/1	0.28	1.71	34,34,34,34	0
86	OHX	5	4244	7/7	0.33	1.71	156,156,156,156	0
86	OHX	5	4122	7/7	0.24	1.71	148,148,148,148	0
86	OHX	6	2123	7/7	0.28	1.70	155,155,155,155	0
86	OHX	5	3977	7/7	0.22	1.70	103,103,103,103	0
85	MG	d6	102	1/1	0.28	1.69	58,58,58,58	0
86	OHX	6	2151	7/7	0.20	1.68	160,160,160,160	0
85	MG	1	3710	1/1	0.18	1.68	42,42,42,42	0
86	OHX	4	223	7/7	0.19	1.68	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	6	2130	7/7	0.30	1.67	144,144,144,144	0
85	MG	6	2040	1/1	0.35	1.67	84,84,84,84	0
86	OHX	1	3872	7/7	0.16	1.64	65,65,65,65	0
85	MG	1	3616	1/1	0.27	1.64	46,46,46,46	0
85	MG	L5	301	1/1	0.59	1.64	71,71,71,71	0
86	OHX	6	2111	7/7	0.20	1.63	121,121,121,121	0
85	MG	5	3719	1/1	0.26	1.62	52,52,52,52	0
86	OHX	5	4017	7/7	0.21	1.61	131,131,131,131	0
86	OHX	6	2122	7/7	0.24	1.60	151,151,151,151	0
85	MG	1	3836	1/1	0.50	1.60	43,43,43,43	0
86	OHX	2	2140	7/7	0.22	1.59	173,173,173,173	0
86	OHX	6	2126	7/7	0.37	1.59	171,171,171,171	0
85	MG	1	3642	1/1	0.18	1.58	67,67,67,67	0
86	OHX	1	4199	7/7	0.26	1.57	178,178,178,178	0
85	MG	5	3489	1/1	0.20	1.57	35,35,35,35	0
86	OHX	1	3984	7/7	0.18	1.57	109,109,109,109	0
86	OHX	4	234	7/7	0.23	1.56	149,149,149,149	0
85	MG	6	2006	1/1	0.30	1.56	63,63,63,63	0
86	OHX	5	4155	7/7	0.24	1.56	128,128,128,128	0
86	OHX	5	4063	7/7	0.18	1.55	155,155,155,155	0
86	OHX	2	2165	7/7	0.28	1.55	166,166,166,166	0
86	OHX	5	4227	7/7	0.24	1.52	180,180,180,180	0
85	MG	1	3724	1/1	0.41	1.52	57,57,57,57	0
86	OHX	1	4100	7/7	0.33	1.52	179,179,179,179	0
86	OHX	6	2104	7/7	0.26	1.52	130,130,130,130	0
86	OHX	5	4088	7/7	0.31	1.51	151,151,151,151	0
86	OHX	1	4010	7/7	0.20	1.51	141,141,141,141	0
85	MG	l5	301	1/1	0.47	1.50	60,60,60,60	0
85	MG	2	1927	1/1	0.32	1.50	37,37,37,37	0
86	OHX	5	4211	7/7	0.21	1.49	117,117,117,117	0
85	MG	M6	201	1/1	0.35	1.48	43,43,43,43	0
86	OHX	L4	403	7/7	0.26	1.48	169,169,169,169	0
85	MG	d3	203	1/1	0.29	1.48	41,41,41,41	0
86	OHX	m8	201	7/7	0.27	1.47	147,147,147,147	0
85	MG	6	1982	1/1	0.45	1.47	52,52,52,52	0
85	MG	1	3740	1/1	0.27	1.47	76,76,76,76	0
85	MG	5	3779	1/1	0.23	1.45	88,88,88,88	0
86	OHX	2	2124	7/7	0.26	1.45	162,162,162,162	0
86	OHX	5	4202	7/7	0.22	1.43	168,168,168,168	0
86	OHX	1	4132	7/7	0.22	1.42	134,134,134,134	0
86	OHX	6	2179	7/7	0.19	1.42	162,162,162,162	0
85	MG	1	3636	1/1	0.28	1.41	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	6	2150	7/7	0.27	1.41	172,172,172,172	0
85	MG	1	3641	1/1	0.34	1.41	57,57,57,57	0
85	MG	5	3542	1/1	0.37	1.39	75,75,75,75	0
85	MG	5	3603	1/1	0.23	1.39	38,38,38,38	0
85	MG	6	2205	1/1	0.30	1.39	59,59,59,59	0
85	MG	1	3472	1/1	0.23	1.38	35,35,35,35	0
85	MG	5	3475	1/1	0.22	1.37	80,80,80,80	0
85	MG	6	2026	1/1	0.24	1.36	98,98,98,98	0
85	MG	M9	202	1/1	0.38	1.35	62,62,62,62	0
86	OHX	5	4087	7/7	0.21	1.35	126,126,126,126	0
85	MG	5	3600	1/1	0.20	1.35	45,45,45,45	0
86	OHX	1	4016	7/7	0.21	1.33	124,124,124,124	0
86	OHX	d9	102	7/7	0.47	1.33	190,190,190,190	0
86	OHX	2	2101	7/7	0.17	1.32	163,163,163,163	0
85	MG	1	3663	1/1	0.23	1.32	36,36,36,36	0
86	OHX	1	4172	7/7	0.18	1.32	111,111,111,111	0
86	OHX	5	4084	7/7	0.26	1.31	115,115,115,115	0
85	MG	2	2004	1/1	0.33	1.31	62,62,62,62	0
85	MG	1	3776	1/1	0.31	1.30	57,57,57,57	0
86	OHX	5	4169	7/7	0.21	1.30	128,128,128,128	0
86	OHX	1	3973	7/7	0.17	1.27	121,121,121,121	0
86	OHX	1	4160	7/7	0.29	1.25	176,176,176,176	0
85	MG	5	3634	1/1	0.18	1.23	36,36,36,36	0
86	OHX	5	4222	7/7	0.33	1.22	174,174,174,174	0
86	OHX	5	4184	7/7	0.34	1.22	141,141,141,141	0
85	MG	1	3647	1/1	0.25	1.21	44,44,44,44	0
85	MG	5	3888	1/1	0.19	1.20	119,119,119,119	0
85	MG	6	2000	1/1	0.18	1.19	102,102,102,102	0
85	MG	5	3429	1/1	0.25	1.17	80,80,80,80	0
86	OHX	5	4027	7/7	0.18	1.16	122,122,122,122	0
85	MG	5	4247	1/1	0.23	1.15	43,43,43,43	0
85	MG	5	3654	1/1	0.18	1.15	32,32,32,32	0
86	OHX	5	4006	7/7	0.20	1.15	120,120,120,120	0
86	OHX	m7	206	7/7	0.28	1.14	147,147,147,147	0
85	MG	1	3681	1/1	0.23	1.13	48,48,48,48	0
86	OHX	1	4030	7/7	0.24	1.12	120,120,120,120	0
85	MG	5	3710	1/1	0.27	1.11	70,70,70,70	0
85	MG	1	3445	1/1	0.20	1.11	52,52,52,52	0
86	OHX	1	3972	7/7	0.19	1.10	114,114,114,114	0
86	OHX	6	2185	7/7	0.18	1.09	189,189,189,189	0
85	MG	2	1992	1/1	0.37	1.08	61,61,61,61	0
86	OHX	l4	402	7/7	0.22	1.07	190,190,190,190	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	2	2087	7/7	0.24	1.07	139,139,139,139	0
85	MG	N3	202	1/1	0.31	1.06	77,77,77,77	0
86	OHX	5	4070	7/7	0.28	1.06	143,143,143,143	0
86	OHX	2	2083	7/7	0.15	1.06	144,144,144,144	0
86	OHX	1	3968	7/7	0.20	1.05	114,114,114,114	0
86	OHX	5	4214	7/7	0.30	1.05	194,194,194,194	0
86	OHX	5	4137	7/7	0.20	1.04	142,142,142,142	0
86	OHX	1	3983	7/7	0.29	1.03	128,128,128,128	0
85	MG	5	3433	1/1	0.21	1.02	33,33,33,33	0
85	MG	2	1954	1/1	0.20	1.02	68,68,68,68	0
85	MG	2	2020	1/1	0.31	1.02	100,100,100,100	0
86	OHX	2	2115	7/7	0.23	1.02	137,137,137,137	0
85	MG	1	3766	1/1	0.24	1.01	49,49,49,49	0
86	OHX	1	4029	7/7	0.21	1.00	138,138,138,138	0
86	OHX	5	4112	7/7	0.19	1.00	145,145,145,145	0
86	OHX	5	4158	7/7	0.17	1.00	161,161,161,161	0
86	OHX	1	4149	7/7	0.42	0.99	162,162,162,162	0
86	OHX	2	2133	7/7	0.23	0.98	167,167,167,167	0
86	OHX	1	4001	7/7	0.24	0.98	128,128,128,128	0
86	OHX	5	4220	7/7	0.28	0.97	169,169,169,169	0
85	MG	5	3701	1/1	0.26	0.97	59,59,59,59	0
86	OHX	1	3884	7/7	0.18	0.96	80,80,80,80	0
86	OHX	2	2111	7/7	0.22	0.96	133,133,133,133	0
86	OHX	5	4125	7/7	0.16	0.96	121,121,121,121	0
86	OHX	5	4035	7/7	0.17	0.95	145,145,145,145	0
85	MG	1	3697	1/1	0.28	0.95	54,54,54,54	0
86	OHX	6	2046	7/7	0.21	0.95	81,81,81,81	0
86	OHX	5	4111	7/7	0.25	0.94	113,113,113,113	0
86	OHX	1	4074	7/7	0.23	0.93	137,137,137,137	0
86	OHX	5	4100	7/7	0.21	0.93	123,123,123,123	0
86	OHX	6	2066	7/7	0.21	0.93	118,118,118,118	0
86	OHX	2	2076	7/7	0.22	0.91	146,146,146,146	0
86	OHX	5	4106	7/7	0.19	0.91	141,141,141,141	0
86	OHX	2	2175	7/7	0.28	0.90	159,159,159,159	0
86	OHX	5	4177	7/7	0.34	0.89	159,159,159,159	0
86	OHX	6	2140	7/7	0.34	0.89	140,140,140,140	0
86	OHX	1	4123	7/7	0.20	0.89	154,154,154,154	0
85	MG	L4	401	1/1	0.24	0.87	68,68,68,68	0
85	MG	1	3487	1/1	0.20	0.87	38,38,38,38	0
86	OHX	1	4048	7/7	0.20	0.87	137,137,137,137	0
86	OHX	6	2201	7/7	0.41	0.86	156,156,156,156	0
86	OHX	5	4051	7/7	0.23	0.85	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	4060	7/7	0.19	0.85	155,155,155,155	0
86	OHX	2	2179	7/7	0.26	0.85	181,181,181,181	0
85	MG	M0	302	1/1	0.24	0.83	45,45,45,45	0
86	OHX	6	2164	7/7	0.31	0.83	164,164,164,164	0
85	MG	5	3599	1/1	0.19	0.83	44,44,44,44	0
86	OHX	2	2065	7/7	0.22	0.81	124,124,124,124	0
86	OHX	1	4165	7/7	0.31	0.81	229,229,229,229	0
85	MG	6	1940	1/1	0.26	0.80	95,95,95,95	0
85	MG	5	3863	1/1	0.18	0.79	29,29,29,29	0
85	MG	1	3721	1/1	0.18	0.78	83,83,83,83	0
88	3J6	1	4213	21/21	0.21	0.78	37,37,37,37	0
86	OHX	6	2105	7/7	0.33	0.77	172,172,172,172	0
86	OHX	d4	201	7/7	0.33	0.77	181,181,181,181	0
85	MG	4	204	1/1	0.40	0.76	70,70,70,70	0
86	OHX	1	3876	7/7	0.17	0.76	64,64,64,64	0
85	MG	5	3527	1/1	0.37	0.76	64,64,64,64	0
86	OHX	5	4075	7/7	0.19	0.75	119,119,119,119	0
86	OHX	5	3995	7/7	0.27	0.75	116,116,116,116	0
85	MG	8	208	1/1	0.28	0.72	50,50,50,50	0
85	MG	6	2044	1/1	0.23	0.72	76,76,76,76	0
85	MG	6	2016	1/1	0.15	0.71	82,82,82,82	0
86	OHX	1	3989	7/7	0.23	0.71	113,113,113,113	0
86	OHX	3	221	7/7	0.18	0.70	140,140,140,140	0
86	OHX	2	2129	7/7	0.25	0.69	212,212,212,212	0
86	OHX	sR	401	7/7	0.24	0.69	177,177,177,177	0
85	MG	5	3493	1/1	0.20	0.69	46,46,46,46	0
86	OHX	6	2148	7/7	0.24	0.68	159,159,159,159	0
86	OHX	6	2192	7/7	0.28	0.67	174,174,174,174	0
85	MG	6	2005	1/1	0.26	0.66	84,84,84,84	0
85	MG	sM	302	1/1	0.28	0.66	51,51,51,51	0
86	OHX	1	4083	7/7	0.28	0.66	162,162,162,162	0
85	MG	1	3482	1/1	0.23	0.66	60,60,60,60	0
86	OHX	2	2058	7/7	0.17	0.66	123,123,123,123	0
85	MG	5	3618	1/1	0.32	0.65	42,42,42,42	0
86	OHX	1	4113	7/7	0.20	0.65	194,194,194,194	0
85	MG	1	4216	1/1	0.22	0.64	32,32,32,32	0
86	OHX	2	2147	7/7	0.18	0.64	182,182,182,182	0
86	OHX	1	3943	7/7	0.18	0.63	106,106,106,106	0
86	OHX	n3	204	7/7	0.19	0.63	125,125,125,125	0
85	MG	6	1983	1/1	0.18	0.60	56,56,56,56	0
86	OHX	5	4195	7/7	0.25	0.60	139,139,139,139	0
86	OHX	1	3958	7/7	0.23	0.59	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	1	3466	1/1	0.19	0.59	48,48,48,48	0
85	MG	1	3582	1/1	0.36	0.58	36,36,36,36	0
85	MG	5	3407	1/1	0.15	0.58	45,45,45,45	0
85	MG	2	1970	1/1	0.28	0.58	90,90,90,90	0
86	OHX	8	229	7/7	0.20	0.57	157,157,157,157	0
85	MG	1	3673	1/1	0.23	0.56	49,49,49,49	0
86	OHX	1	4210	7/7	0.29	0.56	191,191,191,191	0
86	OHX	8	223	7/7	0.13	0.56	135,135,135,135	0
85	MG	5	3796	1/1	0.21	0.56	47,47,47,47	0
86	OHX	5	3999	7/7	0.23	0.56	116,116,116,116	0
86	OHX	6	2135	7/7	0.28	0.55	139,139,139,139	0
86	OHX	1	4007	7/7	0.24	0.55	119,119,119,119	0
86	OHX	1	4019	7/7	0.23	0.54	149,149,149,149	0
86	OHX	2	2112	7/7	0.26	0.53	177,177,177,177	0
85	MG	1	3627	1/1	0.42	0.53	104,104,104,104	0
85	MG	5	3752	1/1	0.21	0.53	55,55,55,55	0
86	OHX	1	4021	7/7	0.21	0.53	140,140,140,140	0
85	MG	5	3769	1/1	0.26	0.52	102,102,102,102	0
86	OHX	5	4081	7/7	0.19	0.51	144,144,144,144	0
86	OHX	5	4057	7/7	0.20	0.51	141,141,141,141	0
85	MG	3	210	1/1	0.22	0.50	70,70,70,70	0
86	OHX	6	2196	7/7	0.23	0.50	190,190,190,190	0
85	MG	1	3434	1/1	0.17	0.48	50,50,50,50	0
86	OHX	1	4088	7/7	0.20	0.47	97,97,97,97	0
86	OHX	6	2160	7/7	0.27	0.47	140,140,140,140	0
86	OHX	5	4238	7/7	0.25	0.46	152,152,152,152	0
85	MG	1	3727	1/1	0.17	0.46	74,74,74,74	0
86	OHX	2	2080	7/7	0.22	0.45	190,190,190,190	0
85	MG	1	3789	1/1	0.26	0.44	55,55,55,55	0
86	OHX	5	4118	7/7	0.19	0.44	166,166,166,166	0
85	MG	L4	402	1/1	0.21	0.43	33,33,33,33	0
86	OHX	2	2151	7/7	0.21	0.42	199,199,199,199	0
86	OHX	1	4156	7/7	0.21	0.42	126,126,126,126	0
86	OHX	5	3920	7/7	0.19	0.40	79,79,79,79	0
86	OHX	5	4072	7/7	0.18	0.38	113,113,113,113	0
86	OHX	6	2182	7/7	0.30	0.37	138,138,138,138	0
86	OHX	2	2142	7/7	0.20	0.35	160,160,160,160	0
86	OHX	2	2072	7/7	0.24	0.34	142,142,142,142	0
85	MG	5	3415	1/1	0.19	0.34	56,56,56,56	0
86	OHX	S6	301	7/7	0.39	0.33	170,170,170,170	0
86	OHX	5	4022	7/7	0.18	0.33	121,121,121,121	0
86	OHX	c5	201	7/7	0.29	0.33	183,183,183,183	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	5	3652	1/1	0.24	0.33	65,65,65,65	0
85	MG	c7	201	1/1	0.23	0.33	80,80,80,80	0
85	MG	5	3686	1/1	0.20	0.32	84,84,84,84	0
86	OHX	4	227	7/7	0.21	0.32	141,141,141,141	0
86	OHX	5	4162	7/7	0.15	0.32	162,162,162,162	0
86	OHX	l9	202	7/7	0.20	0.32	140,140,140,140	0
85	MG	M3	201	1/1	0.17	0.32	46,46,46,46	0
85	MG	5	3635	1/1	0.28	0.31	78,78,78,78	0
85	MG	1	3662	1/1	0.28	0.31	72,72,72,72	0
85	MG	2	1998	1/1	0.31	0.30	74,74,74,74	0
86	OHX	1	3870	7/7	0.20	0.29	64,64,64,64	0
86	OHX	2	2120	7/7	0.18	0.28	148,148,148,148	0
86	OHX	5	4108	7/7	0.19	0.28	125,125,125,125	0
86	OHX	1	3986	7/7	0.20	0.27	134,134,134,134	0
85	MG	1	3800	1/1	0.15	0.27	55,55,55,55	0
85	MG	o1	201	1/1	0.24	0.27	81,81,81,81	0
86	OHX	1	4087	7/7	0.22	0.27	137,137,137,137	0
85	MG	s8	302	1/1	0.19	0.27	54,54,54,54	0
86	OHX	1	4040	7/7	0.21	0.27	126,126,126,126	0
86	OHX	2	2054	7/7	0.18	0.25	152,152,152,152	0
85	MG	5	3696	1/1	0.18	0.23	40,40,40,40	0
85	MG	1	3786	1/1	0.26	0.23	69,69,69,69	0
85	MG	M3	202	1/1	0.40	0.23	90,90,90,90	0
85	MG	L8	301	1/1	0.32	0.23	63,63,63,63	0
86	OHX	6	2194	7/7	0.34	0.23	201,201,201,201	0
85	MG	1	3675	1/1	0.26	0.23	72,72,72,72	0
86	OHX	1	4037	7/7	0.14	0.22	156,156,156,156	0
86	OHX	1	4039	7/7	0.29	0.21	134,134,134,134	0
86	OHX	5	3893	7/7	0.21	0.21	51,51,51,51	0
86	OHX	2	2085	7/7	0.22	0.20	156,156,156,156	0
85	MG	1	3802	1/1	0.19	0.19	52,52,52,52	0
86	OHX	2	2164	7/7	0.19	0.18	187,187,187,187	0
86	OHX	1	4131	7/7	0.34	0.18	167,167,167,167	0
85	MG	5	3611	1/1	0.21	0.18	50,50,50,50	0
86	OHX	5	4123	7/7	0.30	0.17	161,161,161,161	0
86	OHX	1	4035	7/7	0.21	0.17	114,114,114,114	0
85	MG	1	3638	1/1	0.28	0.16	75,75,75,75	0
86	OHX	1	4042	7/7	0.18	0.15	133,133,133,133	0
86	OHX	4	231	7/7	0.16	0.15	145,145,145,145	0
86	OHX	5	3908	7/7	0.15	0.15	67,67,67,67	0
87	ZN	D7	101	1/1	0.24	0.14	153,153,153,153	0
86	OHX	1	4084	7/7	0.18	0.14	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	4190	7/7	0.19	0.13	161,161,161,161	0
86	OHX	5	4119	7/7	0.20	0.12	166,166,166,166	0
85	MG	1	3755	1/1	0.24	0.12	62,62,62,62	0
86	OHX	5	4189	7/7	0.31	0.11	196,196,196,196	0
86	OHX	2	2081	7/7	0.17	0.11	153,153,153,153	0
85	MG	1	3489	1/1	0.19	0.10	40,40,40,40	0
85	MG	M9	201	1/1	0.30	0.08	70,70,70,70	0
86	OHX	2	2144	7/7	0.30	0.08	183,183,183,183	0
85	MG	1	3720	1/1	0.19	0.05	45,45,45,45	0
85	MG	5	3484	1/1	0.23	0.05	77,77,77,77	0
86	OHX	5	4116	7/7	0.20	0.05	152,152,152,152	0
85	MG	5	3446	1/1	0.17	0.05	52,52,52,52	0
85	MG	N3	203	1/1	0.23	0.04	56,56,56,56	0
86	OHX	5	3966	7/7	0.30	0.04	114,114,114,114	0
86	OHX	l3	405	7/7	0.27	0.04	151,151,151,151	0
86	OHX	5	4149	7/7	0.21	0.03	130,130,130,130	0
86	OHX	1	4051	7/7	0.20	0.03	123,123,123,123	0
86	OHX	m0	303	7/7	0.29	0.02	143,143,143,143	0
86	OHX	1	4101	7/7	0.24	0.01	148,148,148,148	0
85	MG	c8	202	1/1	0.37	0.01	61,61,61,61	0
85	MG	6	2014	1/1	0.31	0.00	154,154,154,154	0
86	OHX	m1	202	7/7	0.33	-0.00	164,164,164,164	0
86	OHX	8	219	7/7	0.20	-0.00	129,129,129,129	0
86	OHX	5	4228	7/7	0.22	0.00	119,119,119,119	0
85	MG	5	3760	1/1	0.17	0.00	100,100,100,100	0
86	OHX	6	2152	7/7	0.17	-0.01	145,145,145,145	0
86	OHX	S8	302	7/7	0.28	-0.02	185,185,185,185	0
86	OHX	1	3892	7/7	0.14	-0.03	86,86,86,86	0
86	OHX	6	2102	7/7	0.17	-0.03	133,133,133,133	0
86	OHX	n9	102	7/7	0.14	-0.03	79,79,79,79	0
86	OHX	6	2137	7/7	0.16	-0.04	151,151,151,151	0
85	MG	1	3696	1/1	0.19	-0.05	49,49,49,49	0
86	OHX	1	4103	7/7	0.19	-0.05	131,131,131,131	0
86	OHX	3	219	7/7	0.20	-0.05	129,129,129,129	0
85	MG	1	3643	1/1	0.16	-0.06	66,66,66,66	0
86	OHX	1	4044	7/7	0.24	-0.07	124,124,124,124	0
86	OHX	6	2165	7/7	0.18	-0.07	197,197,197,197	0
86	OHX	L3	405	7/7	0.40	-0.07	171,171,171,171	0
86	OHX	1	4161	7/7	0.20	-0.07	147,147,147,147	0
86	OHX	1	4102	7/7	0.15	-0.07	158,158,158,158	0
86	OHX	6	2141	7/7	0.22	-0.07	156,156,156,156	0
85	MG	1	3739	1/1	0.16	-0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	3999	7/7	0.16	-0.08	119,119,119,119	0
85	MG	1	3436	1/1	0.21	-0.08	44,44,44,44	0
86	OHX	6	2107	7/7	0.16	-0.09	137,137,137,137	0
85	MG	1	3448	1/1	0.15	-0.10	39,39,39,39	0
86	OHX	2	2176	7/7	0.18	-0.10	189,189,189,189	0
85	MG	1	3425	1/1	0.20	-0.10	31,31,31,31	0
85	MG	7	208	1/1	0.15	-0.13	57,57,57,57	0
86	OHX	6	2103	7/7	0.16	-0.13	134,134,134,134	0
86	OHX	1	4049	7/7	0.17	-0.16	160,160,160,160	0
85	MG	5	3723	1/1	0.17	-0.16	62,62,62,62	0
85	MG	2	1942	1/1	0.16	-0.16	76,76,76,76	0
86	OHX	5	3901	7/7	0.16	-0.16	64,64,64,64	0
85	MG	5	3750	1/1	0.18	-0.18	54,54,54,54	0
86	OHX	1	4059	7/7	0.18	-0.19	192,192,192,192	0
86	OHX	1	4144	7/7	0.23	-0.19	172,172,172,172	0
86	OHX	4	225	7/7	0.20	-0.20	118,118,118,118	0
86	OHX	5	4165	7/7	0.26	-0.20	205,205,205,205	0
86	OHX	2	2102	7/7	0.20	-0.21	164,164,164,164	0
86	OHX	5	4082	7/7	0.20	-0.21	128,128,128,128	0
86	OHX	1	4036	7/7	0.22	-0.21	145,145,145,145	0
86	OHX	6	2117	7/7	0.26	-0.21	139,139,139,139	0
86	OHX	5	4032	7/7	0.14	-0.22	137,137,137,137	0
86	OHX	1	3971	7/7	0.21	-0.23	127,127,127,127	0
85	MG	5	3807	1/1	0.18	-0.25	82,82,82,82	0
86	OHX	l5	305	7/7	0.25	-0.25	157,157,157,157	0
85	MG	5	3436	1/1	0.21	-0.28	58,58,58,58	0
86	OHX	5	4008	7/7	0.19	-0.28	101,101,101,101	0
86	OHX	6	2093	7/7	0.18	-0.29	156,156,156,156	0
85	MG	1	3731	1/1	0.18	-0.30	73,73,73,73	0
86	OHX	5	3948	7/7	0.22	-0.31	104,104,104,104	0
85	MG	1	3557	1/1	0.16	-0.32	57,57,57,57	0
85	MG	D3	201	1/1	0.22	-0.32	58,58,58,58	0
85	MG	1	3420	1/1	0.28	-0.33	78,78,78,78	0
85	MG	1	3665	1/1	0.20	-0.33	72,72,72,72	0
85	MG	5	3669	1/1	0.16	-0.33	30,30,30,30	0
85	MG	1	3648	1/1	0.15	-0.34	73,73,73,73	0
86	OHX	1	4002	7/7	0.21	-0.34	112,112,112,112	0
86	OHX	7	223	7/7	0.17	-0.34	118,118,118,118	0
85	MG	m7	202	1/1	0.19	-0.35	32,32,32,32	0
86	OHX	1	4197	7/7	0.18	-0.35	136,136,136,136	0
85	MG	1	3428	1/1	0.18	-0.36	55,55,55,55	0
86	OHX	6	2127	7/7	0.14	-0.36	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	o2	201	7/7	0.18	-0.37	112,112,112,112	0
86	OHX	2	2121	7/7	0.16	-0.37	162,162,162,162	0
86	OHX	5	3958	7/7	0.17	-0.37	104,104,104,104	0
85	MG	1	3729	1/1	0.16	-0.38	68,68,68,68	0
86	OHX	1	3977	7/7	0.16	-0.39	101,101,101,101	0
87	ZN	d6	101	1/1	0.14	-0.39	65,65,65,65	0
85	MG	m7	203	1/1	0.15	-0.39	49,49,49,49	0
86	OHX	5	4236	7/7	0.21	-0.40	101,101,101,101	0
86	OHX	6	2089	7/7	0.17	-0.40	132,132,132,132	0
86	OHX	1	4024	7/7	0.16	-0.42	160,160,160,160	0
85	MG	1	3682	1/1	0.15	-0.42	44,44,44,44	0
86	OHX	2	2067	7/7	0.15	-0.42	157,157,157,157	0
86	OHX	8	217	7/7	0.16	-0.42	64,64,64,64	0
86	OHX	5	4043	7/7	0.15	-0.43	135,135,135,135	0
86	OHX	2	2057	7/7	0.17	-0.44	168,168,168,168	0
85	MG	2	1990	1/1	0.21	-0.44	111,111,111,111	0
85	MG	5	3466	1/1	0.25	-0.44	91,91,91,91	0
86	OHX	1	4023	7/7	0.13	-0.44	156,156,156,156	0
86	OHX	2	2100	7/7	0.20	-0.44	163,163,163,163	0
86	OHX	o7	502	7/7	0.16	-0.45	120,120,120,120	0
86	OHX	5	3897	7/7	0.17	-0.45	59,59,59,59	0
86	OHX	2	2060	7/7	0.17	-0.45	117,117,117,117	0
86	OHX	5	3987	7/7	0.19	-0.46	144,144,144,144	0
85	MG	4	220	1/1	0.16	-0.46	57,57,57,57	0
86	OHX	5	4058	7/7	0.17	-0.46	170,170,170,170	0
85	MG	5	3428	1/1	0.20	-0.46	34,34,34,34	0
86	OHX	m5	303	7/7	0.20	-0.46	149,149,149,149	0
86	OHX	1	4031	7/7	0.19	-0.48	143,143,143,143	0
86	OHX	5	4030	7/7	0.16	-0.49	136,136,136,136	0
86	OHX	D3	202	7/7	0.21	-0.49	160,160,160,160	0
85	MG	5	3839	1/1	0.15	-0.49	58,58,58,58	0
85	MG	1	3488	1/1	0.28	-0.49	53,53,53,53	0
86	OHX	1	4056	7/7	0.18	-0.50	160,160,160,160	0
86	OHX	s8	303	7/7	0.33	-0.50	183,183,183,183	0
86	OHX	2	2025	7/7	0.18	-0.50	96,96,96,96	0
86	OHX	1	3990	7/7	0.18	-0.51	127,127,127,127	0
85	MG	5	3753	1/1	0.17	-0.52	57,57,57,57	0
85	MG	1	3683	1/1	0.18	-0.52	69,69,69,69	0
85	MG	1	3749	1/1	0.15	-0.53	42,42,42,42	0
85	MG	5	3721	1/1	0.17	-0.54	37,37,37,37	0
85	MG	5	3401	1/1	0.16	-0.55	63,63,63,63	0
86	OHX	1	4053	7/7	0.18	-0.55	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	3888	7/7	0.18	-0.55	73,73,73,73	0
86	OHX	1	4089	7/7	0.13	-0.55	145,145,145,145	0
86	OHX	1	4151	7/7	0.17	-0.55	139,139,139,139	0
86	OHX	5	4010	7/7	0.18	-0.55	115,115,115,115	0
86	OHX	1	4090	7/7	0.20	-0.55	175,175,175,175	0
86	OHX	6	2053	7/7	0.14	-0.56	94,94,94,94	0
86	OHX	6	2146	7/7	0.19	-0.56	150,150,150,150	0
86	OHX	1	3924	7/7	0.16	-0.56	119,119,119,119	0
86	OHX	5	3973	7/7	0.15	-0.57	128,128,128,128	0
86	OHX	1	3947	7/7	0.18	-0.57	101,101,101,101	0
86	OHX	2	2114	7/7	0.19	-0.59	178,178,178,178	0
86	OHX	2	2093	7/7	0.17	-0.59	173,173,173,173	0
85	MG	5	3748	1/1	0.15	-0.60	55,55,55,55	0
87	ZN	Q3	501	1/1	0.09	-0.60	70,70,70,70	0
86	OHX	1	3881	7/7	0.15	-0.61	72,72,72,72	0
86	OHX	8	226	7/7	0.16	-0.62	139,139,139,139	0
86	OHX	5	3932	7/7	0.14	-0.62	88,88,88,88	0
86	OHX	5	3917	7/7	0.16	-0.62	79,79,79,79	0
85	MG	7	216	1/1	0.15	-0.63	44,44,44,44	0
86	OHX	5	3907	7/7	0.14	-0.63	70,70,70,70	0
86	OHX	4	224	7/7	0.12	-0.65	122,122,122,122	0
86	OHX	1	4077	7/7	0.14	-0.65	151,151,151,151	0
86	OHX	c8	203	7/7	0.19	-0.65	172,172,172,172	0
86	OHX	C5	201	7/7	0.22	-0.66	191,191,191,191	0
86	OHX	c3	201	7/7	0.24	-0.66	170,170,170,170	0
86	OHX	6	2144	7/7	0.15	-0.66	143,143,143,143	0
86	OHX	1	4124	7/7	0.16	-0.66	161,161,161,161	0
85	MG	1	3666	1/1	0.15	-0.69	54,54,54,54	0
86	OHX	2	2089	7/7	0.16	-0.69	129,129,129,129	0
86	OHX	5	4193	7/7	0.16	-0.70	97,97,97,97	0
86	OHX	5	4013	7/7	0.16	-0.70	116,116,116,116	0
86	OHX	5	3926	7/7	0.14	-0.73	101,101,101,101	0
86	OHX	5	3976	7/7	0.15	-0.73	112,112,112,112	0
86	OHX	5	4052	7/7	0.15	-0.73	156,156,156,156	0
86	OHX	1	4018	7/7	0.18	-0.74	131,131,131,131	0
86	OHX	1	3956	7/7	0.16	-0.75	118,118,118,118	0
86	OHX	1	3895	7/7	0.12	-0.76	82,82,82,82	0
85	MG	1	3736	1/1	0.18	-0.76	66,66,66,66	0
86	OHX	5	3967	7/7	0.09	-0.77	115,115,115,115	0
86	OHX	6	2096	7/7	0.12	-0.77	142,142,142,142	0
86	OHX	2	2055	7/7	0.13	-0.79	130,130,130,130	0
87	ZN	D6	500	1/1	0.12	-0.79	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	3954	7/7	0.16	-0.79	111,111,111,111	0
86	OHX	n6	203	7/7	0.15	-0.80	153,153,153,153	0
86	OHX	5	4235	7/7	0.24	-0.80	245,245,245,245	0
87	ZN	d9	101	1/1	0.11	-0.81	97,97,97,97	0
86	OHX	4	230	7/7	0.10	-0.82	156,156,156,156	0
85	MG	M1	201	1/1	0.16	-0.82	83,83,83,83	0
86	OHX	O1	201	7/7	0.10	-0.82	122,122,122,122	0
86	OHX	5	4059	7/7	0.16	-0.82	127,127,127,127	0
86	OHX	6	2052	7/7	0.18	-0.84	86,86,86,86	0
85	MG	2	1986	1/1	0.21	-0.84	79,79,79,79	0
86	OHX	5	3978	7/7	0.14	-0.84	93,93,93,93	0
86	OHX	2	2130	7/7	0.18	-0.85	127,127,127,127	0
86	OHX	6	2088	7/7	0.15	-0.85	127,127,127,127	0
85	MG	1	3819	1/1	0.25	-0.86	123,123,123,123	0
85	MG	sM	301	1/1	0.15	-0.86	51,51,51,51	0
85	MG	L3	402	1/1	0.13	-0.87	76,76,76,76	0
86	OHX	6	2202	7/7	0.23	-0.88	206,206,206,206	0
85	MG	N8	205	1/1	0.15	-0.88	40,40,40,40	0
85	MG	6	1995	1/1	0.16	-0.89	82,82,82,82	0
86	OHX	Q2	502	7/7	0.15	-0.90	92,92,92,92	0
86	OHX	6	2045	7/7	0.14	-0.91	61,61,61,61	0
86	OHX	q2	502	7/7	0.16	-0.92	94,94,94,94	0
86	OHX	5	3968	7/7	0.13	-0.92	113,113,113,113	0
85	MG	5	3797	1/1	0.12	-0.93	82,82,82,82	0
85	MG	1	3718	1/1	0.17	-0.93	37,37,37,37	0
86	OHX	1	3901	7/7	0.17	-0.94	97,97,97,97	0
86	OHX	5	3895	7/7	0.13	-0.94	70,70,70,70	0
85	MG	M5	301	1/1	0.13	-0.94	49,49,49,49	0
85	MG	5	3421	1/1	0.16	-0.94	43,43,43,43	0
86	OHX	2	2141	7/7	0.17	-0.94	184,184,184,184	0
86	OHX	5	4068	7/7	0.16	-0.94	133,133,133,133	0
86	OHX	3	220	7/7	0.15	-0.95	142,142,142,142	0
86	OHX	5	3900	7/7	0.13	-0.96	71,71,71,71	0
86	OHX	2	2063	7/7	0.13	-0.96	148,148,148,148	0
85	MG	5	3813	1/1	0.17	-0.96	44,44,44,44	0
86	OHX	6	2084	7/7	0.16	-0.96	125,125,125,125	0
86	OHX	L3	404	7/7	0.16	-0.97	123,123,123,123	0
86	OHX	5	4097	7/7	0.12	-0.97	164,164,164,164	0
85	MG	5	3852	1/1	0.10	-0.97	60,60,60,60	0
85	MG	5	3614	1/1	0.14	-0.98	54,54,54,54	0
85	MG	5	3819	1/1	0.21	-0.99	96,96,96,96	0
85	MG	2	1995	1/1	0.13	-1.00	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	o3	203	7/7	0.14	-1.02	120,120,120,120	0
86	OHX	5	4175	7/7	0.22	-1.02	170,170,170,170	0
85	MG	1	3722	1/1	0.16	-1.02	46,46,46,46	0
86	OHX	1	4032	7/7	0.14	-1.02	108,108,108,108	0
86	OHX	C3	202	7/7	0.15	-1.02	181,181,181,181	0
86	OHX	5	3960	7/7	0.17	-1.03	121,121,121,121	0
85	MG	1	3809	1/1	0.37	-1.03	209,209,209,209	0
86	OHX	5	4054	7/7	0.13	-1.03	162,162,162,162	0
86	OHX	1	3875	7/7	0.15	-1.04	71,71,71,71	0
86	OHX	6	2098	7/7	0.17	-1.04	199,199,199,199	0
86	OHX	1	3957	7/7	0.09	-1.05	117,117,117,117	0
86	OHX	6	2116	7/7	0.14	-1.05	152,152,152,152	0
85	MG	M0	301	1/1	0.14	-1.05	85,85,85,85	0
86	OHX	1	4105	7/7	0.17	-1.05	148,148,148,148	0
86	OHX	2	2110	7/7	0.08	-1.06	138,138,138,138	0
86	OHX	n3	203	7/7	0.11	-1.06	117,117,117,117	0
86	OHX	1	3871	7/7	0.12	-1.07	57,57,57,57	0
86	OHX	2	2033	7/7	0.13	-1.07	120,120,120,120	0
86	OHX	7	220	7/7	0.12	-1.08	111,111,111,111	0
86	OHX	2	2024	7/7	0.13	-1.09	90,90,90,90	0
86	OHX	1	3868	7/7	0.13	-1.10	71,71,71,71	0
86	OHX	6	2065	7/7	0.11	-1.11	104,104,104,104	0
86	OHX	6	2128	7/7	0.17	-1.11	133,133,133,133	0
86	OHX	2	2048	7/7	0.10	-1.12	129,129,129,129	0
85	MG	5	3601	1/1	0.09	-1.12	59,59,59,59	0
86	OHX	1	4000	7/7	0.14	-1.12	105,105,105,105	0
86	OHX	6	2157	7/7	0.14	-1.12	119,119,119,119	0
86	OHX	2	2098	7/7	0.08	-1.13	171,171,171,171	0
85	MG	1	3603	1/1	0.15	-1.13	41,41,41,41	0
86	OHX	1	4012	7/7	0.15	-1.13	148,148,148,148	0
86	OHX	1	4041	7/7	0.12	-1.13	144,144,144,144	0
86	OHX	M5	303	7/7	0.19	-1.14	129,129,129,129	0
86	OHX	8	218	7/7	0.07	-1.15	128,128,128,128	0
86	OHX	1	3869	7/7	0.13	-1.16	62,62,62,62	0
87	ZN	Q0	500	1/1	0.14	-1.16	51,51,51,51	0
87	ZN	q0	201	1/1	0.12	-1.17	38,38,38,38	0
86	OHX	5	4232	7/7	0.17	-1.18	162,162,162,162	0
86	OHX	O7	103	7/7	0.08	-1.18	106,106,106,106	0
86	OHX	5	4074	7/7	0.14	-1.19	133,133,133,133	0
86	OHX	5	4033	7/7	0.10	-1.19	144,144,144,144	0
86	OHX	2	2078	7/7	0.17	-1.19	140,140,140,140	0
86	OHX	N9	101	7/7	0.14	-1.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	3948	7/7	0.14	-1.20	129,129,129,129	0
86	OHX	1	4013	7/7	0.10	-1.20	156,156,156,156	0
86	OHX	1	4143	7/7	0.16	-1.20	138,138,138,138	0
86	OHX	1	4034	7/7	0.11	-1.21	165,165,165,165	0
86	OHX	2	2056	7/7	0.12	-1.21	148,148,148,148	0
86	OHX	5	4028	7/7	0.15	-1.21	112,112,112,112	0
86	OHX	1	3936	7/7	0.12	-1.22	108,108,108,108	0
86	OHX	1	3959	7/7	0.17	-1.22	88,88,88,88	0
85	MG	5	3649	1/1	0.16	-1.22	52,52,52,52	0
86	OHX	2	2036	7/7	0.10	-1.24	99,99,99,99	0
85	MG	5	3598	1/1	0.15	-1.24	47,47,47,47	0
86	OHX	1	4017	7/7	0.11	-1.24	168,168,168,168	0
86	OHX	1	4061	7/7	0.12	-1.24	170,170,170,170	0
86	OHX	1	3899	7/7	0.12	-1.24	88,88,88,88	0
86	OHX	4	222	7/7	0.09	-1.25	90,90,90,90	0
87	ZN	e1	501	1/1	0.25	-1.26	204,204,204,204	0
86	OHX	2	2138	7/7	0.15	-1.26	156,156,156,156	0
86	OHX	6	2051	7/7	0.13	-1.28	90,90,90,90	0
86	OHX	6	2071	7/7	0.12	-1.28	161,161,161,161	0
86	OHX	5	4031	7/7	0.13	-1.29	150,150,150,150	0
87	ZN	q3	501	1/1	0.09	-1.30	74,74,74,74	0
86	OHX	1	4178	7/7	0.18	-1.31	247,247,247,247	0
86	OHX	1	4027	7/7	0.14	-1.31	137,137,137,137	0
86	OHX	2	2166	7/7	0.13	-1.31	169,169,169,169	0
85	MG	5	3768	1/1	0.11	-1.31	59,59,59,59	0
86	OHX	7	218	7/7	0.10	-1.31	97,97,97,97	0
86	OHX	1	3964	7/7	0.14	-1.32	108,108,108,108	0
86	OHX	5	4026	7/7	0.10	-1.32	155,155,155,155	0
86	OHX	5	4098	7/7	0.13	-1.35	144,144,144,144	0
86	OHX	6	2109	7/7	0.14	-1.35	142,142,142,142	0
86	OHX	1	3994	7/7	0.14	-1.36	142,142,142,142	0
86	OHX	5	4005	7/7	0.14	-1.38	121,121,121,121	0
85	MG	2	1999	1/1	0.09	-1.39	99,99,99,99	0
86	OHX	1	3908	7/7	0.14	-1.39	90,90,90,90	0
87	ZN	q2	501	1/1	0.14	-1.40	91,91,91,91	0
85	MG	q3	503	1/1	0.18	-1.40	68,68,68,68	0
86	OHX	2	2040	7/7	0.12	-1.41	113,113,113,113	0
86	OHX	1	3979	7/7	0.10	-1.41	120,120,120,120	0
85	MG	5	3724	1/1	0.15	-1.41	40,40,40,40	0
86	OHX	5	3899	7/7	0.16	-1.41	63,63,63,63	0
86	OHX	5	4060	7/7	0.11	-1.41	129,129,129,129	0
85	MG	5	3762	1/1	0.12	-1.42	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	3	216	7/7	0.14	-1.42	129,129,129,129	0
86	OHX	5	3906	7/7	0.11	-1.42	72,72,72,72	0
86	OHX	5	4025	7/7	0.12	-1.42	126,126,126,126	0
85	MG	l5	303	1/1	0.09	-1.42	64,64,64,64	0
86	OHX	5	4124	7/7	0.09	-1.42	151,151,151,151	0
86	OHX	1	3929	7/7	0.12	-1.43	113,113,113,113	0
87	ZN	D9	101	1/1	0.06	-1.45	88,88,88,88	0
86	OHX	1	3866	7/7	0.14	-1.45	50,50,50,50	0
86	OHX	2	2082	7/7	0.10	-1.46	169,169,169,169	0
86	OHX	6	2064	7/7	0.11	-1.46	125,125,125,125	0
86	OHX	l3	404	7/7	0.13	-1.46	111,111,111,111	0
86	OHX	5	4092	7/7	0.14	-1.46	141,141,141,141	0
86	OHX	6	2078	7/7	0.14	-1.47	117,117,117,117	0
86	OHX	2	2034	7/7	0.13	-1.48	116,116,116,116	0
86	OHX	6	2162	7/7	0.26	-1.48	202,202,202,202	0
86	OHX	1	3934	7/7	0.09	-1.49	109,109,109,109	0
86	OHX	5	4078	7/7	0.10	-1.49	145,145,145,145	0
85	MG	5	3857	1/1	0.13	-1.49	65,65,65,65	0
85	MG	1	3422	1/1	0.13	-1.50	36,36,36,36	0
86	OHX	6	2153	7/7	0.14	-1.51	123,123,123,123	0
86	OHX	2	2073	7/7	0.17	-1.51	164,164,164,164	0
86	OHX	2	2099	7/7	0.14	-1.52	135,135,135,135	0
85	MG	5	3847	1/1	0.14	-1.53	57,57,57,57	0
86	OHX	1	4054	7/7	0.13	-1.53	144,144,144,144	0
85	MG	o0	201	1/1	0.15	-1.53	72,72,72,72	0
85	MG	M0	303	1/1	0.21	-1.55	55,55,55,55	0
86	OHX	1	3909	7/7	0.10	-1.55	100,100,100,100	0
85	MG	5	3745	1/1	0.12	-1.56	73,73,73,73	0
86	OHX	5	3998	7/7	0.13	-1.57	117,117,117,117	0
86	OHX	1	3880	7/7	0.09	-1.57	72,72,72,72	0
86	OHX	6	2143	7/7	0.15	-1.57	143,143,143,143	0
86	OHX	2	2023	7/7	0.13	-1.58	77,77,77,77	0
87	ZN	E1	501	1/1	0.07	-1.59	130,130,130,130	0
86	OHX	8	220	7/7	0.10	-1.60	145,145,145,145	0
86	OHX	5	4061	7/7	0.14	-1.60	141,141,141,141	0
86	OHX	2	2156	7/7	0.31	-1.60	249,249,249,249	0
86	OHX	1	3993	7/7	0.14	-1.60	144,144,144,144	0
86	OHX	2	2094	7/7	0.06	-1.61	161,161,161,161	0
86	OHX	2	2132	7/7	0.12	-1.61	165,165,165,165	0
86	OHX	5	4048	7/7	0.13	-1.62	114,114,114,114	0
86	OHX	5	3992	7/7	0.10	-1.62	122,122,122,122	0
85	MG	5	3404	1/1	0.12	-1.62	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	5	4001	7/7	0.16	-1.64	128,128,128,128	0
86	OHX	1	4180	7/7	0.17	-1.65	114,114,114,114	0
86	OHX	5	4020	7/7	0.16	-1.65	123,123,123,123	0
86	OHX	1	3877	7/7	0.13	-1.65	75,75,75,75	0
86	OHX	5	4019	7/7	0.10	-1.65	128,128,128,128	0
86	OHX	2	2047	7/7	0.06	-1.66	140,140,140,140	0
86	OHX	5	3975	7/7	0.11	-1.67	98,98,98,98	0
86	OHX	1	3925	7/7	0.10	-1.67	102,102,102,102	0
86	OHX	2	2043	7/7	0.09	-1.68	123,123,123,123	0
86	OHX	SR	401	7/7	0.12	-1.68	176,176,176,176	0
86	OHX	1	3950	7/7	0.10	-1.68	134,134,134,134	0
86	OHX	2	2068	7/7	0.14	-1.69	169,169,169,169	0
85	MG	1	3441	1/1	0.13	-1.69	43,43,43,43	0
86	OHX	5	3949	7/7	0.12	-1.70	103,103,103,103	0
86	OHX	5	4038	7/7	0.15	-1.70	121,121,121,121	0
86	OHX	5	4126	7/7	0.18	-1.72	198,198,198,198	0
85	MG	1	3606	1/1	0.13	-1.73	62,62,62,62	0
86	OHX	6	2073	7/7	0.07	-1.74	97,97,97,97	0
86	OHX	5	3919	7/7	0.13	-1.74	69,69,69,69	0
86	OHX	1	3967	7/7	0.09	-1.74	130,130,130,130	0
86	OHX	2	2035	7/7	0.12	-1.75	108,108,108,108	0
86	OHX	1	3962	7/7	0.13	-1.75	103,103,103,103	0
86	OHX	1	3886	7/7	0.10	-1.75	80,80,80,80	0
86	OHX	5	3942	7/7	0.08	-1.76	95,95,95,95	0
86	OHX	2	2077	7/7	0.12	-1.77	130,130,130,130	0
86	OHX	2	2107	7/7	0.10	-1.77	127,127,127,127	0
85	MG	5	3458	1/1	0.13	-1.77	73,73,73,73	0
87	ZN	Q2	501	1/1	0.10	-1.77	90,90,90,90	0
86	OHX	8	225	7/7	0.07	-1.78	157,157,157,157	0
85	MG	6	1930	1/1	0.14	-1.78	57,57,57,57	0
86	OHX	6	2054	7/7	0.13	-1.79	83,83,83,83	0
86	OHX	C8	201	7/7	0.06	-1.80	133,133,133,133	0
86	OHX	m0	302	7/7	0.09	-1.81	133,133,133,133	0
86	OHX	5	3953	7/7	0.12	-1.82	86,86,86,86	0
86	OHX	2	2027	7/7	0.10	-1.82	82,82,82,82	0
86	OHX	6	2080	7/7	0.08	-1.82	125,125,125,125	0
85	MG	s1	301	1/1	0.14	-1.83	89,89,89,89	0
86	OHX	5	4036	7/7	0.05	-1.83	164,164,164,164	0
86	OHX	6	2047	7/7	0.14	-1.83	73,73,73,73	0
86	OHX	5	4000	7/7	0.14	-1.85	126,126,126,126	0
85	MG	1	4217	1/1	0.15	-1.88	76,76,76,76	0
86	OHX	5	3930	7/7	0.08	-1.89	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	3928	7/7	0.07	-1.89	98,98,98,98	0
87	ZN	o7	501	1/1	0.09	-1.89	49,49,49,49	0
86	OHX	1	3913	7/7	0.07	-1.90	95,95,95,95	0
86	OHX	6	2062	7/7	0.09	-1.91	105,105,105,105	0
86	OHX	2	2037	7/7	0.09	-1.92	140,140,140,140	0
86	OHX	2	2097	7/7	0.08	-1.94	186,186,186,186	0
85	MG	1	3828	1/1	0.12	-1.95	65,65,65,65	0
86	OHX	1	3921	7/7	0.11	-1.95	125,125,125,125	0
86	OHX	5	3980	7/7	0.07	-1.95	111,111,111,111	0
86	OHX	1	3883	7/7	0.12	-1.95	70,70,70,70	0
86	OHX	7	224	7/7	0.13	-1.96	146,146,146,146	0
86	OHX	1	3938	7/7	0.13	-1.96	111,111,111,111	0
85	MG	5	3815	1/1	0.07	-1.97	72,72,72,72	0
85	MG	6	1996	1/1	0.09	-1.97	62,62,62,62	0
86	OHX	5	3963	7/7	0.09	-1.98	117,117,117,117	0
86	OHX	2	2095	7/7	0.13	-1.98	167,167,167,167	0
86	OHX	1	3867	7/7	0.12	-1.99	55,55,55,55	0
86	OHX	5	3933	7/7	0.10	-1.99	92,92,92,92	0
86	OHX	2	2053	7/7	0.10	-2.00	148,148,148,148	0
86	OHX	6	2056	7/7	0.10	-2.00	104,104,104,104	0
86	OHX	5	3925	7/7	0.12	-2.00	81,81,81,81	0
86	OHX	1	3882	7/7	0.13	-2.01	80,80,80,80	0
85	MG	1	3478	1/1	0.10	-2.01	92,92,92,92	0
86	OHX	2	2031	7/7	0.09	-2.02	125,125,125,125	0
86	OHX	5	3924	7/7	0.13	-2.02	73,73,73,73	0
86	OHX	2	2030	7/7	0.12	-2.04	103,103,103,103	0
85	MG	1	3745	1/1	0.12	-2.04	42,42,42,42	0
86	OHX	5	3904	7/7	0.13	-2.04	62,62,62,62	0
86	OHX	2	2071	7/7	0.15	-2.06	136,136,136,136	0
86	OHX	5	4015	7/7	0.15	-2.07	111,111,111,111	0
86	OHX	1	4192	7/7	0.06	-2.08	178,178,178,178	0
85	MG	5	3636	1/1	0.18	-2.09	60,60,60,60	0
85	MG	5	3469	1/1	0.11	-2.09	109,109,109,109	0
86	OHX	6	2120	7/7	0.13	-2.10	151,151,151,151	0
86	OHX	1	3917	7/7	0.06	-2.13	102,102,102,102	0
86	OHX	5	4016	7/7	0.10	-2.14	133,133,133,133	0
86	OHX	5	3898	7/7	0.12	-2.14	61,61,61,61	0
85	MG	6	1966	1/1	0.13	-2.15	89,89,89,89	0
86	OHX	6	2095	7/7	0.09	-2.15	181,181,181,181	0
86	OHX	6	2133	7/7	0.13	-2.17	145,145,145,145	0
85	MG	5	3817	1/1	0.14	-2.18	60,60,60,60	0
86	OHX	6	2083	7/7	0.09	-2.18	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	3893	7/7	0.11	-2.18	77,77,77,77	0
86	OHX	2	2064	7/7	0.14	-2.21	131,131,131,131	0
86	OHX	1	3891	7/7	0.12	-2.21	73,73,73,73	0
86	OHX	6	2119	7/7	0.09	-2.22	158,158,158,158	0
86	OHX	1	3889	7/7	0.14	-2.22	83,83,83,83	0
86	OHX	7	222	7/7	0.09	-2.24	116,116,116,116	0
86	OHX	6	2050	7/7	0.13	-2.24	79,79,79,79	0
86	OHX	6	2057	7/7	0.09	-2.25	99,99,99,99	0
86	OHX	l5	304	7/7	0.09	-2.26	145,145,145,145	0
85	MG	5	3646	1/1	0.15	-2.27	57,57,57,57	0
85	MG	5	3802	1/1	0.10	-2.27	167,167,167,167	0
86	OHX	1	3988	7/7	0.11	-2.27	132,132,132,132	0
86	OHX	6	2090	7/7	0.08	-2.29	129,129,129,129	0
86	OHX	5	3952	7/7	0.12	-2.30	80,80,80,80	0
86	OHX	1	3919	7/7	0.10	-2.31	109,109,109,109	0
86	OHX	6	2087	7/7	0.05	-2.31	139,139,139,139	0
86	OHX	1	3916	7/7	0.08	-2.32	116,116,116,116	0
87	ZN	O7	101	1/1	0.07	-2.33	42,42,42,42	0
86	OHX	6	2099	7/7	0.06	-2.33	175,175,175,175	0
86	OHX	1	4117	7/7	0.17	-2.35	137,137,137,137	0
86	OHX	3	215	7/7	0.08	-2.36	107,107,107,107	0
86	OHX	1	3949	7/7	0.11	-2.38	123,123,123,123	0
86	OHX	2	2039	7/7	0.07	-2.38	109,109,109,109	0
86	OHX	6	2075	7/7	0.11	-2.39	125,125,125,125	0
86	OHX	1	3997	7/7	0.07	-2.40	176,176,176,176	0
86	OHX	5	3943	7/7	0.09	-2.41	106,106,106,106	0
86	OHX	1	4022	7/7	0.11	-2.42	122,122,122,122	0
86	OHX	5	3962	7/7	0.05	-2.43	116,116,116,116	0
86	OHX	5	3972	7/7	0.12	-2.43	103,103,103,103	0
86	OHX	5	3989	7/7	0.16	-2.43	112,112,112,112	0
86	OHX	1	4003	7/7	0.10	-2.43	130,130,130,130	0
86	OHX	7	219	7/7	0.12	-2.44	106,106,106,106	0
86	OHX	6	2100	7/7	0.10	-2.44	133,133,133,133	0
86	OHX	1	3887	7/7	0.11	-2.44	76,76,76,76	0
86	OHX	1	3874	7/7	0.11	-2.45	69,69,69,69	0
86	OHX	8	221	7/7	0.09	-2.46	136,136,136,136	0
85	MG	1	3812	1/1	0.10	-2.47	40,40,40,40	0
86	OHX	5	4012	7/7	0.06	-2.47	139,139,139,139	0
86	OHX	5	3927	7/7	0.12	-2.47	80,80,80,80	0
86	OHX	2	2032	7/7	0.08	-2.47	115,115,115,115	0
86	OHX	1	3915	7/7	0.10	-2.49	98,98,98,98	0
85	MG	1	3520	1/1	0.09	-2.49	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	1	3910	7/7	0.13	-2.51	83,83,83,83	0
86	OHX	6	2048	7/7	0.11	-2.51	81,81,81,81	0
86	OHX	1	3923	7/7	0.08	-2.51	113,113,113,113	0
86	OHX	5	3923	7/7	0.15	-2.51	105,105,105,105	0
86	OHX	2	2052	7/7	0.14	-2.53	127,127,127,127	0
86	OHX	M0	304	7/7	0.20	-2.53	134,134,134,134	0
85	MG	1	3678	1/1	0.09	-2.54	76,76,76,76	0
86	OHX	1	3894	7/7	0.11	-2.55	80,80,80,80	0
86	OHX	5	4007	7/7	0.06	-2.55	147,147,147,147	0
85	MG	5	3820	1/1	0.09	-2.57	70,70,70,70	0
85	MG	m6	202	1/1	0.07	-2.57	35,35,35,35	0
86	OHX	5	3954	7/7	0.07	-2.58	102,102,102,102	0
86	OHX	1	3998	7/7	0.08	-2.59	164,164,164,164	0
86	OHX	5	4077	7/7	0.15	-2.59	128,128,128,128	0
86	OHX	2	2066	7/7	0.06	-2.61	147,147,147,147	0
86	OHX	1	3951	7/7	0.09	-2.61	130,130,130,130	0
86	OHX	5	4071	7/7	0.08	-2.62	165,165,165,165	0
86	OHX	1	3902	7/7	0.10	-2.62	95,95,95,95	0
86	OHX	6	2068	7/7	0.11	-2.62	101,101,101,101	0
86	OHX	1	3904	7/7	0.08	-2.62	87,87,87,87	0
86	OHX	5	3994	7/7	0.07	-2.62	120,120,120,120	0
86	OHX	2	2026	7/7	0.09	-2.63	96,96,96,96	0
86	OHX	5	3915	7/7	0.10	-2.66	71,71,71,71	0
86	OHX	2	2061	7/7	0.10	-2.66	141,141,141,141	0
85	MG	6	2025	1/1	0.10	-2.67	87,87,87,87	0
86	OHX	1	3961	7/7	0.07	-2.67	123,123,123,123	0
86	OHX	1	3995	7/7	0.07	-2.70	143,143,143,143	0
85	MG	5	3699	1/1	0.11	-2.70	69,69,69,69	0
86	OHX	5	3912	7/7	0.11	-2.70	79,79,79,79	0
86	OHX	5	3936	7/7	0.09	-2.70	103,103,103,103	0
86	OHX	3	217	7/7	0.10	-2.71	121,121,121,121	0
86	OHX	5	4003	7/7	0.12	-2.73	104,104,104,104	0
86	OHX	5	3911	7/7	0.11	-2.74	68,68,68,68	0
86	OHX	4	221	7/7	0.12	-2.80	62,62,62,62	0
86	OHX	5	3951	7/7	0.09	-2.81	97,97,97,97	0
86	OHX	5	3896	7/7	0.10	-2.82	59,59,59,59	0
86	OHX	5	3981	7/7	0.07	-2.82	132,132,132,132	0
86	OHX	5	3983	7/7	0.09	-2.83	115,115,115,115	0
85	MG	5	3827	1/1	0.09	-2.83	84,84,84,84	0
86	OHX	2	2049	7/7	0.10	-2.86	136,136,136,136	0
86	OHX	5	3984	7/7	0.12	-2.86	103,103,103,103	0
86	OHX	5	3959	7/7	0.09	-2.88	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	6	2129	7/7	0.13	-2.88	157,157,157,157	0
86	OHX	5	3905	7/7	0.12	-2.89	65,65,65,65	0
86	OHX	1	3945	7/7	0.09	-2.89	106,106,106,106	0
86	OHX	1	3953	7/7	0.11	-2.90	122,122,122,122	0
86	OHX	5	3991	7/7	0.09	-2.91	119,119,119,119	0
86	OHX	1	3969	7/7	0.08	-2.92	140,140,140,140	0
86	OHX	6	2094	7/7	0.08	-2.94	142,142,142,142	0
86	OHX	5	3913	7/7	0.11	-2.94	77,77,77,77	0
86	OHX	1	3906	7/7	0.11	-2.96	96,96,96,96	0
86	OHX	1	3970	7/7	0.07	-2.99	126,126,126,126	0
86	OHX	5	3929	7/7	0.10	-2.99	85,85,85,85	0
86	OHX	1	3907	7/7	0.10	-3.00	103,103,103,103	0
86	OHX	5	3937	7/7	0.07	-3.00	99,99,99,99	0
86	OHX	2	2045	7/7	0.08	-3.03	116,116,116,116	0
86	OHX	5	4004	7/7	0.08	-3.03	115,115,115,115	0
86	OHX	1	3927	7/7	0.09	-3.04	122,122,122,122	0
86	OHX	5	4002	7/7	0.10	-3.04	81,81,81,81	0
85	MG	5	3650	1/1	0.11	-3.07	41,41,41,41	0
86	OHX	2	2042	7/7	0.05	-3.08	117,117,117,117	0
86	OHX	2	2029	7/7	0.10	-3.08	117,117,117,117	0
86	OHX	1	4136	7/7	0.13	-3.11	115,115,115,115	0
86	OHX	s1	302	7/7	0.09	-3.12	100,100,100,100	0
85	MG	1	3862	1/1	0.09	-3.14	126,126,126,126	0
86	OHX	1	3982	7/7	0.06	-3.16	128,128,128,128	0
86	OHX	5	3947	7/7	0.06	-3.16	103,103,103,103	0
86	OHX	1	3933	7/7	0.13	-3.18	116,116,116,116	0
86	OHX	5	3956	7/7	0.10	-3.20	113,113,113,113	0
86	OHX	1	3905	7/7	0.11	-3.23	98,98,98,98	0
86	OHX	5	3971	7/7	0.08	-3.25	88,88,88,88	0
86	OHX	1	3918	7/7	0.09	-3.26	109,109,109,109	0
86	OHX	1	3930	7/7	0.08	-3.28	115,115,115,115	0
86	OHX	6	2076	7/7	0.08	-3.30	106,106,106,106	0
86	OHX	5	3935	7/7	0.08	-3.30	93,93,93,93	0
86	OHX	6	2114	7/7	0.12	-3.32	151,151,151,151	0
86	OHX	2	2041	7/7	0.07	-3.33	107,107,107,107	0
86	OHX	5	3909	7/7	0.11	-3.33	80,80,80,80	0
85	MG	7	228	1/1	0.13	-3.34	35,35,35,35	0
86	OHX	5	4011	7/7	0.14	-3.34	166,166,166,166	0
86	OHX	1	3878	7/7	0.10	-3.35	67,67,67,67	0
86	OHX	5	3970	7/7	0.10	-3.37	112,112,112,112	0
86	OHX	5	3946	7/7	0.07	-3.38	114,114,114,114	0
86	OHX	1	3960	7/7	0.10	-3.38	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	2	2028	7/7	0.12	-3.40	101,101,101,101	0
86	OHX	5	3997	7/7	0.09	-3.40	122,122,122,122	0
86	OHX	5	4045	7/7	0.07	-3.41	143,143,143,143	0
86	OHX	1	3946	7/7	0.07	-3.42	110,110,110,110	0
86	OHX	1	3940	7/7	0.09	-3.44	109,109,109,109	0
86	OHX	5	3902	7/7	0.09	-3.44	64,64,64,64	0
86	OHX	1	3975	7/7	0.08	-3.47	116,116,116,116	0
86	OHX	6	2072	7/7	0.07	-3.49	154,154,154,154	0
86	OHX	6	2110	7/7	0.13	-3.49	134,134,134,134	0
86	OHX	5	3979	7/7	0.10	-3.49	99,99,99,99	0
86	OHX	1	3963	7/7	0.06	-3.51	136,136,136,136	0
86	OHX	2	2104	7/7	0.22	-3.54	214,214,214,214	0
85	MG	5	3431	1/1	0.13	-3.54	38,38,38,38	0
86	OHX	1	3980	7/7	0.10	-3.59	118,118,118,118	0
86	OHX	1	3890	7/7	0.13	-3.59	84,84,84,84	0
85	MG	5	3785	1/1	0.08	-3.63	53,53,53,53	0
86	OHX	1	3903	7/7	0.10	-3.63	80,80,80,80	0
86	OHX	1	4020	7/7	0.14	-3.65	123,123,123,123	0
86	OHX	1	3879	7/7	0.09	-3.67	71,71,71,71	0
86	OHX	2	2059	7/7	0.08	-3.67	138,138,138,138	0
86	OHX	1	3996	7/7	0.13	-3.68	109,109,109,109	0
86	OHX	1	3987	7/7	0.13	-3.68	127,127,127,127	0
86	OHX	1	3937	7/7	0.10	-3.73	107,107,107,107	0
86	OHX	5	4029	7/7	0.09	-3.75	116,116,116,116	0
86	OHX	5	3955	7/7	0.06	-3.78	100,100,100,100	0
86	OHX	6	2086	7/7	0.12	-3.81	137,137,137,137	0
86	OHX	1	3965	7/7	0.09	-3.81	82,82,82,82	0
86	OHX	1	3966	7/7	0.13	-3.89	114,114,114,114	0
86	OHX	5	4095	7/7	0.13	-3.90	155,155,155,155	0
86	OHX	5	4104	7/7	0.10	-3.90	98,98,98,98	0
86	OHX	5	3950	7/7	0.07	-3.92	96,96,96,96	0
86	OHX	5	4049	7/7	0.05	-3.92	112,112,112,112	0
86	OHX	5	3941	7/7	0.08	-3.96	98,98,98,98	0
86	OHX	1	3942	7/7	0.11	-3.96	114,114,114,114	0
86	OHX	6	2058	7/7	0.07	-3.98	94,94,94,94	0
86	OHX	1	3931	7/7	0.08	-4.02	92,92,92,92	0
86	OHX	1	3944	7/7	0.06	-4.04	115,115,115,115	0
86	OHX	1	4085	7/7	0.16	-4.05	202,202,202,202	0
86	OHX	8	216	7/7	0.09	-4.05	61,61,61,61	0
86	OHX	4	226	7/7	0.07	-4.10	138,138,138,138	0
85	MG	6	2007	1/1	0.13	-4.11	58,58,58,58	0
86	OHX	5	4023	7/7	0.08	-4.11	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	1	3805	1/1	0.12	-4.13	63,63,63,63	0
86	OHX	2	2038	7/7	0.09	-4.15	114,114,114,114	0
86	OHX	5	3945	7/7	0.11	-4.20	109,109,109,109	0
86	OHX	6	2067	7/7	0.05	-4.24	111,111,111,111	0
85	MG	5	3833	1/1	0.10	-4.24	73,73,73,73	0
86	OHX	1	3941	7/7	0.08	-4.25	110,110,110,110	0
86	OHX	6	2063	7/7	0.08	-4.25	118,118,118,118	0
85	MG	5	3804	1/1	0.12	-4.27	96,96,96,96	0
86	OHX	5	3944	7/7	0.10	-4.27	93,93,93,93	0
86	OHX	6	2112	7/7	0.11	-4.28	143,143,143,143	0
86	OHX	m6	203	7/7	0.09	-4.30	109,109,109,109	0
86	OHX	5	3931	7/7	0.07	-4.32	86,86,86,86	0
86	OHX	1	4011	7/7	0.15	-4.32	149,149,149,149	0
86	OHX	5	3934	7/7	0.10	-4.34	90,90,90,90	0
86	OHX	1	3873	7/7	0.09	-4.35	72,72,72,72	0
86	OHX	1	4066	7/7	0.09	-4.35	165,165,165,165	0
86	OHX	1	3912	7/7	0.09	-4.42	112,112,112,112	0
86	OHX	7	221	7/7	0.10	-4.46	109,109,109,109	0
86	OHX	6	2077	7/7	0.08	-4.46	117,117,117,117	0
86	OHX	6	2082	7/7	0.10	-4.48	126,126,126,126	0
86	OHX	5	3993	7/7	0.09	-4.51	99,99,99,99	0
85	MG	1	3806	1/1	0.12	-4.52	69,69,69,69	0
86	OHX	1	3914	7/7	0.07	-4.54	89,89,89,89	0
85	MG	1	3794	1/1	0.09	-4.54	84,84,84,84	0
85	MG	n8	202	1/1	0.12	-4.56	39,39,39,39	0
85	MG	5	3829	1/1	0.12	-4.57	70,70,70,70	0
86	OHX	6	2136	7/7	0.16	-4.59	139,139,139,139	0
86	OHX	5	3969	7/7	0.09	-4.60	113,113,113,113	0
86	OHX	6	2074	7/7	0.09	-4.64	122,122,122,122	0
86	OHX	5	3916	7/7	0.09	-4.68	78,78,78,78	0
86	OHX	5	3988	7/7	0.08	-4.71	121,121,121,121	0
86	OHX	5	3990	7/7	0.05	-4.75	122,122,122,122	0
86	OHX	6	2055	7/7	0.07	-4.76	97,97,97,97	0
86	OHX	5	3965	7/7	0.10	-4.85	98,98,98,98	0
86	OHX	1	3981	7/7	0.09	-4.90	87,87,87,87	0
86	OHX	6	2079	7/7	0.07	-5.01	117,117,117,117	0
86	OHX	5	3964	7/7	0.12	-5.06	113,113,113,113	0
86	OHX	6	2097	7/7	0.16	-5.07	184,184,184,184	0
86	OHX	6	2061	7/7	0.05	-5.08	94,94,94,94	0
86	OHX	5	3961	7/7	0.08	-5.13	102,102,102,102	0
86	OHX	1	3885	7/7	0.07	-5.16	70,70,70,70	0
86	OHX	1	3935	7/7	0.05	-5.16	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
86	OHX	2	2070	7/7	0.05	-5.19	137,137,137,137	0
85	MG	6	2003	1/1	0.18	-5.19	81,81,81,81	0
86	OHX	6	2059	7/7	0.07	-5.20	98,98,98,98	0
86	OHX	6	2049	7/7	0.14	-5.23	80,80,80,80	0
86	OHX	5	3914	7/7	0.08	-5.25	78,78,78,78	0
86	OHX	5	3985	7/7	0.10	-5.27	117,117,117,117	0
86	OHX	1	3939	7/7	0.08	-5.31	105,105,105,105	0
86	OHX	1	3974	7/7	0.09	-5.37	137,137,137,137	0
85	MG	5	3784	1/1	0.09	-5.40	45,45,45,45	0
86	OHX	6	2060	7/7	0.08	-5.41	104,104,104,104	0
85	MG	5	3678	1/1	0.07	-5.48	100,100,100,100	0
86	OHX	5	3921	7/7	0.06	-5.48	92,92,92,92	0
86	OHX	1	3920	7/7	0.07	-5.62	100,100,100,100	0
86	OHX	6	2081	7/7	0.10	-5.62	133,133,133,133	0
86	OHX	3	218	7/7	0.13	-5.72	109,109,109,109	0
86	OHX	2	2044	7/7	0.06	-5.81	118,118,118,118	0
85	MG	1	3406	1/1	0.32	-5.84	129,129,129,129	0
86	OHX	1	4155	7/7	0.11	-5.85	112,112,112,112	0
85	MG	5	3837	1/1	0.07	-6.02	69,69,69,69	0
86	OHX	1	3900	7/7	0.10	-6.05	92,92,92,92	0
86	OHX	5	3928	7/7	0.06	-6.11	96,96,96,96	0
86	OHX	5	3910	7/7	0.07	-6.13	73,73,73,73	0
86	OHX	6	2069	7/7	0.07	-6.33	121,121,121,121	0
86	OHX	6	2091	7/7	0.08	-6.34	118,118,118,118	0
86	OHX	1	3896	7/7	0.06	-6.46	79,79,79,79	0
86	OHX	1	3955	7/7	0.10	-6.60	101,101,101,101	0
86	OHX	5	4209	7/7	0.15	-6.72	195,195,195,195	0
85	MG	5	3758	1/1	0.08	-7.19	47,47,47,47	0
86	OHX	2	2046	7/7	0.10	-7.24	138,138,138,138	0
86	OHX	5	3940	7/7	0.09	-7.47	80,80,80,80	0
86	OHX	6	2085	7/7	0.08	-7.55	119,119,119,119	0
86	OHX	5	3974	7/7	0.10	-7.57	96,96,96,96	0
86	OHX	1	3976	7/7	0.09	-7.62	113,113,113,113	0
85	MG	1	3858	1/1	0.12	-7.87	60,60,60,60	0
86	OHX	6	2092	7/7	0.07	-7.89	147,147,147,147	0
86	OHX	5	3922	7/7	0.07	-7.90	87,87,87,87	0
86	OHX	1	3932	7/7	0.05	-7.97	99,99,99,99	0
86	OHX	5	3938	7/7	0.11	-8.21	95,95,95,95	0
86	OHX	5	3939	7/7	0.08	-8.26	87,87,87,87	0
86	OHX	5	3982	7/7	0.03	-8.32	90,90,90,90	0
86	OHX	2	2050	7/7	0.09	-8.98	131,131,131,131	0
86	OHX	1	3926	7/7	0.06	-9.04	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
85	MG	1	3771	1/1	0.10	-9.40	92,92,92,92	0
86	OHX	1	3922	7/7	0.09	-9.51	113,113,113,113	0
86	OHX	1	3897	7/7	0.09	-11.05	102,102,102,102	0
85	MG	5	3854	1/1	0.13	-12.29	79,79,79,79	0
85	MG	7	214	1/1	0.12	-13.06	78,78,78,78	0
86	OHX	5	3918	7/7	0.08	-13.53	82,82,82,82	0
86	OHX	1	3952	7/7	0.09	-15.65	106,106,106,106	0
85	MG	2	1996	1/1	0.11	-29.42	89,89,89,89	0
86	OHX	5	3957	7/7	0.07	-31.80	95,95,95,95	0
85	MG	6	1998	1/1	0.41	-	127,127,127,127	0
85	MG	4	216	1/1	0.40	-	44,44,44,44	0
85	MG	1	3464	1/1	0.22	-	57,57,57,57	0
85	MG	4	214	1/1	0.32	-	48,48,48,48	0
85	MG	1	3864	1/1	0.37	-	79,79,79,79	0
85	MG	5	3771	1/1	0.60	-	140,140,140,140	0
85	MG	1	3804	1/1	0.06	-	91,91,91,91	0
85	MG	5	3793	1/1	0.22	-	88,88,88,88	0
85	MG	1	3797	1/1	0.21	-	66,66,66,66	0
85	MG	1	3842	1/1	0.34	-	47,47,47,47	0
85	MG	1	3548	1/1	0.77	-	75,75,75,75	0
85	MG	5	3798	1/1	0.15	-	31,31,31,31	0
85	MG	1	3788	1/1	0.52	-	46,46,46,46	0
85	MG	6	2037	1/1	0.48	-	100,100,100,100	0
85	MG	1	3839	1/1	0.74	-	41,41,41,41	0
85	MG	5	3616	1/1	0.71	-	43,43,43,43	0
85	MG	1	3849	1/1	0.73	-	52,52,52,52	0
85	MG	5	3844	1/1	0.60	-	41,41,41,41	0
85	MG	1	3838	1/1	0.34	-	37,37,37,37	0
85	MG	5	3861	1/1	0.66	-	61,61,61,61	0
85	MG	5	3755	1/1	0.34	-	39,39,39,39	0
85	MG	5	3872	1/1	0.75	-	40,40,40,40	0
85	MG	5	3845	1/1	0.14	-	54,54,54,54	0
85	MG	2	1962	1/1	0.11	-	154,154,154,154	0
86	OHX	2	2158	7/7	0.13	-	299,299,299,299	0
85	MG	1	3793	1/1	0.16	-	71,71,71,71	0
85	MG	1	3490	1/1	0.70	-	52,52,52,52	0
85	MG	5	3651	1/1	0.12	-	119,119,119,119	0

6.5 Other polymers (i)

There are no such residues in this entry.